



## Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 12:35 AM UTC

PDB ID : 5OOM / pdb\_00005oom  
EMDB ID : EMD-3843  
Title : Structure of a native assembly intermediate of the human mitochondrial ribosome with unfolded interfacial rRNA  
Authors : Brown, A.; Rathore, S.; Kimanius, D.; Aibara, S.; Bai, X.C.; Rorbach, J.; Amunts, A.; Ramakrishnan, V.  
Deposited on : 2017-08-08  
Resolution : 3.03 Å (reported)  
Based on initial model : 3J9M

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

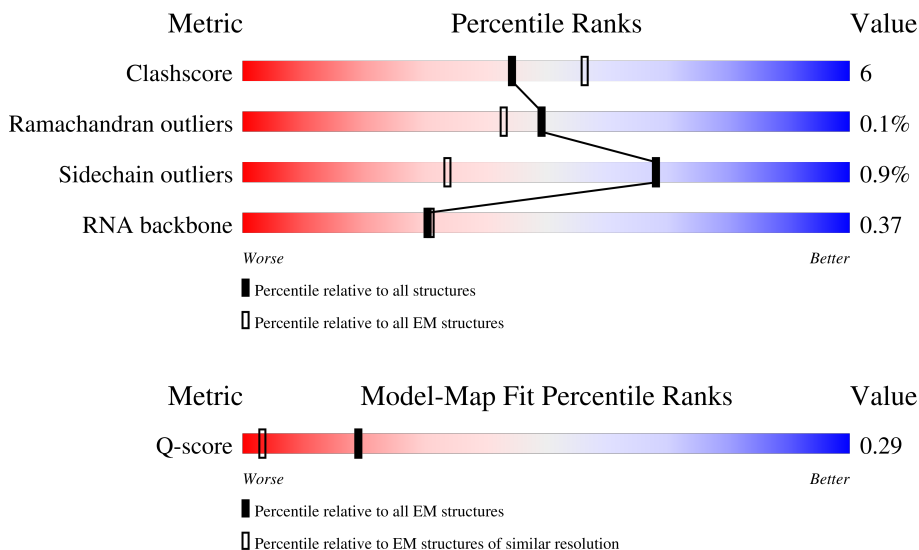
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

# 1 Overall quality at a glance

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

The reported resolution of this entry is 3.03 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	13929 ( 2.53 - 3.53 )

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

Mol	Chain	Length	Quality of chain
1	A	1559	
2	B	69	

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Mol	Chain	Length	Quality of chain
3	D	305	28% 57% 14% 28%
4	E	348	13% 69% 13% 18%
5	F	311	12% 64% 16% 20%
6	H	267	11% 30% 6% 64%
7	I	261	51% 46% 14% 39%
8	J	192	73% 50% 22% 27%
9	K	178	12% 74% 24% ..
10	L	145	24% 61% 19% 21%
11	M	296	17% 81% 16% .
12	N	251	39% 66% 15% 18%
13	O	175	14% 64% 22% . 13%
14	P	180	14% 60% 18% 22%
15	Q	292	15% 60% 14% 26%
16	R	149	19% 86% 6% . 6%
17	S	205	5% 59% 17% 24%
18	T	206	11% 61% 16% 23%
19	U	153	12% 67% 22% . 9%
20	V	216	15% 75% 14% 11%
21	W	148	19% 61% 12% 26%
22	X	256	20% 80% 14% . 5%
23	Y	250	11% 60% 10% 30%
24	Z	161	7% 64% 11% 25%
25	0	188	6% 48% 9% 43%
26	1	65	22% 62% 18% 20%
27	2	92	11% 34% 13% 53%


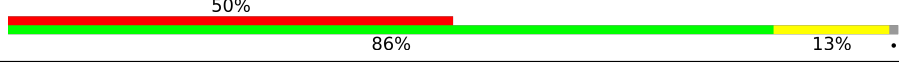
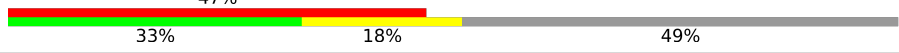
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Mol	Chain	Length	Quality of chain
28	3	188	11% 41% 8% 49%
29	5	423	16% 72% 19% 9%
30	6	380	18% 71% 14% 15%
31	7	338	8% 70% 14% 15%
32	8	206	32% 39% 9% 52%
33	9	137	18% 69% 15% 15%
34	a	142	6% 51% 6% 42%
35	b	215	6% 56% 12% 31%
36	c	332	5% 73% 10% 17%
37	d	306	17% 59% 9% 31%
38	e	279	67% 55% 22% 22%
39	f	212	38% 46% 8% 45%
40	g	166	6% 66% 10% 22%
41	h	158	9% 56% 8% 37%
42	i	128	16% 59% 16% 24%
43	j	123	8% 60% 9% 31%
44	k	112	63% 51% 21% 29%
45	l	138	14% 14% 83%
46	m	128	30% 19% 12% 65%
47	o	102	6% 72% 6% 23%
48	p	206	19% 57% 38%
49	q	222	12% 48% 9% 42%
50	r	196	15% 56% 18% 26%
51	s	439	10% 70% 14% 16%
52	t	28	100% 93% 7%

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Mol	Chain	Length	Quality of chain
53	u	234	
54	v	70	
55	w	156	

## 2 Entry composition i

There are 58 unique types of molecules in this entry. The entry contains 90739 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 RNA chain called 16S ribosomal RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	1092	23184	10409	4202	7481	1092	0	0

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 2 is a RNA chain called mitochondrial tRNAVal.

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

- Molecule 3 is a protein called 39S ribosomal protein L2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	220	1706	1059	339	299	9	0	0

- Molecule 4 is a protein called 39S ribosomal protein L3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	E	285	2258	1457	384	406	11	0	0

- Molecule 5 is a protein called 39S ribosomal protein L4, mitochondrial.

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

- Molecule 6 is a protein called 39S ribosomal protein L9, mitochondrial.

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

- Molecule 7 is a protein called 39S ribosomal protein L10, mitochondrial.

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

- Molecule 8 is a protein called 39S ribosomal protein L11, mitochondrial.

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

- Molecule 9 is a protein called 39S ribosomal protein L13, mitochondrial.

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

- Molecule 10 is a protein called 39S ribosomal protein L14, mitochondrial.

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

- Molecule 11 is a protein called 39S ribosomal protein L15, mitochondrial.

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

- Molecule 12 is a protein called 39S ribosomal protein L16, mitochondrial.

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

- Molecule 13 is a protein called 39S ribosomal protein L17, mitochondrial.

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

- Molecule 14 is a protein called 39S ribosomal protein L18, mitochondrial.

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

- Molecule 15 is a protein called 39S ribosomal protein L19, mitochondrial.

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

- Molecule 16 is a protein called 39S ribosomal protein L20, mitochondrial.

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

- Molecule 17 is a protein called 39S ribosomal protein L21, mitochondrial.

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

- Molecule 18 is a protein called 39S ribosomal protein L22, mitochondrial.

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

- Molecule 19 is a protein called 39S ribosomal protein L23, mitochondrial.

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

- Molecule 20 is a protein called 39S ribosomal protein L24, mitochondrial.

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

- Molecule 21 is a protein called 39S ribosomal protein L27, mitochondrial.

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

- Molecule 22 is a protein called 39S ribosomal protein L28, mitochondrial.

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

- Molecule 23 is a protein called 39S ribosomal protein L47, mitochondrial.

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

- Molecule 24 is a protein called 39S ribosomal protein L30, mitochondrial.

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

- Molecule 25 is a protein called 39S ribosomal protein L32, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	0	108	880	545	172	157	6	0	0

- Molecule 26 is a protein called 39S ribosomal protein L33, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
26	1	52	433	278	83	70	2	0	0

- Molecule 27 is a protein called 39S ribosomal protein L34, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	2	43	Total	C	N	O	S	0	0
			351	218	76	56	1		

- Molecule 28 is a protein called 39S ribosomal protein L35, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	3	95	Total	C	N	O	S	0	0
			831	539	162	127	3		

- Molecule 29 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 30 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 31 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 32 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 33 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 34 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L46, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L49, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L50, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 45 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 46 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 47 is a protein called Ribosomal protein 63, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	o	79	665	420	130	112	3	0	0

- Molecule 48 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 49 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

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

- Molecule 50 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 51 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 52 is a protein called Unknown protein or protein extension.

Mol	Chain	Residues	Atoms				AltConf	Trace
52	t	28	Total	C	N	O	0	0
			140	84	28	28		

- Molecule 53 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 54 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 55 is a protein called Acyl carrier protein, mitochondrial.

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

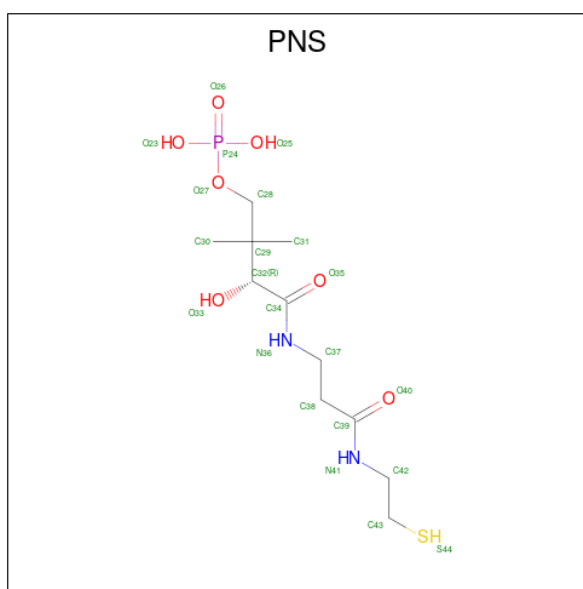
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
56	A	46	Total	Mg	0
			46	46	
56	R	1	Total	Mg	0
			1	1	
56	W	1	Total	Mg	0
			1	1	
56	g	1	Total	Mg	0
			1	1	

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

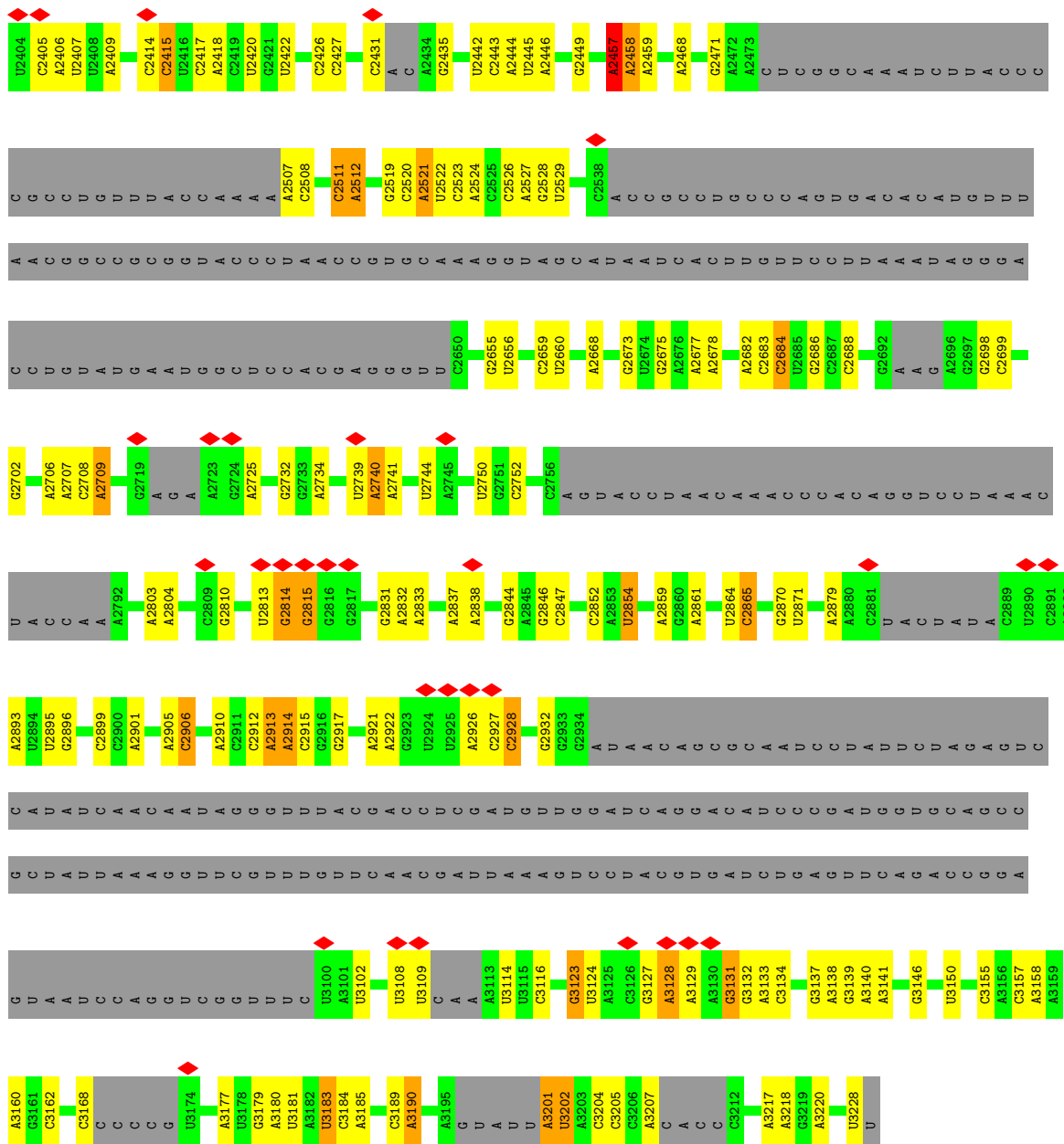
Mol	Chain	Residues	Atoms		AltConf
57	0	1	Total	Zn	0
			1	1	
57	r	1	Total	Zn	0
			1	1	

- Molecule 58 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C<sub>11</sub>H<sub>23</sub>N<sub>2</sub>O<sub>7</sub>PS).

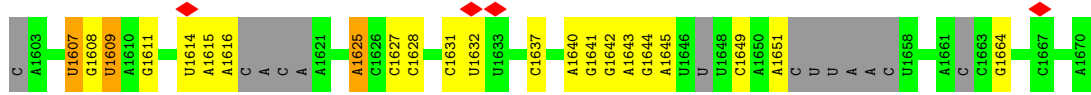


Mol	Chain	Residues	Atoms					AltConf	
			Total	C	N	O	P		S
58	v	1	21	11	2	6	1	1	0

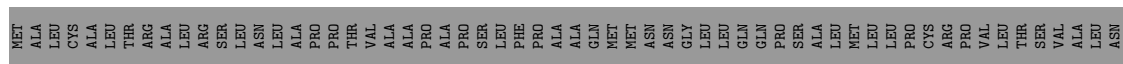


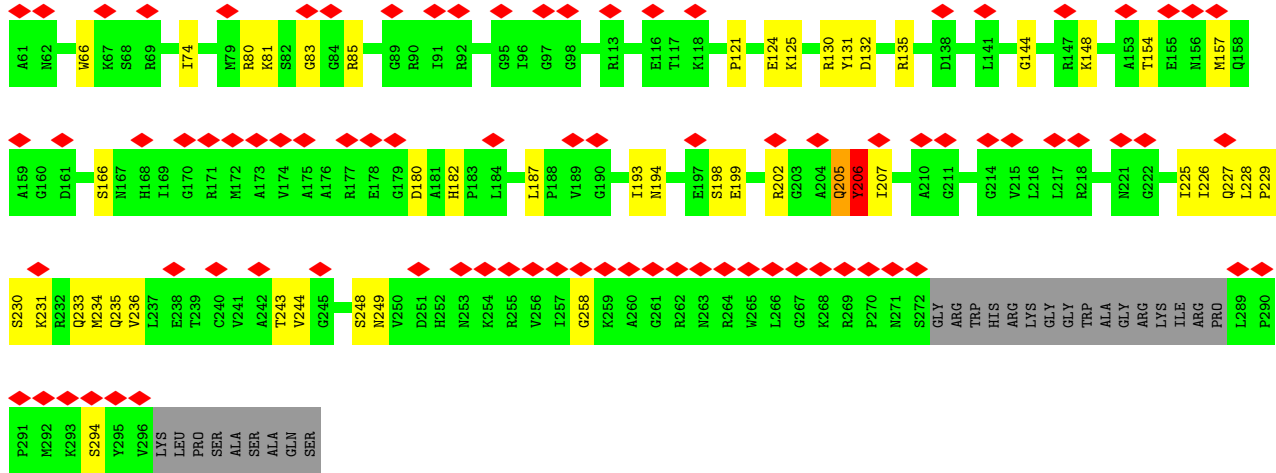


• Molecule 2: mitochondrial tRNAVal

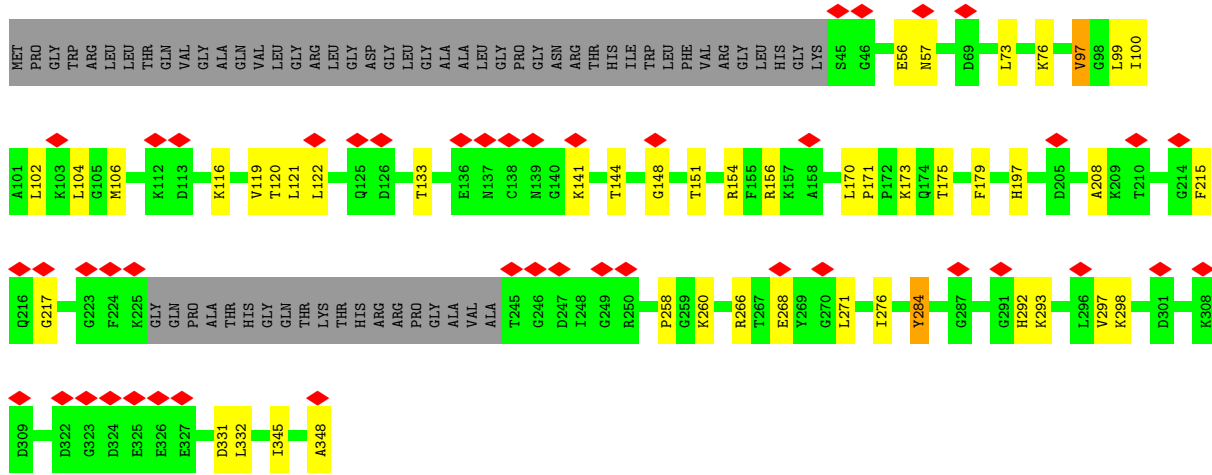


• Molecule 3: 39S ribosomal protein L2, mitochondrial

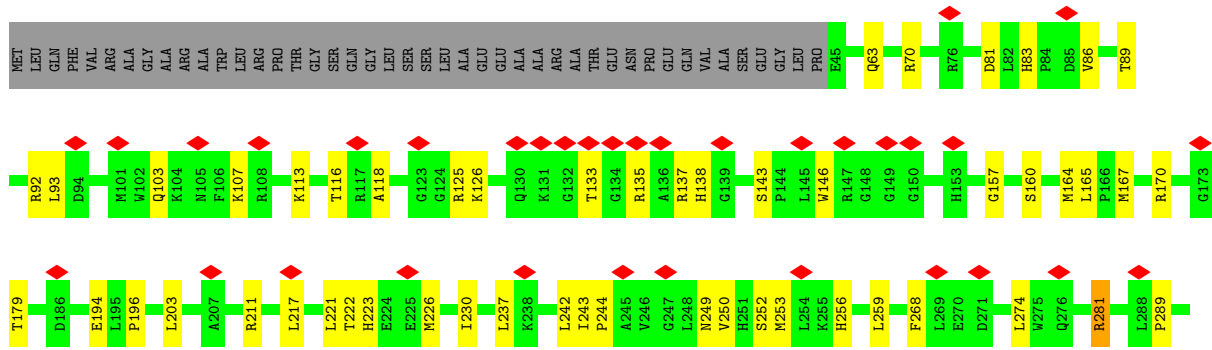




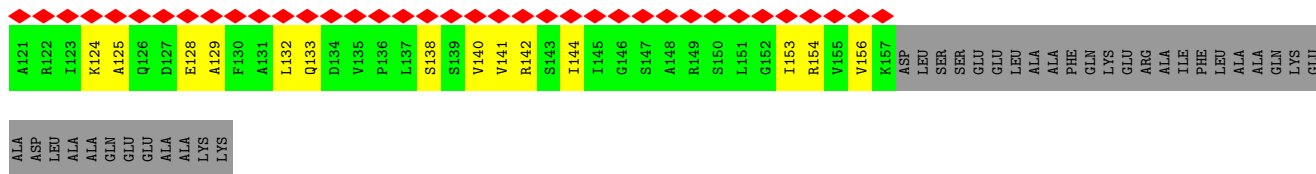
• Molecule 4: 39S ribosomal protein L3, mitochondrial



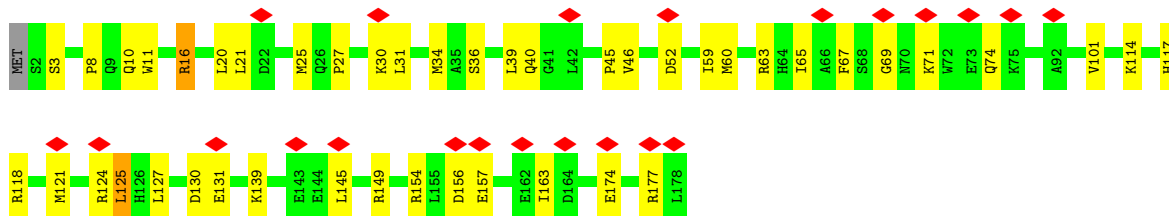
• Molecule 5: 39S ribosomal protein L4, mitochondrial



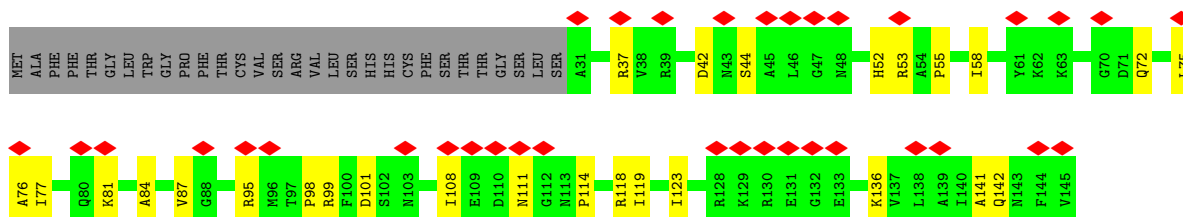




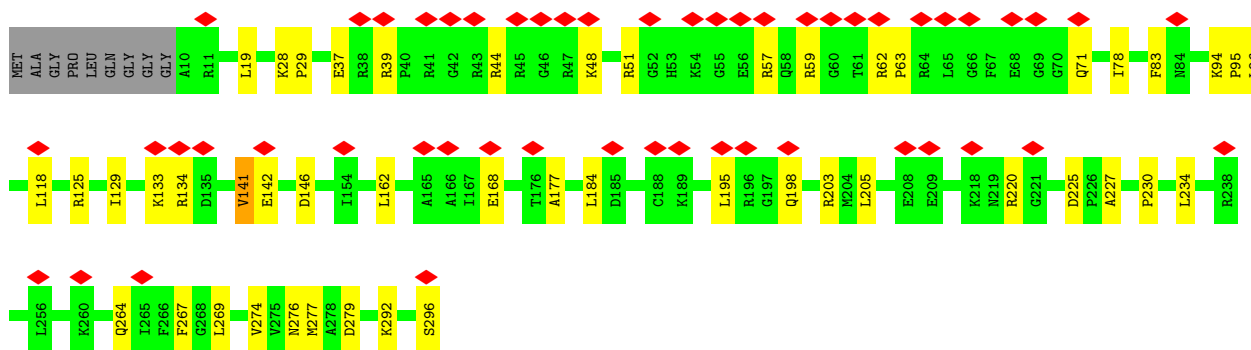
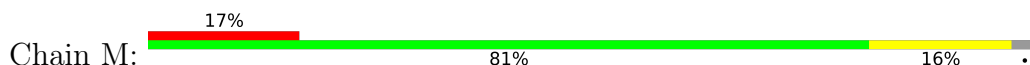
• Molecule 9: 39S ribosomal protein L13, mitochondrial



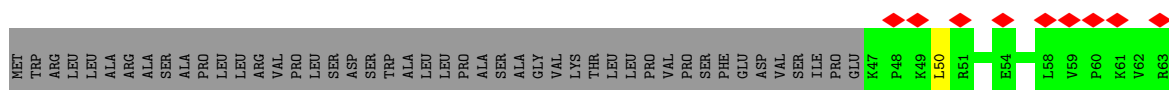
• Molecule 10: 39S ribosomal protein L14, mitochondrial

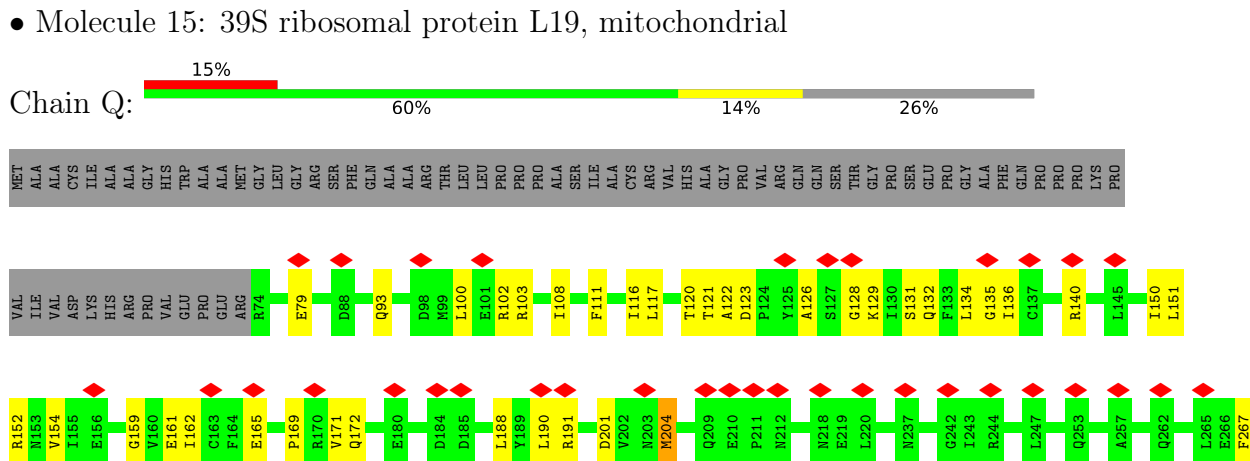
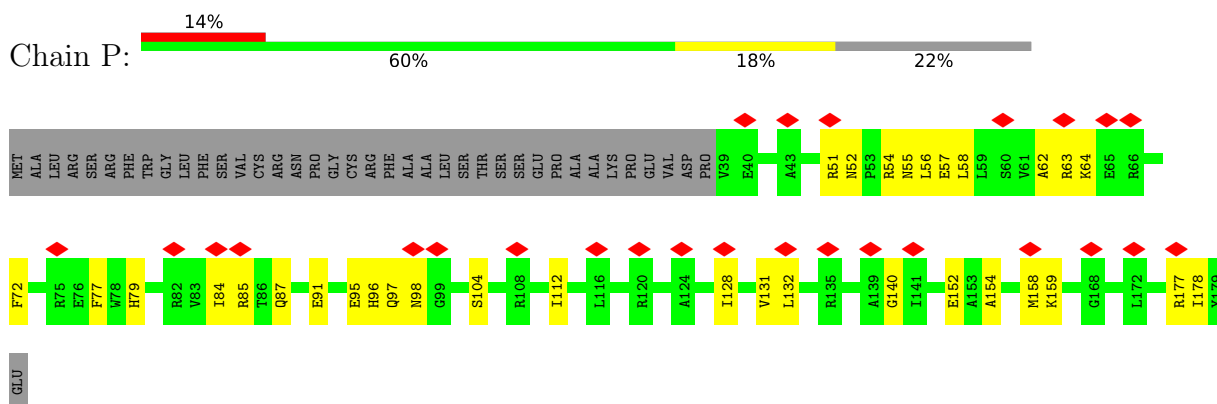
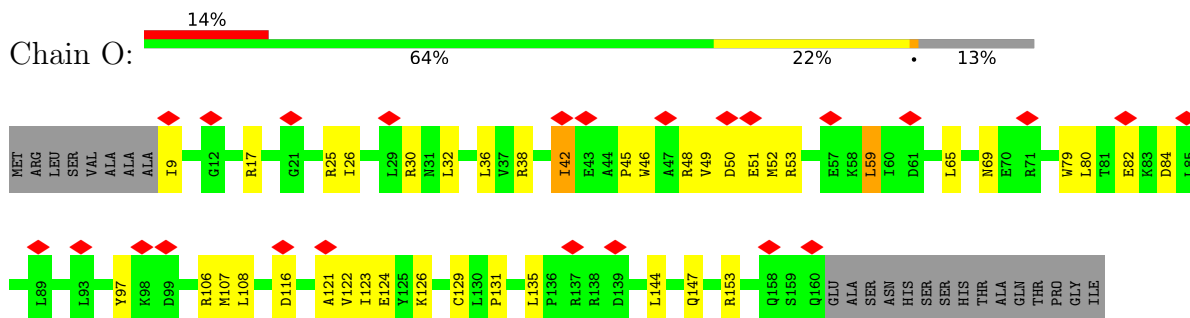
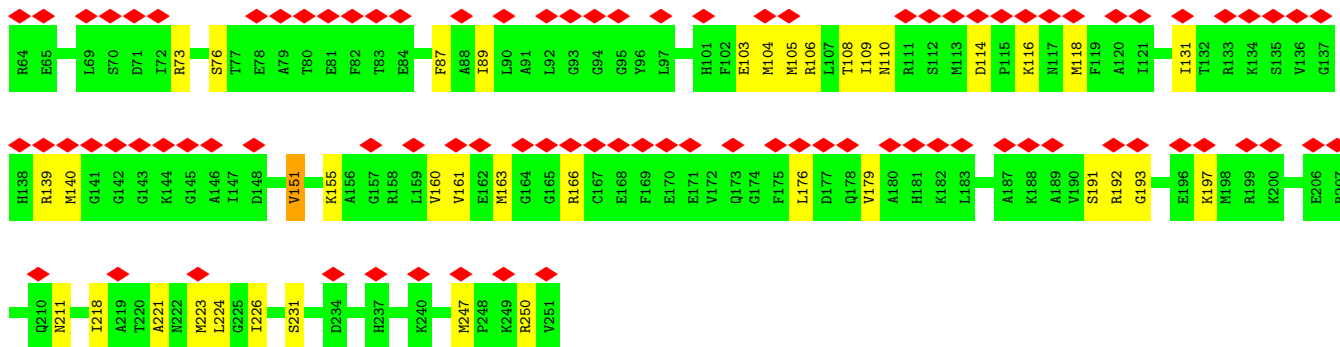


