



Full wwPDB EM Validation Report ⓘ

Mar 26, 2026 – 07:35 PM UTC

PDB ID : 7OIE / pdb_00007oie
EMDB ID : EMD-12927
Title : Cryo-EM structure of late human 39S mitoribosome assembly intermediates, state 5B
Authors : Cheng, J.; Berninghausen, O.; Beckmann, R.
Deposited on : 2021-05-11
Resolution : 3.50 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

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

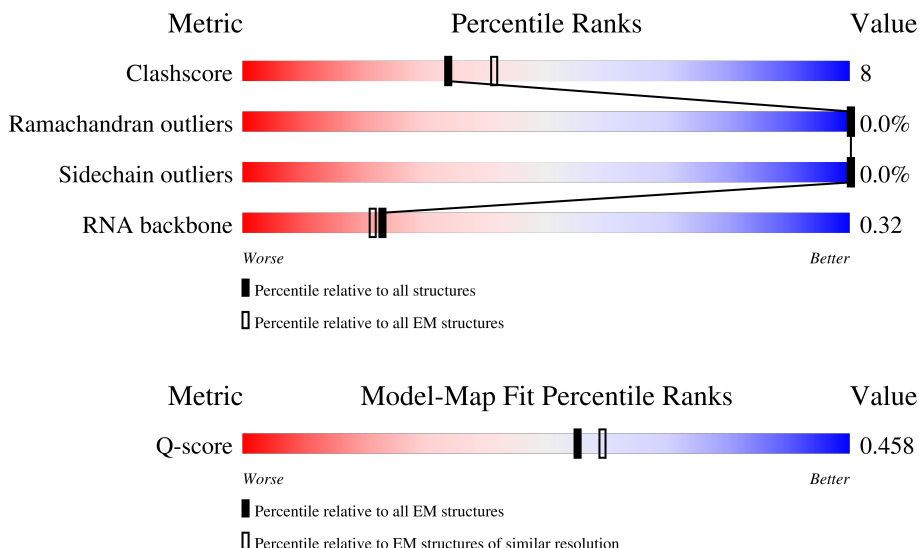
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



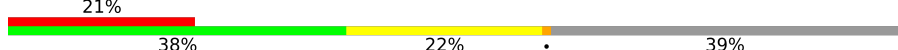
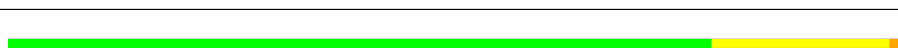
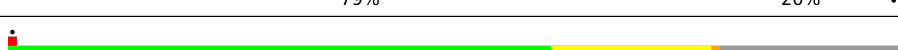
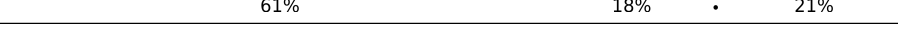
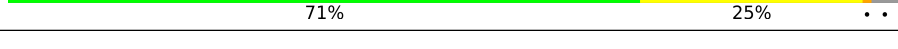
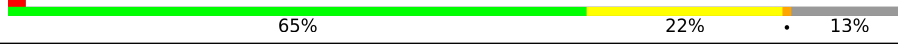
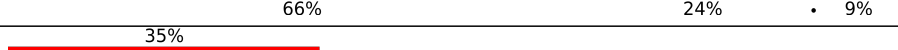
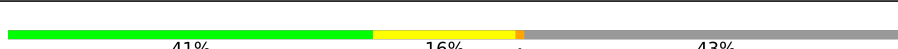
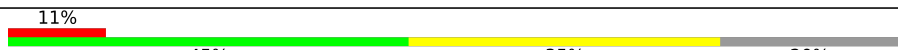
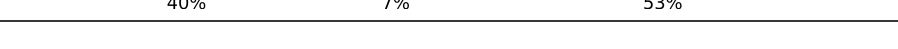
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	13950 (3.00 - 4.00)

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

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

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

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

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Mol	Chain	Length	Quality of chain
54	A	1559	47% 38% 10% 6%
55	B	69	17% 41% 33% 7% 19%

2 Entry composition

There are 58 unique types of molecules in this entry. The entry contains 99578 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

There is a discrepancy between the modelled and reference sequences:

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

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

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

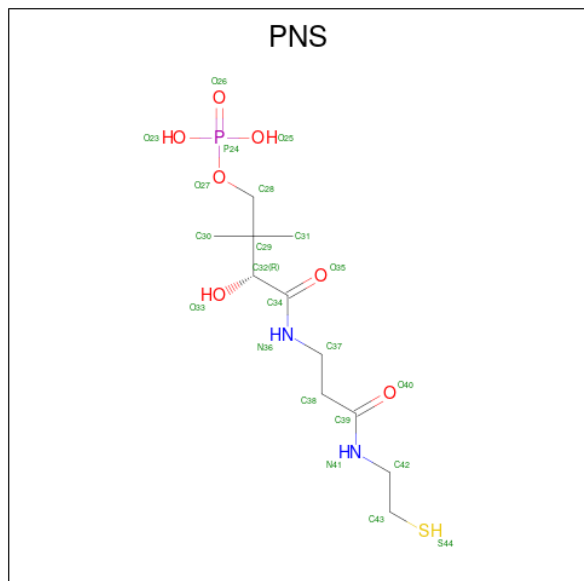
- Molecule 56 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 57 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 58 is 4'-PHOSPHOPANTETHEINE (CCD ID: PNS) (formula: C₁₁H₂₃N₂O₇PS).

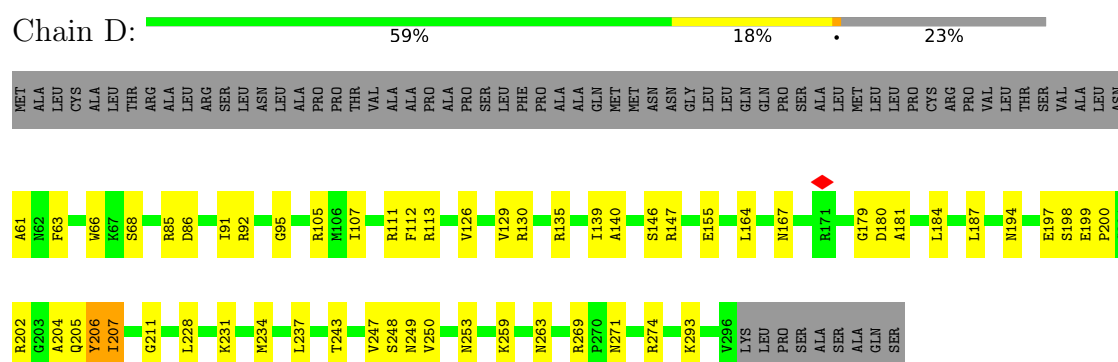


Mol	Chain	Residues	Atoms						AltConf
58	v	1	Total	C	N	O	P	S	0
			21	11	2	6	1	1	

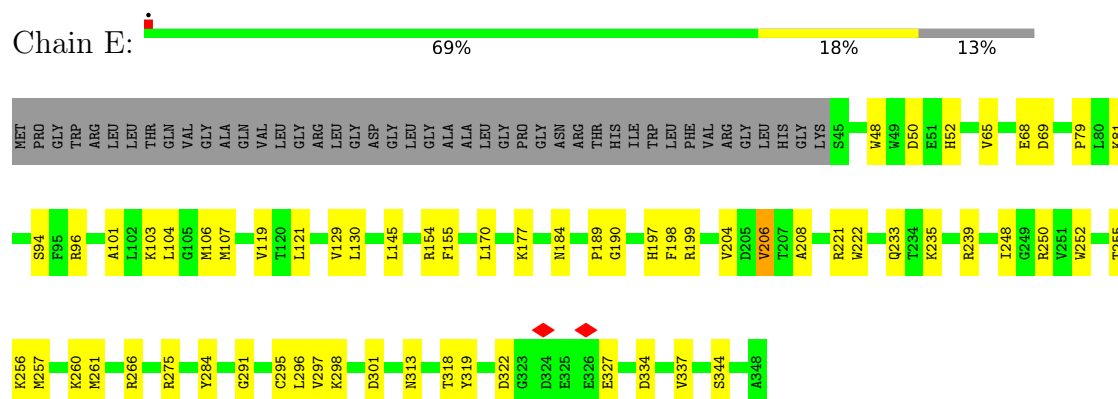
3 Residue-property plots

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.

