



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 03:59 PM UTC

PDB ID : 7OI7 / pdb_00007oi7
EMDB ID : EMD-12920
Title : Cryo-EM structure of late human 39S mitoribosome assembly intermediates, state 2
Authors : Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on : 2021-05-11
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

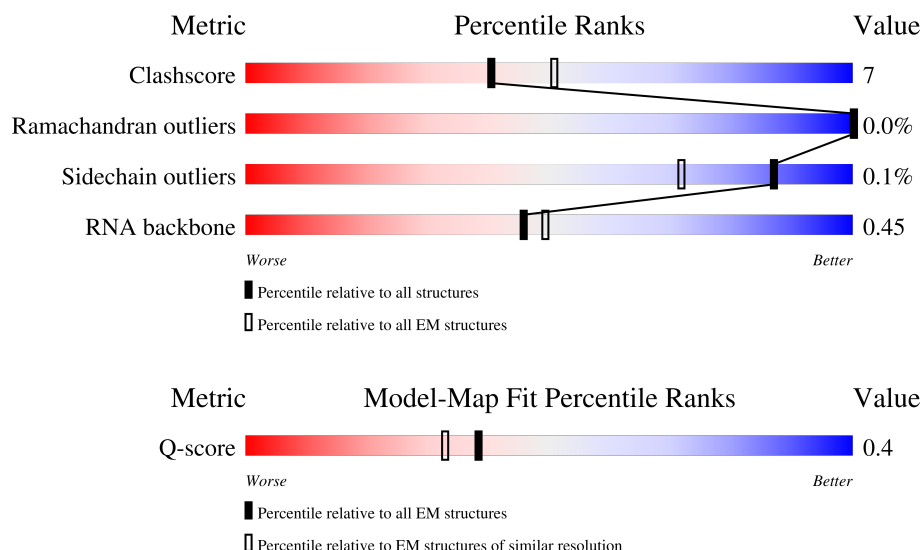
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 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.



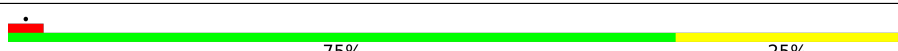
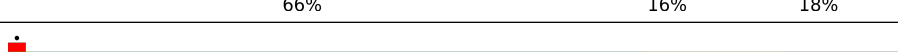
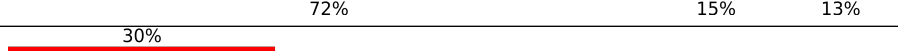
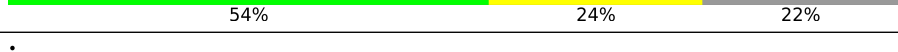
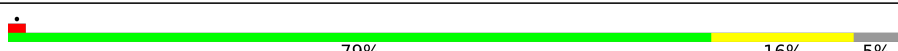
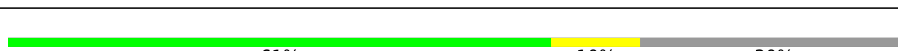
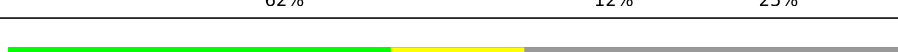
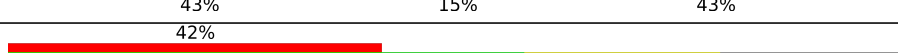
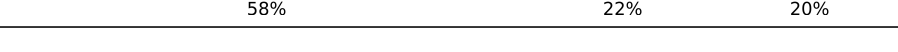
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

Mol	Chain	Length	Quality of chain
1	D	305	
2	E	348	
3	F	311	

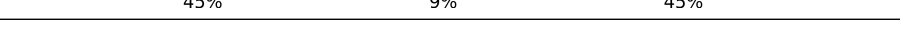
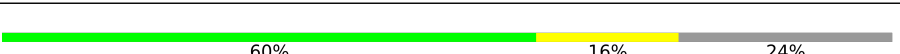
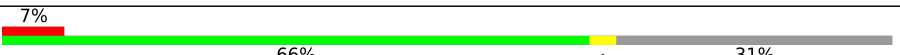
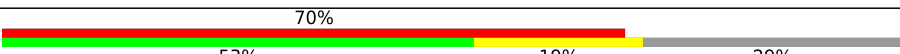
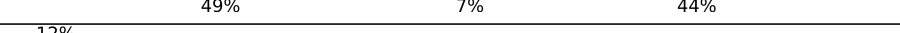
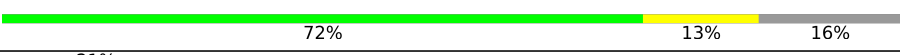
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Mol	Chain	Length	Quality of chain
4	H	267	
5	I	261	
6	J	192	
7	K	178	
8	L	145	
9	M	296	
10	N	251	
11	O	175	
12	P	180	
13	Q	292	
14	R	149	
15	S	205	
16	T	206	
17	U	153	
18	V	216	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	0	188	
24	1	65	
25	2	92	
26	3	188	
27	5	423	
28	6	380	

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Mol	Chain	Length	Quality of chain
29	7	338	
30	8	206	
31	9	137	
32	a	142	
33	b	215	
34	c	332	
35	d	306	
36	e	279	
37	f	212	
38	g	166	
39	h	158	
40	i	128	
41	j	123	
42	k	112	
43	l	138	
44	m	128	
45	o	102	
46	p	206	
47	q	222	
48	r	196	
49	s	439	
50	u	234	
51	v	70	
52	w	156	
53	A	1559	

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Mol	Chain	Length	Quality of chain
54	B	69	46% 33% 42% 6% 19%

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 89747 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called 39S ribosomal protein L2, mitochondrial.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 27 is a protein called 39S ribosomal protein L37, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	5	387	Total	C	N	O	S	0	0
			3156	2039	548	558	11		

- Molecule 28 is a protein called 39S ribosomal protein L38, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	6	324	Total	C	N	O	S	0	0
			2640	1694	470	468	8		

- Molecule 29 is a protein called 39S ribosomal protein L39, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	7	287	Total	C	N	O	S	0	0
			2334	1495	397	425	17		

- Molecule 30 is a protein called 39S ribosomal protein L40, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	8	99	Total	C	N	O	S	0	0
			836	535	144	155	2		

- Molecule 31 is a protein called 39S ribosomal protein L41, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	9	117	Total	C	N	O	S	0	0
			947	614	163	168	2		

- Molecule 32 is a protein called 39S ribosomal protein L42, mitochondrial.

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

- Molecule 33 is a protein called 39S ribosomal protein L43, mitochondrial.

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

- Molecule 34 is a protein called 39S ribosomal protein L44, mitochondrial.

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

- Molecule 35 is a protein called 39S ribosomal protein L45, mitochondrial.

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

- Molecule 36 is a protein called 39S ribosomal protein L46, mitochondrial.

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

- Molecule 37 is a protein called 39S ribosomal protein L48, mitochondrial.

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

- Molecule 38 is a protein called 39S ribosomal protein L49, mitochondrial.

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

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

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

- Molecule 40 is a protein called 39S ribosomal protein L51, mitochondrial.

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

- Molecule 41 is a protein called 39S ribosomal protein L52, mitochondrial.

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

- Molecule 42 is a protein called 39S ribosomal protein L53, mitochondrial.

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

- Molecule 43 is a protein called 39S ribosomal protein L54, mitochondrial.

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

- Molecule 44 is a protein called 39S ribosomal protein L55, mitochondrial.

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

- Molecule 45 is a protein called Ribosomal protein 63, mitochondrial.

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

- Molecule 46 is a protein called Peptidyl-tRNA hydrolase ICT1, mitochondrial.

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

- Molecule 47 is a protein called Growth arrest and DNA damage-inducible proteins-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
47	q	124	Total	C	N	O	S	0	0
			1039	650	200	184	5		

- Molecule 48 is a protein called 39S ribosomal protein S18a, mitochondrial.

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

- Molecule 49 is a protein called 39S ribosomal protein S30, mitochondrial.

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

- Molecule 50 is a protein called Mitochondrial assembly of ribosomal large subunit protein 1.

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

- Molecule 51 is a protein called MIEF1 upstream open reading frame protein.

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

- Molecule 52 is a protein called Acyl carrier protein, mitochondrial.

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

- Molecule 53 is a RNA chain called 16S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
53	A	1054	Total	C	N	O	P	0	0
			22369	10046	4050	7219	1054		

There is a discrepancy between the modelled and reference sequences:

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

- Molecule 54 is a RNA chain called mitochondrial Val tRNA.

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

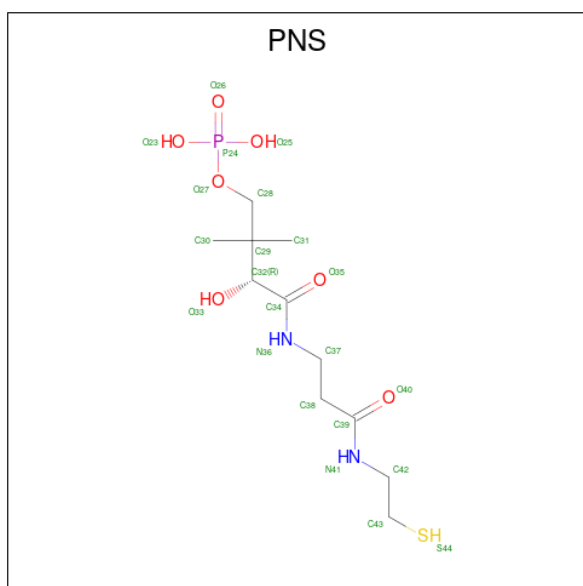
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

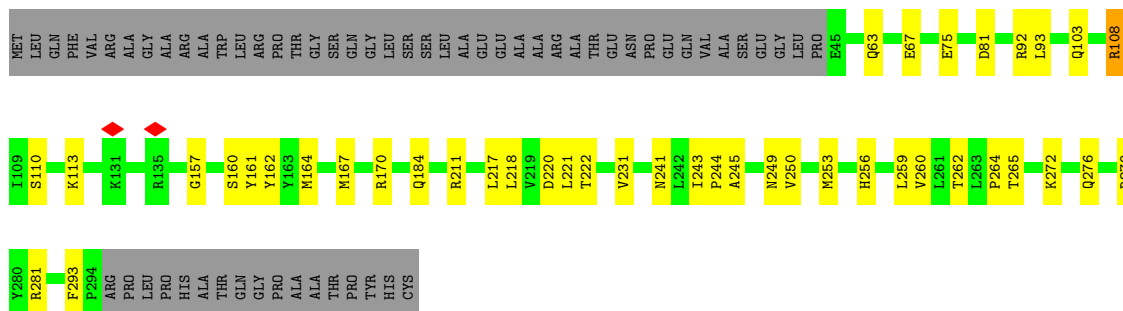
- Molecule 56 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
56	W	1	Total Mg 1 1	0
56	g	1	Total Mg 1 1	0
56	A	47	Total Mg 47 47	0

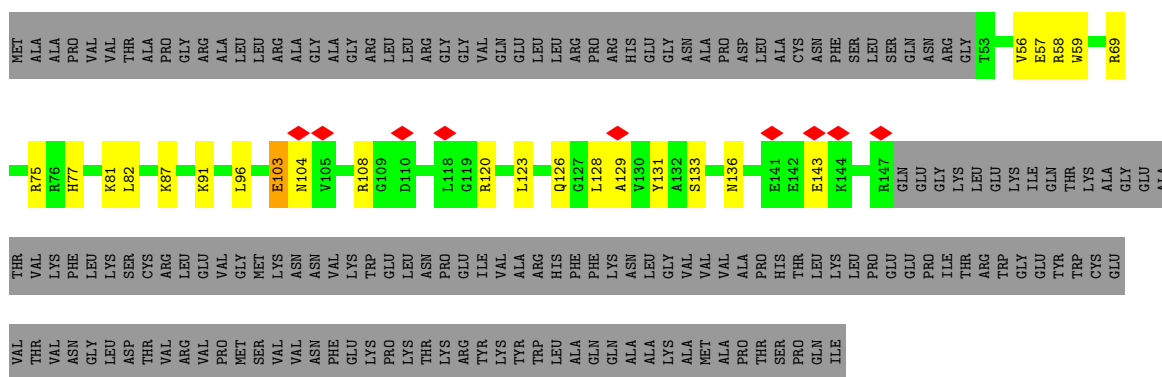
- Molecule 57 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: $C_{11}H_{23}N_2O_7PS$).



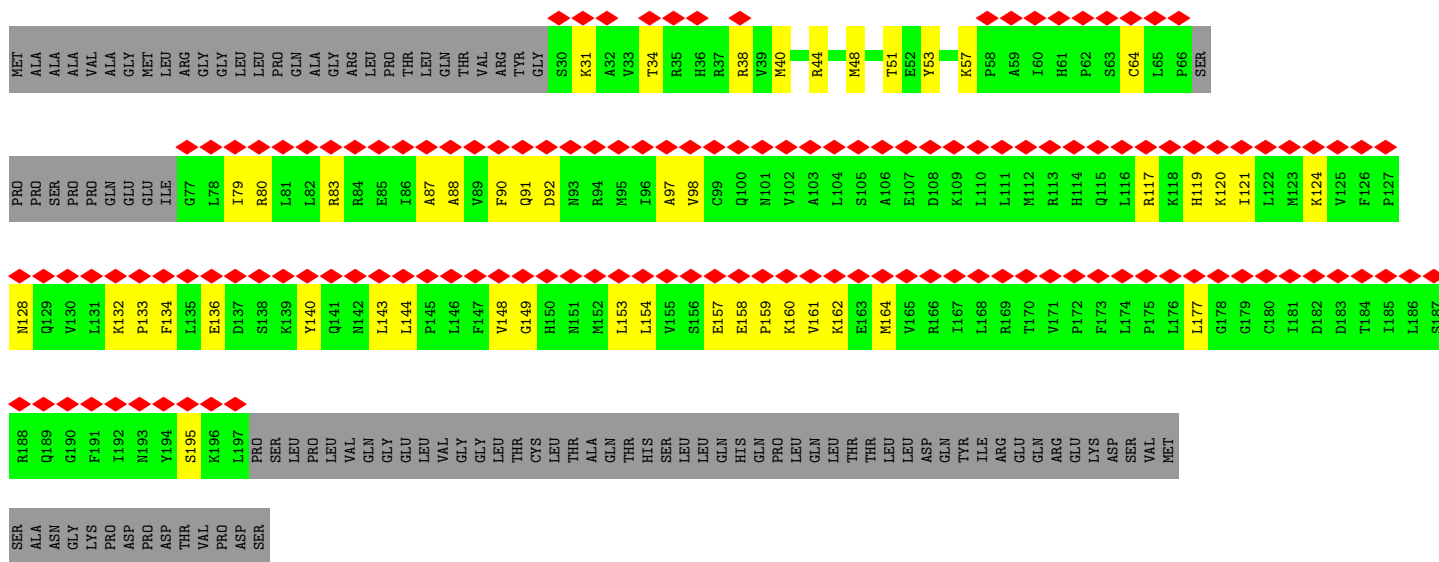
Mol	Chain	Residues	Atoms						AltConf
57	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	



- Molecule 4: 39S ribosomal protein L9, mitochondrial

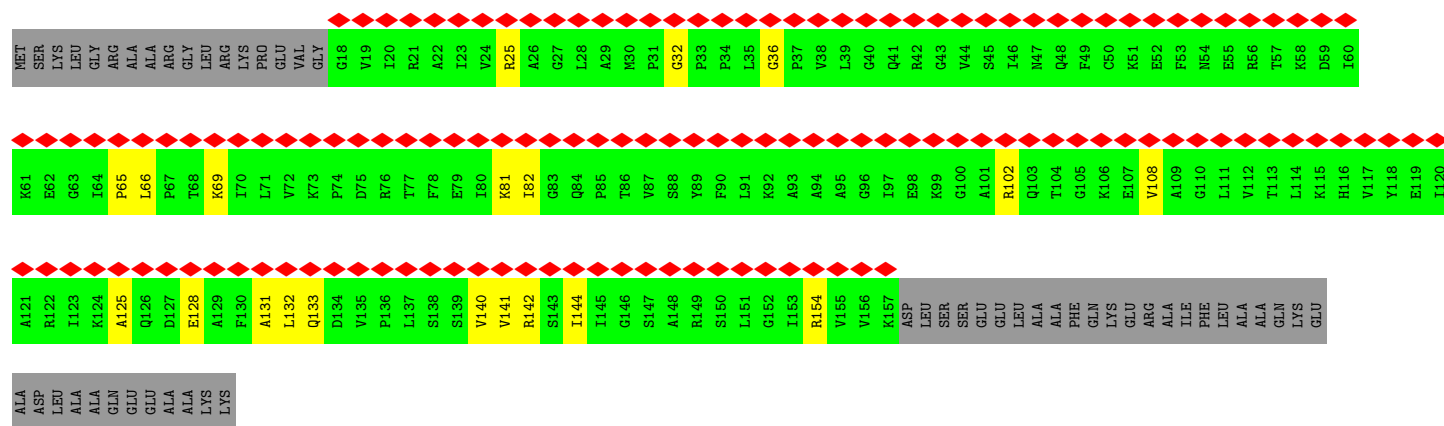


- Molecule 5: 39S ribosomal protein L10, mitochondrial



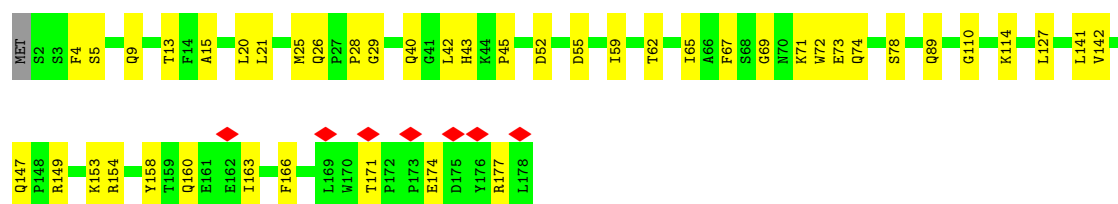
- Molecule 6: 39S ribosomal protein L11, mitochondrial





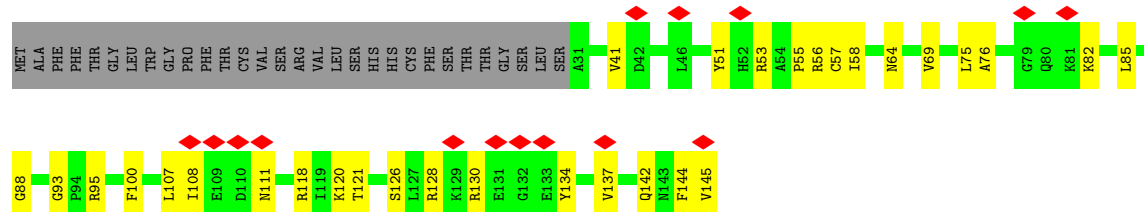
- Molecule 7: 39S ribosomal protein L13, mitochondrial

Chain K: 75% 25%



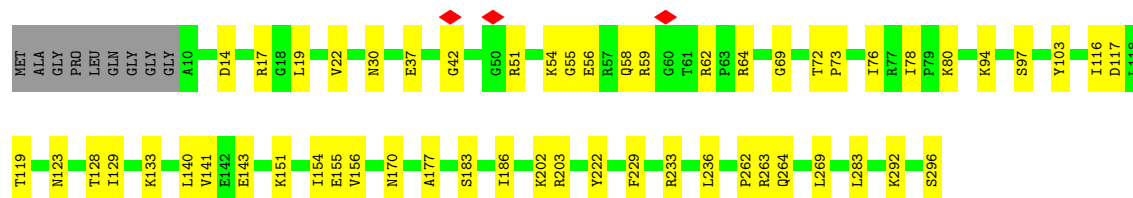
- Molecule 8: 39S ribosomal protein L14, mitochondrial

Chain L: 10% 58% 21% 21%



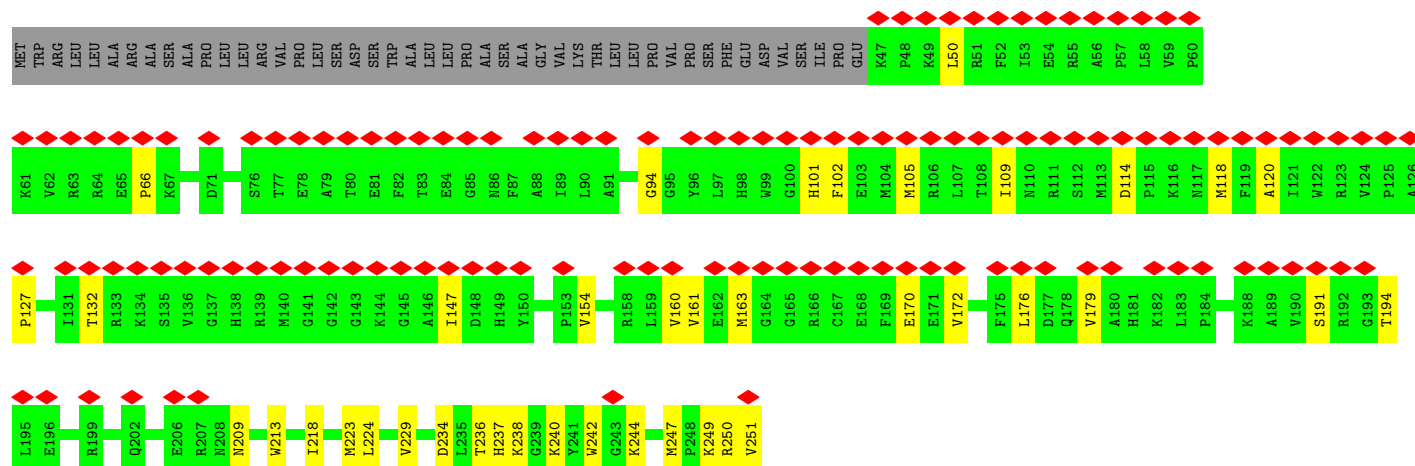
- Molecule 9: 39S ribosomal protein L15, mitochondrial

Chain M: 78% 19%

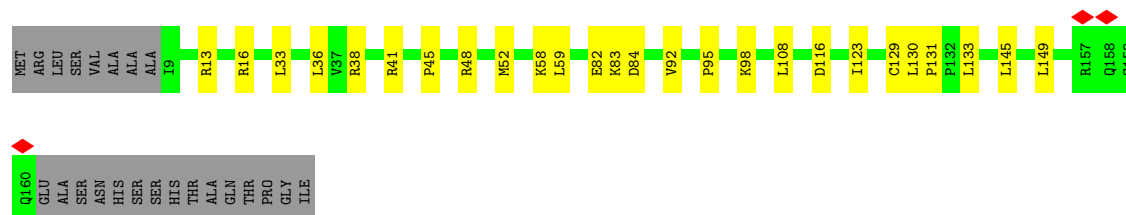


- Molecule 10: 39S ribosomal protein L16, mitochondrial

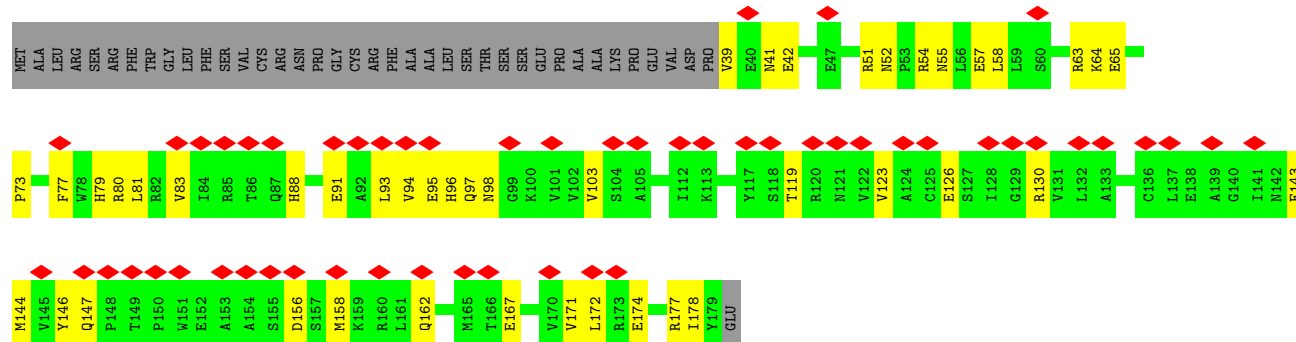
Chain N: 51% 66% 16% 18%



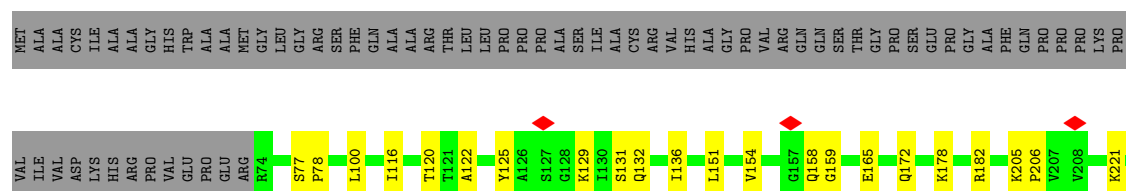
- Molecule 11: 39S ribosomal protein L17, mitochondrial



- Molecule 12: 39S ribosomal protein L18, mitochondrial

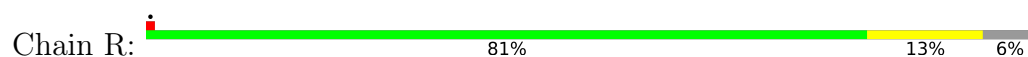


- Molecule 13: 39S ribosomal protein L19, mitochondrial

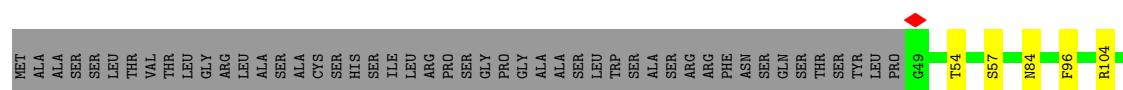




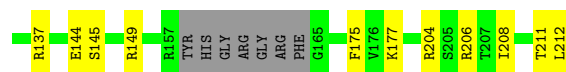
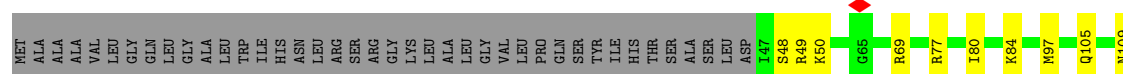
- Molecule 14: 39S ribosomal protein L20, mitochondrial



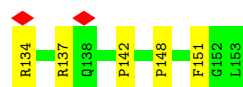
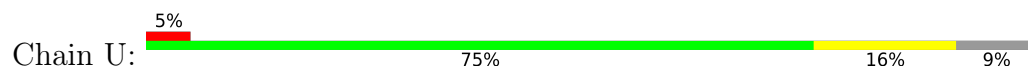
- Molecule 15: 39S ribosomal protein L21, mitochondrial



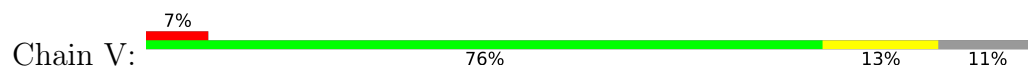
- Molecule 16: 39S ribosomal protein L22, mitochondrial