• Molecule 11: 39S ribosomal protein L15, mitochondrial



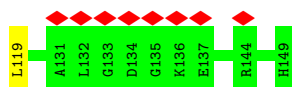
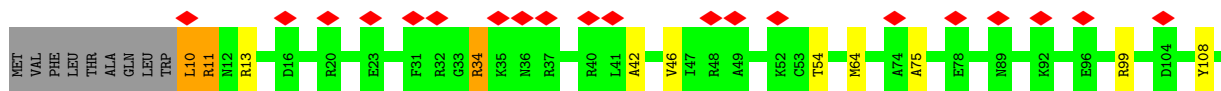
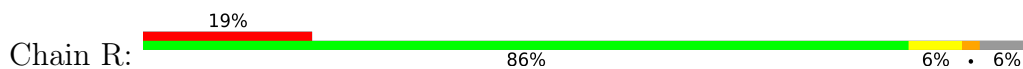
• Molecule 12: 39S ribosomal protein L16, mitochondrial



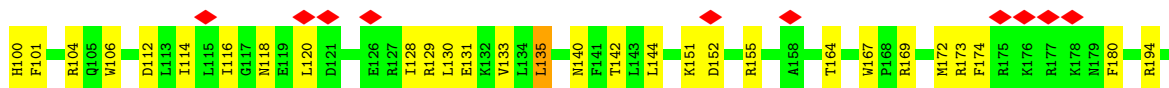
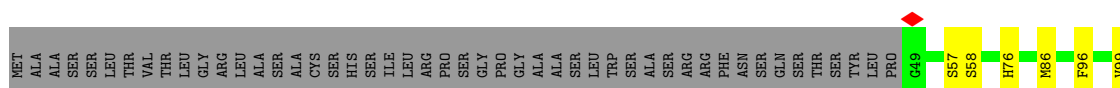




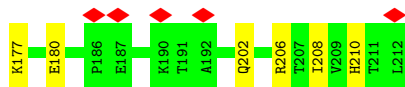
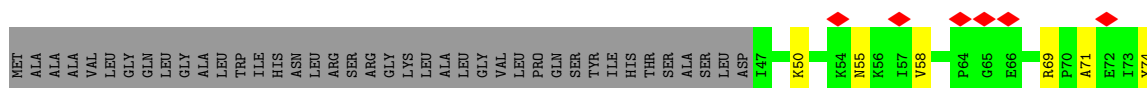
- Molecule 16: 39S ribosomal protein L20, mitochondrial



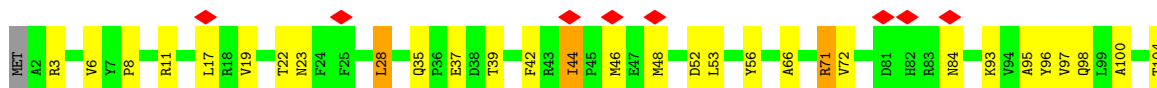
- Molecule 17: 39S ribosomal protein L21, mitochondrial

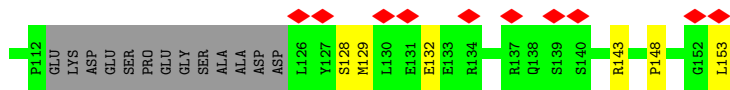


- Molecule 18: 39S ribosomal protein L22, mitochondrial

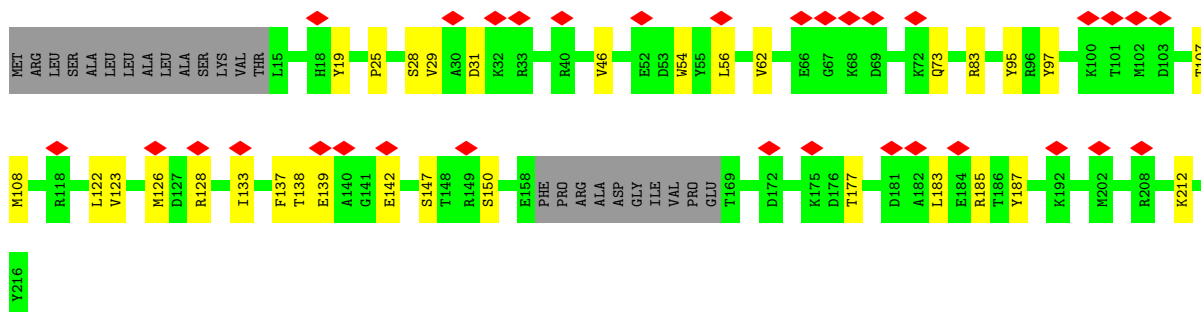
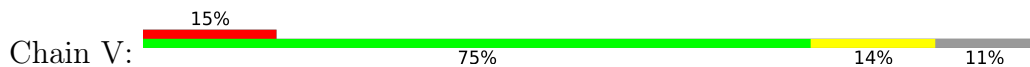


- Molecule 19: 39S ribosomal protein L23, mitochondrial

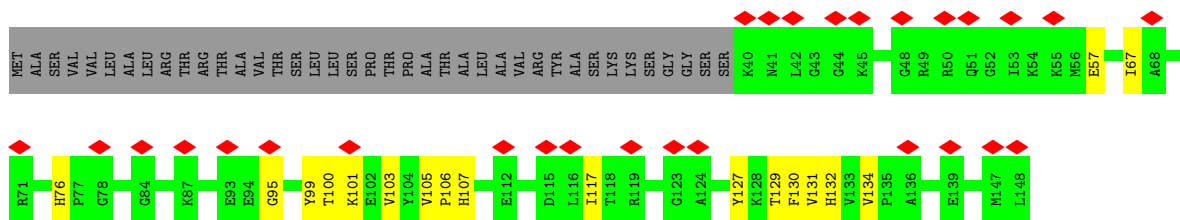




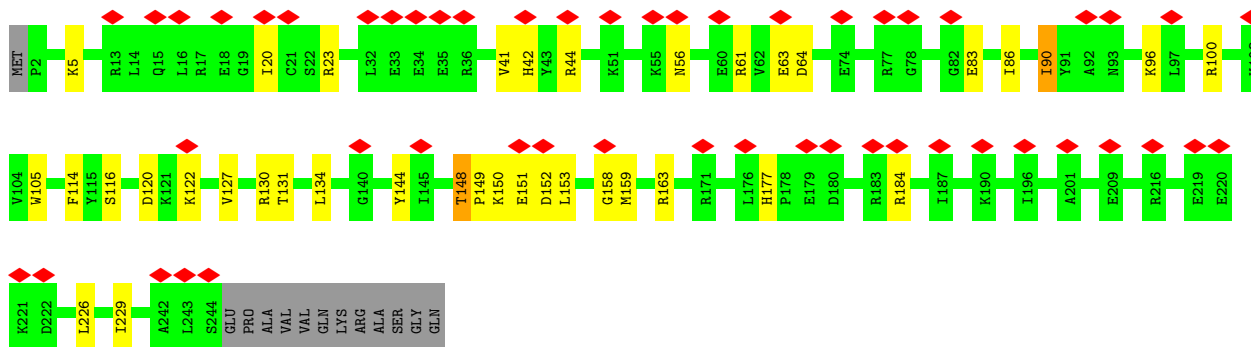
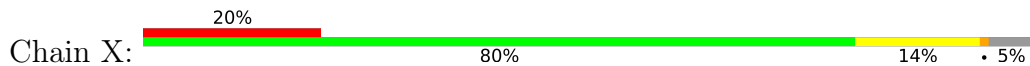
• Molecule 20: 39S ribosomal protein L24, mitochondrial



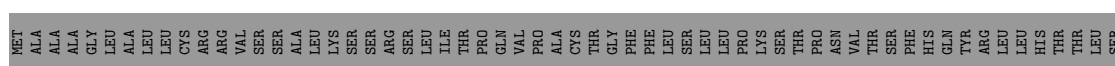
• Molecule 21: 39S ribosomal protein L27, mitochondrial

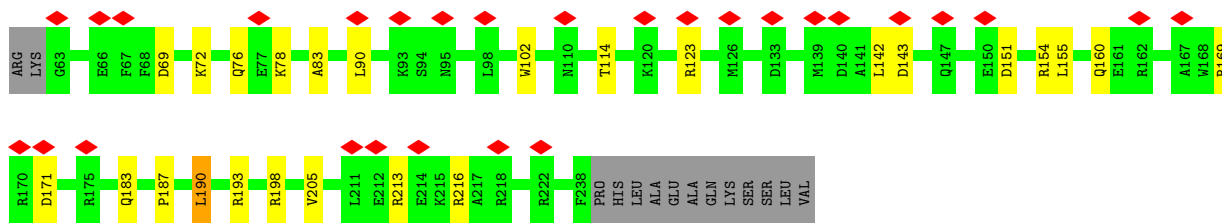


• Molecule 22: 39S ribosomal protein L28, mitochondrial

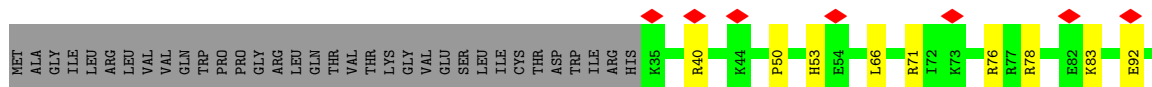


• Molecule 23: 39S ribosomal protein L47, mitochondrial

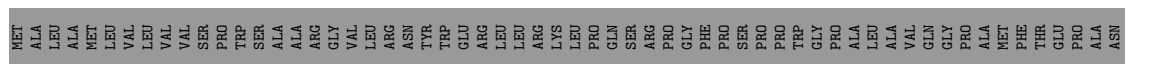




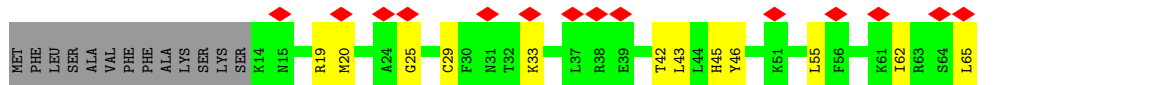
• Molecule 24: 39S ribosomal protein L30, mitochondrial



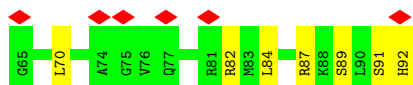
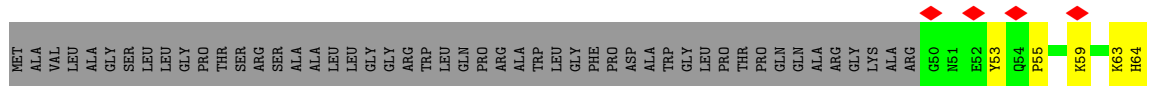
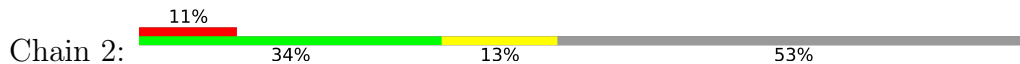
• Molecule 25: 39S ribosomal protein L32, mitochondrial



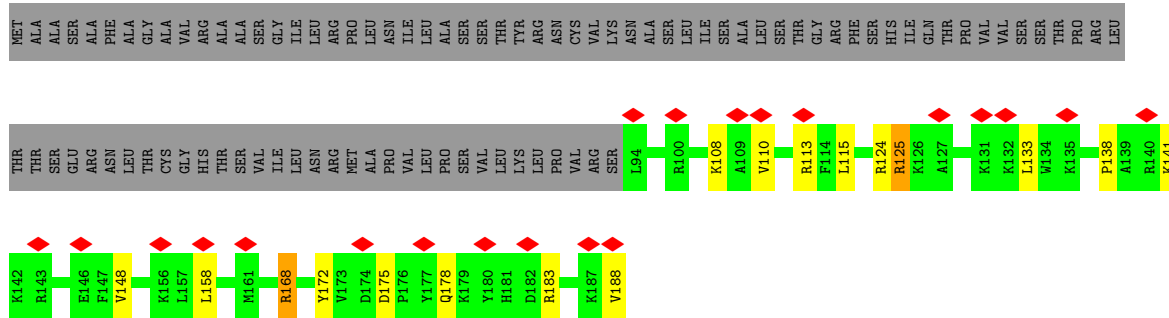
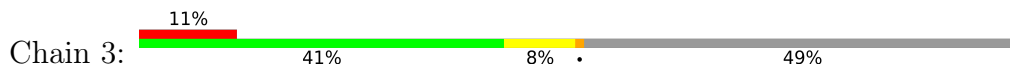
• Molecule 26: 39S ribosomal protein L33, mitochondrial



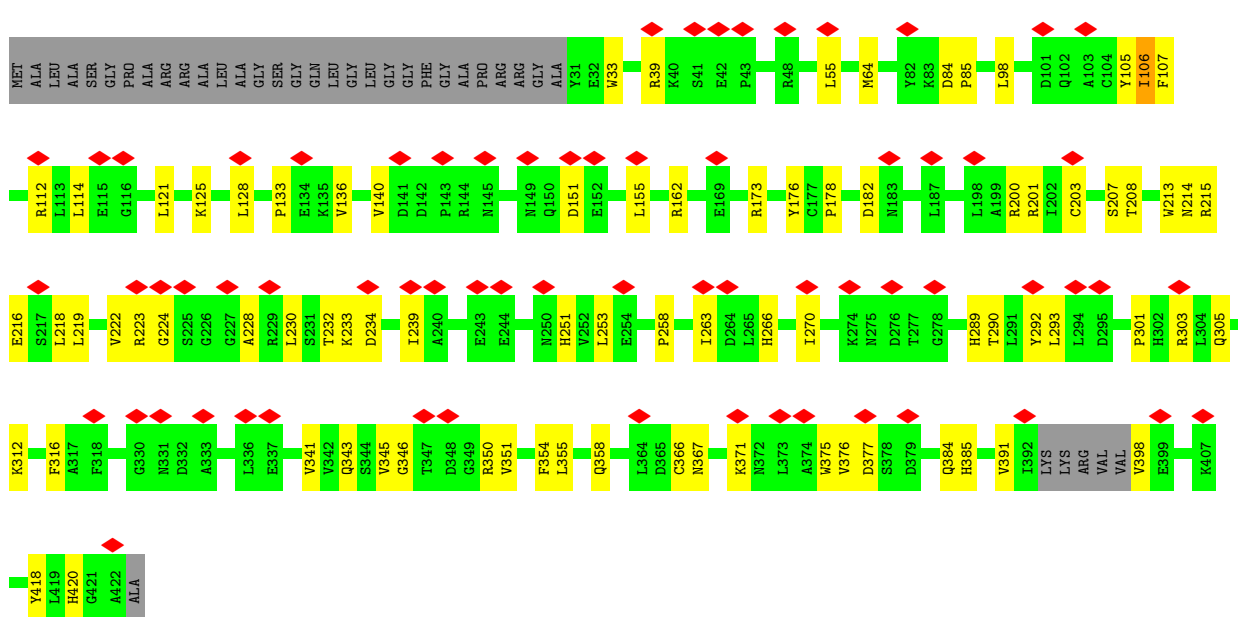
• Molecule 27: 39S ribosomal protein L34, mitochondrial



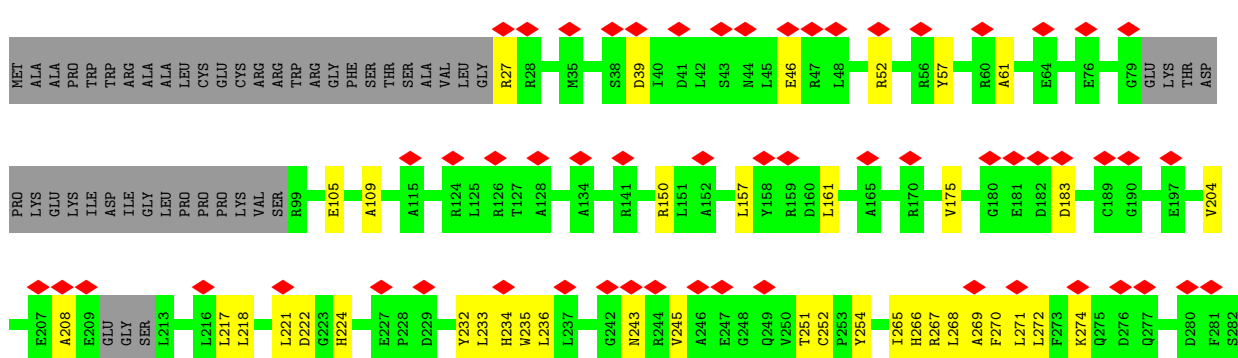
• Molecule 28: 39S ribosomal protein L35, mitochondrial



• Molecule 29: 39S ribosomal protein L37, mitochondrial

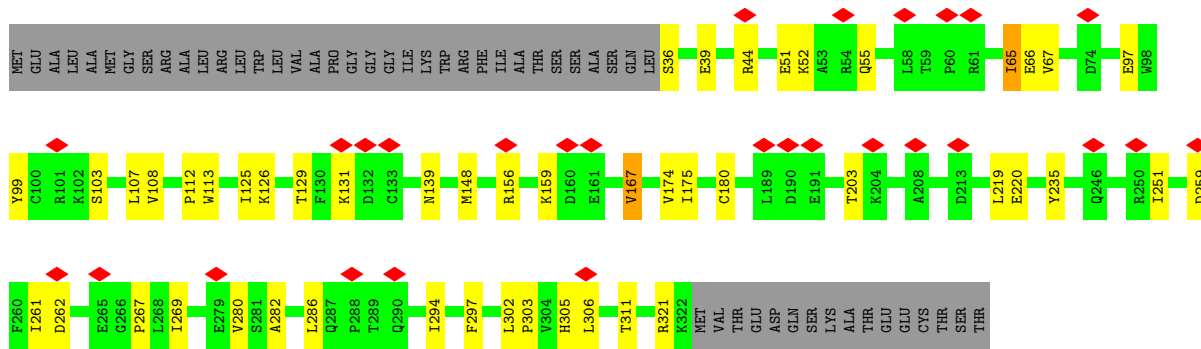


• Molecule 30: 39S ribosomal protein L38, mitochondrial

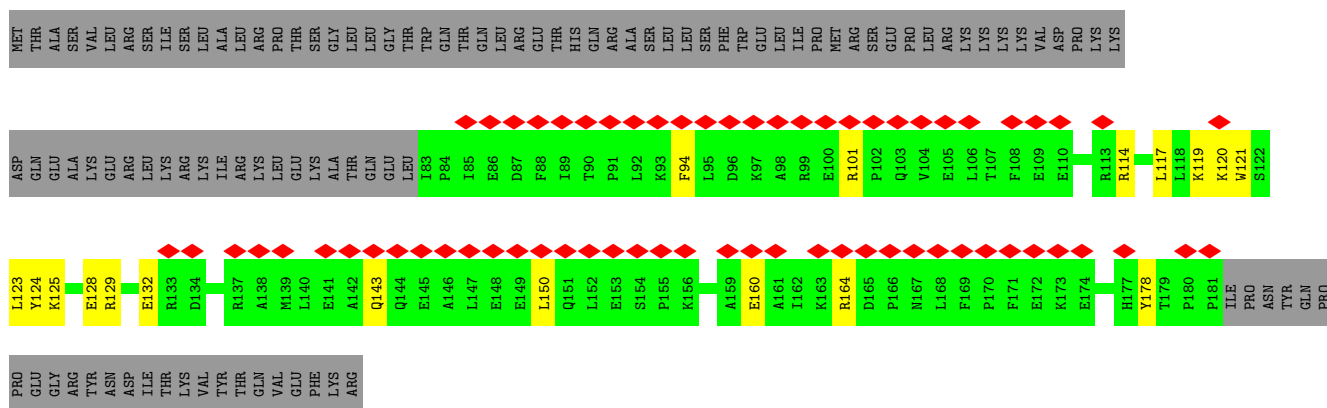
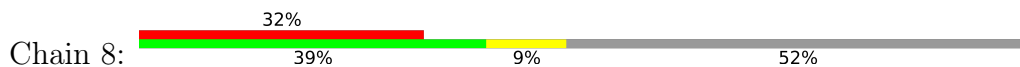




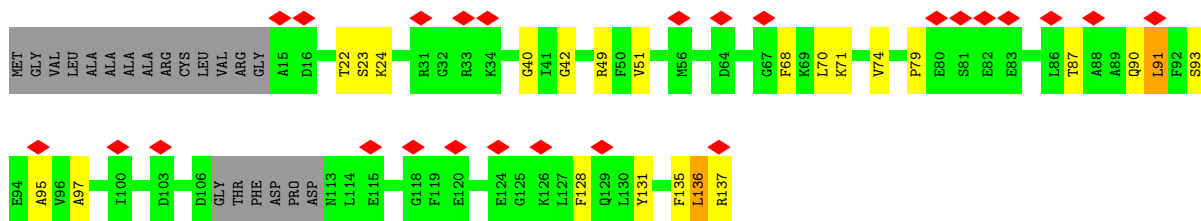
• Molecule 31: 39S ribosomal protein L39, mitochondrial



• Molecule 32: 39S ribosomal protein L40, mitochondrial

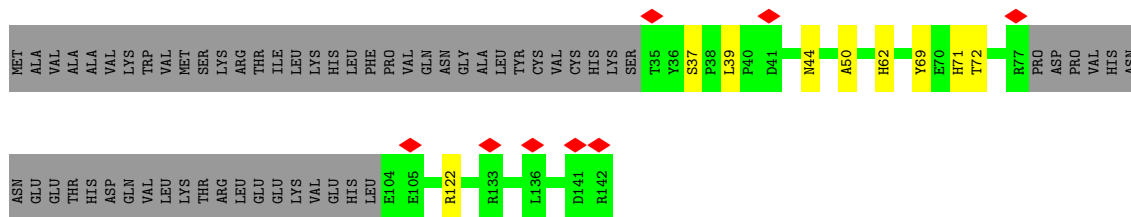


• Molecule 33: 39S ribosomal protein L41, mitochondrial

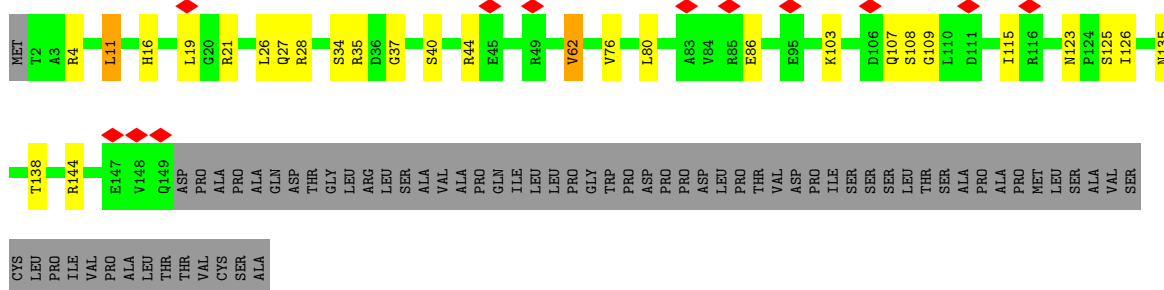


• Molecule 34: 39S ribosomal protein L42, mitochondrial

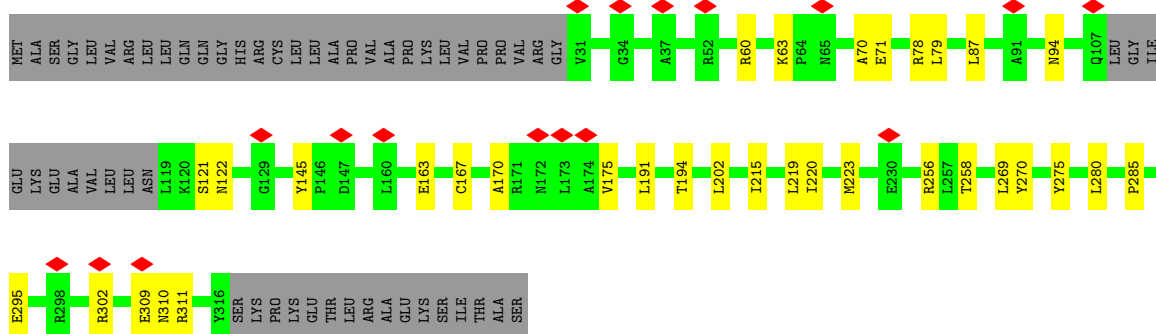
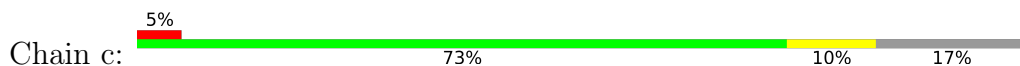




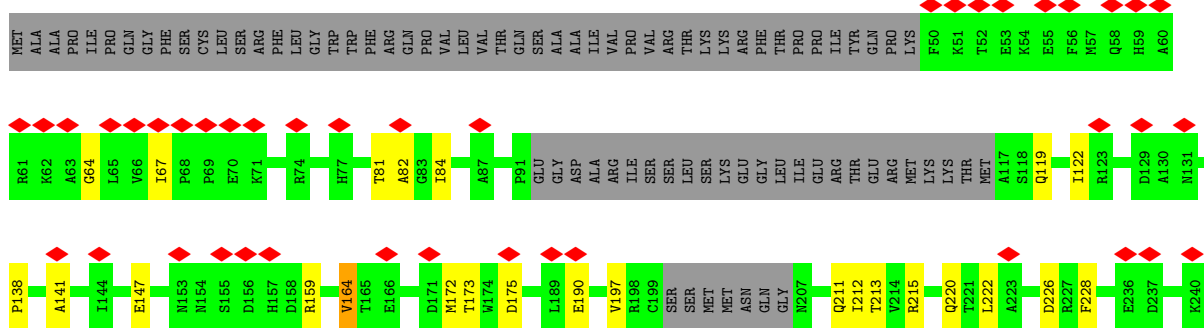
• Molecule 35: 39S ribosomal protein L43, mitochondrial

