



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 02:10 AM UTC

PDB ID : 7QH6 / pdb_00007qh6
EMDB ID : EMD-13965
Title : Cryo-EM structure of the human mtLSU assembly intermediate upon MRM2 depletion - class 1
Authors : Rebelo-Guiomar, P.; Pellegrino, S.; Dent, K.C.; Warren, A.J.; Minczuk, M.
Deposited on : 2021-12-10
Resolution : 3.08 Å(reported)
Based on initial model : 5OOL

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

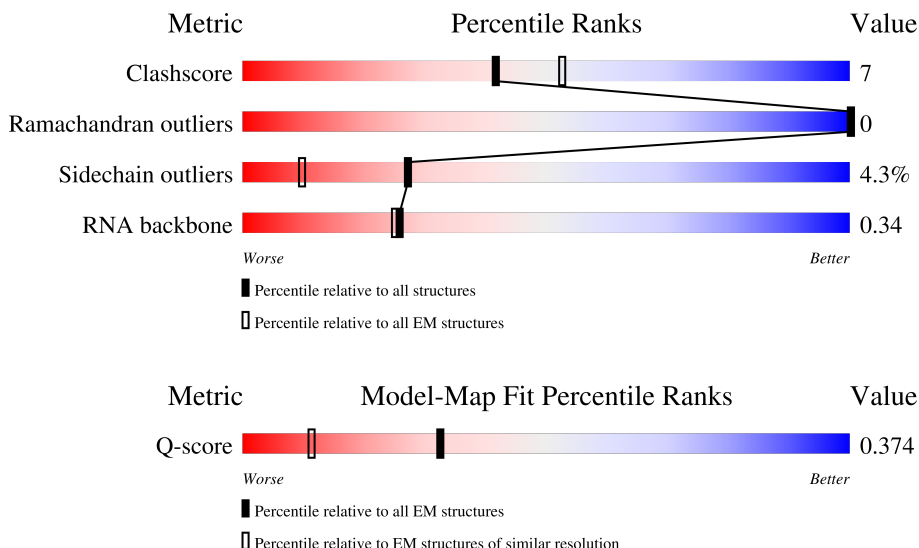
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.08 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.



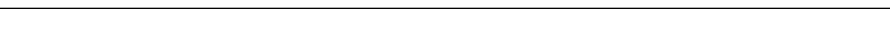
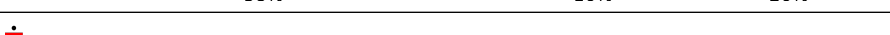
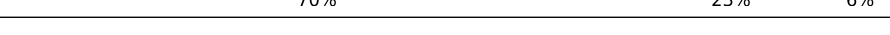
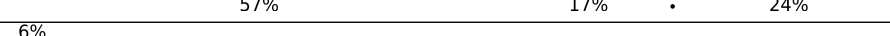
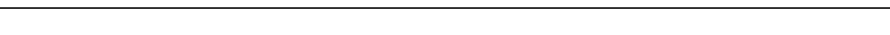
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14000 (2.58 - 3.58)

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	

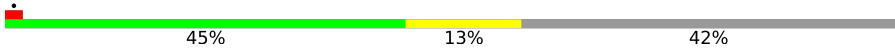
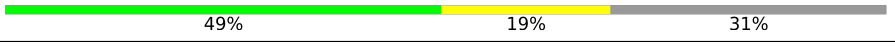
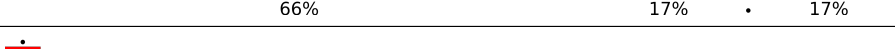
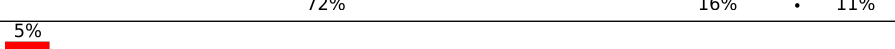
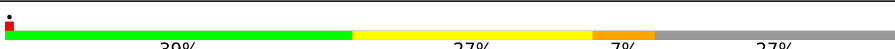
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Mol	Chain	Length	Quality of chain
4	H	267	
5	K	178	
6	L	145	
7	M	296	
8	N	251	
9	O	175	
10	P	180	
11	Q	292	
12	R	149	
13	S	205	
14	T	206	
15	U	153	
16	V	216	
17	W	148	
18	X	256	
19	Y	250	
20	Z	161	
21	0	188	
22	1	65	
23	2	92	
24	3	188	
25	5	423	
26	6	380	
27	7	338	
28	9	137	

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Mol	Chain	Length	Quality of chain
29	a	142	
30	b	215	
31	c	332	
32	d	306	
33	g	166	
34	h	158	
35	i	128	
36	j	123	
37	o	102	
38	p	206	
39	q	222	
40	r	196	
41	s	439	
42	u	234	
43	v	70	
44	w	156	
45	A	1559	
46	B	69	

2 Entry composition

There are 47 unique types of molecules in this entry. The entry contains 83425 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	174	Total	C	N	O	S	0	0
			1349	834	268	240	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	284	Total	C	N	O	S	0	0
			2249	1451	382	405	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	0	0
			784	498	152	134		

- Molecule 5 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L24, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	163	Total	C	N	O	S	0	0
			1333	848	231	247	7		

- Molecule 17 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L30, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	117	Total	C	N	O	S	0	0
			955	610	179	163	3		

- Molecule 21 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	0	108	Total	C	N	O	S	0	0
			880	545	172	157	6		

- Molecule 22 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	1	52	Total	C	N	O	S	0	0
			433	278	83	70	2		

- Molecule 23 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	2	45	Total	C	N	O	S	0	0
			367	227	81	58	1		

- Molecule 24 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 25 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	5	373	Total	C	N	O	S	0	0
			3037	1964	526	536	11		

- Molecule 26 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 27 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 28 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 29 is a protein called 39S ribosomal protein L42, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	a	82	Total	C	N	O	S	0	0
			686	434	124	123	5		

- Molecule 30 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 31 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 32 is a protein called 39S ribosomal protein L45, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	d	185	Total	C	N	O	S	0	0
			1529	989	260	271	9		

- Molecule 33 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 37 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	91	Total	C	N	O	S	0	0
			771	487	156	125	3		

- Molecule 38 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 39 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	q	128	Total	C	N	O	S	0	0
			1076	671	208	192	5		

- Molecule 40 is a protein called 39S ribosomal protein S18a, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	r	130	Total	C	N	O	S	0	0
			1075	683	210	174	8		

- Molecule 41 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 42 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 43 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 44 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 45 is a RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	A	1133	Total	C	N	O	P	0	0
			24063	10801	4361	7768	1133		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3107	U	UNK	conflict	GB 1025814679

- Molecule 46 is a RNA chain called mitochondrial tRNAVal.

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

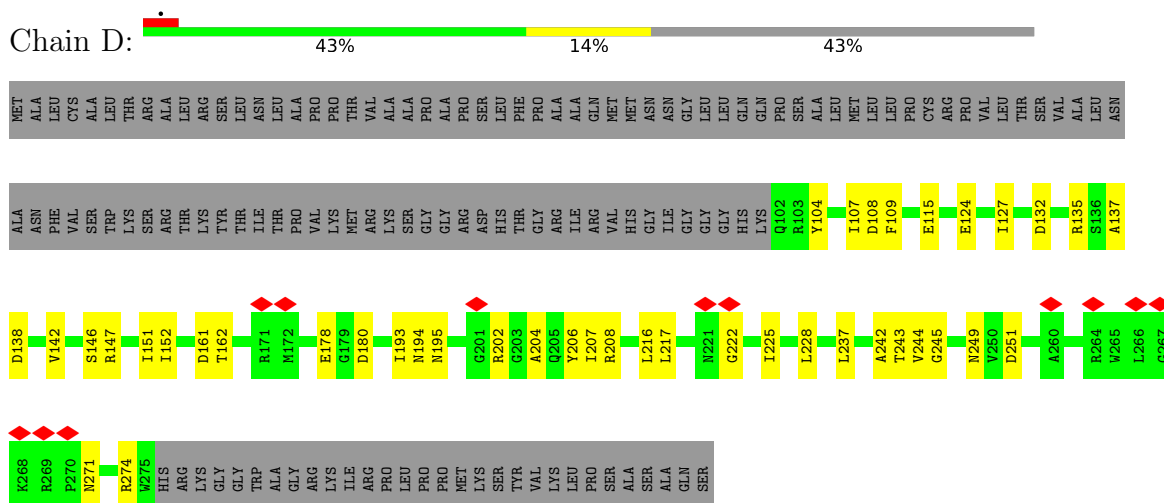
- Molecule 47 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
47	0	1	Total	Zn	0
			1	1	

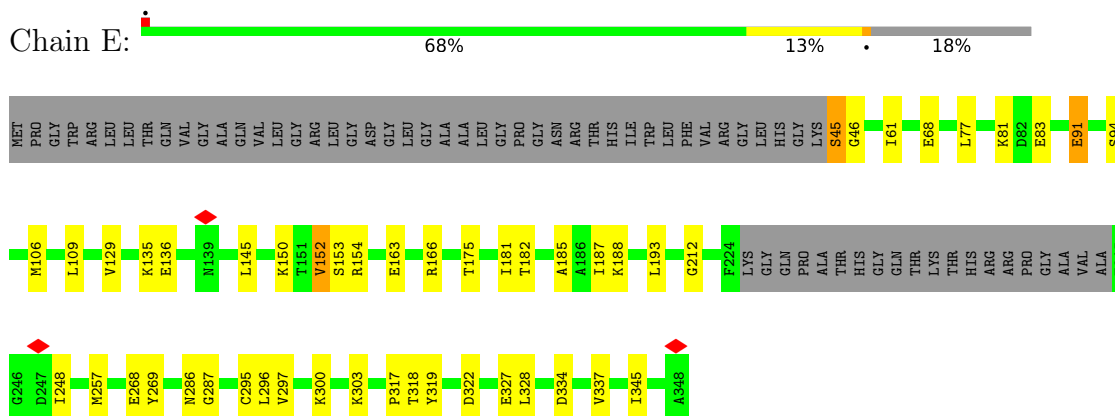
3 Residue-property plots

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.

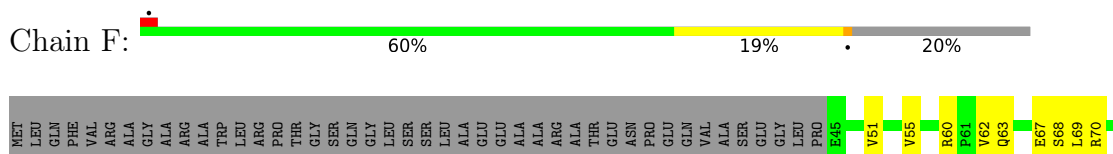
- Molecule 1: 39S ribosomal protein L2, mitochondrial

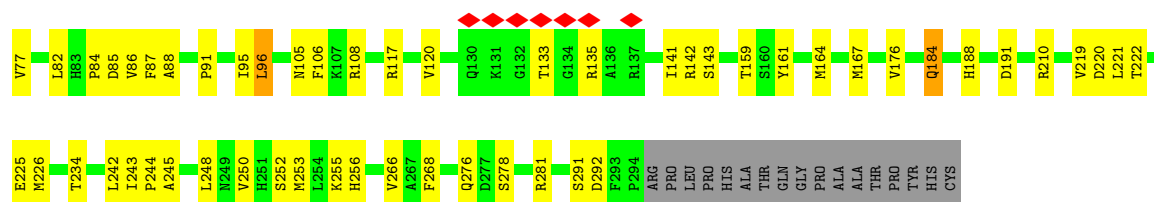


- Molecule 2: 39S ribosomal protein L3, mitochondrial

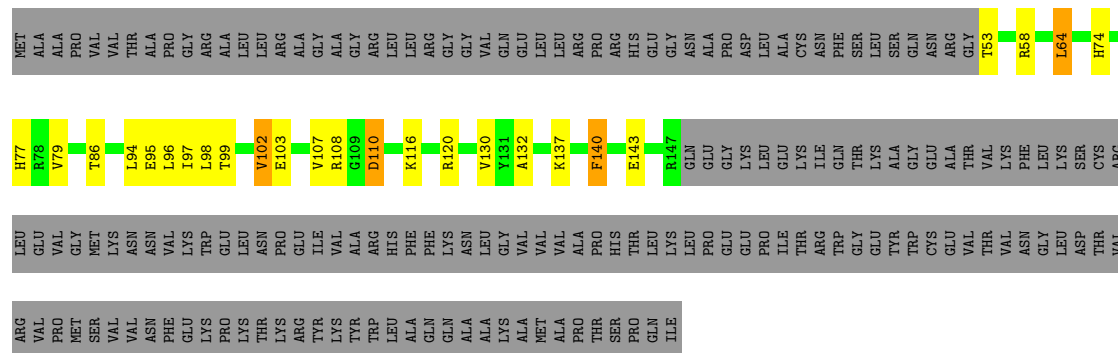


- Molecule 3: 39S ribosomal protein L4, mitochondrial

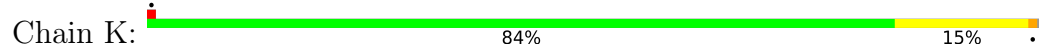




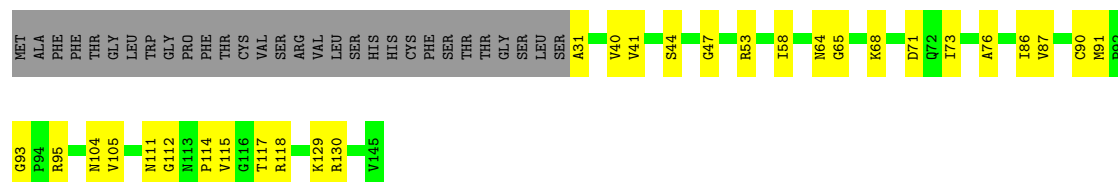
• Molecule 4: 39S ribosomal protein L9, mitochondrial



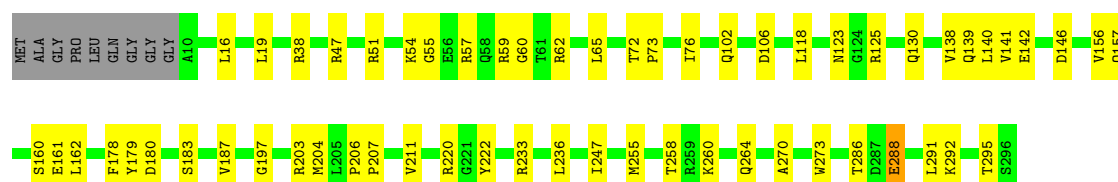
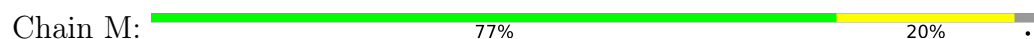
• Molecule 5: 39S ribosomal protein L13, mitochondrial



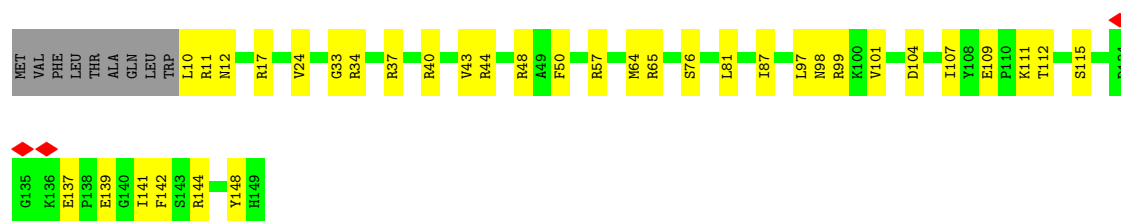
• Molecule 6: 39S ribosomal protein L14, mitochondrial



• Molecule 7: 39S ribosomal protein L15, mitochondrial

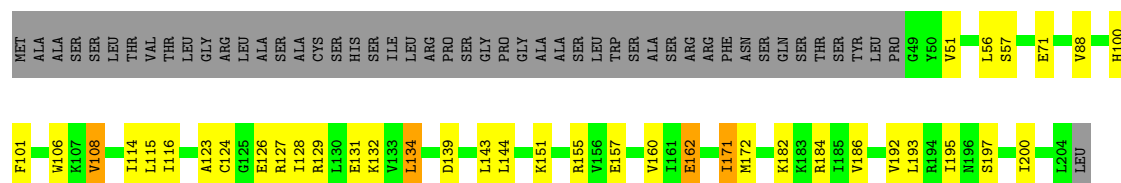


- Chain R: 70% 23% 6%



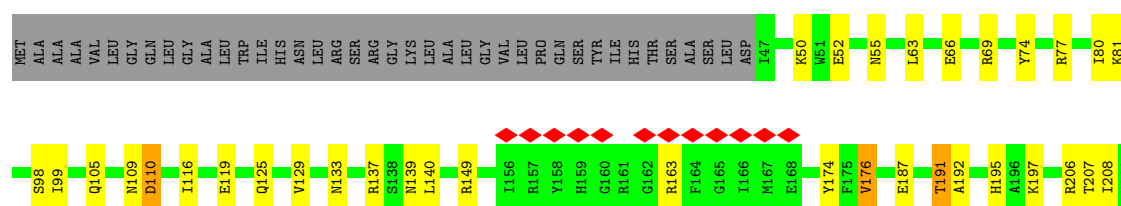
- Molecule 13: 39S ribosomal protein L21, mitochondrial

Chain S:



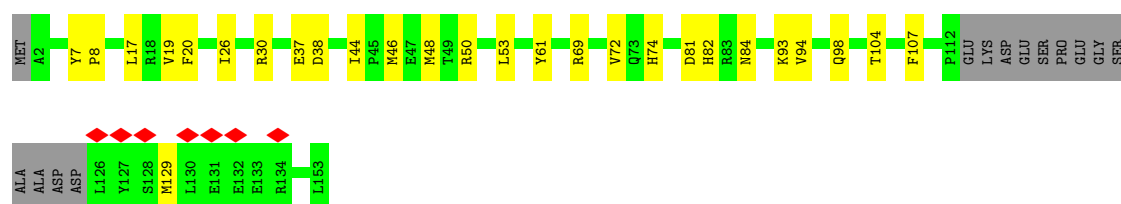
- Molecule 14: 39S ribosomal protein L22, mitochondrial

Chain T:



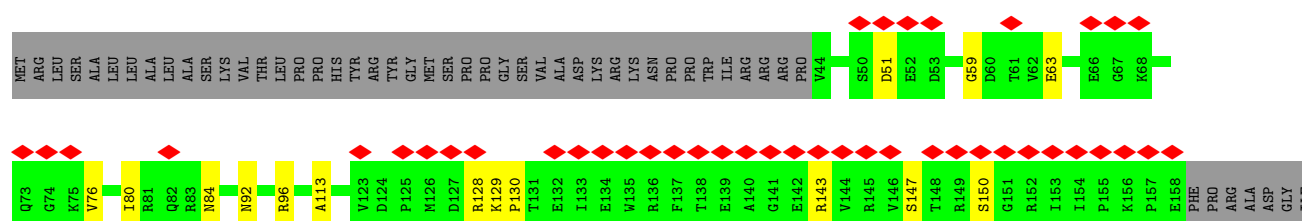
- Molecule 15: 39S ribosomal protein L23, mitochondrial

Chain U:



- Molecule 16: 39S ribosomal protein L24, mitochondrial

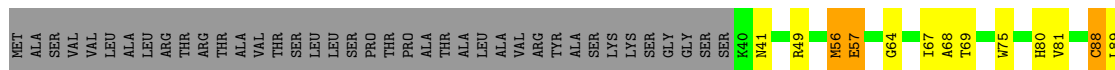
Chain V:





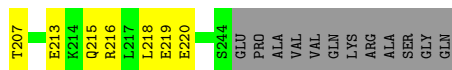
- Molecule 17: 39S ribosomal protein L27, mitochondrial

Chain W: 55% 17% 26%



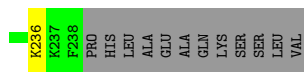
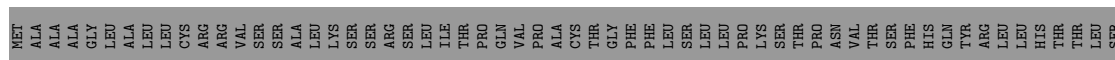
- Molecule 18: 39S ribosomal protein L28, mitochondrial

Chain X: 80% 15% 5%



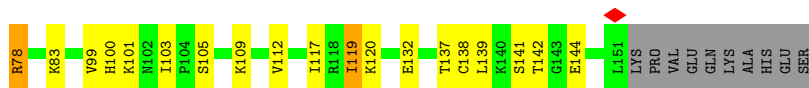
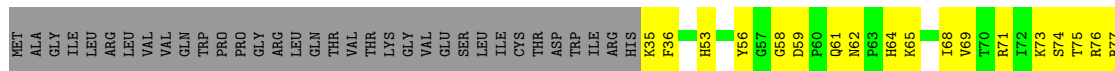
- Molecule 19: 39S ribosomal protein L47, mitochondrial

Chain Y: 56% 14% 30%



- Molecule 20: 39S ribosomal protein L30, mitochondrial

Chain Z: 50% 22% 27%



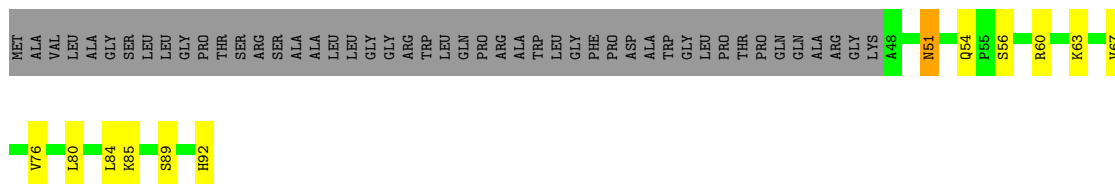
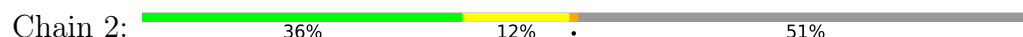
- Molecule 21: 39S ribosomal protein L32, mitochondrial

Chain 0: 41% 15% 43%

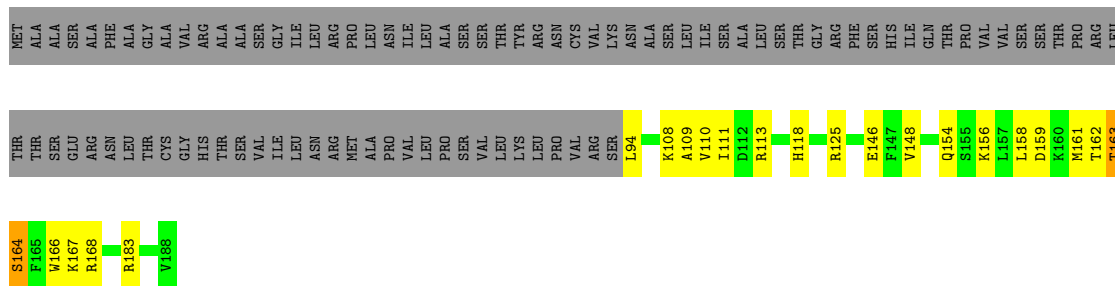
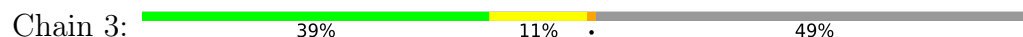
- Molecule 22: 39S ribosomal protein L33, mitochondrial



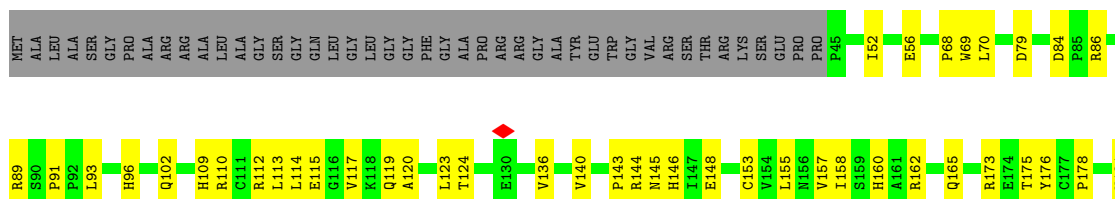
- Molecule 23: 39S ribosomal protein L34, mitochondrial