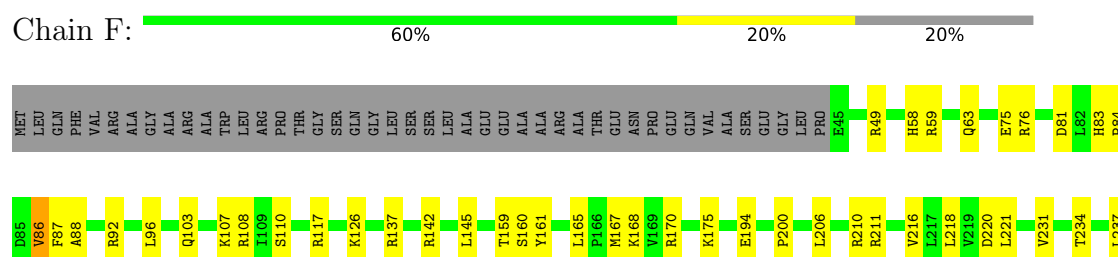
- Molecule 1: 39S ribosomal protein L2, mitochondrial



- Molecule 2: 39S ribosomal protein L3, mitochondrial



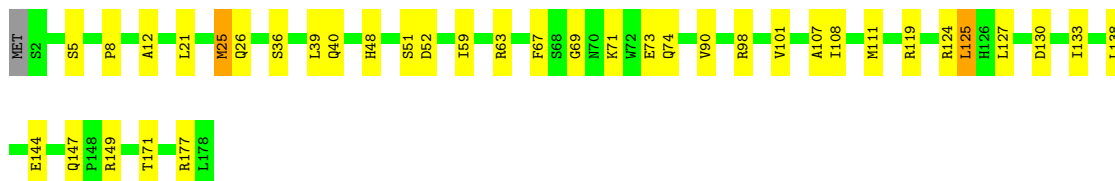
- Molecule 3: 39S ribosomal protein L4, mitochondrial



GLU
ALA
ALA
LYS
LYS

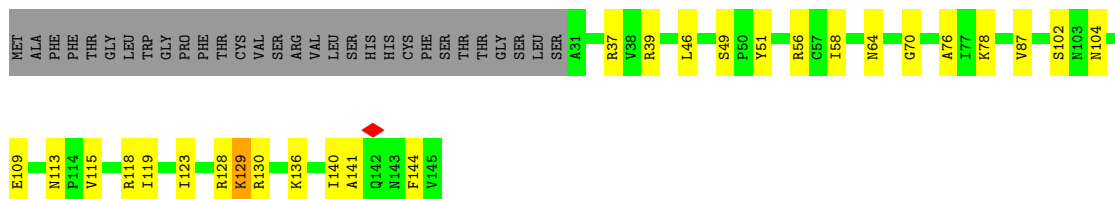
- Molecule 7: 39S ribosomal protein L13, mitochondrial

Chain K:  79% 20% ..



- Molecule 8: 39S ribosomal protein L14, mitochondrial

Chain L:  61% 18% 21%



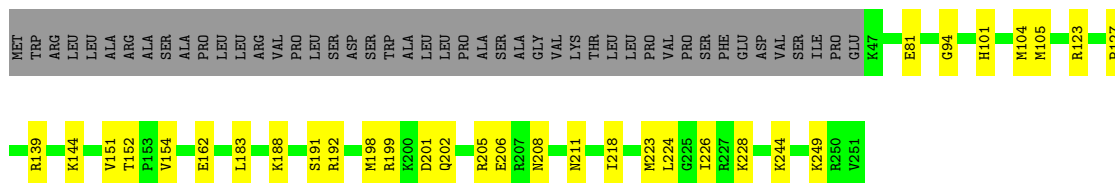
- Molecule 9: 39S ribosomal protein L15, mitochondrial

Chain M:  71% 25% ..



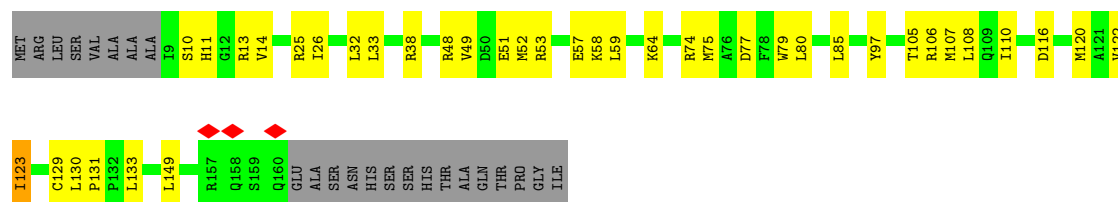
- Molecule 10: 39S ribosomal protein L16, mitochondrial

