



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 02:11 PM UTC

PDB ID : 7OI9 / pdb_00007oi9
EMDB ID : EMD-12922
Title : Cryo-EM structure of late human 39S mitoribosome assembly intermediates, state 3B
Authors : Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on : 2021-05-11
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

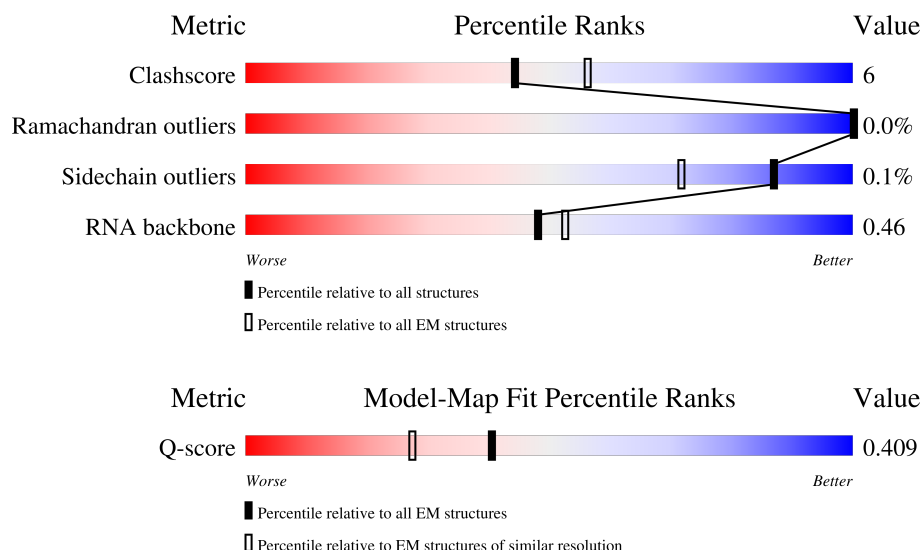
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.30 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.



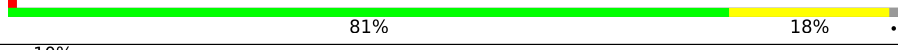
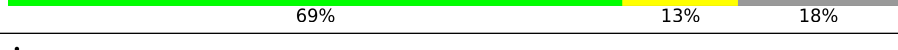
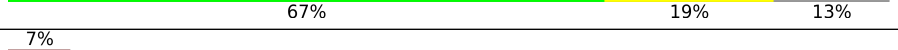
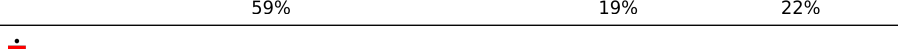
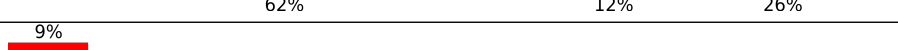
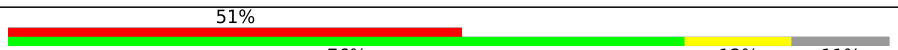
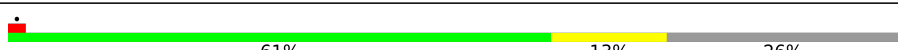
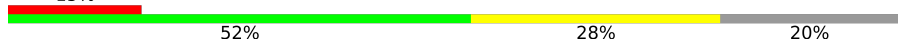
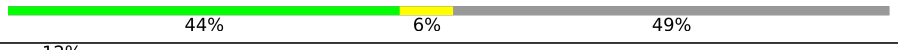
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

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	

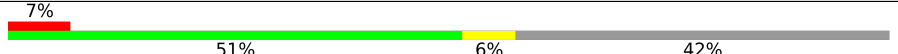
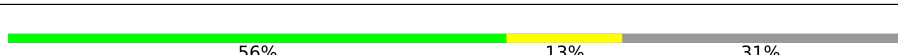
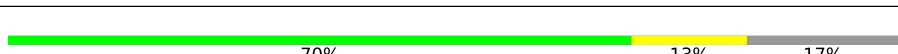
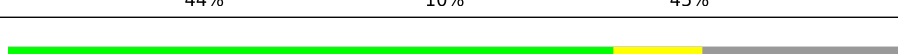
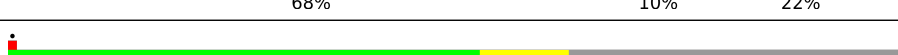
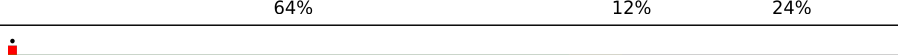
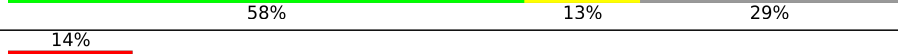
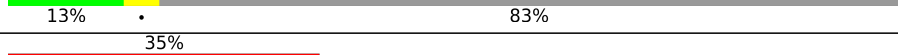
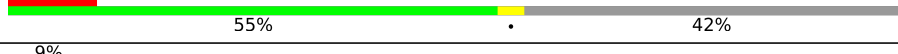
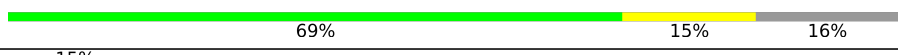
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Mol	Chain	Length	Quality of chain
4	H	267	
5	I	261	
6	J	192	
7	K	178	
8	L	145	
9	M	296	
10	N	251	
11	O	175	
12	P	180	
13	Q	292	
14	R	149	
15	S	205	
16	T	206	
17	U	153	
18	V	216	
19	W	148	
20	X	256	
21	Y	250	
22	Z	161	
23	0	188	
24	1	65	
25	2	92	
26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

2 Entry composition

There are 57 unique types of molecules in this entry. The entry contains 90599 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	128	Total	C	N	O	S	0	0
			1076	671	208	192	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	1092	Total	C	N	O	P	0	0
			23184	10409	4202	7481	1092		

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		

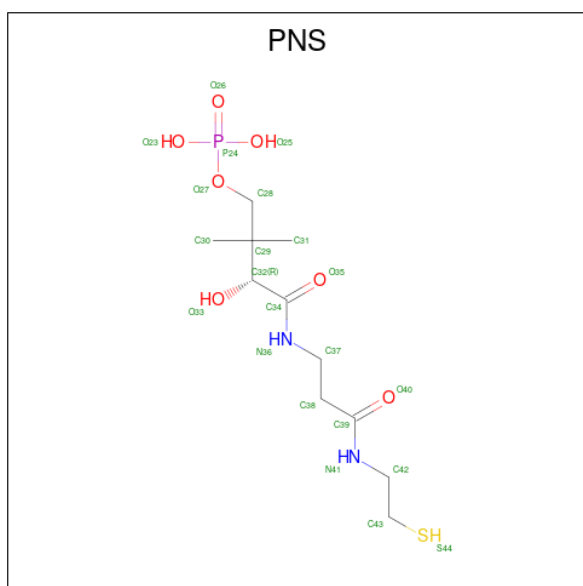
- Molecule 55 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
56	0	1	Total	Zn	0
			1	1	
56	r	1	Total	Zn	0
			1	1	

- Molecule 57 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).



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

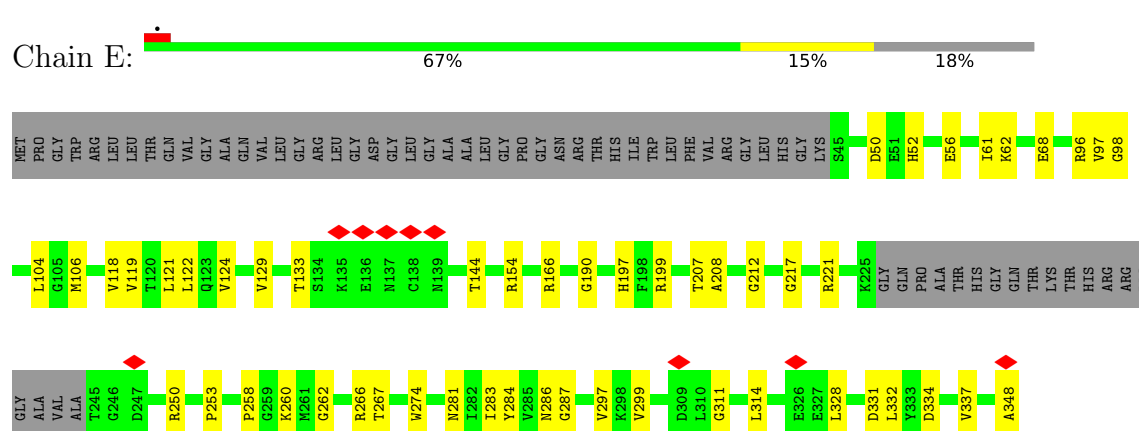
3 Residue-property plots

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

- Molecule 1: 39S ribosomal protein L2, mitochondrial

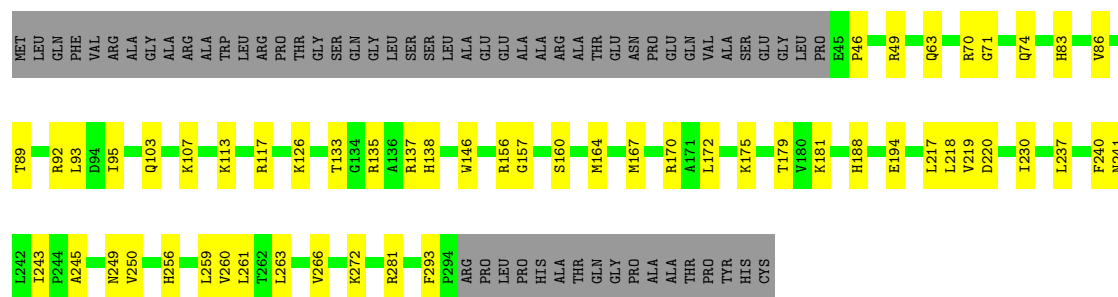


- Molecule 2: 39S ribosomal protein L3, mitochondrial

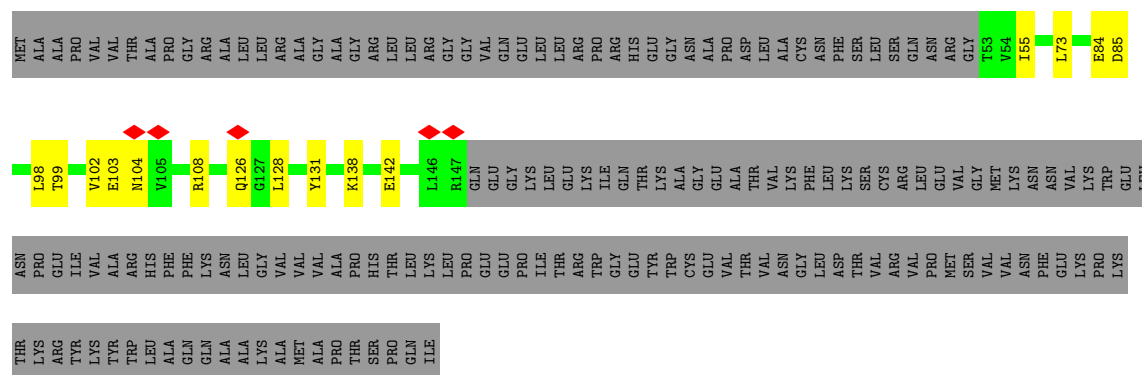


- Molecule 3: 39S ribosomal protein L4, mitochondrial

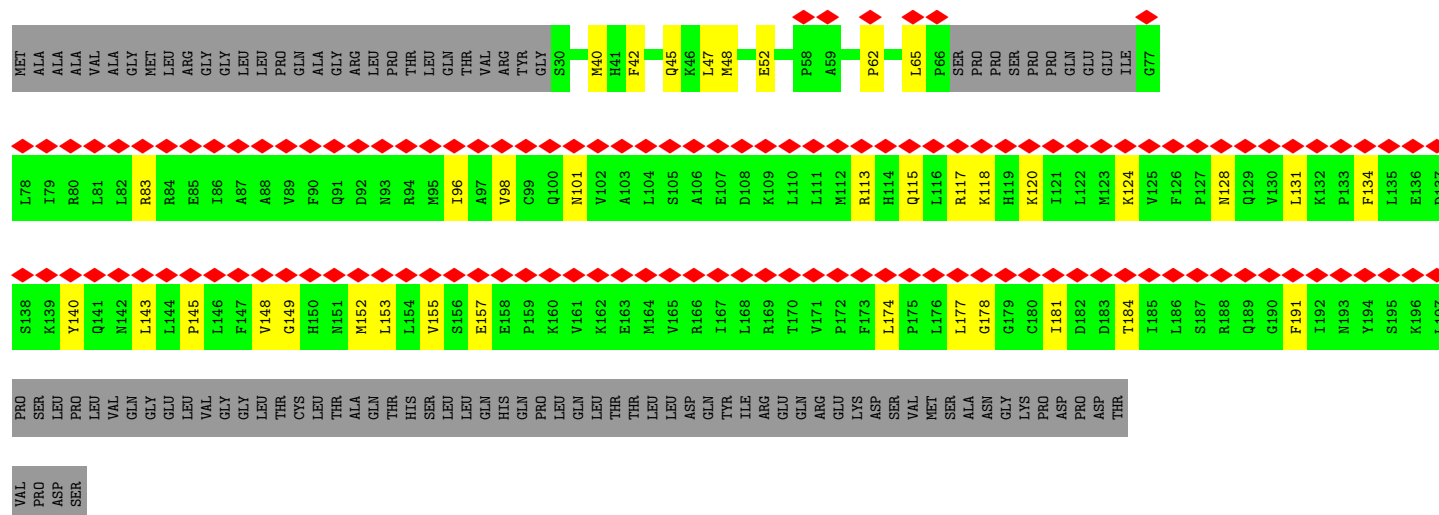




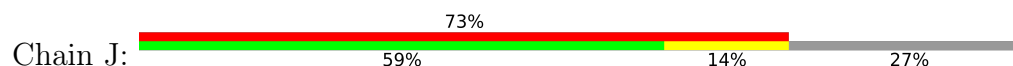
- Molecule 4: 39S ribosomal protein L9, mitochondrial

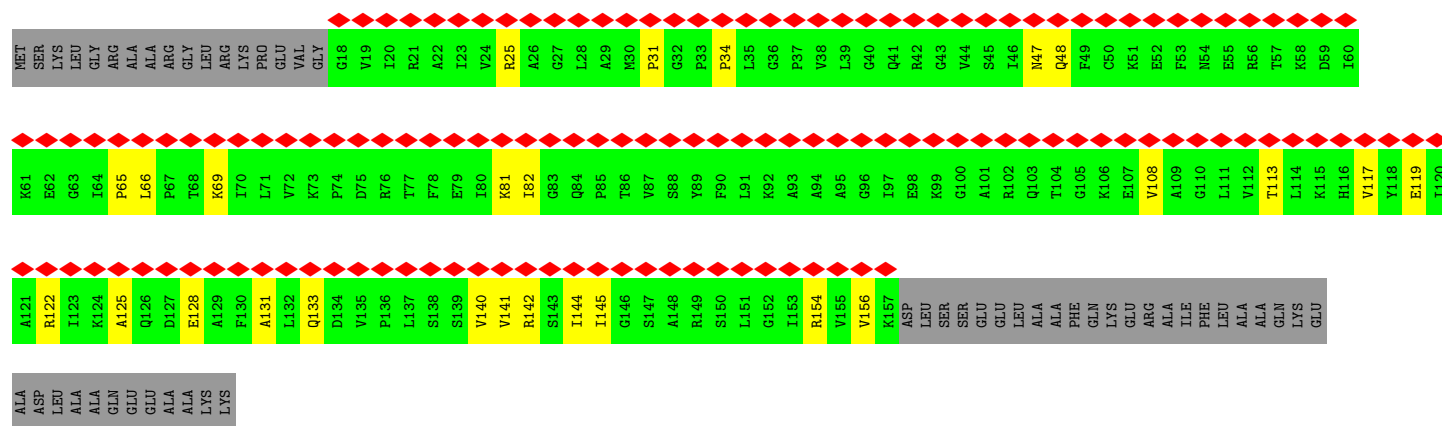


- Molecule 5: 39S ribosomal protein L10, mitochondrial

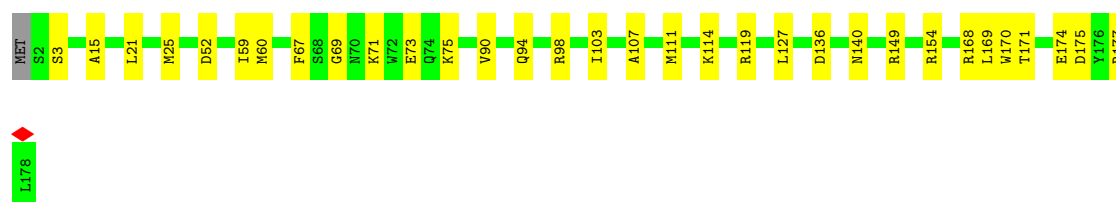
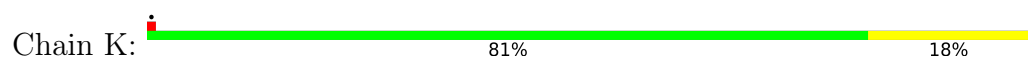


- Molecule 6: 39S ribosomal protein L11, mitochondrial

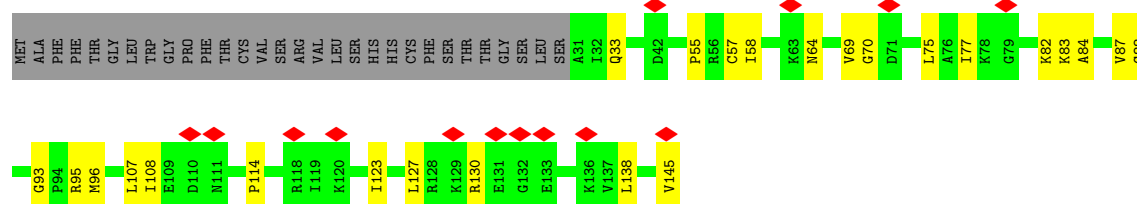




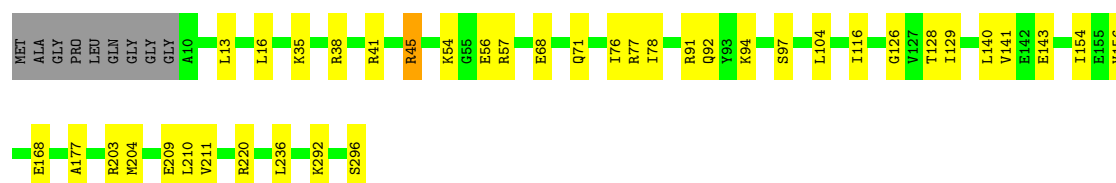
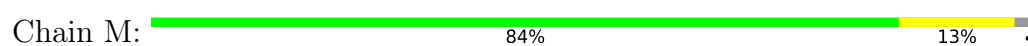
- Molecule 7: 39S ribosomal protein L13, mitochondrial



- Molecule 8: 39S ribosomal protein L14, mitochondrial

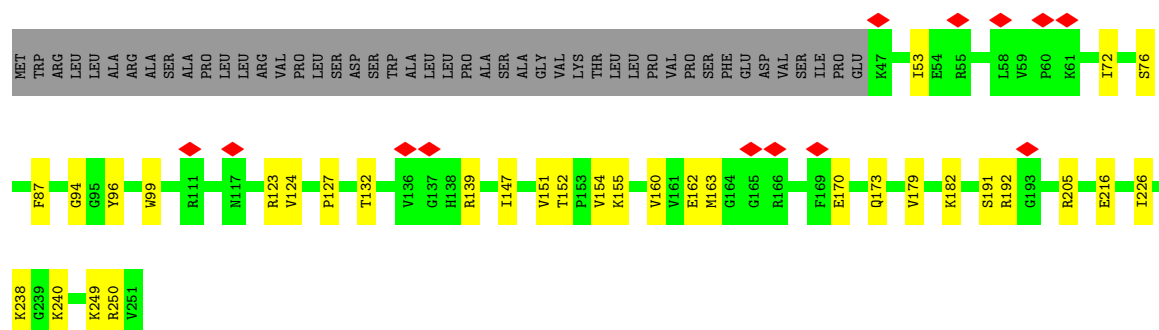


- Molecule 9: 39S ribosomal protein L15, mitochondrial



- Molecule 10: 39S ribosomal protein L16, mitochondrial





- Molecule 11: 39S ribosomal protein L17, mitochondrial



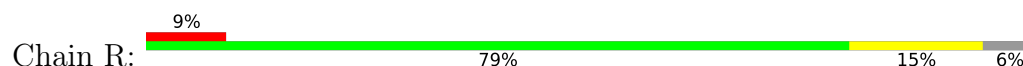
- Molecule 12: 39S ribosomal protein L18, mitochondrial

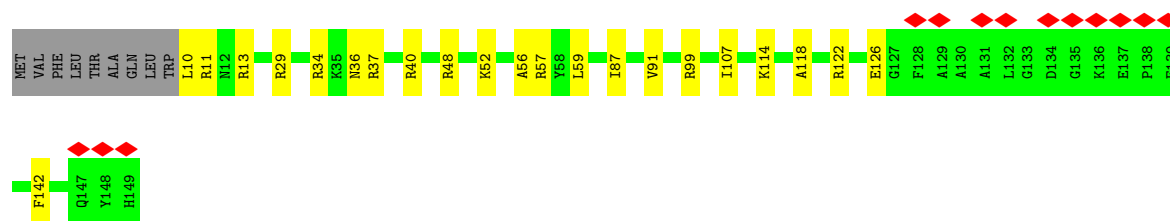


- Molecule 13: 39S ribosomal protein L19, mitochondrial



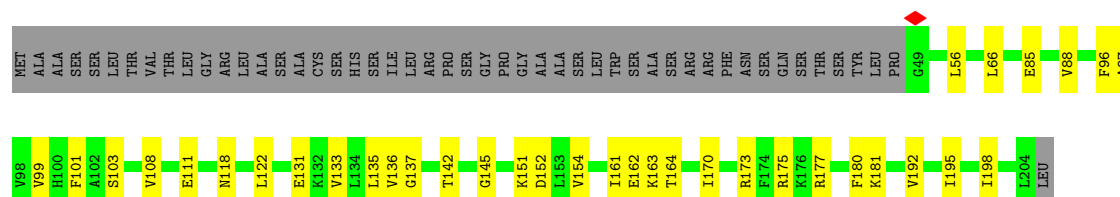
- Molecule 14: 39S ribosomal protein L20, mitochondrial





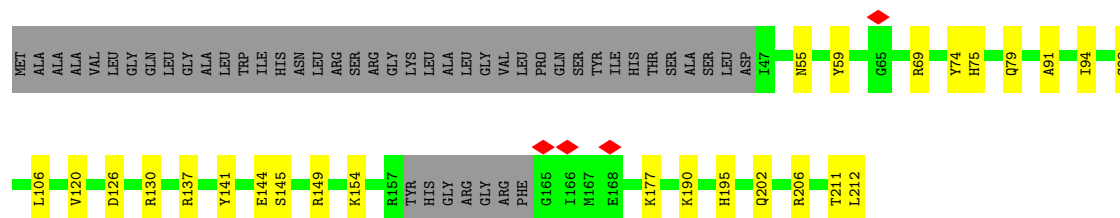
- Molecule 15: 39S ribosomal protein L21, mitochondrial

Chain S: 59% 18% 24%



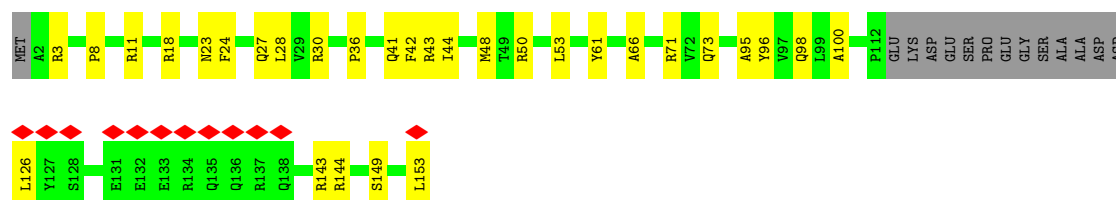
- Molecule 16: 39S ribosomal protein L22, mitochondrial