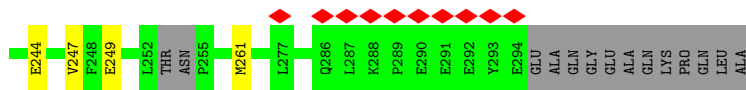


• Molecule 36: 39S ribosomal protein L44, mitochondrial

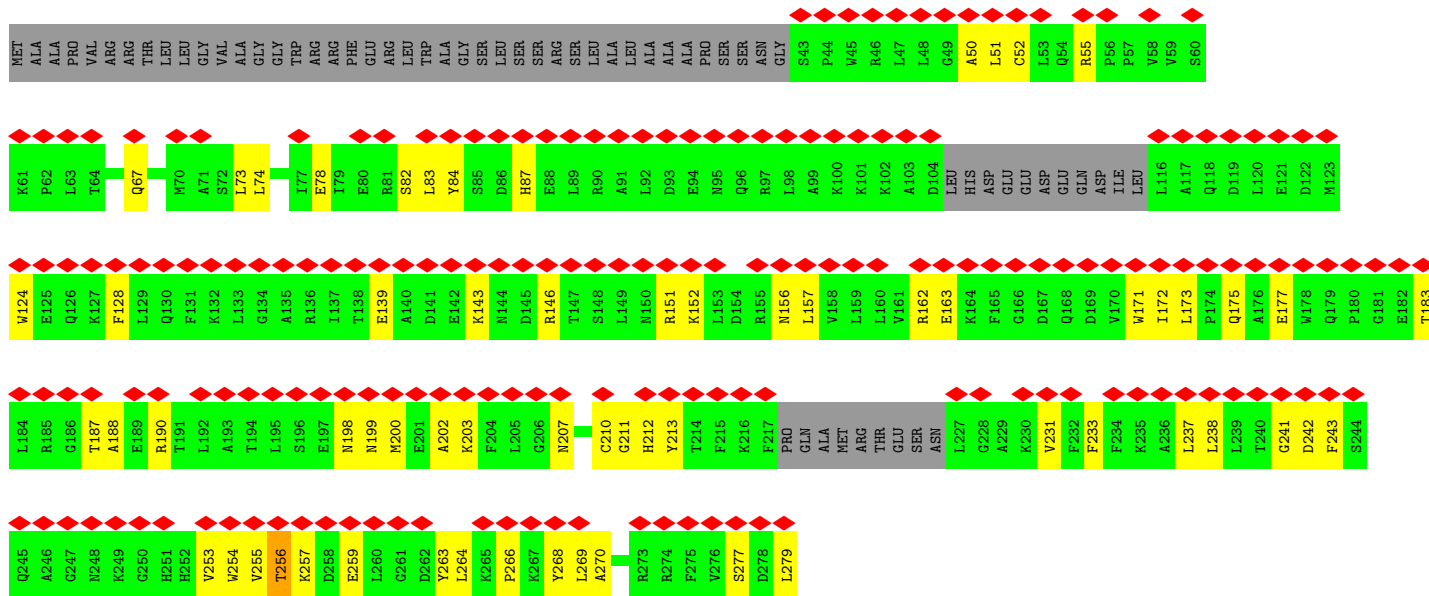


• Molecule 37: 39S ribosomal protein L45, mitochondrial

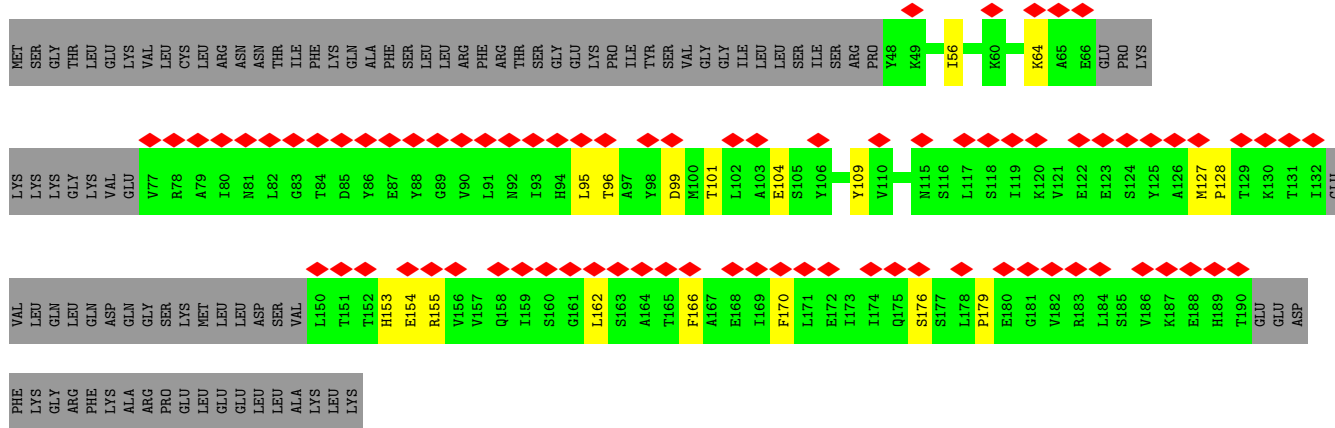
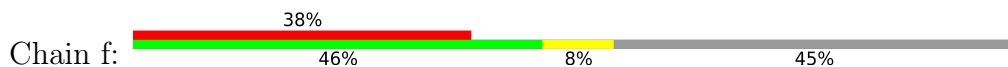




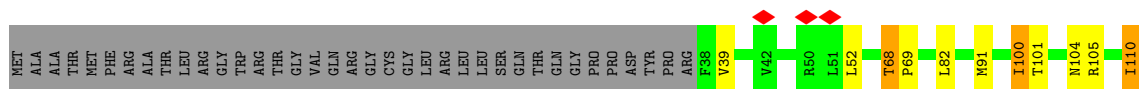
• Molecule 38: 39S ribosomal protein L46, mitochondrial



• Molecule 39: 39S ribosomal protein L48, mitochondrial

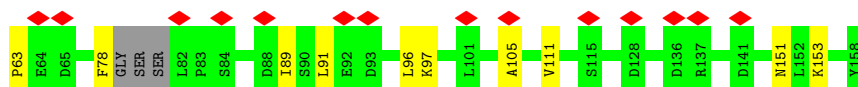
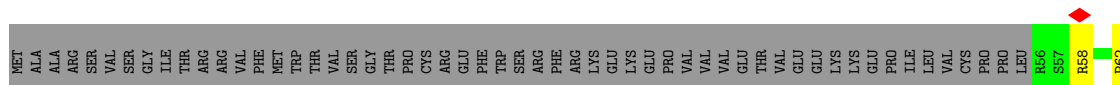


• Molecule 40: 39S ribosomal protein L49, mitochondrial

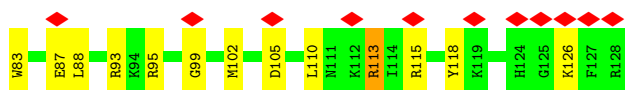
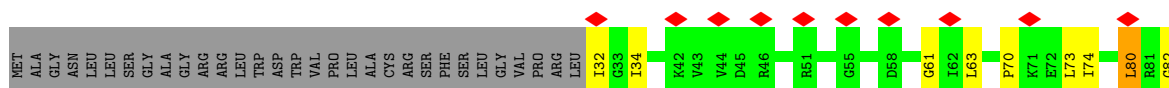




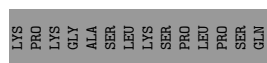
- Molecule 41: 39S ribosomal protein L50, mitochondrial



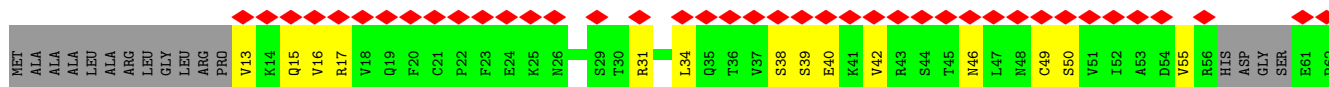
- Molecule 42: 39S ribosomal protein L51, mitochondrial



- Molecule 43: 39S ribosomal protein L52, mitochondrial



- Molecule 44: 39S ribosomal protein L53, mitochondrial



- Molecule 45: 39S ribosomal protein L54, mitochondrial









## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	379869	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 ( $e^-/\text{\AA}^2$ )	1.56	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	130841	Depositor
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.350	Depositor
Minimum map value	-0.156	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.013	Depositor
Recommended contour level	0.075	Depositor
Map size ( $\text{\AA}$ )	373.12, 373.12, 373.12	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.06, 1.06, 1.06	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.84	0/25926	0.62	11/40305 (0.0%)
2	B	0.34	0/1328	0.45	0/2056
3	D	0.56	0/1736	0.73	2/2335 (0.1%)
4	E	0.66	0/2322	0.72	0/3148
5	F	0.89	0/2071	0.81	0/2817
6	H	0.57	0/798	0.76	0/1073
7	I	0.36	0/1308	0.71	3/1761 (0.2%)
8	J	0.24	0/1077	0.60	0/1452
9	K	0.83	0/1495	0.76	0/2029
10	L	0.47	0/904	0.62	0/1218
11	M	0.82	0/2359	0.82	1/3185 (0.0%)
12	N	0.51	0/1697	0.65	0/2281
13	O	0.81	0/1269	0.85	0/1708
14	P	0.61	0/1173	0.70	0/1588
15	Q	0.56	1/1846 (0.1%)	0.70	0/2487
16	R	0.98	0/1174	0.90	3/1572 (0.2%)
17	S	0.89	0/1276	0.82	1/1729 (0.1%)
18	T	0.92	1/1335 (0.1%)	0.78	0/1796
19	U	0.79	0/1183	0.80	0/1600
20	V	0.61	0/1616	0.66	0/2189
21	W	0.80	0/881	0.64	0/1188
22	X	0.63	0/2090	0.71	2/2825 (0.1%)
23	Y	0.78	0/1552	0.71	1/2079 (0.0%)
24	Z	0.80	0/1003	0.77	0/1354
25	0	0.79	0/895	0.77	0/1201
26	1	0.61	0/438	0.76	0/583
27	2	1.04	0/357	0.87	0/475
28	3	0.97	0/852	0.82	0/1136
29	5	0.60	0/3250	0.70	2/4429 (0.0%)
30	6	0.57	0/2726	0.67	2/3715 (0.1%)
31	7	0.60	0/2391	0.69	0/3234
32	8	0.29	0/855	0.54	0/1152

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
33	9	0.70	0/972	0.71	0/1306
34	a	0.75	0/709	0.63	0/963
35	b	0.89	0/1202	0.82	0/1626
36	c	0.74	0/2264	0.73	0/3059
37	d	0.57	0/1790	0.69	0/2423
38	e	0.26	0/1797	0.59	1/2422 (0.0%)
39	f	0.40	0/931	0.57	0/1259
40	g	0.85	0/1102	0.81	0/1503
41	h	0.58	0/847	0.65	0/1150
42	i	0.99	0/849	0.81	0/1135
43	j	0.69	0/698	0.68	0/940
44	k	0.27	0/635	0.63	0/855
45	l	0.22	0/226	0.44	0/299
46	m	0.32	0/379	1.17	6/510 (1.2%)
47	o	0.71	0/682	0.71	0/916
48	p	0.48	0/1071	0.59	0/1433
49	q	0.51	0/1107	0.62	0/1498
50	r	0.64	0/1238	0.69	0/1676
51	s	0.74	0/3114	0.77	0/4225
53	u	0.34	0/949	0.61	0/1281
54	v	0.29	0/597	0.66	0/796
55	w	0.22	0/647	0.61	0/871
All	All	0.72	2/94989 (0.0%)	0.69	35/133846 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
8	J	0	1
26	1	0	1
31	7	0	1
40	g	0	1
46	m	0	1
51	s	0	1
All	All	0	6

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	Q	204	MET	C-N	-5.77	1.21	1.33

*Continued on next page...*

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	T	58	VAL	C-N	-5.13	1.23	1.33

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	205	GLN	N-CA-C	9.18	121.37	111.36
46	m	52	TYR	CA-C-N	8.54	130.51	119.84
46	m	52	TYR	C-N-CA	8.54	130.51	119.84
16	R	34	ARG	CB-CG-CD	-8.43	91.91	111.30
46	m	70	GLU	CA-C-N	8.33	130.25	119.84
46	m	70	GLU	C-N-CA	8.33	130.25	119.84
1	A	1823	A	C2'-C3'-O3'	7.52	120.78	109.50
46	m	53	PRO	O-C-N	-7.17	112.96	122.64
3	D	206	TYR	N-CA-C	6.85	120.30	109.81
1	A	1823	A	P-O3'-C3'	6.84	130.47	120.20
7	I	102	VAL	N-CA-C	-6.72	106.68	113.47
16	R	34	ARG	CG-CD-NE	6.24	125.73	112.00
1	A	1780	U	P-O3'-C3'	6.10	129.35	120.20
1	A	2165	C	P-O3'-C3'	6.00	129.20	120.20
1	A	2165	C	C2'-C3'-O3'	5.77	118.15	109.50
1	A	2243	A	C2'-C3'-O3'	5.68	118.02	109.50
23	Y	205	VAL	N-CA-C	-5.58	106.89	113.42
29	5	345	VAL	CA-C-N	-5.54	118.36	122.18
29	5	345	VAL	C-N-CA	-5.54	118.36	122.18
1	A	1780	U	C2'-C3'-O3'	5.50	117.75	109.50
1	A	2030	U	P-O3'-C3'	5.31	128.16	120.20
1	A	3201	A	P-O3'-C3'	5.29	128.14	120.20
16	R	11	ARG	CG-CD-NE	-5.29	100.36	112.00
1	A	2457	A	P-O3'-C3'	5.29	128.13	120.20
30	6	233	LEU	CA-C-N	-5.26	113.11	122.42
30	6	233	LEU	C-N-CA	-5.26	113.11	122.42
46	m	54	VAL	N-CA-C	5.12	116.12	108.54
17	S	135	LEU	CA-CB-CG	5.07	134.05	116.30
38	e	84	TYR	CA-CB-CG	5.07	123.03	113.90
11	M	134	ARG	CA-CB-CG	5.05	124.21	114.10
1	A	2243	A	P-O3'-C3'	5.05	127.78	120.20
7	I	182	ASP	CA-C-N	5.03	129.55	122.46
7	I	182	ASP	C-N-CA	5.03	129.55	122.46
22	X	148	THR	CA-C-N	5.02	124.92	119.85
22	X	148	THR	C-N-CA	5.02	124.92	119.85

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
26	1	25	GLY	Peptide
31	7	159	LYS	Peptide
8	J	69	LYS	Peptide
40	g	110	ILE	Peptide
46	m	53	PRO	Mainchain
51	s	270	LYS	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	A	23184	0	11795	168	0
2	B	1191	0	607	9	0
3	D	1706	0	1754	38	0
4	E	2258	0	2264	34	0
5	F	2013	0	2044	39	0
6	H	784	0	832	11	0
7	I	1283	0	1369	29	0
8	J	1061	0	1141	29	0
9	K	1451	0	1448	35	0
10	L	889	0	941	19	0
11	M	2305	0	2378	36	0
12	N	1654	0	1681	25	0
13	O	1245	0	1283	32	0
14	P	1148	0	1148	21	0
15	Q	1805	0	1841	33	0
16	R	1153	0	1213	12	0
17	S	1251	0	1322	31	0
18	T	1305	0	1352	25	0
19	U	1154	0	1154	30	0
20	V	1575	0	1583	23	0
21	W	859	0	888	11	0
22	X	2035	0	2054	29	0
23	Y	1517	0	1561	21	0
24	Z	978	0	1029	15	0
25	0	880	0	902	13	0
26	1	433	0	475	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	2	351	0	375	8	0
28	3	831	0	883	15	0
29	5	3156	0	3138	58	0
30	6	2640	0	2464	40	0
31	7	2334	0	2343	32	0
32	8	836	0	844	19	0
33	9	947	0	949	19	0
34	a	686	0	658	8	0
35	b	1178	0	1180	22	0
36	c	2217	0	2220	23	0
37	d	1741	0	1727	19	0
38	e	1762	0	1767	48	0
39	f	915	0	917	22	0
40	g	1067	0	1056	14	0
41	h	827	0	806	8	0
42	i	827	0	856	16	0
43	j	684	0	673	10	0
44	k	627	0	636	13	0
45	l	221	0	227	2	0
46	m	372	0	387	38	0
47	o	665	0	664	5	0
48	p	1058	0	1083	6	0
49	q	1076	0	1049	15	0
50	r	1203	0	1220	31	0
51	s	3036	0	3022	37	0
52	t	140	0	30	1	0
53	u	927	0	921	25	0
54	v	588	0	604	8	0
55	w	638	0	636	17	0
56	A	46	0	0	0	0
56	R	1	0	0	0	0
56	W	1	0	0	0	0
56	g	1	0	0	0	0
57	0	1	0	0	0	0
57	r	1	0	0	0	0
58	v	21	0	21	1	0
All	All	90739	0	79415	1077	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 6.