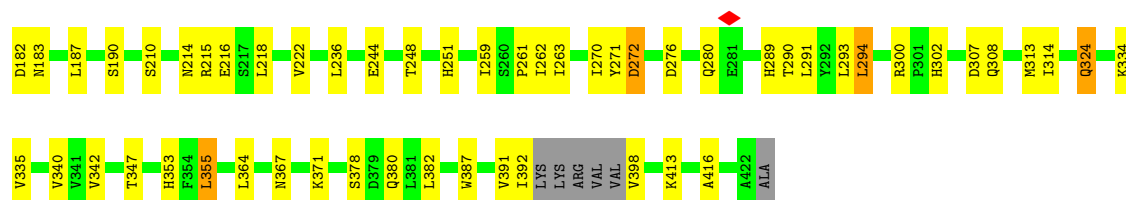


- Molecule 24: 39S ribosomal protein L35, mitochondrial



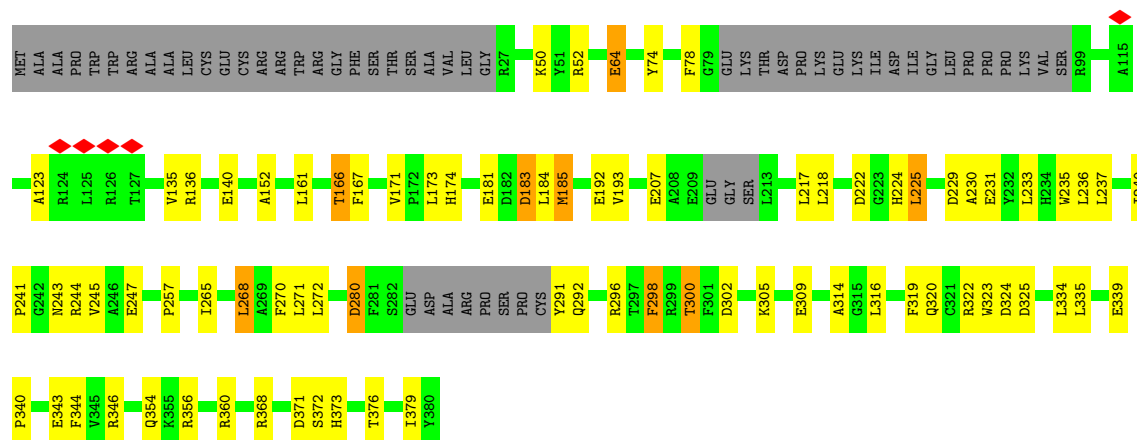
- Molecule 25: 39S ribosomal protein L37, mitochondrial





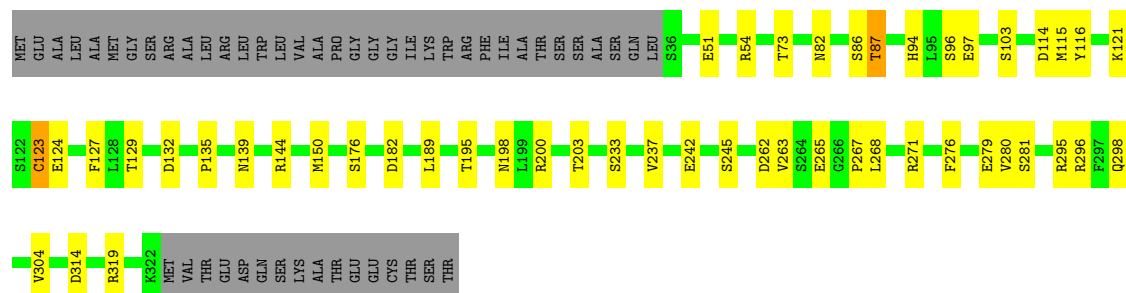
- Molecule 26: 39S ribosomal protein L38, mitochondrial

Chain 6: 64% 19% 15%



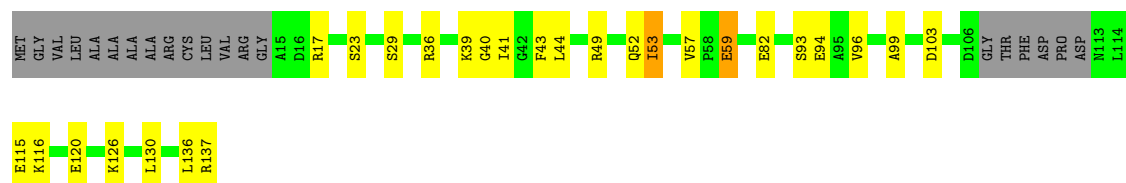
- Molecule 27: 39S ribosomal protein L39, mitochondrial

Chain 7: 70% 14% 15%



- Molecule 28: 39S ribosomal protein L41, mitochondrial

Chain 9: 66% 18% 15%

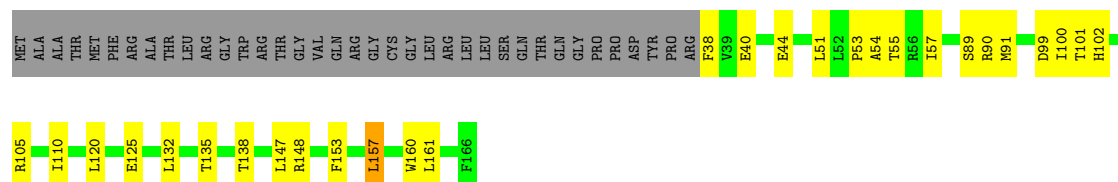


- Molecule 29: 39S ribosomal protein L42, mitochondrial



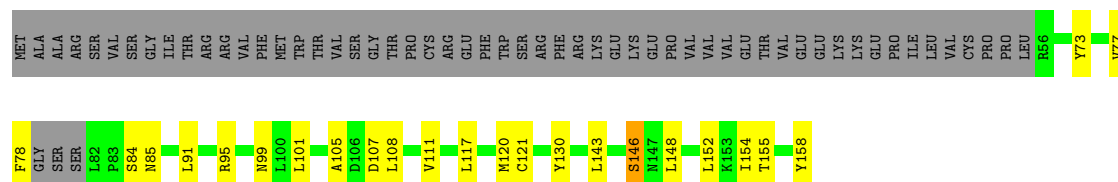
- Molecule 33: 39S ribosomal protein L49, mitochondrial

Chain g: 61% 16% 22%



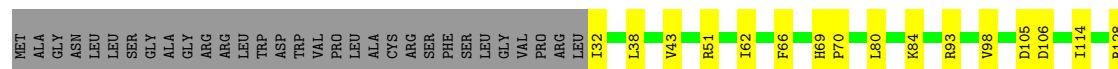
- Molecule 34: 39S ribosomal protein L50, mitochondrial

Chain h: 48% 15% 37%



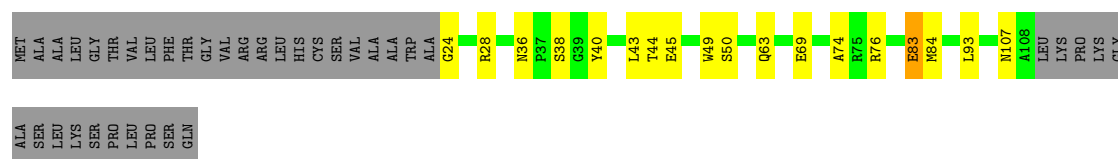
- Molecule 35: 39S ribosomal protein L51, mitochondrial

Chain i: 63% 12% 24%



- Molecule 36: 39S ribosomal protein L52, mitochondrial

Chain j: 54% 14% 31%

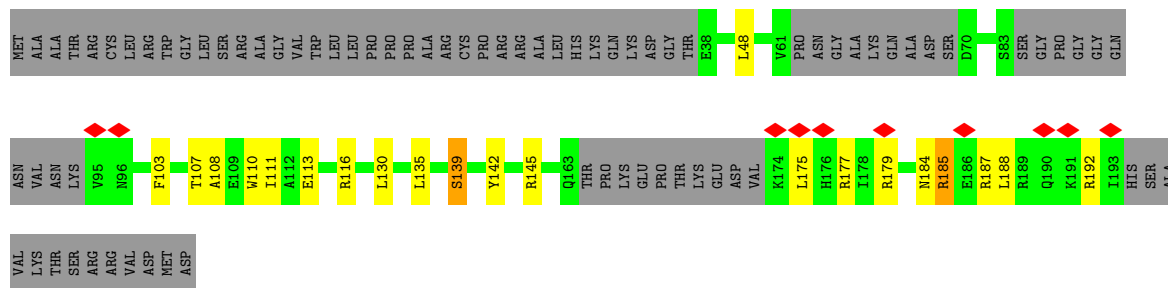


- Molecule 37: Ribosomal protein 63, mitochondrial

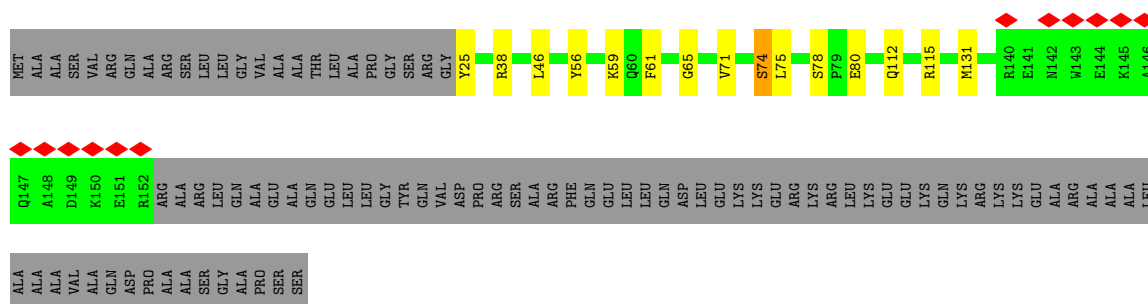
Chain o: 72% 16% 11%



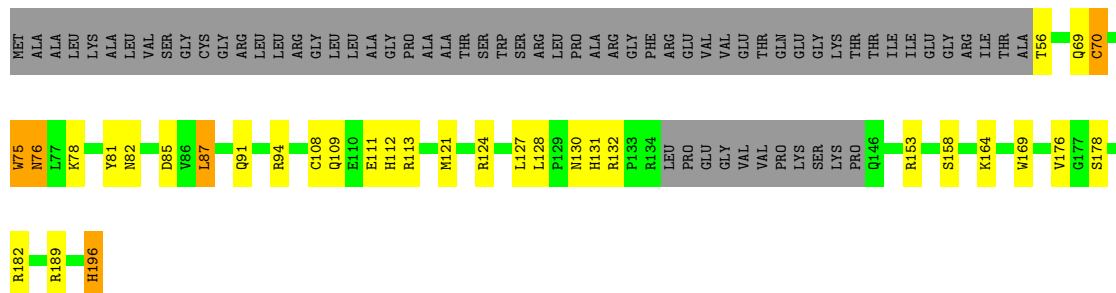
- Molecule 38: Peptidyl-tRNA hydrolase ICT1, mitochondrial



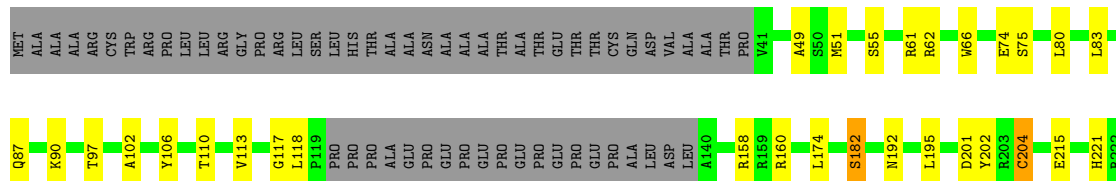
- Molecule 39: Growth arrest and DNA damage-inducible proteins-interacting protein 1



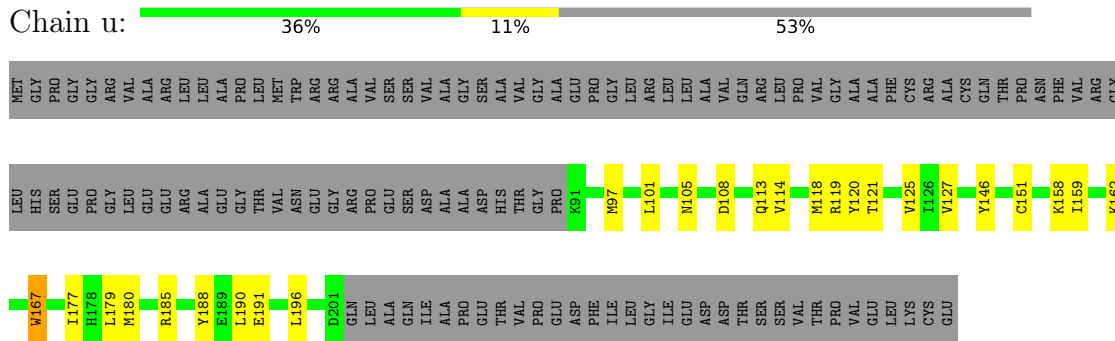
- Molecule 40: 39S ribosomal protein S18a, mitochondrial



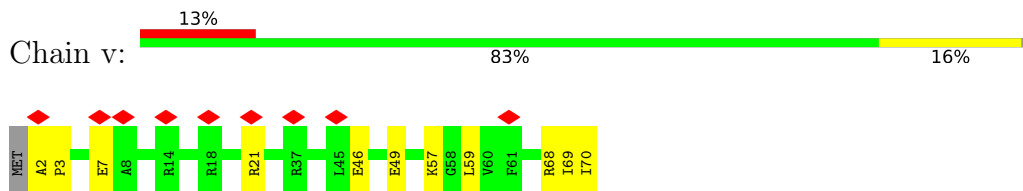
- Molecule 41: 39S ribosomal protein S30, mitochondrial



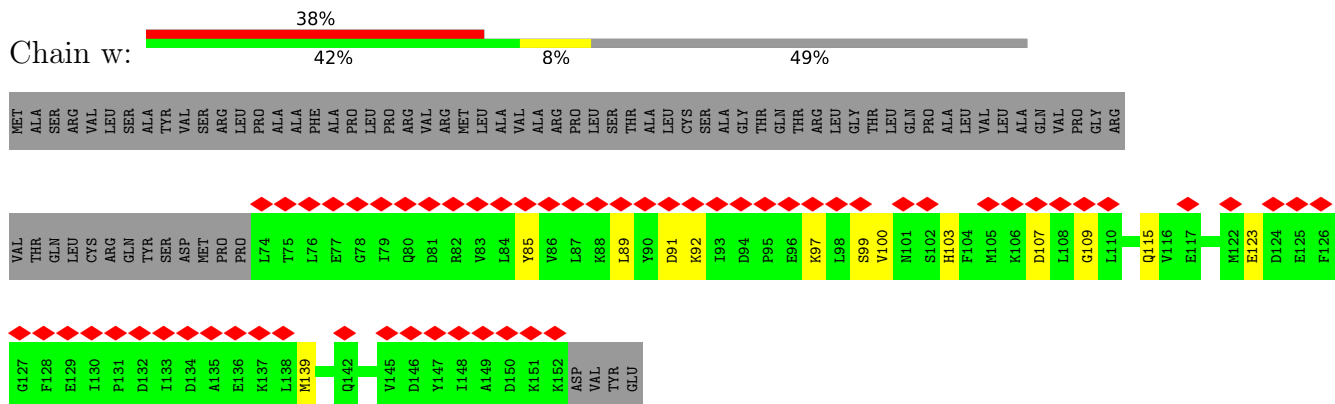
- Molecule 42: Mitochondrial assembly of ribosomal large subunit protein 1



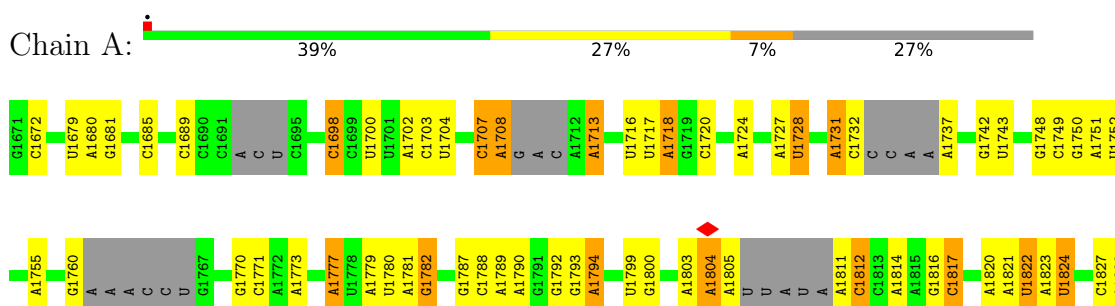
- Molecule 43: MIEF1 upstream open reading frame protein



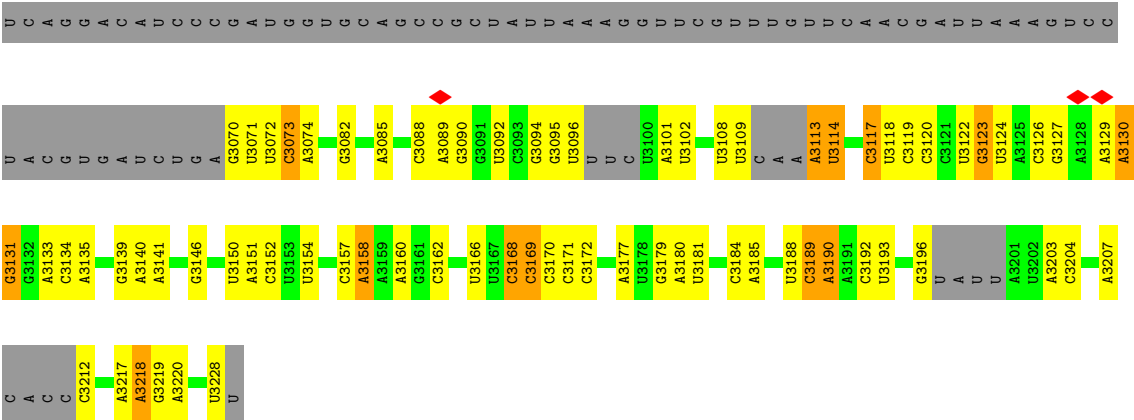
- Molecule 44: Acyl carrier protein, mitochondrial



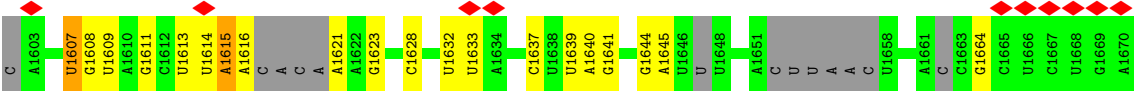
- Molecule 45: 16S ribosomal RNA







● Molecule 46: mitochondrial tRNA^{Val}



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119341	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.5	Depositor
Minimum defocus (nm)	-1000	Depositor
Maximum defocus (nm)	-2600	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.060	Depositor
Minimum map value	-0.020	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.19	0/1371	0.41	0/1848
2	E	0.25	0/2313	0.43	0/3137
3	F	0.35	0/2071	0.47	0/2817
4	H	0.26	0/798	0.47	0/1073
5	K	0.31	0/1495	0.44	0/2029
6	L	0.20	0/904	0.47	0/1218
7	M	0.31	0/2359	0.50	0/3185
8	N	0.22	0/1697	0.42	0/2281
9	O	0.29	0/1269	0.47	0/1708
10	P	0.23	0/1173	0.47	0/1588
11	Q	0.22	0/1846	0.47	0/2487
12	R	0.35	0/1174	0.51	0/1572
13	S	0.32	0/1276	0.52	0/1729
14	T	0.30	0/1402	0.49	0/1886
15	U	0.27	0/1183	0.46	0/1600
16	V	0.17	0/1362	0.34	0/1842
17	W	0.31	0/881	0.50	0/1188
18	X	0.26	0/2090	0.45	0/2825
19	Y	0.30	0/1552	0.45	0/2079
20	Z	0.29	0/979	0.47	0/1321
21	0	0.27	0/895	0.46	0/1201
22	1	0.20	0/438	0.46	0/583
23	2	0.40	0/373	0.60	0/496
24	3	0.38	0/852	0.48	0/1136
25	5	0.20	0/3126	0.42	0/4259
26	6	0.25	0/2726	0.45	0/3715
27	7	0.22	0/2391	0.42	0/3234
28	9	0.27	0/972	0.46	0/1306
29	a	0.29	0/709	0.53	0/963
30	b	0.32	0/1202	0.50	0/1626
31	c	0.26	0/2264	0.42	0/3059
32	d	0.17	0/1573	0.39	0/2134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	g	0.33	0/1102	0.52	0/1503
34	h	0.23	0/847	0.43	0/1150
35	i	0.38	0/849	0.50	0/1135
36	j	0.27	0/698	0.54	0/940
37	o	0.30	0/792	0.46	0/1064
38	p	0.20	0/1071	0.37	0/1433
39	q	0.24	0/1107	0.41	0/1498
40	r	0.24	0/1110	0.45	0/1504
41	s	0.25	0/3114	0.46	0/4225
42	u	0.16	0/949	0.33	0/1281
43	v	0.17	0/597	0.40	0/796
44	w	0.16	0/647	0.37	0/871
45	A	0.30	0/26912	0.39	0/41848
46	B	0.11	0/1328	0.25	0/2056
All	All	0.27	0/87839	0.43	0/124429

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

Mol	Chain	#Chirality outliers	#Planarity outliers
13	S	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
13	S	101	PHE	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	1349	0	1378	28	0
2	E	2249	0	2251	32	0
3	F	2013	0	2044	44	0
4	H	784	0	832	18	0
5	K	1451	0	1448	27	0
6	L	889	0	941	15	0
7	M	2305	0	2378	39	0
8	N	1654	0	1681	17	0
9	O	1245	0	1283	33	0
10	P	1148	0	1148	25	0
11	Q	1805	0	1841	32	0
12	R	1153	0	1214	30	0
13	S	1251	0	1322	28	0
14	T	1368	0	1410	24	0
15	U	1154	0	1154	21	0
16	V	1333	0	1337	15	0
17	W	859	0	888	21	0
18	X	2035	0	2054	20	0
19	Y	1517	0	1561	24	0
20	Z	955	0	1001	27	0
21	0	880	0	902	19	0
22	1	433	0	475	8	0
23	2	367	0	393	11	0
24	3	831	0	883	16	0
25	5	3037	0	3026	63	0
26	6	2640	0	2464	56	0
27	7	2334	0	2343	30	0
28	9	947	0	949	18	0
29	a	686	0	658	12	0
30	b	1178	0	1180	32	0
31	c	2217	0	2220	39	0
32	d	1529	0	1510	29	0
33	g	1067	0	1056	19	0
34	h	827	0	806	13	0
35	i	827	0	857	16	0
36	j	684	0	673	16	0
37	o	771	0	775	16	0
38	p	1058	0	1083	13	0
39	q	1076	0	1049	9	0
40	r	1075	0	1090	24	0
41	s	3036	0	3022	51	0
42	u	927	0	921	18	0
43	v	588	0	604	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
44	w	638	0	637	7	0
45	A	24063	0	12238	221	0
46	B	1191	0	607	6	0
47	0	1	0	0	0	0
All	All	83425	0	71587	1029	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 7.