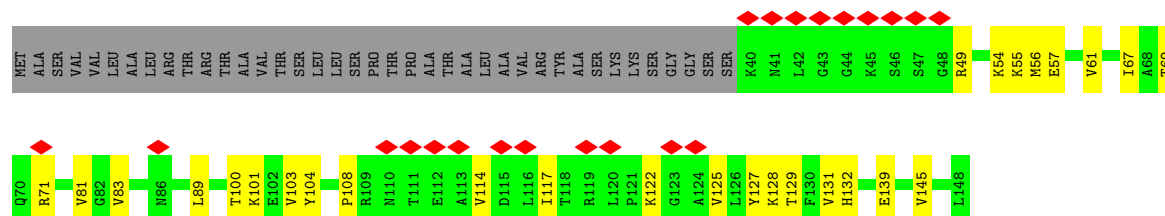
- Molecule 17: 39S ribosomal protein L23, mitochondrial



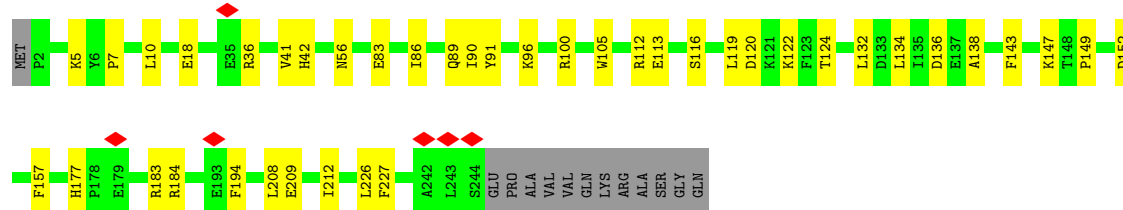
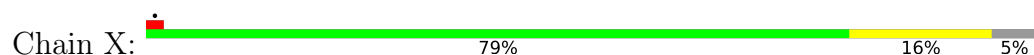
- Molecule 18: 39S ribosomal protein L24, mitochondrial



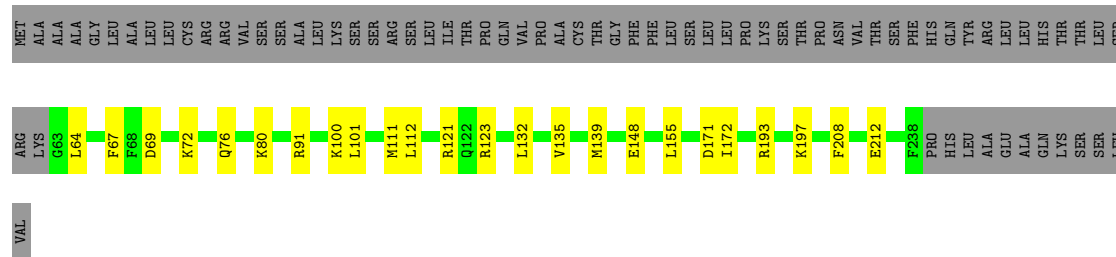
- Molecule 19: 39S ribosomal protein L27, mitochondrial



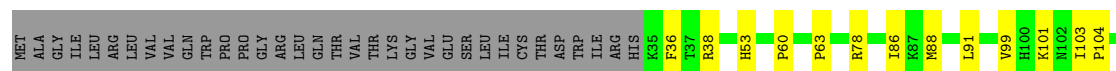
- Molecule 20: 39S ribosomal protein L28, mitochondrial

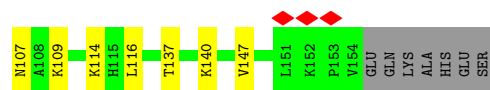


- Molecule 21: 39S ribosomal protein L47, mitochondrial



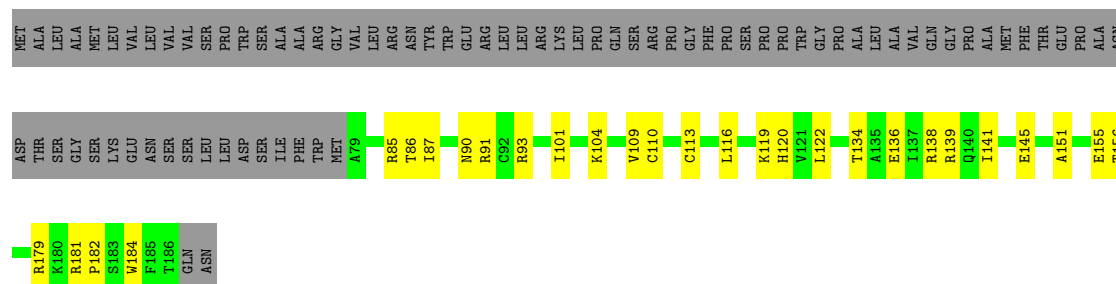
- Molecule 22: 39S ribosomal protein L30, mitochondrial





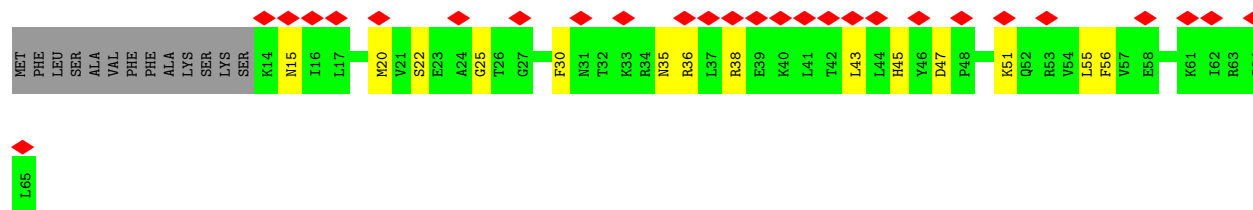
- Molecule 23: 39S ribosomal protein L32, mitochondrial

Chain 0: 43% 15% 43%



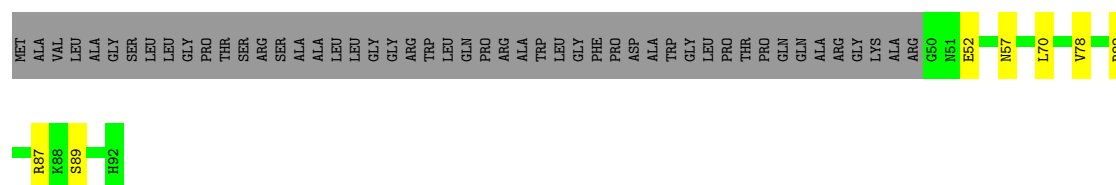
- Molecule 24: 39S ribosomal protein L33, mitochondrial

Chain 1: 42% 58% 22% 20%



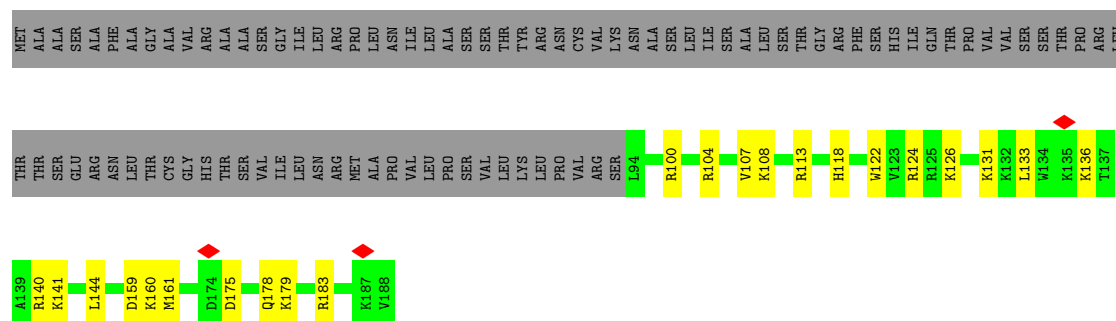
- Molecule 25: 39S ribosomal protein L34, mitochondrial

Chain 2: 39% 8% 53%

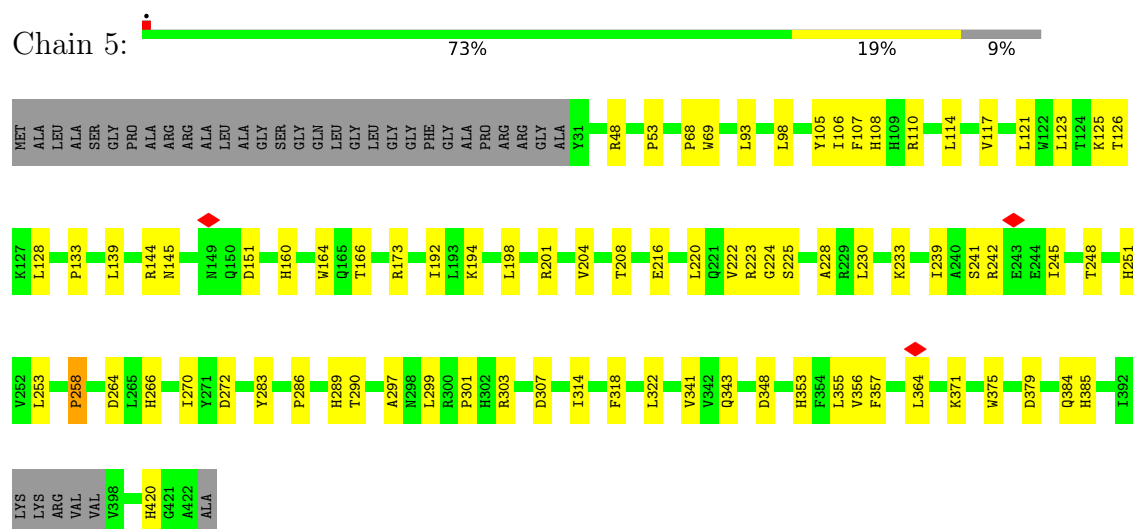


- Molecule 26: 39S ribosomal protein L35, mitochondrial

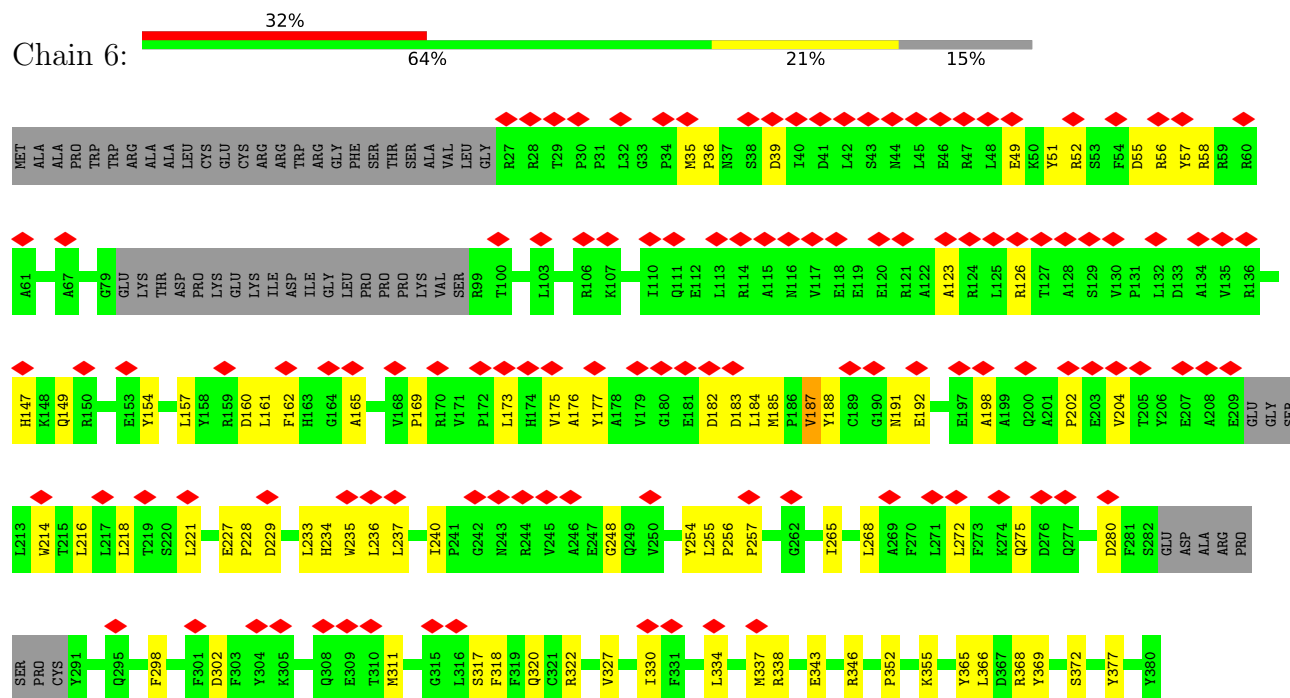
Chain 3: 38% 12% 49%



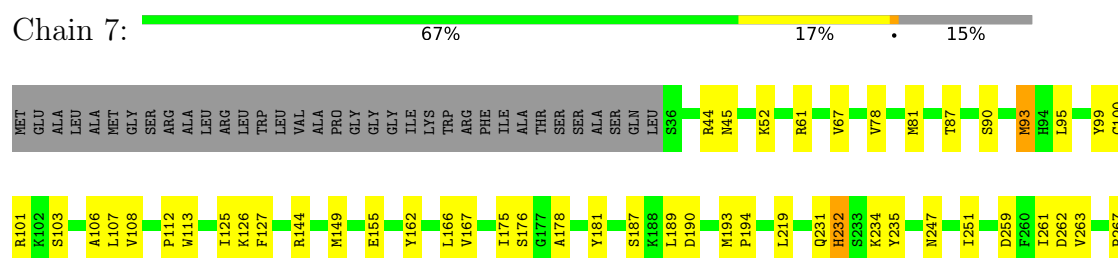
- Molecule 27: 39S ribosomal protein L37, mitochondrial



- Molecule 28: 39S ribosomal protein L38, mitochondrial

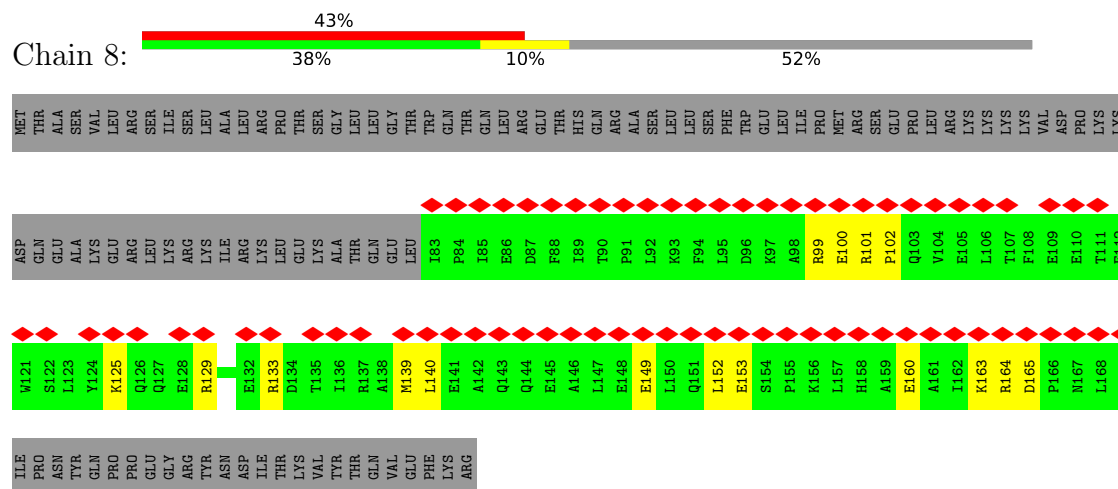


- Molecule 29: 39S ribosomal protein L39, mitochondrial

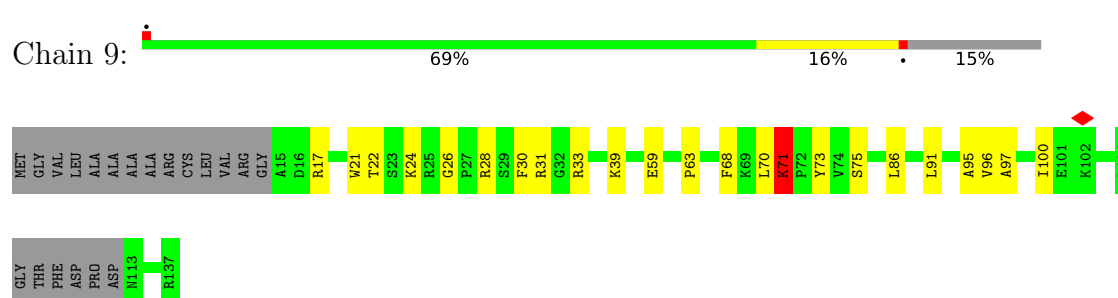




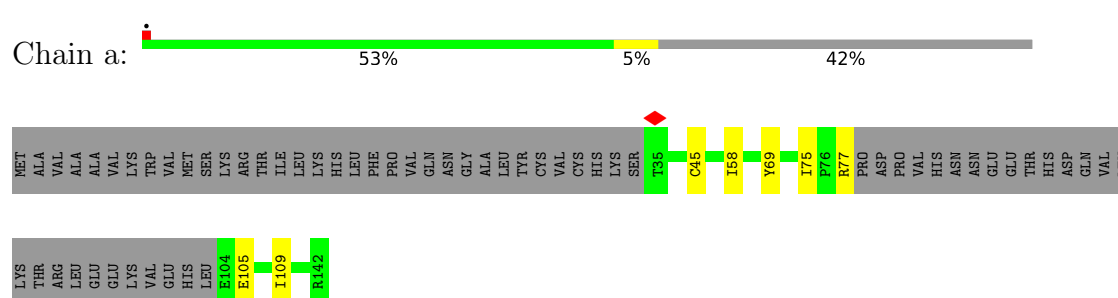
- Molecule 30: 39S ribosomal protein L40, mitochondrial



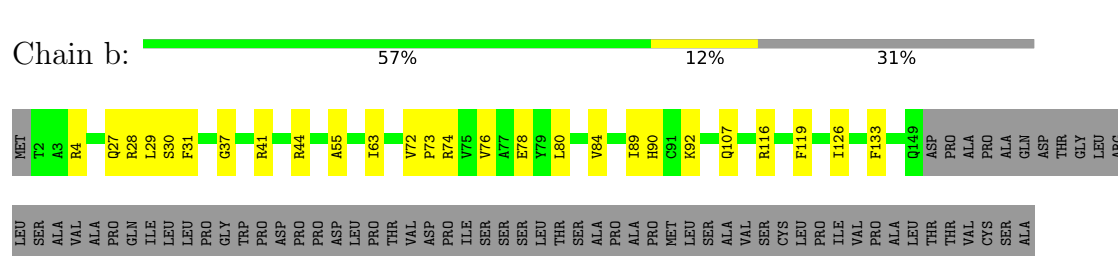
- Molecule 31: 39S ribosomal protein L41, mitochondrial

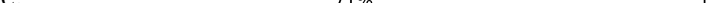


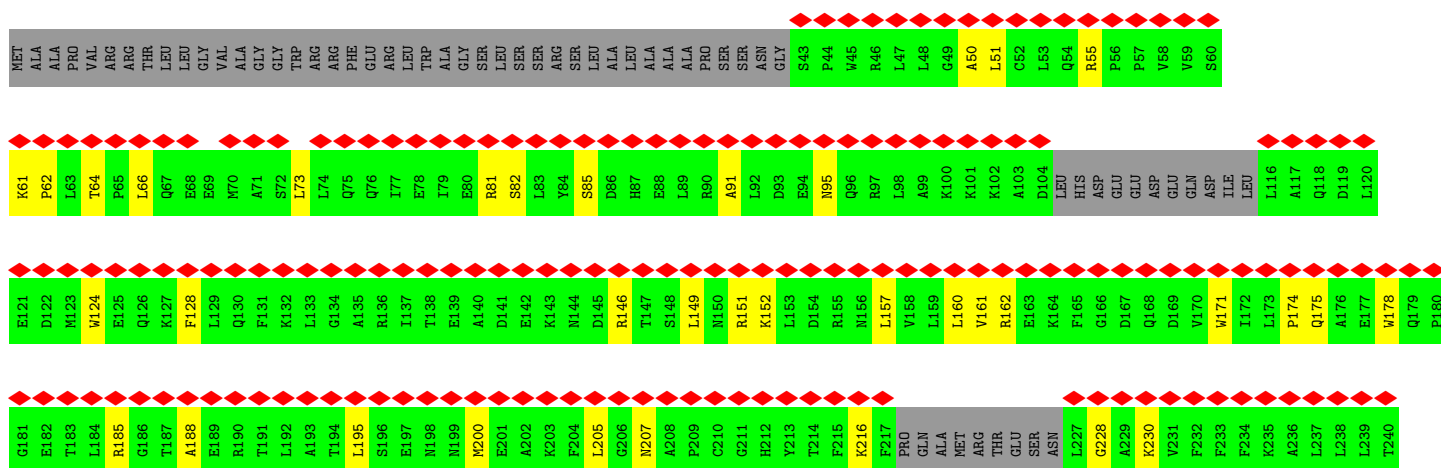
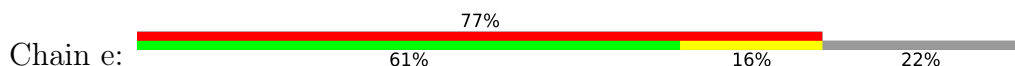
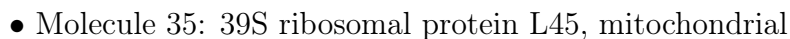
- Molecule 32: 39S ribosomal protein L42, mitochondrial

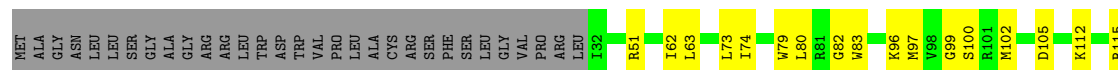


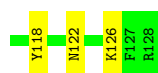
- Molecule 33: 39S ribosomal protein L43, mitochondrial



- Chain c:  71% 11% 17%



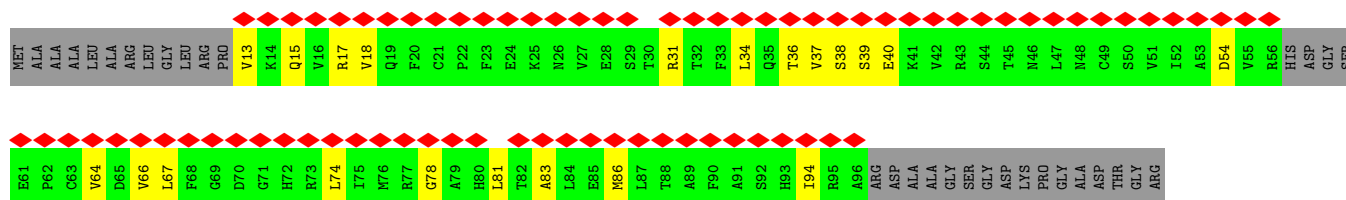




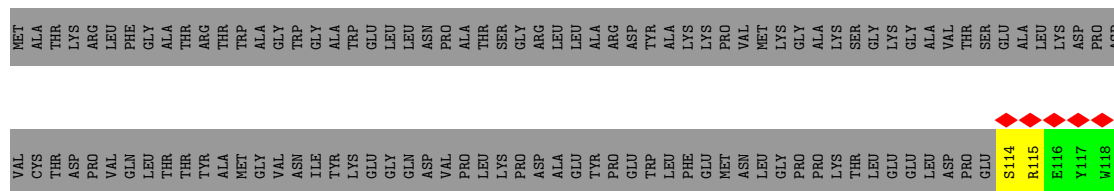
- Molecule 41: 39S ribosomal protein L52, mitochondrial



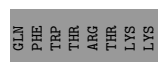
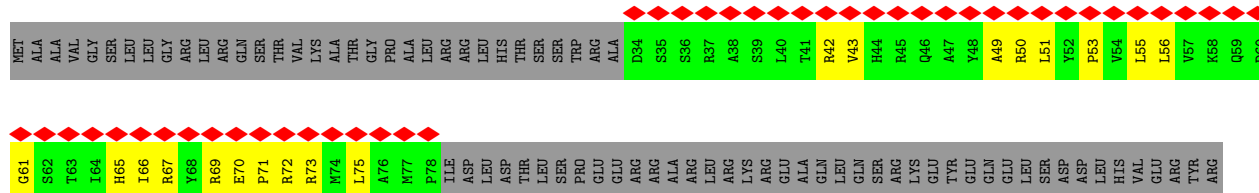
- Molecule 42: 39S ribosomal protein L53, mitochondrial



- Molecule 43: 39S ribosomal protein L54, mitochondrial



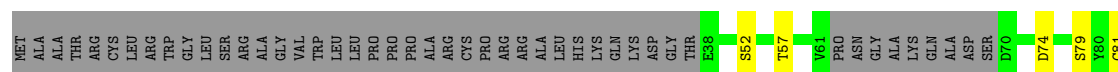
- Molecule 44: 39S ribosomal protein L55, mitochondrial



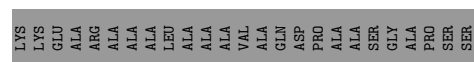
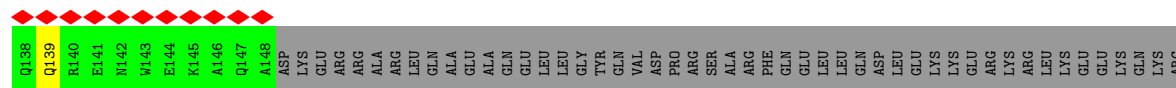
- Molecule 45: Ribosomal protein 63, mitochondrial



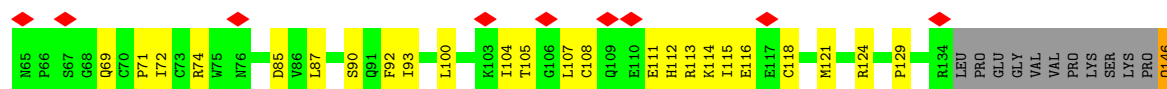
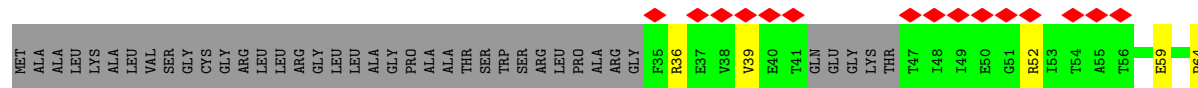
- Molecule 46: Peptidyl-tRNA hydrolase ICT1, mitochondrial



- Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1

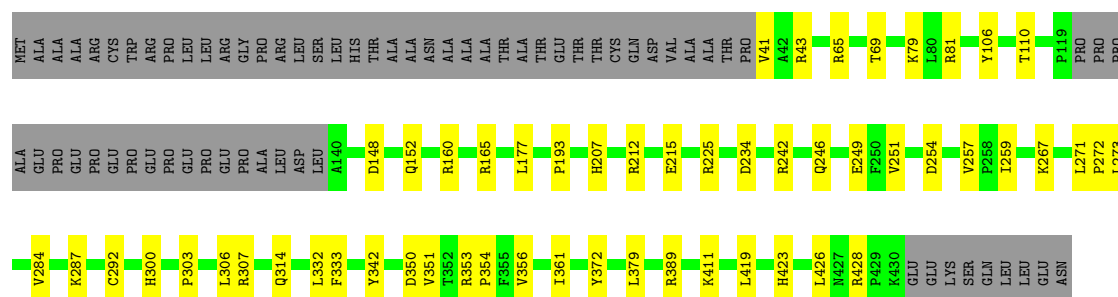


- Molecule 48: 39S ribosomal protein S18a, mitochondrial



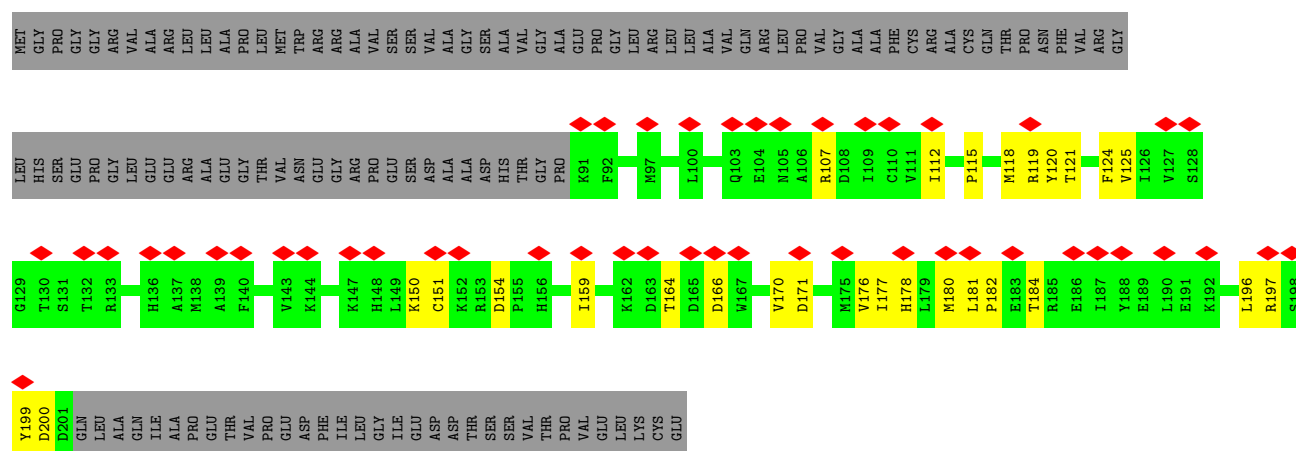
- Molecule 49: 39S ribosomal protein S30, mitochondrial

Chain s: 



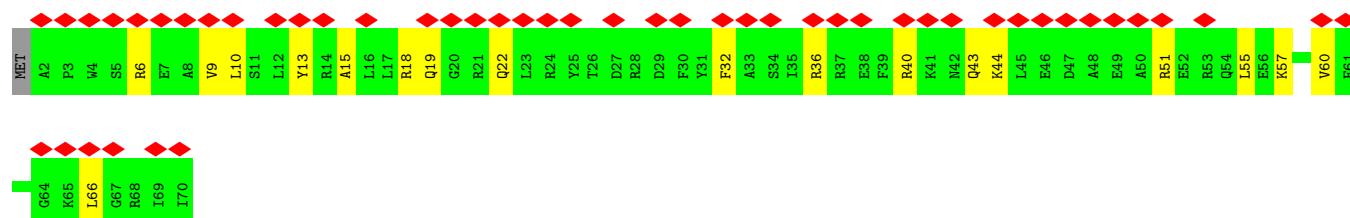
• Molecule 50: Mitochondrial assembly of ribosomal large subunit protein 1

Chain u: 

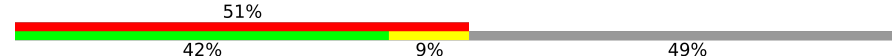


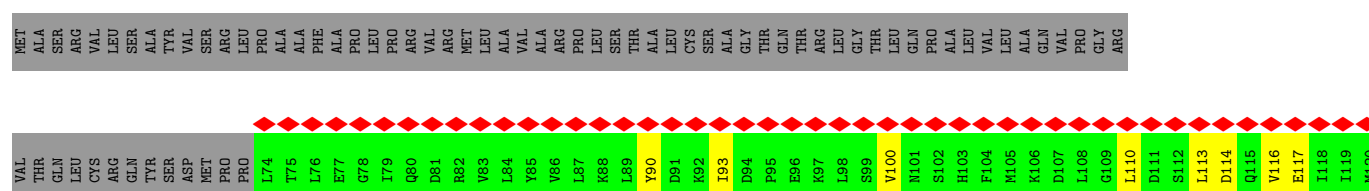
• Molecule 51: MIEF1 upstream open reading frame protein

Chain v: 



• Molecule 52: Acyl carrier protein, mitochondrial

Chain w: 



Chain A:



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76339	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	28	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.910	Depositor
Minimum map value	-0.487	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.018	Depositor
Recommended contour level	0.05	Depositor
Map size ($\text{\AA}$)	390.24, 390.24, 390.24	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.084, 1.084, 1.084	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	D	0.24	0/1736	0.60	0/2335
2	E	0.28	0/2322	0.60	0/3148
3	F	0.37	0/2071	0.58	0/2817
4	H	0.28	0/798	0.78	1/1073 (0.1%)
5	I	0.20	0/1308	0.50	0/1761
6	J	0.18	0/1077	0.50	0/1452
7	K	0.32	0/1495	0.59	0/2029
8	L	0.23	0/904	0.62	0/1218
9	M	0.30	0/2359	0.56	0/3185
10	N	0.21	0/1697	0.54	0/2281
11	O	0.32	0/1269	0.56	0/1708
12	P	0.26	0/1173	0.63	0/1588
13	Q	0.24	0/1846	0.55	0/2487
14	R	0.36	0/1174	0.53	0/1572
15	S	0.33	0/1276	0.64	0/1729
16	T	0.34	0/1335	0.55	0/1796
17	U	0.32	0/1183	0.55	0/1600
18	V	0.22	0/1616	0.47	0/2189
19	W	0.22	0/881	0.54	0/1188
20	X	0.28	0/2090	0.62	2/2825 (0.1%)
21	Y	0.29	0/1552	0.52	0/2079
22	Z	0.24	0/1003	0.53	0/1354
23	0	0.32	0/895	0.59	0/1201
24	1	0.22	0/438	0.59	0/583
25	2	0.39	0/357	0.55	0/475
26	3	0.26	0/852	0.55	0/1136
27	5	0.28	0/3250	0.60	2/4429 (0.0%)
28	6	0.22	0/2726	0.57	0/3715
29	7	0.26	0/2391	0.63	0/3234
30	8	0.21	0/855	0.54	0/1152
31	9	0.32	0/972	0.69	2/1306 (0.2%)
32	a	0.25	0/709	0.48	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.34	0/1202	0.58	0/1626
34	c	0.26	0/2264	0.53	0/3059
35	d	0.24	0/1790	0.60	0/2423
36	e	0.17	0/1797	0.47	0/2422
37	f	0.18	0/931	0.50	0/1259
38	g	0.31	0/1102	0.56	0/1503
39	h	0.26	0/847	0.59	2/1150 (0.2%)
40	i	0.37	0/849	0.50	0/1135
41	j	0.21	0/698	0.41	0/940
42	k	0.19	0/635	0.51	0/855
43	l	0.10	0/226	0.30	0/299
44	m	0.20	0/379	0.56	0/510
45	o	0.25	0/682	0.63	0/916
46	p	0.24	0/1071	0.64	1/1433 (0.1%)
47	q	0.26	0/1070	0.64	2/1450 (0.1%)
48	r	0.28	0/1238	0.65	1/1676 (0.1%)
49	s	0.30	0/3114	0.54	2/4225 (0.0%)
50	u	0.29	0/949	0.77	0/1281
51	v	0.24	0/597	0.70	0/796
52	w	0.24	0/647	0.63	0/871
53	A	0.27	0/25013	0.38	1/38878 (0.0%)
54	B	0.14	0/1328	0.29	0/2056
All	All	0.27	0/94039	0.52	16/132371 (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
3	F	0	1
28	6	0	2
29	7	0	1
31	9	0	1
35	d	0	1
47	q	0	1
All	All	0	7

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	r	64	PRO	CA-N-CD	-9.08	99.29	112.00
27	5	258	PRO	CA-N-CD	-8.70	99.32	111.50
20	X	36	ARG	CA-C-N	7.16	130.66	120.49
20	X	36	ARG	C-N-CA	7.16	130.66	120.49
49	s	251	VAL	N-CA-C	-6.96	103.48	109.19
31	9	71	LYS	CB-CA-C	6.24	118.24	108.88
46	p	186	GLU	N-CA-CB	6.18	119.86	110.28
27	5	258	PRO	N-CD-CG	-6.01	96.59	103.80
4	H	103	GLU	CA-CB-CG	5.80	125.71	114.10
31	9	71	LYS	CA-CB-CG	5.61	125.33	114.10
47	q	139	GLN	CA-C-N	-5.42	111.65	121.14
47	q	139	GLN	C-N-CA	-5.42	111.65	121.14
39	h	71	GLU	CA-CB-CG	5.39	124.89	114.10
39	h	71	GLU	N-CA-CB	5.21	117.78	110.12
49	s	251	VAL	CB-CA-C	5.16	114.39	109.33
53	A	153	A	P-O3'-C3'	5.06	127.78	120.20

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	6	187	VAL	Peptide
28	6	49	GLU	Peptide
29	7	93	MET	Peptide
31	9	71	LYS	Peptide
3	F	108	ARG	Sidechain
35	d	186	VAL	Peptide
47	q	26	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1706	0	1755	37	0
2	E	2258	0	2264	38	0
3	F	2013	0	2044	35	0
4	H	784	0	832	19	0
5	I	1283	0	1369	30	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	J	1061	0	1141	14	0
7	K	1451	0	1448	34	0
8	L	889	0	941	25	0
9	M	2305	0	2378	46	0
10	N	1654	0	1681	27	0
11	O	1245	0	1283	22	0
12	P	1148	0	1148	41	0
13	Q	1805	0	1841	24	0
14	R	1153	0	1214	18	0
15	S	1251	0	1322	28	0
16	T	1305	0	1352	19	0
17	U	1154	0	1154	19	0
18	V	1575	0	1583	22	0
19	W	859	0	888	23	0
20	X	2035	0	2054	34	0
21	Y	1517	0	1561	17	0
22	Z	978	0	1030	16	0
23	0	880	0	902	22	0
24	1	433	0	475	9	0
25	2	351	0	375	8	0
26	3	831	0	883	22	0
27	5	3156	0	3138	56	0
28	6	2640	0	2464	62	0
29	7	2334	0	2343	41	0
30	8	836	0	844	19	0
31	9	947	0	949	23	0
32	a	686	0	658	5	0
33	b	1178	0	1180	20	0
34	c	2217	0	2220	25	0
35	d	1741	0	1727	33	0
36	e	1762	0	1767	34	0
37	f	915	0	917	16	0
38	g	1067	0	1056	20	0
39	h	827	0	806	7	0
40	i	827	0	857	20	0
41	j	684	0	673	4	0
42	k	627	0	636	13	0
43	l	221	0	227	6	0
44	m	372	0	387	17	0
45	o	665	0	664	17	0
46	p	1058	0	1083	18	0
47	q	1039	0	1013	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	r	1203	0	1220	41	0
49	s	3036	0	3022	40	0
50	u	927	0	921	25	0
51	v	588	0	604	18	0
52	w	638	0	636	9	0
53	A	22369	0	11385	236	0
54	B	1191	0	607	18	0
55	O	1	0	0	0	0
55	I	1	0	0	0	0
56	A	47	0	0	0	0
56	W	1	0	0	0	0
56	g	1	0	0	0	0
57	v	21	0	21	5	0
All	All	89747	0	78943	1181	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