Chain T: 65% 13% 23%



- Molecule 17: 39S ribosomal protein L23, mitochondrial

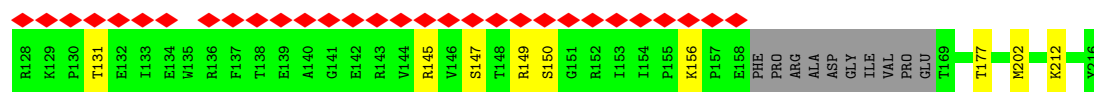
Chain U: 8% 71% 20% 9%



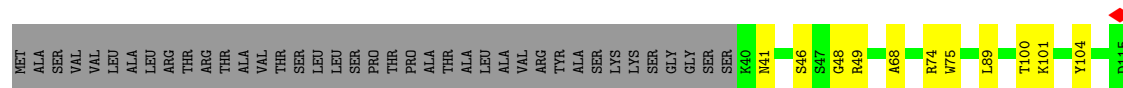
- Molecule 18: 39S ribosomal protein L24, mitochondrial

Chain V: 51% 76% 12% 11%

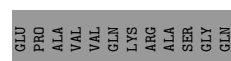
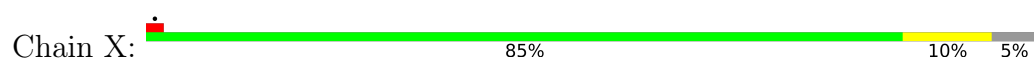




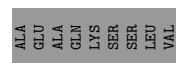
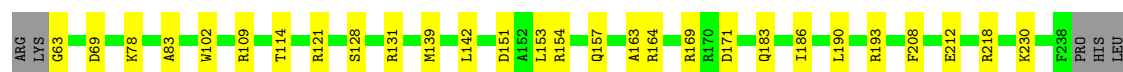
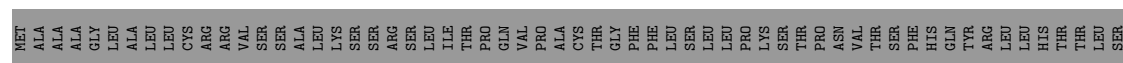
- Molecule 19: 39S ribosomal protein L27, mitochondrial



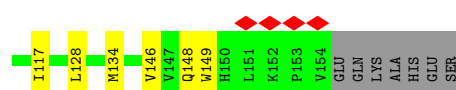
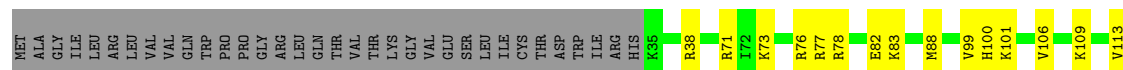
- Molecule 20: 39S ribosomal protein L28, mitochondrial



- Molecule 21: 39S ribosomal protein L47, mitochondrial

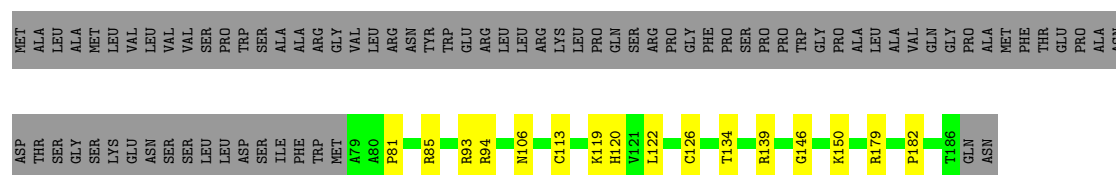


- Molecule 22: 39S ribosomal protein L30, mitochondrial



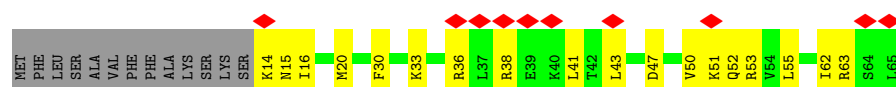
- Molecule 23: 39S ribosomal protein L32, mitochondrial

Chain 0: 



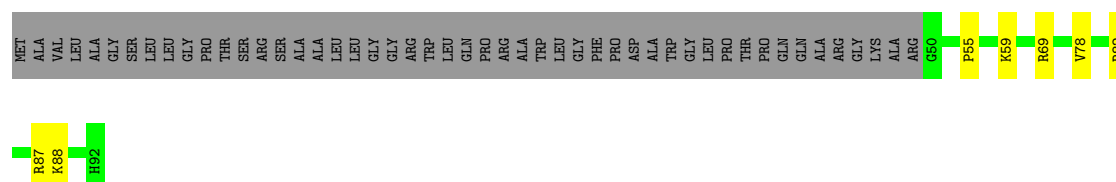
- Molecule 24: 39S ribosomal protein L33, mitochondrial

Chain 1: 

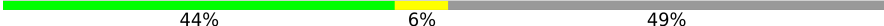


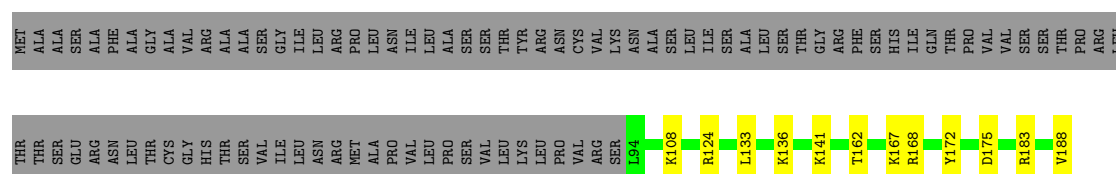
- Molecule 25: 39S ribosomal protein L34, mitochondrial

Chain 2: 



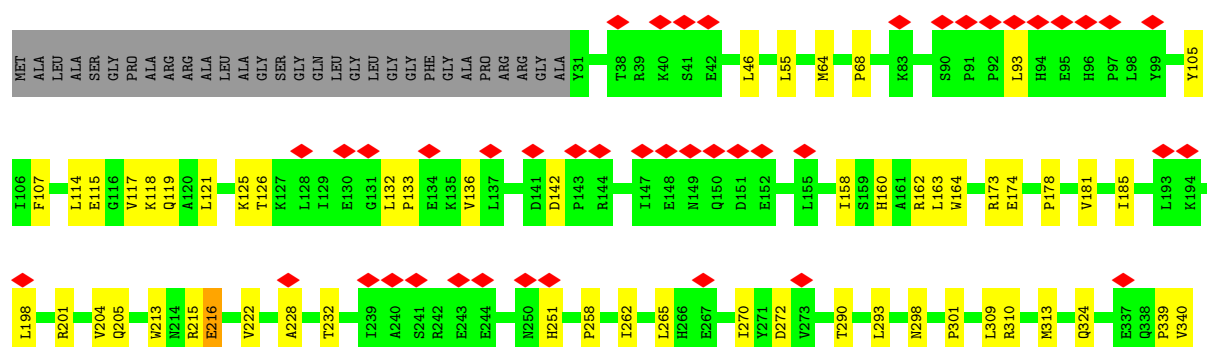
- Molecule 26: 39S ribosomal protein L35, mitochondrial

Chain 3: 



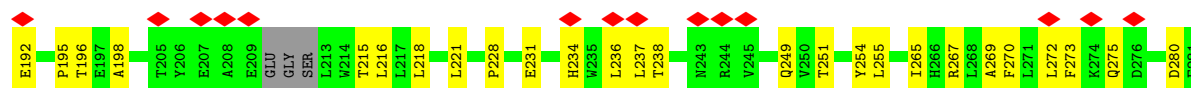
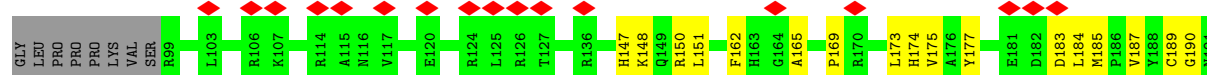
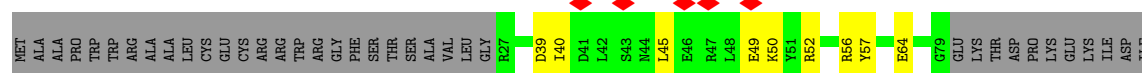
- Molecule 27: 39S ribosomal protein L37, mitochondrial

Chain 5: 

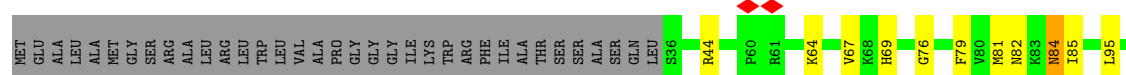




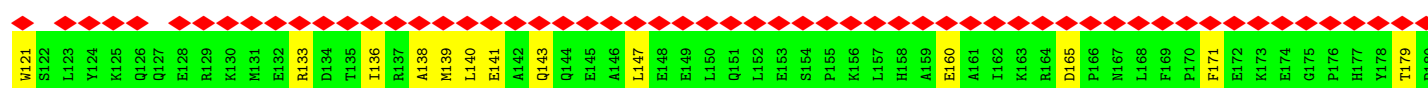
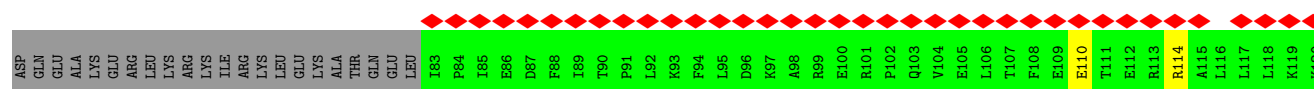
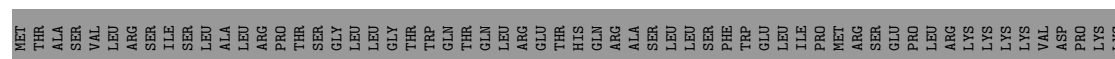
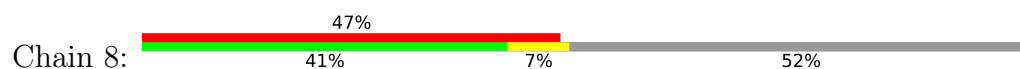
- Molecule 28: 39S ribosomal protein L38, mitochondrial

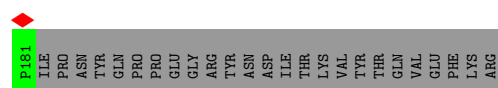


- Molecule 29: 39S ribosomal protein L39, mitochondrial



- Molecule 30: 39S ribosomal protein L40, mitochondrial

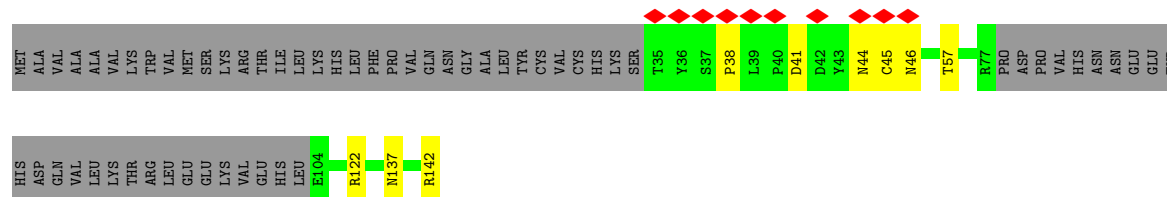




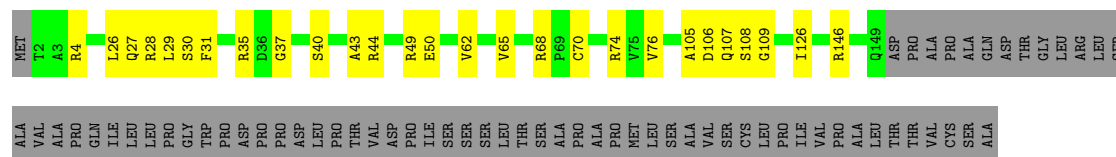
- Molecule 31: 39S ribosomal protein L41, mitochondrial



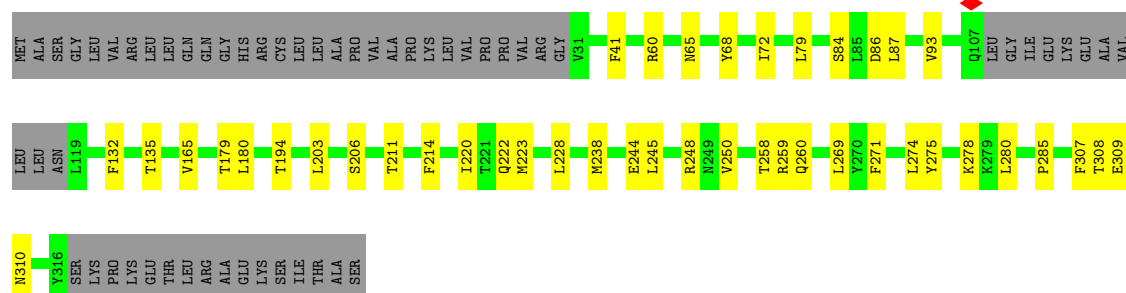
- Molecule 32: 39S ribosomal protein L42, mitochondrial



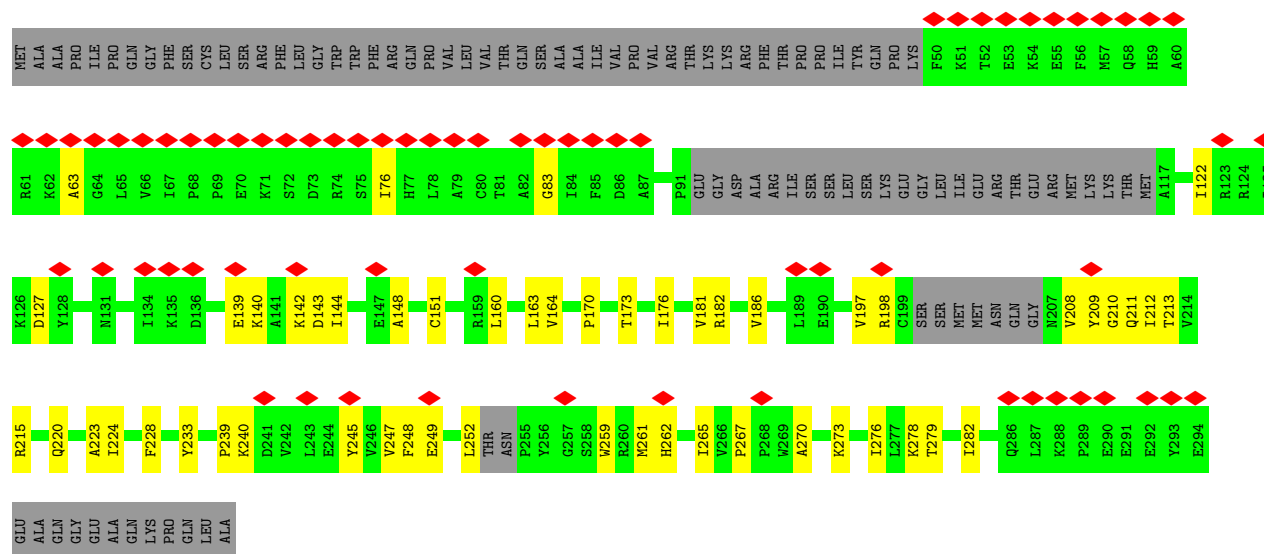
- Molecule 33: 39S ribosomal protein L43, mitochondrial



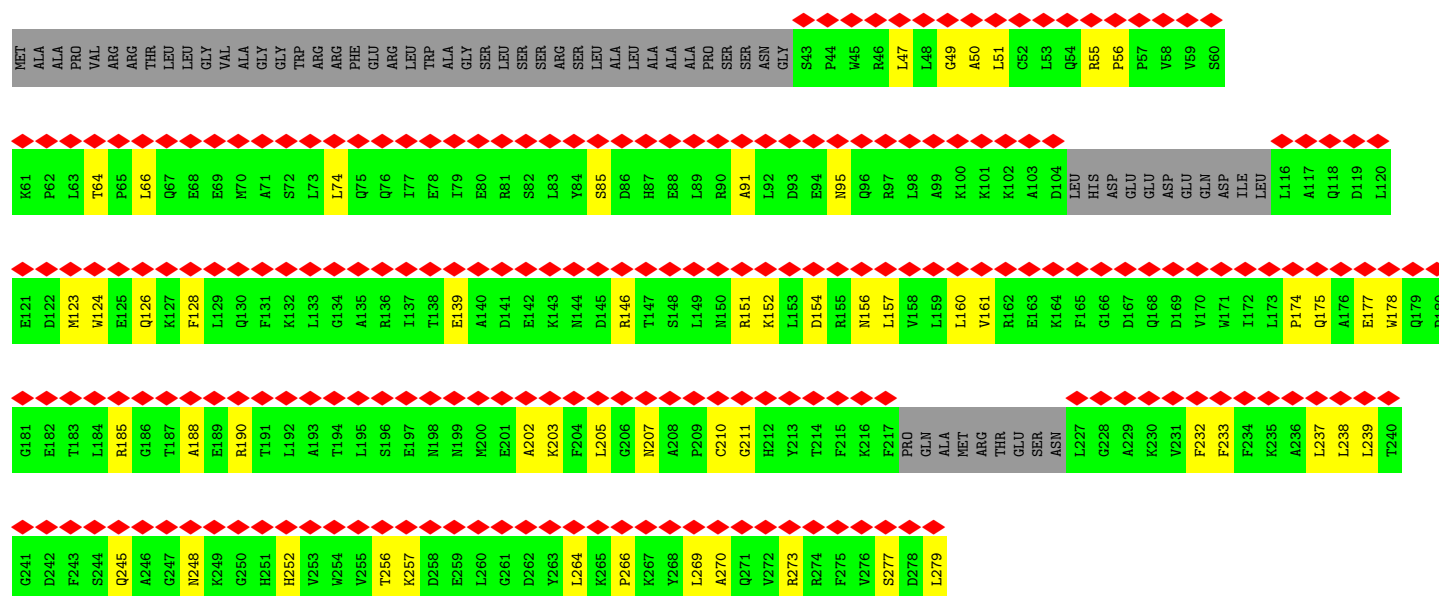
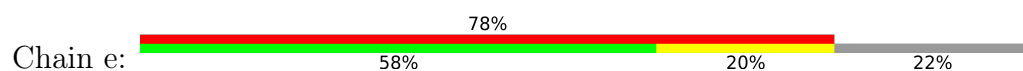
- Molecule 34: 39S ribosomal protein L44, mitochondrial



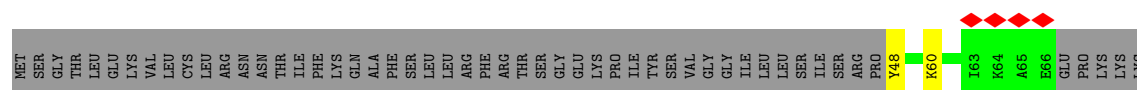
- Molecule 35: 39S ribosomal protein L45, mitochondrial

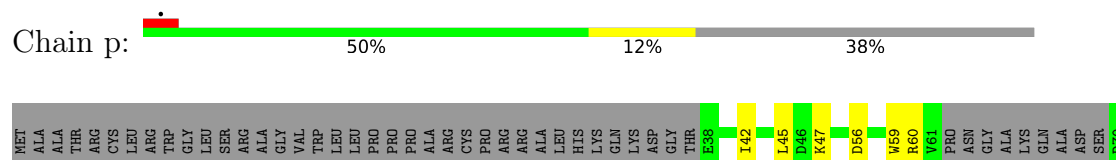


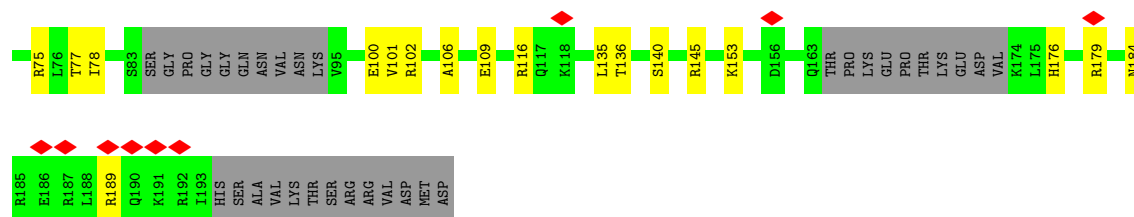
- Molecule 36: 39S ribosomal protein L46, mitochondrial



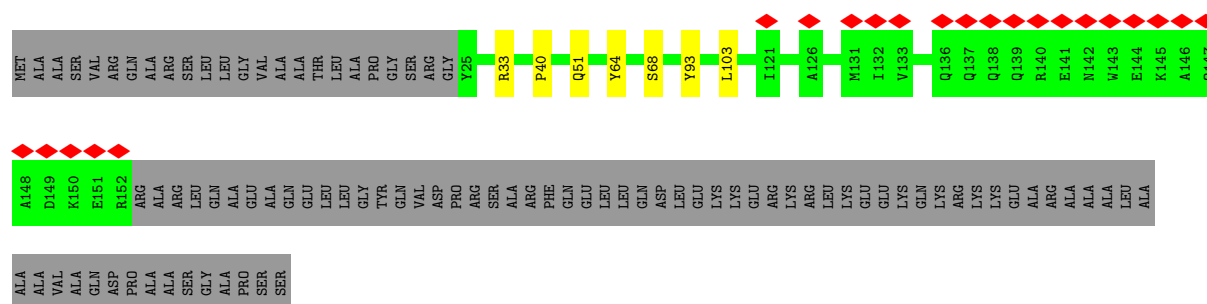
- Molecule 37: 39S ribosomal protein L48, mitochondrial



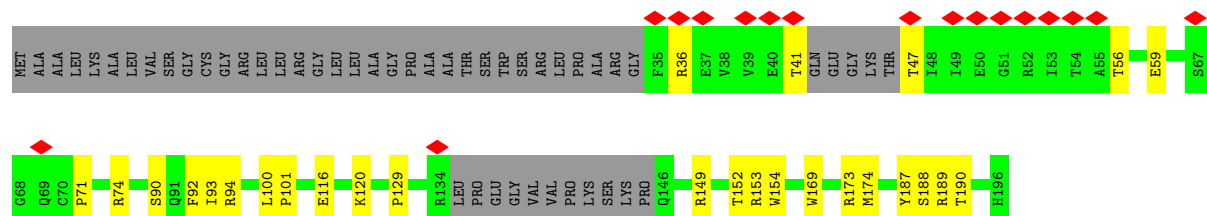




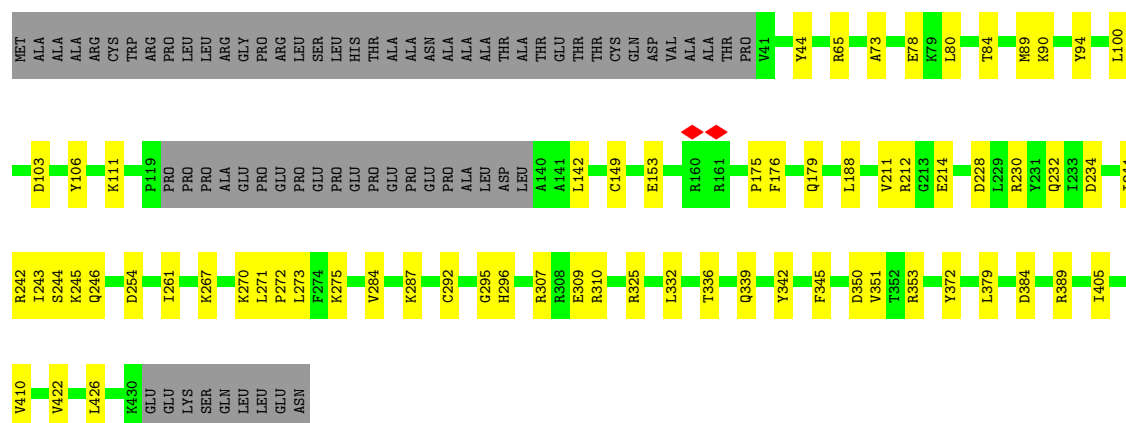
- Molecule 47: Growth arrest and DNA damage-inducible proteins-interacting protein 1