Chain N:  69% 13% 18%

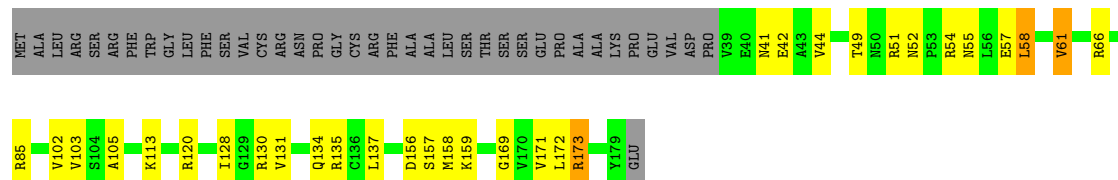


- Molecule 11: 39S ribosomal protein L17, mitochondrial

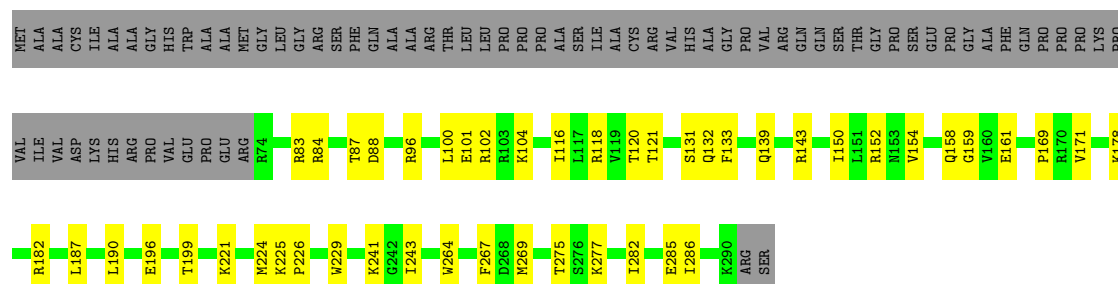
Chain O:  65% 22% 13%



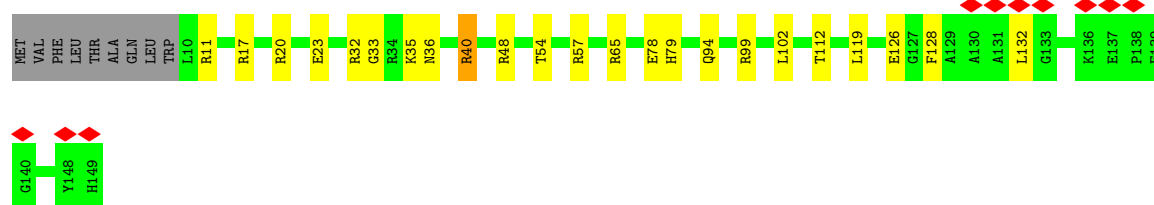
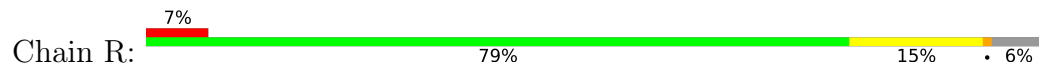
- Molecule 12: 39S ribosomal protein L18, mitochondrial



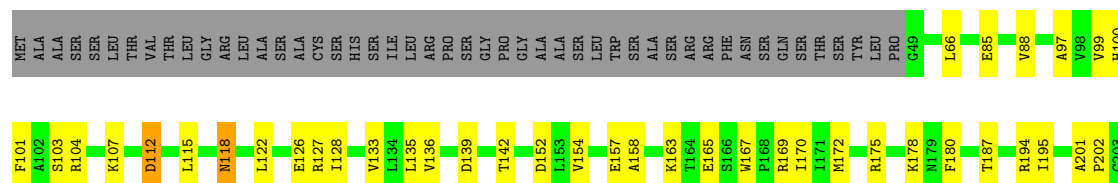
- Molecule 13: 39S ribosomal protein L19, mitochondrial