All (1077) 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)
29:5:105:TYR:CE2	29:5:218:LEU:HD22	1.60	1.34
1:A:3116:C:N4	1:A:3140:A:H61	1.57	1.03
39:f:101:THR:OG1	46:m:67:ARG:NH1	1.90	1.03
46:m:72:ARG:HH21	46:m:75:LEU:HD11	1.20	1.03
1:A:3116:C:H42	1:A:3140:A:N6	1.57	1.01
46:m:51:LEU:HB3	46:m:67:ARG:HB3	1.42	1.01
22:X:144:TYR:O	22:X:148:THR:HG23	1.63	0.98
29:5:105:TYR:CE2	29:5:218:LEU:CD2	2.46	0.97
46:m:55:LEU:HD21	46:m:65:HIS:CD2	2.01	0.95
29:5:105:TYR:HE2	29:5:218:LEU:CD2	1.80	0.93
46:m:50:ARG:HD3	46:m:52:TYR:OH	1.68	0.92
17:S:101:PHE:HD1	17:S:130:LEU:HD22	1.33	0.90
17:S:101:PHE:CE2	17:S:116:ILE:HD13	2.08	0.88
2:B:1607:U:H3	2:B:1664:G:H1	0.89	0.88
38:e:213:TYR:O	38:e:231:VAL:HB	1.73	0.87
38:e:211:GLY:O	38:e:233:PHE:HB2	1.75	0.86
39:f:96:THR:HA	39:f:153:HIS:O	1.75	0.86
29:5:105:TYR:HE2	29:5:218:LEU:HD22	0.99	0.83
20:V:137:PHE:HD2	20:V:142:GLU:O	1.61	0.83
7:I:123:MET:HA	7:I:153:LEU:O	1.79	0.82
29:5:290:THR:HA	29:5:343:GLN:O	1.79	0.82
29:5:105:TYR:CD2	29:5:218:LEU:HD22	2.17	0.80
29:5:293:LEU:O	29:5:346:GLY:HA2	1.83	0.79
15:Q:129:LYS:NZ	53:u:121:THR:O	2.15	0.79
55:w:81:ASP:O	55:w:85:TYR:HB2	1.83	0.78
17:S:101:PHE:CD1	17:S:130:LEU:HD22	2.17	0.77
30:6:270:PHE:HB2	30:6:317:SER:O	1.84	0.77
25:0:179:ARG:HH12	25:0:182:PRO:HG3	1.50	0.76
30:6:157:LEU:O	30:6:161:LEU:HB3	1.86	0.76
1:A:1747:G:N2	1:A:1750:G:O2'	2.19	0.75
20:V:139:GLU:N	20:V:139:GLU:OE1	2.19	0.75
15:Q:123:ASP:OD2	15:Q:126:ALA:N	2.18	0.75
30:6:266:HIS:O	30:6:320:GLN:HA	1.86	0.75
36:c:270:TYR:O	36:c:285:PRO:HA	1.87	0.74
39:f:99:ASP:OD1	46:m:66:ILE:HG23	1.86	0.74
39:f:99:ASP:OD1	46:m:66:ILE:CG2	2.35	0.74
15:Q:152:ARG:NH1	15:Q:190:LEU:O	2.20	0.74
1:A:2140:G:N3	24:Z:76:ARG:NH2	2.36	0.72
29:5:218:LEU:HD12	29:5:218:LEU:O	1.90	0.72
53:u:145:MET:O	53:u:149:LEU:HB2	1.90	0.72
24:Z:99:VAL:O	43:j:76:ARG:NH2	2.23	0.71
29:5:106:ILE:HD11	29:5:223:ARG:HE	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:63:GLN:HG2	5:F:81:ASP:HB3	1.72	0.71
20:V:139:GLU:CD	20:V:139:GLU:H	1.97	0.71
39:f:95:LEU:O	39:f:154:GLU:HA	1.90	0.71
33:9:93:SER:O	33:9:97:ALA:HB3	1.92	0.70
50:r:70:CYS:HB3	50:r:108:CYS:SG	2.32	0.69
38:e:199:ASN:O	38:e:242:ASP:HB2	1.93	0.69
1:A:3116:C:H42	1:A:3140:A:H61	0.78	0.69
7:I:140:TYR:HB3	7:I:143:LEU:HB2	1.73	0.69
25:0:106:ASN:HD22	25:0:118:GLN:HE21	1.38	0.69
35:b:27:GLN:HE21	35:b:80:LEU:HD23	1.59	0.68
15:Q:201:ASP:HB3	15:Q:204:MET:HB3	1.75	0.68
37:d:197:VAL:HG12	37:d:212:ILE:HG12	1.76	0.67
32:8:178:TYR:OH	46:m:65:HIS:ND1	2.18	0.67
15:Q:120:THR:HG22	15:Q:132:GLN:HG2	1.77	0.67
44:k:17:ARG:HB3	44:k:65:ASP:HB3	1.74	0.67
17:S:129:ARG:HE	17:S:155:ARG:HG3	1.60	0.67
23:Y:198:ARG:NH2	27:2:70:LEU:O	2.27	0.67
38:e:55:ARG:HD2	38:e:157:LEU:HD13	1.77	0.67
32:8:143:GLN:HG2	38:e:210:CYS:HA	1.77	0.66
35:b:28:ARG:NH2	36:c:71:GLU:OE2	2.27	0.66
51:s:243:ILE:HG22	51:s:245:LYS:H	1.59	0.66
20:V:137:PHE:CD2	20:V:142:GLU:O	2.45	0.66
2:B:1625:A:H62	14:P:87:GLN:HE22	1.40	0.66
8:J:89:TYR:O	8:J:93:ALA:HB3	1.96	0.66
46:m:51:LEU:HB3	46:m:67:ARG:CB	2.21	0.66
30:6:329:TYR:O	30:6:333:GLN:HB2	1.95	0.66
46:m:56:LEU:HD13	46:m:66:ILE:HD12	1.77	0.66
32:8:128:GLU:HB3	46:m:37:ARG:HH12	1.59	0.66
43:j:45:GLU:OE2	43:j:70:ARG:NH2	2.29	0.66
44:k:34:LEU:HA	44:k:38:SER:HB2	1.78	0.66
53:u:99:SER:O	53:u:103:GLN:HB2	1.96	0.66
7:I:51:THR:OG1	12:N:250:ARG:NH2	2.30	0.65
27:2:59:LYS:O	27:2:63:LYS:HB2	1.97	0.65
37:d:84:ILE:HA	37:d:211:GLN:HE22	1.62	0.65
22:X:150:LYS:HG3	22:X:159:MET:HE2	1.78	0.65
8:J:110:GLY:O	8:J:153:ILE:HA	1.97	0.65
1:A:2064:A:OP1	21:W:101:LYS:NZ	2.29	0.65
22:X:114:PHE:O	22:X:122:LYS:HA	1.97	0.65
55:w:147:TYR:O	55:w:151:LYS:HB2	1.97	0.64
5:F:211:ARG:HH11	41:h:58:ARG:HG3	1.61	0.64
29:5:106:ILE:HG22	29:5:266:HIS:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:32:LEU:HB3	13:O:52:MET:HE2	1.79	0.64
1:A:2702:G:H5'	9:K:114:LYS:HE2	1.77	0.64
5:F:217:LEU:HD11	5:F:243:ILE:HD12	1.80	0.64
29:5:208:THR:HA	29:5:224:GLY:O	1.96	0.64
15:Q:120:THR:HA	15:Q:131:SER:O	1.97	0.64
31:7:203:THR:HG22	31:7:280:VAL:H	1.62	0.64
24:Z:101:LYS:HE3	43:j:80:LEU:HD22	1.78	0.64
31:7:107:LEU:HB2	31:7:126:LYS:HB2	1.79	0.64
11:M:62:ARG:NH1	42:i:126:LYS:O	2.31	0.64
37:d:147:GLU:OE2	37:d:159:ARG:NH1	2.31	0.64
44:k:77:ARG:HB2	50:r:50:GLU:HG2	1.80	0.64
7:I:119:HIS:NE2	7:I:158:GLU:O	2.30	0.64
1:A:2673:G:H5''	18:T:112:LYS:HB2	1.80	0.63
39:f:101:THR:CB	46:m:67:ARG:HH12	2.09	0.63
12:N:87:PHE:HB2	12:N:163:MET:HB2	1.80	0.63
3:D:132:ASP:OD2	3:D:135:ARG:NH1	2.28	0.63
1:A:2292:G:C8	16:R:11:ARG:HB2	2.34	0.63
29:5:230:LEU:O	29:5:289:HIS:HB3	1.99	0.63
14:P:77:PHE:O	14:P:97:GLN:NE2	2.31	0.63
9:K:8:PRO:HG2	36:c:295:GLU:HG3	1.79	0.63
51:s:321:GLU:OE1	51:s:325:ARG:NH2	2.32	0.63
5:F:103:GLN:HE22	5:F:250:VAL:H	1.47	0.62
1:A:1790:A:OP1	27:2:82:ARG:NH1	2.31	0.62
2:B:1643:A:H61	14:P:87:GLN:HE21	1.47	0.62
14:P:52:ASN:HB3	14:P:55:ASN:HB2	1.80	0.62
22:X:163:ARG:HE	29:5:55:LEU:HD22	1.64	0.62
35:b:37:GLY:O	35:b:44:ARG:NH2	2.32	0.62
1:A:2143:G:OP1	17:S:173:ARG:NH2	2.31	0.62
7:I:32:ALA:HB1	12:N:73:ARG:HH21	1.64	0.62
7:I:124:LYS:HB2	7:I:153:LEU:HB2	1.82	0.62
19:U:71:ARG:NH2	19:U:96:TYR:OH	2.33	0.62
38:e:83:LEU:H	46:m:49:ALA:HA	1.64	0.62
39:f:96:THR:HG22	39:f:154:GLU:HG2	1.82	0.62
46:m:50:ARG:HD3	46:m:52:TYR:HH	1.64	0.62
5:F:133:THR:HG21	5:F:135:ARG:HE	1.64	0.62
13:O:25:ARG:NH2	13:O:51:GLU:OE2	2.33	0.62
19:U:128:SER:O	19:U:132:GLU:HB2	2.00	0.61
38:e:213:TYR:HB3	38:e:268:TYR:HD1	1.64	0.61
1:A:2389:C:H5''	29:5:301:PRO:HB3	1.82	0.61
55:w:138:LEU:HD13	55:w:144:ILE:HG12	1.81	0.61
19:U:143:ARG:NH1	31:7:66:GLU:OE1	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:3:183:ARG:NH1	30:6:355:LYS:O	2.34	0.61
3:D:235:GLN:HB3	3:D:294:SER:HA	1.81	0.61
3:D:194:ASN:HA	3:D:207:ILE:CG2	2.30	0.61
35:b:123:ASN:ND2	36:c:309:GLU:OE2	2.30	0.61
1:A:1777:A:N6	1:A:1780:U:OP2	2.34	0.61
3:D:227:GLN:HE21	3:D:231:LYS:HG2	1.65	0.61
18:T:55:ASN:ND2	18:T:74:TYR:O	2.33	0.61
5:F:107:LYS:HG2	42:i:74:ILE:HG22	1.83	0.61
35:b:35:ARG:O	35:b:44:ARG:NH1	2.33	0.61
1:A:2511:C:H3'	1:A:2512:A:H8	1.65	0.60
14:P:58:LEU:HD23	48:p:177:ARG:HH21	1.66	0.60
9:K:154:ARG:HD3	50:r:129:PRO:HG3	1.83	0.60
46:m:54:VAL:HG13	46:m:54:VAL:O	2.02	0.60
50:r:79:HIS:HB3	50:r:184:ASN:HA	1.81	0.60
1:A:1831:G:N7	35:b:4:ARG:NH1	2.49	0.60
24:Z:134:MET:HG2	43:j:75:ARG:HE	1.66	0.60
3:D:194:ASN:HA	3:D:207:ILE:HG21	1.82	0.60
51:s:249:GLU:HA	51:s:356:VAL:HG21	1.84	0.60
54:v:46:GLU:HB2	54:v:51:ARG:HE	1.66	0.60
22:X:20:ILE:HA	22:X:23:ARG:HH11	1.67	0.59
32:8:117:LEU:O	32:8:121:TRP:HB2	2.02	0.59
1:A:1706:C:OP1	23:Y:193:ARG:NH2	2.33	0.59
1:A:2174:G:N2	8:J:102:ARG:O	2.33	0.59
18:T:84:LYS:HD3	18:T:149:ARG:HB3	1.84	0.59
14:P:64:LYS:HA	14:P:97:GLN:HE22	1.67	0.59
28:3:188:VAL:HG11	40:g:104:ASN:HB3	1.84	0.59
37:d:220:GLN:NE2	37:d:244:GLU:OE2	2.34	0.59
1:A:1691:C:O2	23:Y:216:ARG:NH1	2.31	0.59
13:O:49:VAL:HG12	13:O:107:MET:HE2	1.84	0.59
22:X:144:TYR:O	22:X:148:THR:CG2	2.45	0.59
30:6:217:LEU:HD22	30:6:271:LEU:HD12	1.85	0.59
1:A:2147:G:OP1	17:S:104:ARG:NH1	2.36	0.59
9:K:63:ARG:NH1	9:K:130:ASP:OD1	2.36	0.59
39:f:127:MET:HB2	39:f:154:GLU:HB2	1.83	0.59
1:A:2927:C:H2'	1:A:2928:C:H4'	1.84	0.59
19:U:46:MET:HE1	19:U:72:VAL:HG13	1.84	0.59
1:A:2032:G:O2'	1:A:2865:C:O2	2.19	0.58
3:D:194:ASN:OD1	3:D:243:THR:OG1	2.21	0.58
15:Q:152:ARG:HG3	15:Q:161:GLU:HG2	1.85	0.58
17:S:101:PHE:CD1	17:S:130:LEU:CD2	2.85	0.58
22:X:177:HIS:O	22:X:184:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2458:A:OP1	13:O:9:ILE:N	2.37	0.58
2:B:1607:U:O4	2:B:1664:G:O6	2.21	0.58
38:e:279:LEU:HD11	39:f:176:SER:HB2	1.85	0.58
1:A:3146:G:O3'	4:E:266:ARG:NH1	2.36	0.58
10:L:58:ILE:HD11	10:L:76:ALA:HB2	1.84	0.58
14:P:63:ARG:HG2	14:P:177:ARG:HH11	1.69	0.58
16:R:10:LEU:HG	16:R:13:ARG:HD3	1.84	0.58
42:i:87:GLU:OE2	42:i:113:ARG:NH1	2.37	0.58
2:B:1627:C:OP1	32:8:129:ARG:NH1	2.35	0.58
18:T:153:LEU:HB2	18:T:169:LYS:HB2	1.85	0.58
26:l:43:LEU:O	26:l:55:LEU:HA	2.03	0.58
5:F:281:ARG:HD3	11:M:125:ARG:HD3	1.84	0.58
30:6:157:LEU:O	30:6:161:LEU:CB	2.52	0.58
49:q:86:GLU:OE2	49:q:90:ARG:NH2	2.35	0.58
8:J:111:LEU:HG	8:J:154:ARG:HB3	1.86	0.58
10:L:118:ARG:HH12	53:u:189:GLU:HG3	1.69	0.58
17:S:101:PHE:HE2	17:S:116:ILE:HD13	1.65	0.58
20:V:97:TYR:HA	20:V:107:THR:O	2.02	0.58
48:p:75:ARG:HG2	48:p:110:TRP:HE1	1.68	0.58
36:c:145:TYR:OH	36:c:311:ARG:NH1	2.37	0.57
2:B:1642:G:H4'	32:8:119:LYS:HG3	1.85	0.57
3:D:207:ILE:HG22	3:D:207:ILE:O	2.03	0.57
9:K:10:GLN:NE2	18:T:206:ARG:O	2.30	0.57
53:u:123:TYR:HB2	53:u:175:MET:HB3	1.85	0.57
8:J:138:SER:HA	8:J:141:VAL:HG12	1.85	0.57
13:O:45:PRO:HG2	13:O:48:ARG:HD2	1.86	0.57
38:e:156:ASN:ND2	38:e:277:SER:O	2.38	0.57
1:A:3183:U:O2	9:K:177:ARG:NH1	2.36	0.57
7:I:40:MET:HE1	7:I:48:MET:HE2	1.85	0.57
46:m:72:ARG:NH2	46:m:75:LEU:HD11	2.05	0.57
41:h:91:LEU:HD23	41:h:97:LYS:HG3	1.86	0.57
11:M:177:ALA:HB1	11:M:203:ARG:HH12	1.70	0.57
29:5:112:ARG:NH2	29:5:303:ARG:O	2.38	0.57
32:8:114:ARG:HE	38:e:73:LEU:HD11	1.69	0.57
35:b:126:ILE:O	36:c:310:ASN:ND2	2.30	0.57
43:j:63:GLN:OE1	43:j:66:ARG:NH2	2.37	0.57
1:A:1812:C:OP1	18:T:50:LYS:NZ	2.37	0.57
25:0:119:LYS:O	25:0:120:HIS:ND1	2.37	0.57
28:3:175:ASP:HB3	28:3:178:GLN:HB2	1.86	0.57
31:7:107:LEU:HD12	31:7:126:LYS:HD2	1.87	0.57
51:s:246:GLN:OE1	51:s:353:ARG:NH1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:55:PRO:HB3	10:L:77:ILE:HG12	1.87	0.57
19:U:3:ARG:O	19:U:23:ASN:ND2	2.38	0.57
22:X:61:ARG:NH2	22:X:63:GLU:OE2	2.38	0.57
23:Y:123:ARG:HD2	37:d:64:GLY:HA2	1.87	0.57
53:u:101:LEU:HD13	53:u:127:VAL:HG11	1.87	0.57
53:u:168:LEU:HD22	53:u:179:LEU:HD12	1.85	0.57
1:A:1881:A:OP2	40:g:111:ARG:NH2	2.38	0.56
29:5:216:GLU:HA	29:5:216:GLU:OE1	2.05	0.56
54:v:51:ARG:HA	58:v:101:PNS:H422	1.87	0.56
55:w:100:VAL:HB	55:w:142:GLN:HB2	1.87	0.56
1:A:2276:C:H1'	16:R:11:ARG:HH22	1.69	0.56
30:6:218:LEU:HD22	30:6:234:HIS:HB2	1.87	0.56
1:A:2256:U:O2'	17:S:118:ASN:ND2	2.38	0.56
19:U:8:PRO:HA	23:Y:183:GLN:HE22	1.70	0.56
19:U:11:ARG:NH1	20:V:212:LYS:O	2.38	0.56
1:A:2191:A:N6	1:A:2198:A:OP2	2.39	0.56
3:D:199:GLU:HB2	3:D:202:ARG:HB2	1.88	0.56
10:L:99:ARG:NH1	15:Q:161:GLU:OE1	2.39	0.56
22:X:226:LEU:HD12	23:Y:155:LEU:HB3	1.88	0.56
31:7:51:GLU:O	31:7:55:GLN:HB2	2.06	0.56
38:e:266:PRO:HD2	38:e:269:LEU:HB2	1.86	0.56
9:K:174:GLU:HG3	50:r:56:THR:HG21	1.86	0.56
10:L:108:ILE:HA	10:L:114:PRO:HA	1.87	0.56
29:5:350:ARG:NH2	29:5:384:GLN:O	2.38	0.56
32:8:160:GLU:O	38:e:207:ASN:ND2	2.38	0.56
35:b:108:SER:OG	35:b:109:GLY:N	2.38	0.56
44:k:66:VAL:HB	44:k:74:LEU:HB3	1.86	0.56
36:c:163:GLU:O	36:c:167:CYS:HB2	2.06	0.56
1:A:2372:U:O4	19:U:35:GLN:NE2	2.39	0.56
7:I:162:LYS:HD2	7:I:196:LYS:HA	1.88	0.56
11:M:205:LEU:HD13	49:q:96:LEU:HG	1.88	0.56
47:o:89:ALA:O	47:o:93:ASP:HB2	2.06	0.56
20:V:142:GLU:OE1	20:V:142:GLU:HA	2.04	0.56
23:Y:72:LYS:O	23:Y:76:GLN:NE2	2.39	0.56
36:c:121:SER:OG	36:c:122:ASN:N	2.38	0.56
49:q:40:PRO:HG3	49:q:51:GLN:HB3	1.88	0.56
12:N:193:GLY:O	12:N:197:LYS:HB2	2.05	0.56
13:O:38:ARG:NH2	13:O:82:GLU:OE1	2.39	0.56
42:i:99:GLY:HA2	42:i:102:MET:HE3	1.86	0.56
8:J:32:GLY:O	8:J:36:GLY:N	2.33	0.56
15:Q:136:ILE:O	15:Q:151:LEU:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:99:VAL:HG22	17:S:133:VAL:HG12	1.88	0.56
24:Z:71:ARG:NH2	24:Z:92:GLU:O	2.39	0.56
3:D:130:ARG:NH1	3:D:131:TYR:O	2.39	0.55
22:X:41:VAL:HG11	22:X:83:GLU:HB3	1.87	0.55
51:s:211:VAL:HG22	51:s:230:ARG:HG3	1.88	0.55
8:J:29:ALA:HB1	8:J:50:CYS:HB2	1.87	0.55
28:3:172:TYR:HB2	28:3:175:ASP:HB2	1.88	0.55
55:w:148:ILE:HG22	55:w:152:LYS:HE2	1.87	0.55
15:Q:79:GLU:OE2	15:Q:103:ARG:NH2	2.39	0.55
33:9:128:PHE:HD1	33:9:135:PHE:HB3	1.71	0.55
3:D:206:TYR:N	3:D:206:TYR:CD2	2.73	0.55
7:I:87:ALA:HA	7:I:90:PHE:HD2	1.72	0.55
9:K:52:ASP:O	18:T:206:ARG:NH1	2.37	0.55
30:6:204:VAL:HB	30:6:245:VAL:HG21	1.88	0.55
39:f:101:THR:CG2	46:m:67:ARG:NH1	2.69	0.55
1:A:2459:A:N6	1:A:2668:A:O2'	2.39	0.55
1:A:2521:A:OP2	3:D:202:ARG:NH2	2.37	0.55
1:A:3202:U:OP2	4:E:141:LYS:NZ	2.39	0.55
11:M:225:ASP:HB3	11:M:227:ALA:H	1.72	0.55
30:6:175:VAL:HG22	30:6:204:VAL:HG22	1.88	0.55
13:O:26:ILE:HD11	15:Q:268:ASP:HB3	1.88	0.55
19:U:19:VAL:HG22	33:9:136:LEU:HD22	1.89	0.55
49:q:34:ARG:HG3	49:q:38:ARG:HD3	1.88	0.55
22:X:150:LYS:CG	22:X:159:MET:HE2	2.37	0.55
13:O:42:ILE:O	13:O:122:VAL:HA	2.07	0.55
33:9:91:LEU:O	33:9:95:ALA:HB3	2.07	0.55
50:r:70:CYS:SG	50:r:73:CYS:N	2.79	0.55
4:E:171:PRO:O	4:E:173:LYS:NZ	2.40	0.54
12:N:105:MET:HE2	12:N:179:VAL:HG13	1.89	0.54
13:O:131:PRO:HD2	25:0:134:THR:HG22	1.89	0.54
39:f:99:ASP:OD1	46:m:66:ILE:HG22	2.07	0.54
14:P:72:PHE:HB2	21:W:107:HIS:HA	1.88	0.54
3:D:207:ILE:HG12	3:D:229:PRO:HD3	1.90	0.54
3:D:228:LEU:HD11	3:D:234:MET:HE3	1.89	0.54
10:L:123:ILE:HD12	10:L:141:ALA:HB2	1.89	0.54
29:5:341:VAL:HG22	29:5:358:GLN:HG2	1.89	0.54
44:k:76:MET:HG2	50:r:49:ILE:HB	1.88	0.54
50:r:94:ARG:HE	50:r:100:LEU:HD23	1.72	0.54
4:E:268:GLU:HB3	4:E:271:LEU:HD11	1.90	0.54
26:1:20:MET:O	26:1:29:CYS:HA	2.08	0.54
29:5:201:ARG:NH1	29:5:418:TYR:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:7:156:ARG:NH2	31:7:259:ASP:O	2.39	0.54
46:m:55:LEU:CD2	46:m:65:HIS:CD2	2.85	0.54
1:A:2212:C:H2'	1:A:2213:A:H8	1.72	0.54
1:A:2528:G:OP1	3:D:135:ARG:NH2	2.41	0.54
6:H:58:ARG:NH1	6:H:77:HIS:O	2.41	0.54
11:M:146:ASP:N	11:M:146:ASP:OD1	2.41	0.54
34:a:69:TYR:OH	36:c:256:ARG:NH2	2.41	0.54
7:I:191:PHE:O	7:I:195:SER:HB2	2.07	0.54
17:S:174:PHE:HA	17:S:180:PHE:O	2.08	0.54
40:g:110:ILE:HD11	40:g:157:LEU:HD13	1.89	0.54
51:s:165:ARG:O	51:s:307:ARG:NH2	2.38	0.54
53:u:99:SER:O	53:u:103:GLN:CB	2.56	0.54
7:I:191:PHE:O	7:I:195:SER:CB	2.56	0.54
12:N:221:ALA:O	24:Z:114:LYS:NZ	2.37	0.54
14:P:79:HIS:HA	14:P:95:GLU:O	2.08	0.54
15:Q:121:THR:HG22	15:Q:171:VAL:HG12	1.90	0.54
27:2:82:ARG:HE	27:2:87:ARG:HD2	1.72	0.54
29:5:151:ASP:O	29:5:155:LEU:HB2	2.08	0.54
30:6:218:LEU:HA	30:6:269:ALA:O	2.08	0.54
54:v:23:LEU:HD23	54:v:28:ARG:HG2	1.90	0.54
1:A:1745:U:O4	28:3:108:LYS:NZ	2.41	0.54
15:Q:117:LEU:O	15:Q:134:LEU:HA	2.08	0.54
46:m:55:LEU:HD21	46:m:65:HIS:NE2	2.22	0.54
1:A:1884:G:O6	5:F:281:ARG:NH2	2.41	0.53
3:D:198:SER:HB2	3:D:206:TYR:OH	2.08	0.53
3:D:248:SER:OG	3:D:249:ASN:N	2.40	0.53
9:K:156:ASP:OD1	50:r:130:ASN:ND2	2.40	0.53
46:m:56:LEU:HD13	46:m:66:ILE:CD1	2.38	0.53
1:A:1985:G:OP1	1:A:1987:G:O2'	2.25	0.53
1:A:2157:U:H5'	50:r:182:ARG:HH22	1.72	0.53
3:D:124:GLU:HG2	3:D:144:GLY:HA3	1.90	0.53
38:e:124:TRP:CE2	46:m:72:ARG:HG2	2.43	0.53
1:A:1705:A:N6	33:9:40:GLY:O	2.41	0.53
3:D:166:SER:OG	3:D:182:HIS:ND1	2.39	0.53
6:H:75:ARG:HH21	22:X:100:ARG:HH22	1.55	0.53
6:H:98:LEU:HD22	6:H:102:VAL:HG21	1.90	0.53
18:T:69:ARG:NH1	37:d:228:PHE:O	2.42	0.53
28:3:148:VAL:HG13	30:6:360:ARG:HA	1.91	0.53
37:d:190:GLU:OE1	37:d:215:ARG:NH1	2.38	0.53
51:s:325:ARG:O	51:s:328:ALA:HB3	2.08	0.53
4:E:56:GLU:OE2	13:O:153:ARG:NH2	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:128:GLU:HA	8:J:133:GLN:HE21	1.74	0.53
15:Q:111:PHE:O	15:Q:140:ARG:NH1	2.41	0.53
30:6:371:ASP:OD1	30:6:371:ASP:N	2.41	0.53
35:b:80:LEU:HD11	36:c:78:ARG:HD3	1.88	0.53
48:p:100:GLU:OE2	48:p:102:ARG:NH2	2.41	0.53
1:A:2529:U:O2'	3:D:206:TYR:HA	2.07	0.53
1:A:3123:G:N2	1:A:3133:A:OP2	2.42	0.53
3:D:226:ILE:O	3:D:233:GLN:HA	2.08	0.53
38:e:139:GLU:HG2	38:e:152:LYS:HA	1.91	0.53
51:s:242:ARG:NH2	51:s:292:CYS:O	2.41	0.53
4:E:292:HIS:ND1	4:E:293:LYS:O	2.37	0.53
5:F:167:MET:HA	5:F:170:ARG:HE	1.74	0.53
24:Z:78:ARG:HD2	24:Z:116:LEU:HD21	1.90	0.53
41:h:78:PHE:HE2	41:h:89:ILE:HD13	1.73	0.53
1:A:2126:U:O4	24:Z:76:ARG:NH1	2.42	0.53
1:A:2293:A:N6	11:M:37:GLU:OE1	2.41	0.53
1:A:2519:G:N7	3:D:230:SER:OG	2.38	0.53
5:F:223:HIS:HA	5:F:226:MET:HE2	1.90	0.53
17:S:100:HIS:ND1	17:S:100:HIS:O	2.42	0.53
22:X:153:LEU:HD11	22:X:158:GLY:HA3	1.89	0.53
30:6:105:GLU:O	30:6:109:ALA:HB2	2.08	0.53
38:e:151:ARG:HD3	38:e:152:LYS:HG2	1.90	0.53
51:s:419:LEU:O	51:s:423:HIS:ND1	2.36	0.53
1:A:2191:A:OP1	8:J:142:ARG:NH2	2.42	0.53
1:A:2194:U:O2'	1:A:2195:A:O4'	2.27	0.53
8:J:89:TYR:O	8:J:93:ALA:CB	2.56	0.53
9:K:16:ARG:HH22	9:K:124:ARG:HH21	1.55	0.53
29:5:178:PRO:O	29:5:182:ASP:HB2	2.09	0.53
51:s:237:PRO:HG3	51:s:298:GLN:HE21	1.73	0.53
2:B:1637:C:H5'	30:6:52:ARG:HB3	1.90	0.53
5:F:70:ARG:NH1	5:F:194:GLU:OE1	2.41	0.53
9:K:154:ARG:NH1	9:K:157:GLU:OE2	2.41	0.53
1:A:2180:A:H1'	1:A:2206:C:H4'	1.91	0.52
4:E:133:THR:OG1	4:E:144:THR:OG1	2.27	0.52
32:8:117:LEU:O	32:8:121:TRP:CB	2.57	0.52
7:I:83:ARG:HG2	7:I:134:PHE:HE1	1.73	0.52
10:L:72:GLN:HA	10:L:84:ALA:O	2.09	0.52
19:U:44:ILE:HG22	19:U:93:LYS:HB3	1.90	0.52
16:R:54:THR:HG21	17:S:172:MET:H	1.73	0.52
17:S:152:ASP:OD1	17:S:152:ASP:N	2.42	0.52
24:Z:99:VAL:HG12	43:j:80:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:5:213:TRP:O	29:5:219:LEU:HD12	2.09	0.52
49:q:28:ARG:HH12	49:q:31:PRO:HD3	1.74	0.52
1:A:3127:G:H2'	1:A:3128:A:H2'	1.92	0.52
1:A:2511:C:O2'	3:D:258:GLY:N	2.42	0.52
8:J:66:LEU:HB3	8:J:82:ILE:HD11	1.91	0.52
10:L:42:ASP:HB3	10:L:44:SER:H	1.74	0.52
11:M:276:ASN:ND2	11:M:279:ASP:OD1	2.43	0.52
15:Q:103:ARG:NH1	15:Q:108:ILE:HB	2.24	0.52
39:f:99:ASP:CG	46:m:66:ILE:HG23	2.34	0.52
51:s:188:LEU:HD21	51:s:422:VAL:HG13	1.91	0.52
1:A:2192:A:OP2	45:l:119:ARG:NH1	2.43	0.52
17:S:101:PHE:HZ	17:S:120:LEU:HD11	1.74	0.52
32:8:160:GLU:OE1	38:e:207:ASN:ND2	2.36	0.52
3:D:187:LEU:HD21	3:D:244:VAL:HG12	1.91	0.52
5:F:89:THR:H	5:F:179:THR:HG21	1.75	0.52
7:I:83:ARG:O	7:I:87:ALA:CB	2.57	0.52
10:L:95:ARG:HG3	15:Q:165:GLU:OE2	2.10	0.52
11:M:168:GLU:OE1	11:M:220:ARG:NH2	2.38	0.52
30:6:322:ARG:NH1	48:p:181:GLU:OE1	2.43	0.52
50:r:85:ASP:OD1	50:r:85:ASP:N	2.33	0.52
11:M:264:GLN:NE2	11:M:269:LEU:O	2.42	0.52
38:e:146:ARG:HB3	38:e:253:VAL:HG13	1.91	0.52
39:f:101:THR:HG21	46:m:67:ARG:NH1	2.24	0.52
1:A:1889:C:OP1	11:M:133:LYS:NZ	2.39	0.52
12:N:224:LEU:HD11	47:o:38:ARG:HB3	1.92	0.52
36:c:275:TYR:HA	36:c:280:LEU:HA	1.92	0.52
4:E:97:VAL:O	4:E:197:HIS:NE2	2.37	0.52
5:F:160:SER:OG	42:i:83:TRP:O	2.26	0.52
31:7:52:LYS:HG3	31:7:219:LEU:HD11	1.92	0.52
55:w:81:ASP:O	55:w:85:TYR:CB	2.57	0.52
1:A:2310:G:O2'	1:A:2675:G:O6	2.23	0.51
1:A:2395:A:H4'	29:5:350:ARG:HH12	1.75	0.51
1:A:2932:G:OP1	5:F:137:ARG:NH1	2.42	0.51
1:A:3220:A:OP1	4:E:260:LYS:NZ	2.43	0.51
5:F:221:LEU:HD23	5:F:222:THR:HG23	1.91	0.51
17:S:101:PHE:CE2	17:S:116:ILE:CD1	2.90	0.51
19:U:44:ILE:HG23	19:U:48:MET:HB3	1.92	0.51
23:Y:83:ALA:N	33:9:74:VAL:O	2.38	0.51
29:5:107:PHE:HB3	29:5:222:VAL:HG12	1.92	0.51
50:r:99:MET:HG3	50:r:116:GLU:HG2	1.91	0.51
14:P:104:SER:OG	30:6:150:ARG:NH1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:6:265:ILE:HG12	30:6:322:ARG:HG2	1.91	0.51
31:7:131:LYS:HE3	31:7:305:HIS:HB3	1.92	0.51
9:K:21:LEU:HD12	9:K:145:LEU:HD12	1.91	0.51
22:X:64:ASP:OD1	22:X:64:ASP:N	2.37	0.51
1:A:1747:G:OP2	1:A:1749:C:N4	2.43	0.51
8:J:39:LEU:HB3	8:J:44:VAL:HG11	1.91	0.51
19:U:44:ILE:HD11	19:U:53:LEU:HG	1.92	0.51
14:P:152:GLU:HG3	14:P:158:MET:HG3	1.92	0.51
23:Y:143:ASP:OD1	33:9:137:ARG:NH2	2.44	0.51
51:s:405:ILE:HG12	51:s:410:VAL:HG12	1.93	0.51
53:u:108:ASP:O	53:u:127:VAL:HA	2.09	0.51
7:I:128:ASN:HA	7:I:131:LEU:HB3	1.92	0.51
20:V:147:SER:OG	20:V:150:SER:O	2.29	0.51
24:Z:101:LYS:NZ	43:j:83:GLU:OE1	2.44	0.51
38:e:143:LYS:O	38:e:146:ARG:NH1	2.44	0.51
4:E:104:LEU:HB2	4:E:121:LEU:HB2	1.92	0.51
9:K:59:ILE:HB	9:K:127:LEU:HD23	1.93	0.51
4:E:102:LEU:O	4:E:122:LEU:HA	2.11	0.51
4:E:348:ALA:HB2	15:Q:128:GLY:HA3	1.93	0.51
5:F:249:ASN:N	5:F:249:ASN:OD1	2.43	0.51
7:I:37:ARG:HH22	12:N:247:MET:HE3	1.74	0.51
7:I:49:ALA:HB1	47:o:32:LYS:HE2	1.92	0.51
36:c:215:ILE:HG23	36:c:219:LEU:HD12	1.92	0.51
38:e:51:LEU:HD12	38:e:188:ALA:HB1	1.92	0.51
13:O:147:GLN:HE21	31:7:175:ILE:HG12	1.77	0.50
21:W:100:THR:OG1	21:W:132:HIS:NE2	2.39	0.50
21:W:106:PRO:HD2	21:W:117:ILE:HD11	1.93	0.50
55:w:131:PRO:HG2	55:w:134:ASP:HB2	1.93	0.50
1:A:2709:A:H1'	25:0:96:ASN:HD21	1.76	0.50
5:F:81:ASP:OD1	5:F:81:ASP:N	2.42	0.50
20:V:122:LEU:HD12	20:V:133:ILE:HG13	1.93	0.50
46:m:41:THR:OG1	46:m:67:ARG:NH2	2.43	0.50
1:A:2055:U:H2'	1:A:2056:G:H8	1.76	0.50
11:M:19:LEU:HD23	47:o:95:LEU:HD12	1.94	0.50
16:R:64:MET:HE1	18:T:210:HIS:HB3	1.92	0.50
31:7:282:ALA:HB2	31:7:321:ARG:HG2	1.94	0.50
32:8:114:ARG:HG3	38:e:73:LEU:HD21	1.94	0.50
51:s:332:LEU:HD21	51:s:359:ALA:HB2	1.93	0.50
1:A:1718:A:N3	1:A:1911:C:O2'	2.39	0.50
1:A:2010:U:OP2	42:i:115:ARG:NH1	2.43	0.50
23:Y:102:TRP:HE3	23:Y:142:LEU:HD22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:6:335:LEU:HD23	30:6:337:MET:HE2	1.92	0.50
51:s:362:THR:OG1	51:s:363:ASP:N	2.44	0.50
12:N:191:SER:OG	12:N:192:ARG:N	2.43	0.50
23:Y:213:ARG:HA	23:Y:216:ARG:HH21	1.75	0.50
38:e:198:ASN:HD22	38:e:243:PHE:HD1	1.59	0.50
49:q:64:TYR:HB3	49:q:68:SER:HB2	1.92	0.50
4:E:331:ASP:N	4:E:331:ASP:OD1	2.41	0.50
17:S:135:LEU:HD23	17:S:144:LEU:HB3	1.93	0.50
22:X:130:ARG:HE	22:X:134:LEU:HD11	1.77	0.50
51:s:207:HIS:ND1	51:s:234:ASP:OD1	2.44	0.50
1:A:1782:G:O2'	1:A:1793:G:O6	2.26	0.50
1:A:2409:A:O2'	29:5:270:ILE:O	2.30	0.50
5:F:165:LEU:HB2	5:F:170:ARG:HD3	1.94	0.50
8:J:49:PHE:O	8:J:53:PHE:HB2	2.11	0.50
38:e:203:LYS:N	38:e:237:LEU:O	2.45	0.50
53:u:167:TRP:HH2	53:u:190:LEU:HD11	1.77	0.50
5:F:249:ASN:OD1	5:F:252:SER:OG	2.29	0.49
13:O:144:LEU:HD12	31:7:302:LEU:HD23	1.93	0.49
35:b:16:HIS:HB3	35:b:19:LEU:HD12	1.94	0.49
50:r:90:SER:HA	50:r:93:ILE:HD12	1.92	0.49
51:s:240:GLN:HB3	51:s:298:GLN:HG3	1.93	0.49
1:A:2471:G:OP1	10:L:37:ARG:N	2.38	0.49
19:U:66:ALA:HB2	19:U:100:ALA:HB2	1.94	0.49
19:U:153:LEU:HD11	37:d:220:GLN:HB2	1.93	0.49
1:A:2051:A:H2'	1:A:2052:A:C8	2.47	0.49
1:A:2293:A:H2'	11:M:39:ARG:HH12	1.78	0.49
3:D:154:THR:H	3:D:157:MET:HE3	1.77	0.49
19:U:52:ASP:O	19:U:56:TYR:HB2	2.12	0.49
29:5:228:ALA:HB3	29:5:292:TYR:HB2	1.93	0.49
30:6:46:GLU:HG3	39:f:64:LYS:HD2	1.94	0.49
31:7:108:VAL:HG22	31:7:125:ILE:HG12	1.94	0.49
51:s:89:MET:HG3	51:s:275:LYS:HE3	1.93	0.49
51:s:228:ASP:OD1	51:s:228:ASP:N	2.44	0.49
1:A:1977:U:H2'	1:A:1978:A:H8	1.77	0.49
5:F:116:THR:HG23	5:F:118:ALA:H	1.76	0.49
9:K:69:GLY:HA2	50:r:152:THR:HA	1.94	0.49
30:6:183:ASP:HB3	48:p:192:ARG:HG2	1.94	0.49
34:a:72:THR:HG22	36:c:258:THR:HA	1.95	0.49
1:A:2182:G:H1'	1:A:2199:A:H2'	1.93	0.49
37:d:119:GLN:HA	37:d:122:ILE:HD12	1.93	0.49
14:P:56:LEU:HB3	14:P:62:ALA:HB2	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:P:128:ILE:O	14:P:132:LEU:HB2	2.12	0.49
30:6:57:TYR:O	30:6:61:ALA:CB	2.60	0.49
33:9:22:THR:HG23	33:9:24:LYS:H	1.77	0.49
54:v:46:GLU:H	54:v:51:ARG:HH21	1.60	0.49
9:K:3:SER:O	36:c:302:ARG:NH1	2.45	0.49
19:U:153:LEU:HB2	37:d:222:LEU:HD12	1.95	0.49
20:V:29:VAL:HG21	37:d:67:ILE:HG23	1.93	0.49
38:e:183:THR:O	38:e:187:THR:N	2.44	0.49
38:e:256:THR:OG1	38:e:257:LYS:N	2.41	0.49
46:m:54:VAL:N	46:m:66:ILE:O	2.46	0.49
51:s:66:TRP:O	51:s:69:THR:OG1	2.27	0.49
51:s:184:LEU:O	51:s:188:LEU:HB2	2.13	0.49
23:Y:151:ASP:OD1	23:Y:154:ARG:NH1	2.42	0.49
1:A:2318:A:H2'	1:A:2319:A:C8	2.48	0.49
5:F:230:ILE:HG23	5:F:242:LEU:HD11	1.93	0.49
11:M:274:VAL:HG11	49:q:75:LEU:HD13	1.95	0.49
20:V:25:PRO:HG2	20:V:28:SER:HB3	1.95	0.49
30:6:268:LEU:O	30:6:318:PHE:HA	2.12	0.49
40:g:101:THR:O	40:g:105:ARG:HB2	2.13	0.49
49:q:41:ASP:OD1	49:q:41:ASP:N	2.40	0.49
1:A:2349:G:H2'	1:A:2350:A:C8	2.48	0.49
1:A:3179:G:O2'	1:A:3190:A:N6	2.42	0.49
14:P:85:ARG:HD2	14:P:158:MET:HE3	1.95	0.49
15:Q:93:GLN:NE2	15:Q:285:GLU:OE1	2.41	0.49
29:5:136:VAL:HG22	29:5:420:HIS:CD2	2.47	0.49
34:a:71:HIS:HD1	35:b:138:THR:HG1	1.61	0.49
1:A:1871:A:H61	1:A:1901:C:H5'	1.78	0.48
7:I:83:ARG:O	7:I:87:ALA:HB3	2.13	0.48
8:J:43:GLY:HA3	8:J:76:ARG:HH12	1.78	0.48
13:O:50:ASP:HB3	13:O:107:MET:HE1	1.94	0.48
14:P:178:ILE:O	30:6:346:ARG:NH2	2.44	0.48
1:A:2395:A:OP1	29:5:173:ARG:NH2	2.46	0.48
3:D:74:ILE:HD13	3:D:148:LYS:HE3	1.94	0.48
19:U:37:GLU:HB3	19:U:104:THR:HG23	1.95	0.48
23:Y:160:GLN:HG3	33:9:131:TYR:CG	2.48	0.48
25:0:181:ARG:HD3	25:0:182:PRO:HD2	1.95	0.48
30:6:222:ASP:OD1	30:6:222:ASP:N	2.44	0.48
1:A:2173:G:H2'	1:A:2174:G:C8	2.48	0.48
8:J:113:THR:HA	8:J:156:VAL:HB	1.94	0.48
31:7:99:TYR:O	31:7:103:SER:OG	2.28	0.48
32:8:101:ARG:NH2	38:e:82:SER:OG	2.37	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:103:GLU:HG2	6:H:104:ASN:H	1.78	0.48
31:7:44:ARG:HB3	31:7:261:ILE:HD12	1.95	0.48
1:A:1672:C:O2'	18:T:149:ARG:O	2.30	0.48
18:T:75:HIS:HD2	18:T:120:VAL:HG13	1.78	0.48
29:5:354:PHE:HB2	29:5:377:ASP:HB2	1.95	0.48
38:e:74:LEU:O	38:e:78:GLU:HB2	2.13	0.48
44:k:39:SER:OG	44:k:40:GLU:N	2.46	0.48
51:s:142:LEU:HD13	51:s:422:VAL:HG21	1.96	0.48
11:M:94:LYS:HG3	11:M:129:ILE:HG22	1.95	0.48
13:O:46:TRP:HD1	13:O:121:ALA:HB2	1.79	0.48
35:b:11:LEU:HD23	35:b:115:ILE:HD13	1.96	0.48
1:A:2815:G:N7	12:N:139:ARG:NH1	2.61	0.48
20:V:177:THR:HG22	33:9:71:LYS:H	1.79	0.48
55:w:134:ASP:OD2	55:w:147:TYR:OH	2.32	0.48
1:A:2248:U:OP1	16:R:99:ARG:NH2	2.35	0.48
1:A:2367:A:N3	23:Y:123:ARG:NH2	2.61	0.48
1:A:2740:A:N3	1:A:2921:A:O2'	2.46	0.48
18:T:202:GLN:OE1	34:a:122:ARG:NH1	2.47	0.48
31:7:112:PRO:HB2	31:7:267:PRO:HG2	1.94	0.48
38:e:264:LEU:HB3	38:e:269:LEU:HB3	1.96	0.48
1:A:2191:A:H4'	8:J:142:ARG:HG3	1.94	0.48
14:P:96:HIS:ND1	14:P:98:ASN:OD1	2.46	0.48
19:U:42:PHE:HB2	19:U:95:ALA:HB3	1.96	0.48
29:5:293:LEU:HD13	29:5:312:LYS:HE3	1.94	0.48
1:A:1883:G:H5''	40:g:91:MET:HE3	1.96	0.48
1:A:2093:U:O2	1:A:2266:U:O2'	2.31	0.48
18:T:94:ILE:HA	18:T:97:MET:HE2	1.96	0.48
40:g:100:ILE:HA	40:g:105:ARG:O	2.14	0.48
53:u:140:PHE:O	53:u:144:LYS:HB2	2.14	0.48
1:A:1909:A:H61	1:A:2010:U:H3	1.60	0.47
2:B:1609:U:O2	2:B:1616:A:N6	2.47	0.47
4:E:106:MET:HG2	4:E:120:THR:HG22	1.95	0.47
44:k:78:GLY:HA2	44:k:81:LEU:HD13	1.96	0.47
3:D:202:ARG:HE	3:D:205:GLN:NE2	2.11	0.47
31:7:148:MET:HE2	31:7:262:ASP:HB3	1.96	0.47
44:k:15:GLN:HB3	44:k:67:LEU:HB2	1.95	0.47
1:A:1756:A:H2'	1:A:1757:A:H8	1.79	0.47
22:X:149:PRO:HD2	22:X:152:ASP:HB3	1.97	0.47
29:5:200:ARG:NH2	29:5:234:ASP:OD1	2.47	0.47
39:f:101:THR:CB	46:m:67:ARG:NH1	2.72	0.47
46:m:55:LEU:O	46:m:74:MET:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
51:s:105:TRP:HZ3	51:s:268:PRO:HA	1.78	0.47
1:A:1990:G:N2	1:A:1993:A:C2	2.79	0.47
4:E:100:ILE:HA	4:E:297:VAL:O	2.15	0.47
8:J:22:ALA:H	8:J:68:THR:HG22	1.79	0.47
9:K:39:LEU:HD11	9:K:125:LEU:HB2	1.97	0.47
17:S:112:ASP:O	17:S:194:ARG:HA	2.14	0.47
55:w:123:GLU:HG2	55:w:130:ILE:HD12	1.96	0.47
1:A:1883:G:N7	5:F:281:ARG:NH1	2.63	0.47
6:H:98:LEU:HD23	6:H:129:ALA:HB2	1.95	0.47
9:K:21:LEU:HD21	9:K:31:LEU:HD22	1.96	0.47
13:O:49:VAL:HG13	13:O:123:ILE:HG12	1.95	0.47
21:W:76:HIS:HB2	21:W:130:PHE:CD1	2.49	0.47
30:6:355:LYS:HE3	30:6:358:PRO:HA	1.97	0.47
38:e:177:GLU:O	38:e:190:ARG:NH2	2.48	0.47
1:A:2158:U:OP2	50:r:195:TYR:OH	2.29	0.47
24:Z:100:HIS:HB3	24:Z:106:VAL:HG11	1.95	0.47
30:6:221:LEU:HD12	30:6:267:ARG:HG3	1.96	0.47
42:i:105:ASP:OD1	42:i:105:ASP:N	2.41	0.47
1:A:1848:U:OP1	11:M:48:LYS:NZ	2.47	0.47
1:A:2262:C:OP1	17:S:173:ARG:NH1	2.48	0.47
1:A:2684:C:OP1	25:0:86:THR:OG1	2.22	0.47
3:D:66:TRP:HA	3:D:80:ARG:HH11	1.80	0.47
9:K:21:LEU:HD22	9:K:59:ILE:HG12	1.96	0.47
10:L:101:ASP:OD2	15:Q:152:ARG:NH2	2.34	0.47
13:O:79:TRP:NE1	15:Q:267:PHE:O	2.46	0.47
18:T:71:ALA:H	18:T:180:GLU:HB3	1.80	0.47
26:1:19:ARG:HB3	26:1:62:ILE:HD11	1.95	0.47
29:5:33:TRP:O	29:5:39:ARG:NH2	2.47	0.47
29:5:133:PRO:HG3	29:5:239:ILE:HD13	1.96	0.47
51:s:165:ARG:HG2	51:s:307:ARG:HH12	1.79	0.47
51:s:324:PHE:HA	51:s:361:ILE:HD11	1.96	0.47
1:A:2389:C:O2'	29:5:305:GLN:NE2	2.48	0.47
1:A:2854:U:H4'	28:3:138:PRO:HG2	1.97	0.47
9:K:74:GLN:HE21	50:r:159:VAL:HG11	1.80	0.47
13:O:116:ASP:OD1	13:O:116:ASP:N	2.47	0.47
20:V:123:VAL:HG13	20:V:128:ARG:HA	1.97	0.47
30:6:57:TYR:O	30:6:61:ALA:HB2	2.15	0.47
37:d:81:THR:OG1	37:d:249:GLU:OE2	2.26	0.47
1:A:1882:A:N1	1:A:1891:A:O2'	2.44	0.47
1:A:2906:C:O2	26:1:19:ARG:NH2	2.47	0.47
23:Y:69:ASP:OD1	23:Y:69:ASP:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:a:37:SER:OG	34:a:39:LEU:O	2.31	0.47
40:g:125:GLU:HG3	40:g:136:PRO:HD2	1.96	0.47
1:A:1800:G:N1	1:A:1803:A:OP2	2.48	0.47
2:B:1628:C:H5'	32:8:125:LYS:HG2	1.95	0.47
15:Q:131:SER:HB3	53:u:119:ARG:HD3	1.95	0.47
33:9:42:GLY:HA3	33:9:51:VAL:O	2.15	0.47
51:s:371:CYS:HB2	51:s:394:TRP:HB2	1.97	0.47
15:Q:102:ARG:NH1	15:Q:169:PRO:HA	2.30	0.46
38:e:124:TRP:CZ2	46:m:72:ARG:HG2	2.50	0.46
4:E:148:GLY:HA2	4:E:175:THR:O	2.15	0.46
5:F:83:HIS:HB3	5:F:86:VAL:HG12	1.97	0.46
18:T:91:ALA:O	18:T:145:SER:OG	2.32	0.46
44:k:80:HIS:O	50:r:36:ARG:NH1	2.48	0.46
45:l:114:SER:OG	45:l:115:ARG:N	2.42	0.46
1:A:1749:C:OP2	1:A:2899:C:O2'	2.29	0.46
3:D:74:ILE:HD13	3:D:148:LYS:HB2	1.98	0.46
6:H:116:LYS:HD3	6:H:120:ARG:HH22	1.81	0.46
12:N:160:VAL:HG12	12:N:161:VAL:HG23	1.97	0.46
16:R:108:TYR:HD1	35:b:125:SER:HB2	1.80	0.46
19:U:28:LEU:H	23:Y:114:THR:HG22	1.80	0.46
35:b:76:VAL:HG22	35:b:86:GLU:HG3	1.97	0.46
1:A:2422:U:OP2	33:9:24:LYS:NZ	2.48	0.46
1:A:2457:A:O2'	13:O:17:ARG:NH2	2.49	0.46
7:I:52:GLU:O	12:N:211:ASN:ND2	2.43	0.46
11:M:264:GLN:NE2	11:M:267:PHE:O	2.48	0.46
1:A:1737:A:O2'	42:i:93:ARG:NH1	2.45	0.46
29:5:162:ARG:NH2	29:5:176:TYR:OH	2.48	0.46
35:b:21:ARG:NH1	36:c:79:LEU:O	2.47	0.46
38:e:50:ALA:HA	38:e:175:GLN:HA	1.97	0.46
53:u:135:LEU:HD22	53:u:179:LEU:HB3	1.96	0.46
10:L:98:PRO:HA	15:Q:162:ILE:HG13	1.98	0.46
10:L:119:ILE:HG21	10:L:123:ILE:HD11	1.96	0.46
13:O:46:TRP:CD1	13:O:121:ALA:HB2	2.50	0.46
15:Q:154:VAL:HG12	15:Q:159:GLY:HA2	1.98	0.46
32:8:132:GLU:OE1	39:f:109:TYR:OH	2.33	0.46
38:e:266:PRO:O	38:e:270:ALA:N	2.39	0.46
1:A:1924:U:H5''	3:D:81:LYS:HB2	1.97	0.46
1:A:2268:G:N7	11:M:44:ARG:NH1	2.55	0.46
8:J:90:PHE:HE2	8:J:120:ILE:HD13	1.81	0.46
10:L:87:VAL:HG11	10:L:123:ILE:HG12	1.96	0.46
12:N:104:MET:HE3	12:N:108:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:108:LEU:HD13	25:O:122:LEU:HD21	1.96	0.46
20:V:46:VAL:HG11	20:V:83:ARG:HA	1.97	0.46
7:I:119:HIS:HB3	7:I:121:ILE:HG22	1.97	0.46
14:P:154:ALA:HA	14:P:159:LYS:HE3	1.98	0.46
20:V:62:VAL:O	20:V:73:GLN:HA	2.15	0.46
55:w:145:VAL:O	55:w:149:ALA:HB2	2.16	0.46
5:F:143:SER:HG	5:F:146:TRP:CD1	2.34	0.46
19:U:3:ARG:H	19:U:23:ASN:HB3	1.81	0.46
29:5:355:LEU:HD23	29:5:376:VAL:HG12	1.97	0.46
38:e:87:HIS:CG	46:m:71:PRO:HD2	2.51	0.46
53:u:114:VAL:N	53:u:122:ASP:O	2.46	0.46
1:A:1737:A:H61	1:A:1760:G:H1'	1.81	0.46
3:D:125:LYS:HB2	29:5:258:PRO:HD2	1.98	0.46
5:F:160:SER:HB3	42:i:80:LEU:HD13	1.97	0.46
11:M:83:PHE:HB3	28:3:115:LEU:HD13	1.98	0.46
19:U:17:LEU:HD21	33:9:136:LEU:HD12	1.96	0.46
20:V:54:TRP:NE1	20:V:56:LEU:O	2.49	0.46
1:A:1890:C:OP2	28:3:168:ARG:NH2	2.50	0.45
1:A:2016:C:OP2	11:M:59:ARG:NH1	2.41	0.45
1:A:2458:A:O2'	4:E:215:PHE:O	2.33	0.45
32:8:120:LYS:HA	32:8:123:LEU:HD12	1.98	0.45
1:A:2170:G:H4'	8:J:132:LEU:HD11	1.98	0.45
3:D:205:GLN:HB2	3:D:206:TYR:CE2	2.51	0.45
14:P:84:ILE:HB	14:P:91:GLU:HB3	1.98	0.45
41:h:62:PRO:HA	41:h:63:PRO:HD3	1.88	0.45
50:r:72:ILE:HD11	50:r:115:ILE:HD11	1.98	0.45
1:A:2181:A:N6	1:A:2206:C:O2'	2.48	0.45
9:K:27:PRO:HG2	9:K:30:LYS:HB3	1.98	0.45
12:N:131:ILE:HD12	12:N:151:VAL:HG21	1.99	0.45
14:P:112:ILE:HD13	14:P:131:VAL:HG21	1.98	0.45
19:U:129:MET:HA	37:d:82:ALA:HB2	1.98	0.45
38:e:171:TRP:CD1	38:e:263:TYR:HB3	2.51	0.45
7:I:160:LYS:HG2	7:I:163:GLU:HB3	1.99	0.45
9:K:139:LYS:HG2	35:b:144:ARG:HH12	1.82	0.45
32:8:150:LEU:HB2	38:e:212:HIS:HE1	1.81	0.45
34:a:44:ASN:ND2	35:b:135:ASN:OD1	2.49	0.45
39:f:166:PHE:O	39:f:170:PHE:CB	2.65	0.45
46:m:54:VAL:HG21	46:m:72:ARG:HB2	1.98	0.45
1:A:2814:G:H2'	12:N:140:MET:HB2	1.99	0.45
4:E:154:ARG:HB3	31:7:311:THR:HG21	1.99	0.45
10:L:111:ASN:OD1	10:L:111:ASN:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:M:230:PRO:O	11:M:234:LEU:HB2	2.16	0.45
14:P:54:ARG:NH1	14:P:140:GLY:O	2.50	0.45
21:W:103:VAL:HG22	21:W:127:TYR:HE1	1.81	0.45
26:1:45:HIS:CD2	26:1:46:TYR:H	2.34	0.45
30:6:208:ALA:H	30:6:243:ASN:HD21	1.64	0.45
1:A:2116:C:O2'	1:A:2837:A:N3	2.46	0.45
1:A:2165:C:O2'	1:A:2166:C:O4'	2.33	0.45
11:M:78:ILE:O	28:3:113:ARG:NH1	2.49	0.45
17:S:128:ILE:HG23	43:j:49:TRP:HB2	1.98	0.45
18:T:144:GLU:O	18:T:176:VAL:HA	2.17	0.45
22:X:150:LYS:HB2	22:X:159:MET:CE	2.47	0.45
30:6:235:TRP:HB3	30:6:254:TYR:HA	1.99	0.45
37:d:213:THR:HG22	37:d:247:VAL:HG22	1.99	0.45
40:g:111:ARG:NH2	40:g:112:LYS:HD3	2.32	0.45
1:A:1776:G:O6	1:A:1779:A:OP1	2.34	0.45
12:N:89:ILE:HD11	12:N:176:LEU:HD22	1.99	0.45
27:2:64:HIS:HB2	27:2:92:HIS:HD2	1.82	0.45
27:2:91:SER:OG	27:2:92:HIS:N	2.50	0.45
46:m:72:ARG:NE	46:m:75:LEU:HD21	2.32	0.45
51:s:63:ILE:HG21	51:s:382:GLN:HE22	1.82	0.45
1:A:1881:A:H62	40:g:111:ARG:HD3	1.81	0.45
29:5:251:HIS:O	29:5:371:LYS:NZ	2.38	0.45
35:b:28:ARG:HA	35:b:62:VAL:O	2.17	0.45
1:A:1688:A:OP2	22:X:5:LYS:NZ	2.47	0.45
1:A:2395:A:H1'	29:5:385:HIS:HB2	1.98	0.45
20:V:126:MET:SD	20:V:126:MET:N	2.89	0.45
29:5:121:LEU:HD21	29:5:128:LEU:HD13	1.98	0.45
31:7:139:ASN:HB3	31:7:174:VAL:HG21	1.99	0.45
3:D:121:PRO:HB3	3:D:166:SER:HA	1.98	0.45
19:U:28:LEU:HA	19:U:42:PHE:HA	1.99	0.45
22:X:86:ILE:HB	22:X:105:TRP:HB2	1.98	0.45
31:7:36:SER:HB2	31:7:39:GLU:HB2	1.98	0.45
36:c:60:ARG:HD2	36:c:63:LYS:HE3	1.98	0.45
42:i:95:ARG:HB2	42:i:110:LEU:HD21	1.98	0.45
51:s:244:SER:HA	51:s:292:CYS:HA	1.99	0.45
52:t:7:UNK:O	52:t:11:UNK:CB	2.65	0.45
5:F:253:MET:HE3	5:F:259:LEU:HD13	1.99	0.44
9:K:21:LEU:HD11	9:K:34:MET:HE3	2.00	0.44
20:V:19:TYR:OH	20:V:31:ASP:OD2	2.31	0.44
20:V:139:GLU:N	20:V:139:GLU:CD	2.73	0.44
1:A:2127:A:H4'	1:A:2251:A:C5	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:83:GLY:O	3:D:85:ARG:NH1	2.45	0.44
4:E:217:GLY:HA2	4:E:258:PRO:HB3	1.98	0.44
38:e:264:LEU:HD23	38:e:269:LEU:HB3	1.98	0.44
53:u:145:MET:O	53:u:149:LEU:CB	2.64	0.44
54:v:56:GLU:HA	54:v:59:LEU:HD12	2.00	0.44
55:w:79:ILE:HG12	55:w:126:PHE:HZ	1.81	0.44
12:N:114:ASP:H	12:N:118:MET:HE3	1.81	0.44
18:T:97:MET:HE1	18:T:105:GLN:HG3	1.99	0.44
22:X:127:VAL:HG22	22:X:131:THR:HB	1.99	0.44
29:5:350:ARG:HE	29:5:351:VAL:HG23	1.82	0.44
53:u:131:SER:OG	53:u:132:THR:N	2.50	0.44
24:Z:66:LEU:HB2	24:Z:122:LEU:HB3	1.99	0.44
37:d:164:VAL:HG23	37:d:261:MET:HB2	2.00	0.44
53:u:132:THR:O	53:u:136:HIS:HB2	2.18	0.44
13:O:59:LEU:HB2	15:Q:269:MET:HE1	2.00	0.44
21:W:57:GLU:HB2	21:W:99:TYR:HD1	1.83	0.44
29:5:200:ARG:HE	29:5:233:LYS:HD2	1.82	0.44
40:g:39:VAL:HG21	49:q:72:PRO:HB2	1.99	0.44
1:A:1756:A:H2'	1:A:1757:A:C8	2.52	0.44
1:A:2420:U:O2'	33:9:23:SER:OG	2.34	0.44
4:E:56:GLU:OE1	4:E:57:ASN:ND2	2.51	0.44
4:E:119:VAL:HG11	4:E:284:TYR:HB3	1.98	0.44
6:H:59:TRP:HE1	22:X:96:LYS:HE2	1.83	0.44
12:N:116:LYS:O	12:N:166:ARG:NH1	2.51	0.44
13:O:107:MET:HA	13:O:122:VAL:O	2.18	0.44
18:T:133:ASN:HD22	37:d:226:ASP:CG	2.25	0.44
29:5:391:VAL:HG13	29:5:398:VAL:HB	2.00	0.44
46:m:57:VAL:HB	46:m:75:LEU:O	2.18	0.44
49:q:46:LEU:HA	49:q:46:LEU:HD22	1.83	0.44
1:A:1878:U:O3'	5:F:92:ARG:NH2	2.51	0.44
1:A:2034:A:O2'	11:M:71:GLN:OE1	2.29	0.44
1:A:2815:G:O6	12:N:139:ARG:NH2	2.42	0.44
13:O:108:LEU:HD11	13:O:135:LEU:HD23	1.99	0.44
17:S:100:HIS:O	17:S:100:HIS:CG	2.70	0.44
20:V:95:TYR:HB3	20:V:108:MET:SD	2.58	0.44
31:7:303:PRO:HG2	31:7:306:LEU:H	1.83	0.44
55:w:105:MET:HA	55:w:110:LEU:H	1.82	0.44
1:A:2204:U:O2'	1:A:2207:A:N7	2.42	0.44
5:F:126:LYS:NZ	5:F:138:HIS:O	2.42	0.44
11:M:28:LYS:HG2	11:M:29:PRO:HD2	2.00	0.44
21:W:95:GLY:HA3	21:W:134:VAL:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1886:G:H1	42:i:61:GLY:HA3	1.83	0.44
1:A:3181:U:OP1	50:r:94:ARG:NH2	2.51	0.44
14:P:57:GLU:OE2	14:P:96:HIS:NE2	2.51	0.44
18:T:98:SER:OG	31:7:97:GLU:OE1	2.33	0.44
5:F:289:PRO:HD2	11:M:195:LEU:HD11	1.99	0.43
6:H:84:GLU:OE1	22:X:44:ARG:NH2	2.50	0.43
15:Q:152:ARG:NH1	15:Q:191:ARG:HA	2.33	0.43
30:6:161:LEU:HD13	30:6:221:LEU:HD21	2.01	0.43
1:A:3131:G:H3'	1:A:3132:G:H8	1.83	0.43
3:D:202:ARG:HH21	3:D:205:GLN:HE22	1.66	0.43
8:J:25:ARG:HA	8:J:65:PRO:HA	2.01	0.43
8:J:69:LYS:HD3	8:J:129:ALA:HB1	1.99	0.43
18:T:76:CYS:HA	18:T:174:TYR:O	2.18	0.43
22:X:56:ASN:OD1	22:X:56:ASN:N	2.48	0.43
49:q:142:ASN:O	49:q:146:ALA:CB	2.66	0.43
53:u:197:ARG:H	54:v:66:LEU:HD13	1.83	0.43
1:A:1839:C:H5'	9:K:117:HIS:ND1	2.33	0.43
4:E:76:LYS:HG3	4:E:170:LEU:HD21	2.00	0.43
11:M:292:LYS:O	11:M:296:SER:OG	2.31	0.43
22:X:42:HIS:CG	22:X:86:ILE:HD11	2.54	0.43
30:6:39:ASP:OD1	30:6:39:ASP:N	2.51	0.43
38:e:128:PHE:HB2	46:m:73:ARG:CB	2.48	0.43
38:e:162:ARG:HH11	38:e:171:TRP:HB2	1.82	0.43
42:i:70:PRO:O	42:i:73:LEU:HB2	2.17	0.43
1:A:1924:U:H2'	1:A:1925:A:C8	2.53	0.43
13:O:97:TYR:OH	13:O:126:LYS:O	2.28	0.43
17:S:57:SER:OG	17:S:58:SER:N	2.51	0.43
50:r:72:ILE:HD12	50:r:111:GLU:HB3	2.01	0.43
50:r:112:HIS:O	50:r:116:GLU:HB2	2.18	0.43
1:A:2327:U:H4'	13:O:30:ARG:HH21	1.84	0.43
5:F:138:HIS:CD2	5:F:146:TRP:HE1	2.36	0.43
17:S:131:GLU:HG2	17:S:151:LYS:HE2	2.00	0.43
36:c:94:ASN:HA	36:c:122:ASN:HB2	2.00	0.43
46:m:70:GLU:HA	46:m:71:PRO:HD2	1.70	0.43
50:r:93:ILE:HG22	50:r:94:ARG:O	2.19	0.43
1:A:1868:G:N7	11:M:51:ARG:NH2	2.67	0.43
9:K:45:PRO:HB3	16:R:75:ALA:HB2	2.01	0.43
17:S:101:PHE:HB3	17:S:106:TRP:CD1	2.53	0.43
41:h:105:ALA:HB1	41:h:111:VAL:HG22	2.01	0.43
1:A:2241:A:OP1	50:r:150:TYR:OH	2.29	0.43
1:A:2415:C:N4	33:9:49:ARG:HH12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2740:A:H2'	1:A:2741:A:C8	2.53	0.43
17:S:76:HIS:ND1	34:a:50:ALA:HA	2.34	0.43
29:5:114:LEU:HD13	29:5:263:ILE:HG12	2.00	0.43
31:7:286:LEU:HD12	31:7:294:ILE:HB	2.00	0.43
33:9:128:PHE:CD1	33:9:135:PHE:HB3	2.53	0.43
6:H:117:SER:O	6:H:121:ASN:HB2	2.18	0.43
12:N:76:SER:HB3	12:N:155:LYS:HB2	2.00	0.43
31:7:220:GLU:HB3	31:7:251:ILE:HD11	2.00	0.43
1:A:2055:U:H2'	1:A:2056:G:C8	2.52	0.43
1:A:2682:A:H5''	16:R:34:ARG:HH12	1.83	0.43
5:F:237:LEU:O	49:q:25:TYR:N	2.52	0.43
31:7:103:SER:HA	31:7:129:THR:HG22	2.01	0.43
31:7:180:CYS:HA	31:7:297:PHE:O	2.19	0.43
38:e:198:ASN:HD21	38:e:200:MET:HE2	1.83	0.43
38:e:200:MET:HA	38:e:241:GLY:HA2	2.01	0.43
40:g:154:ASP:OD1	40:g:154:ASP:N	2.51	0.43
49:q:142:ASN:O	49:q:146:ALA:HB2	2.19	0.43
1:A:2371:U:H2'	19:U:71:ARG:HD3	2.01	0.43
3:D:180:ASP:OD1	3:D:180:ASP:N	2.39	0.43
17:S:167:TRP:HE1	17:S:169:ARG:HH21	1.67	0.43
25:0:95:ARG:HH11	25:0:95:ARG:HD3	1.71	0.43
32:8:124:TYR:HE2	38:e:67:GLN:HE21	1.67	0.43
1:A:2171:U:C2	1:A:2173:G:H4'	2.54	0.42
7:I:149:GLY:HA3	44:k:31:ARG:HH22	1.84	0.42
8:J:125:ALA:HB2	8:J:140:VAL:HG21	2.00	0.42
12:N:50:LEU:HB2	12:N:110:ASN:HD21	1.84	0.42
13:O:53:ARG:HD2	13:O:107:MET:HE3	2.01	0.42
16:R:42:ALA:O	16:R:46:VAL:HB	2.19	0.42
23:Y:169:ARG:HH22	29:5:64:MET:HB2	1.84	0.42
27:2:89:SER:O	27:2:89:SER:OG	2.36	0.42
29:5:214:ASN:OD1	29:5:219:LEU:HD13	2.17	0.42
29:5:366:CYS:SG	29:5:367:ASN:N	2.92	0.42
50:r:161:PRO:HG2	50:r:163:TYR:CZ	2.54	0.42
51:s:243:ILE:HG13	51:s:296:HIS:HB2	2.01	0.42
1:A:1750:G:OP2	28:3:113:ARG:NH2	2.46	0.42
1:A:2187:C:H2'	1:A:2188:A:C8	2.54	0.42
3:D:66:TRP:HB3	3:D:80:ARG:HE	1.84	0.42
8:J:49:PHE:O	8:J:53:PHE:CB	2.68	0.42
19:U:22:THR:HG21	19:U:56:TYR:HE1	1.83	0.42
29:5:232:THR:OG1	29:5:234:ASP:O	2.33	0.42
38:e:157:LEU:HD23	38:e:254:TRP:HB3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:e:163:GLU:HB2	38:e:172:ILE:HD12	2.01	0.42
53:u:126:ILE:HD13	53:u:178:HIS:HB2	2.01	0.42
1:A:2395:A:O2'	29:5:384:GLN:NE2	2.43	0.42
4:E:208:ALA:HB2	4:E:297:VAL:HG12	2.00	0.42
5:F:113:LYS:HG3	5:F:157:GLY:H	1.83	0.42
10:L:136:LYS:HG2	53:u:167:TRP:NE1	2.34	0.42
11:M:277:MET:HE1	40:g:52:LEU:HD21	2.00	0.42
12:N:103:GLU:OE1	12:N:106:ARG:NH2	2.42	0.42
15:Q:122:ALA:HB2	15:Q:172:GLN:HE22	1.84	0.42
20:V:183:LEU:HD11	33:9:79:PRO:HD2	2.02	0.42
30:6:235:TRP:HA	30:6:252:CYS:O	2.19	0.42
30:6:236:LEU:O	30:6:251:THR:OG1	2.36	0.42
44:k:42:VAL:O	44:k:46:ASN:N	2.41	0.42
46:m:50:ARG:CD	46:m:52:TYR:OH	2.55	0.42
55:w:111:ASP:OD1	55:w:112:SER:N	2.52	0.42
4:E:144:THR:HA	4:E:179:PHE:O	2.20	0.42
23:Y:187:PRO:HD2	23:Y:190:LEU:HD11	2.02	0.42
29:5:125:LYS:HA	29:5:253:LEU:HD21	2.00	0.42
31:7:108:VAL:HB	31:7:113:TRP:CD1	2.54	0.42
31:7:175:ILE:H	31:7:175:ILE:HG13	1.58	0.42
38:e:162:ARG:HD3	38:e:171:TRP:HE3	1.84	0.42
41:h:151:ASN:OD1	41:h:151:ASN:N	2.47	0.42
1:A:1874:A:O2'	1:A:2090:A:O2'	2.23	0.42
1:A:1977:U:H2'	1:A:1978:A:C8	2.55	0.42
1:A:2103:A:H4'	12:N:231:SER:HA	2.01	0.42
1:A:2326:C:OP2	51:s:55:SER:OG	2.31	0.42
3:D:225:ILE:HA	3:D:234:MET:O	2.20	0.42
9:K:67:PHE:HB3	9:K:71:LYS:HB2	2.01	0.42
18:T:144:GLU:HB2	18:T:177:LYS:HB3	2.01	0.42
50:r:40:GLU:HA	50:r:48:ILE:O	2.20	0.42
51:s:253:LEU:HB2	51:s:354:PRO:HD3	2.00	0.42
54:v:54:GLN:HA	54:v:57:LYS:HG2	2.01	0.42
1:A:2682:A:H5''	16:R:34:ARG:NH1	2.34	0.42
8:J:50:CYS:HA	8:J:53:PHE:HB3	2.01	0.42
11:M:118:LEU:HD21	11:M:129:ILE:HD11	2.02	0.42
13:O:84:ASP:OD1	13:O:84:ASP:N	2.50	0.42
38:e:202:ALA:HA	38:e:238:LEU:HA	2.02	0.42
51:s:366:TYR:HA	51:s:400:PRO:HA	2.01	0.42
55:w:103:HIS:CE1	55:w:105:MET:HG2	2.54	0.42
1:A:1753:A:OP1	42:i:118:TYR:OH	2.28	0.42
1:A:1814:A:N3	1:A:1862:U:O2'	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2913:A:H4'	1:A:2914:A:H5''	2.02	0.42
5:F:243:ILE:HG22	5:F:244:PRO:O	2.20	0.42
7:I:96:ILE:HD11	7:I:153:LEU:HD22	2.01	0.42
7:I:121:ILE:HG13	7:I:156:SER:HB2	2.01	0.42
15:Q:150:ILE:HA	15:Q:162:ILE:O	2.20	0.42
18:T:109:ASN:HD21	25:0:101:ILE:HD13	1.85	0.42
22:X:226:LEU:HD23	22:X:229:ILE:HD12	2.02	0.42
31:7:219:LEU:HD23	31:7:219:LEU:HA	1.91	0.42
1:A:3146:G:N2	4:E:268:GLU:OE2	2.46	0.42
13:O:123:ILE:HG21	13:O:123:ILE:HD13	1.76	0.42
27:2:53:TYR:CZ	27:2:55:PRO:HB3	2.55	0.42
30:6:161:LEU:HD21	30:6:271:LEU:HD21	2.02	0.42
31:7:303:PRO:HG2	31:7:306:LEU:HB2	2.02	0.42
38:e:255:VAL:HG13	38:e:259:GLU:HB2	2.01	0.42
41:h:153:LYS:HA	41:h:153:LYS:HD3	1.85	0.42
53:u:118:MET:HE1	54:v:66:LEU:HD22	2.02	0.42
4:E:116:LYS:HD2	15:Q:165:GLU:OE2	2.19	0.42
9:K:118:ARG:HA	9:K:121:MET:HE3	2.01	0.42
29:5:215:ARG:NH2	29:5:366:CYS:O	2.53	0.42
29:5:293:LEU:HD22	29:5:316:PHE:HD2	1.85	0.42
36:c:170:ALA:HB3	36:c:191:LEU:HD21	2.01	0.42
48:p:38:GLU:HB3	48:p:39:PHE:H	1.67	0.42
51:s:145:VAL:HG21	51:s:187:LEU:HD11	2.00	0.42
1:A:2157:U:OP1	50:r:182:ARG:NH1	2.53	0.42
4:E:276:ILE:HG13	4:E:332:LEU:HB2	2.02	0.42
5:F:83:HIS:CG	5:F:274:LEU:HD11	2.55	0.42
16:R:10:LEU:HD13	16:R:10:LEU:HA	1.87	0.42
17:S:86:MET:HE1	17:S:140:ASN:HB2	2.01	0.42
1:A:2442:U:H5''	51:s:85:LYS:HB2	2.01	0.41
6:H:64:LEU:HB2	22:X:63:GLU:OE1	2.20	0.41
9:K:46:VAL:HG13	18:T:208:ILE:HG12	2.01	0.41
10:L:52:HIS:CE1	10:L:53:ARG:HG3	2.55	0.41
25:0:94:ARG:HA	25:0:99:LYS:HD2	2.02	0.41
29:5:203:CYS:O	51:s:179:GLN:NE2	2.52	0.41
55:w:87:LEU:HD13	55:w:98:LEU:HD11	2.01	0.41
4:E:266:ARG:HA	4:E:266:ARG:HD3	1.78	0.41
7:I:191:PHE:O	7:I:195:SER:OG	2.36	0.41
10:L:75:LEU:O	10:L:81:LYS:HA	2.21	0.41
11:M:129:ILE:HG21	11:M:129:ILE:HD13	1.87	0.41
11:M:198:GLN:HE21	49:q:55:ARG:NH1	2.18	0.41
13:O:106:ARG:HG2	13:O:124:GLU:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:6:105:GLU:O	30:6:109:ALA:CB	2.68	0.41
1:A:2142:A:O2'	1:A:2262:C:OP1	2.37	0.41
1:A:2194:U:C4	7:I:125:VAL:HB	2.55	0.41
1:A:2234:C:O2'	1:A:2688:C:O2'	2.32	0.41
15:Q:100:LEU:HD23	15:Q:100:LEU:HA	1.88	0.41
33:9:68:PHE:CE2	33:9:70:LEU:HB2	2.55	0.41
9:K:11:TRP:CD1	36:c:269:LEU:HD23	2.55	0.41
13:O:80:LEU:HD23	13:O:80:LEU:HA	1.94	0.41
19:U:98:GLN:HB3	51:s:100:LEU:HD22	2.01	0.41
25:0:90:ASN:O	25:0:94:ARG:HG2	2.20	0.41
1:A:3116:C:N3	1:A:3140:A:N1	2.68	0.41
3:D:193:ILE:HD11	3:D:226:ILE:HD12	2.03	0.41
4:E:73:LEU:HD11	4:E:151:THR:HG21	2.03	0.41
6:H:55:ILE:HG21	22:X:44:ARG:HD2	2.02	0.41
9:K:74:GLN:HA	50:r:161:PRO:HA	2.03	0.41
28:3:110:VAL:HG13	28:3:158:LEU:HD22	2.02	0.41
4:E:99:LEU:HA	4:E:99:LEU:HD23	1.92	0.41
8:J:32:GLY:HA3	8:J:33:PRO:HD3	1.92	0.41
8:J:124:LYS:HE2	8:J:144:ILE:HG21	2.03	0.41
9:K:20:LEU:HD22	9:K:21:LEU:H	1.86	0.41
11:M:62:ARG:HA	11:M:63:PRO:HD3	1.95	0.41
12:N:218:ILE:HA	12:N:223:MET:HG3	2.03	0.41
21:W:67:ILE:HG21	21:W:131:VAL:HG11	2.02	0.41
21:W:127:TYR:HD2	39:f:56:ILE:HG12	1.86	0.41
1:A:1802:A:OP1	20:V:83:ARG:NH2	2.54	0.41
1:A:2235:C:H4'	50:r:164:LYS:HG2	2.02	0.41
1:A:2837:A:H2'	1:A:2838:A:C8	2.55	0.41
1:A:3205:C:OP2	4:E:298:LYS:NZ	2.54	0.41
11:M:78:ILE:HD13	28:3:124:ARG:HD2	2.03	0.41
11:M:142:GLU:HB2	11:M:162:LEU:HD22	2.03	0.41
17:S:114:ILE:HD13	17:S:114:ILE:HG21	1.79	0.41
18:T:140:LEU:HD23	18:T:180:GLU:HA	2.02	0.41
28:3:133:LEU:HD22	28:3:141:LYS:HG2	2.02	0.41
42:i:32:ILE:HG22	42:i:34:ILE:HG22	2.02	0.41
50:r:41:THR:O	50:r:47:THR:HA	2.20	0.41
1:A:2677:A:H2'	1:A:2678:A:C8	2.55	0.41
5:F:70:ARG:HA	5:F:196:PRO:HD3	2.03	0.41
5:F:252:SER:O	5:F:256:HIS:ND1	2.54	0.41
7:I:178:GLY:HA2	7:I:191:PHE:HE2	1.86	0.41
7:I:188:ARG:HA	7:I:191:PHE:HD2	1.85	0.41
8:J:18:GLY:N	8:J:72:VAL:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:142:GLN:NE2	53:u:197:ARG:O	2.53	0.41
24:Z:50:PRO:HA	24:Z:53:HIS:HD2	1.85	0.41
29:5:133:PRO:HD3	29:5:375:TRP:CG	2.56	0.41
31:7:65:ILE:H	31:7:65:ILE:HG13	1.63	0.41
38:e:74:LEU:HD22	46:m:42:ARG:HB2	2.02	0.41
1:A:2255:C:H5''	43:j:66:ARG:HH11	1.86	0.41
4:E:179:PHE:CE1	4:E:298:LYS:HE3	2.56	0.41
5:F:164:MET:SD	5:F:170:ARG:NH1	2.93	0.41
7:I:119:HIS:HD2	7:I:121:ILE:HB	1.85	0.41
9:K:36:SER:O	9:K:40:GLN:HG3	2.21	0.41
11:M:129:ILE:HD12	11:M:184:LEU:HD11	2.03	0.41
15:Q:188:LEU:HD22	15:Q:191:ARG:HH12	1.86	0.41
17:S:164:THR:HG22	35:b:107:GLN:HB2	2.03	0.41
19:U:148:PRO:HB3	37:d:175:ASP:HB2	2.03	0.41
20:V:185:ARG:NH2	20:V:187:TYR:O	2.54	0.41
26:1:33:LYS:HE3	26:1:65:LEU:HD11	2.03	0.41
30:6:356:ARG:HD2	30:6:356:ARG:HA	1.87	0.41
32:8:94:PHE:HB3	38:e:83:LEU:HD23	2.03	0.41
32:8:164:ARG:NH2	39:f:162:LEU:O	2.54	0.41
35:b:19:LEU:HA	35:b:19:LEU:HD23	1.90	0.41
36:c:70:ALA:HB2	41:h:153:LYS:HE3	2.03	0.41
36:c:220:ILE:O	36:c:223:MET:HG2	2.21	0.41
37:d:172:MET:HG3	37:d:173:THR:HG23	2.03	0.41
39:f:104:GLU:HG3	39:f:155:ARG:HE	1.84	0.41
39:f:127:MET:HE3	39:f:128:PRO:HD2	2.03	0.41
43:j:53:ASP:OD2	43:j:55:ARG:NH2	2.54	0.41
44:k:13:VAL:HG13	44:k:49:CYS:HB2	2.02	0.41
46:m:55:LEU:HD23	46:m:55:LEU:HA	1.94	0.41
51:s:389:ARG:HH21	51:s:389:ARG:HD2	1.71	0.41
53:u:132:THR:O	53:u:136:HIS:CB	2.68	0.41
4:E:345:ILE:H	4:E:345:ILE:HG13	1.68	0.41
13:O:65:LEU:HB3	13:O:69:ASN:HD22	1.85	0.41
17:S:96:PHE:HB3	35:b:126:ILE:HD12	2.03	0.41
21:W:100:THR:O	21:W:129:THR:HA	2.21	0.41
23:Y:171:ASP:OD1	23:Y:171:ASP:N	2.51	0.41
30:6:274:LYS:HG3	30:6:314:ALA:HB2	2.02	0.41
36:c:170:ALA:HB1	36:c:175:VAL:HB	2.02	0.41
44:k:15:GLN:HA	44:k:50:SER:O	2.21	0.41
53:u:140:PHE:HA	53:u:143:VAL:HG12	2.03	0.41
1:A:1679:U:O2'	1:A:1680:A:OP2	2.38	0.40
1:A:1871:A:O2'	1:A:1900:A:N6	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2310:G:N2	1:A:2311:U:O4	2.36	0.40
1:A:3228:U:OP2	4:E:156:ARG:NH2	2.54	0.40
5:F:93:LEU:H	47:o:91:GLN:HE21	1.69	0.40
5:F:268:PHE:HE2	42:i:63:LEU:HD12	1.86	0.40
9:K:163:ILE:HG12	50:r:87:LEU:HD21	2.02	0.40
23:Y:90:LEU:HA	23:Y:90:LEU:HD23	1.88	0.40
31:7:269:ILE:HD13	31:7:269:ILE:HA	1.92	0.40
36:c:122:ASN:HD21	36:c:194:THR:HG22	1.86	0.40
39:f:166:PHE:O	39:f:170:PHE:HB3	2.21	0.40
53:u:125:VAL:HB	53:u:177:ILE:HA	2.02	0.40
1:A:1784:A:O2'	19:U:84:ASN:ND2	2.55	0.40
9:K:25:MET:O	9:K:149:ARG:NH1	2.55	0.40
24:Z:40:ARG:NH2	30:6:27:ARG:HD3	2.36	0.40
29:5:84:ASP:HA	29:5:85:PRO:HD3	1.93	0.40
29:5:203:CYS:HA	29:5:230:LEU:HA	2.03	0.40
30:6:224:HIS:HA	30:6:232:TYR:CE2	2.56	0.40
33:9:87:THR:HG23	33:9:90:GLN:H	1.86	0.40
35:b:34:SER:OG	35:b:40:SER:OG	2.27	0.40
38:e:52:CYS:HB2	38:e:173:LEU:HD21	2.03	0.40
55:w:124:ASP:OD1	55:w:124:ASP:N	2.53	0.40
7:I:117:ARG:NH1	8:J:133:GLN:OE1	2.54	0.40
15:Q:116:ILE:HA	15:Q:135:GLY:O	2.22	0.40
19:U:39:THR:HA	19:U:97:VAL:O	2.21	0.40
24:Z:78:ARG:O	24:Z:83:LYS:NZ	2.55	0.40
29:5:232:THR:HG23	29:5:289:HIS:HB2	2.03	0.40
40:g:68:THR:HG22	40:g:69:PRO:HD2	2.03	0.40
40:g:82:LEU:HD12	40:g:166:PHE:CZ	2.56	0.40
42:i:74:ILE:HD11	42:i:82:GLY:H	1.86	0.40
55:w:82:ARG:HA	55:w:85:TYR:HB3	2.04	0.40
1:A:2180:A:H4'	1:A:2181:A:C8	2.56	0.40
1:A:2235:C:H4'	50:r:164:LYS:HA	2.03	0.40
8:J:24:VAL:HG21	8:J:35:LEU:HD21	2.03	0.40
9:K:65:ILE:HD13	9:K:65:ILE:HG21	1.93	0.40
11:M:95:PRO:HB3	11:M:141:VAL:HG21	2.03	0.40
15:Q:102:ARG:HA	15:Q:102:ARG:HD2	1.96	0.40
17:S:142:THR:HG23	34:a:62:HIS:NE2	2.36	0.40
26:1:42:THR:OG1	49:q:135:TRP:NE1	2.52	0.40
1:A:1884:G:N3	1:A:1895:C:O2'	2.55	0.40
1:A:2196:A:O2'	1:A:2213:A:N1	2.50	0.40
9:K:60:MET:HE3	9:K:131:GLU:HA	2.04	0.40
12:N:105:MET:O	12:N:109:ILE:HB	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:O:129:CYS:SG	25:O:156:THR:OG1	2.80	0.40
18:T:77:ARG:HD3	18:T:120:VAL:HG22	2.03	0.40
19:U:44:ILE:HD13	19:U:44:ILE:HG21	1.80	0.40
22:X:90:ILE:HD13	22:X:90:ILE:HG21	1.91	0.40
22:X:116:SER:O	22:X:120:ASP:N	2.55	0.40
23:Y:78:LYS:HE2	23:Y:78:LYS:HB2	1.91	0.40
28:3:125:ARG:HH21	28:3:125:ARG:HD2	1.66	0.40
29:5:207:SER:HA	51:s:157:LEU:HD11	2.03	0.40
31:7:167:VAL:HG23	31:7:235:TYR:HB3	2.03	0.40
37:d:138:PRO:HA	37:d:141:ALA:HB3	2.04	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	
3	D	216/305 (71%)	203 (94%)	13 (6%)	0	100	100
4	E	281/348 (81%)	273 (97%)	8 (3%)	0	100	100
5	F	248/311 (80%)	234 (94%)	14 (6%)	0	100	100
6	H	93/267 (35%)	85 (91%)	7 (8%)	1 (1%)	11	39
7	I	154/261 (59%)	141 (92%)	13 (8%)	0	100	100
8	J	138/192 (72%)	120 (87%)	18 (13%)	0	100	100
9	K	175/178 (98%)	166 (95%)	9 (5%)	0	100	100
10	L	113/145 (78%)	106 (94%)	7 (6%)	0	100	100
11	M	285/296 (96%)	275 (96%)	10 (4%)	0	100	100
12	N	203/251 (81%)	192 (95%)	11 (5%)	0	100	100
13	O	150/175 (86%)	145 (97%)	5 (3%)	0	100	100
14	P	139/180 (77%)	130 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
15	Q	215/292 (74%)	200 (93%)	15 (7%)	0	100	100
16	R	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
17	S	154/205 (75%)	147 (96%)	7 (4%)	0	100	100
18	T	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
19	U	135/153 (88%)	126 (93%)	9 (7%)	0	100	100
20	V	188/216 (87%)	183 (97%)	5 (3%)	0	100	100
21	W	107/148 (72%)	103 (96%)	4 (4%)	0	100	100
22	X	241/256 (94%)	233 (97%)	8 (3%)	0	100	100
23	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
24	Z	118/161 (73%)	110 (93%)	8 (7%)	0	100	100
25	0	106/188 (56%)	101 (95%)	5 (5%)	0	100	100
26	1	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
27	2	41/92 (45%)	40 (98%)	1 (2%)	0	100	100
28	3	93/188 (50%)	87 (94%)	6 (6%)	0	100	100
29	5	383/423 (90%)	363 (95%)	20 (5%)	0	100	100
30	6	316/380 (83%)	300 (95%)	16 (5%)	0	100	100
31	7	285/338 (84%)	262 (92%)	23 (8%)	0	100	100
32	8	97/206 (47%)	88 (91%)	9 (9%)	0	100	100
33	9	113/137 (82%)	109 (96%)	4 (4%)	0	100	100
34	a	78/142 (55%)	74 (95%)	4 (5%)	0	100	100
35	b	146/215 (68%)	130 (89%)	16 (11%)	0	100	100
36	c	271/332 (82%)	264 (97%)	7 (3%)	0	100	100
37	d	203/306 (66%)	191 (94%)	12 (6%)	0	100	100
38	e	211/279 (76%)	179 (85%)	31 (15%)	1 (0%)	24	57
39	f	110/212 (52%)	98 (89%)	11 (10%)	1 (1%)	14	44
40	g	127/166 (76%)	115 (91%)	12 (9%)	0	100	100
41	h	96/158 (61%)	93 (97%)	3 (3%)	0	100	100
42	i	95/128 (74%)	90 (95%)	5 (5%)	0	100	100
43	j	83/123 (68%)	81 (98%)	2 (2%)	0	100	100
44	k	76/112 (68%)	71 (93%)	5 (7%)	0	100	100
45	l	21/138 (15%)	21 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
46	m	43/128 (34%)	37 (86%)	4 (9%)	2 (5%)	2	10
47	o	77/102 (76%)	76 (99%)	1 (1%)	0	100	100
48	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
49	q	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
50	r	140/196 (71%)	134 (96%)	6 (4%)	0	100	100
51	s	366/439 (83%)	354 (97%)	12 (3%)	0	100	100
53	u	109/234 (47%)	100 (92%)	9 (8%)	0	100	100
54	v	67/70 (96%)	66 (98%)	1 (2%)	0	100	100
55	w	77/156 (49%)	69 (90%)	8 (10%)	0	100	100
All	All	7945/11026 (72%)	7507 (94%)	433 (5%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
46	m	71	PRO
6	H	104	ASN
38	e	256	THR
39	f	179	PRO
46	m	53	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	D	179/245 (73%)	177 (99%)	2 (1%)	65	80
4	E	246/290 (85%)	244 (99%)	2 (1%)	73	83
5	F	217/262 (83%)	214 (99%)	3 (1%)	59	78
6	H	86/228 (38%)	86 (100%)	0	100	100
7	I	145/232 (62%)	144 (99%)	1 (1%)	76	84
8	J	113/150 (75%)	113 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	K	155/156 (99%)	152 (98%)	3 (2%)	50	73
10	L	98/124 (79%)	98 (100%)	0	100	100
11	M	245/249 (98%)	242 (99%)	3 (1%)	63	79
12	N	172/211 (82%)	170 (99%)	2 (1%)	63	79
13	O	133/150 (89%)	130 (98%)	3 (2%)	44	70
14	P	123/155 (79%)	122 (99%)	1 (1%)	73	83
15	Q	199/256 (78%)	199 (100%)	0	100	100
16	R	118/126 (94%)	116 (98%)	2 (2%)	53	75
17	S	141/180 (78%)	141 (100%)	0	100	100
18	T	141/176 (80%)	140 (99%)	1 (1%)	76	84
19	U	124/135 (92%)	120 (97%)	4 (3%)	34	64
20	V	172/191 (90%)	171 (99%)	1 (1%)	78	85
21	W	89/119 (75%)	88 (99%)	1 (1%)	65	80
22	X	219/229 (96%)	217 (99%)	2 (1%)	70	82
23	Y	159/223 (71%)	158 (99%)	1 (1%)	78	85
24	Z	111/147 (76%)	111 (100%)	0	100	100
25	0	97/164 (59%)	97 (100%)	0	100	100
26	1	49/60 (82%)	49 (100%)	0	100	100
27	2	38/72 (53%)	37 (97%)	1 (3%)	40	69
28	3	88/166 (53%)	86 (98%)	2 (2%)	44	70
29	5	348/368 (95%)	345 (99%)	3 (1%)	70	82
30	6	265/332 (80%)	264 (100%)	1 (0%)	84	87
31	7	263/303 (87%)	260 (99%)	3 (1%)	65	80
32	8	91/190 (48%)	91 (100%)	0	100	100
33	9	99/112 (88%)	97 (98%)	2 (2%)	48	73
34	a	78/133 (59%)	78 (100%)	0	100	100
35	b	130/186 (70%)	126 (97%)	4 (3%)	35	65
36	c	241/288 (84%)	239 (99%)	2 (1%)	73	83
37	d	193/274 (70%)	192 (100%)	1 (0%)	81	86
38	e	188/236 (80%)	188 (100%)	0	100	100
39	f	101/188 (54%)	101 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
40	g	119/148 (80%)	116 (98%)	3 (2%)	42	69
41	h	95/148 (64%)	94 (99%)	1 (1%)	65	80
42	i	86/110 (78%)	83 (96%)	3 (4%)	32	62
43	j	68/97 (70%)	68 (100%)	0	100	100
44	k	71/90 (79%)	69 (97%)	2 (3%)	38	67
45	l	23/116 (20%)	23 (100%)	0	100	100
46	m	40/113 (35%)	40 (100%)	0	100	100
47	o	68/87 (78%)	68 (100%)	0	100	100
48	p	117/181 (65%)	117 (100%)	0	100	100
49	q	110/178 (62%)	108 (98%)	2 (2%)	51	74
50	r	133/169 (79%)	132 (99%)	1 (1%)	73	83
51	s	326/381 (86%)	323 (99%)	3 (1%)	70	82
53	u	105/200 (52%)	105 (100%)	0	100	100
54	v	59/60 (98%)	59 (100%)	0	100	100
55	w	73/136 (54%)	72 (99%)	1 (1%)	59	78
All	All	7147/9520 (75%)	7080 (99%)	67 (1%)	68	82