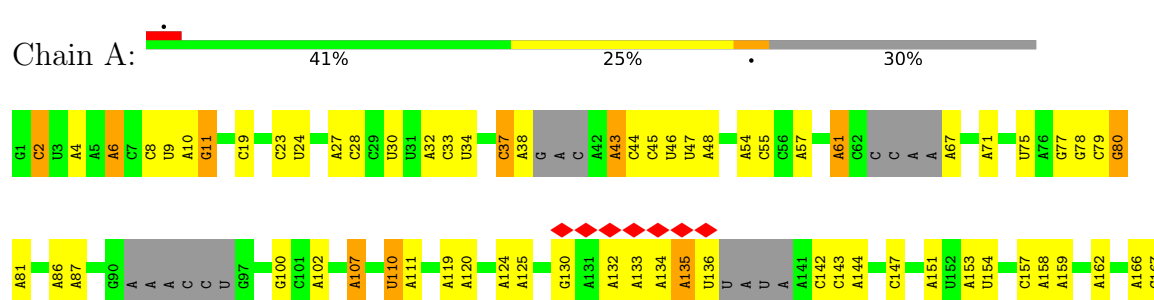
- Molecule 48: 39S ribosomal protein S18a, mitochondrial



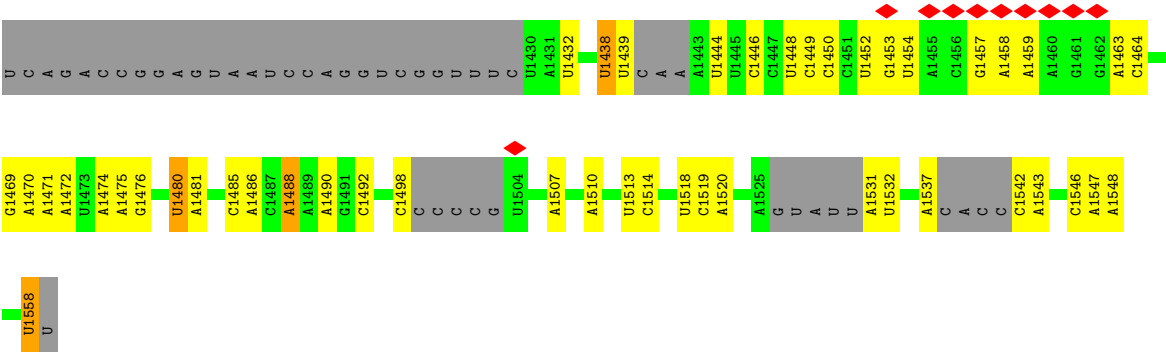
- Molecule 49: 39S ribosomal protein S30, mitochondrial



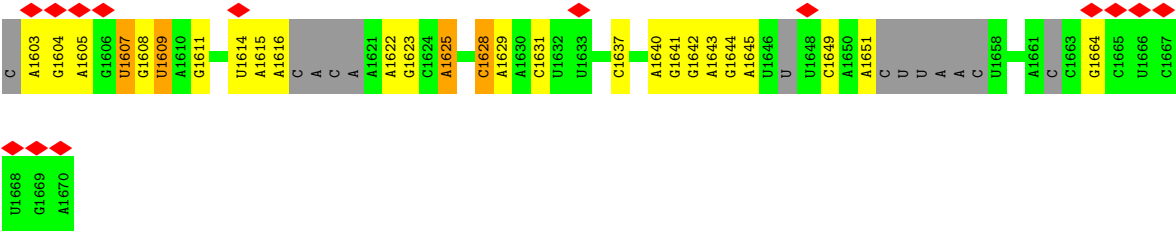
- Molecule 50: Mitochondrial assembly of ribosomal large subunit protein 1







• Molecule 54: mitochondrial Val tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	105924	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	1.004	Depositor
Minimum map value	-0.590	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.021	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: ZN, MG, PNS

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	0.20	0/1736	0.54	0/2335
2	E	0.21	0/2322	0.56	0/3148
3	F	0.24	0/2071	0.54	0/2817
4	H	0.21	0/798	0.66	0/1073
5	I	0.23	0/1308	0.57	0/1761
6	J	0.19	0/1077	0.52	0/1452
7	K	0.18	0/1495	0.46	0/2029
8	L	0.24	0/904	0.63	0/1218
9	M	0.24	0/2359	0.56	0/3185
10	N	0.27	1/1697 (0.1%)	0.53	0/2281
11	O	0.21	0/1269	0.50	0/1708
12	P	0.20	0/1173	0.53	0/1588
13	Q	0.23	0/1846	0.71	4/2487 (0.2%)
14	R	0.22	0/1174	0.49	0/1572
15	S	0.23	0/1276	0.54	0/1729
16	T	0.17	0/1335	0.45	0/1796
17	U	0.20	0/1183	0.50	0/1600
18	V	0.18	0/1616	0.45	0/2189
19	W	0.19	0/881	0.50	0/1188
20	X	0.20	0/2090	0.55	3/2825 (0.1%)
21	Y	0.19	0/1552	0.48	0/2079
22	Z	0.17	0/1003	0.41	0/1354
23	0	0.20	0/895	0.54	0/1201
24	1	0.20	0/438	0.59	0/583
25	2	0.16	0/357	0.44	0/475
26	3	0.16	0/852	0.42	0/1136
27	5	0.19	0/3250	0.51	1/4429 (0.0%)
28	6	0.22	0/2726	0.59	1/3715 (0.0%)
29	7	0.22	0/2391	0.58	1/3234 (0.0%)
30	8	0.20	0/855	0.53	0/1152
31	9	0.21	0/972	0.54	0/1306
32	a	0.18	0/709	0.45	0/963

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	b	0.22	0/1202	0.55	0/1626
34	c	0.20	0/2264	0.54	0/3059
35	d	0.22	0/1790	0.56	0/2423
36	e	0.17	0/1797	0.49	0/2422
37	f	0.19	0/931	0.47	0/1259
38	g	0.21	0/1102	0.51	0/1503
39	h	0.18	0/847	0.45	0/1150
40	i	0.20	0/849	0.47	0/1135
41	j	0.16	0/698	0.43	0/940
42	k	0.19	0/635	0.56	0/855
43	l	0.11	0/226	0.31	0/299
44	m	0.16	0/379	0.41	0/510
45	o	0.21	0/682	0.51	0/916
46	p	0.15	0/1071	0.47	0/1433
47	q	0.18	0/1107	0.44	0/1498
48	r	0.18	0/1238	0.47	0/1676
49	s	0.19	0/3114	0.52	1/4225 (0.0%)
50	u	0.24	0/949	0.70	0/1281
51	v	0.21	0/597	0.54	0/796
52	w	0.20	0/647	0.60	0/871
53	A	0.15	0/25926	0.35	0/40305
54	B	0.14	0/1328	0.30	0/2056
All	All	0.19	1/94989 (0.0%)	0.48	11/133846 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
9	M	0	1
28	6	0	1
35	d	0	1
46	p	0	1
48	r	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	151	VAL	C-N	7.69	1.49	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	Q	204	MET	CA-C-N	14.48	140.35	120.65
13	Q	204	MET	C-N-CA	14.48	140.35	120.65
13	Q	228	PRO	CA-N-CD	-10.62	97.14	112.00
28	6	169	PRO	CA-N-CD	-9.18	99.15	112.00
20	X	36	ARG	CA-C-N	7.18	130.69	120.49
20	X	36	ARG	C-N-CA	7.18	130.69	120.49
13	Q	228	PRO	N-CD-CG	-7.06	92.61	103.20
27	5	262	ILE	N-CA-C	-6.44	105.06	111.88
29	7	242	GLU	N-CA-CB	6.42	119.76	110.20
49	s	175	PRO	CA-N-CD	-6.37	103.09	112.00
20	X	181	PRO	CA-N-CD	-6.31	103.17	112.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
28	6	49	GLU	Peptide
9	M	45	ARG	Sidechain
35	d	186	VAL	Peptide
46	p	59	TRP	Peptide
48	r	173	ARG	Peptide