- Molecule 14: 39S ribosomal protein L20, mitochondrial



- Molecule 15: 39S ribosomal protein L21, mitochondrial



L204
LEU

- Molecule 16: 39S ribosomal protein L22, mitochondrial

Chain T:  68% 9% 23%

MET ALA ALA ASP VAL LEU GLY GLN LEU LEU GLY ALA ALA TRP ILE HIS ASN I26 LEU ARG SER ARG GLY LYS LEU ALA LEU GLY VAL PRO GLN SER TYR ILE HIS THR SER ALA SER LEU ASP ASP 147 V51 E52 K53 R68 R69 E72 C76 D85 Q105 F108 N109 D110

K111 T117 M133 R157 TYR HIS GLY ARG GLY ARG PHE G165 V179 P189 K190 R206 L212

- Molecule 17: 39S ribosomal protein L23, mitochondrial

Chain U:  8% 66% 24% 9%

MET R2 P8 R11 Q16 V19 P20 R21 F24 F25 I26 Q27 L28 V29 R30 P36 T39 F42 R43 I44 P45 M46 E47 M48 T49 D52 L53 Y56 Y61 P64 V65 A66 R71 V72 S76 R80 N84 Y96 V97 A100 F111

F112 GLU LYS ASP SER PRO GLY GLY SER ALA ALA ASP L126 Y127 S128 E131 E132 E133 R134 Q135 Q136 R137 Q138 S139 F151 G152 L153

- Molecule 18: 39S ribosomal protein L24, mitochondrial

Chain V:  35% 69% 20% 11%

MET ARG LEU SER ALA LEU ALA LEU ALA SER ALA LYS VAL THR L15 P16 Y19 R20 Y21 G22 M23 S24 P25 P26 G27 S28 V29 A30 D31 K32 R33 K34 N35 P36 I39 R40 R41 R42 E47 P48 I49 S50 D51 E52 D53 W54 Y55 T61 V62 E63 I64 L65 E66 G67 G71

K72 Q73 G74 K75 V79 Q82 N84 H85 V86 V87 V88 G89 G90 L91 H94 Y96 R96 Y97 I98 G99 Y104 R105 G106 T107 M108 E112 L116 R117 R118 Q119 K121 L122 D124 P125 M126 D127 R128 K129 P130 T131 E132 I133 E134 W135 R136 F137 T138 E139 A140 G141 E142

R143 V144 R145 V146 S147 T148 R149 S150 G151 R152 I153 I154 P155 K156 P157 E158 PHE PRO ARG ALA ASP GLY ILE VAL PRO GLU T169 W170 V179 E180 D181 E184 R185 K212 Y215

- Molecule 19: 39S ribosomal protein L27, mitochondrial

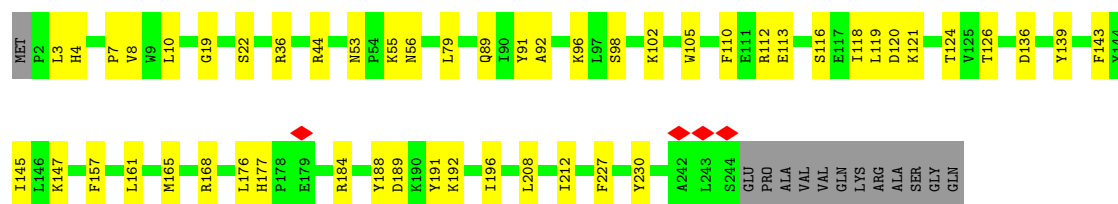
Chain W:  55% 18% 26%

MET ALA SER VAL VAL LEU ALA LEU ARG THR ARG THR ALA VAL THR THR LEU LEU LEU PRO THR PRO ALA THR ALA LEU VAL VAL ARG TYR SER LYS LYS SER GLY SER SER R40 R49 K55 V61 H62 A63 G64 N65 I66 I67 Q70 R71 H72 F73 R74 W75 H76

K87 Y90 E94 G95 T100 K101 V125 F130 V131 H132 V133 V134 K143 L144 V145 A146 M147 L148

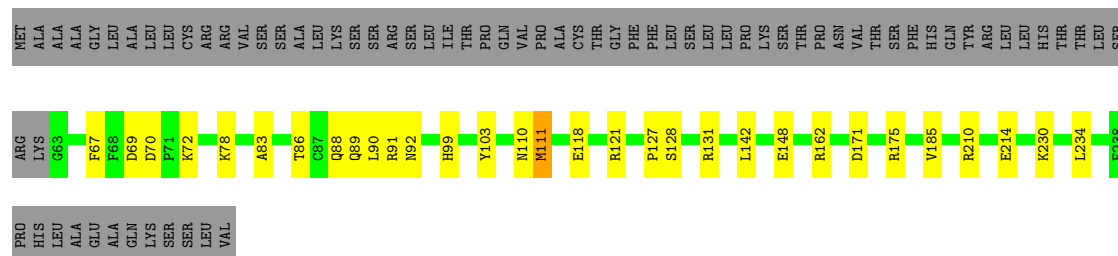
- Molecule 20: 39S ribosomal protein L28, mitochondrial