All (1029) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:234:THR:O	39:q:25:TYR:N	2.10	0.84
18:X:96:LYS:O	45:A:1728:U:O2'	1.95	0.83
9:O:41:ARG:NH2	21:0:134:THR:OG1	2.11	0.83
27:7:135:PRO:O	27:7:139:ASN:ND2	2.11	0.83
9:O:37:VAL:HG21	9:O:80:LEU:HD22	1.62	0.82
30:b:9:ARG:NH1	30:b:111:ASP:O	2.13	0.82
9:O:9:ILE:N	45:A:2458:A:OP1	2.12	0.81
45:A:2093:U:O2	45:A:2266:U:O2'	1.99	0.81
17:W:57:GLU:OE2	45:A:2063:G:O2'	1.99	0.80
5:K:71:LYS:NZ	45:A:2240:C:OP2	2.15	0.80
3:F:281:ARG:NH1	45:A:1883:G:N7	2.29	0.80
36:j:36:ASN:OD1	36:j:38:SER:OG	1.99	0.79
45:A:2925:U:O2'	45:A:2927:C:OP1	2.01	0.79
45:A:1866:U:O2	45:A:2298:A:N6	2.14	0.79
13:S:131:GLU:OE2	36:j:50:SER:OG	2.02	0.78
23:2:85:LYS:NZ	45:A:1792:G:OP2	2.16	0.78
40:r:182:ARG:NH2	45:A:2157:U:OP1	2.17	0.78
1:D:194:ASN:ND2	1:D:245:GLY:O	2.17	0.78
6:L:58:ILE:HD11	6:L:76:ALA:HB2	1.66	0.77
15:U:30:ARG:NH2	19:Y:118:GLU:OE2	2.17	0.77
17:W:101:LYS:NZ	45:A:2064:A:OP1	2.17	0.77
25:5:109:HIS:NE2	45:A:2408:U:O2'	2.15	0.77
45:A:1874:A:O2'	45:A:2090:A:O2'	2.02	0.77
37:o:28:SER:OG	45:A:2154:A:OP1	2.02	0.77
45:A:1874:A:HO2'	45:A:2090:A:HO2'	1.25	0.77
31:c:170:ALA:HB3	31:c:191:LEU:HD21	1.66	0.77
15:U:26:ILE:HD12	15:U:44:ILE:HG22	1.67	0.76
5:K:60:MET:SD	5:K:61:ASN:ND2	2.59	0.76
25:5:215:ARG:NH2	25:5:364:LEU:O	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:A:1822:U:O2	45:A:2707:A:O2'	2.02	0.76
7:M:288:GLU:OE1	7:M:292:LYS:NZ	2.18	0.76
45:A:2863:U:O2	45:A:2869:A:N6	2.19	0.76
3:F:255:LYS:NZ	45:A:2279:U:OP1	2.12	0.76
20:Z:99:VAL:O	36:j:76:ARG:NH2	2.19	0.75
21:O:159:LEU:HD12	21:O:174:ILE:HD11	1.67	0.75
3:F:67:GLU:OE2	3:F:188:HIS:ND1	2.18	0.75
12:R:99:ARG:NH2	45:A:2248:U:OP1	2.19	0.75
38:p:108:ALA:O	38:p:116:ARG:NH2	2.19	0.75
45:A:1811:A:O2'	45:A:1812:C:OP1	2.04	0.75
45:A:3123:G:N2	45:A:3133:A:OP2	2.18	0.75
25:5:300:ARG:NH2	45:A:2395:A:OP2	2.20	0.75
9:O:143:THR:OG1	9:O:146:ASN:OD1	2.05	0.75
7:M:140:LEU:HD23	7:M:156:VAL:HG11	1.69	0.74
26:6:280:ASP:OD1	26:6:280:ASP:N	2.17	0.74
12:R:76:SER:OG	12:R:81:LEU:O	2.02	0.74
5:K:2:SER:OG	31:c:309:GLU:OE2	2.05	0.74
46:B:1607:U:O2	46:B:1664:G:O6	2.05	0.74
30:b:30:SER:OG	31:c:65:ASN:OD1	2.04	0.73
41:s:242:ARG:NH2	41:s:292:CYS:O	2.21	0.73
14:T:110:ASP:OD1	14:T:110:ASP:N	2.21	0.73
22:1:36:ARG:NH1	22:1:64:SER:OG	2.21	0.73
26:6:368:ARG:NH1	45:A:2860:G:OP2	2.21	0.73
2:E:257:MET:SD	45:A:2712:G:N2	2.62	0.73
12:R:57:ARG:NH1	45:A:2144:A:OP1	2.20	0.73
18:X:177:HIS:O	18:X:184:ARG:NH2	2.22	0.73
12:R:40:ARG:O	12:R:44:ARG:NH1	2.22	0.73
17:W:93:GLU:N	17:W:93:GLU:OE1	2.22	0.73
37:o:47:TYR:O	37:o:50:SER:OG	2.06	0.72
18:X:118:ILE:O	18:X:168:ARG:NH1	2.22	0.72
25:5:280:GLN:OE1	41:s:158:ARG:NH1	2.22	0.72
7:M:142:GLU:O	38:p:142:TYR:OH	2.04	0.72
10:P:118:SER:OG	10:P:121:ASN:ND2	2.22	0.72
26:6:305:LYS:NZ	36:j:107:ASN:OD1	2.23	0.72
34:h:105:ALA:HB1	34:h:111:VAL:HG22	1.70	0.72
45:A:1749:C:OP2	45:A:2899:C:O2'	2.07	0.72
45:A:2694:A:O2'	45:A:2695:G:OP1	2.04	0.72
40:r:164:LYS:NZ	45:A:2236:C:OP1	2.22	0.72
43:v:21:ARG:NH2	44:w:123:GLU:OE1	2.22	0.72
23:2:51:ASN:OD1	45:A:2435:G:N2	2.23	0.72
45:A:1718:A:O2'	45:A:1911:C:O2'	1.99	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:X:102:LYS:O	45:A:2745:A:O2'	2.08	0.72
5:K:3:SER:O	31:c:302:ARG:NH1	2.23	0.71
44:w:92:LYS:NZ	44:w:109:GLY:O	2.23	0.71
1:D:204:ALA:O	1:D:208:ARG:NH1	2.23	0.71
5:K:2:SER:OG	5:K:3:SER:N	2.21	0.71
13:S:132:LYS:NZ	36:j:43:LEU:O	2.19	0.71
21:0:139:ARG:NH1	45:A:2322:C:OP2	2.23	0.71
24:3:156:LYS:NZ	45:A:1873:A:O2'	2.24	0.71
3:F:70:ARG:NH1	3:F:191:ASP:OD2	2.23	0.71
10:P:142:ASN:OD1	38:p:184:ASN:ND2	2.24	0.71
12:R:11:ARG:O	31:c:33:LYS:NZ	2.23	0.71
27:7:265:GLU:OE1	27:7:265:GLU:N	2.22	0.71
31:c:227:GLU:OE2	31:c:302:ARG:NE	2.24	0.71
32:d:192:SER:OG	32:d:216:MET:SD	2.48	0.71
16:V:195:GLN:OE1	16:V:195:GLN:N	2.23	0.71
32:d:281:MET:SD	32:d:281:MET:N	2.64	0.71
45:A:1986:A:O2'	45:A:1987:G:OP1	2.08	0.71
21:0:113:CYS:SG	21:0:115:HIS:ND1	2.63	0.71
27:7:200:ARG:NH2	27:7:279:GLU:OE2	2.24	0.71
40:r:70:CYS:SG	40:r:78:LYS:NZ	2.64	0.71
45:A:2824:C:O2'	45:A:2893:A:O2'	2.10	0.70
7:M:130:GLN:OE1	24:3:168:ARG:NH1	2.24	0.70
10:P:85:ARG:NH2	46:B:1640:A:OP1	2.24	0.70
21:0:106:ASN:OD1	45:A:3212:C:O2'	2.10	0.70
25:5:120:ALA:HB3	25:5:314:ILE:HD11	1.73	0.70
15:U:20:PHE:O	19:Y:99:HIS:NE2	2.24	0.70
28:9:115:GLU:OE1	28:9:115:GLU:N	2.25	0.70
25:5:112:ARG:NH2	45:A:2388:A:N7	2.39	0.70
45:A:2721:G:O2'	45:A:2724:G:N2	2.25	0.70
7:M:72:THR:OG1	45:A:2917:G:N7	2.24	0.69
13:S:162:GLU:OE1	30:b:108:SER:OG	2.03	0.69
1:D:104:TYR:OH	45:A:2528:G:OP1	2.09	0.69
5:K:75:LYS:NZ	45:A:2239:A:OP2	2.18	0.69
41:s:295:GLY:N	41:s:339:GLN:OE1	2.25	0.69
7:M:178:PHE:O	7:M:203:ARG:NH1	2.24	0.69
26:6:185:MET:SD	38:p:185:ARG:NH1	2.65	0.69
3:F:184:GLN:NE2	7:M:16:LEU:O	2.26	0.69
25:5:173:ARG:NH2	45:A:2395:A:OP1	2.25	0.69
31:c:100:SER:OG	31:c:182:GLU:OE1	2.08	0.69
2:E:81:LYS:NZ	2:E:322:ASP:OD1	2.26	0.69
8:N:231:SER:OG	8:N:234:ASP:OD1	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5:216:GLU:OE2	25:5:367:ASN:N	2.26	0.69
1:D:271:ASN:ND2	45:A:2510:U:OP1	2.26	0.69
2:E:61:ILE:HD11	9:O:149:LEU:HD22	1.75	0.68
9:O:97:TYR:OH	9:O:126:LYS:O	2.10	0.68
45:A:2310:G:O2'	45:A:2675:G:O6	2.07	0.68
30:b:103:LYS:NZ	30:b:107:GLN:OE1	2.26	0.68
41:s:106:TYR:O	41:s:110:THR:OG1	2.08	0.68
26:6:291:TYR:O	26:6:292:GLN:NE2	2.27	0.68
15:U:48:MET:O	15:U:93:LYS:NZ	2.25	0.68
3:F:105:ASN:OD1	45:A:2289:G:O2'	2.10	0.68
6:L:114:PRO:O	42:u:188:TYR:OH	2.12	0.68
13:S:127:ARG:NE	13:S:157:GLU:OE1	2.27	0.68
16:V:51:ASP:O	16:V:143:ARG:NH2	2.27	0.68
9:O:11:HIS:O	45:A:3158:A:O2'	2.05	0.67
26:6:166:THR:OG1	26:6:167:PHE:N	2.27	0.67
31:c:31:VAL:N	45:A:1773:A:OP2	2.27	0.67
10:P:41:ASN:ND2	26:6:335:LEU:O	2.26	0.67
6:L:90:CYS:SG	11:Q:191:ARG:NH1	2.68	0.67
20:Z:35:LYS:NZ	45:A:2118:U:O2'	2.27	0.67
25:5:110:ARG:NE	45:A:2386:C:O2	2.28	0.67
1:D:115:GLU:OE2	1:D:147:ARG:NH2	2.28	0.67
42:u:127:VAL:HG23	42:u:179:LEU:HD13	1.75	0.67
45:A:2002:G:O2'	45:A:2927:C:N3	2.21	0.67
45:A:2031:A:N6	45:A:2045:A:O4'	2.28	0.67
16:V:206:GLU:OE2	16:V:208:ARG:N	2.27	0.67
45:A:2135:A:OP1	45:A:2136:C:N4	2.20	0.67
41:s:51:MET:O	41:s:62:ARG:NH1	2.27	0.66
2:E:83:GLU:O	2:E:188:LYS:NZ	2.24	0.66
31:c:101:GLU:OE1	31:c:105:ARG:NE	2.28	0.66
18:X:56:ASN:OD1	18:X:57:GLY:N	2.29	0.66
1:D:202:ARG:NH2	45:A:2521:A:OP1	2.29	0.66
5:K:94:GLN:N	5:K:94:GLN:OE1	2.27	0.66
26:6:181:GLU:N	26:6:181:GLU:OE1	2.28	0.66
3:F:220:ASP:O	3:F:245:ALA:N	2.29	0.66
23:2:60:ARG:NE	45:A:1918:G:O6	2.26	0.66
28:9:103:ASP:OD2	28:9:116:LYS:NZ	2.27	0.66
27:7:114:ASP:OD1	27:7:268:LEU:N	2.28	0.66
19:Y:143:ASP:OD2	28:9:137:ARG:NH2	2.30	0.66
15:U:81:ASP:OD1	15:U:82:HIS:ND1	2.29	0.65
43:v:7:GLU:N	43:v:7:GLU:OE1	2.29	0.65
9:O:82:GLU:N	9:O:82:GLU:OE1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:132:GLU:N	20:Z:132:GLU:OE1	2.29	0.65
25:5:110:ARG:NH1	45:A:2408:U:O2	2.29	0.65
26:6:184:LEU:O	38:p:192:ARG:NH2	2.29	0.65
27:7:87:THR:OG1	27:7:115:MET:O	2.13	0.65
1:D:193:ILE:HD11	1:D:242:ALA:HB3	1.77	0.65
15:U:69:ARG:NH2	15:U:98:GLN:OE1	2.30	0.65
25:5:89:ARG:NH2	45:A:1708:A:N1	2.45	0.65
25:5:144:ARG:NH1	25:5:145:ASN:OD1	2.29	0.65
4:H:79:VAL:HG11	18:X:91:TYR:CE2	2.31	0.65
23:2:92:HIS:NE2	45:A:1789:A:OP1	2.30	0.65
41:s:271:LEU:O	41:s:273:LEU:N	2.30	0.65
45:A:1777:A:N6	45:A:1780:U:OP2	2.30	0.65
4:H:58:ARG:NH1	4:H:77:HIS:O	2.30	0.65
7:M:60:GLY:O	35:i:128:ARG:NH2	2.30	0.65
45:A:1884:G:N3	45:A:1895:C:O2'	2.30	0.65
3:F:82:LEU:HD22	3:F:266:VAL:HG21	1.78	0.65
11:Q:96:ARG:NE	11:Q:285:GLU:OE1	2.28	0.65
37:o:37:ARG:NH2	45:A:2151:A:OP1	2.30	0.65
45:A:2507:A:O2'	45:A:2508:C:OP1	2.11	0.65
14:T:149:ARG:NH1	45:A:2305:U:O3'	2.30	0.64
25:5:102:GLN:O	25:5:271:TYR:OH	2.13	0.64
7:M:161:GLU:N	7:M:161:GLU:OE1	2.30	0.64
45:A:1881:A:O2'	45:A:1893:A:N1	2.25	0.64
1:D:124:GLU:OE2	1:D:147:ARG:NH1	2.30	0.64
27:7:121:LYS:NZ	27:7:123:CYS:SG	2.70	0.64
33:g:40:GLU:OE1	33:g:40:GLU:N	2.30	0.64
40:r:124:ARG:NH2	40:r:153:ARG:O	2.30	0.64
45:A:3082:G:N2	45:A:3085:A:OP2	2.30	0.64
20:Z:69:VAL:HG22	20:Z:119:ILE:HG22	1.78	0.64
2:E:135:LYS:NZ	2:E:136:GLU:OE2	2.30	0.64
5:K:158:TYR:HE2	40:r:87:LEU:HD11	1.62	0.64
31:c:83:PHE:CD2	31:c:88:LEU:HD13	2.33	0.64
2:E:268:GLU:OE2	45:A:3146:G:N2	2.21	0.64
31:c:170:ALA:HB1	31:c:175:VAL:HG11	1.79	0.64
32:d:169:PHE:CZ	32:d:173:THR:HG21	2.32	0.64
45:A:1871:A:N6	45:A:1901:C:O2	2.31	0.64
14:T:133:ASN:ND2	32:d:226:ASP:OD2	2.30	0.64
41:s:113:VAL:HG21	41:s:259:ILE:HG23	1.80	0.64
41:s:319:GLN:OE1	41:s:319:GLN:N	2.31	0.64
5:K:30:LYS:NZ	45:A:2240:C:O3'	2.30	0.63
18:X:111:GLU:OE1	18:X:111:GLU:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:146:TYR:OH	10:P:158:MET:SD	2.56	0.63
18:X:97:LEU:HD12	45:A:2919:A:C6	2.33	0.63
45:A:2511:C:N4	45:A:2539:A:O2'	2.31	0.63
2:E:91:GLU:OE2	2:E:94:SER:OG	2.17	0.63
16:V:63:GLU:OE1	16:V:128:ARG:NH2	2.32	0.63
16:V:185:ARG:NH2	16:V:187:TYR:O	2.31	0.63
8:N:118:MET:HE1	8:N:167:CYS:HB3	1.81	0.63
40:r:82:ASN:N	40:r:85:ASP:OD2	2.32	0.63
6:L:31:ALA:N	6:L:91:MET:SD	2.72	0.63
9:O:56:ALA:HB1	9:O:125:TYR:OH	1.99	0.63
45:A:1698:C:O2'	45:A:1702:A:N3	2.30	0.63
3:F:86:VAL:HG13	3:F:87:PHE:HD2	1.63	0.63
9:O:110:ILE:HG13	9:O:122:VAL:HG23	1.81	0.63
28:9:120:GLU:OE1	28:9:126:LYS:NZ	2.31	0.62
41:s:182:SER:OG	41:s:202:TYR:OH	2.17	0.62
7:M:62:ARG:NH2	45:A:2042:U:OP1	2.31	0.62
27:7:51:GLU:OE1	27:7:54:ARG:NH1	2.32	0.62
33:g:110:ILE:HD11	33:g:157:LEU:CD2	2.28	0.62
16:V:59:GLY:N	16:V:76:VAL:O	2.32	0.62
41:s:83:LEU:HD23	41:s:83:LEU:O	2.00	0.62
41:s:350:ASP:OD1	41:s:389:ARG:NH2	2.32	0.62
25:5:293:LEU:HD21	25:5:313:MET:HG2	1.81	0.62
20:Z:78:ARG:O	20:Z:83:LYS:NZ	2.33	0.62
27:7:115:MET:HE1	27:7:127:PHE:HD1	1.64	0.62
36:j:44:THR:O	36:j:63:GLN:NE2	2.32	0.62
45:A:1997:C:OP1	45:A:2500:A:N6	2.33	0.62
29:a:62:HIS:O	29:a:62:HIS:ND1	2.33	0.62
5:K:115:ASN:N	5:K:115:ASN:OD1	2.32	0.61
22:1:55:LEU:HD22	39:q:131:MET:HE1	1.82	0.61
30:b:21:ARG:NE	31:c:217:ASP:OD2	2.32	0.61
6:L:111:ASN:OD1	6:L:112:GLY:N	2.33	0.61
45:A:2016:C:OP1	45:A:2039:A:O2'	2.17	0.61
34:h:95:ARG:NH1	34:h:99:ASN:OD1	2.33	0.61
30:b:114:ARG:NH2	45:A:1832:A:O5'	2.32	0.61
41:s:332:LEU:HD21	41:s:359:ALA:HB2	1.82	0.61
46:B:1609:U:O2	46:B:1616:A:N7	2.34	0.61
26:6:152:ALA:HB2	26:6:316:LEU:HD11	1.83	0.61
27:7:233:SER:O	27:7:237:VAL:HG23	2.01	0.61
45:A:1707:C:O2'	45:A:1708:A:OP2	2.16	0.61
16:V:147:SER:OG	16:V:150:SER:O	2.14	0.61
19:Y:63:GLY:N	19:Y:65:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
42:u:146:TYR:OH	42:u:151:CYS:SG	2.48	0.61
7:M:65:LEU:HD23	24:3:94:LEU:HD21	1.81	0.61
21:0:168:GLN:N	21:0:168:GLN:OE1	2.33	0.61
25:5:302:HIS:O	25:5:302:HIS:ND1	2.34	0.61
8:N:99:TRP:NE1	8:N:103:GLU:OE2	2.34	0.61
13:S:129:ARG:NH2	13:S:151:LYS:O	2.34	0.60
45:A:3113:A:O2'	45:A:3114:U:O5'	2.16	0.60
45:A:2111:C:O2	45:A:2944:C:O2'	2.19	0.60
33:g:110:ILE:HD11	33:g:157:LEU:HD22	1.83	0.60
10:P:86:THR:HG21	46:B:1623:G:H5''	1.82	0.60
41:s:235:ASP:OD1	41:s:236:LYS:N	2.34	0.60
18:X:151:GLU:OE1	18:X:151:GLU:N	2.34	0.60
40:r:176:VAL:HG21	40:r:196:HIS:ND1	2.17	0.60
12:R:139:GLU:OE2	12:R:144:ARG:NE	2.34	0.60
45:A:3180:A:O2'	45:A:3181:U:O4'	2.17	0.60
3:F:86:VAL:HG13	3:F:87:PHE:CD2	2.37	0.59
4:H:110:ASP:OD1	4:H:110:ASP:N	2.32	0.59
25:5:236:LEU:HD21	25:5:289:HIS:NE2	2.17	0.59
42:u:191:GLU:OE1	42:u:191:GLU:N	2.34	0.59
5:K:45:PRO:O	12:R:107:ILE:HD11	2.02	0.59
7:M:140:LEU:CD2	7:M:156:VAL:HG11	2.32	0.59
42:u:196:LEU:HD21	43:v:57:LYS:HG3	1.83	0.59
1:D:146:SER:HA	25:5:263:ILE:HG22	1.84	0.59
42:u:159:ILE:O	42:u:162:LYS:NZ	2.35	0.59
45:A:2934:G:N1	45:A:2938:A:N7	2.50	0.59
17:W:75:TRP:O	17:W:89:LEU:HD11	2.02	0.59
25:5:165:GLN:NE2	41:s:204:CYS:SG	2.75	0.59
38:p:139:SER:O	38:p:139:SER:OG	2.16	0.59
39:q:38:ARG:O	39:q:56:TYR:OH	2.15	0.59
2:E:248:ILE:O	45:A:2715:A:O2'	2.18	0.59
7:M:47:ARG:NH1	45:A:1847:U:OP1	2.33	0.59
11:Q:250:THR:OG1	11:Q:253:GLN:OE1	2.15	0.59
33:g:44:GLU:OE1	33:g:44:GLU:N	2.36	0.59
36:j:24:GLY:O	36:j:28:ARG:NH2	2.36	0.59
5:K:50:LEU:O	45:A:1835:A:N6	2.28	0.59
17:W:148:LEU:O	26:6:339:GLU:N	2.35	0.59
41:s:242:ARG:NH1	41:s:286:SER:OG	2.36	0.59
4:H:103:GLU:N	4:H:103:GLU:OE1	2.36	0.59
11:Q:232:ARG:NH2	45:A:2467:A:OP2	2.36	0.59
20:Z:142:THR:HG23	20:Z:144:GLU:OE1	2.03	0.59
26:6:136:ARG:NH2	26:6:140:GLU:OE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:A:2484:C:O2'	45:A:2485:U:O4'	2.18	0.58
11:Q:152:ARG:NH1	11:Q:190:LEU:O	2.36	0.58
12:R:17:ARG:NH2	45:A:2295:C:OP2	2.36	0.58
31:c:106:GLN:N	31:c:106:GLN:OE1	2.36	0.58
9:O:23:GLU:OE1	9:O:27:HIS:NE2	2.37	0.58
26:6:183:ASP:N	26:6:183:ASP:OD1	2.36	0.58
30:b:77:ALA:HB2	30:b:104:LEU:HD13	1.85	0.58
1:D:161:ASP:OD1	1:D:162:THR:N	2.36	0.58
7:M:51:ARG:NH1	7:M:57:ARG:O	2.37	0.58
11:Q:141:SER:OG	45:A:3152:C:OP1	2.19	0.58
26:6:241:PRO:O	26:6:244:ARG:NH1	2.36	0.58
27:7:176:SER:O	27:7:319:ARG:NH2	2.36	0.58
15:U:81:ASP:OD1	15:U:82:HIS:N	2.35	0.58
12:R:34:ARG:NH2	45:A:2682:A:OP1	2.36	0.58
12:R:112:THR:O	12:R:115:SER:OG	2.16	0.58
28:9:23:SER:OG	45:A:2420:U:O2'	2.22	0.58
3:F:167:MET:HE1	35:i:66:PHE:CE2	2.39	0.58
7:M:73:PRO:HG2	7:M:76:ILE:HD12	1.86	0.58
12:R:139:GLU:N	12:R:139:GLU:OE1	2.36	0.58
27:7:150:MET:HE3	27:7:280:VAL:HG12	1.86	0.58
40:r:69:GLN:O	40:r:69:GLN:NE2	2.37	0.58
14:T:80:ILE:HG23	14:T:116:ILE:HD13	1.86	0.57
14:T:163:ARG:O	45:A:2430:A:N6	2.37	0.57
24:3:110:VAL:HG21	24:3:161:MET:HE3	1.86	0.57
1:D:222:GLY:O	1:D:237:LEU:HD12	2.03	0.57
13:S:100:HIS:ND1	13:S:100:HIS:O	2.35	0.57
18:X:69:ILE:HG22	18:X:86:ILE:CD1	2.34	0.57
2:E:327:GLU:N	2:E:327:GLU:OE2	2.37	0.57
4:H:64:LEU:O	45:A:1755:A:O2'	2.20	0.57
11:Q:154:VAL:HG12	11:Q:198:SER:O	2.04	0.57
13:S:108:VAL:CG1	13:S:195:ILE:HG21	2.34	0.57
24:3:108:LYS:NZ	45:A:1743:U:OP2	2.29	0.57
25:5:251:HIS:O	25:5:371:LYS:NZ	2.26	0.57
26:6:379:ILE:HD13	45:A:1882:A:C6	2.39	0.57
28:9:49:ARG:NH1	45:A:2416:U:O2	2.37	0.57
27:7:195:THR:N	27:7:198:ASN:OD1	2.36	0.57
41:s:160:ARG:NE	45:A:2409:A:OP1	2.38	0.57
45:A:2695:G:OP1	45:A:2941:G:O2'	2.17	0.57
1:D:216:LEU:HD23	1:D:217:LEU:N	2.19	0.57
9:O:62:TYR:OH	11:Q:272:GLU:OE1	2.18	0.57
15:U:61:TYR:OH	19:Y:110:ASN:ND2	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:5:113:LEU:O	25:5:308:GLN:NE2	2.36	0.57
27:7:94:HIS:ND1	32:d:281:MET:SD	2.76	0.57
30:b:34:SER:O	30:b:44:ARG:NH1	2.36	0.57
45:A:1852:C:O4'	45:A:2693:A:N6	2.38	0.57
22:1:34:ARG:NH2	22:1:38:ARG:O	2.38	0.57
38:p:111:ILE:O	38:p:116:ARG:NH2	2.38	0.57
40:r:81:TYR:OH	40:r:111:GLU:OE1	2.08	0.57
44:w:103:HIS:NE2	44:w:139:MET:SD	2.78	0.57
1:D:132:ASP:OD2	1:D:135:ARG:NH1	2.37	0.57
2:E:300:LYS:NZ	45:A:3204:C:OP1	2.30	0.57
45:A:2113:G:H22	45:A:2693:A:H4'	1.70	0.57
10:P:123:VAL:HG21	26:6:123:ALA:HA	1.87	0.57
21:0:119:LYS:O	21:0:120:HIS:ND1	2.38	0.57
17:W:81:VAL:HG11	17:W:131:VAL:HG13	1.86	0.56
12:R:97:LEU:HD22	12:R:101:VAL:HG21	1.86	0.56
26:6:244:ARG:NH1	26:6:247:GLU:OE2	2.37	0.56
2:E:286:ASN:OD1	2:E:287:GLY:N	2.38	0.56
6:L:117:THR:O	6:L:118:ARG:NH2	2.38	0.56
7:M:125:ARG:NH1	33:g:54:ALA:O	2.38	0.56
7:M:220:ARG:NH2	7:M:236:LEU:HD12	2.19	0.56
12:R:104:ASP:CG	14:T:212:LEU:HD13	2.30	0.56
17:W:56:MET:SD	45:A:2063:G:N2	2.77	0.56
27:7:189:LEU:O	27:7:295:ARG:NH2	2.39	0.56
28:9:82:GLU:N	28:9:82:GLU:OE1	2.39	0.56
30:b:116:ARG:O	45:A:2146:A:N6	2.38	0.56
34:h:148:LEU:HD13	34:h:152:LEU:HD22	1.86	0.56
40:r:109:GLN:OE1	40:r:113:ARG:NH1	2.37	0.56
45:A:2822:C:O2'	45:A:2915:C:OP2	2.23	0.56
21:0:99:LYS:NZ	45:A:2710:C:OP1	2.34	0.56
30:b:3:ALA:HB3	45:A:1831:G:OP2	2.06	0.56
45:A:2905:A:O2'	45:A:2906:C:OP1	2.23	0.56
26:6:360:ARG:NH1	45:A:2869:A:N7	2.51	0.56
2:E:212:GLY:N	45:A:3218:A:OP2	2.32	0.56
5:K:46:VAL:HG13	14:T:208:ILE:HD12	1.86	0.56
10:P:68:TRP:HE3	10:P:71:VAL:HG11	1.69	0.56
32:d:166:GLU:OE1	32:d:166:GLU:N	2.39	0.56
45:A:2075:U:O2'	45:A:2833:A:N7	2.34	0.56
1:D:137:ALA:HB1	1:D:152:ILE:HD11	1.87	0.56
3:F:248:LEU:HD13	3:F:253:MET:HE1	1.86	0.56
14:T:105:GLN:NE2	21:0:104:LYS:O	2.38	0.56
19:Y:212:GLU:OE2	19:Y:216:ARG:NH1	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:77:ASP:HA	9:O:86:ILE:HD11	1.86	0.56
16:V:92:ASN:ND2	16:V:113:ALA:O	2.38	0.56
14:T:125:GLN:NE2	14:T:137:ARG:O	2.39	0.56
14:T:129:VAL:HG11	14:T:137:ARG:HG2	1.87	0.56
21:O:110:CYS:O	21:O:114:GLY:N	2.38	0.56
7:M:255:MET:O	7:M:258:THR:OG1	2.23	0.55
18:X:97:LEU:HD12	45:A:2919:A:N1	2.21	0.55
21:O:93:ARG:NH2	45:A:2310:G:OP1	2.36	0.55
41:s:55:SER:OG	45:A:2325:U:OP2	2.24	0.55
45:A:3168:C:O2'	45:A:3169:C:O2	2.23	0.55
26:6:257:PRO:HB3	26:6:268:LEU:HD11	1.88	0.55
31:c:93:VAL:HG11	31:c:119:LEU:HD11	1.88	0.55
41:s:90:LYS:NZ	41:s:232:GLN:OE1	2.32	0.55
11:Q:245:PHE:O	11:Q:249:LEU:N	2.39	0.55
31:c:170:ALA:HB1	31:c:175:VAL:CG1	2.36	0.55
45:A:1835:A:O2'	45:A:1836:A:N7	2.38	0.55
7:M:102:GLN:NE2	7:M:106:ASP:OD1	2.39	0.55
8:N:154:VAL:HG23	8:N:158:ARG:HD3	1.89	0.55
17:W:139:GLU:OE1	17:W:139:GLU:N	2.39	0.55
39:q:112:GLN:OE1	39:q:115:ARG:NE	2.38	0.55