All (1181) 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)
2:E:106:MET:HA	2:E:119:VAL:O	1.17	1.25
1:D:129:VAL:HA	1:D:139:ILE:O	1.31	1.24
53:A:1446:C:H42	53:A:1470:A:N6	1.48	1.10
53:A:1446:C:N4	53:A:1470:A:H61	1.48	1.10
53:A:51:C:H42	53:A:60:U:H3	1.11	0.99
48:r:146:GLN:HE21	48:r:146:GLN:N	1.60	0.98
12:P:81:LEU:HA	12:P:93:LEU:O	1.62	0.98
2:E:106:MET:CA	2:E:119:VAL:O	2.11	0.98
29:7:106:ALA:HA	29:7:126:LYS:O	1.63	0.97
53:A:1454:U:N3	53:A:1463:A:C8	2.31	0.97
54:B:1607:U:H3	54:B:1664:G:H1	1.01	0.96
28:6:216:LEU:O	28:6:236:LEU:HA	1.65	0.96
12:P:79:HIS:HA	12:P:95:GLU:O	1.76	0.85
33:b:31:PHE:HA	33:b:74:ARG:O	1.75	0.85
27:5:290:THR:HA	27:5:343:GLN:O	1.77	0.83
53:A:564:C:HO2'	53:A:1018:C:HO2'	1.24	0.82
12:P:81:LEU:H	12:P:144:MET:HE1	1.45	0.81
44:m:69:ARG:HE	44:m:70:GLU:H	1.26	0.81
1:D:129:VAL:CA	1:D:139:ILE:O	2.25	0.79
34:c:260:GLN:HA	34:c:269:LEU:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:51:ARG:NH1	53:A:198:G:N7	2.32	0.77
35:d:197:VAL:HA	35:d:211:GLN:O	1.85	0.76
25:2:82:ARG:HE	25:2:87:ARG:HD2	1.49	0.75
12:P:52:ASN:HB3	12:P:55:ASN:HB2	1.69	0.74
29:7:107:LEU:HB2	29:7:126:LYS:HB2	1.69	0.74
53:A:51:C:N4	53:A:60:U:H3	1.84	0.73
30:8:139:MET:HE3	37:f:169:ILE:HG23	1.71	0.72
27:5:204:VAL:O	27:5:228:ALA:HA	1.91	0.71
33:b:27:GLN:HE21	33:b:80:LEU:HD23	1.55	0.71
28:6:149:GLN:HE21	28:6:169:PRO:HD2	1.54	0.71
29:7:231:GLN:HE21	29:7:232:HIS:HE1	1.37	0.71
20:X:119:LEU:HD12	27:5:53:PRO:HD2	1.71	0.71
10:N:223:MET:SD	45:o:46:HIS:NE2	2.64	0.71
50:u:125:VAL:HB	50:u:177:ILE:HG22	1.73	0.70
9:M:51:ARG:NH2	53:A:232:C:O2'	2.24	0.70
16:T:84:LYS:HD3	16:T:149:ARG:HB3	1.73	0.70
7:K:69:GLY:HA2	48:r:152:THR:HG22	1.73	0.70
49:s:249:GLU:HA	49:s:356:VAL:HG21	1.74	0.69
33:b:72:VAL:HG13	33:b:90:HIS:HB2	1.74	0.69
4:H:120:ARG:NH2	20:X:136:ASP:OD1	2.25	0.69
22:Z:114:LYS:O	45:o:45:ASN:ND2	2.26	0.68
40:i:51:ARG:NH1	53:A:608:A:OP1	2.25	0.68
42:k:15:GLN:HE22	42:k:17:ARG:HB2	1.59	0.68
1:D:148:LYS:HE3	27:5:114:LEU:HD12	1.75	0.68
8:L:144:PHE:HE1	50:u:120:TYR:HB2	1.59	0.68
50:u:196:LEU:HB3	51:v:57:LYS:HZ1	1.59	0.68
53:A:1454:U:C2	53:A:1463:A:N7	2.62	0.67
35:d:164:VAL:HG13	35:d:261:MET:HB2	1.77	0.67
4:H:126:GLN:HG3	4:H:128:LEU:HD23	1.77	0.66
26:3:183:ARG:NH2	28:6:355:LYS:O	2.28	0.66
38:g:122:LYS:NZ	38:g:126:ASP:OD2	2.26	0.66
35:d:197:VAL:HG12	35:d:212:ILE:HG12	1.78	0.66
53:A:107:A:N6	53:A:110:U:OP2	2.26	0.66
1:D:148:LYS:NZ	27:5:264:ASP:OD1	2.28	0.66
5:I:119:HIS:HB3	5:I:121:ILE:HG22	1.78	0.66
53:A:662:C:H42	53:A:772:U:H3	1.41	0.65
2:E:276:ILE:HD11	2:E:332:LEU:HD12	1.78	0.65
22:Z:53:HIS:CE1	22:Z:60:PRO:HD3	2.30	0.65
17:U:11:ARG:NH2	18:V:212:LYS:O	2.30	0.65
26:3:104:ARG:NH2	26:3:160:LYS:O	2.30	0.65
15:S:104:ARG:NH2	53:A:475:G:N3	2.44	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:3:113:ARG:NH2	53:A:80:G:OP1	2.27	0.65
53:A:201:A:H61	53:A:231:C:H5'	1.62	0.65
45:o:34:ASN:OD1	45:o:37:ARG:NH2	2.30	0.65
48:r:146:GLN:N	48:r:146:GLN:NE2	2.40	0.65
27:5:314:ILE:HD13	27:5:355:LEU:HD11	1.80	0.64
29:7:187:SER:O	29:7:190:ASP:HB2	1.96	0.64
38:g:111:ARG:NH2	53:A:211:A:OP2	2.30	0.64
2:E:74:ALA:HA	2:E:77:LEU:HD23	1.78	0.64
8:L:126:SER:O	8:L:130:ARG:NH1	2.30	0.64
50:u:151:CYS:HB3	50:u:154:ASP:HB2	1.79	0.64
7:K:163:ILE:HA	48:r:87:LEU:HD21	1.80	0.64
29:7:52:LYS:HD2	29:7:219:LEU:HD21	1.78	0.64
53:A:196:U:O2	53:A:628:A:N6	2.31	0.64
15:S:118:ASN:C	15:S:118:ASN:HD22	2.05	0.64
28:6:227:GLU:HG2	28:6:229:ASP:H	1.63	0.63
3:F:281:ARG:NH2	9:M:128:THR:OG1	2.31	0.63
28:6:157:LEU:O	28:6:161:LEU:HB3	1.98	0.63
29:7:286:LEU:HG	29:7:288:PRO:HD2	1.81	0.63
27:5:341:VAL:HA	27:5:357:PHE:O	1.99	0.63
42:k:15:GLN:HB3	42:k:67:LEU:HB2	1.80	0.63
23:0:119:LYS:O	23:0:120:HIS:ND1	2.31	0.63
53:A:1454:U:O2	53:A:1463:A:N7	2.32	0.63
53:A:1457:G:H2'	53:A:1458:A:H2'	1.80	0.63
17:U:151:PHE:O	35:d:273:LYS:NZ	2.31	0.63
34:c:265:THR:HG23	34:c:267:LEU:H	1.63	0.63
9:M:177:ALA:HB1	9:M:203:ARG:HH12	1.63	0.62
30:8:140:LEU:HD22	37:f:169:ILE:HD13	1.81	0.62
27:5:204:VAL:HG11	49:s:152:GLN:HE22	1.63	0.62
41:j:83:GLU:OE1	45:o:66:ARG:NE	2.29	0.62
12:P:177:ARG:NH2	19:W:139:GLU:OE1	2.32	0.62
38:g:86:VAL:HG22	38:g:113:VAL:HG22	1.80	0.62
5:I:51:THR:OG1	10:N:250:ARG:NH2	2.32	0.62
12:P:94:VAL:HB	12:P:103:VAL:HB	1.81	0.62
13:Q:129:LYS:NZ	50:u:121:THR:O	2.33	0.62
2:E:96:ARG:HH21	2:E:202:GLN:HE22	1.48	0.62
20:X:116:SER:O	20:X:120:ASP:HA	1.98	0.62
4:H:131:TYR:O	4:H:136:ASN:ND2	2.26	0.62
49:s:419:LEU:O	49:s:423:HIS:ND1	2.28	0.62
10:N:224:LEU:HD11	45:o:38:ARG:HG2	1.80	0.62
25:2:82:ARG:NH1	53:A:120:A:OP1	2.33	0.62
33:b:29:LEU:HA	33:b:76:VAL:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:217:LEU:HD11	3:F:243:ILE:HD12	1.82	0.61
9:M:80:LYS:HE3	26:3:113:ARG:HH21	1.64	0.61
11:O:45:PRO:HG2	11:O:48:ARG:HD2	1.81	0.61
12:P:167:GLU:O	46:p:187:ARG:NH1	2.32	0.61
34:c:156:LEU:HD22	34:c:231:MET:HE2	1.82	0.61
44:m:70:GLU:OE2	44:m:72:ARG:NH1	2.33	0.61
53:A:495:C:O2	53:A:547:C:N4	2.33	0.61
53:A:1193:U:O2	53:A:1199:A:N6	2.33	0.61
7:K:52:ASP:O	16:T:206:ARG:NH1	2.33	0.61
1:D:124:GLU:OE1	1:D:165:ASN:ND2	2.34	0.61
9:M:55:GLY:O	9:M:59:ARG:NH1	2.33	0.61
25:2:52:GLU:HG3	53:A:249:C:H1'	1.81	0.61
28:6:35:MET:HE3	28:6:36:PRO:HD2	1.83	0.61
45:o:60:ARG:NH1	53:A:409:C:O2	2.34	0.61
49:s:207:HIS:ND1	49:s:234:ASP:OD1	2.33	0.61
12:P:77:PHE:O	12:P:97:GLN:NE2	2.34	0.61
44:m:69:ARG:HH21	44:m:71:PRO:HD3	1.66	0.61
53:A:77:G:N2	53:A:80:G:O2'	2.34	0.61
10:N:240:LYS:NZ	10:N:251:VAL:O	2.33	0.61
30:8:160:GLU:O	36:e:207:ASN:ND2	2.33	0.61
51:v:6:ARG:NH2	57:v:101:PNS:O26	2.33	0.61
27:5:166:THR:O	49:s:287:LYS:NZ	2.34	0.61
1:D:235:GLN:HB3	1:D:294:SER:HA	1.82	0.61
14:R:11:ARG:HB2	53:A:622:G:C8	2.36	0.61
38:g:111:ARG:NH1	53:A:210:C:OP2	2.31	0.61
45:o:71:PHE:HA	45:o:74:ILE:HG22	1.83	0.61
49:s:165:ARG:HH22	53:A:745:C:H3'	1.66	0.61
15:S:184:ARG:NH1	53:A:591:C:O2'	2.33	0.60
53:A:1480:U:H2'	53:A:1481:A:H8	1.66	0.60
46:p:185:ARG:HE	46:p:189:ARG:HH12	1.49	0.60
5:I:87:ALA:O	5:I:91:GLN:NE2	2.34	0.60
48:r:153:ARG:HH22	48:r:195:TYR:HE1	1.48	0.60
5:I:140:TYR:HB3	5:I:143:LEU:HB2	1.83	0.60
8:L:85:LEU:HD13	8:L:137:VAL:HG21	1.82	0.60
14:R:99:ARG:NH1	53:A:578:U:OP1	2.35	0.60
53:A:1446:C:N3	53:A:1470:A:N1	2.49	0.60
28:6:160:ASP:HB3	28:6:221:LEU:HD21	1.82	0.60
9:M:151:LYS:NZ	9:M:170:ASN:O	2.34	0.60
3:F:262:THR:HG22	3:F:264:PRO:HD2	1.84	0.60
29:7:45:ASN:HD21	29:7:259:ASP:HA	1.65	0.60
34:c:275:TYR:HA	34:c:280:LEU:HA	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A:841:C:H3'	53:A:842:A:H8	1.66	0.60
28:6:237:LEU:HB3	28:6:240:ILE:HD11	1.84	0.59
49:s:271:LEU:HD12	49:s:272:PRO:HD2	1.84	0.59
13:Q:120:THR:HG22	13:Q:132:GLN:HG2	1.85	0.59
8:L:69:VAL:HG23	8:L:88:GLY:H	1.68	0.59
10:N:170:GLU:HB3	43:l:132:LEU:HD22	1.84	0.59
26:3:131:LYS:NZ	53:A:1239:G:N7	2.50	0.59
27:5:299:LEU:HB3	27:5:301:PRO:HD2	1.84	0.59
28:6:176:ALA:HB1	28:6:184:LEU:HB3	1.85	0.59
34:c:43:LYS:NZ	53:A:614:C:OP2	2.34	0.59
2:E:133:THR:OG1	2:E:144:THR:OG1	2.20	0.59
3:F:103:GLN:HE22	3:F:249:ASN:HB2	1.68	0.59
5:I:124:LYS:HB2	5:I:153:LEU:HB2	1.85	0.59
23:0:91:ARG:NH1	53:A:148:A:OP2	2.35	0.59
51:v:13:TYR:OH	51:v:36:ARG:NH2	2.35	0.59
3:F:241:ASN:OD1	3:F:256:HIS:NE2	2.35	0.59
8:L:128:ARG:HD3	13:Q:125:TYR:HB3	1.84	0.59
27:5:144:ARG:O	27:5:194:LYS:NZ	2.32	0.59
43:l:120:ARG:NH1	53:A:520:C:OP1	2.35	0.59
53:A:738:U:H2'	53:A:739:A:H8	1.67	0.59
24:l:25:GLY:H	47:q:121:ILE:HD11	1.68	0.59
47:q:59:LYS:NZ	53:A:90:G:OP2	2.30	0.59
53:A:789:A:N6	53:A:998:A:O2'	2.31	0.59
8:L:56:ARG:NH1	53:A:802:A:OP1	2.35	0.59
19:W:54:LYS:HG2	53:A:1192:C:H4'	1.85	0.59
22:Z:78:ARG:HD2	22:Z:116:LEU:HD21	1.83	0.59
38:g:150:LYS:HE3	53:A:382:A:H5''	1.85	0.59
37:f:114:CYS:HA	37:f:119:ILE:HD12	1.84	0.58
2:E:334:ASP:OD1	2:E:335:GLU:N	2.36	0.58
42:k:34:LEU:HA	42:k:38:SER:HB2	1.85	0.58
51:v:40:ARG:O	51:v:44:LYS:NZ	2.31	0.58
53:A:214:G:N3	53:A:225:C:O2'	2.36	0.58
53:A:503:G:H2'	53:A:504:G:C8	2.38	0.58
53:A:132:A:N7	53:A:135:A:N6	2.50	0.58
7:K:174:GLU:O	48:r:36:ARG:NH1	2.36	0.58
16:T:97:MET:HE1	16:T:105:GLN:HG3	1.85	0.58
48:r:173:ARG:HG2	48:r:195:TYR:HB3	1.85	0.58
28:6:218:LEU:HD22	28:6:234:HIS:HB2	1.85	0.58
49:s:193:PRO:HD2	49:s:428:ARG:HH12	1.69	0.58
3:F:262:THR:O	3:F:265:THR:OG1	2.20	0.58
9:M:141:VAL:HG12	9:M:143:GLU:H	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:108:PRO:HA	19:W:114:VAL:HG21	1.86	0.58
36:e:279:LEU:HD11	37:f:176:SER:HB2	1.85	0.58
37:f:163:SER:O	37:f:167:ALA:N	2.34	0.58
20:X:209:GLU:HG3	27:5:69:TRP:CD1	2.39	0.58
27:5:68:PRO:O	53:A:43:A:N6	2.36	0.58
29:7:106:ALA:CA	29:7:126:LYS:O	2.47	0.58
36:e:81:ARG:NH2	44:m:43:VAL:O	2.37	0.58
16:T:69:ARG:NH1	35:d:228:PHE:O	2.36	0.58
28:6:55:ASP:OD1	28:6:58:ARG:NE	2.35	0.58
35:d:213:THR:HG22	35:d:247:VAL:HG22	1.86	0.58
12:P:73:PRO:HB2	12:P:147:GLN:HE21	1.69	0.58
15:S:155:ARG:NH2	15:S:157:GLU:OE2	2.36	0.58
1:D:213:CYS:SG	1:D:246:ARG:NH1	2.77	0.57
7:K:89:GLN:NE2	48:r:163:TYR:O	2.37	0.57
44:m:42:ARG:NH1	54:B:1630:A:OP1	2.37	0.57
9:M:64:ARG:NH1	40:i:122:ASN:O	2.32	0.57
22:Z:99:VAL:O	41:j:76:ARG:NH1	2.36	0.57
29:7:231:GLN:HE21	29:7:232:HIS:CE1	2.21	0.57
17:U:37:GLU:HB3	17:U:104:THR:HG23	1.86	0.57
5:I:133:PRO:HA	5:I:136:GLU:HG2	1.86	0.57
8:L:118:ARG:NH1	50:u:200:ASP:OD1	2.34	0.57
23:0:179:ARG:HH12	23:0:182:PRO:HG3	1.70	0.57
27:5:290:THR:HG22	27:5:343:GLN:HG3	1.85	0.57
3:F:160:SER:OG	40:i:83:TRP:O	2.20	0.57
9:M:51:ARG:HH21	40:i:126:LYS:HB2	1.68	0.57
15:S:129:ARG:HH12	15:S:155:ARG:HG2	1.69	0.57
49:s:106:TYR:O	49:s:110:THR:OG1	2.22	0.57
2:E:213:LYS:HG3	2:E:261:MET:HE2	1.85	0.57
9:M:59:ARG:NH1	53:A:346:C:OP2	2.37	0.57
5:I:148:VAL:O	42:k:31:ARG:NH1	2.38	0.57
7:K:20:LEU:HB2	7:K:141:LEU:HD23	1.84	0.57
39:h:91:LEU:HD23	39:h:97:LYS:HG3	1.85	0.57
5:I:83:ARG:HD3	5:I:134:PHE:HE1	1.70	0.57
14:R:15:THR:HG22	34:c:32:LYS:HB3	1.87	0.57
18:V:126:MET:SD	18:V:126:MET:N	2.77	0.57
48:r:173:ARG:NH1	48:r:196:HIS:O	2.37	0.57
1:D:213:CYS:HB3	1:D:246:ARG:HG2	1.86	0.57
19:W:56:MET:HE2	53:A:393:G:H21	1.70	0.57
22:Z:88:MET:SD	53:A:412:G:N2	2.70	0.57
29:7:112:PRO:HB2	29:7:267:PRO:HG2	1.87	0.57
53:A:1454:U:N3	53:A:1463:A:H8	1.98	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:128:ASN:ND2	5:I:149:GLY:O	2.38	0.57
21:Y:197:LYS:NZ	53:A:29:C:OP2	2.38	0.57
30:8:101:ARG:NH2	36:e:82:SER:OG	2.30	0.57
3:F:231:VAL:HG23	47:q:26:ARG:HG3	1.87	0.56
9:M:51:ARG:HE	40:i:126:LYS:HB2	1.70	0.56
18:V:29:VAL:HG21	35:d:67:ILE:HG23	1.86	0.56
29:7:231:GLN:NE2	29:7:232:HIS:HE1	2.03	0.56
53:A:1063:G:H2'	53:A:1064:A:H8	1.70	0.56
3:F:167:MET:HA	3:F:170:ARG:HE	1.70	0.56
12:P:42:GLU:HB3	28:6:337:MET:HE1	1.87	0.56
15:S:181:LYS:NZ	53:A:626:U:O4	2.38	0.56
26:3:138:PRO:HA	26:3:141:LYS:HG2	1.87	0.56
35:d:140:LYS:O	35:d:143:ASP:HB2	2.06	0.56
4:H:108:ARG:NH2	4:H:143:GLU:OE2	2.38	0.56
6:J:25:ARG:HA	6:J:65:PRO:HA	1.87	0.56
11:O:92:VAL:HG13	23:0:155:GLU:HG2	1.86	0.56
1:D:105:ARG:NH2	53:A:733:G:OP2	2.38	0.56
5:I:161:VAL:HA	5:I:164:MET:HE2	1.87	0.56
48:r:153:ARG:HB3	48:r:154:TRP:HD1	1.71	0.56
53:A:603:A:N1	53:A:623:A:O2'	2.38	0.56
16:T:50:LYS:NZ	53:A:142:C:OP1	2.38	0.56
27:5:173:ARG:NH1	27:5:348:ASP:O	2.39	0.56
31:9:91:LEU:O	31:9:95:ALA:HB3	2.05	0.56
32:a:69:TYR:OH	34:c:256:ARG:NH2	2.39	0.56
53:A:717:U:O2'	53:A:736:A:N6	2.37	0.56
9:M:264:GLN:NE2	9:M:269:LEU:O	2.36	0.56
17:U:65:VAL:HG23	17:U:97:VAL:HG13	1.88	0.56
5:I:88:ALA:O	5:I:92:ASP:HB2	2.06	0.56
5:I:119:HIS:HB2	5:I:160:LYS:HE3	1.87	0.56
8:L:93:GLY:O	8:L:95:ARG:NH2	2.38	0.56
12:P:156:ASP:OD2	28:6:126:ARG:NH1	2.37	0.56
38:g:91:MET:HE3	53:A:213:G:H5''	1.87	0.56
28:6:372:SER:OG	46:p:141:ARG:NH1	2.39	0.55
33:b:28:ARG:NH2	34:c:71:GLU:OE1	2.36	0.55
42:k:66:VAL:HB	42:k:74:LEU:HB3	1.88	0.55
54:B:1610:A:N7	54:B:1612:C:N4	2.53	0.55
53:A:28:C:O2'	53:A:32:A:N3	2.38	0.55
10:N:94:GLY:HA2	10:N:154:VAL:O	2.06	0.55
27:5:106:ILE:HB	27:5:266:HIS:HB3	1.88	0.55
29:7:231:GLN:NE2	29:7:232:HIS:CE1	2.75	0.55
15:S:54:THR:HG22	15:S:57:SER:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:0:85:ARG:NH1	53:A:638:A:OP1	2.40	0.55
53:A:214:G:H1'	53:A:225:C:H1'	1.87	0.55
28:6:216:LEU:O	28:6:236:LEU:CA	2.48	0.55
27:5:160:HIS:HA	27:5:164:TRP:HB2	1.89	0.55
31:9:86:LEU:HD21	31:9:91:LEU:HD12	1.89	0.55
1:D:208:ARG:HH21	53:A:858:G:H3'	1.71	0.55
2:E:129:VAL:HA	2:E:147:VAL:HG22	1.89	0.55
13:Q:205:LYS:HD2	13:Q:206:PRO:HD2	1.88	0.55
16:T:212:LEU:HA	33:b:119:PHE:HE2	1.70	0.55
27:5:270:ILE:O	53:A:739:A:O2'	2.24	0.55
39:h:149:PRO:HG2	39:h:152:LEU:HD23	1.88	0.55
2:E:97:VAL:O	2:E:197:HIS:NE2	2.39	0.55
5:I:117:ARG:NH1	6:J:133:GLN:OE1	2.40	0.55
50:u:200:ASP:HB3	51:v:57:LYS:HE2	1.87	0.55
52:w:147:TYR:O	52:w:151:LYS:HB2	2.06	0.55
3:F:221:LEU:HD23	3:F:222:THR:HG23	1.89	0.55
9:M:14:ASP:OD1	9:M:17:ARG:NH2	2.40	0.55
27:5:283:TYR:OH	49:s:152:GLN:NE2	2.28	0.55
33:b:4:ARG:NH2	53:A:167:C:OP1	2.40	0.55
37:f:163:SER:H	37:f:166:PHE:HB3	1.71	0.55
1:D:141:LEU:HD21	1:D:148:LYS:HG2	1.89	0.54
9:M:62:ARG:NH1	40:i:126:LYS:O	2.40	0.54
27:5:192:ILE:HG13	27:5:198:LEU:HB2	1.88	0.54
35:d:276:ILE:HG22	35:d:278:LYS:H	1.72	0.54
49:s:81:ARG:NH2	53:A:772:U:OP1	2.40	0.54
1:D:202:ARG:O	53:A:851:A:N6	2.41	0.54
30:8:125:LYS:HG2	54:B:1628:C:H5'	1.89	0.54
15:S:169:ARG:HB3	15:S:186:VAL:O	2.07	0.54
48:r:113:ARG:HB3	48:r:180:LEU:HD11	1.89	0.54
1:D:132:ASP:OD2	1:D:135:ARG:NH1	2.39	0.54
19:W:54:LYS:NZ	19:W:69:THR:OG1	2.38	0.54
20:X:226:LEU:HD12	21:Y:155:LEU:HB3	1.89	0.54
24:1:47:ASP:O	24:1:51:LYS:HA	2.07	0.54
36:e:55:ARG:NH1	36:e:149:LEU:O	2.41	0.54
49:s:332:LEU:HD13	49:s:372:TYR:HB2	1.89	0.54
2:E:142:MET:HE2	2:E:182:THR:HA	1.90	0.54
46:p:79:SER:OG	46:p:100:GLU:OE2	2.24	0.54
21:Y:64:LEU:O	21:Y:67:PHE:HB2	2.08	0.54
36:e:152:LYS:HZ3	36:e:256:THR:HG21	1.71	0.54
16:T:149:ARG:O	53:A:2:C:O2'	2.21	0.54
17:U:66:ALA:HB2	17:U:100:ALA:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:27:GLN:OE1	33:b:28:ARG:NH1	2.41	0.54
16:T:48:SER:O	16:T:49:ARG:NH1	2.39	0.54
18:V:156:LYS:NZ	18:V:157:PRO:O	2.41	0.54
8:L:55:PRO:HB2	8:L:75:LEU:HD11	1.90	0.54
8:L:118:ARG:NH1	50:u:200:ASP:O	2.41	0.54
13:Q:116:ILE:HD12	13:Q:178:LYS:HB3	1.89	0.54
7:K:29:GLY:HA3	53:A:570:C:H5'	1.88	0.54
27:5:105:TYR:HB2	27:5:220:LEU:HD23	1.90	0.54
7:K:154:ARG:HD3	48:r:129:PRO:HG3	1.90	0.53
35:d:190:GLU:OE2	35:d:215:ARG:NH1	2.41	0.53
26:3:131:LYS:O	26:3:136:LYS:NZ	2.33	0.53
29:7:93:MET:HB3	29:7:100:CYS:SG	2.48	0.53
48:r:114:LYS:HA	48:r:180:LEU:HD21	1.89	0.53
3:F:103:GLN:HE22	3:F:250:VAL:H	1.56	0.53
12:P:39:VAL:HG12	12:P:41:ASN:H	1.74	0.53
21:Y:72:LYS:O	21:Y:76:GLN:NE2	2.42	0.53
36:e:64:THR:HG22	36:e:66:LEU:H	1.72	0.53
2:E:266:ARG:NH1	53:A:1476:G:O3'	2.41	0.53
7:K:177:ARG:NH2	53:A:1513:U:O2	2.41	0.53
9:M:117:ASP:HA	9:M:155:GLU:HB2	1.89	0.53
26:3:100:ARG:NH1	53:A:84:G:OP1	2.37	0.53
9:M:19:LEU:HD11	45:o:92:LEU:HB3	1.90	0.53
12:P:144:MET:HB3	12:P:172:LEU:HA	1.89	0.53
35:d:81:THR:HB	35:d:262:HIS:HE1	1.73	0.53
36:e:270:ALA:O	36:e:273:ARG:NH1	2.42	0.53
46:p:98:LYS:NZ	46:p:138:GLU:OE2	2.31	0.53
52:w:138:LEU:HD13	52:w:144:ILE:HG12	1.89	0.53
2:E:208:ALA:HB2	2:E:297:VAL:HG12	1.90	0.53
21:Y:193:ARG:NH2	53:A:36:C:OP1	2.41	0.53
42:k:83:ALA:HA	42:k:86:MET:HE2	1.89	0.53
5:I:34:THR:O	10:N:244:LYS:NZ	2.42	0.53
15:S:162:GLU:HG2	15:S:192:VAL:HB	1.89	0.53
53:A:988:U:H3'	53:A:989:C:H2'	1.89	0.53
53:A:1063:G:H2'	53:A:1064:A:C8	2.43	0.53
19:W:49:ARG:HH21	19:W:71:ARG:HH12	1.57	0.53
2:E:104:LEU:HB2	2:E:121:LEU:HB2	1.91	0.53
5:I:132:LYS:NZ	5:I:144:LEU:O	2.41	0.53
9:M:202:LYS:HB2	9:M:263:ARG:HB3	1.91	0.53
28:6:214:TRP:HB2	28:6:240:ILE:HB	1.90	0.53
53:A:521:A:N6	53:A:528:A:OP2	2.42	0.53
2:E:275:ARG:HB3	2:E:284:TYR:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:111:ASN:HB2	50:u:164:THR:HA	1.90	0.53
49:s:41:VAL:O	49:s:43:ARG:NH1	2.42	0.53
9:M:51:ARG:NH2	53:A:232:C:HO2'	2.07	0.52
11:O:58:LYS:HB3	13:Q:269:MET:HE3	1.90	0.52
1:D:217:LEU:HG	1:D:227:GLN:HB2	1.91	0.52
54:B:1607:U:O4	54:B:1664:G:O6	2.27	0.52
5:I:53:TYR:HA	10:N:209:ASN:HD21	1.74	0.52
11:O:131:PRO:HD2	23:O:134:THR:HG22	1.91	0.52
20:X:113:GLU:HG2	20:X:124:THR:HG22	1.90	0.52
48:r:153:ARG:CZ	48:r:179:PRO:HD3	2.39	0.52
8:L:51:TYR:HD1	8:L:53:ARG:H	1.56	0.52
30:8:165:ASP:OD2	36:e:185:ARG:NH1	2.42	0.52
33:b:37:GLY:O	33:b:44:ARG:NH2	2.43	0.52
44:m:51:LEU:HB3	44:m:67:ARG:HB3	1.89	0.52
48:r:124:ARG:NH1	48:r:153:ARG:O	2.41	0.52
3:F:293:PHE:HB2	38:g:55:THR:HG21	1.91	0.52
4:H:96:LEU:HD12	4:H:129:ALA:HB1	1.92	0.52
5:I:31:LYS:O	5:I:38:ARG:NH1	2.43	0.52
25:2:57:ASN:HD22	31:9:26:GLY:HA2	1.74	0.52
29:7:193:MET:HE3	29:7:194:PRO:HD2	1.90	0.52
30:8:133:ARG:HH22	37:f:116:SER:HB2	1.74	0.52
51:v:43:GLN:HA	57:v:101:PNS:H431	1.91	0.52
52:w:100:VAL:HB	52:w:142:GLN:HB2	1.91	0.52
1:D:199:GLU:HB2	1:D:202:ARG:HB2	1.92	0.52
1:D:269:ARG:NH2	53:A:320:G:OP1	2.43	0.52
34:c:60:ARG:NH2	34:c:65:ASN:O	2.43	0.52
49:s:271:LEU:O	49:s:273:LEU:N	2.43	0.52
1:D:189:VAL:HA	1:D:216:LEU:HD22	1.91	0.52
9:M:103:TYR:OH	38:g:93:ASN:OD1	2.26	0.52
12:P:123:VAL:HG21	28:6:123:ALA:HA	1.90	0.52
12:P:146:TYR:OH	12:P:158:MET:SD	2.67	0.52
14:R:76:SER:HB3	14:R:86:LEU:HD22	1.91	0.52
23:O:141:ILE:O	23:O:145:GLU:HB2	2.10	0.52
29:7:87:THR:O	29:7:90:SER:OG	2.24	0.52
26:3:183:ARG:HD2	28:6:366:LEU:HD11	1.92	0.52
53:A:46:U:H3'	53:A:47:U:H4'	1.91	0.52
12:P:126:GLU:OE2	12:P:130:ARG:NE	2.43	0.52
14:R:34:ARG:NH2	53:A:1012:A:OP1	2.39	0.52
24:1:20:MET:HB3	24:1:30:PHE:O	2.10	0.52
36:e:50:ALA:HB2	36:e:175:GLN:HG2	1.91	0.52
3:F:272:LYS:HD2	40:i:63:LEU:HA	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:22:VAL:HG22	45:o:95:LEU:HD11	1.92	0.51
11:O:108:LEU:HD12	11:O:133:LEU:HD13	1.91	0.51
20:X:90:ILE:HD11	20:X:105:TRP:HH2	1.75	0.51
50:u:166:ASP:HB2	50:u:184:THR:HG21	1.92	0.51
53:A:86:A:H2'	53:A:87:A:H8	1.73	0.51
31:9:28:ARG:O	53:A:707:G:O2'	2.27	0.51
36:e:51:LEU:HD12	36:e:188:ALA:HB1	1.91	0.51
49:s:225:ARG:NH1	53:A:779:G:OP2	2.42	0.51
20:X:86:ILE:HB	20:X:105:TRP:HB2	1.92	0.51
29:7:262:ASP:OD1	29:7:263:VAL:N	2.43	0.51
20:X:96:LYS:O	53:A:58:U:O2'	2.22	0.51
29:7:44:ARG:HB3	29:7:261:ILE:HD12	1.93	0.51
44:m:72:ARG:HH21	44:m:75:LEU:HD11	1.76	0.51
1:D:86:ASP:OD1	1:D:92:ARG:NE	2.39	0.51
14:R:57:ARG:NH2	15:S:170:ILE:O	2.35	0.51
38:g:111:ARG:HD3	53:A:211:A:H62	1.76	0.51
51:v:15:ALA:HA	51:v:18:ARG:HG2	1.93	0.51
51:v:19:GLN:HA	51:v:22:GLN:HB2	1.92	0.51
53:A:48:A:N3	53:A:241:C:O2'	2.39	0.51
6:J:128:GLU:HA	6:J:133:GLN:HE21	1.76	0.51
35:d:163:LEU:HD12	35:d:164:VAL:HG23	1.93	0.51
53:A:315:G:OP1	53:A:317:G:O2'	2.28	0.51
53:A:468:U:O2'	53:A:481:A:N3	2.42	0.51
3:F:92:ARG:NH2	53:A:208:U:O3'	2.43	0.51
3:F:220:ASP:O	3:F:245:ALA:N	2.43	0.51
7:K:21:LEU:HB3	7:K:59:ILE:HG12	1.92	0.51
47:q:133:VAL:O	47:q:137:GLN:OE1	2.29	0.51
9:M:140:LEU:HG	9:M:156:VAL:HG11	1.91	0.51
10:N:191:SER:N	10:N:194:THR:OG1	2.44	0.51
21:Y:101:LEU:HD13	31:9:70:LEU:HB3	1.93	0.51
43:l:114:SER:OG	43:l:115:ARG:N	2.44	0.51
53:A:566:C:N4	53:A:1018:C:O2	2.44	0.51
14:R:32:ARG:O	14:R:35:LYS:NZ	2.37	0.51
19:W:55:LYS:HD2	19:W:61:VAL:HG22	1.93	0.51
54:B:1609:U:O2	54:B:1616:A:N6	2.44	0.51
15:S:174:PHE:HA	15:S:180:PHE:O	2.11	0.51
23:0:110:CYS:HB3	23:0:113:CYS:SG	2.51	0.50
43:l:123:LYS:HG2	53:A:527:G:H5'	1.92	0.50
14:R:107:ILE:HG13	16:T:211:THR:HG21	1.92	0.50
20:X:41:VAL:HG11	20:X:83:GLU:HB3	1.93	0.50
28:6:365:TYR:HA	28:6:368:ARG:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:173:THR:HA	35:d:176:ILE:HG22	1.93	0.50
47:q:128:MET:HA	47:q:131:MET:HE2	1.92	0.50
48:r:153:ARG:NE	48:r:177:GLY:O	2.39	0.50
54:B:1628:C:H2'	54:B:1629:A:H8	1.77	0.50
9:M:143:GLU:OE2	28:6:377:TYR:N	2.38	0.50
10:N:176:LEU:HA	10:N:179:VAL:HG12	1.93	0.50
14:R:123:ARG:HE	14:R:143:SER:HA	1.76	0.50
17:U:18:ARG:NH1	31:9:59:GLU:OE1	2.44	0.50
37:f:178:LEU:HD21	37:f:184:LEU:HD21	1.93	0.50
49:s:215:GLU:OE2	49:s:267:LYS:NZ	2.41	0.50
53:A:307:U:H2'	53:A:308:A:H8	1.76	0.50
15:S:132:LYS:NZ	41:j:46:LEU:O	2.44	0.50
1:D:81:LYS:HB2	53:A:254:U:H5''	1.93	0.50
29:7:247:ASN:HD21	29:7:251:ILE:H	1.60	0.50
35:d:127:ASP:N	35:d:127:ASP:OD1	2.44	0.50
12:P:83:VAL:HA	12:P:91:GLU:O	2.12	0.50
13:Q:131:SER:HB3	50:u:119:ARG:HD3	1.93	0.50
16:T:50:LYS:NZ	53:A:1:G:OP1	2.38	0.50
19:W:101:LYS:HD3	19:W:129:THR:HG22	1.92	0.50
36:e:160:LEU:HD11	36:e:264:LEU:HD11	1.94	0.50
36:e:266:PRO:HD2	36:e:269:LEU:HB2	1.94	0.50
48:r:69:GLN:NE2	48:r:108:CYS:SG	2.84	0.50
53:A:1257:C:H2'	53:A:1258:C:H4'	1.94	0.50
1:D:207:ILE:HD13	1:D:214:GLY:HA3	1.92	0.50
1:D:237:LEU:HD23	1:D:239:THR:H	1.77	0.50
13:Q:235:ARG:HH12	53:A:796:A:H5''	1.76	0.50
15:S:118:ASN:C	15:S:118:ASN:ND2	2.70	0.50
26:3:108:LYS:NZ	53:A:75:U:O4	2.35	0.50
49:s:242:ARG:NH1	49:s:292:CYS:O	2.45	0.50
5:I:44:ARG:HG2	10:N:242:TRP:HZ3	1.76	0.50
11:O:16:ARG:NE	53:A:786:U:OP1	2.44	0.50
14:R:100:LYS:NZ	14:R:104:ASP:OD2	2.45	0.50
53:A:204:A:HO2'	53:A:420:A:HO2'	1.58	0.50
8:L:53:ARG:NH1	53:A:980:C:O2'	2.45	0.50
22:Z:101:LYS:HB3	22:Z:103:ILE:HG12	1.93	0.50
33:b:41:ARG:HA	33:b:44:ARG:HE	1.76	0.50
53:A:362:G:O2'	53:A:1195:C:O2	2.29	0.50
2:E:217:GLY:HA2	2:E:258:PRO:HB3	1.94	0.49
8:L:57:CYS:SG	8:L:58:ILE:N	2.85	0.49
19:W:100:THR:OG1	19:W:132:HIS:NE2	2.42	0.49
26:3:118:HIS:NE2	53:A:221:A:OP1	2.34	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:u:112:ILE:HG23	50:u:124:PHE:HB3	1.93	0.49
3:F:113:LYS:HD2	3:F:157:GLY:HA2	1.94	0.49
26:3:126:LYS:HD3	26:3:144:LEU:HA	1.94	0.49
46:p:128:ASN:OD1	46:p:129:ARG:N	2.44	0.49
2:E:182:THR:OG1	2:E:184:ASN:OD1	2.25	0.49
29:7:166:LEU:HD22	29:7:181:TYR:HE2	1.76	0.49
42:k:18:VAL:HG23	42:k:64:VAL:HG22	1.95	0.49
48:r:90:SER:HA	48:r:93:ILE:HD12	1.94	0.49
8:L:130:ARG:HG3	8:L:134:TYR:HE2	1.78	0.49
15:S:96:PHE:HB3	33:b:126:ILE:HD13	1.94	0.49
17:U:27:GLN:HG3	17:U:43:ARG:HB2	1.94	0.49
4:H:91:LYS:HE3	53:A:1084:A:H5''	1.95	0.49
11:O:13:ARG:NH2	53:A:993:C:OP1	2.43	0.49
17:U:54:ARG:HH12	49:s:314:GLN:NE2	2.09	0.49
28:6:157:LEU:O	28:6:161:LEU:CB	2.60	0.49
4:H:57:GLU:O	4:H:81:LYS:N	2.39	0.49
30:8:113:ARG:HE	30:8:116:LEU:HD12	1.77	0.49
36:e:205:LEU:HD21	37:f:175:GLN:HE22	1.75	0.49
9:M:222:TYR:HE1	9:M:262:PRO:HB3	1.77	0.49
22:Z:63:PRO:HG2	45:o:53:TYR:HA	1.93	0.49
47:q:79:PRO:HB2	47:q:83:ARG:HH12	1.77	0.49
48:r:85:ASP:OD1	48:r:85:ASP:N	2.45	0.49
7:K:62:THR:HG21	7:K:127:LEU:HD22	1.94	0.49
9:M:283:LEU:HD12	38:g:39:VAL:HB	1.94	0.49
12:P:39:VAL:HB	12:P:42:GLU:HG2	1.95	0.49
20:X:147:LYS:HG3	20:X:194:PHE:HZ	1.77	0.49
20:X:227:PHE:HE2	31:9:96:VAL:HG21	1.76	0.49
31:9:91:LEU:O	31:9:95:ALA:CB	2.61	0.49
53:A:455:C:OP2	53:A:593:C:O2'	2.31	0.49
4:H:133:SER:HG	4:H:136:ASN:H	1.61	0.49
10:N:234:ASP:HA	10:N:237:HIS:HB2	1.94	0.49
11:O:145:LEU:H	29:7:306:LEU:HD23	1.78	0.49
17:U:24:PHE:HB2	17:U:45:PRO:HG3	1.95	0.49
17:U:24:PHE:HE2	17:U:48:MET:HE3	1.78	0.49
20:X:116:SER:O	20:X:120:ASP:CA	2.61	0.49
20:X:147:LYS:HG3	20:X:194:PHE:CZ	2.47	0.49
28:6:198:ALA:O	28:6:254:TYR:OH	2.30	0.49
28:6:265:ILE:HG22	28:6:322:ARG:HG2	1.94	0.49
29:7:176:SER:O	29:7:319:ARG:NH1	2.46	0.49
40:i:118:TYR:OH	53:A:83:A:OP1	2.22	0.49
11:O:84:ASP:HB3	23:0:151:ALA:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:136:ILE:O	13:Q:151:LEU:HA	2.12	0.48
18:V:27:GLY:O	18:V:32:LYS:NZ	2.46	0.48
23:0:93:ARG:NH2	53:A:640:G:OP2	2.46	0.48
26:3:133:LEU:HA	26:3:136:LYS:HB2	1.94	0.48
27:5:123:LEU:HD22	27:5:220:LEU:HD11	1.95	0.48
38:g:96:VAL:HG12	38:g:110:ILE:HG12	1.94	0.48
5:I:160:LYS:NZ	5:I:164:MET:SD	2.78	0.48
9:M:56:GLU:OE1	53:A:370:G:O2'	2.30	0.48
15:S:54:THR:OG1	48:r:85:ASP:OD2	2.26	0.48
27:5:121:LEU:HD11	27:5:128:LEU:HB2	1.96	0.48
35:d:225:TYR:HA	35:d:231:LEU:HA	1.95	0.48
7:K:13:THR:HG21	16:T:208:ILE:HD11	1.95	0.48
20:X:143:PHE:O	20:X:147:LYS:HB2	2.13	0.48
21:Y:172:ILE:HD12	25:2:70:LEU:HD13	1.96	0.48
28:6:330:ILE:HD12	28:6:334:LEU:HD21	1.94	0.48
35:d:208:VAL:HB	35:d:252:LEU:HB2	1.94	0.48
46:p:182:ASN:OD1	46:p:185:ARG:NH2	2.46	0.48
53:A:1082:C:H2'	53:A:1083:A:H8	1.78	0.48
3:F:67:GLU:HG2	3:F:75:GLU:HB3	1.95	0.48
27:5:239:ILE:HD12	27:5:356:VAL:HG11	1.95	0.48
35:d:160:LEU:O	35:d:164:VAL:N	2.46	0.48
53:A:214:G:O2'	53:A:225:C:O2	2.30	0.48
53:A:533:G:N2	53:A:539:G:O6	2.46	0.48
28:6:327:VAL:HA	28:6:330:ILE:HG22	1.94	0.48
46:p:140:SER:OG	46:p:142:TYR:O	2.30	0.48
48:r:153:ARG:NH1	53:A:488:U:O2'	2.46	0.48
51:v:40:ARG:HH21	52:w:113:LEU:HD13	1.78	0.48
1:D:194:ASN:HD22	1:D:247:VAL:HG22	1.79	0.48
6:J:131:ALA:HB3	53:A:499:A:H4'	1.96	0.48
31:9:24:LYS:NZ	53:A:752:U:OP2	2.45	0.48
46:p:74:ASP:OD1	46:p:74:ASP:N	2.45	0.48
53:A:130:G:N1	53:A:133:A:OP2	2.36	0.48
1:D:126:VAL:HA	1:D:142:VAL:HG22	1.95	0.48
1:D:154:THR:N	1:D:157:MET:SD	2.83	0.48
27:5:125:LYS:NZ	27:5:364:LEU:HA	2.29	0.48
35:d:63:ALA:HA	53:A:678:A:H1'	1.96	0.48
37:f:101:THR:OG1	44:m:67:ARG:NH1	2.47	0.48
6:J:142:ARG:NH2	53:A:521:A:OP1	2.47	0.48
11:O:129:CYS:SG	23:0:156:THR:OG1	2.65	0.48
16:T:204:ARG:NH2	34:c:287:GLU:OE1	2.46	0.48
20:X:7:PRO:HB3	40:i:100:SER:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:181:SER:OG	34:c:182:GLU:N	2.46	0.48
50:u:178:HIS:HB3	50:u:180:MET:HE1	1.94	0.48
7:K:160:GLN:HA	7:K:163:ILE:HD12	1.94	0.48
9:M:42:GLY:HA2	53:A:352:G:H5'	1.96	0.48
19:W:122:LYS:HD3	28:6:51:TYR:HE1	1.78	0.48
33:b:89:ILE:HA	33:b:92:LYS:HD2	1.95	0.48
39:h:77:VAL:HG13	39:h:78:PHE:HD2	1.78	0.48
50:u:115:PRO:HG3	51:v:66:LEU:HA	1.96	0.48
3:F:241:ASN:HD22	47:q:25:TYR:N	2.11	0.48
18:V:199:MET:HA	18:V:202:MET:HB2	1.94	0.48
20:X:5:LYS:HE3	47:q:46:LEU:HD11	1.96	0.48
31:9:68:PHE:CZ	31:9:70:LEU:HB2	2.49	0.48
2:E:218:VAL:HG23	2:E:222:TRP:HD1	1.79	0.47
10:N:114:ASP:H	10:N:118:MET:HE2	1.78	0.47
26:3:122:TRP:NE1	26:3:159:ASP:OD1	2.40	0.47
30:8:149:GLU:HA	30:8:152:LEU:HG	1.96	0.47
42:k:54:ASP:N	42:k:54:ASP:OD1	2.46	0.47
12:P:58:LEU:HD13	28:6:322:ARG:HH21	1.78	0.47
27:5:133:PRO:HG3	27:5:239:ILE:HG21	1.96	0.47
48:r:153:ARG:HD2	48:r:154:TRP:CD1	2.49	0.47
50:u:107:ARG:NH2	50:u:182:PRO:HD3	2.29	0.47
53:A:358:G:N2	53:A:594:A:OP2	2.35	0.47
53:A:416:A:H2'	53:A:417:U:C6	2.49	0.47
1:D:130:ARG:NH1	53:A:718:A:O2'	2.47	0.47
2:E:266:ARG:HH12	53:A:1477:G:P	2.37	0.47
17:U:142:PRO:HB2	35:d:282:ILE:HG12	1.96	0.47
18:V:56:LEU:HD23	18:V:86:VAL:HG11	1.96	0.47
22:Z:53:HIS:HE1	22:Z:60:PRO:HD3	1.77	0.47
31:9:97:ALA:HA	31:9:100:ILE:HG22	1.96	0.47
36:e:178:TRP:HZ2	36:e:230:LYS:HZ1	1.61	0.47
50:u:125:VAL:O	50:u:177:ILE:HA	2.13	0.47
53:A:1542:C:H3'	53:A:1543:A:H8	1.80	0.47
4:H:75:ARG:NH2	20:X:100:ARG:HH22	2.13	0.47
8:L:145:VAL:O	50:u:119:ARG:NH2	2.46	0.47
17:U:41:GLN:NE2	53:A:700:A:OP1	2.30	0.47
28:6:162:PHE:HB3	28:6:165:ALA:HB3	1.96	0.47
53:A:640:G:O2'	53:A:1005:G:O6	2.29	0.47
12:P:63:ARG:NH1	19:W:139:GLU:OE2	2.46	0.47
17:U:79:ARG:NH2	53:A:696:G:OP1	2.47	0.47
29:7:178:ALA:HB2	29:7:320:SER:HB2	1.96	0.47
36:e:85:SER:HB2	44:m:49:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:K:110:GLY:O	7:K:114:LYS:NZ	2.38	0.47
12:P:144:MET:HG2	12:P:172:LEU:HD23	1.95	0.47
13:Q:255:LYS:HA	13:Q:258:GLN:HB2	1.97	0.47
29:7:155:GLU:HB2	29:7:166:LEU:HD11	1.97	0.47
3:F:276:GLN:O	38:g:90:ARG:NH2	2.48	0.47
4:H:56:VAL:HG12	4:H:82:LEU:HA	1.95	0.47
4:H:120:ARG:CZ	20:X:132:LEU:HB3	2.45	0.47
5:I:98:VAL:HG13	5:I:177:LEU:HB3	1.97	0.47
12:P:42:GLU:OE1	28:6:338:ARG:NH2	2.47	0.47
13:Q:282:ILE:O	13:Q:286:ILE:HG12	2.15	0.47
15:S:134:LEU:HB3	15:S:148:LEU:HD23	1.95	0.47
18:V:177:THR:HG22	31:9:71:LYS:H	1.79	0.47
20:X:89:GLN:HG2	20:X:100:ARG:HH11	1.78	0.47
22:Z:137:THR:HG22	22:Z:147:VAL:HA	1.96	0.47
27:5:125:LYS:HZ2	27:5:364:LEU:HA	1.79	0.47
29:7:144:ARG:NH1	29:7:267:PRO:O	2.48	0.47
34:c:179:THR:HG23	34:c:194:THR:HG21	1.96	0.47
40:i:97:MET:HE2	40:i:97:MET:HB3	1.78	0.47
42:k:78:GLY:HA2	42:k:81:LEU:HD13	1.97	0.47
43:l:133:SER:O	53:A:530:A:O2'	2.33	0.47
53:A:79:C:H4'	53:A:80:G:H8	1.79	0.47
8:L:126:SER:HA	13:Q:125:TYR:CZ	2.50	0.47
10:N:213:TRP:HB3	10:N:218:ILE:HD11	1.97	0.47
18:V:212:LYS:HB3	18:V:212:LYS:HE3	1.74	0.47
25:2:78:VAL:O	25:2:82:ARG:HG2	2.14	0.47
28:6:175:VAL:HG22	28:6:204:VAL:HG22	1.97	0.47
40:i:96:LYS:HE2	40:i:96:LYS:HB3	1.69	0.47
50:u:166:ASP:HA	50:u:181:LEU:HD23	1.97	0.47
53:A:361:A:N6	53:A:374:A:O2'	2.47	0.47
11:O:83:LYS:HA	11:O:83:LYS:HD3	1.72	0.47
15:S:118:ASN:OD1	53:A:586:U:O2'	2.30	0.47
30:8:114:ARG:HE	36:e:73:LEU:HD11	1.80	0.47
36:e:157:LEU:HD12	36:e:254:TRP:HB3	1.97	0.47
48:r:168:ARG:NH1	53:A:567:A:OP1	2.47	0.47
2:E:116:LYS:NZ	13:Q:165:GLU:OE1	2.43	0.47
7:K:171:THR:HG22	48:r:59:GLU:HG3	1.97	0.47
13:Q:235:ARG:NH2	53:A:796:A:OP1	2.42	0.47
21:Y:69:ASP:HB3	21:Y:111:MET:HE2	1.96	0.47
22:Z:109:LYS:NZ	53:A:411:U:O2	2.45	0.47
27:5:233:LYS:HA	27:5:286:PRO:HD2	1.97	0.47
1:D:137:ALA:HB3	1:D:152:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:300:HIS:HB2	49:s:361:ILE:HG22	1.97	0.46
51:v:51:ARG:HH11	57:v:101:PNS:H432	1.79	0.46
4:H:103:GLU:CD	4:H:104:ASN:H	2.23	0.46
6:J:102:ARG:NH1	53:A:516:C:O2	2.48	0.46
7:K:43:HIS:NE2	7:K:55:ASP:OD2	2.43	0.46
9:M:94:LYS:HG3	9:M:129:ILE:HG22	1.98	0.46
10:N:172:VAL:HG12	10:N:176:LEU:HG	1.96	0.46
22:Z:114:LYS:NZ	45:o:42:GLU:OE2	2.36	0.46
26:3:136:LYS:HG2	26:3:140:ARG:HD3	1.96	0.46
49:s:106:TYR:O	49:s:110:THR:CB	2.64	0.46
49:s:165:ARG:O	49:s:307:ARG:NH2	2.48	0.46
49:s:303:PRO:HD2	49:s:306:LEU:HD12	1.96	0.46