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	39	0
2	E	2258	0	2264	36	0
3	F	2013	0	2044	40	0
4	H	784	0	832	9	0
5	I	1283	0	1369	24	0
6	J	1061	0	1141	17	0
7	K	1451	0	1448	25	0
8	L	889	0	941	17	0
9	M	2305	0	2378	32	0
10	N	1654	0	1681	19	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
11	O	1245	0	1283	26	0
12	P	1148	0	1148	25	0
13	Q	1805	0	1841	24	0
14	R	1153	0	1214	19	0
15	S	1251	0	1322	28	0
16	T	1305	0	1352	19	0
17	U	1154	0	1154	26	0
18	V	1575	0	1583	18	0
19	W	859	0	888	18	0
20	X	2035	0	2054	18	0
21	Y	1517	0	1561	22	0
22	Z	978	0	1030	19	0
23	0	880	0	902	14	0
24	1	433	0	475	14	0
25	2	351	0	375	9	0
26	3	831	0	883	9	0
27	5	3156	0	3138	52	0
28	6	2640	0	2464	53	0
29	7	2334	0	2343	39	0
30	8	836	0	844	12	0
31	9	947	0	949	16	0
32	a	686	0	658	8	0
33	b	1178	0	1180	24	0
34	c	2217	0	2220	28	0
35	d	1741	0	1727	38	0
36	e	1762	0	1767	40	0
37	f	915	0	917	17	0
38	g	1067	0	1056	12	0
39	h	827	0	806	12	0
40	i	827	0	857	17	0
41	j	684	0	673	10	0
42	k	627	0	636	10	0
43	l	221	0	227	5	0
44	m	372	0	387	9	0
45	o	665	0	664	10	0
46	p	1058	0	1083	14	0
47	q	1076	0	1049	7	0
48	r	1203	0	1220	23	0
49	s	3036	0	3022	41	0
50	u	927	0	921	22	0
51	v	588	0	604	17	0
52	w	638	0	636	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
53	A	23184	0	11797	232	0
54	B	1191	0	607	10	0
55	A	47	0	0	0	0
55	W	1	0	0	0	0
55	g	1	0	0	0	0
56	0	1	0	0	0	0
56	r	1	0	0	0	0
57	v	21	0	21	4	0
All	All	90599	0	79391	1073	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (1073) 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)
1:D:129:VAL:HA	1:D:139:ILE:O	1.25	1.28
2:E:106:MET:HA	2:E:119:VAL:O	1.06	1.19
28:6:216:LEU:O	28:6:236:LEU:HA	1.40	1.17
53:A:1446:C:N4	53:A:1470:A:H61	1.48	1.11
2:E:106:MET:CA	2:E:119:VAL:O	2.00	1.09
53:A:1446:C:H42	53:A:1470:A:N6	1.49	1.08
54:B:1607:U:H3	54:B:1664:G:H1	1.04	1.01
53:A:662:C:N4	53:A:772:U:O4	2.00	0.94
33:b:31:PHE:HA	33:b:74:ARG:O	1.68	0.94
27:5:290:THR:HA	27:5:343:GLN:O	1.68	0.92
1:D:129:VAL:CA	1:D:139:ILE:O	2.18	0.90
53:A:1454:U:N3	53:A:1463:A:C8	2.38	0.90
36:e:211:GLY:O	36:e:233:PHE:HB2	1.72	0.88
29:7:106:ALA:HA	29:7:126:LYS:O	1.74	0.88
28:6:270:PHE:HB2	28:6:317:SER:O	1.81	0.81
33:b:29:LEU:HA	33:b:76:VAL:O	1.81	0.79
34:c:260:GLN:HA	34:c:269:LEU:O	1.83	0.79
35:d:197:VAL:HA	35:d:211:GLN:O	1.83	0.78
9:M:38:ARG:HE	9:M:45:ARG:HH21	1.31	0.76
17:U:44:ILE:HG23	17:U:48:MET:HB3	1.69	0.74
27:5:160:HIS:HA	27:5:164:TRP:HB2	1.69	0.74
11:O:45:PRO:HG2	11:O:48:ARG:HD2	1.71	0.73
52:w:147:TYR:O	52:w:151:LYS:HB2	1.90	0.72
49:s:242:ARG:HA	49:s:295:GLY:HA2	1.72	0.72
5:I:124:LYS:HB2	5:I:153:LEU:HB2	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:109:ARG:NH1	21:Y:139:MET:SD	2.65	0.70
53:A:669:G:H21	53:A:757:C:H5'	1.58	0.68
23:0:119:LYS:O	23:0:120:HIS:ND1	2.27	0.68
51:v:6:ARG:NH2	57:v:101:PNS:O26	2.26	0.68
53:A:107:A:N6	53:A:110:U:OP2	2.27	0.67
35:d:197:VAL:HG12	35:d:212:ILE:HG12	1.75	0.67
23:0:146:GLY:O	23:0:150:LYS:NZ	2.26	0.67
16:T:144:GLU:HG3	16:T:177:LYS:HE2	1.76	0.66
15:S:136:VAL:HG21	15:S:154:VAL:HG21	1.77	0.66
34:c:275:TYR:HA	34:c:280:LEU:HA	1.78	0.66
50:u:107:ARG:NH1	50:u:129:GLY:O	2.29	0.66
53:A:77:G:N2	53:A:80:G:O2'	2.29	0.66
12:P:142:ASN:OD1	46:p:184:ASN:ND2	2.28	0.66
22:Z:99:VAL:O	41:j:76:ARG:NH1	2.29	0.65
12:P:52:ASN:ND2	28:6:265:ILE:O	2.30	0.65
6:J:119:GLU:O	6:J:122:ARG:NH1	2.28	0.65
49:s:405:ILE:HG12	49:s:410:VAL:HG12	1.78	0.65
53:A:1454:U:C2	53:A:1463:A:N7	2.65	0.65
40:i:74:ILE:HD11	40:i:82:GLY:H	1.60	0.65
3:F:281:ARG:NH2	9:M:128:THR:OG1	2.30	0.64
47:q:64:TYR:HB3	47:q:68:SER:HB2	1.79	0.64
27:5:117:VAL:O	27:5:121:LEU:HB2	1.97	0.64
3:F:217:LEU:HD11	3:F:243:ILE:HD12	1.78	0.64
29:7:166:LEU:HD22	29:7:181:TYR:HE2	1.62	0.64
2:E:311:GLY:HA2	2:E:314:LEU:HD13	1.79	0.64
18:V:80:ILE:HB	18:V:85:TRP:HB2	1.80	0.64
42:k:15:GLN:HG3	42:k:67:LEU:HB2	1.80	0.64
12:P:52:ASN:OD1	28:6:267:ARG:NH1	2.26	0.64
35:d:139:GLU:O	35:d:142:LYS:HB3	1.98	0.64
24:1:15:ASN:HD21	24:1:33:LYS:HD3	1.61	0.64
33:b:31:PHE:HB2	33:b:65:VAL:HG12	1.80	0.64
49:s:307:ARG:HD2	49:s:309:GLU:HB2	1.77	0.64
13:Q:177:VAL:HG13	13:Q:206:PRO:HA	1.80	0.63
7:K:69:GLY:HA2	48:r:152:THR:HG22	1.80	0.63
18:V:56:LEU:HD11	18:V:76:VAL:HG21	1.80	0.63
53:A:564:C:HO2'	53:A:1018:C:HO2'	1.43	0.63
12:P:97:GLN:NE2	12:P:98:ASN:OD1	2.31	0.63
35:d:182:ARG:HB3	35:d:223:ALA:HB3	1.81	0.63
2:E:104:LEU:HB2	2:E:121:LEU:HB2	1.81	0.63
12:P:52:ASN:HB2	12:P:55:ASN:HB2	1.79	0.63
17:U:66:ALA:HB2	17:U:100:ALA:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:166:SER:HG	1:D:182:HIS:HD1	1.46	0.63
53:A:1457:G:H2'	53:A:1458:A:H2'	1.81	0.62
27:5:115:GLU:HB3	27:5:118:LYS:HB3	1.80	0.62
28:6:218:LEU:HA	28:6:269:ALA:O	1.98	0.62
20:X:61:ARG:NH2	20:X:63:GLU:OE1	2.32	0.62
27:5:158:ILE:O	27:5:162:ARG:HB3	2.00	0.62
46:p:135:LEU:HD12	46:p:153:LYS:HE3	1.81	0.62
53:A:130:G:H22	53:A:133:A:H5'	1.63	0.62
18:V:105:ARG:HE	35:d:170:PRO:HB2	1.64	0.62
15:S:161:ILE:HG22	15:S:162:GLU:HG3	1.82	0.62
51:v:15:ALA:O	51:v:19:GLN:NE2	2.33	0.62
42:k:34:LEU:HA	42:k:38:SER:HB2	1.82	0.62
53:A:1176:G:O2'	53:A:1243:A:N6	2.33	0.62
28:6:148:LYS:NZ	28:6:189:CYS:SG	2.72	0.61
49:s:188:LEU:HD12	49:s:426:LEU:HD21	1.82	0.61
9:M:77:ARG:NH1	53:A:1247:G:O6	2.33	0.61
49:s:228:ASP:O	49:s:230:ARG:NH1	2.34	0.61
53:A:1454:U:O2	53:A:1463:A:N7	2.33	0.61
17:U:42:PHE:HB2	17:U:95:ALA:HB3	1.81	0.61
19:W:143:LYS:HE2	28:6:345:VAL:HG21	1.83	0.61
10:N:139:ARG:NH1	53:A:1145:G:N7	2.49	0.61
20:X:59:ARG:NH2	47:q:93:TYR:OH	2.32	0.61
22:Z:101:LYS:HE3	41:j:80:LEU:HD22	1.81	0.61
19:W:101:LYS:NZ	53:A:394:A:OP1	2.34	0.61
14:R:114:LYS:NZ	32:a:45:CYS:SG	2.63	0.61
21:Y:218:ARG:NH2	40:i:105:ASP:OD1	2.34	0.61
9:M:141:VAL:HG12	9:M:143:GLU:H	1.66	0.60
17:U:18:ARG:NH1	31:9:59:GLU:OE2	2.34	0.60
48:r:169:TRP:O	53:A:485:A:N6	2.33	0.60
10:N:216:GLU:HG2	10:N:238:LYS:HG2	1.82	0.60
53:A:55:C:O2	53:A:1251:A:N6	2.33	0.60
53:A:495:C:O2	53:A:547:C:N4	2.34	0.60
17:U:44:ILE:HD11	17:U:53:LEU:HD22	1.82	0.60
15:S:103:SER:OG	53:A:475:G:N2	2.34	0.60
29:7:116:TYR:OH	29:7:271:ARG:NH2	2.35	0.60
49:s:211:VAL:HG22	49:s:230:ARG:HG3	1.83	0.60
1:D:124:GLU:HG3	1:D:144:GLY:HA3	1.82	0.60
23:0:85:ARG:NH1	53:A:638:A:OP1	2.35	0.60
17:U:30:ARG:O	21:Y:121:ARG:NH1	2.35	0.60
49:s:244:SER:HA	49:s:292:CYS:HA	1.81	0.60
7:K:15:ALA:HB3	34:c:269:LEU:HD12	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:R:122:ARG:HB2	32:a:38:PRO:HB3	1.83	0.60
49:s:336:THR:HA	49:s:339:GLN:HE21	1.66	0.60
14:R:29:ARG:NH1	14:R:36:ASN:O	2.34	0.60
44:m:72:ARG:HH21	44:m:75:LEU:HD11	1.66	0.60
48:r:41:THR:O	48:r:47:THR:HA	2.01	0.60
13:Q:108:ILE:HG23	13:Q:174:ILE:HD11	1.83	0.59
29:7:69:HIS:O	29:7:76:GLY:N	2.36	0.59
35:d:213:THR:HG22	35:d:247:VAL:HG22	1.84	0.59
1:D:87:HIS:ND1	53:A:853:C:O2	2.35	0.59
25:2:82:ARG:NH1	53:A:120:A:OP1	2.35	0.59
52:w:87:LEU:HB3	52:w:98:LEU:HD21	1.83	0.59
3:F:133:THR:HG22	3:F:135:ARG:H	1.67	0.59
14:R:99:ARG:NH2	53:A:578:U:OP1	2.32	0.59
15:S:118:ASN:ND2	53:A:586:U:O2'	2.35	0.59
50:u:109:ILE:HA	50:u:127:VAL:HG12	1.84	0.59
53:A:214:G:H1'	53:A:225:C:H1'	1.83	0.59
15:S:163:LYS:HB2	33:b:106:ASP:HB3	1.84	0.59
28:6:234:HIS:ND1	28:6:255:LEU:O	2.35	0.59
35:d:198:ARG:HB2	35:d:211:GLN:HB2	1.84	0.59
36:e:146:ARG:HA	36:e:151:ARG:HD2	1.84	0.59
18:V:25:PRO:HG2	18:V:28:SER:HB3	1.85	0.59
30:8:165:ASP:OD2	36:e:185:ARG:NH1	2.36	0.59
1:D:113:ARG:O	1:D:147:ARG:NH2	2.36	0.58
3:F:49:ARG:HD3	3:F:263:LEU:HD22	1.85	0.58
5:I:148:VAL:O	42:k:31:ARG:NH1	2.36	0.58
49:s:212:ARG:HD3	49:s:379:LEU:HD12	1.85	0.58
23:0:113:CYS:HB3	23:0:126:CYS:SG	2.44	0.58
27:5:68:PRO:O	53:A:43:A:N6	2.37	0.58
49:s:232:GLN:NE2	49:s:234:ASP:OD1	2.36	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
27:5:324:GLN:HE22	27:5:340:VAL:HG11	1.68	0.58
30:8:160:GLU:OE1	36:e:207:ASN:ND2	2.36	0.58
37:f:114:CYS:HA	37:f:119:ILE:HD12	1.85	0.58
53:A:566:C:N4	53:A:1018:C:O2	2.36	0.58
27:5:215:ARG:HE	27:5:216:GLU:HG2	1.68	0.58
20:X:77:ARG:NH2	27:5:46:LEU:O	2.30	0.58
16:T:149:ARG:O	53:A:2:C:O2'	2.22	0.58
27:5:132:LEU:HD12	27:5:136:VAL:HG21	1.86	0.58
28:6:52:ARG:HB3	54:B:1637:C:H5'	1.86	0.58
34:c:244:GLU:OE1	34:c:248:ARG:NH2	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:w:138:LEU:HD13	52:w:144:ILE:HG12	1.86	0.58
3:F:92:ARG:NH2	53:A:208:U:O3'	2.37	0.58
17:U:11:ARG:NH1	18:V:212:LYS:O	2.37	0.57
20:X:177:HIS:O	20:X:184:ARG:NH1	2.37	0.57
1:D:111:ARG:O	1:D:165:ASN:ND2	2.38	0.57
1:D:235:GLN:HB2	1:D:294:SER:HA	1.86	0.57
2:E:133:THR:OG1	2:E:144:THR:OG1	2.21	0.57
5:I:117:ARG:NH1	6:J:133:GLN:OE1	2.38	0.57
5:I:128:ASN:ND2	5:I:149:GLY:O	2.37	0.57
15:S:162:GLU:HB2	15:S:192:VAL:HB	1.85	0.57
38:g:111:ARG:NH2	53:A:211:A:OP2	2.37	0.57
51:v:54:GLN:HG2	51:v:57:LYS:HE2	1.85	0.57
11:O:64:LYS:NZ	11:O:97:TYR:O	2.36	0.57
25:2:59:LYS:NZ	53:A:310:A:OP2	2.37	0.57
42:k:16:VAL:HG12	42:k:66:VAL:HG22	1.87	0.57
43:l:120:ARG:NH1	53:A:520:C:OP1	2.36	0.57
51:v:13:TYR:OH	51:v:36:ARG:NH2	2.37	0.57
51:v:43:GLN:HA	57:v:101:PNS:H431	1.85	0.57
51:v:44:LYS:NZ	52:w:111:ASP:OD2	2.37	0.57
1:D:202:ARG:O	53:A:851:A:N6	2.36	0.57
3:F:71:GLY:HA3	3:F:74:GLN:HB2	1.86	0.57
3:F:167:MET:HA	3:F:170:ARG:HE	1.68	0.57
36:e:152:LYS:HZ3	36:e:256:THR:HG21	1.68	0.57
9:M:57:ARG:NH2	53:A:425:U:OP2	2.37	0.57
12:P:39:VAL:HG12	12:P:41:ASN:H	1.69	0.57
53:A:423:U:O2	53:A:596:U:O2'	2.22	0.57
50:u:194:TRP:HA	50:u:197:ARG:HH11	1.69	0.57
53:A:769:U:H2'	53:A:770:G:H8	1.69	0.57
3:F:217:LEU:HD23	3:F:259:LEU:HD12	1.86	0.57
15:S:101:PHE:HE2	41:j:49:TRP:HB3	1.70	0.57
22:Z:71:ARG:NH2	53:A:470:G:OP2	2.38	0.57
53:A:385:U:H2'	53:A:386:G:H8	1.70	0.57
12:P:39:VAL:HB	12:P:42:GLU:HG2	1.87	0.57
22:Z:109:LYS:NZ	53:A:388:C:O2	2.33	0.57
50:u:135:LEU:HD12	50:u:179:LEU:HB3	1.86	0.57
7:K:119:ARG:NH2	53:A:1035:U:OP2	2.37	0.57
22:Z:77:ARG:NH1	53:A:466:C:OP2	2.38	0.57
29:7:167:VAL:HG23	29:7:235:TYR:HB3	1.87	0.57
29:7:189:LEU:O	29:7:295:ARG:NH2	2.38	0.57
51:v:14:ARG:NH1	52:w:132:ASP:OD2	2.38	0.57
12:P:146:TYR:OH	12:P:158:MET:SD	2.63	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:16:ILE:HD11	24:1:36:ARG:HE	1.68	0.56
42:k:80:HIS:O	48:r:36:ARG:NH1	2.38	0.56
5:I:101:ASN:HD22	5:I:174:LEU:HD21	1.71	0.56
5:I:120:LYS:NZ	5:I:157:GLU:OE1	2.38	0.56
11:O:139:ASP:OD2	29:7:131:LYS:NZ	2.38	0.56
16:T:94:ILE:HD13	16:T:106:LEU:HD11	1.87	0.56
35:d:140:LYS:O	35:d:143:ASP:HB2	2.05	0.56
27:5:204:VAL:O	27:5:228:ALA:HA	2.05	0.56
12:P:51:ARG:NH1	28:6:228:PRO:O	2.38	0.56
50:u:93:ASP:H	50:u:96:MET:HE2	1.70	0.56
12:P:49:THR:HG21	28:6:228:PRO:HB3	1.87	0.56
26:3:162:THR:OG1	26:3:167:LYS:NZ	2.37	0.56
29:7:262:ASP:OD1	29:7:263:VAL:N	2.38	0.56
53:A:405:U:O2'	53:A:1163:A:N7	2.35	0.56
2:E:50:ASP:OD2	11:O:138:ARG:NH2	2.37	0.56
11:O:26:ILE:HD13	13:Q:264:TRP:HB2	1.88	0.56
29:7:203:THR:HG22	29:7:280:VAL:H	1.70	0.56
35:d:148:ALA:O	35:d:151:CYS:HB2	2.05	0.56
8:L:87:VAL:HG11	8:L:123:ILE:HD12	1.88	0.56
17:U:71:ARG:NH1	17:U:73:GLN:OE1	2.39	0.56
7:K:73:GLU:OE2	48:r:149:ARG:NH2	2.36	0.56
10:N:123:ARG:NH1	10:N:162:GLU:OE1	2.39	0.56
11:O:125:TYR:O	11:O:128:ASN:ND2	2.39	0.56
19:W:74:ARG:HG3	53:A:395:A:C4	2.41	0.56
27:5:163:LEU:O	49:s:287:LYS:NZ	2.38	0.56
33:b:65:VAL:HG23	39:h:154:ILE:HG23	1.88	0.55
53:A:130:G:N1	53:A:133:A:OP2	2.39	0.55
53:A:1065:G:H1	53:A:1254:U:H3	1.53	0.55
2:E:96:ARG:NH2	2:E:197:HIS:O	2.37	0.55
7:K:60:MET:HE1	33:b:146:ARG:HE	1.71	0.55
9:M:54:LYS:NZ	53:A:349:G:N7	2.45	0.55
36:e:279:LEU:HD11	37:f:176:SER:HB2	1.89	0.55
53:A:1446:C:N3	53:A:1470:A:N1	2.54	0.55
11:O:130:LEU:HD22	23:0:134:THR:HG23	1.88	0.55
16:T:202:GLN:OE1	32:a:122:ARG:NH2	2.39	0.55
21:Y:193:ARG:NH2	53:A:37:C:OP1	2.39	0.55
5:I:48:MET:O	10:N:250:ARG:NH2	2.34	0.55
9:M:168:GLU:OE2	9:M:220:ARG:NH2	2.38	0.55
24:1:47:ASP:O	24:1:51:LYS:N	2.39	0.55
38:g:100:ILE:HA	38:g:105:ARG:O	2.06	0.55
3:F:63:GLN:OE1	39:h:97:LYS:NZ	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:272:LYS:HD2	40:i:63:LEU:HA	1.89	0.55
21:Y:151:ASP:OD1	21:Y:154:ARG:NH2	2.40	0.55
21:Y:163:ALA:HB1	31:9:133:ARG:HG3	1.89	0.55
20:X:116:SER:O	20:X:120:ASP:HA	2.07	0.55
37:f:95:LEU:O	37:f:154:GLU:HA	2.07	0.55
39:h:148:LEU:HD22	39:h:152:LEU:HD22	1.88	0.55
40:i:36:LEU:HD21	53:A:143:C:H41	1.72	0.55
53:A:1070:A:N3	53:A:1251:A:O2'	2.39	0.55
33:b:30:SER:H	33:b:76:VAL:H	1.54	0.55
53:A:1152:C:O2'	53:A:1245:C:OP2	2.24	0.55
3:F:86:VAL:HG23	3:F:175:LYS:HG2	1.87	0.55
14:R:10:LEU:HD22	14:R:13:ARG:HD3	1.89	0.55
6:J:25:ARG:HA	6:J:65:PRO:HA	1.89	0.55
10:N:87:PHE:HB2	10:N:163:MET:HB2	1.89	0.55
13:Q:86:ARG:HH22	53:A:1546:C:H4'	1.71	0.55
16:T:69:ARG:NH1	35:d:228:PHE:O	2.40	0.55
50:u:121:THR:HG21	50:u:176:VAL:HB	1.89	0.55
1:D:79:MET:HE3	1:D:104:TYR:HB2	1.88	0.55
21:Y:157:GLN:HE22	31:9:119:PHE:HA	1.71	0.55
23:0:81:PRO:O	53:A:1009:U:O2'	2.25	0.55
27:5:345:VAL:HG21	27:5:414:PHE:HE1	1.72	0.55
28:6:175:VAL:HB	28:6:187:VAL:HB	1.89	0.55
30:8:133:ARG:HA	30:8:136:ILE:HG12	1.88	0.55
36:e:74:LEU:HD22	44:m:42:ARG:HB3	1.89	0.55
1:D:132:ASP:OD2	1:D:135:ARG:NH1	2.38	0.54
3:F:137:ARG:NH1	53:A:1262:G:OP1	2.40	0.54
19:W:49:ARG:NE	53:A:1156:G:OP1	2.40	0.54
35:d:210:GLY:O	35:d:249:GLU:HA	2.06	0.54
7:K:168:ARG:HH12	7:K:170:TRP:CD1	2.25	0.54
24:1:14:LYS:NZ	53:A:1179:G:OP1	2.40	0.54
36:e:64:THR:HG22	36:e:66:LEU:H	1.72	0.54
49:s:243:ILE:HG22	49:s:245:LYS:H	1.73	0.54
4:H:73:LEU:HD21	20:X:65:VAL:HG11	1.89	0.54
27:5:107:PHE:HB3	27:5:222:VAL:HG12	1.89	0.54
36:e:50:ALA:HB2	36:e:175:GLN:HG2	1.89	0.54
36:e:245:GLN:OE1	36:e:248:ASN:ND2	2.41	0.54
10:N:205:ARG:NH2	10:N:249:LYS:O	2.40	0.54
24:1:47:ASP:O	24:1:51:LYS:CA	2.55	0.54
33:b:4:ARG:NH2	53:A:167:C:OP1	2.40	0.54
19:W:121:PRO:HG2	28:6:40:ILE:HD12	1.89	0.54
27:5:115:GLU:HB2	27:5:119:GLN:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:149:CYS:SG	49:s:179:GLN:NE2	2.80	0.54
27:5:125:LYS:HE2	27:5:371:LYS:HG2	1.89	0.54
28:6:237:LEU:HA	28:6:249:GLN:O	2.08	0.54
21:Y:186:ILE:HD12	21:Y:190:LEU:HD12	1.90	0.54
36:e:202:ALA:HB2	36:e:238:LEU:HD23	1.89	0.54
11:O:52:MET:HE1	11:O:123:ILE:HG21	1.89	0.54
17:U:8:PRO:HA	21:Y:183:GLN:HE22	1.73	0.54
49:s:332:LEU:HD13	49:s:372:TYR:HB2	1.90	0.54
53:A:841:C:H3'	53:A:842:A:H8	1.73	0.54
9:M:104:LEU:HD11	9:M:126:GLY:HA3	1.90	0.54
14:R:57:ARG:NH2	15:S:170:ILE:O	2.40	0.54
27:5:174:GLU:OE2	27:5:298:ASN:ND2	2.41	0.54
28:6:292:GLN:HG3	28:6:294:ALA:H	1.73	0.54
37:f:125:TYR:O	37:f:155:ARG:NH1	2.41	0.54
1:D:235:GLN:HE21	1:D:292:MET:HE2	1.73	0.53
2:E:274:TRP:NE1	2:E:286:ASN:OD1	2.41	0.53
50:u:143:VAL:HG11	50:u:159:ILE:HD11	1.90	0.53
22:Z:38:ARG:NH1	53:A:405:U:OP1	2.40	0.53
24:1:47:ASP:O	24:1:51:LYS:HA	2.08	0.53
30:8:139:MET:HE1	37:f:169:ILE:HG12	1.89	0.53
1:D:154:THR:H	1:D:157:MET:HE2	1.73	0.53
30:8:171:PHE:HE1	36:e:203:LYS:HG2	1.73	0.53
52:w:82:ARG:NH2	52:w:125:GLU:OE1	2.42	0.53
19:W:75:TRP:HB2	19:W:89:LEU:HD11	1.91	0.53
21:Y:230:LYS:NZ	53:A:10:A:OP2	2.41	0.53
36:e:177:GLU:O	36:e:190:ARG:NH2	2.42	0.53
40:i:36:LEU:HD23	53:A:6:A:H1'	1.90	0.53
13:Q:238:PHE:HB3	13:Q:240:ILE:HG12	1.89	0.53
15:S:181:LYS:NZ	53:A:626:U:O4	2.39	0.53
50:u:196:LEU:HD11	50:u:199:TYR:HB2	1.91	0.53
14:R:48:ARG:NH2	53:A:174:A:OP2	2.39	0.53
22:Z:99:VAL:HG12	41:j:80:LEU:HD12	1.90	0.53
31:9:53:ILE:HD12	31:9:56:MET:HE2	1.91	0.53
35:d:181:VAL:HG23	35:d:224:ILE:HG12	1.91	0.53
53:A:521:A:N6	53:A:528:A:OP2	2.42	0.53
3:F:156:ARG:O	40:i:90:ARG:NH1	2.42	0.53
7:K:114:LYS:NZ	53:A:1032:G:OP1	2.41	0.53
20:X:86:ILE:HB	20:X:105:TRP:HB2	1.90	0.53
29:7:64:LYS:NZ	35:d:276:ILE:O	2.42	0.53
36:e:205:LEU:HD21	37:f:175:GLN:HE22	1.73	0.53
2:E:68:GLU:OE2	2:E:154:ARG:NH1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:220:ASP:O	3:F:245:ALA:N	2.42	0.53
13:Q:155:ILE:HG22	13:Q:156:GLU:HG2	1.90	0.53
16:T:79:GLN:HE21	16:T:79:GLN:HA	1.74	0.53
17:U:126:LEU:HD11	35:d:76:ILE:HD12	1.91	0.53
23:O:139:ARG:NH2	53:A:652:C:OP1	2.42	0.53
35:d:208:VAL:HB	35:d:252:LEU:HB2	1.91	0.53
53:A:615:U:H2'	53:A:616:A:H8	1.73	0.53
5:I:140:TYR:HB3	5:I:143:LEU:HB2	1.91	0.52
15:S:131:GLU:OE2	15:S:151:LYS:NZ	2.42	0.52
38:g:101:THR:O	38:g:105:ARG:HB2	2.09	0.52
40:i:93:ARG:NH1	53:A:67:A:O2'	2.42	0.52
27:5:384:GLN:NE2	53:A:725:A:O2'	2.38	0.52
34:c:60:ARG:NH2	34:c:65:ASN:O	2.41	0.52
28:6:221:LEU:HD23	28:6:231:GLU:HG2	1.91	0.52
34:c:93:VAL:HG12	34:c:180:LEU:HD22	1.91	0.52
3:F:188:HIS:HB2	3:F:260:VAL:HG22	1.92	0.52
4:H:99:THR:O	4:H:108:ARG:NH1	2.43	0.52
25:2:82:ARG:HH21	25:2:87:ARG:HD3	1.74	0.52
26:3:133:LEU:HD22	26:3:141:LYS:HG2	1.91	0.52
29:7:106:ALA:O	29:7:113:TRP:HB2	2.09	0.52
38:g:56:ARG:NH1	38:g:57:ILE:O	2.39	0.52
3:F:160:SER:HB3	40:i:80:LEU:HD13	1.91	0.52
5:I:128:ASN:HA	5:I:131:LEU:HB3	1.91	0.52
18:V:177:THR:O	31:9:75:SER:OG	2.27	0.52
27:5:205:GLN:HA	27:5:228:ALA:H	1.74	0.52
49:s:142:LEU:HD13	49:s:422:VAL:HG21	1.92	0.52
51:v:40:ARG:HH21	52:w:113:LEU:HD13	1.74	0.52
2:E:166:ARG:NH1	29:7:314:ASP:OD2	2.43	0.52
28:6:302:ASP:HA	28:6:305:LYS:HG2	1.92	0.52
40:i:45:ASP:O	40:i:51:ARG:NH1	2.42	0.52
49:s:272:PRO:O	53:A:704:A:N6	2.34	0.52
5:I:101:ASN:HB2	5:I:152:MET:HG3	1.90	0.52
17:U:3:ARG:O	17:U:23:ASN:ND2	2.42	0.52
19:W:100:THR:OG1	19:W:132:HIS:NE2	2.39	0.52
53:A:789:A:N6	53:A:998:A:O2'	2.43	0.52
8:L:69:VAL:HG23	8:L:88:GLY:H	1.74	0.52
19:W:41:ASN:HD21	53:A:1171:U:H3'	1.75	0.52
50:u:127:VAL:HG23	50:u:179:LEU:HD13	1.90	0.52
54:B:1628:C:H2'	54:B:1629:A:H8	1.75	0.52
12:P:126:GLU:OE2	12:P:130:ARG:NE	2.43	0.52
23:O:106:ASN:OD1	53:A:1542:C:O2'	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:b:26:LEU:HD22	33:b:105:ALA:HA	1.91	0.52
48:r:153:ARG:NH2	53:A:489:U:OP2	2.43	0.52
49:s:310:ARG:HH22	53:A:747:C:H2'	1.75	0.52
9:M:94:LYS:HG3	9:M:129:ILE:HG22	1.92	0.51
15:S:173:ARG:NH2	53:A:473:G:OP1	2.40	0.51
24:l:50:VAL:HG12	24:l:52:GLN:HB2	1.91	0.51