16:V:194:LEU:HD13	19:Y:95:ASN:OD1	2.07	0.55
26:6:224:HIS:CD2	26:6:230:ALA:HB3	2.42	0.55
33:g:99:ASP:OD1	33:g:100:ILE:N	2.40	0.55
41:s:300:HIS:HB2	41:s:361:ILE:HG22	1.89	0.55
4:H:98:LEU:HD22	4:H:102:VAL:HG21	1.89	0.55
12:R:33:GLY:O	12:R:37:ARG:NH2	2.40	0.55
18:X:79:LEU:HD21	18:X:158:GLY:CA	2.37	0.55
32:d:154:ASN:O	32:d:155:SER:OG	2.20	0.55
41:s:49:ALA:O	41:s:61:ARG:NH1	2.40	0.55
31:c:68:TYR:CE2	31:c:72:ILE:HD11	2.42	0.55
35:i:32:ILE:HD11	45:A:1814:A:C8	2.42	0.55
45:A:2054:U:O2'	45:A:2055:U:O4'	2.15	0.55
15:U:129:MET:SD	32:d:78:LEU:HD11	2.47	0.54
18:X:213:GLU:OE1	18:X:216:ARG:NH2	2.38	0.54
25:5:157:VAL:HG22	25:5:183:ASN:OD1	2.07	0.54
28:9:40:GLY:O	28:9:41:ILE:HD13	2.07	0.54
30:b:45:GLU:CD	30:b:94:VAL:HG22	2.32	0.54
31:c:276:CYS:SG	31:c:279:LYS:NZ	2.80	0.54
7:M:54:LYS:NZ	45:A:2019:G:N7	2.56	0.54
19:Y:105:LEU:HD22	19:Y:135:VAL:HG23	1.89	0.54
45:A:3127:G:N2	45:A:3130:A:OP2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:68:ILE:CD1	20:Z:139:LEU:HD21	2.36	0.54
23:2:63:LYS:NZ	45:A:1918:G:OP1	2.30	0.54
39:q:71:VAL:O	39:q:74:SER:OG	2.26	0.54
45:A:1824:U:O2'	45:A:2705:U:O2	2.25	0.54
4:H:120:ARG:NH1	18:X:136:ASP:OD2	2.41	0.54
25:5:153:CYS:O	25:5:157:VAL:HG23	2.08	0.54
45:A:2430:A:OP1	45:A:2433:C:N4	2.40	0.54
5:K:174:GLU:N	5:K:174:GLU:OE1	2.39	0.54
19:Y:94:SER:OG	19:Y:95:ASN:N	2.39	0.54
25:5:68:PRO:O	45:A:1713:A:N6	2.40	0.54
25:5:120:ALA:O	25:5:124:THR:HG22	2.07	0.54
26:6:218:LEU:HD13	26:6:270:PHE:CE1	2.42	0.54
31:c:68:TYR:CZ	31:c:72:ILE:HD11	2.43	0.54
33:g:57:ILE:CD1	33:g:91:MET:HE2	2.38	0.54
40:r:158:SER:OG	45:A:3189:C:OP2	2.22	0.54
45:A:1926:A:H2	45:A:1978:A:H61	1.54	0.54
2:E:166:ARG:NH2	27:7:314:ASP:OD1	2.41	0.54
13:S:160:VAL:HG12	13:S:193:LEU:CD2	2.37	0.54
26:6:161:LEU:HD11	26:6:271:LEU:HD11	1.89	0.54
17:W:41:ASN:ND2	45:A:2841:U:OP2	2.41	0.54
37:o:16:GLN:NE2	45:A:2691:U:OP1	2.41	0.54
41:s:225:ARG:NH2	45:A:2449:G:OP2	2.40	0.54
3:F:167:MET:HE1	35:i:66:PHE:CZ	2.43	0.54
12:R:37:ARG:NH1	45:A:1816:G:OP2	2.41	0.54
15:U:17:LEU:HD11	28:9:136:LEU:HD12	1.89	0.54
15:U:37:GLU:HB3	15:U:104:THR:HG23	1.90	0.54
26:6:235:TRP:CE3	26:6:237:LEU:HD23	2.43	0.54
26:6:268:LEU:HD12	26:6:319:PHE:CZ	2.43	0.54
30:b:70:CYS:SG	30:b:71:CYS:N	2.80	0.54
10:P:61:VAL:HG11	26:6:344:PHE:CE2	2.43	0.54
14:T:149:ARG:O	45:A:1672:C:O2'	2.23	0.54
19:Y:153:LEU:HD23	28:9:130:LEU:HD21	1.90	0.54
7:M:207:PRO:O	7:M:211:VAL:HG23	2.07	0.53
21:0:167:GLU:OE1	21:0:167:GLU:N	2.40	0.53
5:K:46:VAL:HG13	14:T:208:ILE:CD1	2.39	0.53
10:P:92:ALA:C	10:P:93:LEU:HD22	2.33	0.53
8:N:124:VAL:HG12	8:N:152:THR:HG21	1.90	0.53
25:5:69:TRP:O	25:5:70:LEU:HD12	2.09	0.53
25:5:93:LEU:HG	25:5:270:ILE:HD12	1.89	0.53
2:E:45:SER:OG	2:E:46:GLY:N	2.38	0.53
15:U:26:ILE:HD12	15:U:44:ILE:CG2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:Y:218:ARG:NH1	35:i:105:ASP:OD2	2.40	0.53
40:r:69:GLN:NE2	40:r:108:CYS:SG	2.81	0.53
2:E:150:LYS:CB	2:E:296:LEU:HD21	2.38	0.53
8:N:96:TYR:HB3	8:N:151:VAL:HG11	1.91	0.53
10:P:59:LEU:O	10:P:60:SER:OG	2.22	0.53
41:s:320:ILE:O	41:s:323:VAL:HG12	2.08	0.53
4:H:107:VAL:HG22	4:H:108:ARG:H	1.71	0.53
9:O:50:ASP:OD1	9:O:107:MET:HE1	2.08	0.53
22:1:42:THR:HB	22:1:55:LEU:HD21	1.90	0.53
26:6:173:LEU:HD23	26:6:174:HIS:N	2.23	0.53
45:A:2503:A:N6	45:A:2505:A:N3	2.57	0.53
13:S:155:ARG:NH1	13:S:157:GLU:OE2	2.41	0.53
1:D:142:VAL:HG11	1:D:151:ILE:HD11	1.91	0.53
10:P:58:LEU:O	38:p:177:ARG:NH1	2.41	0.53
23:2:54:GLN:OE1	23:2:54:GLN:N	2.41	0.53
36:j:45:GLU:N	36:j:45:GLU:OE1	2.42	0.53
41:s:102:ALA:HB1	41:s:106:TYR:CE2	2.44	0.53
3:F:142:ARG:NH2	45:A:1794:A:OP1	2.39	0.53
5:K:170:TRP:NE1	40:r:91:GLN:O	2.37	0.53
6:L:68:LYS:N	6:L:71:ASP:OD2	2.39	0.53
1:D:178:GLU:O	1:D:244:VAL:HG23	2.09	0.52
1:D:194:ASN:OD1	1:D:243:THR:OG1	2.27	0.52
4:H:95:GLU:OE1	4:H:132:ALA:HB3	2.09	0.52
30:b:65:VAL:HG22	34:h:154:ILE:HG22	1.91	0.52
32:d:276:ILE:HG22	32:d:278:LYS:H	1.73	0.52
38:p:110:TRP:CH2	38:p:111:ILE:HD11	2.44	0.52
1:D:137:ALA:CB	1:D:152:ILE:HD11	2.39	0.52
25:5:117:VAL:N	25:5:307:ASP:OD2	2.43	0.52
40:r:112:HIS:NE2	45:A:3181:U:O2'	2.41	0.52
42:u:108:ASP:OD2	42:u:185:ARG:NH1	2.42	0.52
3:F:226:MET:HE1	3:F:244:PRO:HD3	1.91	0.52
5:K:140:ASN:OD1	31:c:263:GLY:N	2.43	0.52
14:T:55:ASN:ND2	14:T:74:TYR:O	2.41	0.52
11:Q:252:GLN:OE1	11:Q:255:LYS:NZ	2.28	0.52
29:a:47:VAL:HG12	29:a:62:HIS:HB3	1.92	0.52
31:c:61:SER:O	31:c:61:SER:OG	2.22	0.52
45:A:2445:U:O2	45:A:2447:A:N6	2.43	0.52
45:A:2520:C:O2	45:A:2528:G:N2	2.42	0.52
5:K:36:SER:O	5:K:40:GLN:NE2	2.42	0.52
27:7:129:THR:OG1	27:7:132:ASP:OD1	2.24	0.52
30:b:67:SER:OG	34:h:155:THR:O	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:b:120:HIS:O	30:b:120:HIS:ND1	2.42	0.52
3:F:51:VAL:HG11	3:F:55:VAL:HG21	1.91	0.52
38:p:113:GLU:OE1	38:p:116:ARG:NH1	2.42	0.52
41:s:260:GLU:N	41:s:260:GLU:OE1	2.41	0.52
19:Y:130:GLU:N	19:Y:130:GLU:OE1	2.42	0.52
33:g:120:LEU:HD23	33:g:120:LEU:O	2.09	0.52
45:A:2282:C:O2	45:A:2284:C:N4	2.38	0.52
1:D:115:GLU:N	1:D:115:GLU:OE1	2.41	0.52
42:u:113:GLN:NE2	42:u:114:VAL:O	2.43	0.52
14:T:139:ASN:C	14:T:140:LEU:HD12	2.35	0.52
17:W:57:GLU:N	17:W:57:GLU:OE1	2.43	0.52
21:0:176:GLU:N	21:0:176:GLU:OE1	2.43	0.52
32:d:169:PHE:CE1	32:d:173:THR:HG21	2.45	0.52
45:A:2138:U:O2'	45:A:2151:A:N3	2.37	0.52
45:A:3130:A:O2'	45:A:3131:G:OP1	2.25	0.52
4:H:53:THR:HG1	4:H:86:THR:HG1	1.54	0.51
19:Y:191:ASN:OD1	19:Y:192:LYS:N	2.43	0.51
26:6:193:VAL:N	26:6:320:GLN:O	2.41	0.51
3:F:164:MET:HE1	35:i:70:PRO:HB2	1.92	0.51
13:S:116:ILE:HD11	13:S:193:LEU:HD12	1.90	0.51
13:S:171:ILE:HD11	13:S:186:VAL:HG21	1.91	0.51
2:E:175:THR:HB	2:E:296:LEU:HD22	1.92	0.51
12:R:10:LEU:N	45:A:1771:C:O3'	2.42	0.51
25:5:334:LYS:NZ	25:5:335:VAL:O	2.27	0.51
42:u:167:TRP:NE1	42:u:180:MET:SD	2.83	0.51
10:P:83:VAL:HG21	10:P:158:MET:HE1	1.93	0.51
23:2:67:VAL:HG12	23:2:67:VAL:O	2.10	0.51
36:j:36:ASN:ND2	45:A:2148:A:N3	2.58	0.51
45:A:2653:C:O2'	45:A:2654:U:OP1	2.25	0.51
1:D:127:ILE:HD11	25:5:114:LEU:HD21	1.93	0.51
9:O:69:ASN:OD1	9:O:70:GLU:N	2.44	0.51
24:3:108:LYS:HZ3	45:A:1743:U:P	2.33	0.51
32:d:152:LEU:HD23	32:d:181:VAL:HG11	1.93	0.51
36:j:84:MET:HE2	37:o:53:TYR:HD2	1.75	0.51
41:s:234:ASP:OD1	41:s:234:ASP:N	2.40	0.51
26:6:217:LEU:HD23	26:6:218:LEU:N	2.24	0.51
14:T:99:ILE:HD13	14:T:125:GLN:NE2	2.26	0.51
41:s:74:GLU:OE1	41:s:74:GLU:N	2.44	0.51
3:F:117:ARG:NH2	45:A:1906:G:OP2	2.39	0.51
10:P:86:THR:HG22	10:P:87:GLN:H	1.76	0.51
14:T:63:LEU:N	14:T:66:GLU:OE2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:U:50:ARG:NH2	45:A:2373:A:OP1	2.44	0.51
29:a:44:ASN:ND2	30:b:135:ASN:OD1	2.44	0.51
31:c:83:PHE:CE2	31:c:88:LEU:HD13	2.46	0.51
42:u:97:MET:HE1	42:u:177:ILE:HG21	1.92	0.51
19:Y:171:ASP:OD2	19:Y:175:ARG:NE	2.39	0.50
2:E:145:LEU:HD13	2:E:181:ILE:HD13	1.92	0.50
13:S:108:VAL:HG13	13:S:195:ILE:HG21	1.93	0.50
15:U:44:ILE:HD13	15:U:53:LEU:HD22	1.92	0.50
35:i:93:ARG:NH2	45:A:1737:A:O2'	2.43	0.50
41:s:97:THR:HG21	41:s:106:TYR:OH	2.12	0.50
41:s:192:ASN:CG	41:s:195:LEU:HD13	2.37	0.50
8:N:160:VAL:HG12	8:N:161:VAL:HG23	1.93	0.50
25:5:272:ASP:OD1	25:5:272:ASP:N	2.44	0.50
31:c:170:ALA:CB	31:c:191:LEU:HD21	2.39	0.50
2:E:334:ASP:HB3	2:E:337:VAL:HG23	1.92	0.50
20:Z:138:CYS:SG	20:Z:139:LEU:N	2.85	0.50
27:7:82:ASN:N	27:7:86:SER:OG	2.44	0.50
42:u:125:VAL:HB	42:u:177:ILE:HG22	1.93	0.50
45:A:2282:C:O2'	45:A:2284:C:N4	2.44	0.50
45:A:2925:U:O2'	45:A:2926:A:O5'	2.29	0.50
5:K:176:TYR:OH	40:r:94:ARG:NH2	2.44	0.50
14:T:81:LYS:NZ	45:A:2675:G:OP2	2.43	0.50
20:Z:62:ASN:O	20:Z:62:ASN:ND2	2.42	0.50
12:R:24:VAL:HG11	12:R:43:VAL:HG22	1.93	0.50
25:5:143:PRO:O	25:5:146:HIS:ND1	2.45	0.50
9:O:41:ARG:NH1	9:O:131:PRO:O	2.41	0.50
18:X:79:LEU:HD21	18:X:158:GLY:HA3	1.93	0.50
32:d:125:ILE:HD13	32:d:250:LYS:HZ1	1.77	0.50
40:r:127:LEU:C	40:r:128:LEU:HD12	2.37	0.50
3:F:252:SER:O	3:F:256:HIS:ND1	2.43	0.50
21:O:166:SER:OG	21:O:167:GLU:OE1	2.29	0.50
26:6:272:LEU:O	26:6:314:ALA:N	2.41	0.50
31:c:38:ALA:HB1	35:i:38:LEU:HD23	1.94	0.50
12:R:17:ARG:NH1	45:A:2295:C:OP1	2.45	0.49
13:S:160:VAL:HG12	13:S:193:LEU:HD21	1.93	0.49
20:Z:109:LYS:NZ	45:A:2058:C:O2	2.39	0.49
38:p:48:LEU:HD23	38:p:48:LEU:O	2.11	0.49
11:Q:132:GLN:O	42:u:119:ARG:NH2	2.45	0.49
41:s:117:GLY:C	41:s:118:LEU:HD12	2.37	0.49
16:V:129:LYS:NZ	16:V:130:PRO:O	2.43	0.49
25:5:313:MET:HE2	25:5:355:LEU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:9:93:SER:OG	28:9:94:GLU:OE1	2.30	0.49
8:N:171:GLU:HG3	8:N:172:VAL:HG13	1.94	0.49
10:P:61:VAL:HG13	26:6:346:ARG:HH22	1.77	0.49
19:Y:154:ARG:HH11	19:Y:163:ALA:HB2	1.76	0.49
5:K:46:VAL:HG12	5:K:46:VAL:O	2.13	0.49
13:S:51:VAL:HG11	13:S:57:SER:HB2	1.95	0.49
18:X:173:ASP:O	18:X:188:TYR:OH	2.30	0.49
43:v:49:GLU:OE1	43:v:49:GLU:N	2.43	0.49
3:F:161:TYR:OH	45:A:2291:A:OP1	2.22	0.49
3:F:278:SER:OG	3:F:278:SER:O	2.31	0.49
31:c:280:LEU:HD12	31:c:282:ALA:H	1.78	0.49
33:g:147:LEU:HD23	33:g:148:ARG:N	2.27	0.49
41:s:238:ASN:OD1	41:s:301:LEU:N	2.46	0.49
11:Q:123:ASP:OD1	11:Q:131:SER:OG	2.31	0.49
25:5:261:PRO:O	25:5:262:ILE:HD13	2.12	0.49
26:6:371:ASP:OD1	26:6:372:SER:N	2.42	0.49
34:h:143:LEU:O	34:h:146:SER:OG	2.30	0.49
46:B:1615:A:N1	46:B:1621:A:O2'	2.41	0.49
2:E:303:LYS:NZ	45:A:3203:A:OP1	2.46	0.49
6:L:104:ASN:OD1	11:Q:158:GLN:NE2	2.46	0.49
9:O:67:ASP:OD1	9:O:67:ASP:N	2.46	0.49
20:Z:36:PHE:N	45:A:2119:U:O2	2.43	0.49
20:Z:120:LYS:NZ	37:o:44:GLU:OE2	2.23	0.49
30:b:144:ARG:NH2	30:b:147:GLU:OE1	2.41	0.49
44:w:85:TYR:CE2	44:w:89:LEU:HD11	2.47	0.49
2:E:181:ILE:CG2	2:E:185:ALA:HB3	2.43	0.48
13:S:100:HIS:CD2	36:j:43:LEU:HD22	2.48	0.48
20:Z:74:SER:N	45:A:2139:U:OP2	2.45	0.48
26:6:233:LEU:O	26:6:296:ARG:NH1	2.46	0.48
20:Z:59:ASP:OD1	20:Z:59:ASP:N	2.46	0.48
27:7:242:GLU:O	27:7:245:SER:OG	2.28	0.48
45:A:1782:G:N2	45:A:1794:A:OP2	2.40	0.48
45:A:2519:G:N1	45:A:2530:A:N7	2.61	0.48
2:E:181:ILE:HG22	2:E:182:THR:O	2.12	0.48
4:H:53:THR:OG1	4:H:86:THR:OG1	2.25	0.48
19:Y:69:ASP:OD1	19:Y:69:ASP:N	2.47	0.48
20:Z:101:LYS:NZ	36:j:83:GLU:OE2	2.24	0.48
31:c:295:GLU:O	31:c:299:VAL:HG23	2.13	0.48
41:s:51:MET:SD	41:s:61:ARG:NH2	2.87	0.48
26:6:302:ASP:N	26:6:302:ASP:OD1	2.46	0.48
29:a:119:THR:HG22	29:a:120:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c:213:LEU:HD22	31:c:216:ARG:NH1	2.29	0.48
40:r:132:ARG:NH2	45:A:3192:C:OP1	2.45	0.48
45:A:2344:C:O2'	45:A:2345:G:OP1	2.23	0.48
45:A:2661:U:HO2'	45:A:3160:A:HO2'	1.62	0.48
1:D:195:ASN:N	1:D:207:ILE:O	2.45	0.48
3:F:164:MET:HE3	35:i:69:HIS:HE1	1.78	0.48
11:Q:184:ASP:OD2	11:Q:189:TYR:OH	2.30	0.48
21:0:108:ASP:OD2	21:0:119:LYS:NZ	2.40	0.48
22:1:34:ARG:CD	22:1:41:LEU:HD21	2.42	0.48
24:3:109:ALA:HB1	24:3:113:ARG:HH12	1.78	0.48
25:5:84:ASP:OD2	25:5:86:ARG:NH2	2.46	0.48
31:c:86:ASP:OD1	31:c:87:LEU:N	2.47	0.48
45:A:1787:G:N2	45:A:1790:A:OP2	2.39	0.48
3:F:292:ASP:OD1	33:g:55:THR:OG1	2.30	0.48
25:5:69:TRP:C	25:5:70:LEU:HD12	2.37	0.48
40:r:169:TRP:O	45:A:2155:A:N6	2.46	0.48
41:s:229:LEU:H	41:s:229:LEU:HD23	1.78	0.48
17:W:115:ASP:O	17:W:118:THR:OG1	2.24	0.48
27:7:144:ARG:NH2	27:7:267:PRO:O	2.46	0.48
27:7:262:ASP:OD1	27:7:263:VAL:N	2.39	0.48
27:7:276:PHE:HB2	27:7:304:VAL:HG12	1.96	0.48
34:h:77:VAL:HG23	34:h:78:PHE:CD2	2.49	0.48
13:S:143:LEU:CD1	13:S:200:ILE:HD11	2.44	0.48
14:T:174:TYR:CE2	14:T:176:VAL:HG13	2.49	0.48
17:W:68:ALA:HB1	17:W:75:TRP:CE3	2.49	0.48
24:3:148:VAL:HG13	26:6:360:ARG:HA	1.95	0.48
25:5:114:LEU:HD23	25:5:115:GLU:N	2.29	0.48
25:5:181:VAL:CG1	25:5:347:THR:HG21	2.44	0.48
2:E:109:LEU:HD21	2:E:337:VAL:HG22	1.96	0.48
30:b:66:ASN:C	30:b:67:SER:HG	2.21	0.48
45:A:2029:A:OP2	45:A:2263:C:N4	2.47	0.48
4:H:94:LEU:HD22	4:H:116:LYS:HA	1.96	0.48
19:Y:215:LYS:NZ	23:2:84:LEU:O	2.47	0.48
22:1:34:ARG:NE	22:1:41:LEU:HD21	2.29	0.48
14:T:69:ARG:NH1	32:d:228:PHE:O	2.47	0.47
24:3:183:ARG:NH1	26:6:354:GLN:OE1	2.47	0.47
45:A:2083:U:O4	45:A:2084:A:N6	2.47	0.47
6:L:53:ARG:NH2	45:A:2650:C:O3'	2.47	0.47
9:O:53:ARG:HH11	9:O:107:MET:HE2	1.80	0.47
11:Q:121:THR:HG22	11:Q:171:VAL:HG12	1.97	0.47
13:S:128:ILE:HD12	36:j:49:TRP:CE3	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:V:191:LEU:O	19:Y:153:LEU:HD21	2.13	0.47
20:Z:99:VAL:O	20:Z:100:HIS:ND1	2.47	0.47
31:c:97:TYR:CE2	31:c:180:LEU:HD13	2.48	0.47
43:v:46:GLU:OE1	43:v:46:GLU:N	2.46	0.47
2:E:269:TYR:O	45:A:3166:U:O2'	2.24	0.47
8:N:218:ILE:HG23	8:N:223:MET:HB2	1.97	0.47
10:P:156:ASP:OD1	10:P:157:SER:N	2.47	0.47
11:Q:156:GLU:N	11:Q:156:GLU:OE1	2.48	0.47
15:U:8:PRO:HG2	15:U:17:LEU:HD13	1.96	0.47
24:3:163:THR:HG21	45:A:1742:G:H5''	1.95	0.47
41:s:195:LEU:HD11	41:s:296:HIS:CE1	2.49	0.47
1:D:180:ASP:O	1:D:244:VAL:HG22	2.15	0.47
7:M:123:ASN:ND2	33:g:51:LEU:O	2.47	0.47
10:P:52:ASN:ND2	26:6:265:ILE:O	2.45	0.47
3:F:167:MET:HE2	3:F:276:GLN:OE1	2.15	0.47
9:O:17:ARG:NH2	45:A:2457:A:N3	2.63	0.47
30:b:136:LYS:O	31:c:259:ARG:NH2	2.46	0.47
1:D:138:ASP:OD2	1:D:249:ASN:ND2	2.46	0.47
3:F:84:PRO:O	3:F:88:ALA:N	2.47	0.47
6:L:87:VAL:HG23	6:L:87:VAL:O	2.15	0.47
8:N:78:GLU:OE1	8:N:78:GLU:N	2.48	0.47
23:2:89:SER:OG	28:9:17:ARG:NH2	2.46	0.47
32:d:235:GLN:OE1	32:d:236:GLU:N	2.47	0.47
33:g:160:TRP:HE3	33:g:161:LEU:HD12	1.78	0.47
37:o:27:VAL:O	37:o:27:VAL:HG13	2.15	0.47
37:o:67:ARG:NH1	45:A:2082:G:N7	2.62	0.47
2:E:345:ILE:HD11	11:Q:170:ARG:HB3	1.96	0.47
7:M:203:ARG:NE	7:M:264:GLN:O	2.44	0.47
9:O:43:GLU:HG2	9:O:122:VAL:HG22	1.96	0.47
11:Q:76:LEU:HD11	11:Q:80:PHE:HD2	1.79	0.47
26:6:171:VAL:HG11	26:6:272:LEU:CD2	2.45	0.47
27:7:124:GLU:OE2	27:7:124:GLU:N	2.48	0.47
27:7:281:SER:HG	27:7:298:GLN:C	2.17	0.47
31:c:172:ASN:O	31:c:173:LEU:HD12	2.15	0.47
32:d:157:HIS:O	32:d:161:HIS:ND1	2.48	0.47
32:d:235:GLN:HB3	32:d:238:VAL:HG22	1.97	0.47
39:q:78:SER:OG	39:q:80:GLU:OE2	2.17	0.47
41:s:314:GLN:N	41:s:314:GLN:OE1	2.48	0.47
45:A:1814:A:N3	45:A:1862:U:O2'	2.43	0.47
45:A:2498:U:O4	45:A:2505:A:N7	2.48	0.47
11:Q:165:GLU:OE1	11:Q:168:ASN:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:77:ARG:NE	14:T:119:GLU:OE2	2.47	0.47
15:U:7:TYR:HD2	15:U:17:LEU:HD21	1.80	0.47
20:Z:64:HIS:CE1	37:o:51:MET:HE2	2.49	0.47
31:c:301:LEU:HD23	31:c:301:LEU:O	2.14	0.47
11:Q:117:LEU:HB3	11:Q:174:ILE:HD11	1.96	0.47
40:r:130:ASN:OD1	40:r:131:HIS:ND1	2.45	0.47
32:d:168:CYS:SG	32:d:172:MET:HE2	2.55	0.47
38:p:175:LEU:O	38:p:179:ARG:NE	2.48	0.47
45:A:2457:A:O2'	45:A:2458:A:OP2	2.26	0.47
4:H:97:ILE:HG13	4:H:132:ALA:HB2	1.97	0.46
27:7:116:TYR:OH	27:7:271:ARG:NH2	2.48	0.46
11:Q:176:VAL:HG23	11:Q:176:VAL:O	2.15	0.46
2:E:150:LYS:HB3	2:E:296:LEU:HD21	1.98	0.46
3:F:117:ARG:NH1	45:A:1905:C:OP1	2.48	0.46
25:5:380:GLN:OE1	25:5:413:LYS:NZ	2.44	0.46
41:s:350:ASP:OD1	41:s:351:VAL:N	2.47	0.46
10:P:145:VAL:HG13	10:P:174:GLU:CD	2.41	0.46
14:T:133:ASN:ND2	14:T:133:ASN:O	2.48	0.46
20:Z:141:SER:N	36:j:40:TYR:OH	2.49	0.46
25:5:324:GLN:OE1	25:5:340:VAL:HG11	2.15	0.46
32:d:127:ASP:OD1	32:d:128:TYR:N	2.47	0.46
43:v:68:ARG:NH1	43:v:69:ILE:O	2.48	0.46
45:A:2282:C:HO2'	45:A:2283:C:P	2.38	0.46
3:F:222:THR:OG1	3:F:225:GLU:OE1	2.27	0.46
28:9:57:VAL:O	28:9:59:GLU:N	2.48	0.46
41:s:288:THR:HG22	41:s:342:TYR:HE1	1.79	0.46
45:A:3117:C:H42	45:A:3139:G:H1	1.62	0.46
8:N:124:VAL:CG1	8:N:152:THR:HG21	2.46	0.46
13:S:143:LEU:HD23	29:a:59:VAL:HG22	1.97	0.46
28:9:41:ILE:HG21	28:9:57:VAL:HG22	1.97	0.46
35:i:51:ARG:NE	45:A:2278:A:OP1	2.48	0.46
45:A:2384:A:H61	45:A:2409:A:N6	2.13	0.46
7:M:179:TYR:OH	7:M:260:LYS:NZ	2.34	0.46
12:R:12:ASN:ND2	45:A:2293:A:O4'	2.47	0.46
42:u:196:LEU:HD21	43:v:57:LYS:CG	2.45	0.46
45:A:1983:U:O2	45:A:1988:G:O2'	2.30	0.46
2:E:150:LYS:HB2	2:E:296:LEU:HD21	1.95	0.46
15:U:19:VAL:HG23	15:U:19:VAL:O	2.14	0.46
16:V:96:ARG:NH2	45:A:1804:A:O4'	2.49	0.46
17:W:134:VAL:HG22	26:6:78:PHE:CZ	2.51	0.46
20:Z:64:HIS:HD1	37:o:51:MET:HE2	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:O:87:ILE:HD13	45:A:1817:C:OP1	2.16	0.46
26:6:298:PHE:CZ	26:6:300:THR:HG23	2.51	0.46
41:s:87:GLN:OE1	45:A:2441:C:O2'	2.11	0.46
45:A:1793:G:O2'	45:A:1794:A:O4'	2.34	0.46
4:H:74:HIS:NE2	45:A:1731:A:OP1	2.47	0.46
12:R:50:PHE:HD2	13:S:172:MET:HE2	1.81	0.46
24:3:109:ALA:O	24:3:113:ARG:NH1	2.46	0.46
24:3:163:THR:HG22	24:3:164:SER:H	1.81	0.46
26:6:222:ASP:OD1	26:6:222:ASP:N	2.47	0.46
32:d:148:ALA:HB2	32:d:163:LEU:HD23	1.98	0.46
1:D:107:ILE:HG22	1:D:108:ASP:N	2.31	0.46
1:D:107:ILE:HG21	1:D:109:PHE:CE1	2.50	0.46
45:A:2037:U:O2'	45:A:2038:U:O5'	2.32	0.46
2:E:319:TYR:OH	2:E:328:LEU:HD23	2.15	0.45
3:F:164:MET:HE3	35:i:69:HIS:CE1	2.51	0.45
7:M:38:ARG:NH1	45:A:2269:G:OP2	2.49	0.45
10:P:81:LEU:HD23	10:P:82:ARG:N	2.31	0.45
26:6:52:ARG:NH2	46:B:1637:C:OP1	2.49	0.45
26:6:324:ASP:OD1	26:6:325:ASP:N	2.47	0.45
29:a:73:LYS:NZ	30:b:141:ARG:O	2.32	0.45
30:b:11:LEU:HD23	30:b:12:ALA:N	2.31	0.45
41:s:253:LEU:HD23	41:s:254:ASP:N	2.32	0.45
1:D:206:TYR:CD1	1:D:228:LEU:HD21	2.51	0.45
35:i:105:ASP:OD1	35:i:106:ASP:N	2.49	0.45
41:s:332:LEU:HD13	41:s:372:TYR:HB2	1.98	0.45