53:A:511:A:N6	53:A:536:C:O2'	2.48	0.46
12:P:80:ARG:O	12:P:94:VAL:HA	2.15	0.46
15:S:152:ASP:OD1	15:S:152:ASP:N	2.48	0.46
18:V:150:SER:HB3	18:V:152:ARG:HH12	1.80	0.46
26:3:107:VAL:HG21	26:3:161:MET:HE3	1.96	0.46
30:8:152:LEU:HD12	30:8:153:GLU:HG3	1.96	0.46
11:O:130:LEU:HD12	23:O:134:THR:HG22	1.98	0.46
19:W:71:ARG:NH2	53:A:1222:A:O4'	2.48	0.46
20:X:177:HIS:CE1	20:X:183:ARG:HH12	2.34	0.46
22:Z:86:ILE:HG23	22:Z:91:LEU:HB2	1.97	0.46
24:1:45:HIS:ND1	53:A:1182:C:O2'	2.38	0.46
35:d:147:GLU:O	35:d:151:CYS:N	2.44	0.46
36:e:91:ALA:O	36:e:95:ASN:ND2	2.37	0.46
40:i:79:TRP:HH2	53:A:15:C:H5'	1.79	0.46
48:r:105:THR:HG23	48:r:107:LEU:HG	1.98	0.46
9:M:54:LYS:NZ	53:A:349:G:OP2	2.47	0.46
9:M:292:LYS:O	9:M:296:SER:OG	2.31	0.46
12:P:81:LEU:N	12:P:144:MET:HE1	2.22	0.46
12:P:146:TYR:HE2	12:P:162:GLN:HE21	1.63	0.46
17:U:48:MET:HE2	17:U:53:LEU:HA	1.96	0.46
27:5:117:VAL:N	27:5:307:ASP:OD2	2.47	0.46
29:7:149:MET:HE2	29:7:272:THR:HG22	1.97	0.46
33:b:116:ARG:HH21	53:A:163:C:H3'	1.80	0.46
34:c:259:ARG:HB2	34:c:271:PHE:HB2	1.97	0.46
35:d:182:ARG:HB2	35:d:223:ALA:HB3	1.97	0.46
38:g:91:MET:HG3	53:A:213:G:H5'	1.98	0.46
38:g:110:ILE:HD12	38:g:147:LEU:HD23	1.98	0.46
10:N:132:THR:HG22	10:N:147:ILE:HA	1.97	0.46
27:5:297:ALA:HB3	27:5:303:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:129:ARG:NH1	54:B:1627:C:OP1	2.47	0.46
31:9:21:TRP:HZ2	31:9:30:PHE:HD1	1.63	0.46
40:i:112:LYS:NZ	53:A:339:G:OP1	2.43	0.46
46:p:151:LEU:HD23	46:p:154:ILE:HD12	1.97	0.46
53:A:1131:A:H2'	53:A:1132:A:C8	2.51	0.46
13:Q:122:ALA:HB2	13:Q:172:GLN:HE22	1.81	0.46
23:0:87:ILE:O	23:0:91:ARG:HB2	2.16	0.46
27:5:93:LEU:HB3	27:5:270:ILE:HD11	1.97	0.46
30:8:179:THR:OG1	44:m:61:GLY:O	2.30	0.46
32:a:75:ILE:HD11	32:a:77:ARG:HH22	1.80	0.46
49:s:110:THR:HG23	49:s:333:PHE:CG	2.51	0.46
50:u:118:MET:SD	50:u:197:ARG:NE	2.89	0.46
10:N:160:VAL:HG12	10:N:161:VAL:HG23	1.97	0.46
27:5:245:ILE:O	27:5:248:THR:OG1	2.30	0.46
28:6:216:LEU:HD23	28:6:240:ILE:HG13	1.98	0.46
30:8:99:ARG:HH12	30:8:102:PRO:HB3	1.81	0.46
43:l:123:LYS:NZ	53:A:521:A:N7	2.58	0.46
9:M:229:PHE:O	9:M:233:ARG:HG3	2.16	0.46
40:i:115:ARG:NH1	53:A:340:U:OP2	2.43	0.46
51:v:51:ARG:HH11	57:v:101:PNS:C39	2.29	0.46
52:w:90:TYR:HD2	52:w:93:ILE:HG12	1.81	0.46
2:E:148:GLY:HA2	2:E:175:THR:O	2.16	0.46
7:K:26:GLN:NE2	7:K:147:GLN:OE1	2.49	0.46
7:K:71:LYS:HG2	48:r:174:MET:SD	2.56	0.46
12:P:144:MET:O	12:P:174:GLU:N	2.49	0.46
27:5:208:THR:HG22	27:5:225:SER:HA	1.98	0.46
28:6:52:ARG:HB3	54:B:1637:C:H5'	1.98	0.46
33:b:30:SER:HB2	33:b:76:VAL:HB	1.97	0.46
4:H:59:TRP:HZ3	20:X:91:TYR:H	1.64	0.45
10:N:236:THR:O	10:N:238:LYS:NZ	2.40	0.45
20:X:149:PRO:HD2	20:X:152:ASP:HB3	1.98	0.45
42:k:39:SER:OG	42:k:40:GLU:N	2.49	0.45
49:s:272:PRO:O	53:A:704:A:N6	2.42	0.45
9:M:76:ILE:HA	26:3:113:ARG:HH11	1.81	0.45
28:6:176:ALA:HA	28:6:185:MET:O	2.16	0.45
30:8:174:GLU:HA	37:f:183:ARG:HA	1.98	0.45
53:A:1059:U:O4	53:A:1060:A:N6	2.50	0.45
6:J:108:VAL:HG21	6:J:154:ARG:HG2	1.98	0.45
12:P:58:LEU:HD11	28:6:265:ILE:HG21	1.99	0.45
30:8:163:LYS:O	36:e:207:ASN:ND2	2.49	0.45
51:v:9:VAL:HG22	51:v:55:LEU:HD11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A:247:A:O2'	53:A:313:U:O4	2.31	0.45
9:M:183:SER:HA	9:M:186:ILE:HD12	1.97	0.45
11:O:36:LEU:HD13	11:O:123:ILE:HG23	1.99	0.45
12:P:65:GLU:H	12:P:97:GLN:HE22	1.65	0.45
12:P:96:HIS:ND1	12:P:98:ASN:OD1	2.49	0.45
28:6:173:LEU:HD22	28:6:317:SER:HB3	1.98	0.45
28:6:233:LEU:HB3	28:6:298:PHE:HE1	1.81	0.45
28:6:352:PRO:O	28:6:369:TYR:OH	2.30	0.45
38:g:39:VAL:HG11	47:q:72:PRO:HB2	1.98	0.45
53:A:1007:A:H2'	53:A:1008:A:C8	2.52	0.45
2:E:131:LYS:HG2	2:E:146:SER:OG	2.17	0.45
13:Q:244:ARG:HH12	13:Q:246:ASP:HB3	1.82	0.45
22:Z:104:PRO:HA	22:Z:107:ASN:HB2	1.98	0.45
23:0:86:THR:O	23:0:90:ASN:ND2	2.50	0.45
48:r:188:SER:OG	48:r:189:ARG:N	2.49	0.45
1:D:227:GLN:HA	1:D:227:GLN:NE2	2.32	0.45
5:I:162:LYS:HG2	5:I:195:SER:HB3	1.99	0.45
6:J:69:LYS:HB3	6:J:81:LYS:HB3	1.99	0.45
7:K:114:LYS:HE2	53:A:1032:G:H5'	1.98	0.45
8:L:120:LYS:HA	8:L:142:GLN:HE22	1.81	0.45
8:L:130:ARG:HG3	8:L:134:TYR:CE2	2.51	0.45
25:2:87:ARG:NH2	53:A:122:G:N7	2.63	0.45
36:e:256:THR:OG1	36:e:257:LYS:N	2.50	0.45
48:r:118:CYS:HA	48:r:121:MET:HG2	1.99	0.45
51:v:10:LEU:HD22	52:w:116:VAL:HG21	1.98	0.45
7:K:15:ALA:HB3	34:c:269:LEU:HD22	1.99	0.45
11:O:33:LEU:HD21	11:O:59:LEU:HD13	1.97	0.45
13:Q:250:THR:HG23	13:Q:253:GLN:H	1.82	0.45
14:R:65:ARG:HH21	14:R:99:ARG:NH1	2.15	0.45
20:X:134:LEU:O	20:X:138:ALA:CB	2.64	0.45
34:c:86:ASP:N	34:c:86:ASP:OD1	2.50	0.45
45:o:56:ARG:NH2	53:A:390:A:O4'	2.48	0.45
50:u:199:TYR:HB2	51:v:57:LYS:HZ2	1.81	0.45
53:A:144:A:N3	53:A:192:U:O2'	2.45	0.45
53:A:648:A:H2'	53:A:649:A:C8	2.52	0.45
4:H:69:ARG:HA	4:H:69:ARG:HD2	1.75	0.45
10:N:101:HIS:O	10:N:105:MET:HG2	2.17	0.45
31:9:22:THR:HG23	31:9:24:LYS:H	1.82	0.45
40:i:73:LEU:HD11	47:q:31:PRO:HG3	1.98	0.45
49:s:212:ARG:HD3	49:s:379:LEU:HD12	1.98	0.45
53:A:472:A:O2'	53:A:592:C:OP1	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:ILE:HA	2:E:297:VAL:O	2.17	0.45
15:S:158:ALA:HB2	15:S:195:ILE:HD13	1.99	0.45
20:X:177:HIS:O	20:X:184:ARG:NH1	2.41	0.45
21:Y:112:LEU:HB3	21:Y:132:LEU:HD12	1.99	0.45
28:6:188:TYR:HE2	28:6:191:ASN:HB3	1.81	0.45
47:q:128:MET:HE3	47:q:128:MET:HB3	1.90	0.45
48:r:71:PRO:HD2	48:r:107:LEU:HD23	1.98	0.45
2:E:102:LEU:HD11	2:E:150:LYS:HD2	1.99	0.45
12:P:64:LYS:HA	12:P:97:GLN:HE22	1.81	0.45
18:V:202:MET:HE1	31:9:63:PRO:HA	2.00	0.45
27:5:251:HIS:O	27:5:371:LYS:NZ	2.38	0.45
29:7:81:MET:HB2	29:7:81:MET:HE3	1.60	0.45
36:e:61:LYS:HD3	36:e:62:PRO:HD2	1.99	0.45
46:p:52:SER:HB2	46:p:57:THR:HG21	1.97	0.45
2:E:78:CYS:SG	2:E:81:LYS:NZ	2.73	0.44
5:I:57:LYS:HA	5:I:57:LYS:HD2	1.82	0.44
20:X:208:LEU:O	20:X:212:ILE:HG13	2.17	0.44
21:Y:91:ARG:NE	21:Y:148:GLU:OE2	2.47	0.44
36:e:146:ARG:HA	36:e:151:ARG:HD2	1.97	0.44
49:s:148:ASP:O	49:s:152:GLN:HB2	2.17	0.44
53:A:1451:C:O2	53:A:1465:A:N6	2.40	0.44
2:E:264:ILE:HD11	2:E:266:ARG:HH21	1.82	0.44
4:H:58:ARG:NH1	4:H:77:HIS:O	2.50	0.44
8:L:100:PHE:HB3	13:Q:158:GLN:HE21	1.83	0.44
35:d:196:GLN:O	35:d:212:ILE:HA	2.17	0.44
53:A:615:U:H2'	53:A:616:A:H8	1.82	0.44
8:L:58:ILE:HD11	8:L:76:ALA:HB2	1.98	0.44
16:T:144:GLU:HB2	16:T:177:LYS:HB3	1.98	0.44
18:V:36:PRO:HG2	18:V:39:ILE:HG23	1.98	0.44
19:W:103:VAL:HG12	19:W:127:TYR:HE1	1.82	0.44
24:1:35:ASN:HB2	24:1:38:ARG:HG2	2.00	0.44
27:5:223:ARG:HH11	53:A:739:A:H5''	1.81	0.44
44:m:56:LEU:HA	44:m:75:LEU:HB2	1.99	0.44
50:u:171:ASP:HA	50:u:176:VAL:HG23	1.99	0.44
53:A:512:G:H1'	53:A:529:A:H2'	1.99	0.44
5:I:90:PHE:HE2	5:I:134:PHE:HB3	1.82	0.44
7:K:40:GLN:HB2	7:K:42:LEU:HD23	2.00	0.44
27:5:139:LEU:O	27:5:145:ASN:ND2	2.51	0.44
29:7:45:ASN:ND2	29:7:259:ASP:OD1	2.50	0.44
29:7:101:ARG:O	29:7:305:HIS:NE2	2.38	0.44
29:7:108:VAL:HB	29:7:113:TRP:CD1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:100:GLU:HG2	30:8:101:ARG:HE	1.82	0.44
31:9:24:LYS:HG2	53:A:751:G:H5'	1.98	0.44
47:q:42:PRO:HB3	47:q:52:LEU:HD11	1.99	0.44
2:E:123:GLN:HG3	2:E:282:ILE:HD13	1.99	0.44
5:I:31:LYS:NZ	53:A:436:A:N7	2.65	0.44
5:I:64:CYS:SG	48:r:69:GLN:NE2	2.86	0.44
13:Q:100:LEU:HD11	13:Q:286:ILE:HD13	2.00	0.44
21:Y:171:ASP:OD1	21:Y:171:ASP:N	2.50	0.44
26:3:124:ARG:NH2	53:A:1198:C:OP1	2.50	0.44
28:6:280:ASP:OD1	28:6:280:ASP:N	2.50	0.44
34:c:273:GLY:HA2	34:c:283:GLU:HA	1.99	0.44
44:m:56:LEU:HD13	44:m:66:ILE:HD12	2.00	0.44
54:B:1642:G:H2'	54:B:1643:A:C8	2.53	0.44
1:D:147:ARG:NH1	1:D:149:ARG:HE	2.16	0.44
6:J:25:ARG:HG2	6:J:65:PRO:HB3	2.00	0.44
7:K:5:SER:HB3	34:c:302:ARG:HH22	1.82	0.44
12:P:171:VAL:HG21	46:p:180:ILE:HD13	1.98	0.44
18:V:136:ARG:HD2	18:V:146:VAL:HG21	1.99	0.44
28:6:302:ASP:N	28:6:302:ASP:OD1	2.51	0.44
53:A:374:A:H2'	53:A:375:A:C8	2.53	0.44
4:H:59:TRP:HE1	4:H:81:LYS:HD3	1.83	0.44
11:O:38:ARG:NH1	11:O:82:GLU:OE1	2.50	0.44
31:9:39:LYS:HD3	53:A:35:A:C8	2.53	0.44
34:c:121:SER:OG	34:c:122:ASN:N	2.49	0.44
36:e:152:LYS:HB2	36:e:157:LEU:HD21	1.99	0.44
48:r:112:HIS:HA	48:r:115:ILE:HG22	1.99	0.44
8:L:82:LYS:NZ	8:L:108:ILE:O	2.48	0.44
12:P:51:ARG:NH1	28:6:228:PRO:O	2.51	0.44
18:V:144:VAL:HG21	18:V:153:ILE:HD13	1.99	0.44
27:5:107:PHE:HD2	27:5:222:VAL:HG23	1.83	0.44
53:A:112:G:O2'	53:A:123:G:O6	2.29	0.44
2:E:184:ASN:OD1	2:E:185:ALA:N	2.51	0.44
3:F:93:LEU:HB2	45:o:91:GLN:HE21	1.83	0.44
9:M:119:THR:O	9:M:123:ASN:HB2	2.18	0.44
12:P:54:ARG:HH12	12:P:79:HIS:CE1	2.35	0.44
15:S:188:THR:HG21	53:A:474:A:H1'	2.00	0.44
21:Y:123:ARG:HD3	35:d:64:GLY:HA2	2.00	0.44
28:6:39:ASP:N	28:6:39:ASP:OD1	2.50	0.44
28:6:188:TYR:CE2	28:6:191:ASN:HB3	2.53	0.44
39:h:139:LYS:HD2	39:h:142:GLU:HB3	2.00	0.44
53:A:1488:A:H2'	53:A:1489:A:H8	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:B:1663:C:H2'	54:B:1664:G:H8	1.83	0.44
1:D:123:GLU:HG2	27:5:258:PRO:HB3	2.00	0.43
3:F:218:LEU:HD23	3:F:260:VAL:HB	2.00	0.43
22:Z:140:LYS:HB3	22:Z:140:LYS:HE2	1.82	0.43
27:5:241:SER:OG	27:5:242:ARG:N	2.49	0.43
27:5:289:HIS:ND1	27:5:290:THR:HG23	2.33	0.43
29:7:61:ARG:NH2	35:d:235:GLN:OE1	2.49	0.43
35:d:183:TRP:HD1	35:d:222:LEU:HD13	1.83	0.43
46:p:97:SER:OG	46:p:98:LYS:N	2.51	0.43
1:D:74:ILE:HG12	1:D:148:LYS:HB2	2.00	0.43
6:J:32:GLY:O	6:J:36:GLY:N	2.48	0.43
6:J:132:LEU:HD11	53:A:500:G:H4'	1.99	0.43
7:K:142:VAL:HG11	33:b:133:PHE:HE1	1.83	0.43
9:M:76:ILE:HA	26:3:113:ARG:NH1	2.33	0.43
10:N:120:ALA:HB2	10:N:163:MET:HG3	2.00	0.43
18:V:149:ARG:HB2	18:V:152:ARG:HH22	1.83	0.43
26:3:175:ASP:HB3	26:3:178:GLN:HB2	2.00	0.43
36:e:200:MET:HA	36:e:241:GLY:HA2	2.00	0.43
42:k:36:THR:HG23	42:k:37:VAL:HG13	2.00	0.43
49:s:350:ASP:OD2	49:s:351:VAL:N	2.48	0.43
53:A:632:U:H2'	53:A:633:A:C8	2.52	0.43
53:A:1454:U:C4	53:A:1463:A:H8	2.36	0.43
1:D:183:PRO:HA	1:D:241:VAL:HA	1.99	0.43
2:E:257:MET:HB2	2:E:257:MET:HE3	1.81	0.43
3:F:93:LEU:HD13	45:o:95:LEU:HD13	2.00	0.43
3:F:162:TYR:CE1	3:F:164:MET:HE3	2.53	0.43
3:F:253:MET:HG2	3:F:259:LEU:HD12	2.00	0.43
11:O:52:MET:HE1	11:O:123:ILE:HG21	2.00	0.43
19:W:114:VAL:HA	19:W:117:ILE:HD12	2.00	0.43
21:Y:135:VAL:O	21:Y:139:MET:HG2	2.18	0.43
29:7:103:SER:HB2	29:7:127:PHE:HB3	2.00	0.43
50:u:159:ILE:HG12	50:u:170:VAL:HG22	2.00	0.43
1:D:183:PRO:HG3	1:D:241:VAL:HG22	2.01	0.43
2:E:142:MET:HE3	2:E:143:ALA:H	1.82	0.43
7:K:153:LYS:HG3	7:K:158:TYR:CE1	2.53	0.43
16:T:105:GLN:NE2	23:0:104:LYS:O	2.37	0.43
20:X:113:GLU:OE1	20:X:122:LYS:HB3	2.18	0.43
30:8:114:ARG:HG3	36:e:73:LEU:HD21	1.99	0.43
46:p:104:HIS:HB3	46:p:107:THR:HG22	2.00	0.43
50:u:150:LYS:HD3	50:u:151:CYS:H	1.84	0.43
2:E:212:GLY:HA2	2:E:262:GLY:HA3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:54:ARG:HA	12:P:57:GLU:HG2	2.00	0.43
16:T:77:ARG:HB3	16:T:80:ILE:HD11	2.00	0.43
16:T:145:SER:HA	16:T:175:PHE:O	2.19	0.43
17:U:134:ARG:HA	17:U:137:ARG:HG3	2.00	0.43
23:O:181:ARG:HD3	23:O:182:PRO:HD2	2.01	0.43
34:c:79:LEU:HD13	34:c:214:PHE:HE1	1.83	0.43
53:A:3:U:O2	53:A:145:A:N6	2.52	0.43
2:E:221:ARG:HA	2:E:261:MET:SD	2.59	0.43
3:F:108:ARG:HD3	3:F:161:TYR:CD2	2.53	0.43
7:K:67:PHE:HB2	7:K:72:TRP:CD1	2.53	0.43
20:X:112:ARG:HD3	20:X:112:ARG:HA	1.80	0.43
20:X:157:PHE:CD1	27:5:48:ARG:HG2	2.54	0.43
27:5:384:GLN:NE2	53:A:725:A:O2'	2.42	0.43
28:6:175:VAL:HB	28:6:187:VAL:HB	2.00	0.43
29:7:67:VAL:O	29:7:78:VAL:HA	2.18	0.43
31:9:17:ARG:HH21	53:A:119:A:H5''	1.83	0.43
32:a:105:GLU:HG3	32:a:109:ILE:HD12	2.01	0.43
53:A:201:A:O2'	53:A:230:A:N6	2.52	0.43
1:D:215:VAL:HB	1:D:227:GLN:HB3	2.00	0.43
9:M:202:LYS:HE3	9:M:263:ARG:HH21	1.83	0.43
10:N:50:LEU:HD21	10:N:120:ALA:HB3	2.01	0.43
12:P:88:HIS:O	12:P:119:THR:OG1	2.35	0.43
29:7:287:GLN:CD	29:7:288:PRO:HD3	2.43	0.43
34:c:161:THR:O	34:c:192:GLN:NE2	2.51	0.43
38:g:117:ILE:HD13	38:g:142:GLU:HB2	1.99	0.43
48:r:189:ARG:NH2	53:A:574:U:O2'	2.51	0.43
4:H:59:TRP:CE2	4:H:81:LYS:HB2	2.54	0.43
7:K:4:PHE:HB2	7:K:9:GLN:HB2	1.99	0.43
11:O:95:PRO:O	11:O:98:LYS:NZ	2.45	0.43
35:d:267:PRO:HG2	35:d:270:ALA:HB2	2.00	0.43
46:p:106:ALA:O	46:p:116:ARG:NH1	2.52	0.43
49:s:249:GLU:HB3	49:s:354:PRO:HG2	2.00	0.43
49:s:332:LEU:HD23	49:s:332:LEU:HA	1.89	0.43
53:A:385:U:H2'	53:A:386:G:H8	1.84	0.43
12:P:178:ILE:HG22	28:6:346:ARG:HH22	1.84	0.43
28:6:173:LEU:HD12	28:6:272:LEU:HD13	1.99	0.43
29:7:167:VAL:HG23	29:7:235:TYR:HB3	2.00	0.43
35:d:147:GLU:HA	35:d:150:LEU:HB2	1.99	0.43
45:o:54:MET:HE2	45:o:54:MET:HB3	1.95	0.43
53:A:415:A:H2'	53:A:416:A:C8	2.53	0.43
12:P:88:HIS:NE2	54:B:1644:G:O6	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:c:148:MET:HE3	34:c:148:MET:HB3	1.80	0.43
44:m:50:ARG:HB2	44:m:69:ARG:NH1	2.33	0.43
54:B:1622:A:H2'	54:B:1623:G:C8	2.54	0.43
3:F:110:SER:O	3:F:110:SER:OG	2.37	0.42
20:X:56:ASN:ND2	53:A:75:U:OP1	2.52	0.42
35:d:142:LYS:O	35:d:145:PHE:HB3	2.19	0.42
45:o:37:ARG:O	45:o:41:ILE:HG12	2.18	0.42
53:A:411:U:H2'	53:A:412:G:C8	2.54	0.42
1:D:157:MET:HE3	1:D:163:ILE:HD11	2.01	0.42
7:K:28:PRO:HG3	7:K:65:ILE:HG21	2.00	0.42
11:O:116:ASP:OD2	53:A:783:G:O2'	2.23	0.42
27:5:385:HIS:HB2	53:A:725:A:H1'	2.01	0.42
53:A:18:A:H2'	53:A:19:C:H4'	2.01	0.42
53:A:43:A:H2'	53:A:44:C:C2	2.54	0.42
53:A:49:G:H2'	53:A:50:C:H6	1.84	0.42
1:D:111:ARG:HA	1:D:111:ARG:HD2	1.91	0.42
4:H:123:LEU:HB3	4:H:129:ALA:HB2	2.01	0.42
5:I:79:ILE:HG23	5:I:80:ARG:HD3	2.01	0.42
7:K:127:LEU:HD23	7:K:127:LEU:HA	1.86	0.42
12:P:57:GLU:OE2	28:6:154:TYR:OH	2.38	0.42
13:Q:154:VAL:HA	13:Q:159:GLY:HA2	2.00	0.42
15:S:133:VAL:HG21	15:S:154:VAL:HG11	2.00	0.42
16:T:206:ARG:HA	53:A:164:U:C4	2.54	0.42
17:U:32:GLY:HA2	21:Y:121:ARG:HH22	1.85	0.42
26:3:179:LYS:HB3	26:3:179:LYS:HE3	1.90	0.42
29:7:285:ASN:HD21	29:7:295:ARG:HH21	1.67	0.42
34:c:137:LEU:HB3	34:c:157:VAL:HG22	2.01	0.42
40:i:74:ILE:HD11	40:i:82:GLY:N	2.34	0.42
53:A:501:U:C2	53:A:503:G:H4'	2.54	0.42
7:K:25:MET:O	7:K:149:ARG:NH1	2.53	0.42
7:K:78:SER:OG	53:A:565:C:N3	2.50	0.42
10:N:229:VAL:O	53:A:432:A:O2'	2.37	0.42
20:X:42:HIS:CG	20:X:86:ILE:HD11	2.54	0.42
28:6:234:HIS:ND1	28:6:255:LEU:O	2.53	0.42
35:d:186:VAL:HG13	35:d:219:ARG:HB3	2.01	0.42
36:e:174:PRO:HB3	36:e:195:LEU:HD23	2.01	0.42
51:v:32:PHE:O	51:v:36:ARG:HG2	2.19	0.42
53:A:424:G:H2'	53:A:425:U:C6	2.54	0.42
1:D:197:GLU:HB2	1:D:240:CYS:HB2	2.00	0.42
7:K:73:GLU:OE1	48:r:149:ARG:NH2	2.39	0.42
15:S:163:LYS:HG2	15:S:191:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:T:109:ASN:HD21	23:O:101:ILE:HD13	1.84	0.42
31:9:31:ARG:O	53:A:750:U:O2'	2.27	0.42
33:b:55:ALA:HB2	33:b:63:ILE:HD12	2.01	0.42
42:k:18:VAL:HG11	42:k:34:LEU:HD13	2.01	0.42
49:s:65:ARG:O	49:s:69:THR:HG23	2.19	0.42
52:w:114:ASP:HA	52:w:117:GLU:HG3	2.00	0.42
53:A:1488:A:H2'	53:A:1489:A:C8	2.55	0.42
8:L:82:LYS:NZ	8:L:107:LEU:HB3	2.34	0.42
9:M:69:GLY:O	53:A:365:U:O2'	2.32	0.42
9:M:78:ILE:HD13	26:3:124:ARG:HD3	2.00	0.42
14:R:34:ARG:HG2	14:R:37:ARG:HH21	1.84	0.42
24:1:22:SER:HA	24:1:56:PHE:CD1	2.55	0.42
27:5:108:HIS:CE1	27:5:110:ARG:HB3	2.54	0.42
27:5:208:THR:HA	27:5:224:GLY:O	2.19	0.42
53:A:431:C:H2'	53:A:432:A:H8	1.83	0.42
53:A:539:G:H3'	53:A:540:C:H5''	2.02	0.42
3:F:243:ILE:HG22	3:F:244:PRO:O	2.20	0.42
7:K:45:PRO:HB2	14:R:107:ILE:HD13	2.01	0.42
10:N:102:PHE:HE2	10:N:127:PRO:HG3	1.83	0.42
24:1:43:LEU:O	24:1:55:LEU:HA	2.18	0.42
36:e:216:LYS:HG2	36:e:228:GLY:HA2	2.01	0.42
48:r:71:PRO:HG3	48:r:74:ARG:HH21	1.84	0.42
8:L:41:VAL:HG11	8:L:121:THR:H	1.84	0.42
9:M:30:ASN:ND2	53:A:207:U:O3'	2.53	0.42
12:P:143:PHE:HB3	12:P:174:GLU:HA	2.02	0.42
13:Q:221:LYS:HB3	13:Q:244:ARG:HG2	2.01	0.42
19:W:125:VAL:HA	28:6:57:TYR:HE1	1.85	0.42
22:Z:38:ARG:HE	22:Z:38:ARG:HB2	1.74	0.42
27:5:151:ASP:OD1	27:5:151:ASP:N	2.52	0.42
28:6:268:LEU:O	28:6:318:PHE:HA	2.19	0.42
33:b:78:GLU:HG2	33:b:84:VAL:HG22	2.01	0.42
48:r:72:ILE:HG13	48:r:111:GLU:OE2	2.20	0.42
49:s:426:LEU:HD23	49:s:426:LEU:HA	1.94	0.42
52:w:129:GLU:HG2	52:w:151:LYS:HZ3	1.85	0.42
2:E:141:LYS:NZ	53:A:1532:U:OP2	2.53	0.42
10:N:105:MET:O	10:N:109:ILE:HG12	2.18	0.42
14:R:99:ARG:HG2	53:A:478:A:OP1	2.20	0.42
18:V:94:HIS:NE2	53:A:135:A:OP2	2.51	0.42
18:V:146:VAL:HG12	18:V:153:ILE:HG12	2.02	0.42
18:V:170:TRP:HE1	21:Y:80:LYS:NZ	2.18	0.42
20:X:7:PRO:HD2	20:X:10:LEU:HD22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:47:ASP:O	24:1:51:LYS:CA	2.67	0.42
27:5:201:ARG:HB2	27:5:230:LEU:HD21	2.02	0.42
28:6:192:GLU:HG3	28:6:320:GLN:HB2	2.01	0.42
29:7:99:TYR:O	29:7:103:SER:OG	2.31	0.42
34:c:81:GLU:OE1	34:c:81:GLU:N	2.53	0.42
35:d:165:THR:HG23	35:d:260:ARG:HB2	2.01	0.42
35:d:198:ARG:HB2	35:d:211:GLN:HB3	2.00	0.42
36:e:124:TRP:HB3	44:m:73:ARG:HG3	2.02	0.42
53:A:374:A:H2'	53:A:375:A:H8	1.84	0.42
13:Q:287:GLU:HA	13:Q:290:LYS:HZ3	1.85	0.42
16:T:137:ARG:NH1	29:7:95:LEU:O	2.53	0.42
17:U:148:PRO:HB3	35:d:175:ASP:HB2	2.01	0.42
18:V:134:GLU:N	18:V:134:GLU:OE2	2.52	0.42
30:8:164:ARG:HE	37:f:86:TYR:C	2.27	0.42
37:f:104:GLU:HG3	37:f:155:ARG:HE	1.85	0.42
53:A:67:A:N6	53:A:90:G:H1'	2.35	0.42
53:A:542:C:H2'	53:A:543:A:H8	1.83	0.42
54:B:1663:C:H2'	54:B:1664:G:C8	2.54	0.42
2:E:61:ILE:HD11	11:O:149:LEU:HD11	2.01	0.41
19:W:101:LYS:HD2	37:f:56:ILE:HG21	2.02	0.41
27:5:353:HIS:CE1	27:5:379:ASP:H	2.38	0.41
28:6:235:TRP:HE3	28:6:237:LEU:HD13	1.85	0.41
49:s:257:VAL:HG12	49:s:259:ILE:H	1.84	0.41
1:D:126:VAL:HG13	1:D:140:ALA:HB1	2.03	0.41
3:F:160:SER:HB3	40:i:80:LEU:HD13	2.01	0.41
3:F:167:MET:HG3	40:i:62:ILE:HG22	2.01	0.41
6:J:141:VAL:HA	6:J:144:ILE:HG12	2.02	0.41
9:M:97:SER:HA	9:M:141:VAL:HB	2.03	0.41
11:O:131:PRO:HB3	23:0:184:TRP:HZ3	1.85	0.41
18:V:61:THR:HG23	18:V:123:VAL:HB	2.02	0.41
21:Y:208:PHE:O	21:Y:212:GLU:HG2	2.20	0.41
31:9:33:ARG:NH1	53:A:31:U:O4	2.53	0.41
53:A:165:A:O2'	53:A:166:A:N7	2.51	0.41
7:K:74:GLN:HA	48:r:161:PRO:HA	2.02	0.41
9:M:37:GLU:HB3	53:A:230:A:H5''	2.01	0.41
15:S:201:ALA:HA	15:S:202:PRO:HD3	1.91	0.41
19:W:83:VAL:HG22	19:W:89:LEU:HD13	2.02	0.41
29:7:106:ALA:HB1	29:7:125:ILE:HG23	2.02	0.41
31:9:71:LYS:O	31:9:73:TYR:N	2.53	0.41
36:e:128:PHE:HE1	44:m:55:LEU:HD12	1.85	0.41
49:s:411:LYS:HE2	49:s:411:LYS:HB2	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A:740:U:H2'	53:A:741:U:H6	1.86	0.41
5:I:97:ALA:HB3	5:I:154:LEU:HB2	2.01	0.41
6:J:66:LEU:HD22	6:J:82:ILE:HD11	2.03	0.41
9:M:72:THR:HA	9:M:73:PRO:HD3	1.94	0.41
11:O:108:LEU:HD13	23:O:122:LEU:HD21	2.02	0.41
12:P:103:VAL:HA	28:6:147:HIS:HE2	1.85	0.41
37:f:81:ASN:HB3	37:f:86:TYR:HD1	1.85	0.41
38:g:104:ASN:HD22	53:A:419:U:H1'	1.84	0.41
39:h:90:SER:OG	39:h:122:ARG:NH2	2.53	0.41
39:h:120:MET:HE2	39:h:120:MET:HB3	1.79	0.41
44:m:53:PRO:HB2	44:m:65:HIS:HD2	1.85	0.41
53:A:575:A:H1'	53:A:576:A:C8	2.55	0.41
53:A:722:U:H2'	53:A:724:A:H62	1.86	0.41
2:E:76:LYS:HG3	2:E:170:LEU:HD21	2.02	0.41
15:S:164:THR:HG22	33:b:107:GLN:HB2	2.03	0.41
19:W:56:MET:HG3	19:W:57:GLU:N	2.36	0.41
19:W:67:ILE:HG21	19:W:131:VAL:HG21	2.03	0.41
25:2:82:ARG:NH2	25:2:89:SER:O	2.54	0.41
28:6:56:ARG:NE	54:B:1625:A:OP1	2.53	0.41
28:6:182:ASP:OD1	28:6:183:ASP:N	2.54	0.41
36:e:161:VAL:HG23	36:e:174:PRO:HG3	2.03	0.41
49:s:254:ASP:HA	49:s:389:ARG:HG2	2.01	0.41
53:A:79:C:OP2	53:A:1229:C:O2'	2.27	0.41
53:A:197:A:N1	53:A:349:G:O2'	2.47	0.41
53:A:1474:A:H2'	53:A:1475:A:H8	1.86	0.41
10:N:66:PRO:HB2	53:A:436:A:H5''	2.03	0.41
15:S:108:VAL:HG12	15:S:114:ILE:HD11	2.01	0.41
28:6:185:MET:HE1	46:p:189:ARG:HA	2.02	0.41
54:B:1621:A:H61	54:B:1645:A:H3'	1.85	0.41
17:U:54:ARG:HH12	49:s:314:GLN:CD	2.29	0.41
19:W:145:VAL:HG21	28:6:343:GLU:HB2	2.02	0.41
28:6:256:PRO:HA	28:6:257:PRO:HD3	1.89	0.41
28:6:275:GLN:HG3	28:6:311:MET:HE1	2.02	0.41
29:7:175:ILE:O	29:7:319:ARG:NH2	2.54	0.41
34:c:227:GLU:OE1	34:c:302:ARG:NH2	2.54	0.41
38:g:142:GLU:HG3	45:o:88:ILE:HG13	2.03	0.41
54:B:1604:G:H2'	54:B:1605:A:H8	1.86	0.41
5:I:120:LYS:NZ	5:I:157:GLU:OE1	2.35	0.41
7:K:166:PHE:HB2	48:r:87:LEU:HD22	2.01	0.41
14:R:119:LEU:HD11	32:a:58:ILE:HD13	2.02	0.41
15:S:178:LYS:NZ	53:A:455:C:H5'	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:157:LEU:HB3	36:e:254:TRP:HB3	2.02	0.41
50:u:196:LEU:HD11	51:v:60:VAL:HG23	2.03	0.41
52:w:93:ILE:HG22	52:w:110:LEU:HD21	2.03	0.41
2:E:221:ARG:NH2	53:A:1438:U:OP2	2.54	0.41
5:I:158:GLU:HA	5:I:159:PRO:HD3	1.85	0.41
6:J:125:ALA:HB2	6:J:140:VAL:HG21	2.03	0.41
17:U:28:LEU:HA	17:U:42:PHE:HA	2.02	0.41
19:W:128:LYS:HE2	19:W:128:LYS:HB3	1.93	0.41
23:0:136:GLU:HG3	23:0:139:ARG:HH21	1.84	0.41
24:1:15:ASN:O	24:1:36:ARG:NH2	2.50	0.41
29:7:162:TYR:HB3	29:7:189:LEU:HD11	2.02	0.41
40:i:105:ASP:OD1	40:i:105:ASP:N	2.54	0.41
42:k:13:VAL:HB	42:k:94:ILE:HD11	2.02	0.41
46:p:100:GLU:HB3	46:p:136:THR:HG22	2.03	0.41
48:r:92:PHE:HE2	48:r:107:LEU:HD21	1.86	0.41
49:s:177:LEU:HD23	49:s:177:LEU:HA	1.90	0.41
53:A:241:C:H2'	53:A:242:A:C8	2.56	0.41
54:B:1603:A:H2'	54:B:1604:G:C8	2.56	0.41
2:E:298:LYS:NZ	53:A:1534:C:OP1	2.49	0.41
3:F:167:MET:HE3	3:F:279:ARG:NH2	2.35	0.41
3:F:211:ARG:HB2	39:h:58:ARG:NH2	2.35	0.41
9:M:133:LYS:NZ	53:A:219:C:OP1	2.47	0.41
12:P:65:GLU:H	12:P:97:GLN:NE2	2.18	0.41
15:S:169:ARG:NH2	53:A:475:G:OP1	2.54	0.41
27:5:318:PHE:CZ	27:5:322:LEU:HD12	2.56	0.41
27:5:355:LEU:HA	27:5:375:TRP:O	2.20	0.41
35:d:121:SER:HB3	35:d:197:VAL:HG23	2.03	0.41
46:p:81:CYS:O	46:p:98:LYS:HB3	2.21	0.41
48:r:113:ARG:HA	48:r:116:GLU:HG2	2.03	0.41
49:s:284:VAL:HG12	49:s:342:TYR:HE2	1.85	0.41
53:A:86:A:H2'	53:A:87:A:C8	2.54	0.41
8:L:64:ASN:HD21	53:A:1472:A:H5''	1.86	0.40
21:Y:100:LYS:HE2	31:9:68:PHE:CE2	2.56	0.40
27:5:125:LYS:NZ	27:5:364:LEU:HD13	2.36	0.40
27:5:125:LYS:HA	27:5:253:LEU:HD21	2.03	0.40
44:m:70:GLU:O	44:m:72:ARG:N	2.54	0.40
53:A:402:A:H2'	53:A:403:A:C8	2.56	0.40
4:H:87:LYS:HE2	4:H:87:LYS:HB3	1.83	0.40
5:I:40:MET:HE1	5:I:48:MET:HE2	2.04	0.40
9:M:236:LEU:HD23	9:M:236:LEU:HA	1.79	0.40
10:N:94:GLY:CA	10:N:154:VAL:O	2.68	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:91:VAL:HG11	41:j:24:GLY:HA3	2.02	0.40
15:S:175:ARG:HB2	15:S:180:PHE:HB3	2.02	0.40
19:W:81:VAL:HG11	19:W:131:VAL:HG13	2.04	0.40
20:X:18:GLU:OE2	53:A:19:C:N4	2.54	0.40
20:X:116:SER:O	20:X:120:ASP:N	2.55	0.40
27:5:121:LEU:HD13	27:5:126:THR:OG1	2.21	0.40
28:6:177:TYR:CE1	28:6:202:PRO:HG3	2.55	0.40
29:7:234:LYS:H	29:7:234:LYS:HG2	1.76	0.40
34:c:242:VAL:HG12	34:c:246:LYS:NZ	2.36	0.40
40:i:99:GLY:HA2	40:i:102:MET:HE3	2.02	0.40
49:s:160:ARG:NH2	53:A:739:A:OP1	2.38	0.40
49:s:246:GLN:OE1	49:s:353:ARG:NH1	2.54	0.40
53:A:169:C:H2'	53:A:170:C:C6	2.56	0.40
53:A:381:A:H2'	53:A:382:A:C8	2.55	0.40
53:A:457:A:H4'	53:A:581:A:C5	2.55	0.40
53:A:1070:A:H2'	53:A:1071:A:H8	1.86	0.40
3:F:249:ASN:OD1	3:F:249:ASN:N	2.54	0.40
9:M:116:ILE:HB	9:M:154:ILE:HA	2.04	0.40
14:R:114:LYS:HD3	32:a:45:CYS:SG	2.61	0.40
22:Z:36:PHE:O	53:A:449:U:O2'	2.37	0.40
27:5:98:LEU:HD13	27:5:272:ASP:HB2	2.03	0.40
38:g:97:TYR:O	38:g:108:THR:HA	2.21	0.40
51:v:43:GLN:HG2	57:v:101:PNS:H431	2.03	0.40
53:A:1070:A:H2'	53:A:1071:A:C8	2.56	0.40
53:A:1447:C:N3	53:A:1469:G:N1	2.41	0.40
2:E:248:ILE:O	53:A:1045:A:O2'	2.39	0.40
3:F:63:GLN:HG2	3:F:81:ASP:HB3	2.03	0.40
9:M:58:GLN:NE2	53:A:350:U:O4	2.55	0.40
10:N:247:MET:HE3	10:N:249:LYS:HB3	2.04	0.40
11:O:41:ARG:HB3	23:0:138:ARG:HH22	1.85	0.40
13:Q:77:SER:HA	13:Q:78:PRO:HD3	1.95	0.40
18:V:145:ARG:NH2	18:V:155:PRO:O	2.54	0.40
18:V:170:TRP:HZ3	31:9:75:SER:HB2	1.87	0.40
23:0:109:VAL:HA	23:0:116:LEU:HA	2.03	0.40
27:5:223:ARG:HH12	53:A:740:U:P	2.43	0.40
33:b:30:SER:H	33:b:76:VAL:H	1.68	0.40
36:e:162:ARG:HD3	36:e:171:TRP:CE3	2.56	0.40
37:f:95:LEU:O	37:f:154:GLU:HA	2.21	0.40
38:g:132:LEU:HD21	38:g:153:PHE:HZ	1.85	0.40
48:r:39:VAL:HG21	48:r:52:ARG:HD2	2.04	0.40
48:r:100:LEU:HD22	48:r:104:ILE:HG21	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:103:GLN:NE2	3:F:249:ASN:HB2	2.35	0.40
3:F:108:ARG:NH2	53:A:99:C:H2'	2.36	0.40
13:Q:182:ARG:HA	13:Q:182:ARG:HD3	1.91	0.40
14:R:83:TYR:OH	14:R:99:ARG:NH1	2.55	0.40
19:W:104:TYR:O	28:6:57:TYR:OH	2.35	0.40
27:5:343:GLN:HE22	27:5:420:HIS:HB3	1.87	0.40
28:6:240:ILE:HD13	28:6:248:GLY:HA3	2.02	0.40
33:b:73:PRO:HG2	33:b:89:ILE:HG13	2.04	0.40
36:e:162:ARG:HD3	36:e:171:TRP:HE3	1.86	0.40
49:s:79:LYS:HB3	49:s:79:LYS:HE3	1.92	0.40
50:u:150:LYS:HD3	50:u:151:CYS:N	2.36	0.40
53:A:616:A:H2'	53:A:617:U:C6	2.56	0.40
53:A:1464:C:H6	53:A:1464:C:H2'	1.74	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	216/305 (71%)	201 (93%)	14 (6%)	1 (0%)	24	57
2	E	281/348 (81%)	274 (98%)	7 (2%)	0	100	100
3	F	248/311 (80%)	239 (96%)	9 (4%)	0	100	100
4	H	93/267 (35%)	89 (96%)	4 (4%)	0	100	100
5	I	154/261 (59%)	142 (92%)	12 (8%)	0	100	100
6	J	138/192 (72%)	127 (92%)	11 (8%)	0	100	100
7	K	175/178 (98%)	167 (95%)	8 (5%)	0	100	100
8	L	113/145 (78%)	108 (96%)	5 (4%)	0	100	100
9	M	285/296 (96%)	271 (95%)	14 (5%)	0	100	100
10	N	203/251 (81%)	198 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	O	150/175 (86%)	145 (97%)	5 (3%)	0	100	100
12	P	139/180 (77%)	134 (96%)	5 (4%)	0	100	100
13	Q	215/292 (74%)	206 (96%)	9 (4%)	0	100	100
14	R	138/149 (93%)	133 (96%)	5 (4%)	0	100	100
15	S	154/205 (75%)	149 (97%)	5 (3%)	0	100	100
16	T	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
17	U	135/153 (88%)	127 (94%)	8 (6%)	0	100	100
18	V	188/216 (87%)	180 (96%)	8 (4%)	0	100	100
19	W	107/148 (72%)	102 (95%)	5 (5%)	0	100	100
20	X	241/256 (94%)	237 (98%)	4 (2%)	0	100	100
21	Y	174/250 (70%)	168 (97%)	6 (3%)	0	100	100
22	Z	118/161 (73%)	110 (93%)	8 (7%)	0	100	100
23	0	106/188 (56%)	102 (96%)	4 (4%)	0	100	100
24	1	50/65 (77%)	49 (98%)	1 (2%)	0	100	100
25	2	41/92 (45%)	41 (100%)	0	0	100	100
26	3	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
27	5	383/423 (90%)	366 (96%)	16 (4%)	1 (0%)	36	67
28	6	316/380 (83%)	299 (95%)	17 (5%)	0	100	100
29	7	285/338 (84%)	265 (93%)	20 (7%)	0	100	100
30	8	97/206 (47%)	90 (93%)	7 (7%)	0	100	100
31	9	113/137 (82%)	105 (93%)	8 (7%)	0	100	100
32	a	78/142 (55%)	76 (97%)	2 (3%)	0	100	100
33	b	146/215 (68%)	138 (94%)	8 (6%)	0	100	100
34	c	271/332 (82%)	262 (97%)	9 (3%)	0	100	100
35	d	203/306 (66%)	197 (97%)	6 (3%)	0	100	100
36	e	211/279 (76%)	196 (93%)	15 (7%)	0	100	100
37	f	110/212 (52%)	103 (94%)	7 (6%)	0	100	100
38	g	127/166 (76%)	119 (94%)	8 (6%)	0	100	100
39	h	96/158 (61%)	93 (97%)	3 (3%)	0	100	100
40	i	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
41	j	83/123 (68%)	83 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
42	k	76/112 (68%)	73 (96%)	3 (4%)	0	100	100
43	l	21/138 (15%)	21 (100%)	0	0	100	100
44	m	43/128 (34%)	38 (88%)	5 (12%)	0	100	100
45	o	77/102 (76%)	75 (97%)	2 (3%)	0	100	100
46	p	119/206 (58%)	118 (99%)	1 (1%)	0	100	100
47	q	122/222 (55%)	121 (99%)	1 (1%)	0	100	100
48	r	140/196 (71%)	134 (96%)	6 (4%)	0	100	100
49	s	366/439 (83%)	355 (97%)	11 (3%)	0	100	100
50	u	109/234 (47%)	100 (92%)	9 (8%)	0	100	100
51	v	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
52	w	77/156 (49%)	73 (95%)	4 (5%)	0	100	100
All	All	7941/11026 (72%)	7598 (96%)	341 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
27	5	216	GLU
1	D	207	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	179/245 (73%)	178 (99%)	1 (1%)	78	79
2	E	246/290 (85%)	246 (100%)	0	100	100
3	F	217/262 (83%)	216 (100%)	1 (0%)	81	80
4	H	86/228 (38%)	86 (100%)	0	100	100
5	I	145/232 (62%)	145 (100%)	0	100	100
6	J	113/150 (75%)	113 (100%)	0	100	100
7	K	155/156 (99%)	155 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	L	98/124 (79%)	98 (100%)	0	100	100
9	M	245/249 (98%)	245 (100%)	0	100	100
10	N	172/211 (82%)	172 (100%)	0	100	100
11	O	133/150 (89%)	133 (100%)	0	100	100
12	P	123/155 (79%)	123 (100%)	0	100	100
13	Q	199/256 (78%)	199 (100%)	0	100	100
14	R	118/126 (94%)	118 (100%)	0	100	100
15	S	141/180 (78%)	139 (99%)	2 (1%)	59	71
16	T	141/176 (80%)	141 (100%)	0	100	100
17	U	124/135 (92%)	124 (100%)	0	100	100
18	V	172/191 (90%)	172 (100%)	0	100	100
19	W	89/119 (75%)	89 (100%)	0	100	100
20	X	219/229 (96%)	219 (100%)	0	100	100
21	Y	159/223 (71%)	159 (100%)	0	100	100
22	Z	111/147 (76%)	111 (100%)	0	100	100
23	0	97/164 (59%)	97 (100%)	0	100	100
24	1	49/60 (82%)	49 (100%)	0	100	100
25	2	38/72 (53%)	38 (100%)	0	100	100
26	3	88/166 (53%)	88 (100%)	0	100	100
27	5	348/368 (95%)	348 (100%)	0	100	100
28	6	265/332 (80%)	265 (100%)	0	100	100
29	7	263/303 (87%)	261 (99%)	2 (1%)	73	77
30	8	91/190 (48%)	91 (100%)	0	100	100
31	9	99/112 (88%)	99 (100%)	0	100	100
32	a	78/133 (59%)	78 (100%)	0	100	100
33	b	130/186 (70%)	130 (100%)	0	100	100
34	c	241/288 (84%)	241 (100%)	0	100	100
35	d	193/274 (70%)	193 (100%)	0	100	100
36	e	188/236 (80%)	188 (100%)	0	100	100
37	f	101/188 (54%)	101 (100%)	0	100	100
38	g	119/148 (80%)	119 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
39	h	95/148 (64%)	95 (100%)	0	100	100
40	i	86/110 (78%)	86 (100%)	0	100	100
41	j	68/97 (70%)	68 (100%)	0	100	100
42	k	71/90 (79%)	71 (100%)	0	100	100
43	l	23/116 (20%)	23 (100%)	0	100	100
44	m	40/113 (35%)	40 (100%)	0	100	100
45	o	68/87 (78%)	68 (100%)	0	100	100
46	p	117/181 (65%)	117 (100%)	0	100	100
47	q	106/178 (60%)	106 (100%)	0	100	100
48	r	133/169 (79%)	132 (99%)	1 (1%)	73	77
49	s	326/381 (86%)	326 (100%)	0	100	100
50	u	105/200 (52%)	105 (100%)	0	100	100
51	v	59/60 (98%)	59 (100%)	0	100	100
52	w	73/136 (54%)	73 (100%)	0	100	100
All	All	7143/9520 (75%)	7136 (100%)	7 (0%)	87	87