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	206	TYR
3	D	236	VAL
4	E	97	VAL
4	E	284	TYR
5	F	125	ARG
5	F	203	LEU
5	F	281	ARG
7	I	146	LEU
9	K	16	ARG
9	K	101	VAL
9	K	125	LEU
11	M	57	ARG
11	M	96	LEU
11	M	141	VAL
12	N	151	VAL
12	N	226	ILE
13	O	36	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
13	O	42	ILE
13	O	59	LEU
14	P	51	ARG
16	R	10	LEU
16	R	119	LEU
18	T	176	VAL
19	U	6	VAL
19	U	28	LEU
19	U	44	ILE
19	U	71	ARG
20	V	138	THR
21	W	105	VAL
22	X	90	ILE
22	X	151	GLU
23	Y	190	LEU
27	2	84	LEU
28	3	125	ARG
28	3	168	ARG
29	5	98	LEU
29	5	106	ILE
29	5	140	VAL
30	6	272	LEU
31	7	65	ILE
31	7	67	VAL
31	7	167	VAL
33	9	91	LEU
33	9	136	LEU
35	b	11	LEU
35	b	26	LEU
35	b	62	VAL
35	b	103	LYS
36	c	87	LEU
36	c	202	LEU
37	d	164	VAL
40	g	68	THR
40	g	100	ILE
40	g	137	VAL
41	h	96	LEU
42	i	80	LEU
42	i	88	LEU
42	i	113	ARG
44	k	16	VAL