42:u:120:TYR:CD2	42:u:121:THR:HG22	2.51	0.45
3:F:67:GLU:OE1	3:F:210:ARG:NH1	2.45	0.45
13:S:182:LYS:NZ	45:A:2025:C:OP2	2.41	0.45
25:5:214:ASN:ND2	25:5:218:LEU:O	2.47	0.45
28:9:96:VAL:O	28:9:99:ALA:N	2.49	0.45
1:D:274:ARG:NH1	45:A:1992:C:O2	2.50	0.45
3:F:141:ILE:HD11	45:A:1793:G:OP1	2.16	0.45
7:M:291:LEU:O	7:M:295:THR:OG1	2.33	0.45
18:X:160:ASP:OD1	18:X:163:ARG:NH1	2.47	0.45
24:3:154:GLN:O	24:3:158:LEU:HD13	2.17	0.45
25:5:178:PRO:HA	25:5:181:VAL:HG22	1.99	0.45
26:6:161:LEU:HD11	26:6:271:LEU:HD21	1.99	0.45
28:9:43:PHE:HE1	28:9:53:ILE:HD11	1.82	0.45
32:d:192:SER:OG	32:d:215:ARG:O	2.34	0.45
34:h:108:LEU:HD12	34:h:130:TYR:CE2	2.51	0.45
41:s:374:LEU:HD12	41:s:391:ASN:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:73:ILE:HG21	6:L:86:ILE:HD11	1.99	0.45
12:R:112:THR:N	30:b:127:GLN:OE1	2.42	0.45
18:X:161:LEU:HD23	25:5:52:ILE:HD12	1.98	0.45
30:b:93:SER:N	30:b:96:GLU:OE2	2.50	0.45
41:s:225:ARG:NH1	45:A:2449:G:OP2	2.50	0.45
45:A:3070:G:O2'	45:A:3073:C:OP2	2.34	0.45
3:F:60:ARG:NH1	34:h:121:CYS:SG	2.85	0.45
5:K:2:SER:O	5:K:3:SER:OG	2.20	0.45
17:W:64:GLY:O	45:A:2860:G:O2'	2.34	0.45
20:Z:71:ARG:NH1	20:Z:73:LYS:O	2.47	0.45
44:w:97:LYS:NZ	44:w:107:ASP:OD2	2.49	0.45
20:Z:137:THR:HG21	36:j:74:ALA:HB2	1.99	0.45
21:0:183:SER:OG	32:d:292:GLU:OE1	2.26	0.45
31:c:96:CYS:O	31:c:100:SER:OG	2.35	0.45
42:u:114:VAL:HG13	42:u:118:MET:HE3	1.99	0.45
45:A:1707:C:HO2'	45:A:1708:A:P	2.39	0.45
7:M:180:ASP:OD2	7:M:204:MET:N	2.46	0.45
9:O:29:LEU:HD23	9:O:55:TYR:CE2	2.52	0.45
30:b:65:VAL:CG2	34:h:154:ILE:HG22	2.46	0.45
32:d:125:ILE:HD11	32:d:199:CYS:HA	1.98	0.45
15:U:7:TYR:CD2	15:U:17:LEU:HD21	2.52	0.45
42:u:113:GLN:HB2	43:v:70:ILE:HD12	1.99	0.45
45:A:2381:A:N6	45:A:2412:A:N1	2.65	0.45
45:A:2481:A:O2'	45:A:2482:A:O4'	2.27	0.45
13:S:139:ASP:OD2	31:c:310:ASN:ND2	2.50	0.45
20:Z:64:HIS:ND1	37:o:51:MET:HE2	2.32	0.45
31:c:301:LEU:HD21	31:c:305:TYR:CE2	2.53	0.45
40:r:75:TRP:O	40:r:76:ASN:ND2	2.50	0.45
28:9:43:PHE:CE1	28:9:53:ILE:HD11	2.52	0.44
33:g:125:GLU:OE2	33:g:135:THR:OG1	2.35	0.44
5:K:51:SER:O	14:T:206:ARG:NH1	2.50	0.44
16:V:178:SER:OG	16:V:180:GLU:OE2	2.27	0.44
18:X:171:ARG:NH2	18:X:173:ASP:OD1	2.50	0.44
45:A:3196:G:OP1	45:A:3196:G:N2	2.45	0.44
12:R:142:PHE:CE1	29:a:58:ILE:HD11	2.52	0.44
19:Y:154:ARG:O	19:Y:158:THR:N	2.45	0.44
24:3:111:ILE:HD12	24:3:166:TRP:CD2	2.53	0.44
27:7:203:THR:HG22	27:7:279:GLU:HA	2.00	0.44
31:c:280:LEU:HD12	31:c:282:ALA:N	2.33	0.44
45:A:2414:C:O2'	45:A:2415:C:OP2	2.29	0.44
9:O:39:HIS:ND1	45:A:2321:A:N1	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Z:56:TYR:O	20:Z:58:GLY:N	2.50	0.44
25:5:187:LEU:O	25:5:190:SER:OG	2.29	0.44
29:a:141:ASP:OD2	30:b:117:LYS:NZ	2.45	0.44
34:h:73:TYR:OH	34:h:107:ASP:OD2	2.25	0.44
34:h:84:SER:OG	34:h:85:ASN:N	2.50	0.44
9:O:54:GLY:C	11:Q:270:MET:HE1	2.43	0.44
13:S:134:LEU:HD23	13:S:134:LEU:H	1.82	0.44
20:Z:68:ILE:HD11	20:Z:139:LEU:HD21	2.00	0.44
30:b:141:ARG:NH1	30:b:149:GLN:O	2.46	0.44
2:E:152:VAL:HG12	2:E:153:SER:H	1.83	0.44
25:5:160:HIS:NE2	41:s:201:ASP:OD1	2.48	0.44
26:6:64:GLU:N	26:6:64:GLU:OE1	2.51	0.44
3:F:219:VAL:HG11	3:F:248:LEU:HD21	2.00	0.44
19:Y:205:VAL:HG12	19:Y:209:LEU:CD1	2.48	0.44
25:5:136:VAL:HG22	25:5:416:ALA:HB1	1.99	0.44
35:i:32:ILE:HD12	35:i:32:ILE:N	2.32	0.44
3:F:243:ILE:HG22	3:F:244:PRO:O	2.18	0.44
3:F:291:SER:OG	33:g:53:PRO:O	2.34	0.44
10:P:79:HIS:O	10:P:145:VAL:HG22	2.18	0.44
12:R:48:ARG:NH2	45:A:1844:A:OP2	2.50	0.44
42:u:101:LEU:O	42:u:105:ASN:N	2.51	0.44
44:w:91:ASP:OD1	44:w:92:LYS:N	2.51	0.44
7:M:59:ARG:NH1	45:A:2016:C:OP2	2.46	0.43
25:5:222:VAL:O	25:5:222:VAL:HG13	2.18	0.43
27:7:200:ARG:O	27:7:203:THR:OG1	2.28	0.43
27:7:281:SER:N	27:7:298:GLN:O	2.44	0.43
39:q:59:LYS:NZ	45:A:1760:G:OP2	2.34	0.43
2:E:187:ILE:HD11	2:E:317:PRO:HA	2.00	0.43
3:F:91:PRO:O	3:F:176:VAL:HG13	2.17	0.43
8:N:123:ARG:O	8:N:158:ARG:NH2	2.50	0.43
45:A:1868:G:H21	45:A:1868:G:P	2.41	0.43
3:F:221:LEU:HD11	3:F:268:PHE:CD2	2.53	0.43
5:K:73:GLU:N	5:K:73:GLU:OE1	2.50	0.43
26:6:217:LEU:HD23	26:6:218:LEU:H	1.82	0.43
26:6:217:LEU:HD21	26:6:233:LEU:HB2	1.99	0.43
41:s:227:ASP:OD1	41:s:228:ASP:N	2.51	0.43
41:s:345:PHE:CD2	41:s:351:VAL:HG12	2.53	0.43
2:E:187:ILE:N	2:E:187:ILE:HD12	2.33	0.43
3:F:167:MET:HE3	35:i:62:ILE:HG22	1.99	0.43
9:O:44:ALA:HB3	9:O:49:VAL:CG2	2.48	0.43
12:R:148:TYR:OH	29:a:56:ARG:NE	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:6:207:GLU:N	26:6:207:GLU:OE1	2.51	0.43
17:W:80:HIS:HA	17:W:92:LEU:HD12	1.99	0.43
25:5:355:LEU:C	25:5:355:LEU:HD23	2.44	0.43
33:g:57:ILE:HD11	33:g:91:MET:HE2	2.00	0.43
41:s:302:LEU:HD11	41:s:324:PHE:CE1	2.53	0.43
42:u:190:LEU:HD22	42:u:190:LEU:H	1.84	0.43
4:H:132:ALA:HB1	4:H:137:LYS:HE3	2.00	0.43
10:P:154:ALA:O	10:P:159:LYS:NZ	2.51	0.43
13:S:143:LEU:HD11	13:S:200:ILE:HD11	2.00	0.43
25:5:181:VAL:HG11	25:5:347:THR:HG21	2.00	0.43
32:d:122:ILE:HG23	32:d:126:LYS:HE3	2.01	0.43
6:L:64:ASN:OD1	6:L:65:GLY:N	2.49	0.43
8:N:163:MET:HE1	8:N:176:LEU:HD11	2.00	0.43
32:d:214:VAL:HG23	32:d:216:MET:HE1	2.01	0.43
41:s:257:VAL:HG22	41:s:259:ILE:HG22	1.99	0.43
43:v:2:ALA:HB3	43:v:3:PRO:HD3	2.00	0.43
3:F:51:VAL:HG11	3:F:55:VAL:CG2	2.49	0.43
4:H:102:VAL:HG12	4:H:103:GLU:H	1.84	0.43
10:P:115:HIS:CD2	26:6:135:VAL:HG22	2.54	0.43
17:W:88:CYS:SG	45:A:2872:C:O2'	2.74	0.43
25:5:294:LEU:N	25:5:294:LEU:HD23	2.34	0.43
30:b:48:GLU:N	30:b:48:GLU:OE1	2.52	0.43
25:5:392:ILE:O	25:5:398:VAL:HG11	2.19	0.43
26:6:229:ASP:OD1	26:6:230:ALA:N	2.52	0.43
27:7:103:SER:OG	27:7:115:MET:HE3	2.19	0.43
27:7:115:MET:HE1	27:7:127:PHE:CD1	2.50	0.43
41:s:201:ASP:OD2	41:s:242:ARG:NE	2.48	0.43
8:N:175:PHE:O	8:N:179:VAL:HG23	2.18	0.43
25:5:119:GLN:O	25:5:123:LEU:HD23	2.19	0.43
41:s:80:LEU:HD22	41:s:282:ILE:HG21	2.00	0.43
7:M:19:LEU:HD13	37:o:92:LEU:O	2.19	0.42
11:Q:119:VAL:HG22	11:Q:174:ILE:HD13	2.00	0.42
11:Q:171:VAL:O	11:Q:171:VAL:HG23	2.18	0.42
12:R:65:ARG:NH1	45:A:2148:A:OP2	2.52	0.42
25:5:155:LEU:HA	25:5:158:ILE:HG22	2.00	0.42
9:O:29:LEU:HD21	9:O:51:GLU:HB3	2.01	0.42
29:a:54:ASP:OD1	29:a:56:ARG:N	2.45	0.42
31:c:148:MET:HE1	31:c:156:LEU:HD12	2.02	0.42
32:d:125:ILE:HD11	32:d:199:CYS:CA	2.50	0.42
36:j:93:LEU:C	36:j:93:LEU:HD12	2.44	0.42
45:A:2238:A:N6	45:A:2239:A:N1	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:106:TRP:CE3	13:S:114:ILE:HG23	2.54	0.42
24:3:159:ASP:O	24:3:167:LYS:NZ	2.33	0.42
30:b:21:ARG:NH1	31:c:79:LEU:O	2.51	0.42
5:K:158:TYR:CE2	40:r:87:LEU:HD11	2.48	0.42
37:o:101:TRP:O	37:o:102:SER:OG	2.25	0.42
7:M:55:GLY:O	7:M:59:ARG:NH1	2.52	0.42
7:M:233:ARG:HH22	7:M:247:ILE:HD11	1.85	0.42
11:Q:116:ILE:C	11:Q:117:LEU:HD12	2.44	0.42
11:Q:201:ASP:OD1	11:Q:201:ASP:N	2.52	0.42
13:S:171:ILE:HD13	45:A:2143:G:H4'	2.02	0.42
22:1:34:ARG:HD3	22:1:41:LEU:HD21	2.01	0.42
25:5:79:ASP:OD1	25:5:79:ASP:N	2.53	0.42
33:g:110:ILE:HD12	33:g:147:LEU:HD22	2.00	0.42
7:M:146:ASP:N	7:M:146:ASP:OD1	2.51	0.42
11:Q:106:LEU:HD22	11:Q:172:GLN:O	2.19	0.42
20:Z:53:HIS:ND1	37:o:47:TYR:OH	2.42	0.42
20:Z:117:ILE:O	37:o:45:ASN:ND2	2.47	0.42
26:6:343:GLU:OE1	26:6:343:GLU:N	2.53	0.42
27:7:182:ASP:OD1	27:7:296:ARG:NE	2.37	0.42
45:A:1880:C:O2'	45:A:1884:G:OP1	2.37	0.42
45:A:1985:G:OP1	45:A:1987:G:O2'	2.31	0.42
2:E:68:GLU:OE1	2:E:154:ARG:NH1	2.52	0.42
7:M:157:GLN:OE1	7:M:157:GLN:N	2.52	0.42
8:N:124:VAL:HG21	8:N:160:VAL:HG13	2.01	0.42
9:O:79:TRP:O	9:O:80:LEU:HD23	2.19	0.42
13:S:171:ILE:HD12	13:S:184:ARG:HD3	2.02	0.42
17:W:67:ILE:HD12	17:W:131:VAL:HG21	2.01	0.42
22:1:36:ARG:C	22:1:37:LEU:HD22	2.44	0.42
25:5:236:LEU:HD21	25:5:289:HIS:CD2	2.55	0.42
31:c:287:GLU:OE1	31:c:287:GLU:N	2.49	0.42
37:o:98:THR:HG22	37:o:98:THR:O	2.20	0.42
45:A:3179:G:H21	45:A:3190:A:H62	1.67	0.42
15:U:30:ARG:NH1	15:U:107:PHE:O	2.53	0.42
19:Y:158:THR:HG22	19:Y:158:THR:O	2.20	0.42
10:P:136:CYS:SG	10:P:137:LEU:N	2.93	0.42
32:d:262:HIS:O	32:d:263:THR:HG23	2.20	0.42
41:s:301:LEU:HD12	41:s:362:THR:O	2.20	0.42
11:Q:118:ARG:O	11:Q:174:ILE:HD12	2.20	0.42
11:Q:227:LYS:O	11:Q:229:TRP:N	2.53	0.42
13:S:123:ALA:N	13:S:126:GLU:OE1	2.53	0.42
29:a:47:VAL:HG12	29:a:62:HIS:CB	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:d:280:VAL:HG12	32:d:281:MET:O	2.20	0.42
4:H:99:THR:HG22	4:H:99:THR:O	2.20	0.41
7:M:197:GLY:O	39:q:75:LEU:HD12	2.20	0.41
33:g:132:LEU:HD11	33:g:153:PHE:CZ	2.55	0.41
39:q:61:PHE:O	39:q:65:GLY:N	2.52	0.41
40:r:189:ARG:NH1	45:A:2245:A:O2'	2.53	0.41
45:A:2459:A:N6	45:A:2668:A:O2'	2.52	0.41
45:A:2691:U:H2'	45:A:2692:G:O4'	2.19	0.41
9:O:108:LEU:HD13	21:0:122:LEU:HD11	2.02	0.41
12:R:141:ILE:HD12	12:R:141:ILE:N	2.35	0.41
13:S:115:LEU:HD12	13:S:192:VAL:HG12	2.02	0.41
14:T:191:THR:OG1	14:T:192:ALA:N	2.53	0.41
17:W:144:LEU:HD23	17:W:144:LEU:O	2.19	0.41
21:0:82:LYS:NZ	45:A:2719:G:O3'	2.51	0.41
3:F:62:VAL:HG12	3:F:63:GLN:N	2.35	0.41
6:L:44:SER:OG	6:L:115:VAL:HG12	2.19	0.41
11:Q:258:GLN:O	11:Q:261:ASN:ND2	2.54	0.41
16:V:198:VAL:HG21	19:Y:99:HIS:ND1	2.34	0.41
23:2:63:LYS:NZ	45:A:1917:A:OP1	2.37	0.41
30:b:45:GLU:OE2	30:b:94:VAL:HG13	2.20	0.41
9:O:101:THR:O	9:O:101:THR:OG1	2.33	0.41
25:5:259:ILE:HG23	25:5:263:ILE:HD13	2.02	0.41
26:6:265:ILE:N	26:6:265:ILE:HD12	2.36	0.41
34:h:101:LEU:HD21	34:h:120:MET:HE1	2.02	0.41
5:K:136:ASP:OD1	5:K:136:ASP:N	2.51	0.41
12:R:137:GLU:N	12:R:137:GLU:OE1	2.54	0.41
19:Y:173:PHE:HB3	23:2:80:LEU:HD21	2.03	0.41
20:Z:103:ILE:HD11	45:A:2081:U:O2'	2.20	0.41
25:5:291:LEU:HD23	25:5:342:VAL:CG1	2.51	0.41
33:g:101:THR:HG22	33:g:102:HIS:ND1	2.35	0.41
40:r:87:LEU:HD12	40:r:87:LEU:H	1.85	0.41
45:A:2328:C:O2'	45:A:2329:C:O5'	2.36	0.41
7:M:138:VAL:HG12	7:M:139:GLN:N	2.34	0.41
12:R:64:MET:HE2	14:T:210:HIS:CG	2.55	0.41
17:W:96:ILE:HG21	17:W:98:ARG:NH2	2.36	0.41
24:3:118:HIS:NE2	45:A:1891:A:OP1	2.41	0.41
25:5:162:ARG:NH2	25:5:176:TYR:OH	2.53	0.41
26:6:372:SER:OG	26:6:373:HIS:N	2.53	0.41
3:F:96:LEU:CD2	3:F:250:VAL:HG13	2.51	0.41
8:N:50:LEU:HD21	8:N:120:ALA:HB3	2.03	0.41
8:N:209:ASN:HD22	8:N:209:ASN:C	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:O:44:ALA:HB3	9:O:49:VAL:HG23	2.01	0.41
25:5:91:PRO:O	25:5:96:HIS:NE2	2.47	0.41
41:s:215:GLU:HB3	41:s:229:LEU:HD22	2.02	0.41
41:s:356:VAL:O	41:s:357:SER:OG	2.34	0.41
2:E:129:VAL:HG13	2:E:193:LEU:HD11	2.02	0.41
3:F:95:ILE:HD11	45:A:1879:G:H5'	2.01	0.41
5:K:91:THR:OG1	5:K:94:GLN:OE1	2.39	0.41
15:U:72:VAL:HG23	15:U:72:VAL:O	2.19	0.41
19:Y:111:MET:SD	19:Y:112:LEU:HD12	2.60	0.41
45:A:2341:C:O2'	45:A:2342:U:OP2	2.38	0.41
5:K:34:MET:HE3	5:K:148:PRO:HB3	2.02	0.41
9:O:53:ARG:HB2	9:O:123:ILE:HD12	2.02	0.41
9:O:108:LEU:HD12	9:O:133:LEU:HD13	2.03	0.41
9:O:114:SER:O	9:O:117:ARG:NH1	2.54	0.41
11:Q:90:LEU:O	11:Q:90:LEU:HD23	2.21	0.41
29:a:75:ILE:HD12	31:c:255:SER:OG	2.21	0.41
30:b:36:ASP:OD1	30:b:36:ASP:N	2.52	0.41
32:d:173:THR:O	32:d:177:LYS:N	2.52	0.41
45:A:2145:G:O2'	45:A:2147:G:OP1	2.38	0.41
1:D:225:ILE:HD12	1:D:225:ILE:N	2.36	0.41
6:L:40:VAL:HG11	6:L:47:GLY:HA3	2.02	0.41
7:M:286:THR:HG22	33:g:38:PHE:C	2.46	0.41
18:X:215:GLN:NE2	18:X:219:GLU:OE2	2.50	0.41
45:A:2004:G:H2'	45:A:2005:C:O4'	2.21	0.41
3:F:68:SER:OG	3:F:69:LEU:N	2.53	0.40
6:L:93:GLY:O	6:L:95:ARG:NH2	2.50	0.40
7:M:206:PRO:HG2	7:M:211:VAL:HG22	2.02	0.40
25:5:290:THR:C	25:5:291:LEU:HD22	2.46	0.40
25:5:313:MET:HE1	25:5:353:HIS:O	2.20	0.40
26:6:225:LEU:HD11	26:6:340:PRO:HG3	2.03	0.40
26:6:240:ILE:HG21	26:6:245:VAL:HA	2.02	0.40
44:w:99:SER:OG	44:w:100:VAL:N	2.54	0.40
10:P:70:THR:HG22	10:P:70:THR:O	2.20	0.40
15:U:46:MET:SD	28:9:36:ARG:NE	2.87	0.40
32:d:223:ALA:HB2	32:d:236:GLU:HA	2.03	0.40
35:i:43:VAL:O	35:i:43:VAL:HG13	2.22	0.40
40:r:121:MET:SD	40:r:178:SER:OG	2.79	0.40
9:O:29:LEU:HD23	9:O:55:TYR:CD2	2.57	0.40
11:Q:121:THR:HG21	11:Q:164:PHE:CE1	2.57	0.40
12:R:111:LYS:N	30:b:127:GLN:OE1	2.55	0.40
26:6:224:HIS:HD2	26:6:230:ALA:HB3	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:A:2878:G:O6	45:A:2879:A:N6	2.54	0.40
3:F:62:VAL:HG21	3:F:88:ALA:HB2	2.04	0.40
7:M:162:LEU:HD21	38:p:145:ARG:HE	1.87	0.40
10:P:77:PHE:HB3	10:P:145:VAL:HG21	2.03	0.40
16:V:80:ILE:O	16:V:84:ASN:N	2.52	0.40
17:W:102:GLU:OE2	26:6:74:TYR:N	2.54	0.40
25:5:378:SER:O	25:5:380:GLN:NE2	2.52	0.40
35:i:51:ARG:NH2	45:A:2278:A:OP1	2.53	0.40
45:A:2944:C:H42	45:A:2981:A:H61	1.69	0.40
4:H:97:ILE:HG21	4:H:140:PHE:HD2	1.86	0.40
7:M:270:ALA:HB3	7:M:273:TRP:CE2	2.56	0.40
12:R:98:ASN:OD1	12:R:101:VAL:HG22	2.22	0.40
17:W:49:ARG:NH1	45:A:2827:A:OP1	2.55	0.40
25:5:244:GLU:O	25:5:248:THR:HG23	2.22	0.40
25:5:387:TRP:HZ3	25:5:391:VAL:HG11	1.86	0.40
30:b:45:GLU:OE2	30:b:94:VAL:HG22	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	172/305 (56%)	158 (92%)	14 (8%)	0	100	100
2	E	280/348 (80%)	262 (94%)	18 (6%)	0	100	100
3	F	248/311 (80%)	230 (93%)	18 (7%)	0	100	100
4	H	93/267 (35%)	86 (92%)	7 (8%)	0	100	100
5	K	175/178 (98%)	161 (92%)	14 (8%)	0	100	100
6	L	113/145 (78%)	105 (93%)	8 (7%)	0	100	100
7	M	285/296 (96%)	265 (93%)	20 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	N	203/251 (81%)	189 (93%)	14 (7%)	0	100	100
9	O	150/175 (86%)	142 (95%)	8 (5%)	0	100	100
10	P	139/180 (77%)	132 (95%)	7 (5%)	0	100	100
11	Q	215/292 (74%)	198 (92%)	17 (8%)	0	100	100
12	R	138/149 (93%)	128 (93%)	10 (7%)	0	100	100
13	S	154/205 (75%)	144 (94%)	10 (6%)	0	100	100
14	T	164/206 (80%)	152 (93%)	12 (7%)	0	100	100
15	U	135/153 (88%)	128 (95%)	7 (5%)	0	100	100
16	V	159/216 (74%)	150 (94%)	9 (6%)	0	100	100
17	W	107/148 (72%)	100 (94%)	7 (6%)	0	100	100
18	X	241/256 (94%)	229 (95%)	12 (5%)	0	100	100
19	Y	174/250 (70%)	165 (95%)	9 (5%)	0	100	100
20	Z	115/161 (71%)	107 (93%)	8 (7%)	0	100	100
21	0	106/188 (56%)	102 (96%)	4 (4%)	0	100	100
22	1	50/65 (77%)	45 (90%)	5 (10%)	0	100	100
23	2	43/92 (47%)	36 (84%)	7 (16%)	0	100	100
24	3	93/188 (50%)	89 (96%)	4 (4%)	0	100	100
25	5	369/423 (87%)	342 (93%)	27 (7%)	0	100	100
26	6	316/380 (83%)	290 (92%)	26 (8%)	0	100	100
27	7	285/338 (84%)	262 (92%)	23 (8%)	0	100	100
28	9	113/137 (82%)	107 (95%)	6 (5%)	0	100	100
29	a	78/142 (55%)	72 (92%)	6 (8%)	0	100	100
30	b	146/215 (68%)	132 (90%)	14 (10%)	0	100	100
31	c	271/332 (82%)	258 (95%)	13 (5%)	0	100	100
32	d	177/306 (58%)	166 (94%)	11 (6%)	0	100	100
33	g	127/166 (76%)	120 (94%)	7 (6%)	0	100	100
34	h	96/158 (61%)	90 (94%)	6 (6%)	0	100	100
35	i	95/128 (74%)	85 (90%)	10 (10%)	0	100	100
36	j	83/123 (68%)	79 (95%)	4 (5%)	0	100	100
37	o	89/102 (87%)	81 (91%)	8 (9%)	0	100	100
38	p	119/206 (58%)	112 (94%)	7 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	q	126/222 (57%)	119 (94%)	7 (6%)	0	100	100
40	r	126/196 (64%)	118 (94%)	8 (6%)	0	100	100
41	s	366/439 (83%)	340 (93%)	26 (7%)	0	100	100
42	u	109/234 (47%)	98 (90%)	11 (10%)	0	100	100
43	v	67/70 (96%)	62 (92%)	5 (8%)	0	100	100
44	w	77/156 (49%)	67 (87%)	10 (13%)	0	100	100
All	All	6987/9498 (74%)	6503 (93%)	484 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	140/245 (57%)	139 (99%)	1 (1%)	76	80
2	E	245/290 (84%)	236 (96%)	9 (4%)	30	58
3	F	217/262 (83%)	205 (94%)	12 (6%)	19	47
4	H	86/228 (38%)	79 (92%)	7 (8%)	11	34
5	K	155/156 (99%)	152 (98%)	3 (2%)	50	70
6	L	98/124 (79%)	94 (96%)	4 (4%)	27	56
7	M	245/249 (98%)	238 (97%)	7 (3%)	37	63
8	N	172/211 (82%)	167 (97%)	5 (3%)	37	63
9	O	133/150 (89%)	125 (94%)	8 (6%)	17	45
10	P	123/155 (79%)	116 (94%)	7 (6%)	18	46
11	Q	199/256 (78%)	195 (98%)	4 (2%)	48	69
12	R	118/126 (94%)	116 (98%)	2 (2%)	53	71
13	S	141/180 (78%)	131 (93%)	10 (7%)	13	39
14	T	146/176 (83%)	135 (92%)	11 (8%)	12	37
15	U	124/135 (92%)	120 (97%)	4 (3%)	34	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	146/191 (76%)	143 (98%)	3 (2%)	47	68
17	W	89/119 (75%)	83 (93%)	6 (7%)	15	41
18	X	219/229 (96%)	207 (94%)	12 (6%)	19	47
19	Y	159/223 (71%)	152 (96%)	7 (4%)	25	54
20	Z	108/147 (74%)	99 (92%)	9 (8%)	10	33
21	0	97/164 (59%)	89 (92%)	8 (8%)	10	34
22	1	49/60 (82%)	49 (100%)	0	100	100
23	2	39/72 (54%)	36 (92%)	3 (8%)	12	36
24	3	88/166 (53%)	83 (94%)	5 (6%)	18	46
25	5	335/368 (91%)	323 (96%)	12 (4%)	31	58
26	6	265/332 (80%)	245 (92%)	20 (8%)	12	37
27	7	263/303 (87%)	258 (98%)	5 (2%)	50	70
28	9	99/112 (88%)	93 (94%)	6 (6%)	17	44
29	a	78/133 (59%)	72 (92%)	6 (8%)	12	36
30	b	130/186 (70%)	123 (95%)	7 (5%)	20	48
31	c	241/288 (84%)	230 (95%)	11 (5%)	24	53
32	d	170/274 (62%)	168 (99%)	2 (1%)	63	75
33	g	119/148 (80%)	114 (96%)	5 (4%)	26	55
34	h	95/148 (64%)	91 (96%)	4 (4%)	26	55
35	i	86/110 (78%)	82 (95%)	4 (5%)	23	52
36	j	68/97 (70%)	66 (97%)	2 (3%)	37	63
37	o	78/87 (90%)	73 (94%)	5 (6%)	16	42
38	p	117/181 (65%)	109 (93%)	8 (7%)	14	40
39	q	110/178 (62%)	108 (98%)	2 (2%)	51	70
40	r	119/169 (70%)	113 (95%)	6 (5%)	22	50
41	s	326/381 (86%)	313 (96%)	13 (4%)	28	56
42	u	105/200 (52%)	103 (98%)	2 (2%)	50	70
43	v	59/60 (98%)	58 (98%)	1 (2%)	53	71
44	w	73/136 (54%)	72 (99%)	1 (1%)	59	73
All	All	6272/8205 (76%)	6003 (96%)	269 (4%)	27	55