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	205	GLN
3	F	184	GLN
15	S	84	ASN
15	S	118	ASN
29	7	232	HIS
29	7	284	HIS
48	r	146	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	195	ASN
1	D	205	GLN
1	D	249	ASN
2	E	202	GLN
3	F	103	GLN
3	F	228	GLN

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Mol	Chain	Res	Type
4	H	100	GLN
5	I	43	GLN
5	I	91	GLN
5	I	115	GLN
5	I	189	GLN
6	J	103	GLN
7	K	26	GLN
9	M	84	ASN
9	M	114	GLN
11	O	147	GLN
12	P	97	GLN
12	P	147	GLN
12	P	162	GLN
13	Q	158	GLN
14	R	89	ASN
15	S	91	GLN
15	S	190	GLN
16	T	62	GLN
16	T	75	HIS
16	T	210	HIS
18	V	73	GLN
19	W	51	GLN
19	W	72	HIS
19	W	110	ASN
20	X	4	HIS
20	X	27	HIS
20	X	94	ASN
20	X	177	HIS
20	X	215	GLN
20	X	237	GLN
21	Y	76	GLN
21	Y	157	GLN
22	Z	67	HIS
23	0	170	GLN
27	5	150	GLN
27	5	165	GLN
27	5	275	ASN
27	5	324	GLN
28	6	69	HIS
28	6	149	GLN
28	6	200	GLN
28	6	307	HIS