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Mol	Chain	Res	Type
44	k	55	VAL
49	q	46	LEU
49	q	82	LEU
50	r	86	VAL
51	s	299	PHE
51	s	360	VAL
51	s	361	ILE
55	w	106	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (84) such sidechains are listed below:

Mol	Chain	Res	Type
3	D	205	GLN
3	D	227	GLN
4	E	52	HIS
4	E	184	ASN
5	F	58	HIS
5	F	188	HIS
5	F	223	HIS
6	H	121	ASN
7	I	141	GLN
7	I	189	GLN
9	K	160	GLN
10	L	59	HIS
10	L	80	GLN
10	L	142	GLN
11	M	114	GLN
11	M	198	GLN
13	O	147	GLN
13	O	150	GLN
14	P	87	GLN
14	P	97	GLN
14	P	115	HIS
16	R	63	ASN
16	R	77	GLN
16	R	89	ASN
16	R	125	HIS
17	S	118	ASN
17	S	140	ASN
18	T	75	HIS
18	T	210	HIS
19	U	4	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
19	U	55	ASN
19	U	82	HIS
19	U	101	HIS
20	V	92	ASN
21	W	62	HIS
21	W	72	HIS
21	W	80	HIS
22	X	46	HIS
22	X	237	GLN
22	X	240	GLN
23	Y	117	GLN
23	Y	207	HIS
24	Z	100	HIS
24	Z	107	ASN
25	0	106	ASN
25	0	168	GLN
29	5	109	HIS
29	5	266	HIS
29	5	269	ASN
29	5	275	ASN
29	5	305	GLN
29	5	308	GLN
29	5	353	HIS
30	6	243	ASN
30	6	277	GLN
30	6	359	HIS
31	7	45	ASN
31	7	55	GLN
32	8	143	GLN
35	b	27	GLN
35	b	102	GLN
37	d	167	HIS
37	d	251	GLN
38	e	67	GLN
38	e	198	ASN
38	e	212	HIS
39	f	112	ASN
41	h	87	GLN
42	i	120	HIS
42	i	124	HIS
43	j	105	GLN
44	k	15	GLN