37:f:163:SER:O	37:f:167:ALA:N	2.39	0.51
53:A:472:A:O2'	53:A:592:C:OP1	2.27	0.51
29:7:144:ARG:NH1	29:7:171:GLU:OE1	2.43	0.51
3:F:93:LEU:HD12	45:o:91:GLN:HG2	1.91	0.51
29:7:282:ALA:HB2	29:7:321:ARG:HG2	1.91	0.51
2:E:221:ARG:NH2	53:A:1438:U:O4'	2.43	0.51
6:J:31:PRO:HB2	6:J:34:PRO:HG2	1.91	0.51
49:s:65:ARG:NH2	53:A:776:A:OP1	2.43	0.51
1:D:202:ARG:NH2	53:A:851:A:OP2	2.42	0.51
2:E:266:ARG:NH1	53:A:1476:G:O3'	2.44	0.51
6:J:128:GLU:HA	6:J:133:GLN:HE21	1.75	0.51
13:Q:150:ILE:HA	13:Q:162:ILE:O	2.11	0.51
15:S:175:ARG:HB2	15:S:180:PHE:HB3	1.91	0.51
17:U:28:LEU:O	21:Y:114:THR:OG1	2.26	0.51
28:6:185:MET:HE1	46:p:189:ARG:HG3	1.92	0.51
37:f:101:THR:OG1	44:m:67:ARG:NH1	2.43	0.51
23:0:179:ARG:HH12	23:0:182:PRO:HG3	1.75	0.51
25:2:82:ARG:HE	25:2:87:ARG:HD3	1.76	0.51
49:s:111:LYS:NZ	49:s:384:ASP:OD1	2.36	0.51
13:Q:129:LYS:NZ	50:u:121:THR:O	2.35	0.51
28:6:292:GLN:HB3	28:6:295:GLN:HG2	1.92	0.51
53:A:201:A:H61	53:A:231:C:H5'	1.76	0.51
19:W:125:VAL:HA	28:6:57:TYR:HE1	1.75	0.51
34:c:308:THR:HG22	34:c:310:ASN:H	1.76	0.51
36:e:124:TRP:HB3	44:m:73:ARG:HG3	1.92	0.51
53:A:1454:U:N3	53:A:1463:A:H8	2.04	0.51
1:D:90:ARG:NH1	53:A:314:A:OP1	2.42	0.51
9:M:38:ARG:HE	9:M:45:ARG:NH2	2.06	0.51
23:0:119:LYS:C	23:0:120:HIS:HD1	2.18	0.51
26:3:172:TYR:HB2	26:3:175:ASP:HB2	1.93	0.51
36:e:51:LEU:HD12	36:e:188:ALA:HB1	1.92	0.51
26:3:188:VAL:HG11	38:g:104:ASN:HB3	1.93	0.51
29:7:152:CYS:SG	29:7:156:ARG:NH1	2.84	0.51
11:O:13:ARG:NH2	53:A:993:C:OP1	2.44	0.50
14:R:40:ARG:NH1	53:A:626:U:O2'	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:44:VAL:HG11	18:V:83:ARG:HE	1.75	0.50
18:V:145:ARG:HH22	18:V:156:LYS:HA	1.74	0.50
26:3:108:LYS:NZ	53:A:75:U:O4	2.36	0.50
36:e:152:LYS:HB2	36:e:157:LEU:HD11	1.93	0.50
3:F:89:THR:H	3:F:179:THR:HG21	1.76	0.50
16:T:137:ARG:NH2	29:7:95:LEU:O	2.44	0.50
29:7:106:ALA:CA	29:7:126:LYS:O	2.54	0.50
53:A:28:C:O2'	53:A:32:A:N3	2.40	0.50
14:R:126:GLU:HA	15:S:66:LEU:HD11	1.93	0.50
40:i:72:GLU:OE1	47:q:33:ARG:NH2	2.42	0.50
4:H:131:TYR:HD2	20:X:139:TYR:HA	1.75	0.50
7:K:177:ARG:NH2	53:A:1513:U:O2	2.43	0.50
10:N:179:VAL:HA	10:N:182:LYS:HZ2	1.76	0.50
14:R:107:ILE:HG13	16:T:211:THR:HG21	1.92	0.50
29:7:44:ARG:HB3	29:7:261:ILE:HD13	1.93	0.50
53:A:512:G:H1'	53:A:529:A:H2'	1.93	0.50
9:M:177:ALA:HB1	9:M:203:ARG:HH12	1.76	0.50
16:T:79:GLN:HA	16:T:79:GLN:NE2	2.26	0.50
17:U:48:MET:HE2	17:U:53:LEU:HA	1.92	0.50
3:F:241:ASN:OD1	3:F:256:HIS:NE2	2.37	0.50
6:J:142:ARG:NH2	53:A:521:A:OP1	2.44	0.50
27:5:114:LEU:HD22	53:A:718:A:H62	1.76	0.50
28:6:196:THR:OG1	28:6:324:ASP:OD2	2.26	0.50
10:N:170:GLU:HA	10:N:173:GLN:HB2	1.92	0.50
28:6:273:PHE:HA	28:6:313:PRO:HA	1.93	0.50
28:6:365:TYR:HA	28:6:368:ARG:HD3	1.92	0.50
36:e:55:ARG:HH21	36:e:157:LEU:HD13	1.77	0.50
36:e:270:ALA:O	36:e:273:ARG:NH1	2.44	0.50
53:A:1257:C:H2'	53:A:1258:C:H4'	1.94	0.50
19:W:68:ALA:HB3	19:W:89:LEU:HD12	1.94	0.50
30:8:140:LEU:HD22	37:f:169:ILE:HD13	1.94	0.50
41:j:88:LEU:HD21	45:o:54:MET:HG2	1.94	0.50
2:E:331:ASP:N	2:E:331:ASP:OD1	2.44	0.49
14:R:114:LYS:HE2	32:a:44:ASN:HB3	1.94	0.49
29:7:193:MET:HE1	29:7:285:ASN:HD21	1.77	0.49
53:A:11:G:C6	53:A:102:A:N1	2.80	0.49
22:Z:82:GLU:HG2	22:Z:113:VAL:HG12	1.94	0.49
39:h:86:TRP:H	39:h:86:TRP:CD1	2.30	0.49
49:s:246:GLN:OE1	49:s:353:ARG:NH1	2.45	0.49
50:u:190:LEU:HA	50:u:193:LEU:HD23	1.93	0.49
50:u:197:ARG:HG2	51:v:66:LEU:HB3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:w:111:ASP:OD1	52:w:112:SER:N	2.45	0.49
53:A:307:U:H2'	53:A:308:A:H8	1.77	0.49
20:X:92:ALA:HB3	20:X:98:SER:HB2	1.94	0.49
53:A:1152:C:H5''	53:A:1153:U:H5	1.76	0.49
27:5:173:ARG:NH1	27:5:348:ASP:O	2.44	0.49
43:l:131:ARG:HA	43:l:134:LYS:HE3	1.94	0.49
53:A:722:U:H2'	53:A:724:A:H62	1.77	0.49
1:D:264:ARG:HE	53:A:304:A:H4'	1.76	0.49
11:O:108:LEU:HD13	23:O:122:LEU:HD21	1.94	0.49
12:P:82:ARG:HH12	12:P:84:ILE:HD11	1.77	0.49
12:P:85:ARG:HD2	12:P:158:MET:HE3	1.94	0.49
36:e:266:PRO:HD2	36:e:269:LEU:HB2	1.95	0.49
37:f:158:GLN:NE2	37:f:160:SER:OG	2.45	0.49
57:v:101:PNS:O27	57:v:101:PNS:O33	2.27	0.49
2:E:212:GLY:HA2	2:E:262:GLY:HA3	1.95	0.49
11:O:145:LEU:HD11	29:7:308:ALA:HB2	1.95	0.49
27:5:301:PRO:HD3	53:A:720:A:H4'	1.94	0.49
28:6:198:ALA:O	28:6:254:TYR:OH	2.30	0.49
29:7:81:MET:HG2	35:d:279:THR:HB	1.95	0.49
29:7:194:PRO:HG2	29:7:283:VAL:HG21	1.94	0.49
36:e:91:ALA:O	36:e:95:ASN:ND2	2.36	0.49
9:M:140:LEU:HG	9:M:156:VAL:HG11	1.94	0.49
14:R:11:ARG:HB2	53:A:622:G:C8	2.46	0.49
35:d:144:ILE:HG23	35:d:163:LEU:HD22	1.95	0.49
36:e:123:MET:HA	36:e:126:GLN:HG2	1.95	0.49
54:B:1607:U:O4	54:B:1664:G:O6	2.30	0.49
21:Y:83:ALA:N	31:9:74:VAL:O	2.43	0.49
3:F:107:LYS:HG2	40:i:74:ILE:HG22	1.95	0.49
6:J:128:GLU:OE1	6:J:133:GLN:NE2	2.46	0.49
17:U:61:TYR:O	21:Y:63:GLY:N	2.45	0.49
29:7:108:VAL:HB	29:7:113:TRP:CD1	2.48	0.49
4:H:103:GLU:HG2	4:H:104:ASN:H	1.77	0.49
53:A:573:A:H4'	53:A:574:U:H5'	1.95	0.49
1:D:252:HIS:HE1	1:D:255:ARG:HH22	1.61	0.48
9:M:71:GLN:OE1	53:A:364:A:O2'	2.31	0.48
9:M:116:ILE:HB	9:M:154:ILE:HA	1.94	0.48
24:1:62:ILE:HG21	53:A:1238:U:H4'	1.95	0.48
35:d:176:ILE:HD11	35:d:181:VAL:HB	1.95	0.48
22:Z:149:TRP:NE1	41:j:45:GLU:OE1	2.28	0.48
29:7:99:TYR:O	29:7:103:SER:OG	2.28	0.48
46:p:78:ILE:HG22	46:p:101:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:s:295:GLY:N	49:s:339:GLN:OE1	2.46	0.48
53:A:738:U:H2'	53:A:739:A:H8	1.77	0.48
1:D:142:VAL:O	1:D:148:LYS:HA	2.13	0.48
3:F:219:VAL:HB	3:F:261:LEU:HD23	1.95	0.48
10:N:76:SER:HB3	10:N:155:LYS:HB2	1.94	0.48
28:6:56:ARG:NE	54:B:1625:A:OP1	2.44	0.48
28:6:192:GLU:HG3	28:6:320:GLN:HB2	1.95	0.48
53:A:77:G:OP2	53:A:79:C:N4	2.46	0.48
6:J:131:ALA:HB3	53:A:499:A:H4'	1.95	0.48
8:L:93:GLY:O	8:L:95:ARG:NH2	2.47	0.48
13:Q:221:LYS:HB3	13:Q:244:ARG:HG2	1.95	0.48
16:T:55:ASN:ND2	16:T:74:TYR:O	2.40	0.48
20:X:116:SER:O	20:X:120:ASP:CA	2.62	0.48
35:d:209:TYR:O	35:d:211:GLN:NE2	2.42	0.48
43:l:123:LYS:HG2	53:A:527:G:H5'	1.95	0.48
51:v:39:PHE:HE1	51:v:54:GLN:HE22	1.60	0.48
7:K:3:SER:HA	34:c:309:GLU:HG3	1.96	0.48
7:K:59:ILE:HB	7:K:127:LEU:HD23	1.95	0.48
10:N:94:GLY:HA2	10:N:154:VAL:O	2.12	0.48
12:P:154:ALA:HA	12:P:159:LYS:HE3	1.95	0.48
16:T:75:HIS:HD2	16:T:120:VAL:HG13	1.78	0.48
18:V:20:ARG:NH2	53:A:132:A:OP1	2.44	0.48
29:7:132:ASP:HB3	29:7:135:PRO:HB3	1.94	0.48
37:f:81:ASN:HB3	37:f:86:TYR:CE1	2.49	0.48
3:F:175:LYS:O	3:F:179:THR:HG23	2.14	0.48
6:J:108:VAL:HG21	6:J:154:ARG:HG2	1.95	0.48
8:L:145:VAL:O	50:u:119:ARG:NH2	2.47	0.48
21:Y:153:LEU:HG	31:9:130:LEU:HD11	1.95	0.48
34:c:220:ILE:HG13	34:c:223:MET:HE3	1.96	0.48
35:d:83:GLY:O	35:d:262:HIS:NE2	2.39	0.48
40:i:61:GLY:HA3	53:A:216:G:H1	1.79	0.48
50:u:102:ARG:NH2	51:v:25:TYR:O	2.40	0.48
12:P:65:GLU:OE2	12:P:68:TRP:NE1	2.42	0.48
17:U:41:GLN:HE21	17:U:96:TYR:HE2	1.62	0.48
23:0:94:ARG:NH2	53:A:640:G:OP2	2.46	0.48
53:A:381:A:H2'	53:A:382:A:C8	2.48	0.48
7:K:71:LYS:HG2	48:r:174:MET:HE2	1.96	0.48
27:5:310:ARG:NH2	27:5:378:SER:OG	2.47	0.48
37:f:124:SER:OG	37:f:155:ARG:NH2	2.47	0.48
53:A:132:A:N7	53:A:135:A:N6	2.62	0.48
1:D:248:SER:OG	1:D:249:ASN:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:Y:128:SER:OG	21:Y:131:ARG:NE	2.41	0.48
23:O:120:HIS:CD2	53:A:1543:A:H4'	2.48	0.48
31:9:22:THR:HG23	31:9:24:LYS:H	1.79	0.48
48:r:116:GLU:O	48:r:120:LYS:HG2	2.14	0.48
53:A:985:G:N2	53:A:989:C:O2'	2.46	0.48
5:I:40:MET:HB2	5:I:45:GLN:HG3	1.95	0.47
5:I:101:ASN:HA	5:I:174:LEU:HD11	1.96	0.47
8:L:96:MET:HG3	13:Q:170:ARG:HH22	1.79	0.47
24:1:63:ARG:NH2	53:A:1240:A:OP1	2.46	0.47
41:j:76:ARG:NH2	53:A:413:U:OP1	2.46	0.47
49:s:254:ASP:HA	49:s:389:ARG:HG3	1.96	0.47
53:A:119:A:N3	53:A:245:C:O2'	2.42	0.47
1:D:124:GLU:HA	27:5:258:PRO:HG3	1.96	0.47
5:I:62:PRO:HA	5:I:65:LEU:HD12	1.96	0.47
6:J:25:ARG:HG2	6:J:65:PRO:HB3	1.96	0.47
18:V:131:THR:HG22	18:V:149:ARG:HH11	1.78	0.47
52:w:87:LEU:HD23	52:w:98:LEU:HD11	1.96	0.47
53:A:1134:A:H2'	53:A:1135:A:H8	1.78	0.47
7:K:174:GLU:HG3	48:r:56:THR:HG21	1.96	0.47
19:W:121:PRO:HD2	19:W:124:ALA:HB2	1.96	0.47
21:Y:69:ASP:OD1	21:Y:69:ASP:N	2.44	0.47
23:O:93:ARG:NH2	53:A:640:G:OP2	2.47	0.47
53:A:1260:U:H2'	53:A:1261:A:H8	1.78	0.47
16:T:91:ALA:O	16:T:145:SER:OG	2.32	0.47
31:9:24:LYS:NZ	53:A:752:U:OP2	2.48	0.47
2:E:348:ALA:HB2	13:Q:128:GLY:HA3	1.97	0.47
9:M:41:ARG:NE	53:A:624:A:OP2	2.37	0.47
52:w:114:ASP:HA	52:w:117:GLU:HG3	1.95	0.47
3:F:126:LYS:NZ	3:F:138:HIS:O	2.42	0.47
6:J:69:LYS:HB3	6:J:81:LYS:HB3	1.97	0.47
11:O:116:ASP:OD2	53:A:783:G:O2'	2.32	0.47
17:U:98:GLN:HB3	49:s:100:LEU:HD12	1.96	0.47
36:e:202:ALA:HA	36:e:239:LEU:H	1.80	0.47
53:A:79:C:OP2	53:A:1229:C:O2'	2.26	0.47
2:E:208:ALA:HB2	2:E:297:VAL:HG12	1.96	0.47
5:I:145:PRO:O	42:k:26:ASN:ND2	2.42	0.47
7:K:67:PHE:HE2	7:K:103:ILE:HD13	1.79	0.47
8:L:108:ILE:HA	8:L:114:PRO:HA	1.97	0.47
9:M:220:ARG:HH22	9:M:236:LEU:HD12	1.80	0.47
12:P:88:HIS:O	12:P:119:THR:OG1	2.30	0.47
24:1:20:MET:HB3	24:1:30:PHE:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:l:43:LEU:O	24:l:55:LEU:HA	2.14	0.47
28:6:50:LYS:O	28:6:52:ARG:NH1	2.48	0.47
35:d:276:ILE:HG22	35:d:278:LYS:H	1.80	0.47
53:A:1140:G:H2'	53:A:1141:G:H8	1.79	0.47
9:M:292:LYS:O	9:M:296:SER:OG	2.32	0.47
3:F:138:HIS:CD2	3:F:146:TRP:HE1	2.32	0.47
9:M:97:SER:HA	9:M:141:VAL:HB	1.96	0.47
20:X:23:ARG:NH1	20:X:219:GLU:OE2	2.48	0.47
28:6:173:LEU:O	28:6:174:HIS:ND1	2.47	0.47
29:7:79:PHE:HB3	29:7:81:MET:HE3	1.96	0.47
52:w:104:PHE:HD1	52:w:110:LEU:HD12	1.80	0.47
53:A:661:C:H5'	53:A:774:A:H62	1.80	0.47
1:D:246:ARG:NH2	53:A:861:U:O4	2.48	0.47
14:R:57:ARG:NH1	53:A:474:A:OP1	2.42	0.47
16:T:98:SER:HA	16:T:141:TYR:HA	1.97	0.47
27:5:353:HIS:CE1	27:5:379:ASP:H	2.33	0.47
33:b:27:GLN:OE1	33:b:28:ARG:NH2	2.48	0.47
38:g:105:ARG:HD2	53:A:382:A:H5'	1.97	0.47
39:h:66:LEU:HD21	39:h:130:TYR:HB3	1.97	0.47
42:k:39:SER:OG	42:k:40:GLU:N	2.48	0.47
53:A:48:A:N3	53:A:241:C:O2'	2.40	0.47
1:D:208:ARG:HB2	53:A:859:U:H2'	1.96	0.46
9:M:68:GLU:OE2	9:M:71:GLN:NE2	2.46	0.46
9:M:292:LYS:HB3	9:M:292:LYS:HE2	1.71	0.46
29:7:84:ASN:O	29:7:84:ASN:ND2	2.37	0.46
42:k:66:VAL:HB	42:k:74:LEU:HB3	1.97	0.46
51:v:51:ARG:HG3	57:v:101:PNS:H422	1.97	0.46
53:A:241:C:H2'	53:A:242:A:H8	1.79	0.46
2:E:97:VAL:O	2:E:197:HIS:NE2	2.48	0.46
7:K:52:ASP:O	16:T:206:ARG:NH1	2.47	0.46
9:M:38:ARG:HD2	9:M:45:ARG:HE	1.80	0.46
11:O:91:GLN:NE2	49:s:44:TYR:OH	2.48	0.46
27:5:339:PRO:HB2	27:5:358:GLN:HE22	1.79	0.46
38:g:87:ARG:HB2	38:g:112:LYS:HB3	1.97	0.46
2:E:221:ARG:NH1	2:E:260:LYS:O	2.48	0.46
9:M:91:ARG:NE	9:M:210:LEU:HD11	2.31	0.46
13:Q:122:ALA:HB2	13:Q:172:GLN:HE22	1.80	0.46
31:9:126:LYS:HB3	31:9:126:LYS:HE2	1.76	0.46
35:d:220:GLN:O	35:d:239:PRO:HA	2.15	0.46
43:l:133:SER:O	53:A:530:A:O2'	2.33	0.46
46:p:106:ALA:O	46:p:116:ARG:NH1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A:368:U:O4	53:A:1141:G:O2'	2.33	0.46
53:A:991:U:H2'	53:A:992:A:H8	1.81	0.46
22:Z:88:MET:SD	53:A:412:G:N2	2.73	0.46
24:1:47:ASP:HB2	24:1:50:VAL:HB	1.98	0.46
28:6:360:ARG:NH1	53:A:1198:C:OP2	2.45	0.46
29:7:67:VAL:HG12	29:7:123:CYS:H	1.80	0.46
35:d:245:TYR:HB2	35:d:265:ILE:HB	1.97	0.46
48:r:94:ARG:HE	48:r:100:LEU:HD23	1.81	0.46
48:r:188:SER:OG	48:r:190:THR:O	2.33	0.46
50:u:125:VAL:HB	50:u:177:ILE:HG13	1.98	0.46
53:A:1260:U:H2'	53:A:1261:A:C8	2.50	0.46
7:K:21:LEU:HB3	7:K:59:ILE:HG12	1.97	0.46
13:Q:119:VAL:HG23	13:Q:174:ILE:HG22	1.98	0.46
17:U:24:PHE:HE2	17:U:48:MET:HE3	1.80	0.46
27:5:385:HIS:HB2	53:A:725:A:H1'	1.98	0.46
53:A:237:A:N3	53:A:1260:U:O2'	2.41	0.46
53:A:1007:A:H2'	53:A:1008:A:C8	2.51	0.46
3:F:261:LEU:HD13	3:F:266:VAL:HG12	1.98	0.46
18:V:87:VAL:HG22	18:V:114:PRO:HB3	1.97	0.46
18:V:147:SER:OG	18:V:150:SER:O	2.30	0.46
27:5:117:VAL:O	27:5:121:LEU:CB	2.63	0.46
3:F:83:HIS:HB3	3:F:86:VAL:HG12	1.97	0.46
8:L:55:PRO:HB3	8:L:77:ILE:HG12	1.97	0.46
11:O:59:LEU:HB2	13:Q:269:MET:HE1	1.97	0.46
17:U:50:ARG:NH2	53:A:703:A:OP1	2.49	0.46
28:6:327:VAL:HA	28:6:330:ILE:HD12	1.97	0.46
29:7:142:TYR:HB2	29:7:269:ILE:HD11	1.98	0.46
30:8:143:GLN:HG2	36:e:210:CYS:HA	1.98	0.46
33:b:26:LEU:HD21	33:b:29:LEU:HD11	1.97	0.46
49:s:270:LYS:HA	49:s:270:LYS:HD3	1.81	0.46
50:u:184:THR:HA	50:u:187:ILE:HG12	1.97	0.46
51:v:23:LEU:HD23	51:v:28:ARG:HG2	1.97	0.46
51:v:36:ARG:O	51:v:40:ARG:N	2.48	0.46
53:A:241:C:H2'	53:A:242:A:C8	2.51	0.46
53:A:411:U:H2'	53:A:412:G:C8	2.51	0.46
53:A:801:G:N2	53:A:985:G:OP2	2.48	0.46
8:L:82:LYS:HD3	8:L:107:LEU:HD22	1.98	0.46
8:L:83:LYS:HG3	8:L:108:ILE:HG23	1.97	0.46
20:X:116:SER:O	20:X:120:ASP:N	2.49	0.46
50:u:108:ASP:OD2	50:u:185:ARG:NH1	2.49	0.46
53:A:511:A:N6	53:A:536:C:O2'	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:82:ARG:HH11	12:P:93:LEU:HD12	1.81	0.46
16:T:190:LYS:HG3	16:T:195:HIS:CE1	2.50	0.46
22:Z:76:ARG:NH2	53:A:470:G:N3	2.63	0.46
30:8:179:THR:OG1	44:m:61:GLY:O	2.28	0.46
53:A:27:A:N3	53:A:33:C:O2'	2.48	0.46
53:A:144:A:N3	53:A:192:U:O2'	2.46	0.46
53:A:416:A:H2'	53:A:417:U:C6	2.50	0.46
35:d:160:LEU:O	35:d:164:VAL:N	2.44	0.46
36:e:161:VAL:HG23	36:e:174:PRO:HG3	1.98	0.46
45:o:55:THR:HG22	45:o:58:GLN:HG3	1.97	0.46
1:D:225:ILE:HA	1:D:234:MET:O	2.16	0.45
12:P:63:ARG:HA	12:P:177:ARG:HE	1.81	0.45
13:Q:79:GLU:HA	13:Q:143:ARG:HD3	1.98	0.45
13:Q:100:LEU:HD12	13:Q:286:ILE:HD13	1.99	0.45
15:S:164:THR:HG22	33:b:107:GLN:HB2	1.98	0.45
46:p:176:HIS:HA	46:p:179:ARG:HD2	1.99	0.45
1:D:81:LYS:HB2	53:A:254:U:H5''	1.97	0.45
3:F:103:GLN:HE22	3:F:250:VAL:H	1.64	0.45
27:5:142:ASP:OD1	27:5:142:ASP:N	2.50	0.45
33:b:37:GLY:H	33:b:44:ARG:HH12	1.63	0.45
35:d:267:PRO:HG2	35:d:270:ALA:HB2	1.98	0.45
53:A:86:A:H2'	53:A:87:A:H8	1.81	0.45
1:D:218:ARG:O	1:D:225:ILE:HB	2.16	0.45
2:E:122:LEU:HB2	2:E:283:ILE:HB	1.97	0.45
7:K:25:MET:O	7:K:149:ARG:NH1	2.48	0.45
11:O:9:ILE:N	53:A:788:A:OP1	2.49	0.45
18:V:64:ILE:HD11	18:V:88:VAL:HG11	1.98	0.45
49:s:153:GLU:HG3	49:s:176:PHE:HB2	1.99	0.45
34:c:86:ASP:N	34:c:86:ASP:OD1	2.49	0.45
35:d:215:ARG:HG2	35:d:245:TYR:CE1	2.51	0.45
38:g:154:ASP:OD1	38:g:154:ASP:N	2.48	0.45
48:r:153:ARG:HG2	48:r:154:TRP:CD1	2.51	0.45
3:F:113:LYS:HD2	3:F:157:GLY:HA2	1.99	0.45
5:I:115:GLN:O	5:I:118:LYS:NZ	2.36	0.45
14:R:118:ALA:HB1	32:a:38:PRO:HG2	1.99	0.45
28:6:39:ASP:OD1	28:6:39:ASP:N	2.50	0.45
35:d:173:THR:HA	35:d:176:ILE:HG22	1.98	0.45
2:E:199:ARG:HD3	2:E:199:ARG:HA	1.74	0.45
3:F:237:LEU:HD13	3:F:240:PHE:HD2	1.81	0.45
7:K:90:VAL:HG13	7:K:94:GLN:HB2	1.98	0.45
16:T:154:LYS:NZ	53:A:634:G:OP1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:d:63:ALA:HA	53:A:678:A:H1'	1.99	0.45
1:D:87:HIS:CD2	1:D:88:THR:HG23	2.52	0.45
1:D:210:ALA:HB1	1:D:249:ASN:HB3	1.98	0.45
22:Z:117:ILE:O	45:o:45:ASN:ND2	2.46	0.45
27:5:178:PRO:HA	27:5:181:VAL:HG12	1.97	0.45
28:6:280:ASP:OD1	28:6:280:ASP:N	2.49	0.45
46:p:42:ILE:HD12	46:p:47:LYS:HD3	1.98	0.45
53:A:640:G:O2'	53:A:1005:G:O6	2.33	0.45
9:M:211:VAL:HG13	47:q:103:LEU:HD11	1.98	0.45
27:5:198:LEU:HD21	27:5:419:LEU:HD13	1.98	0.45
28:6:195:PRO:HA	28:6:198:ALA:HB3	1.97	0.45
40:i:115:ARG:HG3	53:A:61:A:N1	2.31	0.45
53:A:247:A:O5'	53:A:314:A:N6	2.50	0.45
3:F:218:LEU:HD23	3:F:260:VAL:HB	1.98	0.45
8:L:33:GLN:NE2	53:A:800:G:H1'	2.32	0.45
9:M:92:GLN:OE1	26:3:168:ARG:NH2	2.50	0.45
19:W:125:VAL:HG21	28:6:64:GLU:HG3	1.99	0.45
26:3:183:ARG:NH2	28:6:355:LYS:O	2.49	0.45
27:5:343:GLN:NE2	27:5:417:LEU:O	2.49	0.45
53:A:1075:A:H61	53:A:1133:A:H2	1.64	0.45
53:A:1480:U:H2'	53:A:1481:A:H8	1.82	0.45
5:I:47:LEU:HD12	10:N:226:ILE:HD13	1.98	0.45
6:J:47:ASN:OD1	6:J:48:GLN:N	2.50	0.45
14:R:34:ARG:HG2	14:R:37:ARG:HH21	1.81	0.45
15:S:137:GLY:HA3	15:S:142:THR:HG22	1.98	0.45
29:7:220:GLU:HG3	29:7:253:LYS:HG2	1.99	0.45
34:c:228:LEU:HB2	34:c:307:PHE:CD2	2.52	0.45
37:f:60:LYS:HD3	53:A:397:C:H5'	1.99	0.45
5:I:96:ILE:HG13	5:I:155:VAL:HG12	2.00	0.44
5:I:98:VAL:HG13	5:I:177:LEU:HB3	1.98	0.44
33:b:108:SER:OG	33:b:109:GLY:N	2.50	0.44
36:e:49:GLY:HA2	36:e:232:PHE:HB2	1.98	0.44
43:l:123:LYS:NZ	53:A:521:A:N7	2.61	0.44
50:u:124:PHE:HE2	50:u:178:HIS:CE1	2.34	0.44
3:F:117:ARG:NH1	53:A:235:C:OP1	2.47	0.44
5:I:181:ILE:O	5:I:184:THR:OG1	2.30	0.44
10:N:53:ILE:O	10:N:99:TRP:NE1	2.44	0.44
36:e:160:LEU:HD11	36:e:264:LEU:HD11	1.99	0.44
49:s:214:GLU:HA	49:s:228:ASP:HA	1.98	0.44
53:A:1542:C:H3'	53:A:1543:A:H8	1.82	0.44
54:B:1609:U:O2	54:B:1616:A:N6	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:20:LEU:N	11:O:24:SER:OG	2.39	0.44
22:Z:78:ARG:O	22:Z:83:LYS:NZ	2.50	0.44
45:o:54:MET:HB3	45:o:58:GLN:HB2	1.98	0.44
49:s:103:ASP:OD1	49:s:325:ARG:NH1	2.45	0.44
49:s:241:ILE:O	49:s:296:HIS:N	2.40	0.44
52:w:148:ILE:HG22	52:w:152:LYS:HE2	1.99	0.44
53:A:415:A:H2'	53:A:416:A:C8	2.53	0.44
54:B:1642:G:H2'	54:B:1643:A:C8	2.51	0.44
1:D:181:ALA:HB2	1:D:243:THR:HG22	2.00	0.44
17:U:149:SER:O	35:d:273:LYS:NZ	2.50	0.44
19:W:48:GLY:HA3	53:A:1165:C:H5''	2.00	0.44
38:g:91:MET:HE3	53:A:213:G:H5'	2.00	0.44
3:F:113:LYS:HG3	3:F:157:GLY:H	1.82	0.44
26:3:133:LEU:HD23	26:3:136:LYS:HD2	2.00	0.44
27:5:133:PRO:HD3	27:5:375:TRP:CG	2.53	0.44
34:c:206:SER:O	34:c:206:SER:OG	2.31	0.44
34:c:260:GLN:CA	34:c:269:LEU:O	2.61	0.44
52:w:78:GLY:O	52:w:82:ARG:HB2	2.17	0.44
1:D:252:HIS:HE1	1:D:255:ARG:NH2	2.16	0.44
2:E:328:LEU:HD22	2:E:332:LEU:HD11	2.00	0.44
17:U:27:GLN:HG3	17:U:43:ARG:HB2	2.00	0.44
17:U:36:PRO:HD3	49:s:270:LYS:HB3	1.99	0.44
27:5:354:PHE:HB2	27:5:377:ASP:HB2	2.00	0.44
32:a:41:ASP:HB3	32:a:46:ASN:HA	2.00	0.44
34:c:259:ARG:HD2	34:c:271:PHE:HD2	1.82	0.44
53:A:212:A:N1	53:A:221:A:O2'	2.48	0.44
53:A:1070:A:H2'	53:A:1071:A:C8	2.53	0.44
8:L:127:LEU:HD12	8:L:138:LEU:HD12	1.99	0.44
11:O:62:TYR:OH	13:Q:272:GLU:OE2	2.31	0.44
22:Z:73:LYS:NZ	53:A:468:U:OP1	2.41	0.44
27:5:309:LEU:O	27:5:313:MET:HG2	2.17	0.44
28:6:374:GLU:OE2	46:p:140:SER:OG	2.27	0.44
29:7:107:LEU:HD23	29:7:126:LYS:HE3	2.00	0.44
49:s:267:LYS:HE2	49:s:267:LYS:HB3	1.77	0.44