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Mol	Chain	Res	Type
29	7	45	ASN
29	7	232	HIS
29	7	255	HIS
36	e	248	ASN
38	g	106	GLN
39	h	99	ASN
40	i	120	HIS
42	k	15	GLN
42	k	80	HIS
43	l	135	ASN
44	m	46	GLN
44	m	65	HIS
45	o	58	GLN
45	o	96	ASN
46	p	96	ASN
46	p	163	GLN
47	q	142	ASN
49	s	152	GLN
49	s	191	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1032/1559 (66%)	250 (24%)	11 (1%)
54	B	51/69 (73%)	14 (27%)	1 (1%)
All	All	1083/1628 (66%)	264 (24%)	12 (1%)

All (264) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	5	A
53	A	6	A
53	A	7	C
53	A	8	C
53	A	9	U
53	A	11	G
53	A	19	C
53	A	23	C
53	A	24	U
53	A	30	U
53	A	34	U

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Mol	Chain	Res	Type
53	A	37	C
53	A	38	A
53	A	43	A
53	A	44	C
53	A	45	C
53	A	46	U
53	A	47	U
53	A	54	A
53	A	57	A
53	A	58	U
53	A	61	A
53	A	71	A
53	A	78	G
53	A	80	G
53	A	81	A
53	A	100	G
53	A	111	A
53	A	124	A
53	A	130	G
53	A	133	A
53	A	134	A
53	A	135	A
53	A	136	U
53	A	142	C
53	A	151	A
53	A	153	A
53	A	154	U
53	A	157	C
53	A	158	A
53	A	159	A
53	A	162	A
53	A	166	A
53	A	173	U
53	A	174	A
53	A	197	A
53	A	199	A
53	A	200	A
53	A	201	A
53	A	202	U
53	A	208	U
53	A	212	A
53	A	213	G

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Mol	Chain	Res	Type
53	A	216	G
53	A	218	G
53	A	222	A
53	A	223	A
53	A	231	C
53	A	232	C
53	A	233	C
53	A	248	G
53	A	257	G
53	A	303	G
53	A	315	G
53	A	316	A
53	A	317	G
53	A	322	C
53	A	330	C
53	A	331	C
53	A	332	G
53	A	345	G
53	A	351	U
53	A	352	G
53	A	360	U
53	A	361	A
53	A	362	G
53	A	366	C
53	A	367	U
53	A	369	A
53	A	389	C
53	A	390	A
53	A	395	A
53	A	404	A
53	A	409	C
53	A	413	U
53	A	427	A
53	A	441	C
53	A	443	G
53	A	454	A
53	A	455	C
53	A	456	U
53	A	466	C
53	A	471	U
53	A	472	A
53	A	477	G

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Mol	Chain	Res	Type
53	A	484	A
53	A	487	U
53	A	488	U
53	A	489	U
53	A	493	A
53	A	496	C
53	A	498	U
53	A	501	U
53	A	502	A
53	A	503	G
53	A	504	G
53	A	510	A
53	A	511	A
53	A	512	G
53	A	513	C
53	A	514	A
53	A	517	C
53	A	520	C
53	A	523	U
53	A	524	U
53	A	525	A
53	A	527	G
53	A	528	A
53	A	530	A
53	A	534	U
53	A	540	C
53	A	546	A
53	A	565	C
53	A	567	A
53	A	569	A
53	A	571	A
53	A	573	A
53	A	574	U
53	A	575	A
53	A	589	C
53	A	591	C
53	A	592	C
53	A	593	C
53	A	594	A
53	A	613	C
53	A	614	C
53	A	615	U

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Mol	Chain	Res	Type
53	A	627	A
53	A	629	U
53	A	630	G
53	A	651	A
53	A	652	C
53	A	654	U
53	A	662	C
53	A	675	G
53	A	701	U
53	A	703	A
53	A	704	A
53	A	711	A
53	A	714	A
53	A	720	A
53	A	723	C
53	A	726	C
53	A	731	A
53	A	734	U
53	A	735	C
53	A	736	A
53	A	737	U
53	A	744	C
53	A	745	C
53	A	746	U
53	A	747	C
53	A	748	A
53	A	756	C
53	A	757	C
53	A	761	C
53	A	765	G
53	A	771	C
53	A	773	C
53	A	774	A
53	A	776	A
53	A	788	A
53	A	798	A
53	A	838	C
53	A	841	C
53	A	842	A
53	A	850	C
53	A	851	A
53	A	852	U

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Mol	Chain	Res	Type
53	A	853	C
53	A	854	A
53	A	856	C
53	A	857	A
53	A	866	G
53	A	985	G
53	A	986	U
53	A	990	U
53	A	1013	C
53	A	1014	C
53	A	1016	G
53	A	1028	G
53	A	1029	C
53	A	1036	A
53	A	1037	A
53	A	1038	C
53	A	1039	A
53	A	1055	A
53	A	1062	G
53	A	1069	U
53	A	1070	A
53	A	1073	U
53	A	1075	A
53	A	1080	U
53	A	1134	A
53	A	1182	C
53	A	1183	A
53	A	1184	U
53	A	1191	A
53	A	1194	U
53	A	1195	C
53	A	1200	G
53	A	1201	U
53	A	1202	C
53	A	1209	A
53	A	1222	A
53	A	1223	A
53	A	1225	U
53	A	1231	A
53	A	1236	C
53	A	1240	A
53	A	1243	A

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Mol	Chain	Res	Type
53	A	1245	C
53	A	1247	G
53	A	1252	A
53	A	1253	G
53	A	1256	A
53	A	1258	C
53	A	1438	U
53	A	1439	U
53	A	1444	U
53	A	1452	U
53	A	1453	G
53	A	1459	A
53	A	1464	C
53	A	1469	G
53	A	1480	U
53	A	1488	A
53	A	1490	A
53	A	1492	C
53	A	1498	C
53	A	1507	A
53	A	1510	A
53	A	1514	C
53	A	1519	C
53	A	1520	A
53	A	1532	U
53	A	1537	A
53	A	1547	A
53	A	1548	A
53	A	1558	U
54	B	1607	U
54	B	1608	G
54	B	1609	U
54	B	1611	G
54	B	1614	U
54	B	1615	A
54	B	1631	C
54	B	1639	U
54	B	1640	A
54	B	1641	G
54	B	1644	G
54	B	1645	A
54	B	1649	C

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Mol	Chain	Res	Type
54	B	1651	A

All (12) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	A	43	A
53	A	135	A
53	A	153	A
53	A	360	U
53	A	502	A
53	A	516	C
53	A	573	A
53	A	787	A
53	A	837	A
53	A	1235	A
53	A	1531	A
54	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	$\# Z > 2$
57	PNS	v	101	-	14,20,21	2.21	3 (21%)	18,26,29	1.41	3 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	PNS	v	101	-	-	11/24/26/27	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	v	101	PNS	C39-N41	5.71	1.46	1.33
57	v	101	PNS	C34-N36	5.08	1.45	1.33
57	v	101	PNS	O35-C34	-2.26	1.19	1.23

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	v	101	PNS	C37-C38-C39	-3.77	106.11	112.39
57	v	101	PNS	C42-N41-C39	2.40	127.29	122.82
57	v	101	PNS	C37-N36-C34	-2.09	118.80	122.55

There are no chirality outliers.

All (11) torsion outliers are listed below:

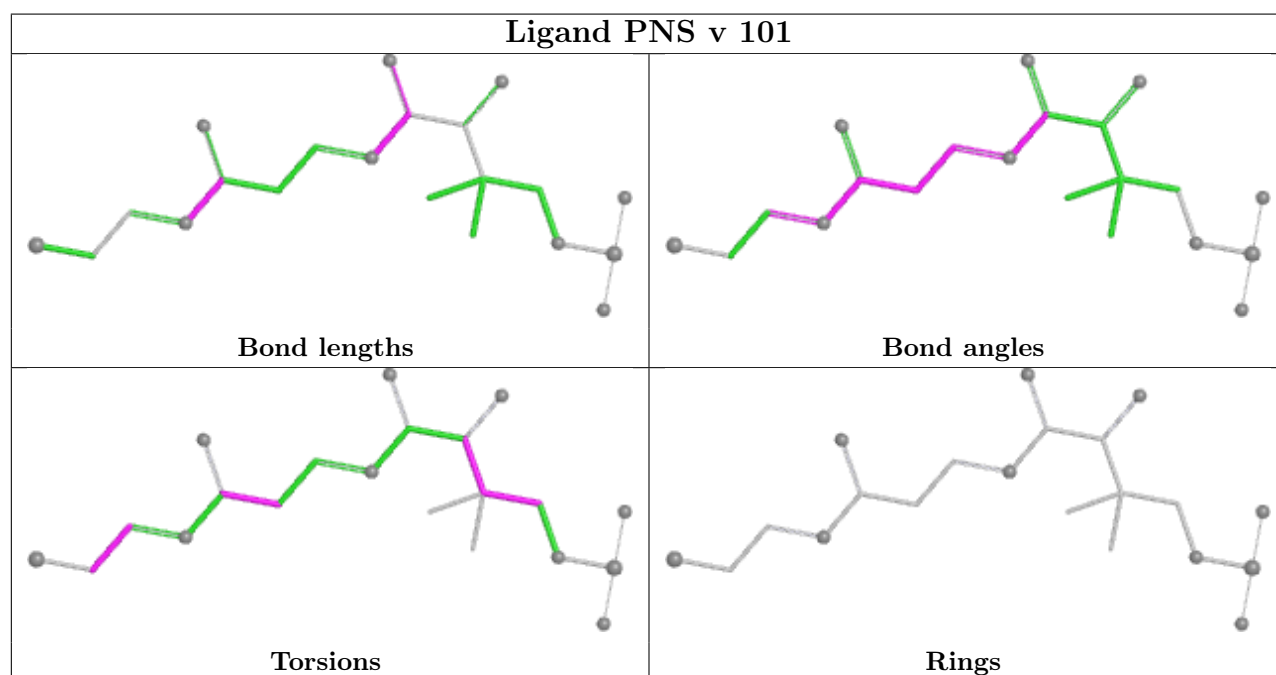
Mol	Chain	Res	Type	Atoms
57	v	101	PNS	O27-C28-C29-C30
57	v	101	PNS	O27-C28-C29-C31
57	v	101	PNS	O27-C28-C29-C32
57	v	101	PNS	C28-C29-C32-O33
57	v	101	PNS	C30-C29-C32-O33
57	v	101	PNS	C31-C29-C32-O33
57	v	101	PNS	N41-C42-C43-S44
57	v	101	PNS	C37-C38-C39-O40
57	v	101	PNS	C31-C29-C32-C34
57	v	101	PNS	C28-C29-C32-C34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

There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	v	101	PNS	5	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 [i](#)

There are no chain breaks in this entry.

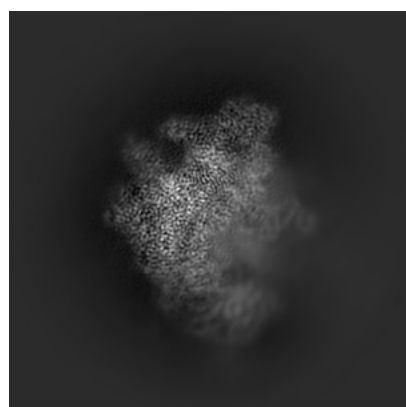
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12920. These allow visual inspection of the internal detail of the map and identification of artifacts.

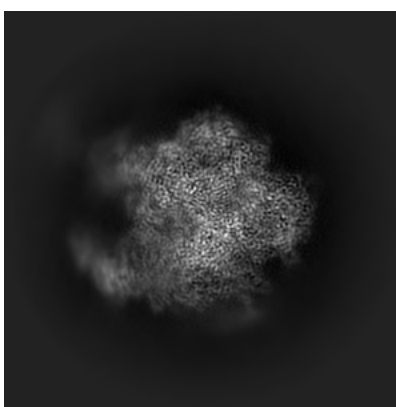
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

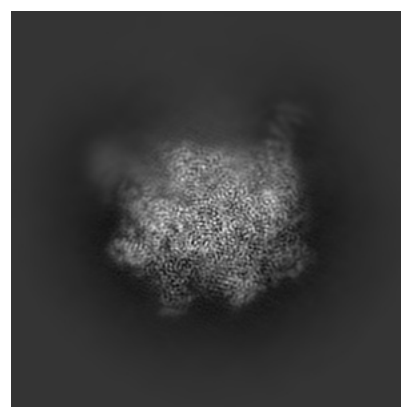
6.1.1 Primary map



X



Y



Z

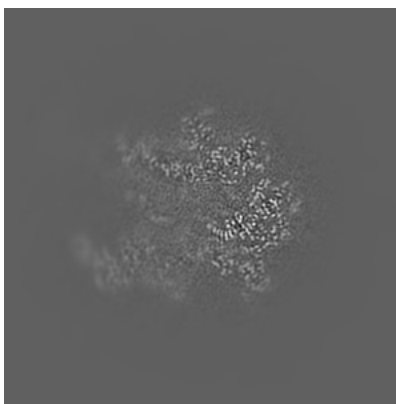
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

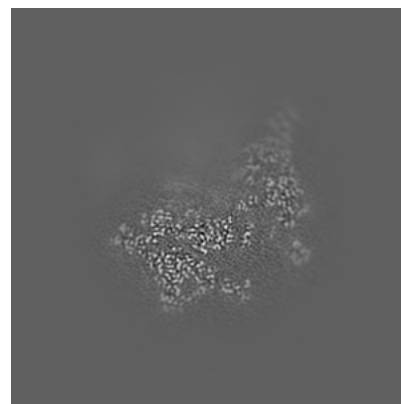
6.2.1 Primary map



X Index: 180



Y Index: 180

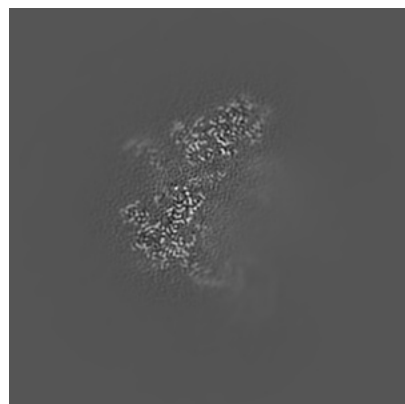


Z Index: 180

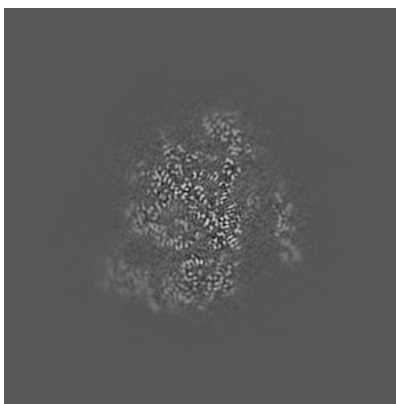
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

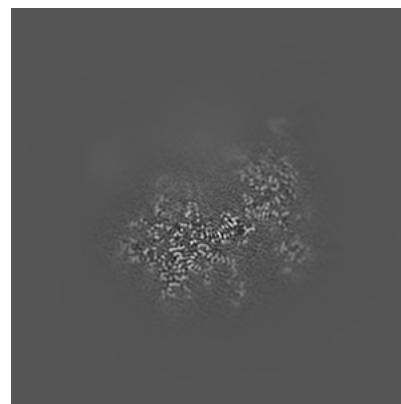
6.3.1 Primary map



X Index: 191



Y Index: 146

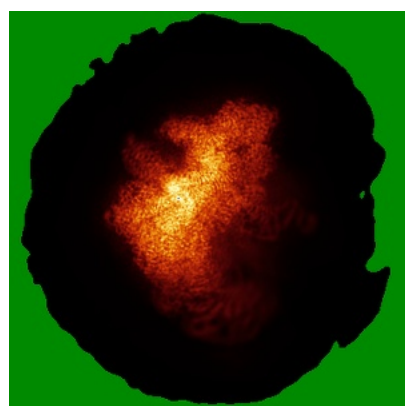


Z Index: 188

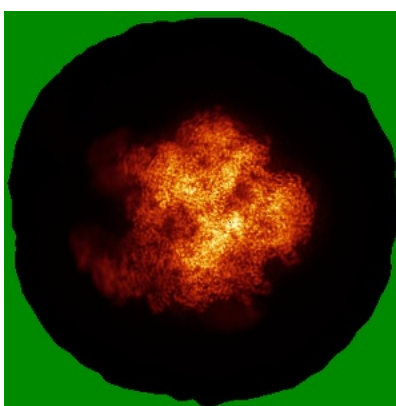
The images above show the largest variance slices of the map in three orthogonal directions.