Chain X: 



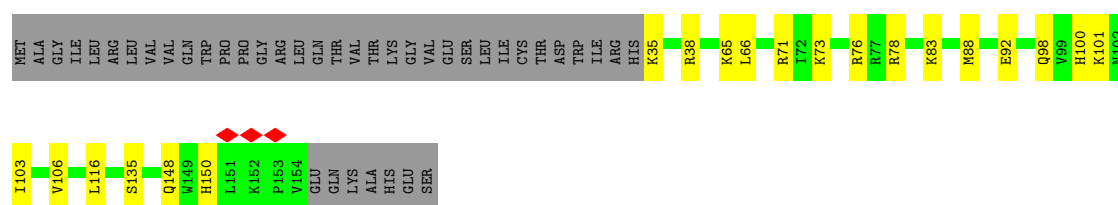
- Molecule 21: 39S ribosomal protein L47, mitochondrial

Chain Y: 

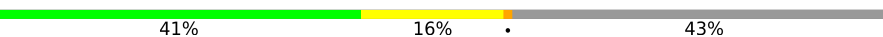


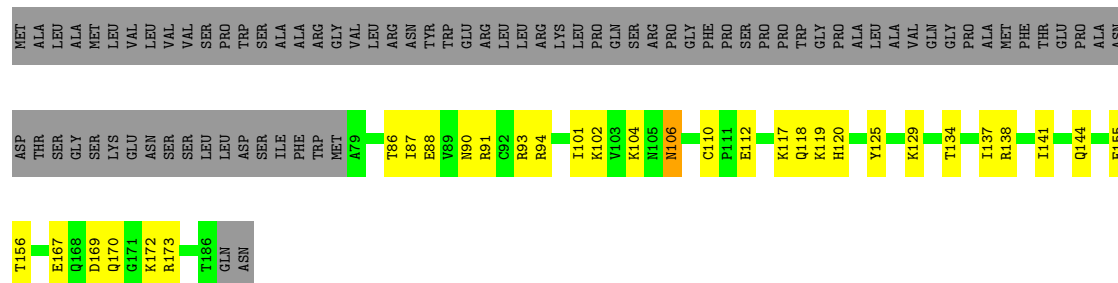
- Molecule 22: 39S ribosomal protein L30, mitochondrial

Chain Z: 



- Molecule 23: 39S ribosomal protein L32, mitochondrial

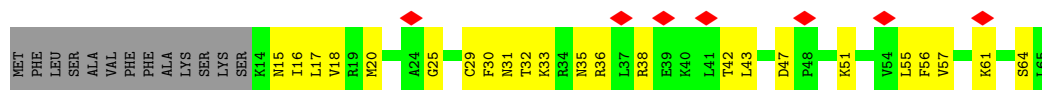
Chain 0: 



- Molecule 24: 39S ribosomal protein L33, mitochondrial

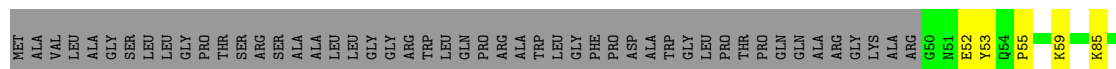
Chain 1: 





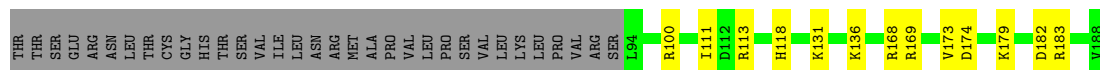
- Molecule 25: 39S ribosomal protein L34, mitochondrial

Chain 2: 40% 7% 53%



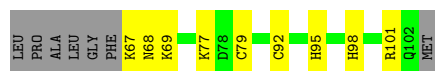
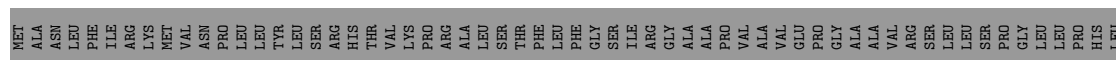
- Molecule 26: 39S ribosomal protein L35, mitochondrial