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Mol	Chain	Res	Type
48	p	184	ASN
49	q	134	ASN
49	q	139	GLN
49	q	142	ASN
50	r	112	HIS
51	s	298	GLN
51	s	315	ASN
51	s	343	GLN
51	s	382	GLN
53	u	136	HIS
54	v	63	ASN
55	w	115	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	1071/1559 (68%)	303 (28%)	17 (1%)
2	B	51/69 (73%)	15 (29%)	1 (1%)
All	All	1122/1628 (68%)	318 (28%)	18 (1%)

All (318) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1676	A
1	A	1677	C
1	A	1678	C
1	A	1679	U
1	A	1681	G
1	A	1689	C
1	A	1694	U
1	A	1700	U
1	A	1701	U
1	A	1703	C
1	A	1704	U
1	A	1707	C
1	A	1708	A
1	A	1713	A
1	A	1714	C
1	A	1715	C
1	A	1716	U
1	A	1717	U

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1719	G
1	A	1724	A
1	A	1727	A
1	A	1728	U
1	A	1731	A
1	A	1741	A
1	A	1748	G
1	A	1750	G
1	A	1751	A
1	A	1760	G
1	A	1770	G
1	A	1773	A
1	A	1775	A
1	A	1780	U
1	A	1781	A
1	A	1791	G
1	A	1794	A
1	A	1803	A
1	A	1804	A
1	A	1805	A
1	A	1806	U
1	A	1812	C
1	A	1813	C
1	A	1817	C
1	A	1820	A
1	A	1823	A
1	A	1824	U
1	A	1827	C
1	A	1828	A
1	A	1829	A
1	A	1832	A
1	A	1836	A
1	A	1844	A
1	A	1849	C
1	A	1861	U
1	A	1867	A
1	A	1869	A
1	A	1870	A
1	A	1871	A
1	A	1872	U
1	A	1874	A
1	A	1875	C

*Continued on next page...*

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	1878	U
1	A	1882	A
1	A	1883	G
1	A	1887	A
1	A	1888	G
1	A	1890	C
1	A	1892	A
1	A	1893	A
1	A	1901	C
1	A	1903	C
1	A	1914	A
1	A	1918	G
1	A	1927	G
1	A	1975	U
1	A	1985	G
1	A	1987	G
1	A	1992	C
1	A	1994	A
1	A	2000	C
1	A	2001	C
1	A	2002	G
1	A	2004	G
1	A	2015	G
1	A	2020	U
1	A	2021	U
1	A	2022	G
1	A	2023	U
1	A	2027	A
1	A	2028	G
1	A	2029	A
1	A	2030	U
1	A	2031	A
1	A	2032	G
1	A	2036	C
1	A	2037	U
1	A	2039	A
1	A	2041	U
1	A	2053	U
1	A	2055	U
1	A	2060	A
1	A	2065	A
1	A	2074	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2079	C
1	A	2083	U
1	A	2085	A
1	A	2095	U
1	A	2105	G
1	A	2113	G
1	A	2124	A
1	A	2125	C
1	A	2126	U
1	A	2132	A
1	A	2134	A
1	A	2142	A
1	A	2147	G
1	A	2154	A
1	A	2156	A
1	A	2157	U
1	A	2158	U
1	A	2159	U
1	A	2161	A
1	A	2163	A
1	A	2166	C
1	A	2168	U
1	A	2171	U
1	A	2172	A
1	A	2173	G
1	A	2174	G
1	A	2180	A
1	A	2181	A
1	A	2182	G
1	A	2183	C
1	A	2187	C
1	A	2190	C
1	A	2193	U
1	A	2194	U
1	A	2195	A
1	A	2197	G
1	A	2198	A
1	A	2200	A
1	A	2204	U
1	A	2207	A
1	A	2210	C
1	A	2216	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2237	A
1	A	2239	A
1	A	2241	A
1	A	2243	A
1	A	2244	U
1	A	2245	A
1	A	2257	C
1	A	2259	C
1	A	2261	C
1	A	2262	C
1	A	2263	C
1	A	2264	A
1	A	2281	A
1	A	2283	C
1	A	2284	C
1	A	2285	U
1	A	2290	A
1	A	2296	U
1	A	2297	A
1	A	2299	U
1	A	2300	G
1	A	2306	A
1	A	2313	A
1	A	2315	A
1	A	2321	A
1	A	2323	A
1	A	2324	U
1	A	2332	C
1	A	2335	A
1	A	2342	U
1	A	2345	G
1	A	2371	U
1	A	2374	A
1	A	2375	C
1	A	2381	A
1	A	2387	U
1	A	2389	C
1	A	2390	A
1	A	2393	C
1	A	2396	C
1	A	2401	A
1	A	2405	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2406	A
1	A	2407	U
1	A	2414	C
1	A	2415	C
1	A	2417	C
1	A	2418	A
1	A	2426	C
1	A	2427	C
1	A	2431	C
1	A	2435	G
1	A	2443	C
1	A	2444	A
1	A	2445	U
1	A	2446	A
1	A	2449	G
1	A	2457	A
1	A	2458	A
1	A	2468	A
1	A	2508	C
1	A	2511	C
1	A	2512	A
1	A	2520	C
1	A	2521	A
1	A	2522	U
1	A	2523	C
1	A	2524	A
1	A	2526	C
1	A	2527	A
1	A	2655	G
1	A	2656	U
1	A	2659	C
1	A	2660	U
1	A	2683	C
1	A	2684	C
1	A	2686	G
1	A	2698	G
1	A	2699	C
1	A	2706	A
1	A	2707	A
1	A	2708	C
1	A	2709	A
1	A	2725	A

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	2732	G
1	A	2734	A
1	A	2739	U
1	A	2740	A
1	A	2744	U
1	A	2750	U
1	A	2752	C
1	A	2803	A
1	A	2804	A
1	A	2810	G
1	A	2813	U
1	A	2814	G
1	A	2815	G
1	A	2831	G
1	A	2832	A
1	A	2833	A
1	A	2844	G
1	A	2846	G
1	A	2847	C
1	A	2852	C
1	A	2854	U
1	A	2859	A
1	A	2861	A
1	A	2864	U
1	A	2865	C
1	A	2870	G
1	A	2871	U
1	A	2879	A
1	A	2893	A
1	A	2895	U
1	A	2896	G
1	A	2901	A
1	A	2906	C
1	A	2910	A
1	A	2912	C
1	A	2913	A
1	A	2914	A
1	A	2915	C
1	A	2917	G
1	A	2922	A
1	A	2926	A
1	A	2928	C

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	3102	U
1	A	3108	U
1	A	3109	U
1	A	3114	U
1	A	3123	G
1	A	3124	U
1	A	3128	A
1	A	3129	A
1	A	3131	G
1	A	3134	C
1	A	3137	G
1	A	3138	A
1	A	3139	G
1	A	3141	A
1	A	3150	U
1	A	3155	C
1	A	3157	C
1	A	3158	A
1	A	3160	A
1	A	3162	C
1	A	3168	C
1	A	3177	A
1	A	3180	A
1	A	3183	U
1	A	3184	C
1	A	3185	A
1	A	3189	C
1	A	3190	A
1	A	3202	U
1	A	3204	C
1	A	3207	A
1	A	3217	A
1	A	3218	A
2	B	1607	U
2	B	1608	G
2	B	1609	U
2	B	1611	G
2	B	1614	U
2	B	1615	A
2	B	1625	A
2	B	1631	C
2	B	1632	U

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Mol	Chain	Res	Type
2	B	1640	A
2	B	1641	G
2	B	1644	G
2	B	1645	A
2	B	1649	C
2	B	1651	A

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1703	C
1	A	1713	A
1	A	1772	A
1	A	1780	U
1	A	1805	A
1	A	1823	A
1	A	2030	U
1	A	2125	C
1	A	2165	C
1	A	2172	A
1	A	2186	C
1	A	2243	A
1	A	2444	A
1	A	2457	A
1	A	2507	A
1	A	2905	A
1	A	3201	A
2	B	1607	U

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

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

#### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

#### 5.6 Ligand geometry [i](#)

Of 52 ligands modelled in this entry, 51 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
58	PNS	v	101	-	14,20,21	2.18	4 (28%)	18,26,29	1.12	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
58	PNS	v	101	-	-	7/24/26/27	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	v	101	PNS	C34-N36	5.16	1.45	1.33
58	v	101	PNS	C39-N41	5.10	1.45	1.33
58	v	101	PNS	O40-C39	-2.23	1.18	1.23
58	v	101	PNS	O35-C34	-2.21	1.19	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	v	101	PNS	C31-C29-C32	2.63	113.25	108.77

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
58	v	101	PNS	C28-C29-C32-O33
58	v	101	PNS	C28-C29-C32-C34
58	v	101	PNS	C31-C29-C32-O33
58	v	101	PNS	N41-C42-C43-S44
58	v	101	PNS	C30-C29-C32-O33
58	v	101	PNS	C31-C29-C32-C34

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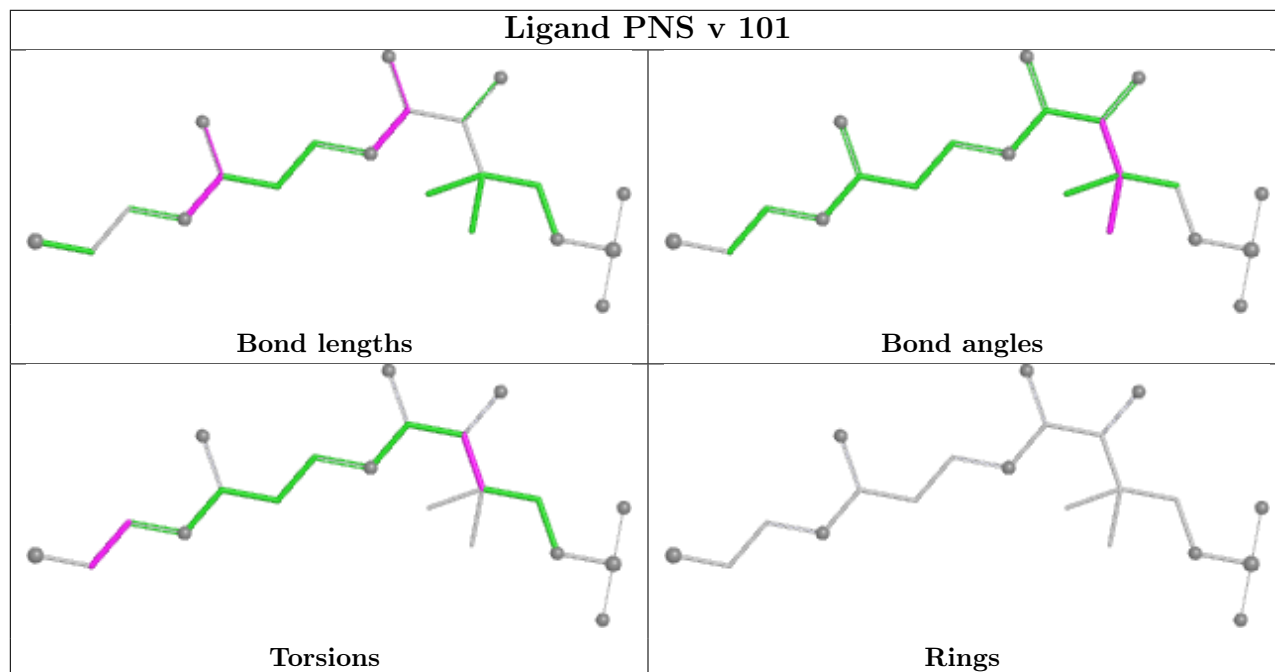
Mol	Chain	Res	Type	Atoms
58	v	101	PNS	C30-C29-C32-C34

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
58	v	101	PNS	1	0

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



## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	Z	1
42	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	Z	151:LEU	C	152:LYS	N	1.17
1	i	68:LYS	C	69:HIS	N	1.16

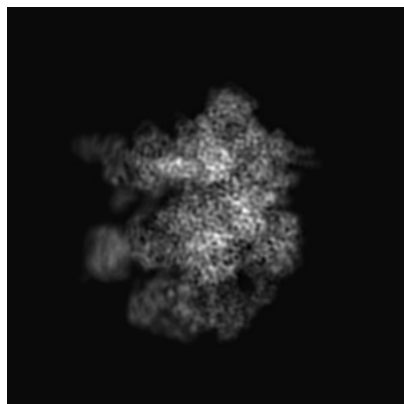
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3843. These allow visual inspection of the internal detail of the map and identification of artifacts.

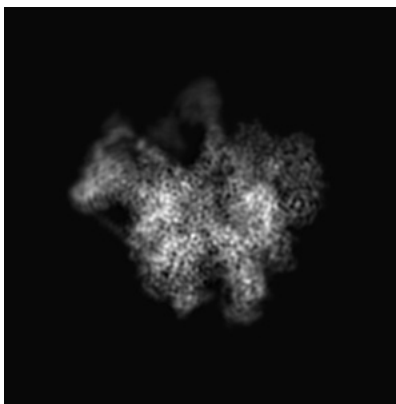
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

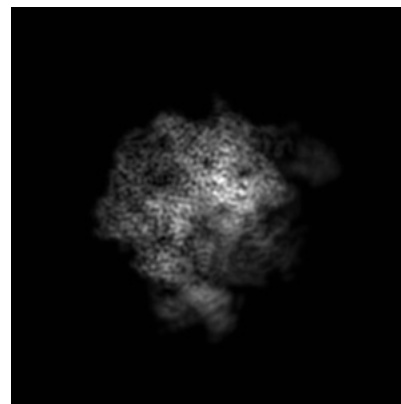
#### 6.1.1 Primary map



X

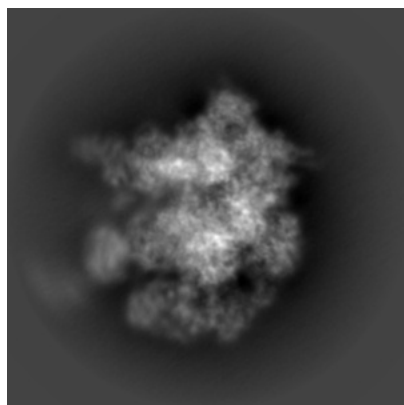


Y

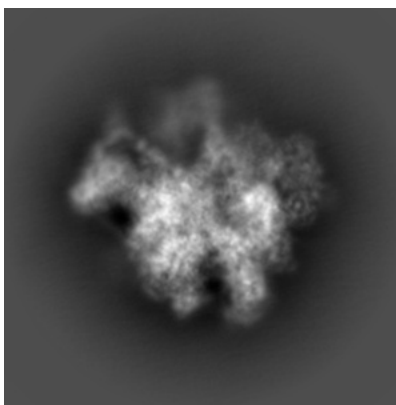


Z

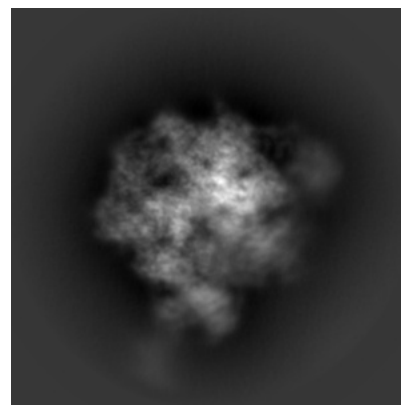
#### 6.1.2 Raw map



X



Y

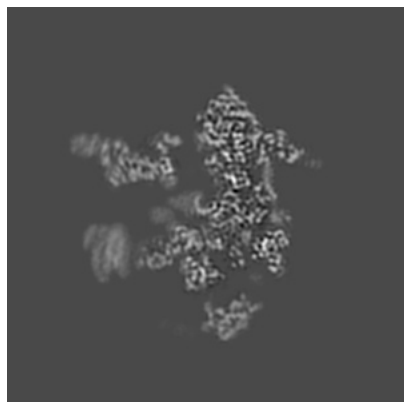


Z

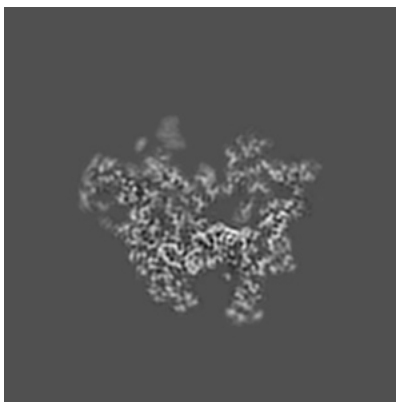
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

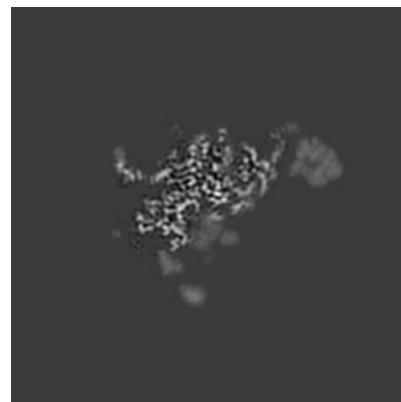
### 6.2.1 Primary map



X Index: 176

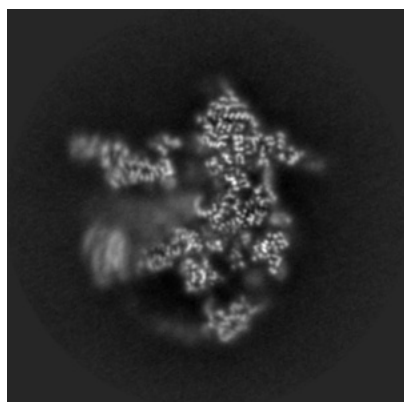


Y Index: 176

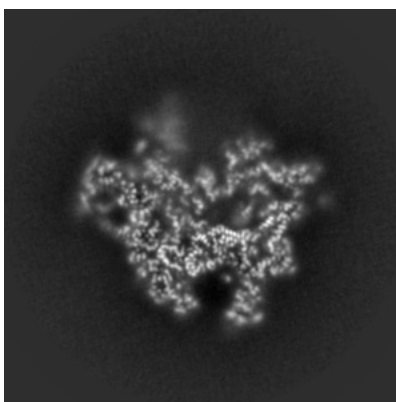


Z Index: 176

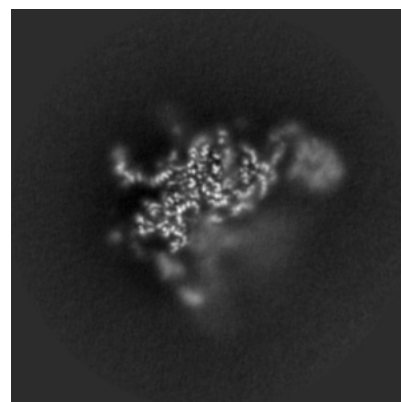
### 6.2.2 Raw map



X Index: 176



Y Index: 176

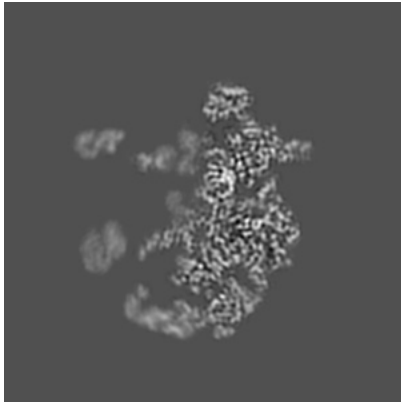


Z Index: 176

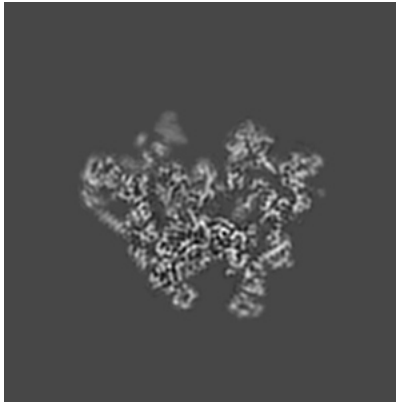
The images above show central slices of the map in three orthogonal directions.

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

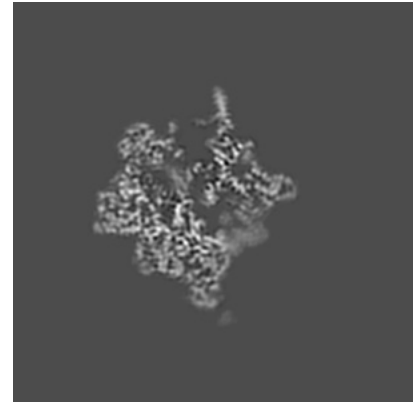
### 6.3.1 Primary map



X Index: 188

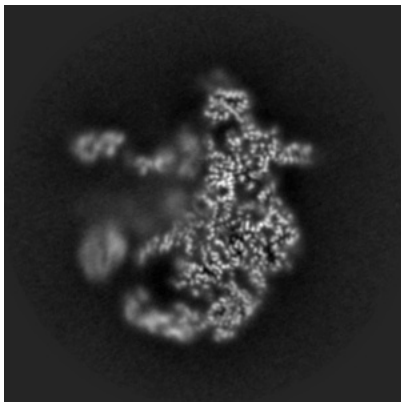


Y Index: 179

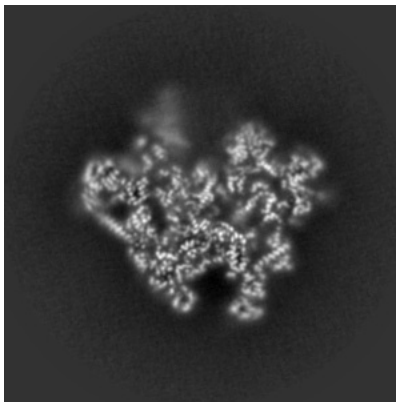


Z Index: 214

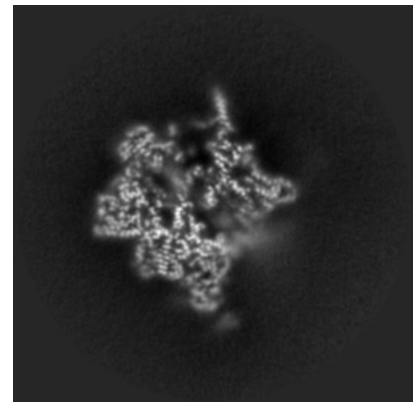
### 6.3.2 Raw map



X Index: 187



Y Index: 180

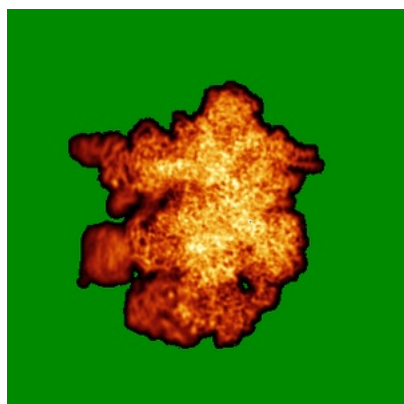


Z Index: 214

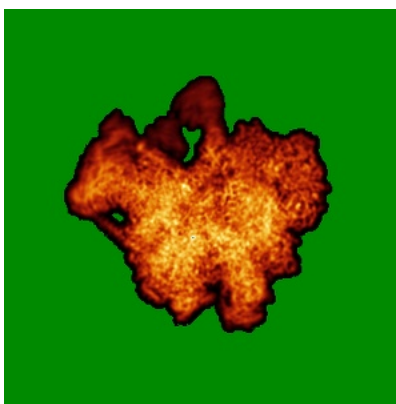
The images above show the largest variance slices of the map in three orthogonal directions.

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

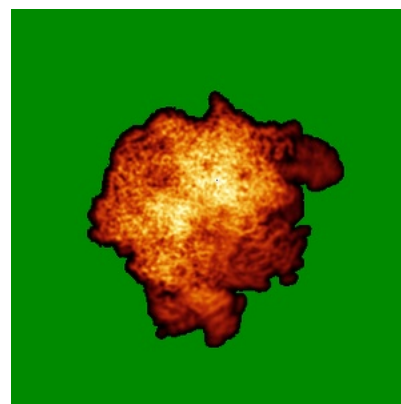
### 6.4.1 Primary map



X

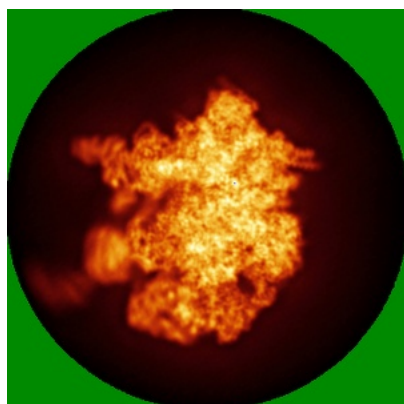


Y

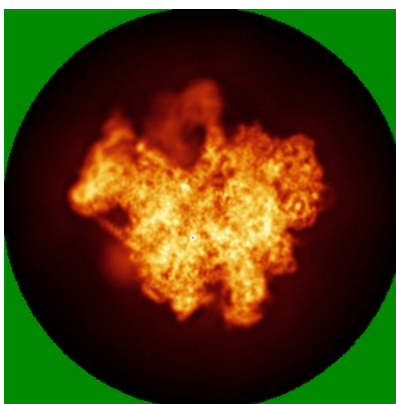


Z

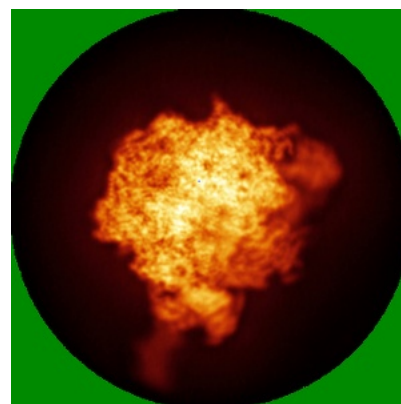
### 6.4.2 Raw map



X



Y

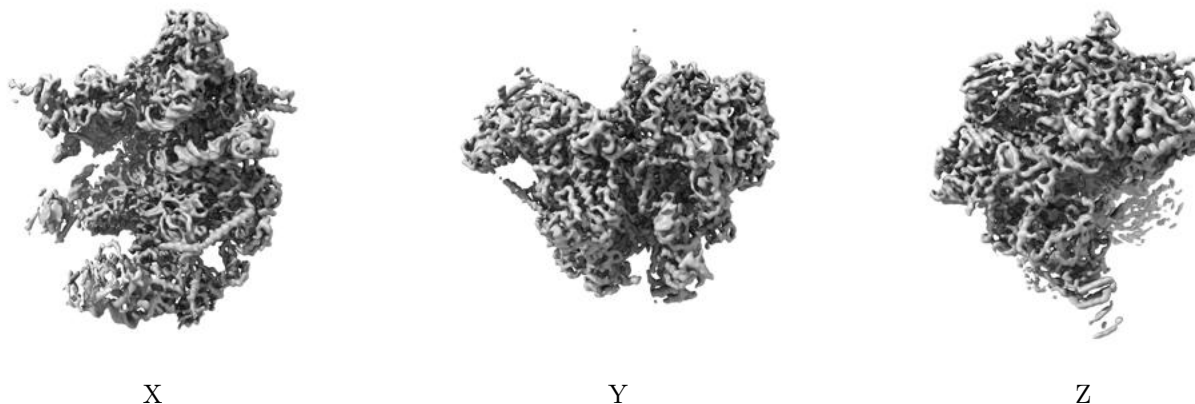


Z

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

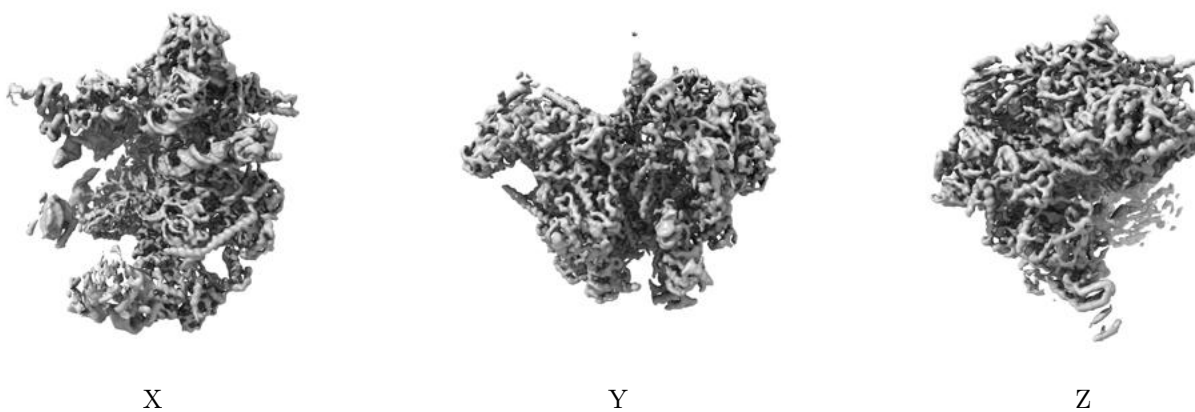
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.075. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