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

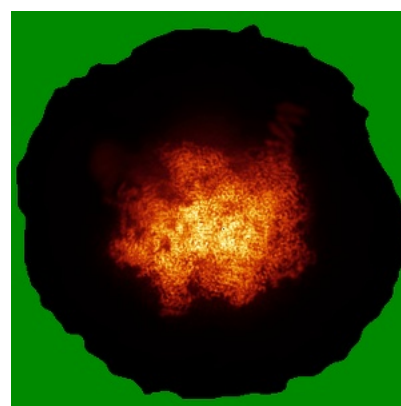
6.4.1 Primary map



X



Y

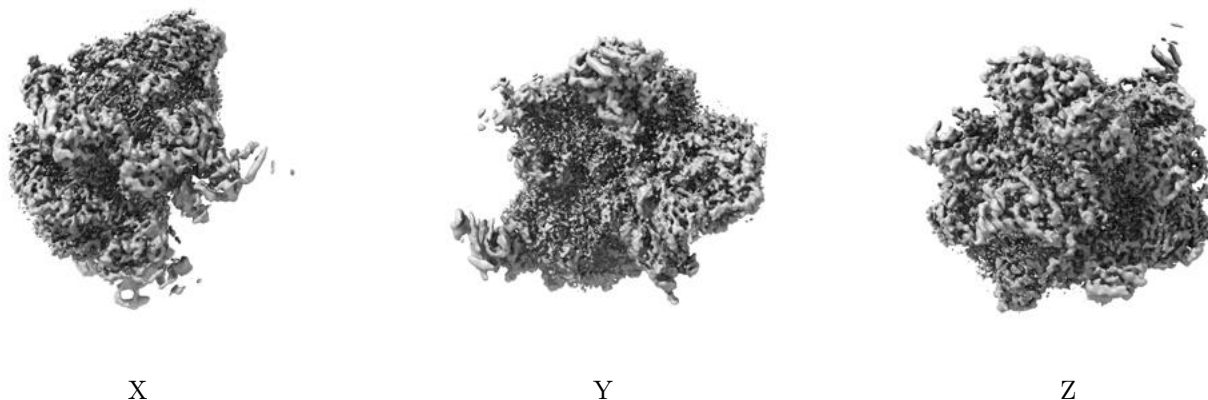


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

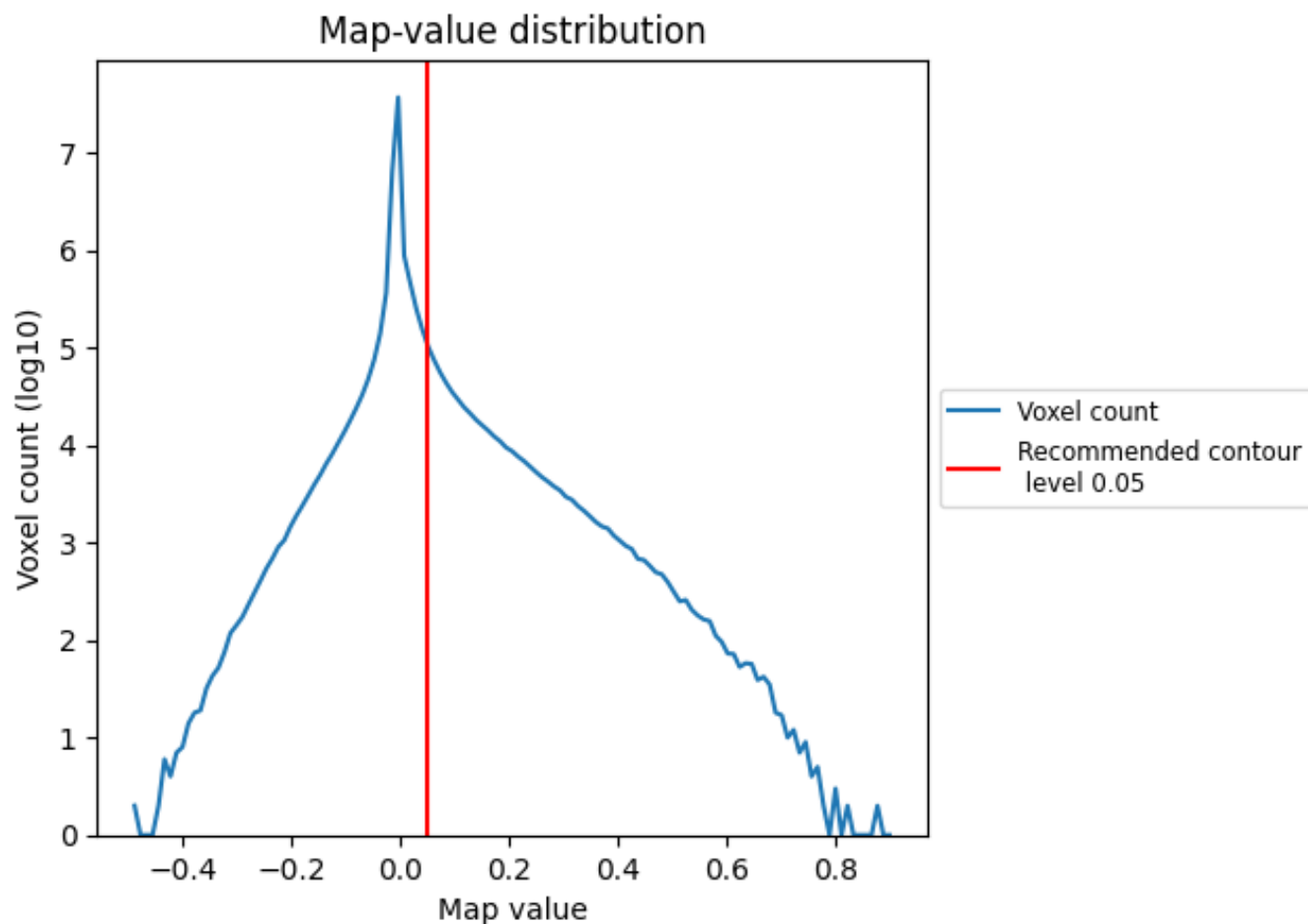
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

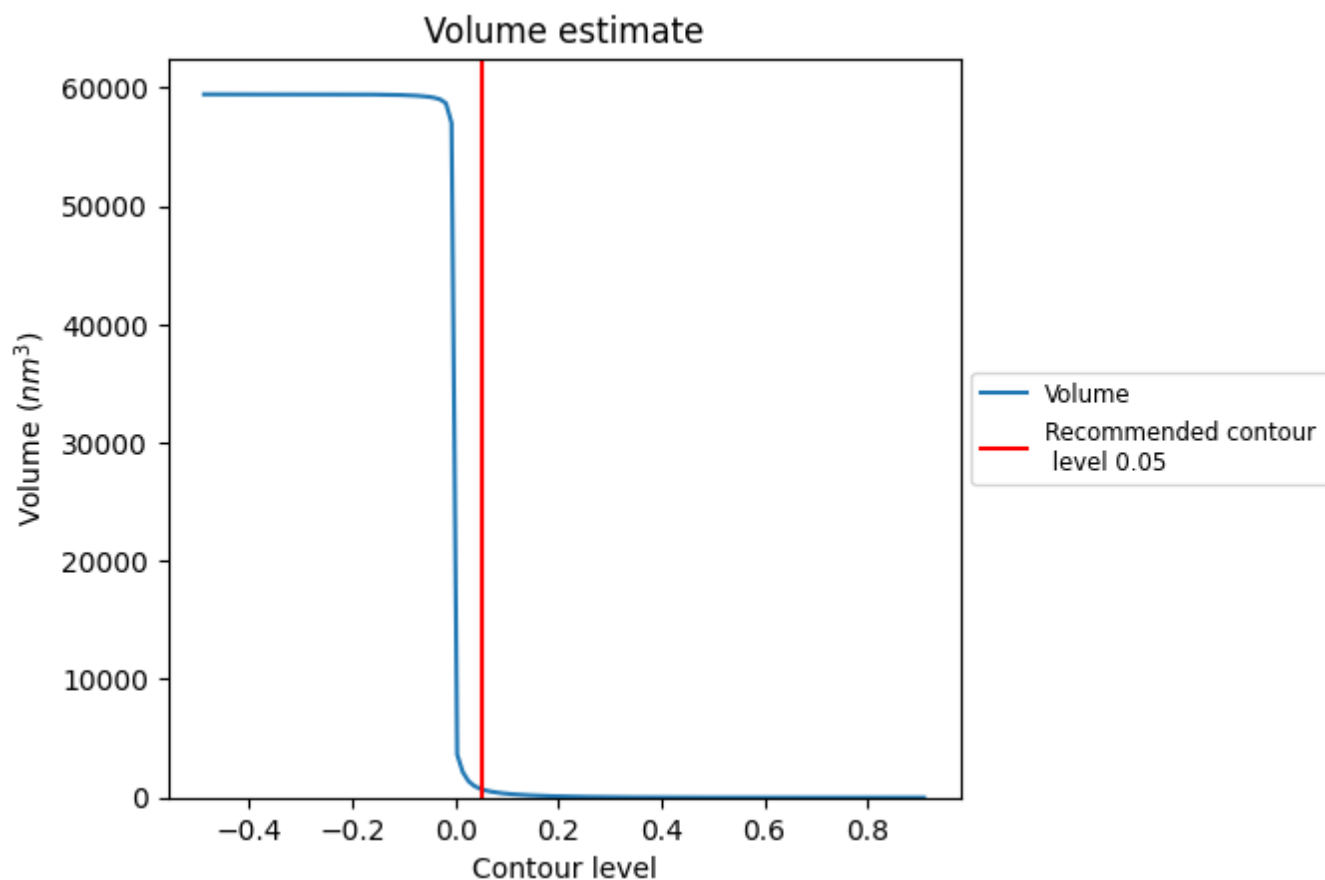
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

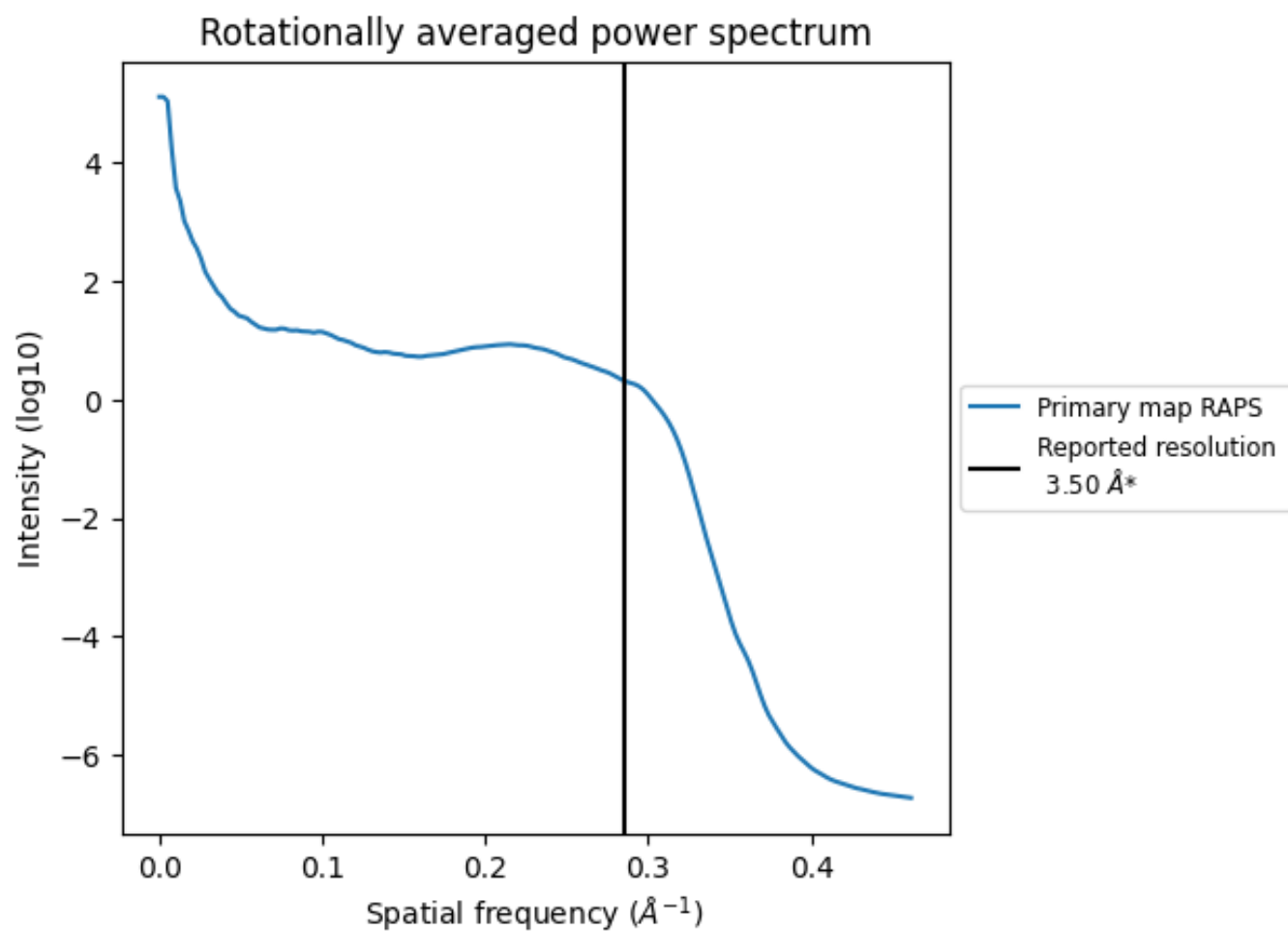
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 728 nm^3 ; this corresponds to an approximate mass of 657 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

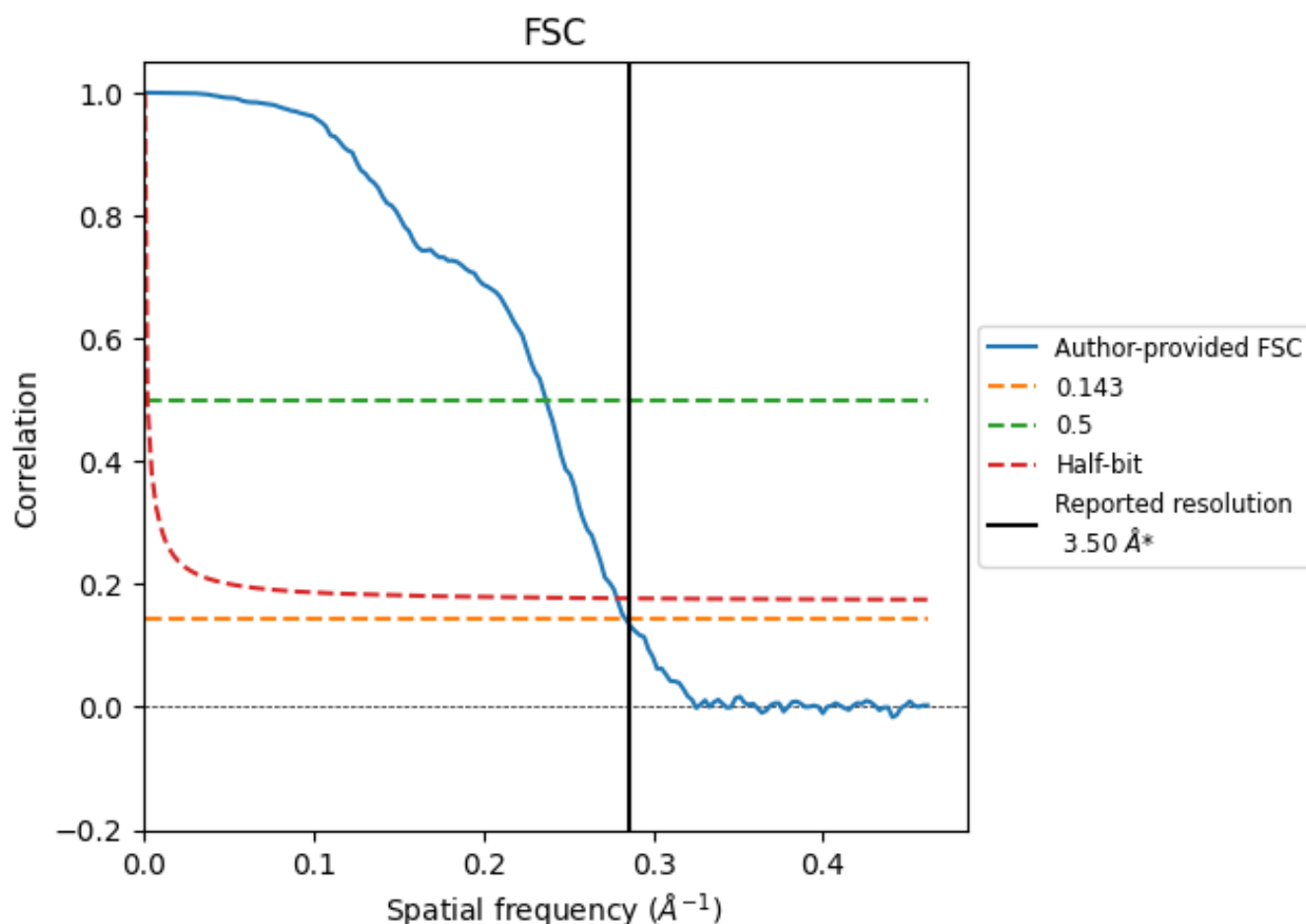


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8.2 Resolution estimates [i](#)

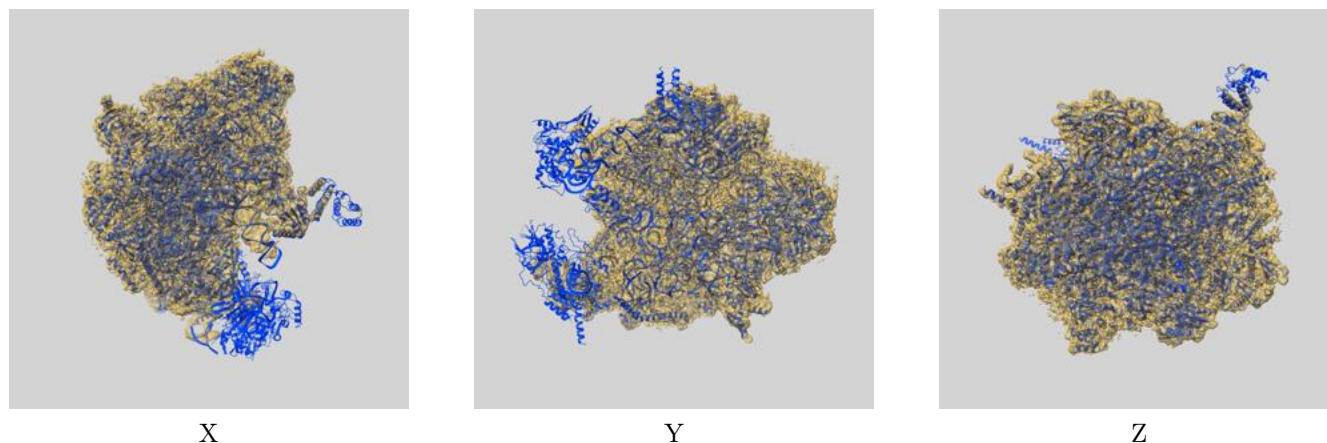
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.52	4.22	3.59
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

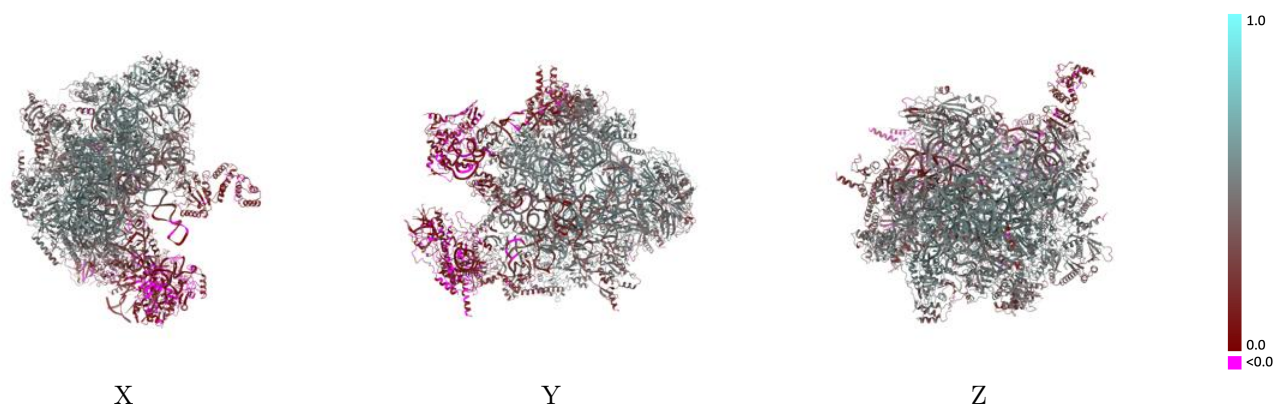
This section contains information regarding the fit between EMDB map EMD-12920 and PDB model 7OI7. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)



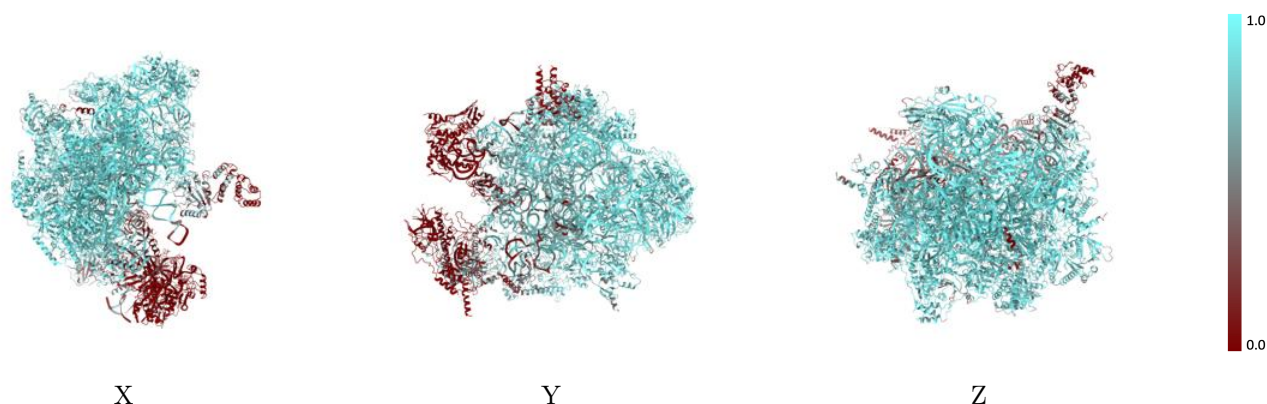
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



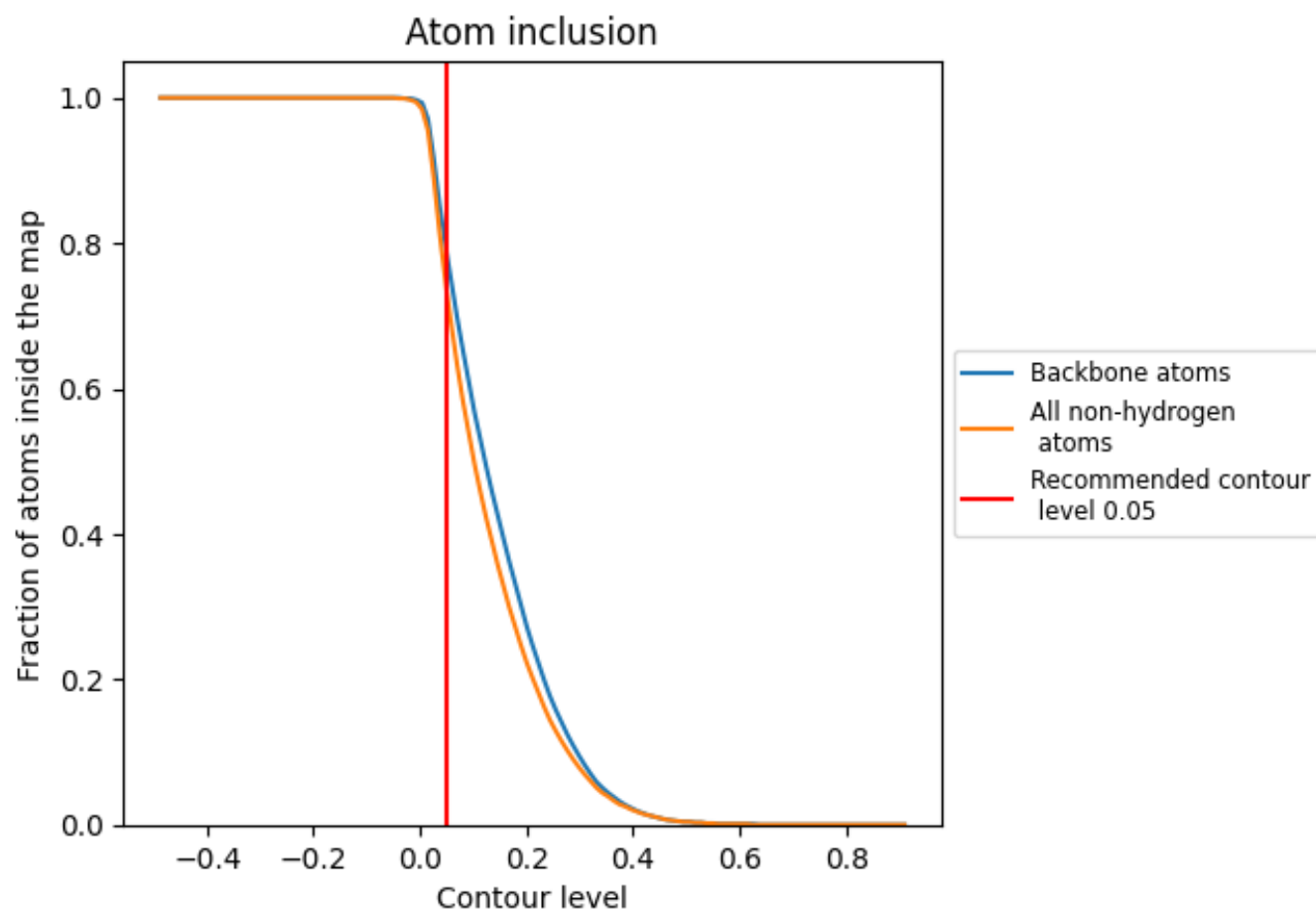
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 73% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7340	 0.4000
0	 0.8910	 0.5030
1	 0.3760	 0.2290
2	 0.9790	 0.5950
3	 0.8780	 0.5180
5	 0.8650	 0.4580
6	 0.5450	 0.2340
7	 0.8280	 0.4370
8	 0.0810	 0.1010
9	 0.8600	 0.4780
A	 0.8260	 0.4300
B	 0.4080	 0.1440
D	 0.7700	 0.4150
E	 0.8590	 0.4580
F	 0.9180	 0.5320
H	 0.7400	 0.3860
I	 0.1190	 0.1300
J	 0.0000	 0.0330
K	 0.8690	 0.4760
L	 0.6840	 0.3590
M	 0.8720	 0.4900
N	 0.3240	 0.2550
O	 0.9130	 0.5170
P	 0.5500	 0.1990
Q	 0.8330	 0.4390
R	 0.9110	 0.5290
S	 0.8790	 0.4920
T	 0.9250	 0.5450
U	 0.8780	 0.5050
V	 0.7540	 0.4350
W	 0.6730	 0.3590
X	 0.8420	 0.4540
Y	 0.9130	 0.5190
Z	 0.8240	 0.4360
a	 0.8900	 0.5040



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Chain	Atom inclusion	Q-score
b	 0.9270	 0.5320
c	 0.8800	 0.4810
d	 0.7090	 0.3880
e	 0.0120	 0.0750
f	 0.0800	 0.0810
g	 0.9240	 0.5130
h	 0.8660	 0.4410
i	 0.9300	 0.5590
j	 0.7930	 0.4410
k	 0.0200	 0.0840
l	 0.0340	 0.0630
m	 0.0000	 0.0670
o	 0.8830	 0.4720
p	 0.6840	 0.3380
q	 0.7050	 0.3830
r	 0.7420	 0.3510
s	 0.9040	 0.5100
u	 0.4420	 0.2130
v	 0.2290	 0.1960
w	 0.0160	 0.1370