Chain 3: 44% 7% 49%



- Molecule 27: 39S ribosomal protein L36, mitochondrial

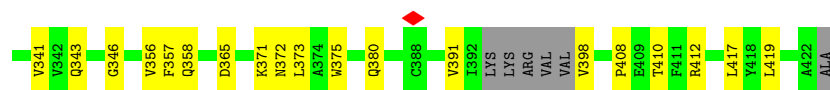
Chain 4: 26% 9% 65%



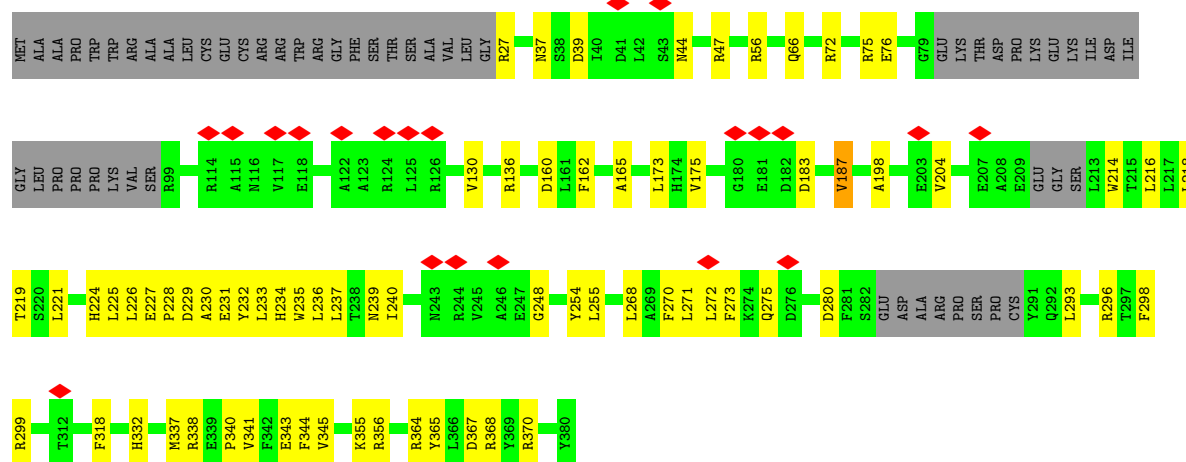
- Molecule 28: 39S ribosomal protein L37, mitochondrial