All (269) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	251	ASP
2	E	45	SER
2	E	77	LEU
2	E	91	GLU
2	E	106	MET
2	E	152	VAL
2	E	163	GLU
2	E	295	CYS
2	E	297	VAL
2	E	318	THR
3	F	77	VAL
3	F	85	ASP
3	F	96	LEU
3	F	106	PHE
3	F	108	ARG
3	F	120	VAL
3	F	133	THR
3	F	135	ARG
3	F	143	SER
3	F	159	THR
3	F	184	GLN
3	F	242	LEU
4	H	64	LEU
4	H	96	LEU
4	H	102	VAL
4	H	110	ASP
4	H	130	VAL
4	H	140	PHE
4	H	143	GLU
5	K	101	VAL
5	K	115	ASN
5	K	157	GLU
6	L	41	VAL
6	L	105	VAL
6	L	129	LYS
6	L	130	ARG
7	M	118	LEU
7	M	141	VAL
7	M	160	SER
7	M	183	SER
7	M	187	VAL
7	M	222	TYR
7	M	288	GLU

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Mol	Chain	Res	Type
8	N	90	LEU
8	N	196	GLU
8	N	201	ASP
8	N	209	ASN
8	N	247	MET
9	O	25	ARG
9	O	33	LEU
9	O	42	ILE
9	O	67	ASP
9	O	101	THR
9	O	150	GLN
9	O	155	ASP
9	O	158	GLN
10	P	47	GLU
10	P	57	GLU
10	P	59	LEU
10	P	86	THR
10	P	106	SER
10	P	136	CYS
10	P	155	SER
11	Q	87	THR
11	Q	119	VAL
11	Q	199	THR
11	Q	270	MET
12	R	87	ILE
12	R	109	GLU
13	S	56	LEU
13	S	71	GLU
13	S	88	VAL
13	S	108	VAL
13	S	124	CYS
13	S	134	LEU
13	S	144	LEU
13	S	162	GLU
13	S	171	ILE
13	S	197	SER
14	T	50	LYS
14	T	52	GLU
14	T	98	SER
14	T	109	ASN
14	T	110	ASP
14	T	176	VAL