9:M:209:GLU:HB2	9:M:210:LEU:HD12	2.00	0.44
12:P:79:HIS:HA	12:P:95:GLU:O	2.18	0.44
12:P:104:SER:OG	28:6:147:HIS:NE2	2.51	0.44
22:Z:128:LEU:HD12	41:j:78:VAL:HG23	2.00	0.44
28:6:190:GLY:N	28:6:318:PHE:O	2.42	0.44
34:c:41:PHE:HE1	40:i:36:LEU:HD13	1.83	0.44
2:E:52:HIS:CD2	29:7:306:LEU:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:207:THR:HB	2:E:267:THR:HG23	2.00	0.44
6:J:113:THR:HA	6:J:156:VAL:HB	2.00	0.44
9:M:56:GLU:HG3	53:A:345:G:H5'	2.00	0.44
17:U:143:ARG:HG3	35:d:282:ILE:HD11	2.00	0.44
42:k:18:VAL:HG23	42:k:64:VAL:HG22	1.99	0.44
45:o:42:GLU:HG3	45:o:46:HIS:CE1	2.53	0.44
49:s:89:MET:HG3	49:s:275:LYS:HE3	2.00	0.44
53:A:192:U:H2'	53:A:193:A:C8	2.53	0.44
53:A:192:U:H2'	53:A:193:A:H8	1.82	0.44
54:B:1622:A:H2'	54:B:1623:G:C8	2.51	0.44
19:W:46:SER:OG	53:A:1156:G:OP2	2.33	0.43
39:h:66:LEU:HD13	39:h:108:LEU:HD21	2.00	0.43
49:s:80:LEU:O	49:s:84:THR:OG1	2.33	0.43
49:s:271:LEU:O	49:s:273:LEU:N	2.50	0.43
53:A:607:U:H2'	53:A:608:A:H8	1.83	0.43
2:E:118:VAL:HG23	2:E:287:GLY:HA2	2.00	0.43
16:T:212:LEU:O	32:a:142:ARG:NH1	2.50	0.43
18:V:96:ARG:CZ	53:A:135:A:H1'	2.49	0.43
19:W:120:LEU:O	28:6:50:LYS:NZ	2.40	0.43
19:W:145:VAL:HG11	28:6:343:GLU:HG3	1.98	0.43
48:r:94:ARG:HH21	48:r:101:PRO:HD3	1.84	0.43
14:R:122:ARG:HD2	14:R:142:PHE:CE2	2.53	0.43
20:X:6:TYR:CG	20:X:14:LEU:HD11	2.52	0.43
24:1:53:ARG:NH2	53:A:1209:A:O2'	2.51	0.43
28:6:177:TYR:O	28:6:184:LEU:HA	2.19	0.43
50:u:151:CYS:HB3	50:u:154:ASP:HB2	2.00	0.43
53:A:713:U:O4	53:A:714:A:N6	2.51	0.43
1:D:95:GLY:HA2	1:D:269:ARG:HB2	2.00	0.43
20:X:163:ARG:HD2	27:5:55:LEU:HD22	2.00	0.43
29:7:276:PHE:HB2	29:7:304:VAL:HG12	2.01	0.43
31:9:31:ARG:HD2	53:A:751:G:H4'	1.99	0.43
53:A:501:U:C2	53:A:503:G:H4'	2.53	0.43
10:N:132:THR:HG22	10:N:147:ILE:HA	2.00	0.43
15:S:145:GLY:HA2	32:a:57:THR:HA	2.01	0.43
15:S:162:GLU:HB3	15:S:164:THR:HG23	2.00	0.43
27:5:201:ARG:HB3	27:5:232:THR:HG22	2.00	0.43
28:6:275:GLN:HG3	28:6:311:MET:HE1	2.00	0.43
46:p:77:THR:HB	46:p:102:ARG:HG3	2.01	0.43
51:v:36:ARG:HE	51:v:40:ARG:NH1	2.16	0.43
52:w:100:VAL:HB	52:w:142:GLN:HB2	2.00	0.43
2:E:121:LEU:HD22	2:E:284:TYR:CE1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:221:ARG:NH2	53:A:1438:U:OP2	2.52	0.43
2:E:250:ARG:HH12	2:E:253:PRO:HD3	1.83	0.43
7:K:169:LEU:HD12	48:r:92:PHE:HE2	1.83	0.43
10:N:124:VAL:HG23	10:N:160:VAL:HA	2.01	0.43
18:V:95:TYR:C	18:V:96:ARG:HD2	2.43	0.43
20:X:42:HIS:CG	20:X:86:ILE:HD11	2.53	0.43
20:X:161:LEU:O	20:X:165:MET:HG3	2.18	0.43
53:A:696:G:H2'	53:A:697:A:C8	2.54	0.43
15:S:177:ARG:H	53:A:176:C:P	2.41	0.43
18:V:202:MET:HB3	18:V:202:MET:HE3	1.82	0.43
19:W:104:TYR:HB2	19:W:128:LYS:HG2	2.00	0.43
20:X:53:ASN:OD1	20:X:53:ASN:N	2.52	0.43
28:6:215:THR:HG22	28:6:238:THR:HA	2.00	0.43
35:d:164:VAL:HG23	35:d:261:MET:HB2	2.00	0.43
5:I:113:ARG:O	5:I:117:ARG:HB2	2.18	0.43
19:W:121:PRO:HG3	28:6:45:LEU:HD23	2.01	0.43
27:5:272:ASP:OD1	27:5:272:ASP:N	2.51	0.43
28:6:216:LEU:O	28:6:236:LEU:CA	2.34	0.43
30:8:138:ALA:O	30:8:141:GLU:HG3	2.19	0.43
34:c:84:SER:HB2	34:c:87:LEU:HB3	2.00	0.43
52:w:90:TYR:CE2	52:w:92:LYS:HG2	2.53	0.43
53:A:457:A:H4'	53:A:581:A:C5	2.54	0.43
3:F:249:ASN:OD1	3:F:249:ASN:N	2.51	0.43
14:R:56:ALA:HA	14:R:59:LEU:HB2	2.00	0.43
15:S:108:VAL:HG12	15:S:198:ILE:HD11	2.00	0.43
53:A:1474:A:H2'	53:A:1475:A:H8	1.84	0.43
3:F:46:PRO:HB3	39:h:98:PHE:CE2	2.54	0.43
3:F:293:PHE:HB2	38:g:55:THR:HG21	2.01	0.43
5:I:52:GLU:OE2	10:N:250:ARG:NH2	2.52	0.43
11:O:110:ILE:HG13	11:O:122:VAL:HG23	2.00	0.43
16:T:126:ASP:HB3	16:T:130:ARG:HH12	1.83	0.43
24:1:38:ARG:HH22	24:1:41:LEU:HD22	1.84	0.43
27:5:93:LEU:HB3	27:5:270:ILE:HD11	2.01	0.43
27:5:105:TYR:HB3	27:5:265:LEU:HB3	2.00	0.43
28:6:215:THR:O	28:6:272:LEU:HA	2.19	0.43
53:A:455:C:OP2	53:A:593:C:O2'	2.24	0.43
53:A:1448:U:H2'	53:A:1449:C:H6	1.84	0.43
3:F:164:MET:HE1	40:i:70:PRO:HB2	2.01	0.42
8:L:84:ALA:HA	8:L:108:ILE:HG22	2.01	0.42
18:V:46:VAL:HG11	18:V:83:ARG:HA	2.00	0.42
27:5:121:LEU:HD12	27:5:126:THR:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:e:257:LYS:HE2	36:e:273:ARG:HD2	2.00	0.42
38:g:94:ILE:HG22	38:g:96:VAL:HG23	2.00	0.42
38:g:117:ILE:HD13	38:g:142:GLU:HA	2.00	0.42
53:A:1485:C:H2'	53:A:1486:A:C8	2.53	0.42
2:E:56:GLU:OE1	11:O:141:HIS:ND1	2.52	0.42
6:J:66:LEU:HD22	6:J:82:ILE:HD11	2.01	0.42
15:S:99:VAL:HG22	15:S:133:VAL:HG23	2.01	0.42
18:V:25:PRO:HA	18:V:26:PRO:HD3	1.92	0.42
21:Y:208:PHE:O	21:Y:212:GLU:HG2	2.19	0.42
33:b:30:SER:O	33:b:74:ARG:O	2.36	0.42
33:b:68:ARG:HD2	33:b:70:CYS:HB3	2.01	0.42
36:e:55:ARG:NH1	36:e:56:PRO:O	2.52	0.42
49:s:350:ASP:OD1	49:s:389:ARG:NH1	2.51	0.42
53:A:431:C:H2'	53:A:432:A:H8	1.83	0.42
49:s:94:TYR:O	49:s:106:TYR:OH	2.28	0.42
53:A:242:A:H2'	53:A:243:G:C8	2.54	0.42
1:D:133:PRO:HG3	53:A:732:A:H3'	2.01	0.42
1:D:235:GLN:NE2	1:D:292:MET:HE2	2.34	0.42
7:K:175:ASP:OD2	48:r:36:ARG:NH1	2.52	0.42
27:5:380:GLN:HB3	27:5:410:THR:HG22	2.02	0.42
34:c:203:LEU:HD13	34:c:211:THR:HG21	2.02	0.42
36:e:47:LEU:HB3	36:e:178:TRP:CE2	2.55	0.42
48:r:189:ARG:HH21	53:A:574:U:HO2'	1.64	0.42
53:A:217:A:O2'	53:A:218:G:O5'	2.37	0.42
53:A:347:U:H2'	53:A:348:G:C8	2.54	0.42
4:H:98:LEU:HD22	4:H:102:VAL:HG21	2.02	0.42
13:Q:284:LYS:HA	13:Q:284:LYS:HD3	1.83	0.42
44:m:70:GLU:O	44:m:72:ARG:N	2.52	0.42
53:A:1134:A:H2'	53:A:1135:A:C8	2.54	0.42
1:D:105:ARG:HH22	1:D:130:ARG:HE	1.68	0.42
2:E:334:ASP:HB3	2:E:337:VAL:HG13	2.00	0.42
34:c:68:TYR:CZ	34:c:72:ILE:HD11	2.55	0.42
35:d:197:VAL:CA	35:d:211:GLN:O	2.61	0.42
6:J:141:VAL:HA	6:J:144:ILE:HG12	2.02	0.42
7:K:90:VAL:HG11	7:K:98:ARG:HH11	1.85	0.42
7:K:136:ASP:O	7:K:140:ASN:ND2	2.52	0.42
15:S:111:GLU:N	15:S:195:ILE:O	2.53	0.42
16:T:59:TYR:HD2	35:d:228:PHE:HA	1.85	0.42
21:Y:102:TRP:HE3	21:Y:142:LEU:HD22	1.84	0.42
22:Z:146:VAL:HG12	22:Z:148:GLN:H	1.83	0.42
27:5:350:ARG:HH12	27:5:381:LEU:HD22	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:8:110:GLU:O	30:8:114:ARG:HG2	2.20	0.42
33:b:35:ARG:HH22	39:h:156:TRP:HB3	1.85	0.42
34:c:179:THR:HG22	34:c:194:THR:HG21	2.00	0.42
49:s:73:ALA:HB1	49:s:78:GLU:HG3	2.02	0.42
53:A:1140:G:H2'	53:A:1141:G:C8	2.54	0.42
54:B:1604:G:H2'	54:B:1605:A:H8	1.85	0.42
2:E:98:GLY:HA3	2:E:299:VAL:O	2.20	0.42
11:O:11:HIS:O	53:A:1488:A:O2'	2.29	0.42
11:O:150:GLN:O	11:O:154:GLN:HG2	2.19	0.42
17:U:153:LEU:HA	35:d:240:LYS:NZ	2.35	0.42
36:e:139:GLU:HG2	36:e:152:LYS:HA	2.02	0.42
44:m:51:LEU:HB3	44:m:67:ARG:HB3	2.02	0.42
1:D:118:LYS:NZ	1:D:122:PHE:HB3	2.35	0.42
4:H:126:GLN:HG3	4:H:128:LEU:HD23	2.01	0.42
6:J:125:ALA:HB2	6:J:140:VAL:HG21	2.02	0.42
9:M:204:MET:HE1	47:q:93:TYR:CD2	2.54	0.42
14:R:48:ARG:HG2	14:R:52:LYS:HE2	2.01	0.42
15:S:152:ASP:OD1	15:S:152:ASP:N	2.49	0.42
31:9:131:TYR:HA	31:9:132:PRO:HA	1.93	0.42
34:c:245:LEU:HG	34:c:250:VAL:HB	2.01	0.42
3:F:95:ILE:HD13	3:F:172:LEU:HD22	2.01	0.42
4:H:85:ASP:OD1	53:A:1126:G:O2'	2.36	0.42
7:K:107:ALA:O	7:K:111:MET:HG2	2.20	0.42
7:K:154:ARG:HD2	48:r:129:PRO:HG3	2.01	0.42
29:7:82:ASN:HB3	29:7:85:ILE:HD13	2.02	0.42
33:b:28:ARG:HA	33:b:62:VAL:O	2.19	0.42
33:b:49:ARG:HG2	33:b:50:GLU:HG2	2.01	0.42
36:e:256:THR:OG1	36:e:257:LYS:N	2.48	0.42
49:s:90:LYS:HD2	49:s:232:GLN:HB2	2.00	0.42
49:s:261:ILE:H	49:s:261:ILE:HD12	1.85	0.42
53:A:374:A:H2'	53:A:375:A:H8	1.85	0.42
14:R:87:ILE:O	14:R:91:VAL:HG23	2.20	0.41
15:S:96:PHE:HB3	33:b:126:ILE:HD13	2.02	0.41
21:Y:164:ARG:NH1	53:A:27:A:OP2	2.41	0.41
28:6:162:PHE:HB3	28:6:165:ALA:HB3	2.02	0.41
36:e:248:ASN:HB2	36:e:252:HIS:HE1	1.85	0.41
36:e:264:LEU:HD23	36:e:269:LEU:HB3	2.02	0.41
1:D:212:THR:HG21	53:A:860:A:H5''	2.02	0.41
2:E:217:GLY:HA2	2:E:258:PRO:HB3	2.02	0.41
3:F:70:ARG:NH2	3:F:194:GLU:OE2	2.53	0.41
10:N:72:ILE:HD11	10:N:96:TYR:CE1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:O:152:LEU:HD13	29:7:319:ARG:HB2	2.02	0.41
13:Q:179:LEU:HD13	13:Q:209:GLN:HG2	2.02	0.41
17:U:153:LEU:O	35:d:233:TYR:OH	2.39	0.41
25:2:55:PRO:HG3	53:A:758:C:H5'	2.02	0.41
27:5:251:HIS:O	27:5:371:LYS:NZ	2.51	0.41
29:7:132:ASP:OD1	29:7:133:CYS:N	2.51	0.41
31:9:128:PHE:HD1	31:9:135:PHE:HB3	1.85	0.41
33:b:40:SER:O	33:b:43:ALA:HB3	2.20	0.41
53:A:1070:A:H2'	53:A:1071:A:H8	1.84	0.41
5:I:178:GLY:HA2	5:I:191:PHE:HE2	1.86	0.41
30:8:121:TRP:NE1	36:e:66:LEU:HG	2.35	0.41
45:o:34:ASN:ND2	53:A:483:A:OP2	2.48	0.41
2:E:266:ARG:HD3	2:E:266:ARG:HA	1.81	0.41
8:L:55:PRO:HB2	8:L:75:LEU:HD11	2.03	0.41
9:M:13:LEU:HD23	9:M:16:LEU:HD12	2.02	0.41
22:Z:134:MET:HG2	41:j:75:ARG:HE	1.86	0.41
25:2:88:LYS:HB3	31:9:18:MET:HE1	2.01	0.41
27:5:345:VAL:HG12	27:5:354:PHE:HD1	1.86	0.41
29:7:172:VAL:HG21	29:7:180:CYS:HB2	2.02	0.41
51:v:29:ASP:OD1	51:v:30:PHE:N	2.54	0.41
52:w:98:LEU:HD12	52:w:98:LEU:HA	1.95	0.41
53:A:539:G:H3'	53:A:540:C:H5''	2.03	0.41
4:H:138:LYS:O	4:H:142:GLU:HG2	2.20	0.41
15:S:97:ALA:HA	15:S:135:LEU:O	2.20	0.41
17:U:144:ARG:HA	17:U:144:ARG:HD2	1.76	0.41
37:f:163:SER:H	37:f:166:PHE:HB3	1.86	0.41
48:r:71:PRO:HG3	48:r:74:ARG:HH22	1.85	0.41
53:A:1131:A:H2'	53:A:1132:A:C8	2.55	0.41
53:A:1448:U:H2'	53:A:1449:C:C6	2.56	0.41
7:K:75:LYS:HB2	48:r:174:MET:HE1	2.02	0.41
7:K:171:THR:HG23	48:r:59:GLU:HG3	2.03	0.41
9:M:204:MET:HE1	47:q:93:TYR:CE2	2.56	0.41
11:O:58:LYS:HA	11:O:61:ASP:HB2	2.02	0.41
22:Z:100:HIS:HB3	22:Z:106:VAL:HG11	2.02	0.41
27:5:350:ARG:HG3	27:5:351:VAL:HG23	2.03	0.41
33:b:68:ARG:HA	39:h:157:SER:HB3	2.01	0.41
36:e:156:ASN:ND2	36:e:277:SER:O	2.54	0.41
39:h:140:PHE:O	39:h:144:SER:OG	2.35	0.41
53:A:738:U:H2'	53:A:739:A:C8	2.54	0.41
10:N:191:SER:OG	10:N:192:ARG:N	2.53	0.41
12:P:56:LEU:HB3	12:P:62:ALA:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:2:82:ARG:HH12	31:9:17:ARG:HH12	1.68	0.41
27:5:270:ILE:O	53:A:739:A:O2'	2.38	0.41
29:7:216:PHE:CE1	29:7:257:ILE:HG12	2.55	0.41
50:u:196:LEU:HD21	51:v:57:LYS:HB2	2.02	0.41
2:E:61:ILE:HD11	11:O:149:LEU:HD12	2.01	0.41
2:E:129:VAL:O	2:E:190:GLY:N	2.53	0.41
3:F:181:LYS:HA	3:F:181:LYS:HD2	1.94	0.41
11:O:55:TYR:CZ	13:Q:270:MET:HG2	2.55	0.41
12:P:81:LEU:HD11	12:P:165:MET:HE3	2.03	0.41
27:5:181:VAL:O	27:5:185:ILE:HG12	2.21	0.41
35:d:127:ASP:N	35:d:127:ASP:OD1	2.52	0.41
35:d:248:PHE:HD2	35:d:259:TRP:HB3	1.85	0.41
36:e:154:ASP:OD1	36:e:154:ASP:N	2.54	0.41
46:p:56:ASP:O	46:p:60:ARG:HD2	2.20	0.41
46:p:100:GLU:HG3	46:p:136:THR:HG22	2.02	0.41
52:w:119:ILE:HD13	52:w:122:MET:HE1	2.02	0.41
53:A:258:A:H2'	53:A:259:A:H8	1.85	0.41
1:D:111:ARG:C	1:D:165:ASN:HD21	2.28	0.41
2:E:124:VAL:HB	2:E:281:ASN:HB3	2.03	0.41
3:F:218:LEU:HD13	3:F:230:ILE:HD11	2.03	0.41
4:H:55:ILE:HB	4:H:84:GLU:HB3	2.02	0.41
5:I:42:PHE:CE1	45:o:25:ARG:HG2	2.56	0.41
5:I:83:ARG:HG2	5:I:134:PHE:HE1	1.86	0.41
8:L:82:LYS:NZ	8:L:107:LEU:HB3	2.36	0.41
15:S:175:ARG:NH2	53:A:592:C:O2'	2.54	0.41
20:X:230:TYR:HB3	31:9:92:PHE:CE2	2.56	0.41
25:2:78:VAL:O	25:2:82:ARG:HG2	2.21	0.41
27:5:213:TRP:HZ3	27:5:222:VAL:HG22	1.85	0.41
27:5:293:LEU:O	27:5:346:GLY:HA2	2.20	0.41
48:r:90:SER:HA	48:r:93:ILE:HD12	2.02	0.41
53:A:679:G:H2'	53:A:680:A:C8	2.56	0.41
1:D:91:ILE:HG13	53:A:319:C:OP1	2.21	0.41
15:S:122:LEU:HD21	41:j:49:TRP:CH2	2.56	0.41
21:Y:169:ARG:HH22	27:5:64:MET:HB2	1.86	0.41
25:2:69:ARG:NH2	53:A:246:G:OP1	2.49	0.41
28:6:147:HIS:O	28:6:151:LEU:HG	2.21	0.41
34:c:132:PHE:HA	34:c:135:THR:HG22	2.03	0.41
39:h:127:LEU:HD23	39:h:127:LEU:HA	1.90	0.41
53:A:616:A:H2'	53:A:617:U:C6	2.56	0.41
53:A:991:U:H2'	53:A:992:A:C8	2.55	0.41
8:L:57:CYS:SG	8:L:58:ILE:N	2.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:76:ILE:HD12	53:A:80:G:H5''	2.04	0.40
9:M:78:ILE:HD13	26:3:124:ARG:HD2	2.03	0.40
12:P:104:SER:OG	28:6:150:ARG:NH1	2.54	0.40
15:S:56:LEU:O	48:r:187:TYR:OH	2.24	0.40
17:U:28:LEU:HA	17:U:42:PHE:HA	2.03	0.40
34:c:238:MET:HE1	34:c:274:LEU:HD21	2.03	0.40
37:f:155:ARG:NH1	37:f:156:VAL:O	2.52	0.40
40:i:116:TYR:OH	53:A:199:A:N6	2.47	0.40
45:o:36:ILE:O	45:o:40:GLU:HG3	2.21	0.40
47:q:40:PRO:HG3	47:q:51:GLN:HB3	2.03	0.40
49:s:284:VAL:HG12	49:s:342:TYR:HE2	1.85	0.40
50:u:147:LYS:NZ	53:A:1450:C:OP1	2.48	0.40
8:L:64:ASN:HD21	53:A:1472:A:H5''	1.87	0.40
11:O:15:PHE:HE1	13:Q:271:ARG:HD2	1.87	0.40
13:Q:201:ASP:HB3	13:Q:204:MET:HB2	2.04	0.40
33:b:44:ARG:NH2	45:o:99:LYS:O	2.55	0.40
33:b:68:ARG:O	33:b:70:CYS:N	2.54	0.40
34:c:165:VAL:HG13	34:c:222:GLN:HG3	2.02	0.40
34:c:259:ARG:HD2	34:c:271:PHE:CD2	2.57	0.40
36:e:85:SER:HB2	44:m:50:ARG:H	1.86	0.40
36:e:203:LYS:N	36:e:237:LEU:O	2.50	0.40
37:f:90:VAL:HG12	37:f:158:GLN:HE21	1.87	0.40
40:i:74:ILE:HD11	40:i:82:GLY:N	2.33	0.40
46:p:45:LEU:HD23	46:p:45:LEU:HA	1.92	0.40
52:w:124:ASP:OD1	52:w:124:ASP:N	2.54	0.40
54:B:1603:A:H2'	54:B:1604:G:C8	2.57	0.40
9:M:35:LYS:N	53:A:229:G:O2'	2.54	0.40
12:P:81:LEU:HA	12:P:93:LEU:O	2.21	0.40
12:P:147:GLN:N	12:P:147:GLN:OE1	2.55	0.40
13:Q:136:ILE:O	13:Q:151:LEU:HA	2.21	0.40
15:S:85:GLU:HA	15:S:88:VAL:HG12	2.03	0.40
21:Y:78:LYS:HE2	21:Y:78:LYS:HB2	1.75	0.40
34:c:278:LYS:HE3	34:c:278:LYS:HA	2.03	0.40
37:f:48:TYR:N	53:A:395:A:OP1	2.55	0.40
46:p:75:ARG:NH1	46:p:109:GLU:OE1	2.54	0.40
49:s:345:PHE:CD2	49:s:351:VAL:HG23	2.56	0.40
50:u:192:LYS:NZ	50:u:200:ASP:HB2	2.36	0.40
53:A:191:U:H2'	53:A:192:U:C6	2.55	0.40
1:D:108:ASP:OD2	1:D:113:ARG:NH2	2.55	0.40
2:E:62:LYS:HD3	53:A:1558:U:H4'	2.03	0.40
10:N:127:PRO:HA	10:N:152:THR:HG23	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:Q:119:VAL:HG11	13:Q:164:PHE:CE2	2.56	0.40
21:Y:171:ASP:OD1	21:Y:171:ASP:N	2.54	0.40
22:Z:109:LYS:HE3	53:A:412:G:H1'	2.03	0.40
29:7:107:LEU:HB3	29:7:126:LYS:HB2	2.02	0.40
34:c:79:LEU:HD13	34:c:214:PHE:HE1	1.86	0.40
34:c:258:THR:HG22	34:c:259:ARG:HG3	2.04	0.40
36:e:128:PHE:HE1	44:m:55:LEU:HD12	1.86	0.40
42:k:82:THR:HB	48:r:36:ARG:HH22	1.87	0.40
53:A:510:A:H1'	53:A:536:C:H4'	2.02	0.40
53:A:1029:C:H2'	53:A:1030:G:H8	1.87	0.40
1:D:148:LYS:HD3	27:5:114:LEU:HD21	2.04	0.40
6:J:117:VAL:HG11	6:J:145:ILE:HD11	2.03	0.40
8:L:70:GLY:HA3	8:L:130:ARG:NH2	2.37	0.40
10:N:240:LYS:HB2	10:N:240:LYS:HE3	1.77	0.40
28:6:183:ASP:OD1	28:6:183:ASP:N	2.54	0.40
28:6:236:LEU:HB3	28:6:251:THR:OG1	2.22	0.40
28:6:371:ASP:OD1	28:6:371:ASP:N	2.50	0.40
28:6:374:GLU:OE1	46:p:145:ARG:NH2	2.55	0.40
30:8:147:LEU:HD23	30:8:147:LEU:HA	1.90	0.40
34:c:271:PHE:CE1	34:c:285:PRO:HB3	2.56	0.40
35:d:122:ILE:HG13	35:d:197:VAL:HG21	2.04	0.40
39:h:120:MET:H	39:h:120:MET:HG2	1.77	0.40
53:A:254:U:H2'	53:A:255:A:C8	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	216/305 (71%)	204 (94%)	11 (5%)	1 (0%)	24 55
2	E	281/348 (81%)	273 (97%)	8 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	F	248/311 (80%)	241 (97%)	7 (3%)	0	100	100
4	H	93/267 (35%)	90 (97%)	3 (3%)	0	100	100
5	I	154/261 (59%)	142 (92%)	12 (8%)	0	100	100
6	J	138/192 (72%)	131 (95%)	7 (5%)	0	100	100
7	K	175/178 (98%)	169 (97%)	6 (3%)	0	100	100
8	L	113/145 (78%)	105 (93%)	8 (7%)	0	100	100
9	M	285/296 (96%)	276 (97%)	9 (3%)	0	100	100
10	N	203/251 (81%)	199 (98%)	4 (2%)	0	100	100
11	O	150/175 (86%)	144 (96%)	6 (4%)	0	100	100
12	P	139/180 (77%)	131 (94%)	8 (6%)	0	100	100
13	Q	215/292 (74%)	210 (98%)	5 (2%)	0	100	100
14	R	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
15	S	154/205 (75%)	150 (97%)	4 (3%)	0	100	100
16	T	155/206 (75%)	152 (98%)	3 (2%)	0	100	100
17	U	135/153 (88%)	129 (96%)	6 (4%)	0	100	100
18	V	188/216 (87%)	184 (98%)	4 (2%)	0	100	100
19	W	107/148 (72%)	103 (96%)	4 (4%)	0	100	100
20	X	241/256 (94%)	235 (98%)	6 (2%)	0	100	100
21	Y	174/250 (70%)	170 (98%)	4 (2%)	0	100	100
22	Z	118/161 (73%)	113 (96%)	5 (4%)	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%)	92 (99%)	1 (1%)	0	100	100
27	5	383/423 (90%)	365 (95%)	17 (4%)	1 (0%)	36	65
28	6	316/380 (83%)	301 (95%)	15 (5%)	0	100	100
29	7	285/338 (84%)	273 (96%)	12 (4%)	0	100	100
30	8	97/206 (47%)	92 (95%)	5 (5%)	0	100	100
31	9	113/137 (82%)	107 (95%)	6 (5%)	0	100	100
32	a	78/142 (55%)	75 (96%)	3 (4%)	0	100	100
33	b	146/215 (68%)	135 (92%)	11 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	c	271/332 (82%)	266 (98%)	5 (2%)	0	100	100
35	d	203/306 (66%)	195 (96%)	8 (4%)	0	100	100
36	e	211/279 (76%)	192 (91%)	19 (9%)	0	100	100
37	f	110/212 (52%)	100 (91%)	10 (9%)	0	100	100
38	g	127/166 (76%)	124 (98%)	3 (2%)	0	100	100
39	h	96/158 (61%)	90 (94%)	6 (6%)	0	100	100
40	i	95/128 (74%)	93 (98%)	2 (2%)	0	100	100
41	j	83/123 (68%)	82 (99%)	1 (1%)	0	100	100
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%)	36 (84%)	7 (16%)	0	100	100
45	o	77/102 (76%)	75 (97%)	2 (3%)	0	100	100
46	p	119/206 (58%)	115 (97%)	4 (3%)	0	100	100
47	q	126/222 (57%)	124 (98%)	2 (2%)	0	100	100
48	r	140/196 (71%)	133 (95%)	7 (5%)	0	100	100
49	s	366/439 (83%)	355 (97%)	11 (3%)	0	100	100
50	u	109/234 (47%)	104 (95%)	5 (5%)	0	100	100
51	v	67/70 (96%)	65 (97%)	2 (3%)	0	100	100
52	w	77/156 (49%)	71 (92%)	6 (8%)	0	100	100
All	All	7945/11026 (72%)	7631 (96%)	312 (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	81
2	E	246/290 (85%)	246 (100%)	0	100	100
3	F	217/262 (83%)	217 (100%)	0	100	100
4	H	86/228 (38%)	86 (100%)	0	100	100
5	I	145/232 (62%)	145 (100%)	0	100	100
6	J	113/150 (75%)	113 (100%)	0	100	100
7	K	155/156 (99%)	155 (100%)	0	100	100
8	L	98/124 (79%)	98 (100%)	0	100	100
9	M	245/249 (98%)	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%)	141 (100%)	0	100	100
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%)	262 (100%)	1 (0%)	84	84
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%)	77 (99%)	1 (1%)	61	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
39	h	95/148 (64%)	94 (99%)	1 (1%)	65	76
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	110/178 (62%)	110 (100%)	0	100	100
48	r	133/169 (79%)	133 (100%)	0	100	100
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	7147/9520 (75%)	7143 (100%)	4 (0%)	87	90