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

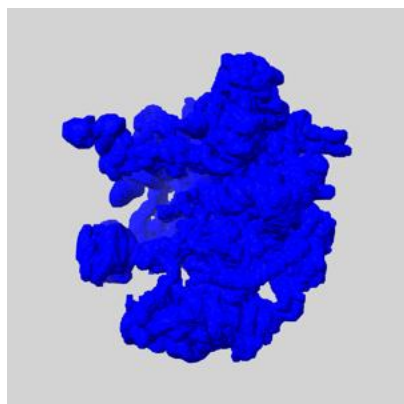
## 6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

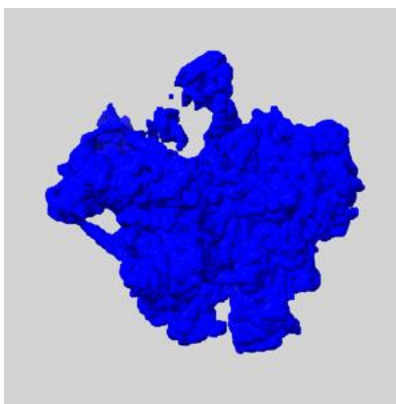
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

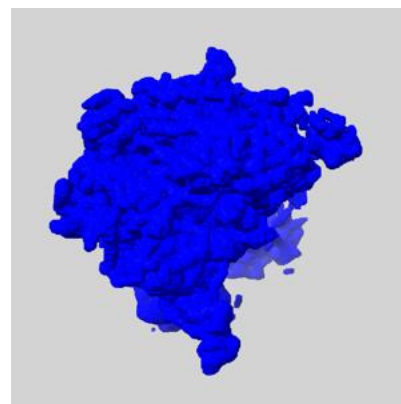
### 6.6.1 emd\_3843\_msk\_1.map [i](#)



X



Y

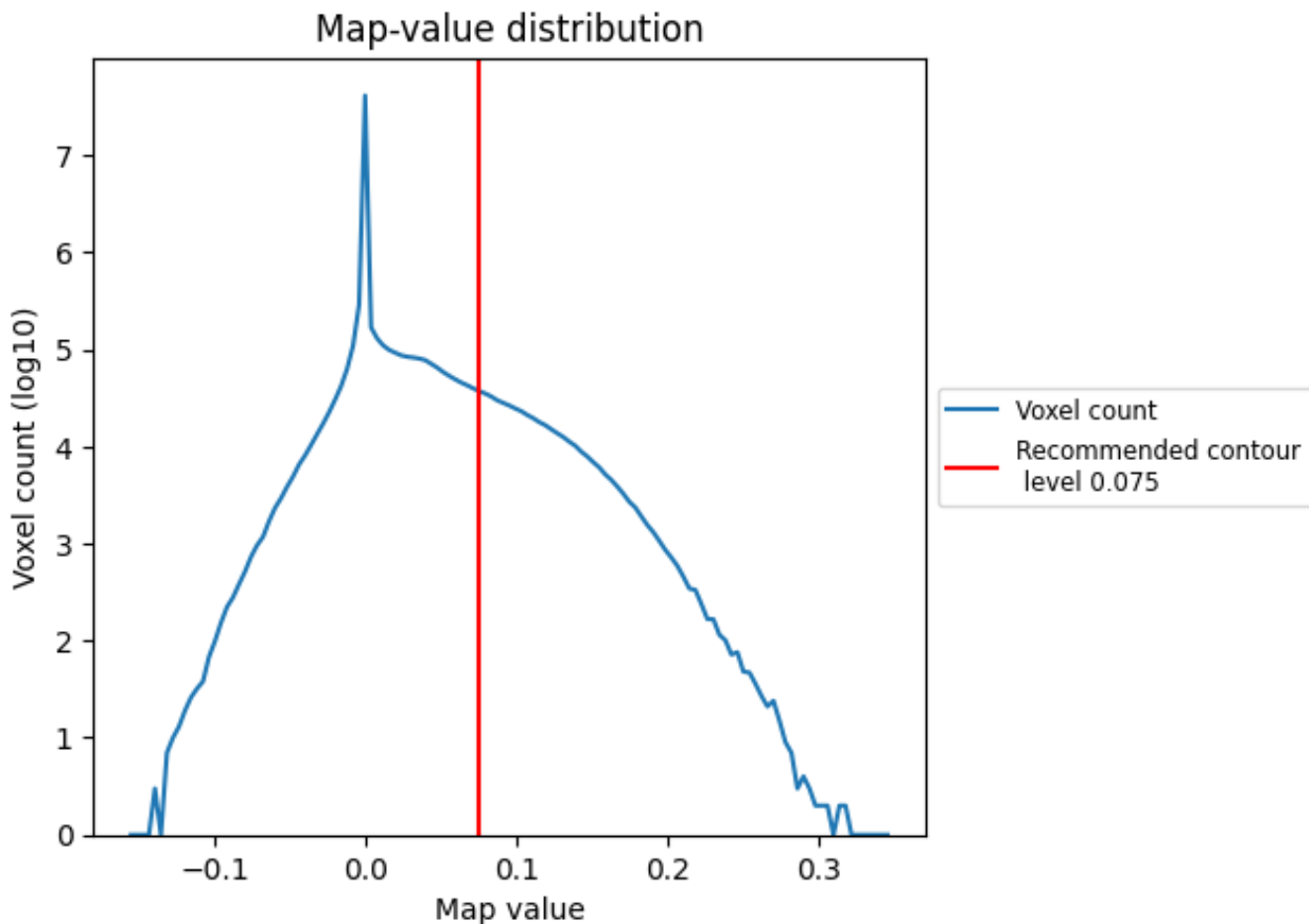


Z

## 7 Map analysis [i](#)

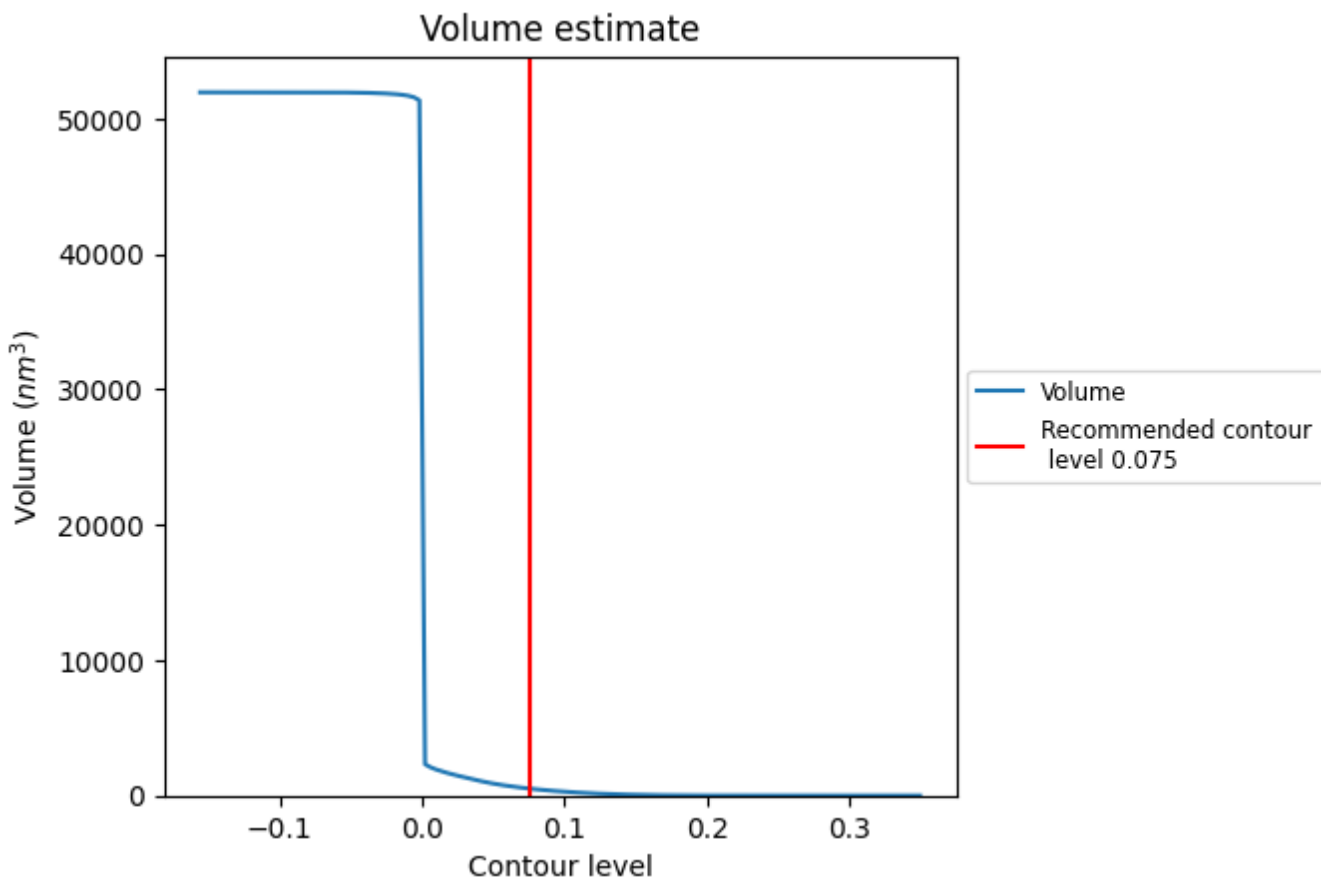
This section contains the results of statistical analysis of the map.

### 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.

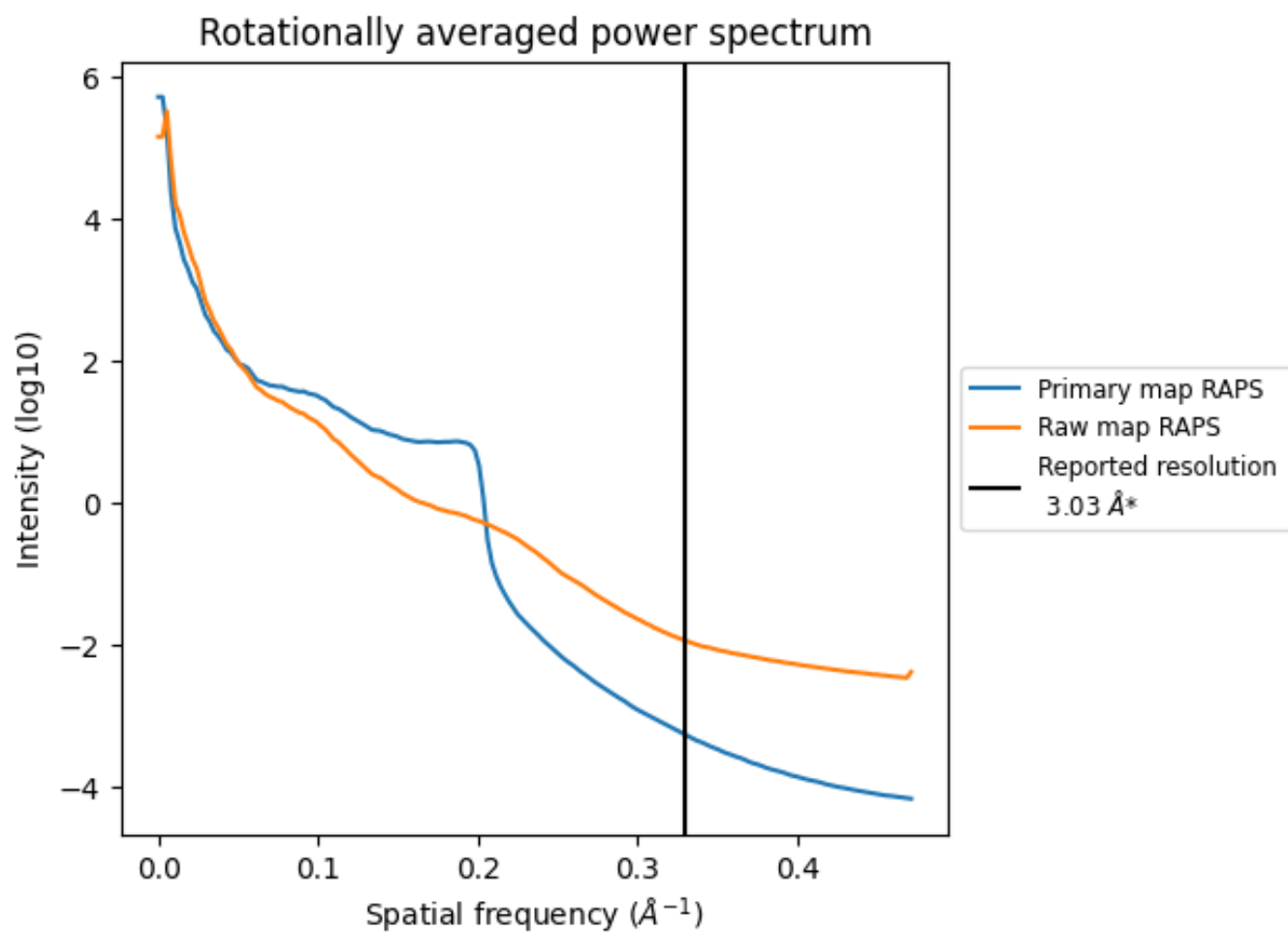
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 519 nm<sup>3</sup>; this corresponds to an approximate mass of 469 kDa.

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

### 7.3 Rotationally averaged power spectrum i

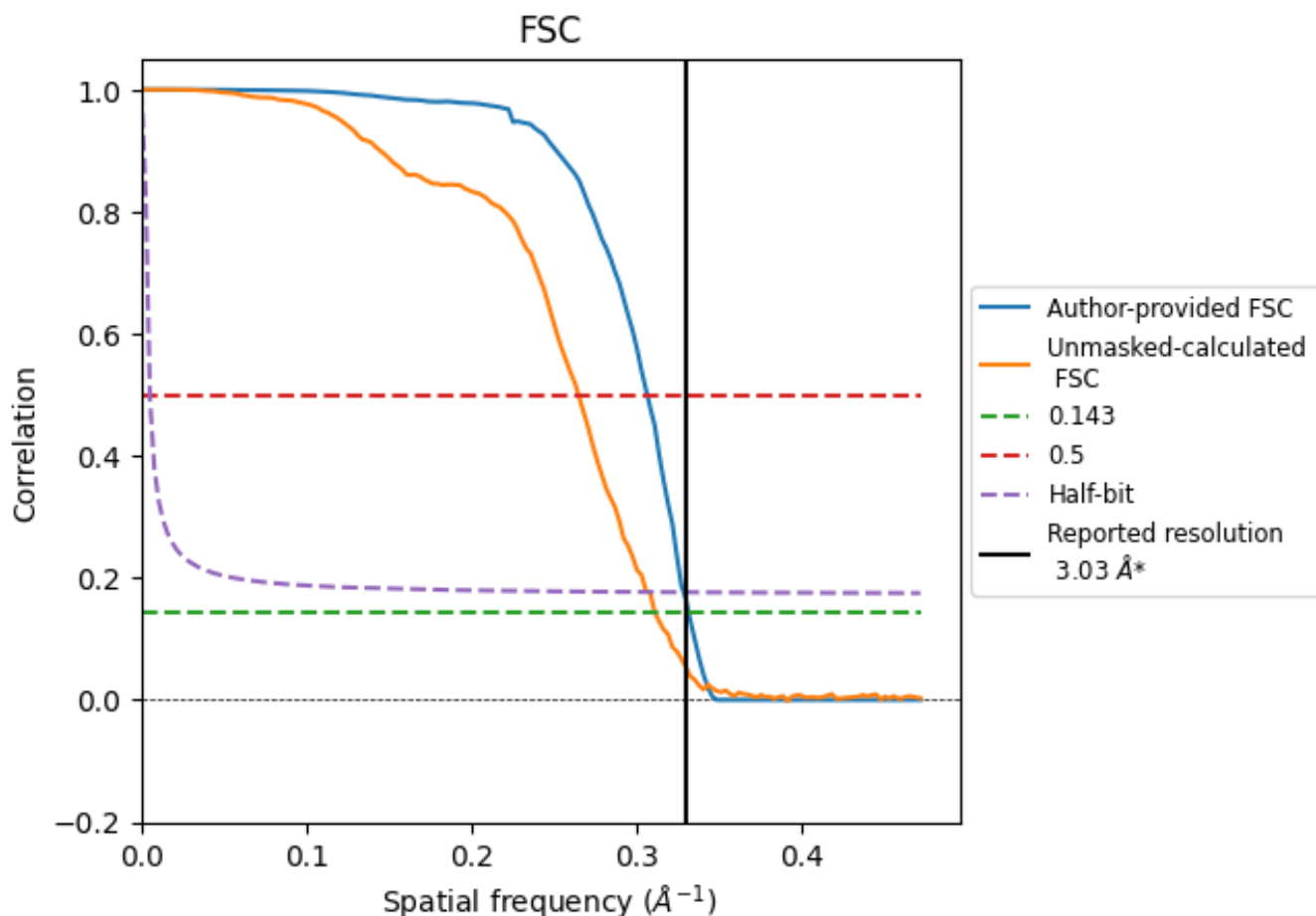


\*Reported resolution corresponds to spatial frequency of 0.330 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.330 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

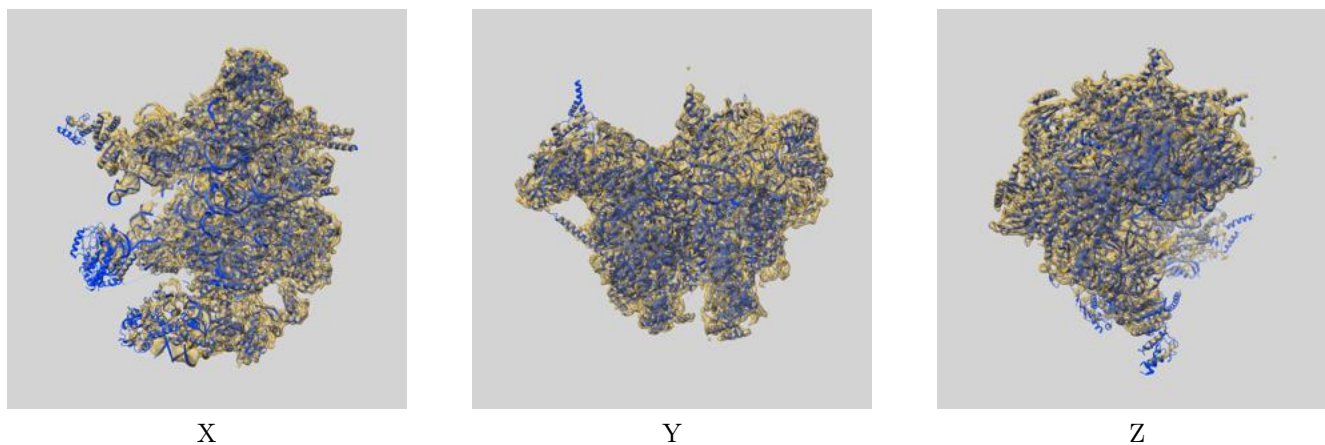
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.03	-	-
Author-provided FSC curve	3.02	3.26	3.05
Unmasked-calculated*	3.22	3.78	3.26

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

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

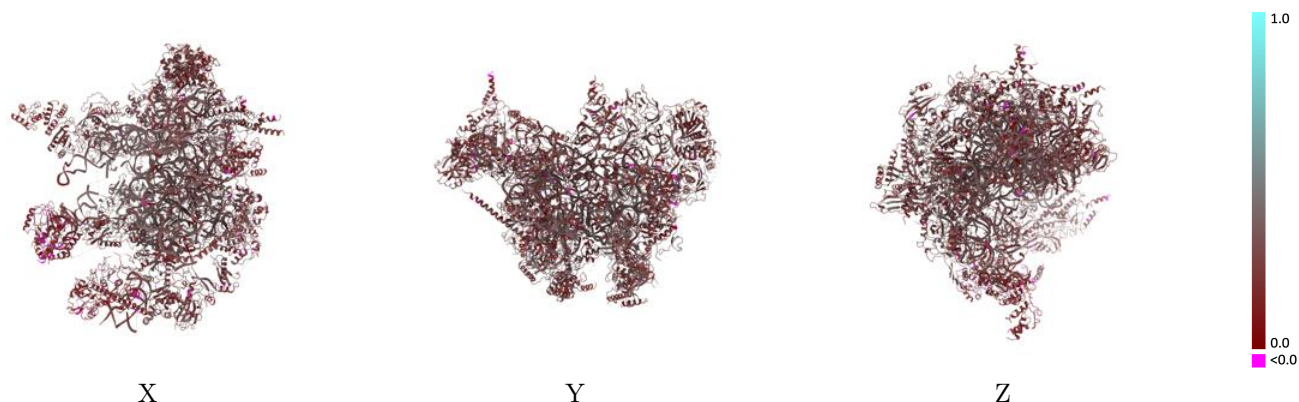
This section contains information regarding the fit between EMDB map EMD-3843 and PDB model 5OOM. Per-residue inclusion information can be found in section 3 on page 16.

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



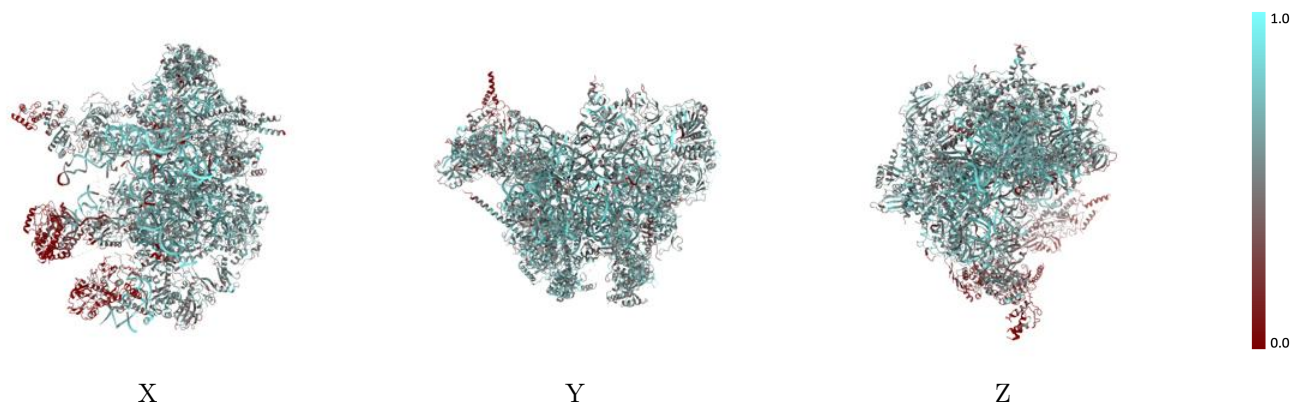
The images above show the 3D surface view of the map at the recommended contour level 0.075 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



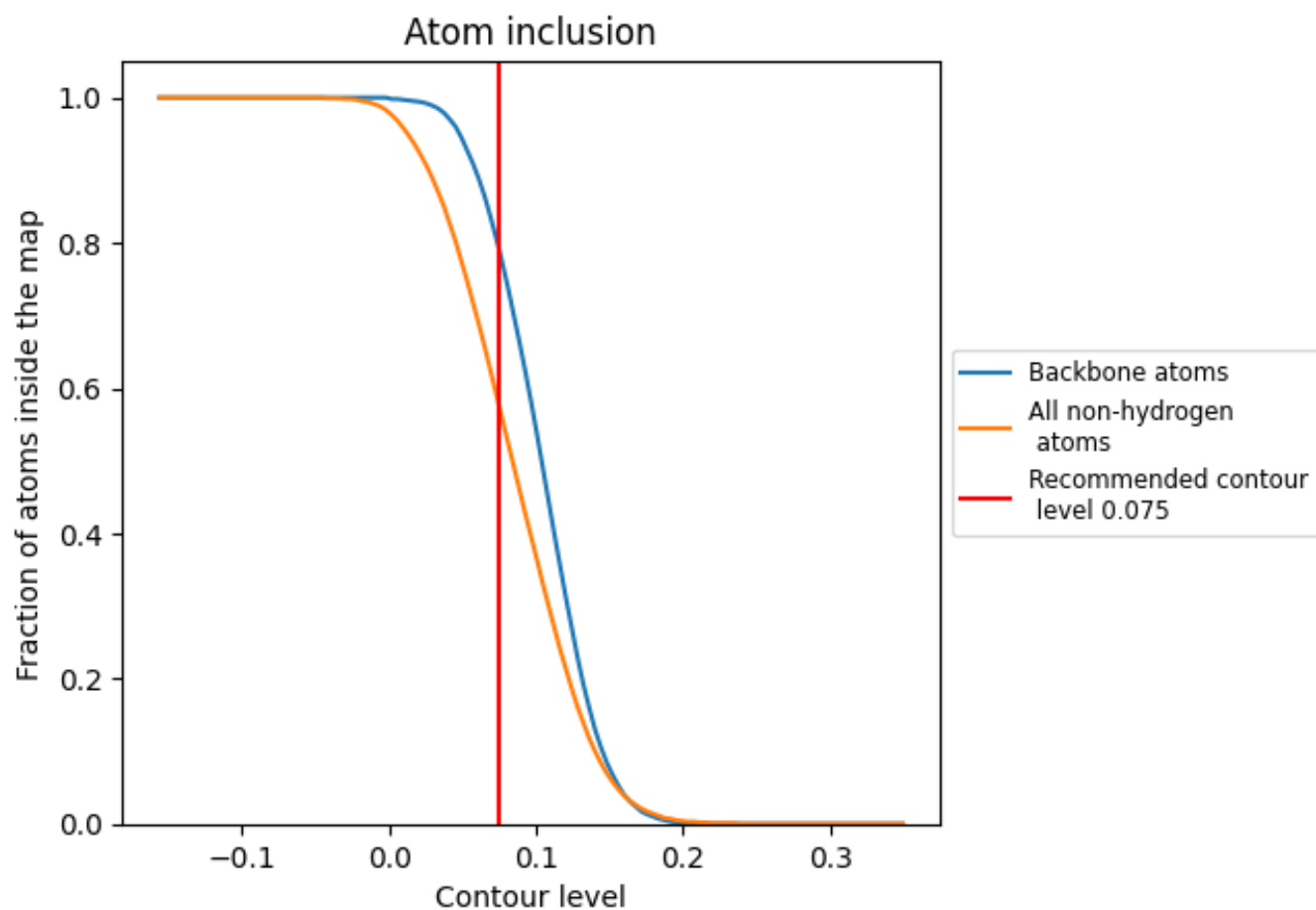
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.075).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 58% 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 (0.075) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5760	 0.2900
0	 0.5830	 0.2950
1	 0.5190	 0.2800
2	 0.5730	 0.2750
3	 0.5400	 0.2880
5	 0.5640	 0.2750
6	 0.5640	 0.2930
7	 0.5810	 0.2940
8	 0.2810	 0.2180
9	 0.5800	 0.2950
A	 0.7380	 0.3310
B	 0.7360	 0.2960
D	 0.4550	 0.2710
E	 0.5670	 0.3030
F	 0.5890	 0.2970
H	 0.5050	 0.2710
I	 0.1400	 0.1770
J	 0.0000	 0.1210
K	 0.6000	 0.2990
L	 0.4680	 0.2880
M	 0.5740	 0.2790
N	 0.4270	 0.2890
O	 0.6000	 0.2980
P	 0.5560	 0.2740
Q	 0.5530	 0.2920
R	 0.5650	 0.2810
S	 0.6020	 0.3110
T	 0.5800	 0.2970
U	 0.5890	 0.2890
V	 0.5720	 0.3020
W	 0.5130	 0.2790
X	 0.5500	 0.2680
Y	 0.5890	 0.2640
Z	 0.5750	 0.3070
a	 0.5960	 0.3120



*Continued on next page...*

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Chain	Atom inclusion	Q-score
b	 0.6260	 0.3150
c	 0.6150	 0.2960
d	 0.5280	 0.3020
e	 0.1520	 0.1760
f	 0.2930	 0.2410
g	 0.6430	 0.3100
h	 0.5750	 0.2920
i	 0.5600	 0.2750
j	 0.5960	 0.2910
k	 0.1660	 0.2010
l	 0.2430	 0.1580
m	 0.1870	 0.2490
o	 0.6320	 0.2870
p	 0.5200	 0.2680
q	 0.5550	 0.2750
r	 0.5650	 0.3100
s	 0.5970	 0.2770
t	 0.0000	 0.1400
u	 0.5090	 0.2500
v	 0.4010	 0.1980
w	 0.0820	 0.1790