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Mol	Chain	Res	Type
14	T	187	GLU
14	T	191	THR
14	T	195	HIS
14	T	197	LYS
14	T	207	THR
15	U	38	ASP
15	U	74	HIS
15	U	84	ASN
15	U	94	VAL
16	V	194	LEU
16	V	200	GLU
16	V	213	VAL
17	W	56	MET
17	W	57	GLU
17	W	69	THR
17	W	88	CYS
17	W	126	LEU
17	W	145	VAL
18	X	11	TRP
18	X	14	LEU
18	X	95	ASP
18	X	101	LEU
18	X	137	GLU
18	X	154	CYS
18	X	167	LEU
18	X	182	GLU
18	X	200	GLU
18	X	207	THR
18	X	218	LEU
18	X	220	GLU
19	Y	86	THR
19	Y	96	GLU
19	Y	98	LEU
19	Y	113	LEU
19	Y	209	LEU
19	Y	223	LYS
19	Y	236	LYS
20	Z	61	GLN
20	Z	65	LYS
20	Z	75	THR
20	Z	76	ARG
20	Z	77	ARG

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Mol	Chain	Res	Type
20	Z	78	ARG
20	Z	105	SER
20	Z	112	VAL
20	Z	119	ILE
21	0	88	GLU
21	0	91	ARG
21	0	96	ASN
21	0	109	VAL
21	0	110	CYS
21	0	117	LYS
21	0	145	GLU
21	0	164	THR
23	2	51	ASN
23	2	56	SER
23	2	76	VAL
24	3	125	ARG
24	3	146	GLU
24	3	162	THR
24	3	163	THR
24	3	164	SER
25	5	56	GLU
25	5	140	VAL
25	5	148	GLU
25	5	175	THR
25	5	182	ASP
25	5	210	SER
25	5	272	ASP
25	5	276	ASP
25	5	294	LEU
25	5	324	GLN
25	5	355	LEU
25	5	382	LEU
26	6	50	LYS
26	6	64	GLU
26	6	166	THR
26	6	183	ASP
26	6	185	MET
26	6	192	GLU
26	6	225	LEU
26	6	231	GLU
26	6	236	LEU
26	6	243	ASN

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Mol	Chain	Res	Type
26	6	268	LEU
26	6	280	ASP
26	6	298	PHE
26	6	300	THR
26	6	309	GLU
26	6	322	ARG
26	6	323	TRP
26	6	334	LEU
26	6	356	ARG
26	6	376	THR
27	7	73	THR
27	7	87	THR
27	7	96	SER
27	7	97	GLU
27	7	123	CYS
28	9	29	SER
28	9	39	LYS
28	9	44	LEU
28	9	52	GLN
28	9	53	ILE
28	9	59	GLU
29	a	53	SER
29	a	64	SER
29	a	65	VAL
29	a	70	GLU
29	a	72	THR
29	a	111	GLN
30	b	2	THR
30	b	48	GLU
30	b	50	GLU
30	b	58	ASN
30	b	99	THR
30	b	119	PHE
30	b	122	ASP
31	c	39	PHE
31	c	43	LYS
31	c	82	ASN
31	c	100	SER
31	c	169	VAL
31	c	178	LEU
31	c	198	VAL
31	c	238	MET

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Mol	Chain	Res	Type
31	c	254	GLU
31	c	258	THR
31	c	280	LEU
32	d	186	VAL
32	d	281	MET
33	g	89	SER
33	g	90	ARG
33	g	105	ARG
33	g	138	THR
33	g	157	LEU
34	h	91	LEU
34	h	117	LEU
34	h	146	SER
34	h	158	TYR
35	i	80	LEU
35	i	84	LYS
35	i	98	VAL
35	i	114	ILE
36	j	69	GLU
36	j	83	GLU
37	o	28	SER
37	o	51	MET
37	o	54	MET
37	o	74	ILE
37	o	81	LYS
38	p	103	PHE
38	p	107	THR
38	p	130	LEU
38	p	135	LEU
38	p	139	SER
38	p	185	ARG
38	p	187	ARG
38	p	188	LEU
39	q	46	LEU
39	q	74	SER
40	r	56	THR
40	r	70	CYS
40	r	75	TRP
40	r	76	ASN
40	r	87	LEU
40	r	196	HIS
41	s	66	TRP

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Mol	Chain	Res	Type
41	s	75	SER
41	s	174	LEU
41	s	182	SER
41	s	204	CYS
41	s	221	HIS
41	s	223	ARG
41	s	229	LEU
41	s	243	ILE
41	s	271	LEU
41	s	371	CYS
41	s	376	THR
41	s	401	LEU
42	u	158	LYS
42	u	167	TRP
43	v	59	LEU
44	w	115	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	241	ASN
6	L	103	ASN
7	M	26	ASN
7	M	219	ASN
7	M	276	ASN
8	N	173	GLN
10	P	121	ASN
10	P	142	ASN
11	Q	213	GLN
12	R	22	GLN
14	T	125	GLN
18	X	241	GLN
19	Y	89	GLN
19	Y	207	HIS
24	3	178	GLN
25	5	338	GLN
26	6	191	ASN
26	6	239	ASN
26	6	292	GLN
26	6	359	HIS
27	7	277	GLN
28	9	123	GLN

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Mol	Chain	Res	Type
29	a	44	ASN
30	b	17	ASN
31	c	222	GLN
32	d	262	HIS
35	i	59	ASN
38	p	152	GLN
38	p	184	ASN
40	r	76	ASN
41	s	281	HIS
41	s	296	HIS
41	s	300	HIS
41	s	375	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
45	A	1113/1559 (71%)	358 (32%)	15 (1%)
46	B	51/69 (73%)	13 (25%)	0
All	All	1164/1628 (71%)	371 (31%)	15 (1%)

All (371) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
45	A	1679	U
45	A	1680	A
45	A	1681	G
45	A	1685	C
45	A	1689	C
45	A	1698	C
45	A	1700	U
45	A	1703	C
45	A	1704	U
45	A	1707	C
45	A	1708	A
45	A	1713	A
45	A	1716	U
45	A	1717	U
45	A	1718	A
45	A	1720	C
45	A	1724	A
45	A	1727	A

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Mol	Chain	Res	Type
45	A	1728	U
45	A	1731	A
45	A	1732	C
45	A	1748	G
45	A	1750	G
45	A	1751	A
45	A	1752	U
45	A	1770	G
45	A	1777	A
45	A	1779	A
45	A	1781	A
45	A	1782	G
45	A	1788	C
45	A	1794	A
45	A	1799	U
45	A	1800	G
45	A	1803	A
45	A	1804	A
45	A	1805	A
45	A	1812	C
45	A	1817	C
45	A	1820	A
45	A	1821	A
45	A	1822	U
45	A	1823	A
45	A	1824	U
45	A	1827	C
45	A	1828	A
45	A	1829	A
45	A	1832	A
45	A	1836	A
45	A	1844	A
45	A	1849	C
45	A	1853	A
45	A	1854	U
45	A	1855	A
45	A	1856	A
45	A	1867	A
45	A	1869	A
45	A	1870	A
45	A	1871	A
45	A	1872	U

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Mol	Chain	Res	Type
45	A	1873	A
45	A	1877	U
45	A	1878	U
45	A	1882	A
45	A	1883	G
45	A	1886	G
45	A	1887	A
45	A	1893	A
45	A	1903	C
45	A	1912	A
45	A	1914	A
45	A	1918	G
45	A	1930	C
45	A	1933	C
45	A	1934	U
45	A	1972	A
45	A	1974	A
45	A	1985	G
45	A	1986	A
45	A	1987	G
45	A	1992	C
45	A	1993	A
45	A	1994	A
45	A	1995	A
45	A	2000	C
45	A	2002	G
45	A	2003	A
45	A	2015	G
45	A	2016	C
45	A	2017	U
45	A	2019	G
45	A	2022	G
45	A	2025	C
45	A	2028	G
45	A	2029	A
45	A	2030	U
45	A	2031	A
45	A	2032	G
45	A	2034	A
45	A	2036	C
45	A	2037	U
45	A	2039	A

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Mol	Chain	Res	Type
45	A	2053	U
45	A	2055	U
45	A	2059	C
45	A	2060	A
45	A	2065	A
45	A	2066	C
45	A	2074	A
45	A	2080	U
45	A	2083	U
45	A	2085	A
45	A	2089	U
45	A	2096	U
45	A	2105	G
45	A	2113	G
45	A	2126	U
45	A	2129	G
45	A	2132	A
45	A	2135	A
45	A	2139	U
45	A	2141	U
45	A	2147	G
45	A	2154	A
45	A	2156	A
45	A	2157	U
45	A	2233	U
45	A	2237	A
45	A	2238	A
45	A	2241	A
45	A	2245	A
45	A	2246	A
45	A	2250	A
45	A	2257	C
45	A	2260	A
45	A	2261	C
45	A	2262	C
45	A	2263	C
45	A	2278	A
45	A	2282	C
45	A	2283	C
45	A	2284	C
45	A	2297	A
45	A	2299	U

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Mol	Chain	Res	Type
45	A	2300	G
45	A	2306	A
45	A	2307	U
45	A	2309	A
45	A	2317	G
45	A	2321	A
45	A	2322	C
45	A	2324	U
45	A	2329	C
45	A	2331	C
45	A	2332	C
45	A	2342	U
45	A	2344	C
45	A	2345	G
45	A	2364	C
45	A	2369	A
45	A	2370	A
45	A	2372	U
45	A	2373	A
45	A	2374	A
45	A	2375	C
45	A	2377	G
45	A	2379	C
45	A	2384	A
45	A	2386	C
45	A	2387	U
45	A	2388	A
45	A	2389	C
45	A	2390	A
45	A	2391	A
45	A	2392	U
45	A	2393	C
45	A	2394	A
45	A	2395	A
45	A	2396	C
45	A	2399	A
45	A	2401	A
45	A	2404	U
45	A	2407	U
45	A	2409	A
45	A	2415	C
45	A	2416	U

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Mol	Chain	Res	Type
45	A	2417	C
45	A	2418	A
45	A	2426	C
45	A	2433	C
45	A	2442	U
45	A	2444	A
45	A	2446	A
45	A	2451	A
45	A	2453	G
45	A	2458	A
45	A	2484	C
45	A	2500	A
45	A	2501	C
45	A	2502	C
45	A	2504	A
45	A	2508	C
45	A	2511	C
45	A	2519	G
45	A	2520	C
45	A	2521	A
45	A	2523	C
45	A	2524	A
45	A	2525	C
45	A	2526	C
45	A	2527	A
45	A	2529	U
45	A	2531	U
45	A	2540	C
45	A	2654	U
45	A	2656	U
45	A	2658	U
45	A	2659	C
45	A	2660	U
45	A	2675	G
45	A	2678	A
45	A	2683	C
45	A	2686	G
45	A	2689	C
45	A	2694	A
45	A	2695	G
45	A	2696	A
45	A	2699	C

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Mol	Chain	Res	Type
45	A	2706	A
45	A	2709	A
45	A	2710	C
45	A	2718	C
45	A	2720	A
45	A	2722	A
45	A	2723	A
45	A	2724	G
45	A	2725	A
45	A	2726	C
45	A	2731	U
45	A	2732	G
45	A	2735	G
45	A	2739	U
45	A	2740	A
45	A	2743	U
45	A	2750	U
45	A	2755	A
45	A	2756	C
45	A	2801	A
45	A	2810	G
45	A	2813	U
45	A	2814	G
45	A	2815	G
45	A	2829	C
45	A	2831	G
45	A	2832	A
45	A	2833	A
45	A	2844	G
45	A	2847	C
45	A	2848	A
45	A	2849	G
45	A	2851	A
45	A	2852	C
45	A	2853	A
45	A	2854	U
45	A	2855	G
45	A	2856	C
45	A	2861	A
45	A	2864	U
45	A	2865	C
45	A	2869	A

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Mol	Chain	Res	Type
45	A	2880	A
45	A	2891	C
45	A	2895	U
45	A	2906	C
45	A	2907	U
45	A	2908	U
45	A	2909	G
45	A	2910	A
45	A	2911	C
45	A	2913	A
45	A	2916	G
45	A	2917	G
45	A	2918	A
45	A	2919	A
45	A	2922	A
45	A	2924	U
45	A	2925	U
45	A	2926	A
45	A	2928	C
45	A	2930	U
45	A	2932	G
45	A	2934	G
45	A	2935	A
45	A	2937	A
45	A	2938	A
45	A	2940	A
45	A	2943	G
45	A	2946	A
45	A	2947	U
45	A	2951	A
45	A	2974	A
45	A	2975	G
45	A	2977	G
45	A	2982	C
45	A	2983	G
45	A	3071	U
45	A	3072	U
45	A	3073	C
45	A	3074	A
45	A	3088	C
45	A	3089	A
45	A	3090	G

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Mol	Chain	Res	Type
45	A	3092	U
45	A	3094	G
45	A	3095	G
45	A	3096	U
45	A	3101	A
45	A	3102	U
45	A	3108	U
45	A	3109	U
45	A	3114	U
45	A	3118	U
45	A	3119	C
45	A	3120	C
45	A	3122	U
45	A	3123	G
45	A	3124	U
45	A	3126	C
45	A	3129	A
45	A	3131	G
45	A	3134	C
45	A	3135	A
45	A	3140	A
45	A	3141	A
45	A	3150	U
45	A	3151	A
45	A	3154	U
45	A	3157	C
45	A	3158	A
45	A	3162	C
45	A	3168	C
45	A	3169	C
45	A	3170	C
45	A	3171	C
45	A	3172	C
45	A	3177	A
45	A	3184	C
45	A	3185	A
45	A	3188	U
45	A	3189	C
45	A	3190	A
45	A	3193	U
45	A	3207	A
45	A	3217	A

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Mol	Chain	Res	Type
45	A	3218	A
45	A	3219	G
45	A	3220	A
45	A	3228	U
46	B	1607	U
46	B	1608	G
46	B	1611	G
46	B	1613	U
46	B	1614	U
46	B	1615	A
46	B	1628	C
46	B	1632	U
46	B	1633	U
46	B	1639	U
46	B	1641	G
46	B	1644	G
46	B	1645	A

All (15) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
45	A	2030	U
45	A	2245	A
45	A	2344	C
45	A	2414	C
45	A	2457	A
45	A	2507	A
45	A	2530	A
45	A	2653	C
45	A	2905	A
45	A	2925	U
45	A	3113	A
45	A	3117	C
45	A	3123	G
45	A	3130	A
45	A	3168	C

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

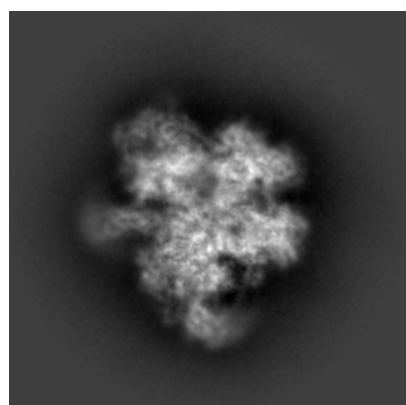
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13965. These allow visual inspection of the internal detail of the map and identification of artifacts.

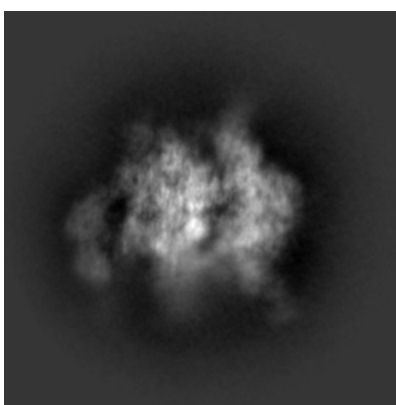
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

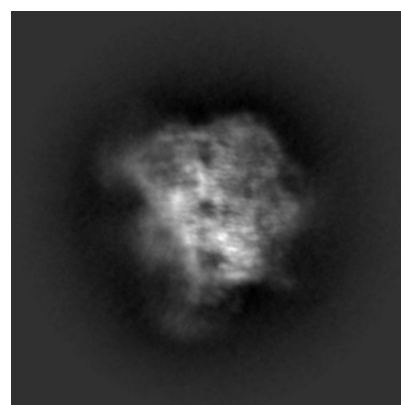
6.1.1 Primary map



X



Y

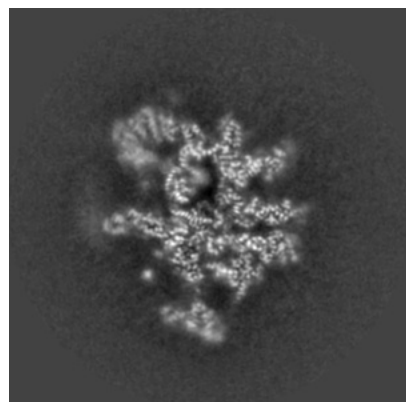


Z

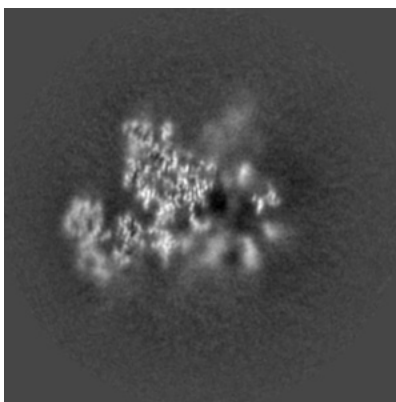
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

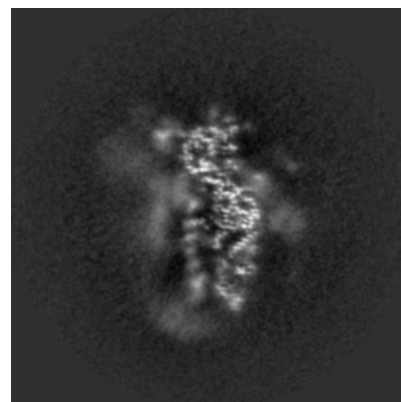
6.2.1 Primary map



X Index: 180



Y Index: 180

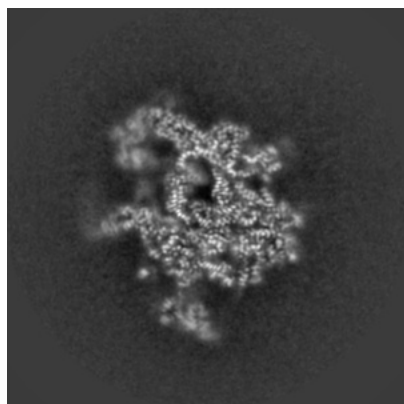


Z Index: 180

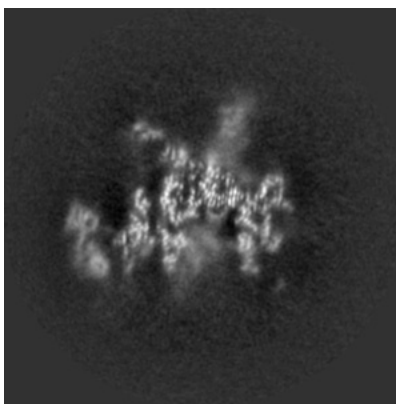
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

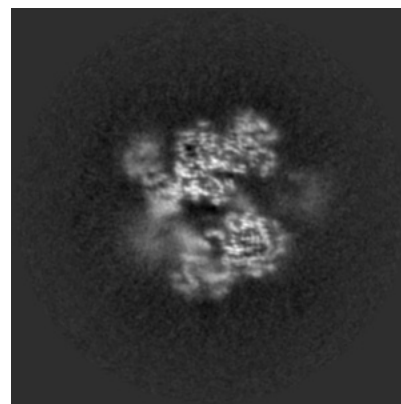
6.3.1 Primary map



X Index: 186



Y Index: 191

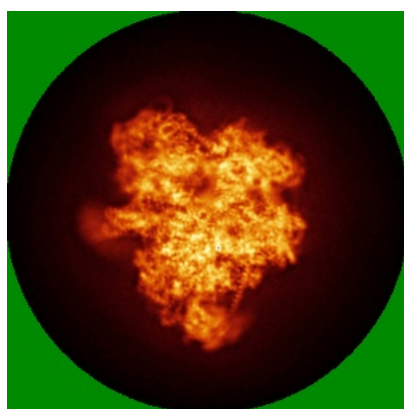


Z Index: 221

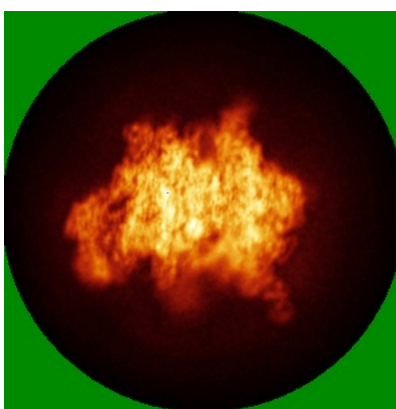
The images above show the largest variance slices of the map in three orthogonal directions.