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	252	HIS
29	7	84	ASN
32	a	137	ASN
39	h	87	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (65) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	128	GLN

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Mol	Chain	Res	Type
1	D	165	ASN
2	E	128	HIS
3	F	105	ASN
3	F	188	HIS
7	K	9	GLN
8	L	104	ASN
8	L	143	ASN
9	M	102	GLN
9	M	264	GLN
11	O	128	ASN
12	P	97	GLN
13	Q	107	HIS
13	Q	213	GLN
13	Q	258	GLN
15	S	118	ASN
16	T	75	HIS
16	T	109	ASN
16	T	133	ASN
16	T	195	HIS
17	U	27	GLN
17	U	82	HIS
17	U	101	HIS
18	V	18	HIS
19	W	41	ASN
20	X	4	HIS
20	X	108	GLN
21	Y	117	GLN
21	Y	157	GLN
23	0	140	GLN
24	1	15	ASN
27	5	156	ASN
27	5	324	GLN
27	5	343	GLN
27	5	353	HIS
27	5	372	ASN
28	6	200	GLN
28	6	243	ASN
28	6	292	GLN
28	6	333	GLN
28	6	359	HIS
29	7	277	GLN
29	7	285	ASN

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Mol	Chain	Res	Type
33	b	120	HIS
33	b	129	GLN
34	c	80	GLN
35	d	157	HIS
36	e	67	GLN
36	e	248	ASN
36	e	252	HIS
37	f	112	ASN
37	f	158	GLN
39	h	87	GLN
39	h	99	ASN
41	j	30	GLN
41	j	31	GLN
41	j	99	GLN
47	q	142	ASN
48	r	123	HIS
49	s	71	HIS
49	s	179	GLN
49	s	298	GLN
49	s	397	GLN
51	v	43	GLN
51	v	54	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
53	A	1071/1559 (68%)	254 (23%)	12 (1%)
54	B	51/69 (73%)	15 (29%)	1 (1%)
All	All	1122/1628 (68%)	269 (23%)	13 (1%)

All (269) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
53	A	2	C
53	A	4	A
53	A	6	A
53	A	8	C
53	A	9	U
53	A	11	G
53	A	19	C
53	A	23	C

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Mol	Chain	Res	Type
53	A	24	U
53	A	30	U
53	A	34	U
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	61	A
53	A	71	A
53	A	78	G
53	A	80	G
53	A	81	A
53	A	100	G
53	A	107	A
53	A	111	A
53	A	124	A
53	A	125	A
53	A	134	A
53	A	135	A
53	A	136	U
53	A	142	C
53	A	147	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	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

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Mol	Chain	Res	Type
53	A	212	A
53	A	213	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	315	G
53	A	317	G
53	A	322	C
53	A	324	A
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	366	C
53	A	367	U
53	A	369	A
53	A	389	C
53	A	390	A
53	A	391	C
53	A	395	A
53	A	404	A
53	A	409	C
53	A	410	U
53	A	413	U
53	A	415	A
53	A	427	A
53	A	443	G
53	A	454	A
53	A	456	U
53	A	472	A
53	A	477	G
53	A	484	A
53	A	487	U

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Mol	Chain	Res	Type
53	A	489	U
53	A	490	A
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	571	A
53	A	573	A
53	A	574	U
53	A	575	A
53	A	582	C
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
53	A	620	A
53	A	627	A

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Mol	Chain	Res	Type
53	A	629	U
53	A	630	G
53	A	651	A
53	A	652	C
53	A	662	C
53	A	672	U
53	A	675	G
53	A	701	U
53	A	704	A
53	A	705	C
53	A	710	C
53	A	711	A
53	A	717	U
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	756	C
53	A	757	C
53	A	761	C
53	A	765	G
53	A	774	A
53	A	776	A
53	A	781	A
53	A	782	A
53	A	788	A
53	A	798	A
53	A	802	A
53	A	803	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	1036	A
53	A	1037	A
53	A	1039	A
53	A	1049	G
53	A	1062	G
53	A	1070	A
53	A	1073	U
53	A	1080	U
53	A	1086	C
53	A	1133	A
53	A	1134	A
53	A	1140	G
53	A	1144	G
53	A	1161	G
53	A	1162	A
53	A	1163	A
53	A	1174	G
53	A	1177	C
53	A	1182	C
53	A	1184	U
53	A	1189	A
53	A	1194	U
53	A	1195	C
53	A	1199	A
53	A	1201	U
53	A	1222	A
53	A	1223	A
53	A	1225	U
53	A	1226	G
53	A	1231	A

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Mol	Chain	Res	Type
53	A	1236	C
53	A	1240	A
53	A	1242	C
53	A	1243	A
53	A	1247	G
53	A	1249	A
53	A	1252	A
53	A	1253	G
53	A	1256	A
53	A	1258	C
53	A	1432	U
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	1471	A
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	1518	U
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

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Mol	Chain	Res	Type
54	B	1625	A
54	B	1628	C
54	B	1631	C
54	B	1640	A
54	B	1641	G
54	B	1644	G
54	B	1645	A
54	B	1649	C
54	B	1651	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
53	A	43	A
53	A	110	U
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	2.22	3 (21%)	18,26,29	0.97	0

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	5.55	1.46	1.33
57	v	101	PNS	C34-N36	5.12	1.45	1.33
57	v	101	PNS	O35-C34	-2.21	1.19	1.23

There are no bond angle outliers.

There are no chirality outliers.

All (11) torsion outliers are listed below:

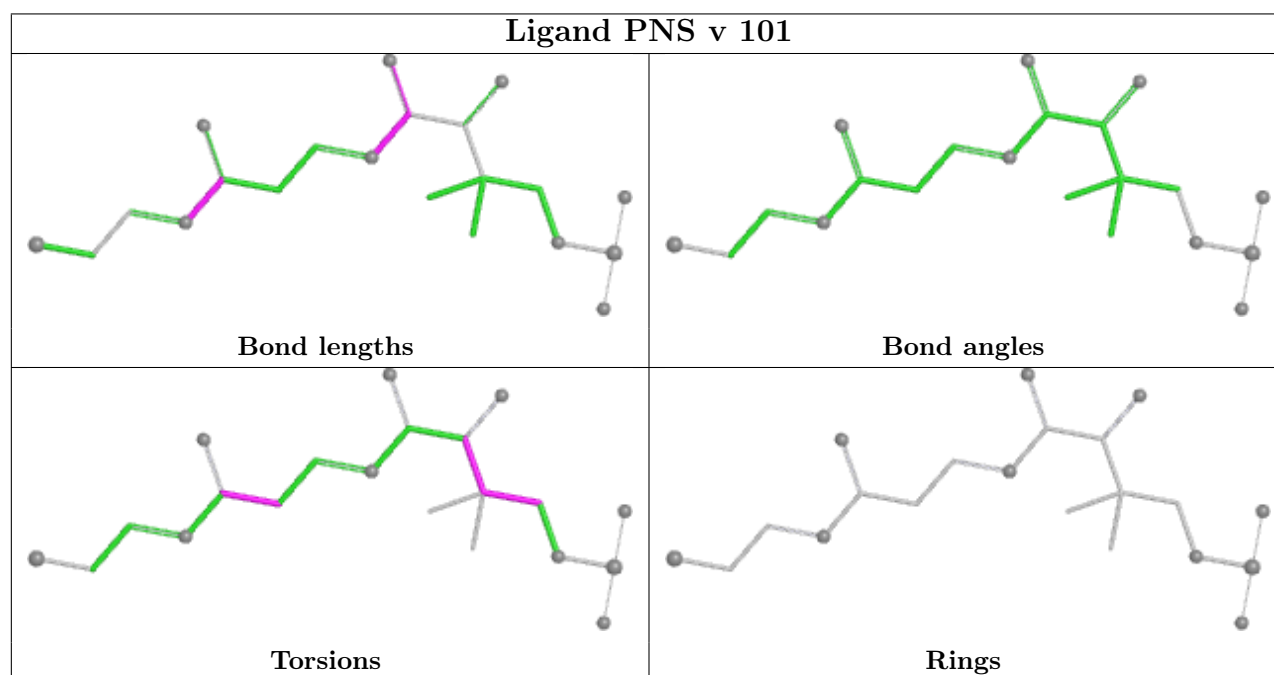
Mol	Chain	Res	Type	Atoms
57	v	101	PNS	O27-C28-C29-C30
57	v	101	PNS	O27-C28-C29-C31
57	v	101	PNS	O27-C28-C29-C32
57	v	101	PNS	C28-C29-C32-O33
57	v	101	PNS	C28-C29-C32-C34
57	v	101	PNS	C31-C29-C32-O33
57	v	101	PNS	C31-C29-C32-C34
57	v	101	PNS	C30-C29-C32-O33
57	v	101	PNS	C37-C38-C39-O40
57	v	101	PNS	C37-C38-C39-N41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

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	v	101	PNS	4	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.

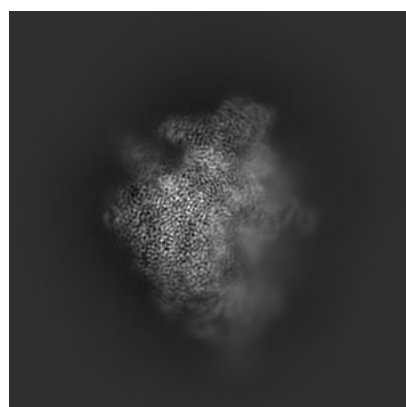
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12922. These allow visual inspection of the internal detail of the map and identification of artifacts.

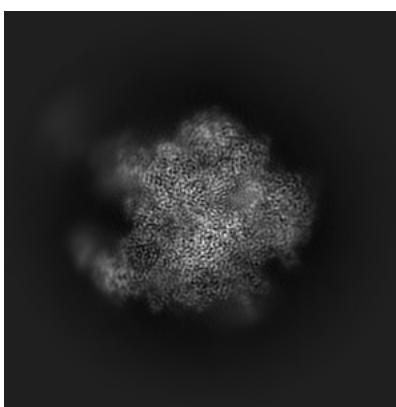
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

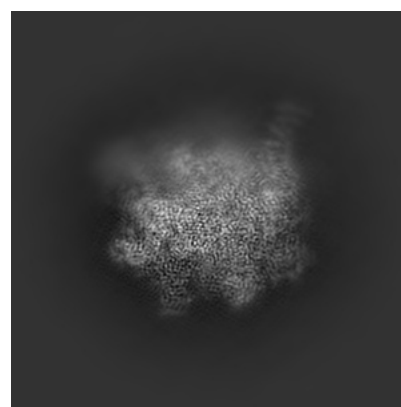
6.1.1 Primary map



X



Y

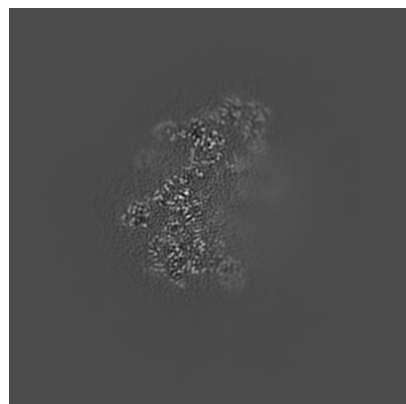


Z

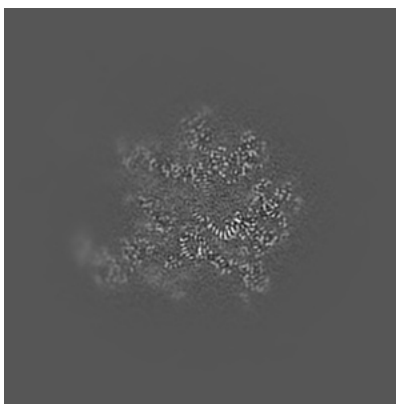
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

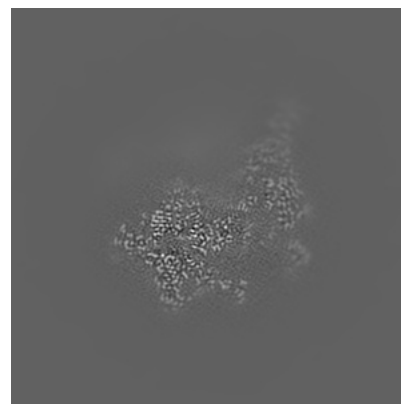
6.2.1 Primary map



X Index: 180



Y Index: 180

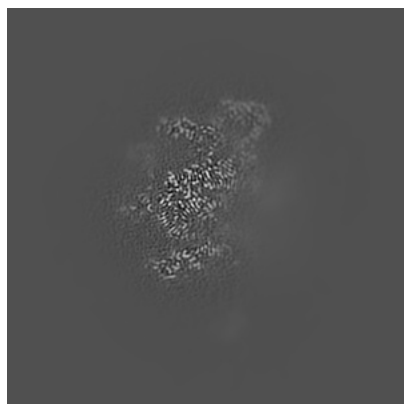


Z Index: 180

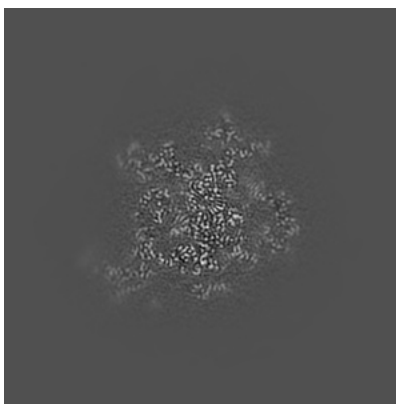
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

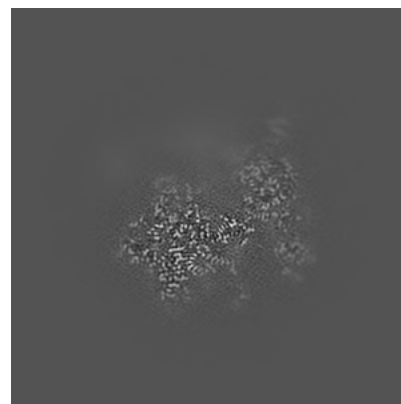
6.3.1 Primary map



X Index: 168



Y Index: 160

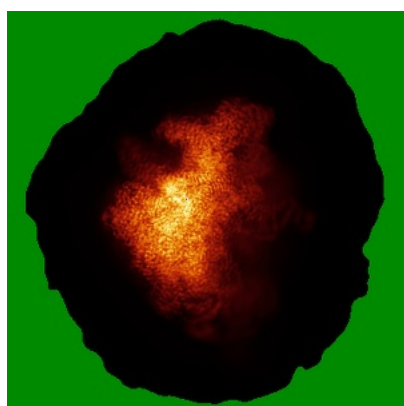


Z Index: 187

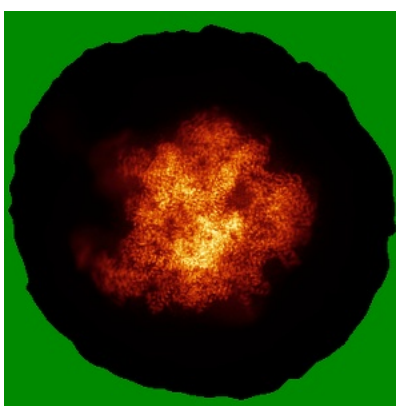
The images above show the largest variance slices of the map in three orthogonal directions.

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

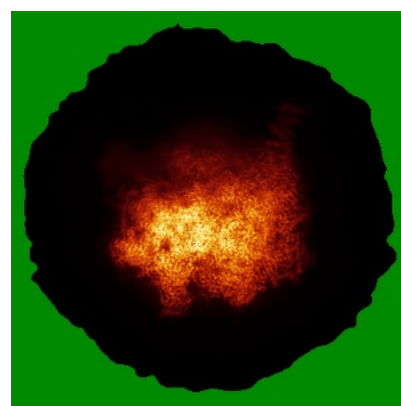
6.4.1 Primary map



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

This section was not generated.