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

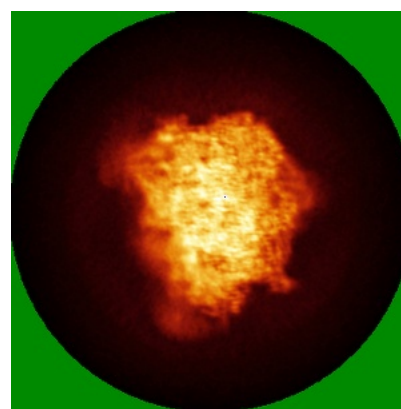
6.4.1 Primary map



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](#)

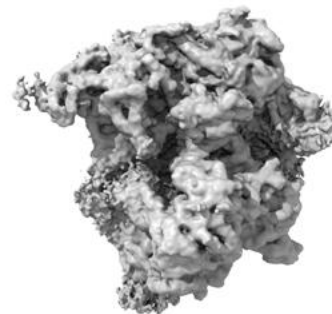
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

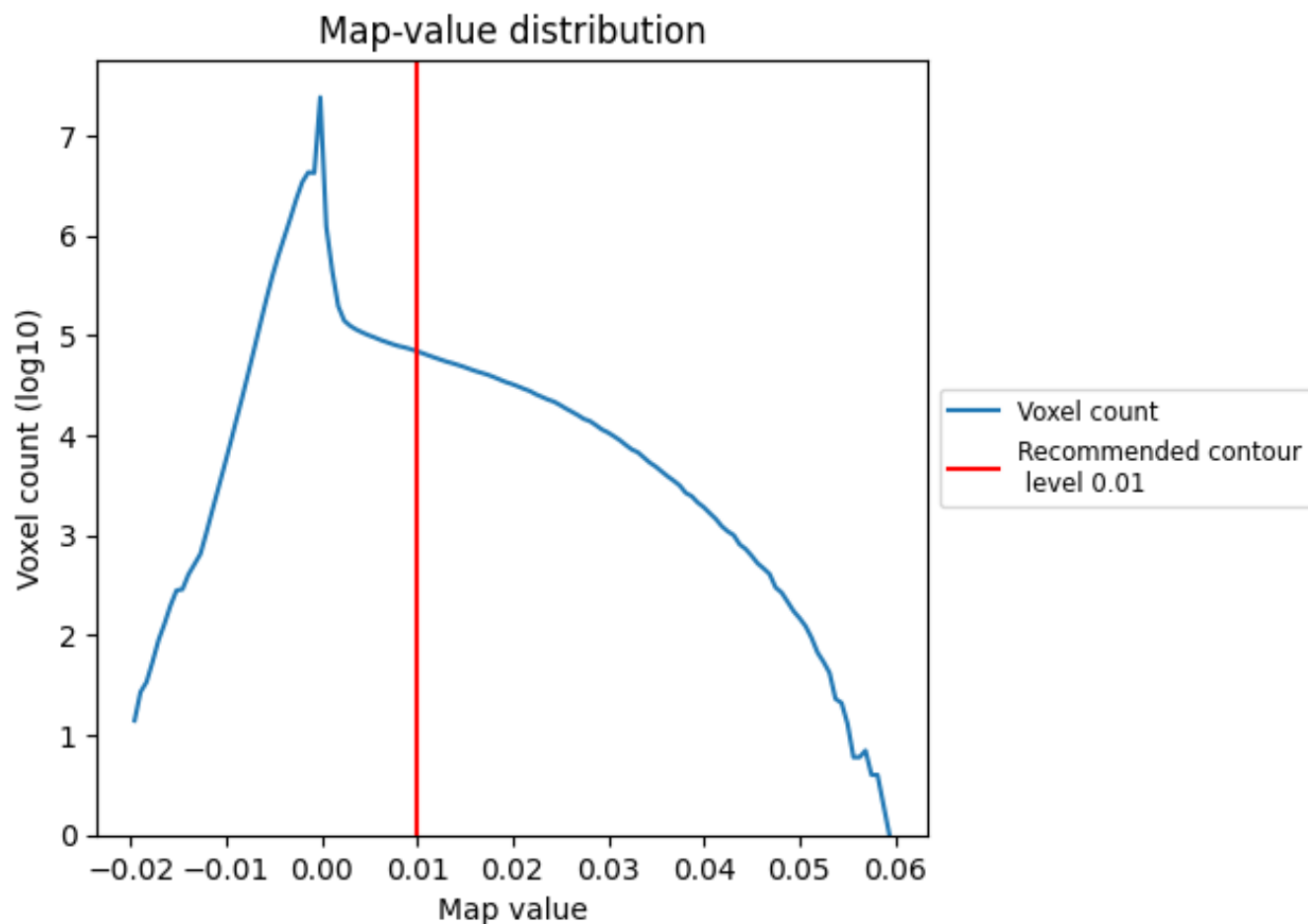
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

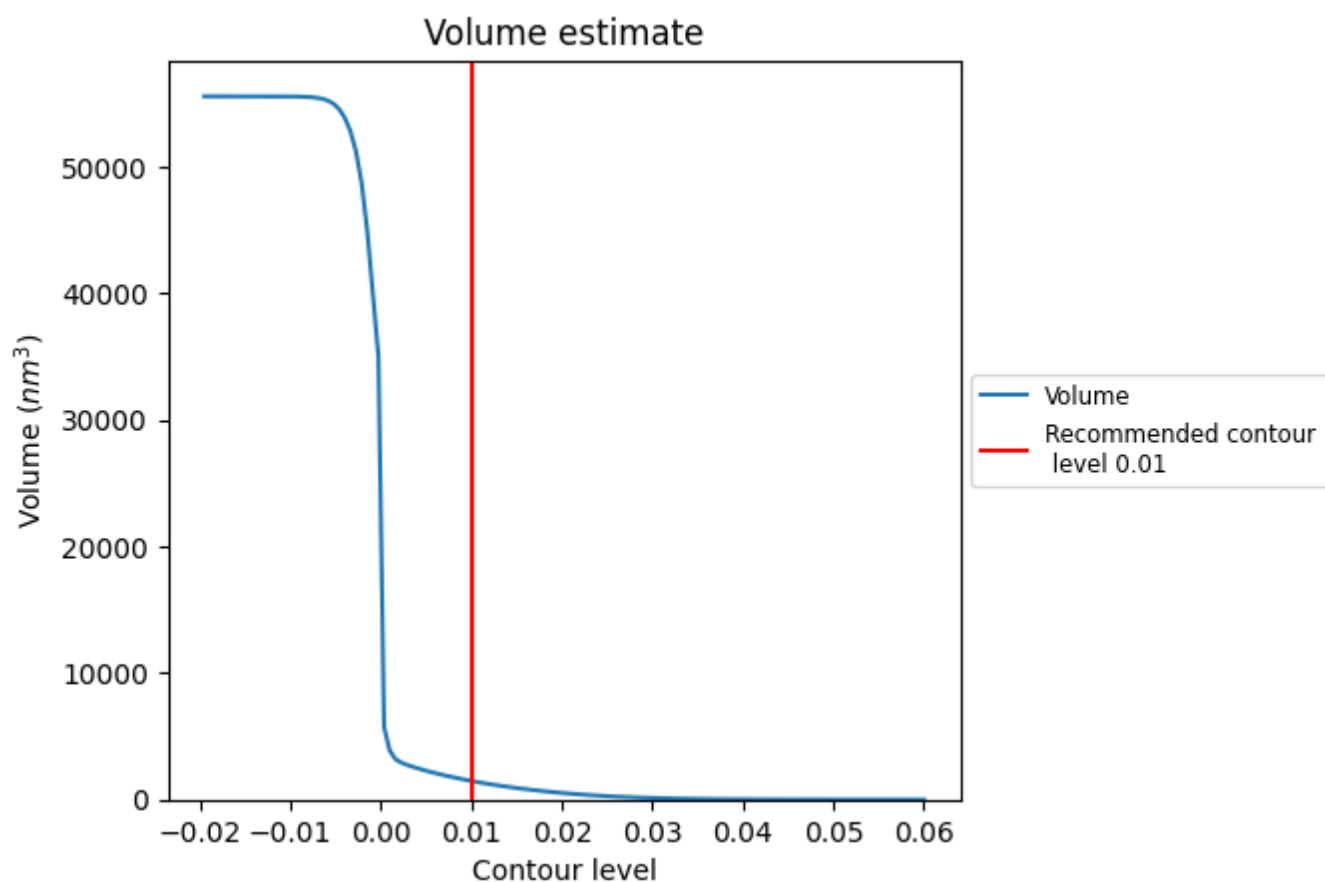
This section contains the results of statistical analysis of the map.

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.

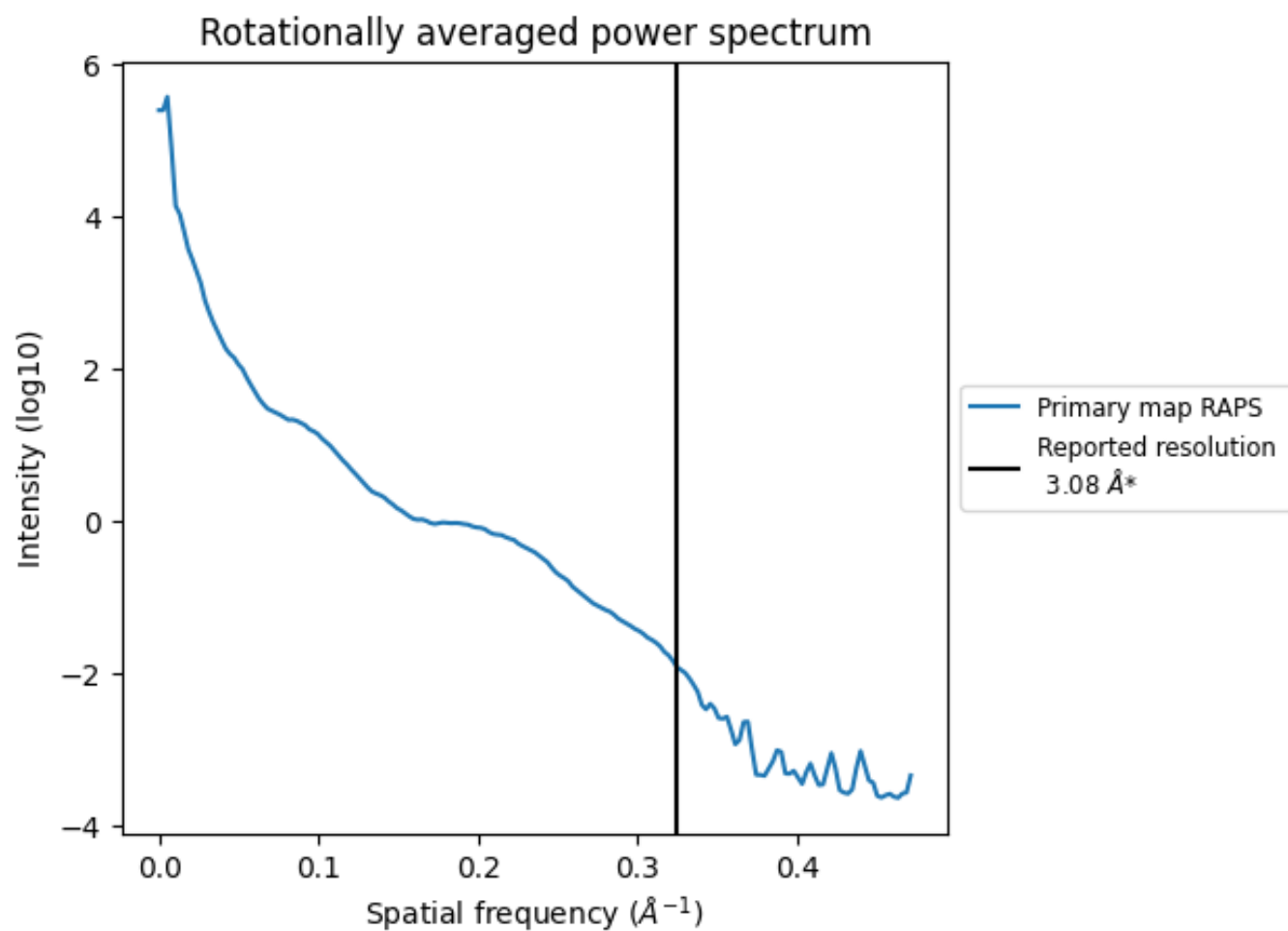
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1470 nm³; this corresponds to an approximate mass of 1328 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 ⓘ

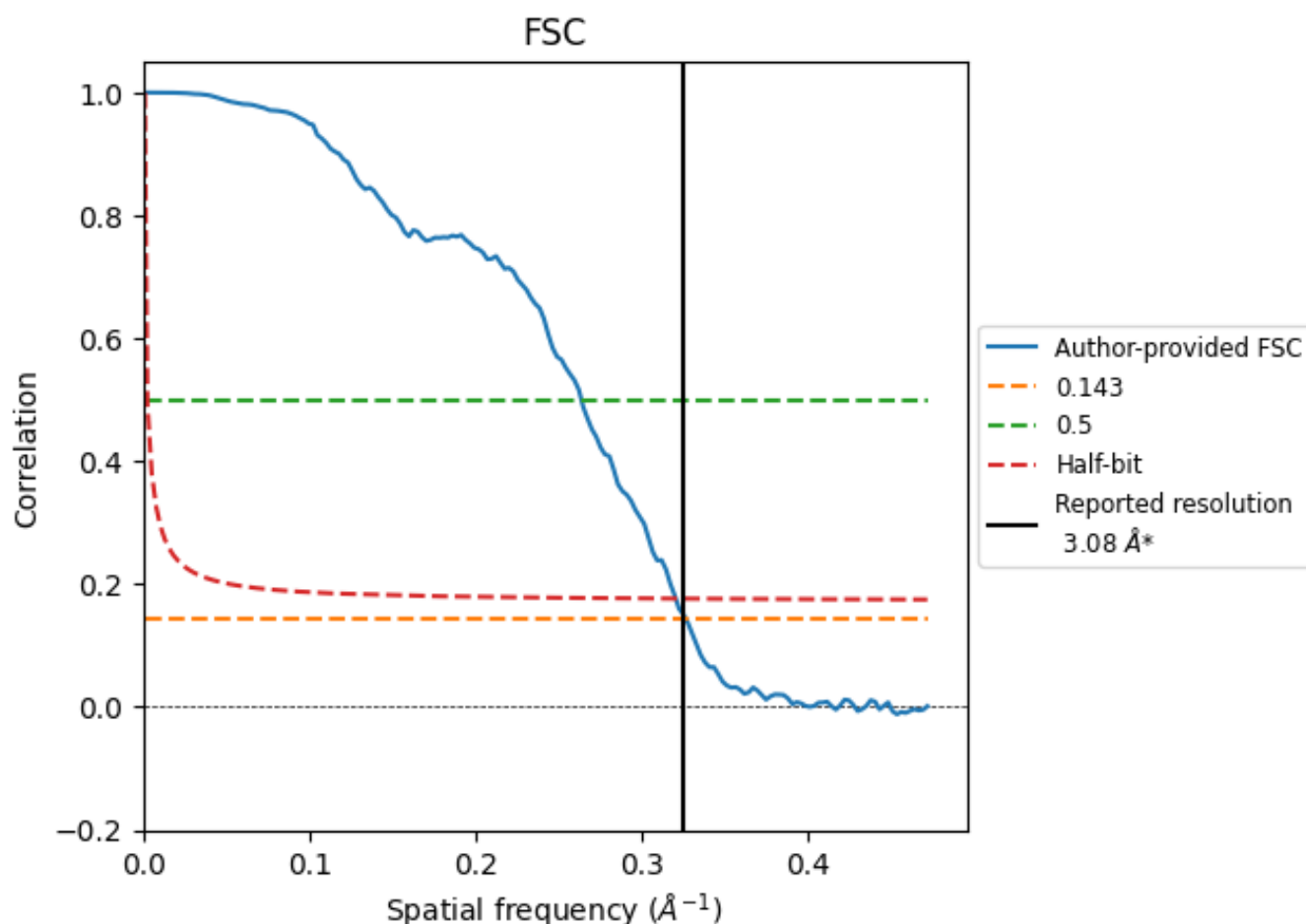


*Reported resolution corresponds to spatial frequency of 0.325 Å⁻¹

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 0.325 Å⁻¹

8.2 Resolution estimates [i](#)

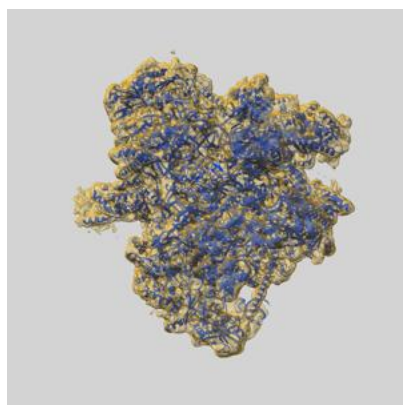
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.08	-	-
Author-provided FSC curve	3.06	3.79	3.12
Unmasked-calculated*	-	-	-

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

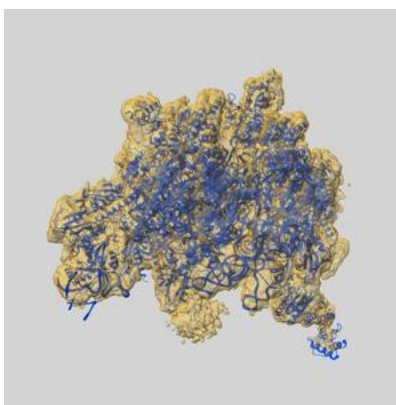
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-13965 and PDB model 7QH6. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

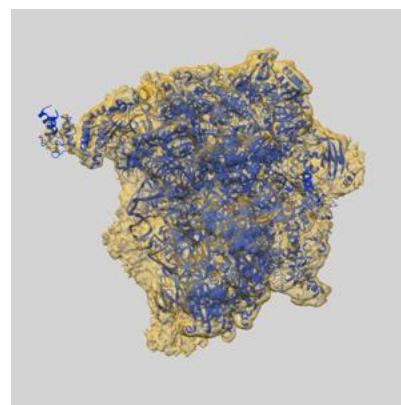
9.1 Map-model overlay [i](#)



X



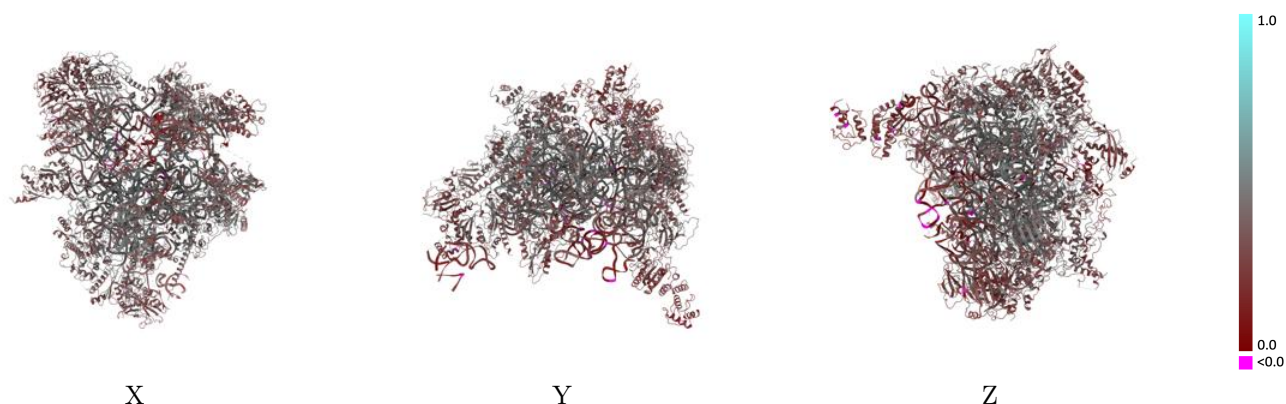
Y



Z

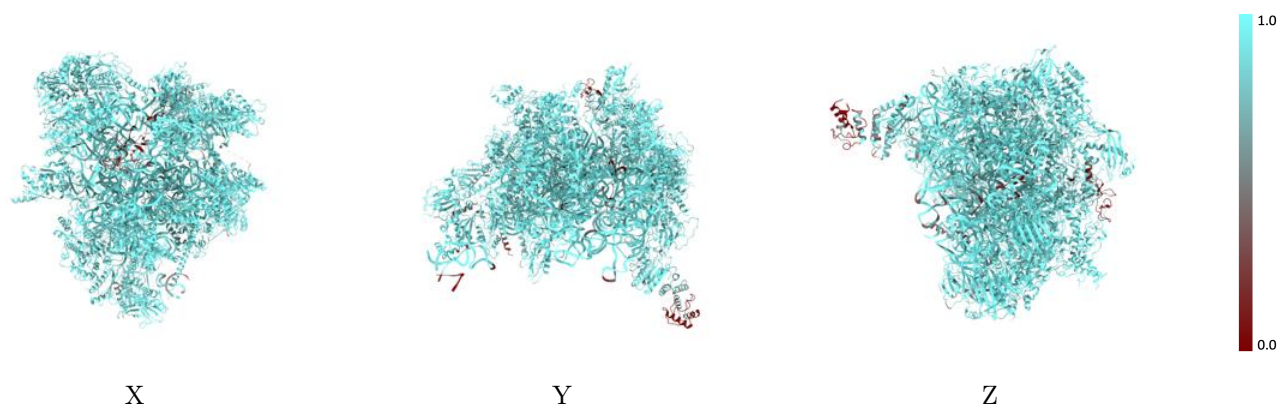
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



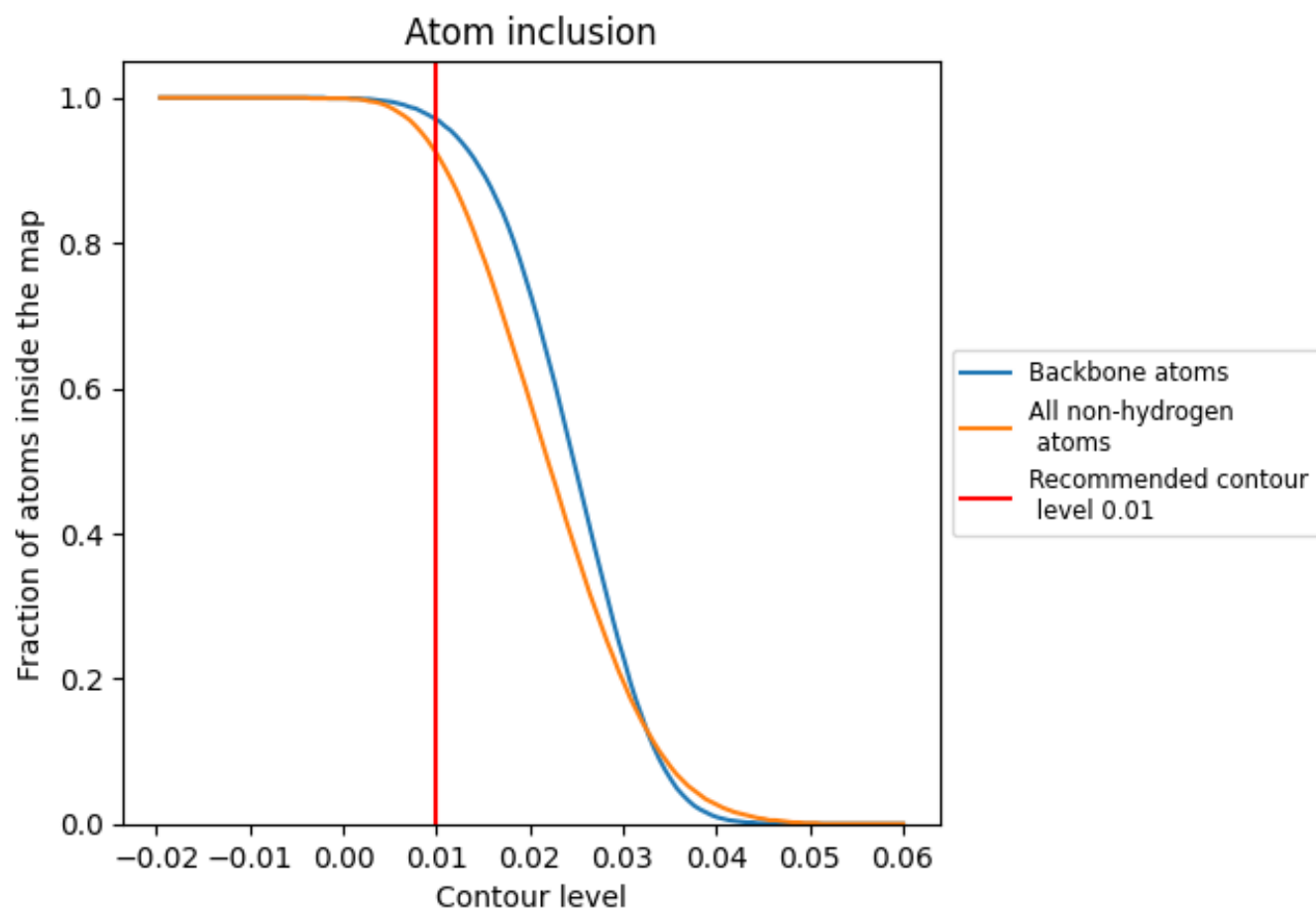
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 92% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9240	 0.3740
0	 0.9370	 0.3980
1	 0.9290	 0.2150
2	 0.9430	 0.4390
3	 0.9370	 0.4640
5	 0.9170	 0.3150
6	 0.9370	 0.3440
7	 0.9400	 0.3480
9	 0.9450	 0.3830
A	 0.9680	 0.3810
B	 0.7940	 0.2040
D	 0.8890	 0.2740
E	 0.9460	 0.3950
F	 0.9210	 0.4450
H	 0.9160	 0.3710
K	 0.9420	 0.4230
L	 0.9270	 0.3380
M	 0.9310	 0.4290
N	 0.9270	 0.3690
O	 0.9440	 0.4180
P	 0.9450	 0.3540
Q	 0.8990	 0.3710
R	 0.9070	 0.4310
S	 0.9340	 0.4330
T	 0.8600	 0.3980
U	 0.8950	 0.3940
V	 0.6720	 0.2610
W	 0.9540	 0.4380
X	 0.9210	 0.3890
Y	 0.9560	 0.3990
Z	 0.9050	 0.4340
a	 0.9100	 0.4070
b	 0.9720	 0.4450
c	 0.9480	 0.3890
d	 0.8900	 0.2920



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Chain	Atom inclusion	Q-score
g	 0.9650	 0.4300
h	 0.9430	 0.3700
i	 0.9590	 0.4550
j	 0.9110	 0.4070
o	 0.9120	 0.3760
p	 0.8080	 0.3460
q	 0.8080	 0.3250
r	 0.9610	 0.3730
s	 0.9360	 0.3940
u	 0.9150	 0.2750
v	 0.6880	 0.2350
w	 0.1750	 0.1840