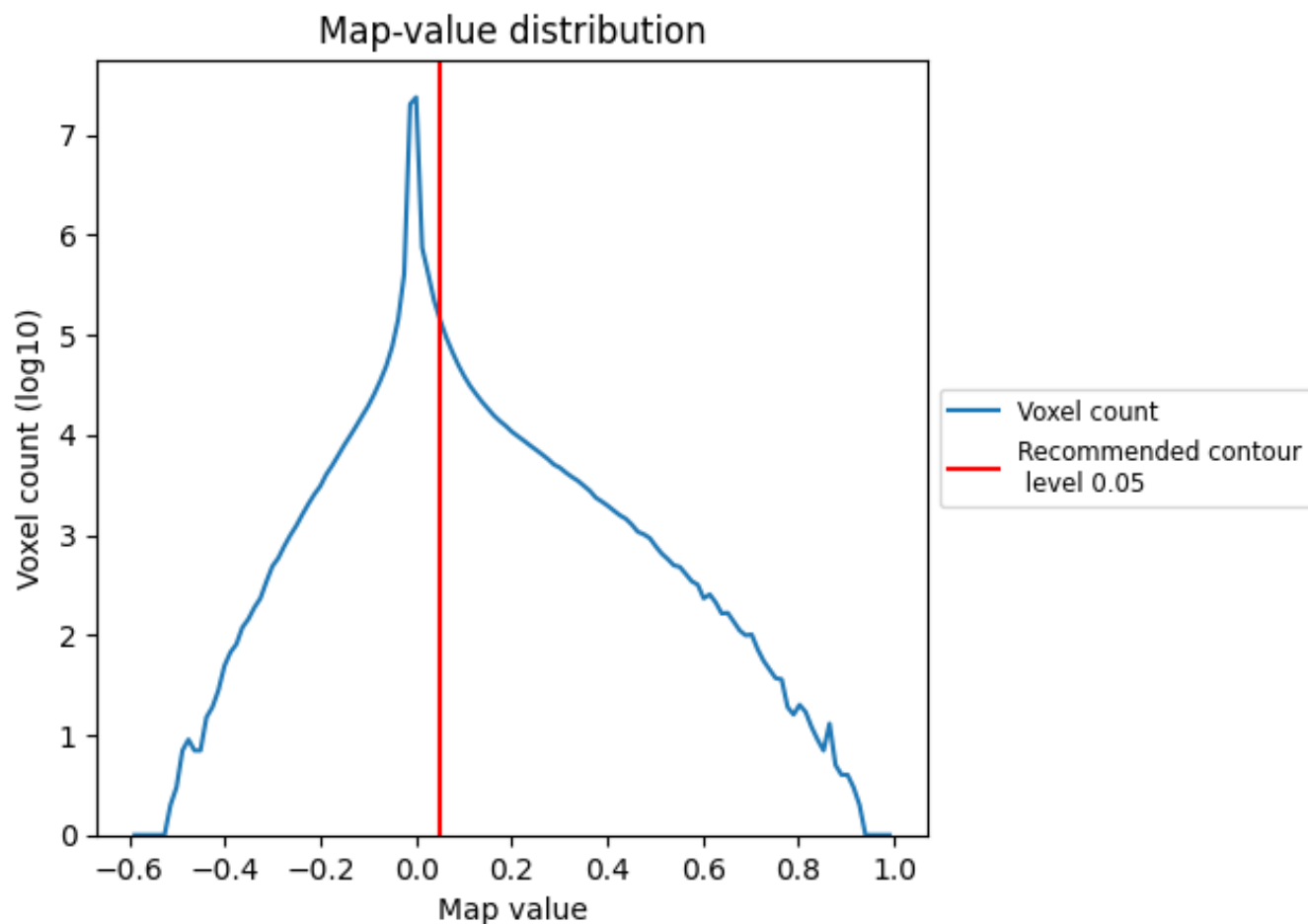
6.6 Mask visualisation

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

7 Map analysis [i](#)

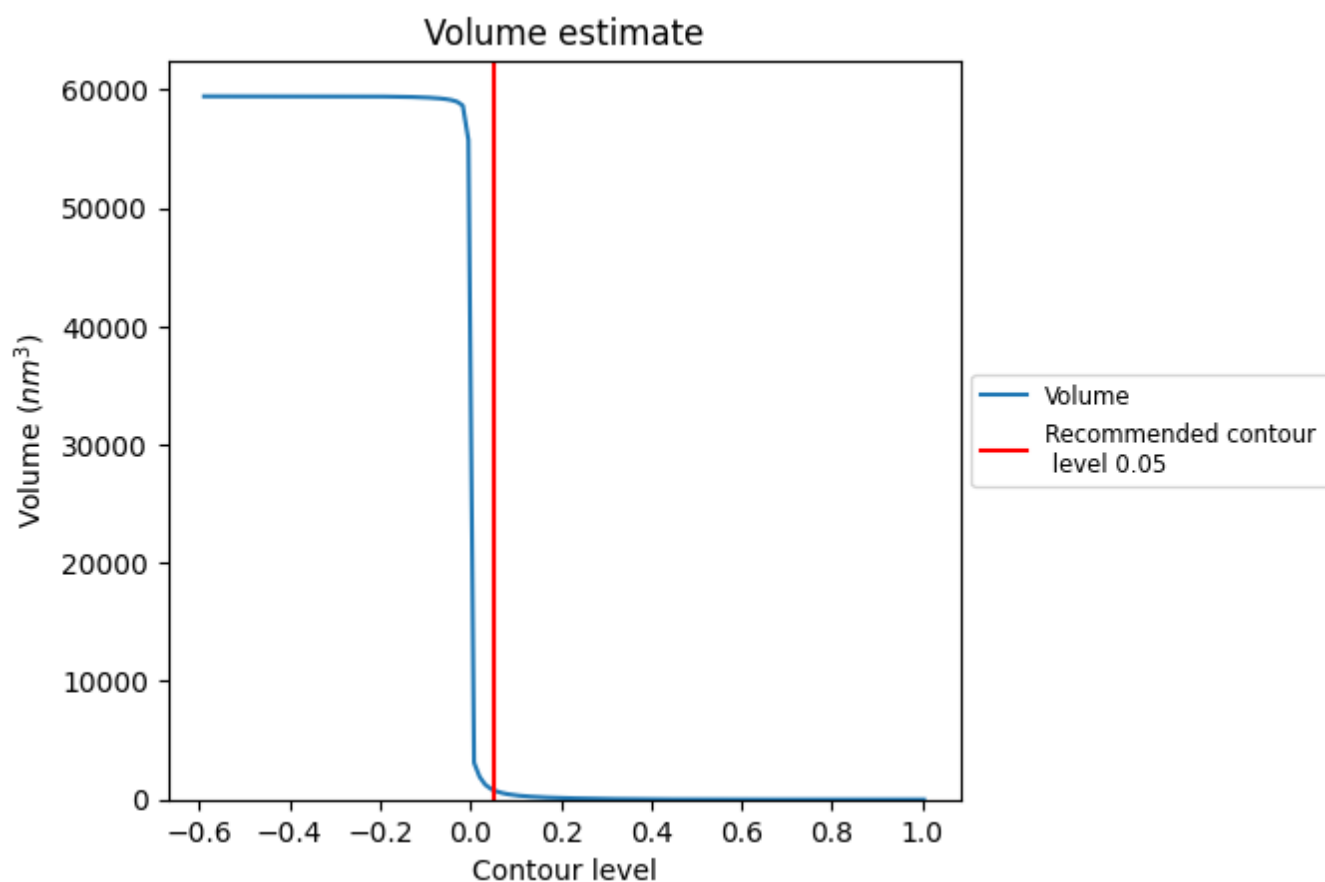
This section contains the results of statistical analysis of the map.

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.

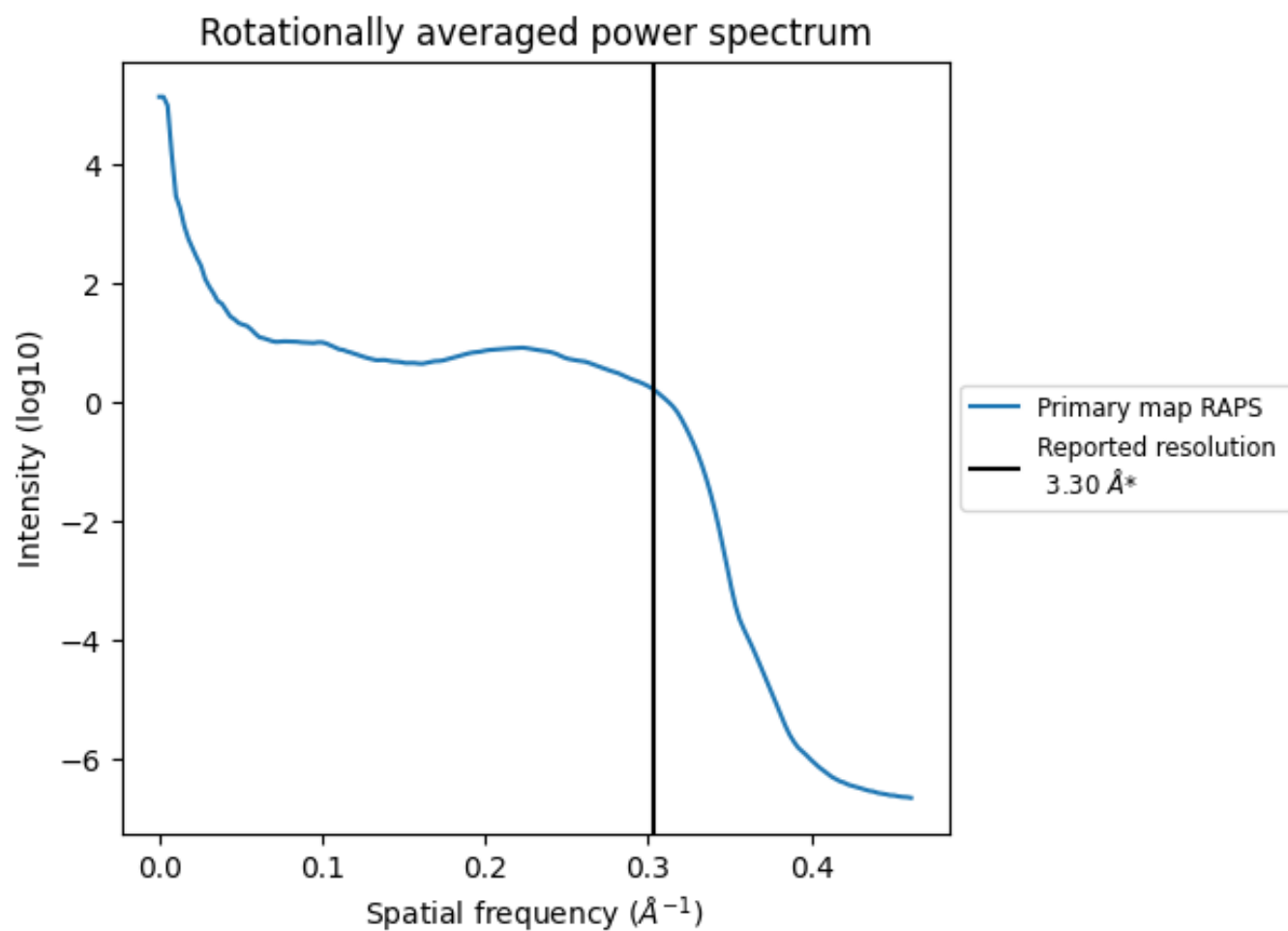
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 823 nm^3 ; this corresponds to an approximate mass of 743 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 ⓘ

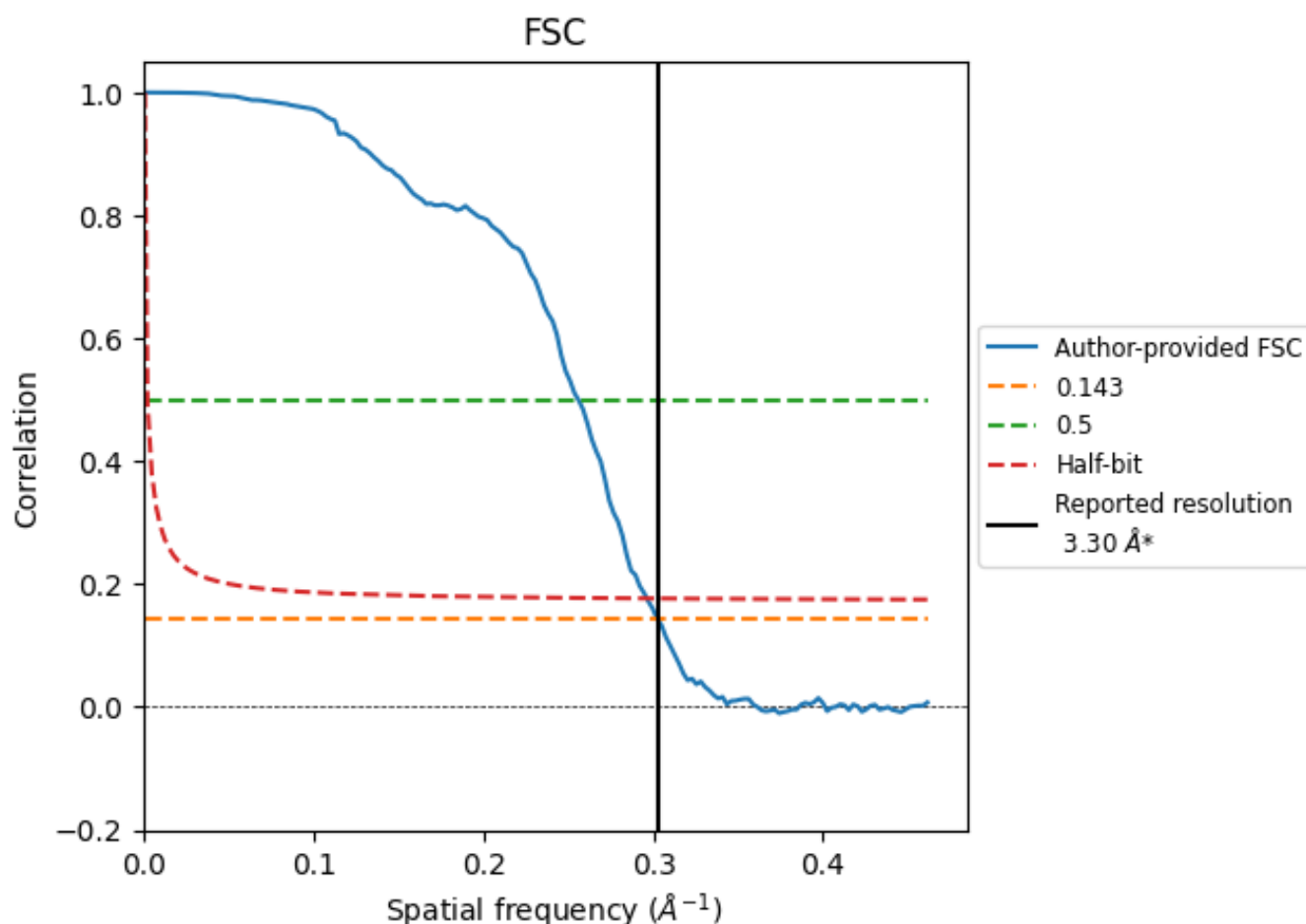


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

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 0.303 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.91	3.37
Unmasked-calculated*	-	-	-

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

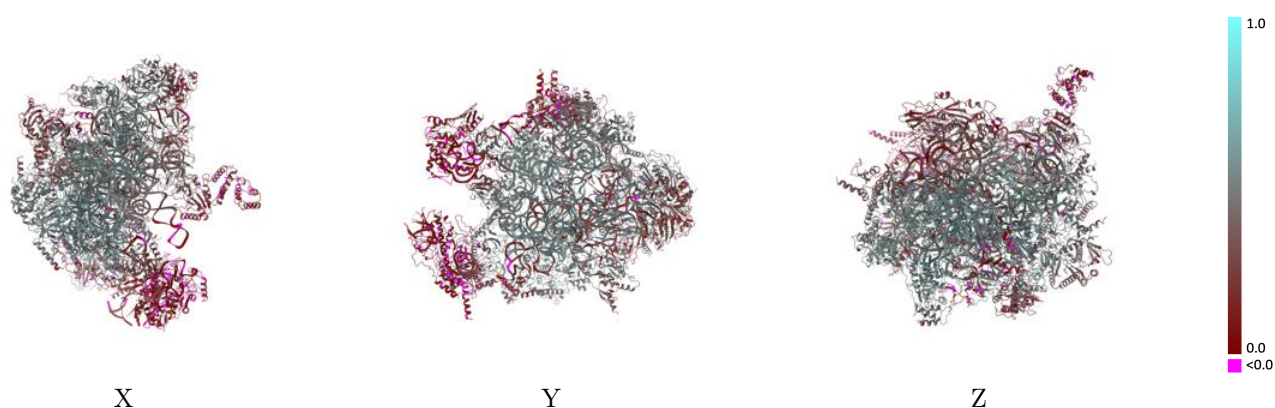
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-12922 and PDB model 7OI9. Per-residue inclusion information can be found in section 3 on page 15.

9.1 Map-model overlay [i](#)

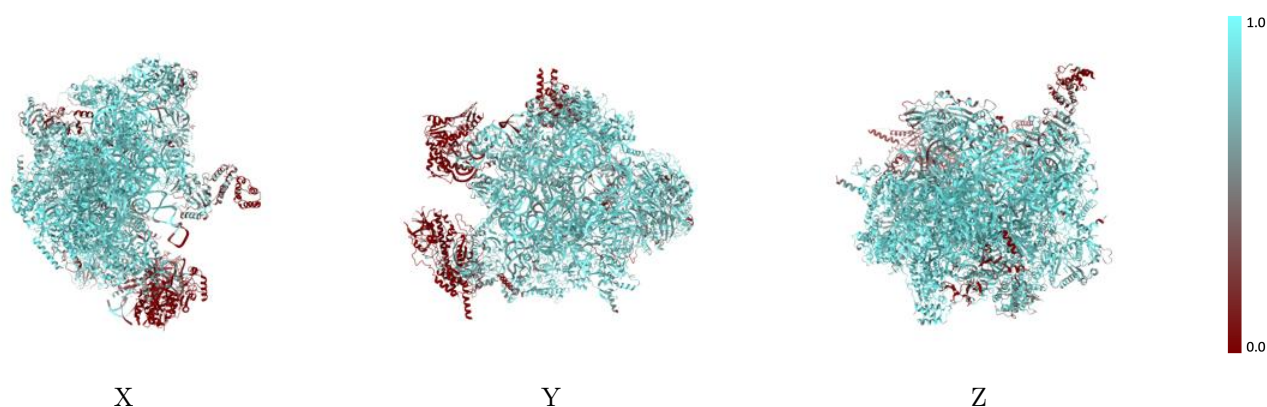
This section was not generated.

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



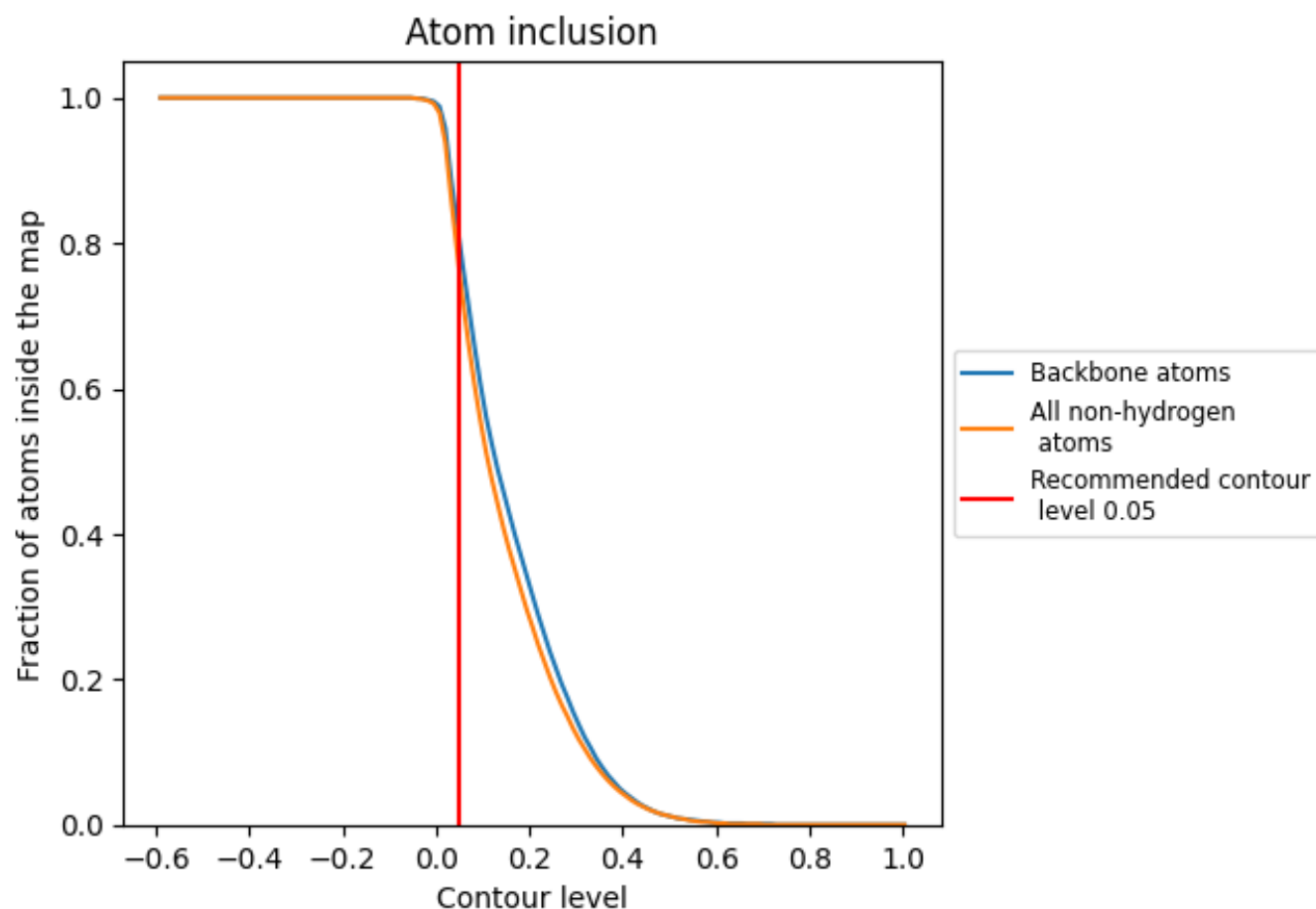
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 81% of all backbone atoms, 76% 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	 0.7620	 0.4090
0	 0.8820	 0.4820
1	 0.5880	 0.2410
2	 0.9380	 0.5650
3	 0.9610	 0.5860
5	 0.7000	 0.3130
6	 0.7530	 0.3270
7	 0.8020	 0.4060
8	 0.0290	 0.1390
9	 0.8800	 0.4740
A	 0.8780	 0.4450
B	 0.6440	 0.1820
D	 0.6420	 0.3060
E	 0.8650	 0.4640
F	 0.9450	 0.5600
H	 0.8070	 0.4310
I	 0.1830	 0.1810
J	 0.0000	 0.0650
K	 0.9040	 0.5190
L	 0.6890	 0.3370
M	 0.9360	 0.5420
N	 0.7910	 0.4240
O	 0.8990	 0.5060
P	 0.7810	 0.3590
Q	 0.8040	 0.4120
R	 0.8430	 0.5100
S	 0.9070	 0.5170
T	 0.9010	 0.5270
U	 0.8330	 0.4740
V	 0.3820	 0.2610
W	 0.9050	 0.5160
X	 0.8770	 0.4900
Y	 0.8900	 0.5010
Z	 0.8620	 0.5020
a	 0.7980	 0.4330



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Chain	Atom inclusion	Q-score
b	 0.9230	 0.5320
c	 0.8880	 0.4910
d	 0.5570	 0.2700
e	 0.0000	 0.0870
f	 0.1350	 0.1590
g	 0.9260	 0.5370
h	 0.8530	 0.4350
i	 0.9410	 0.5730
j	 0.8580	 0.4970
k	 0.1680	 0.1660
l	 0.1650	 0.1020
m	 0.0000	 0.0900
o	 0.9140	 0.5160
p	 0.7960	 0.4140
q	 0.7380	 0.4050
r	 0.8160	 0.4240
s	 0.8780	 0.4760
u	 0.5330	 0.2320
v	 0.3060	 0.1590
w	 0.0410	 0.1140