Chain 5: 5% 68% 23% 9%

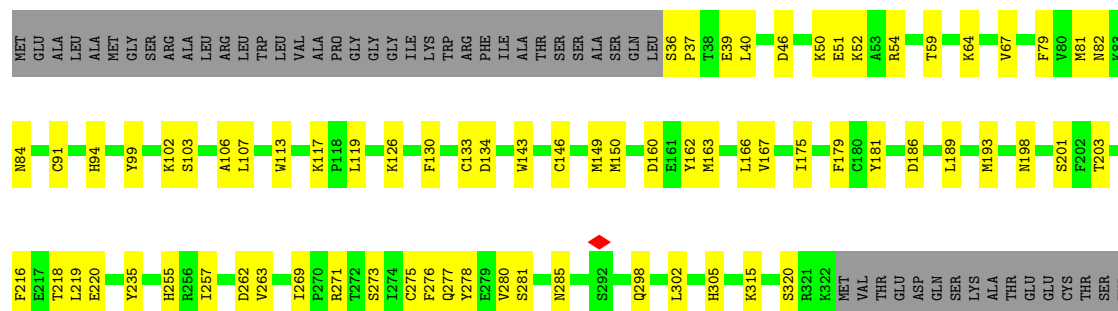




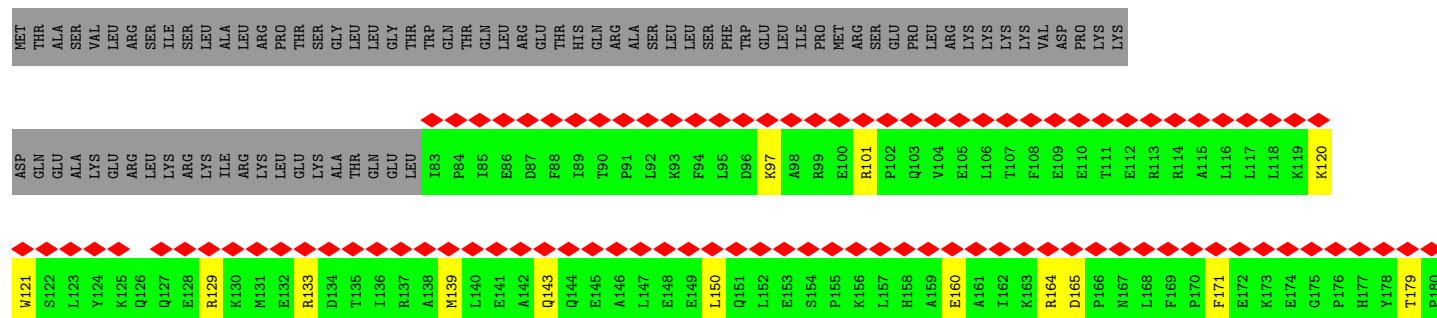
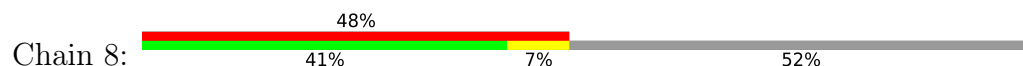
- Molecule 29: 39S ribosomal protein L38, mitochondrial

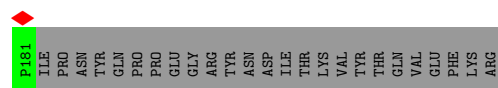


- Molecule 30: 39S ribosomal protein L39, mitochondrial

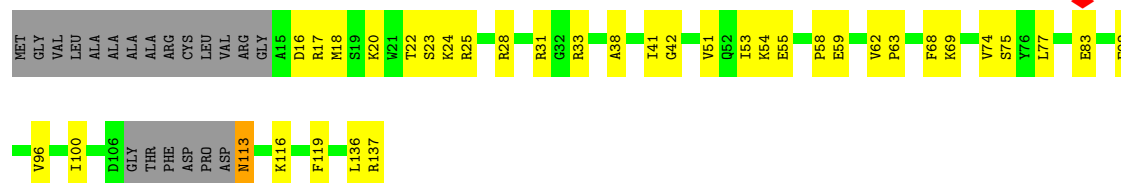


- Molecule 31: 39S ribosomal protein L40, mitochondrial

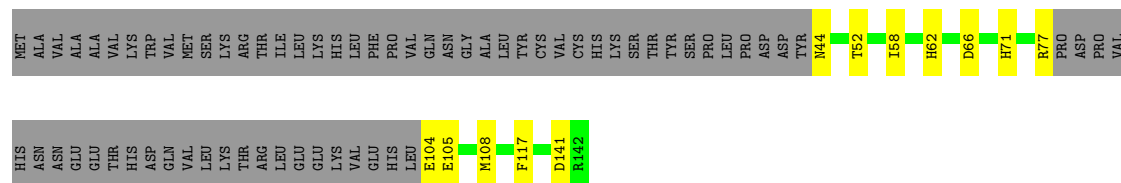




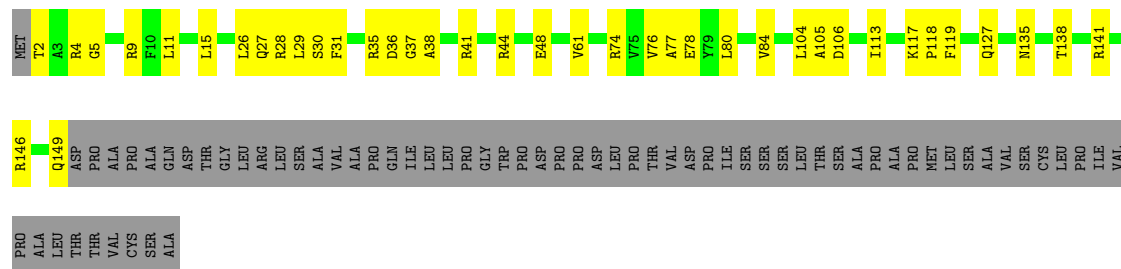
- Molecule 32: 39S ribosomal protein L41, mitochondrial



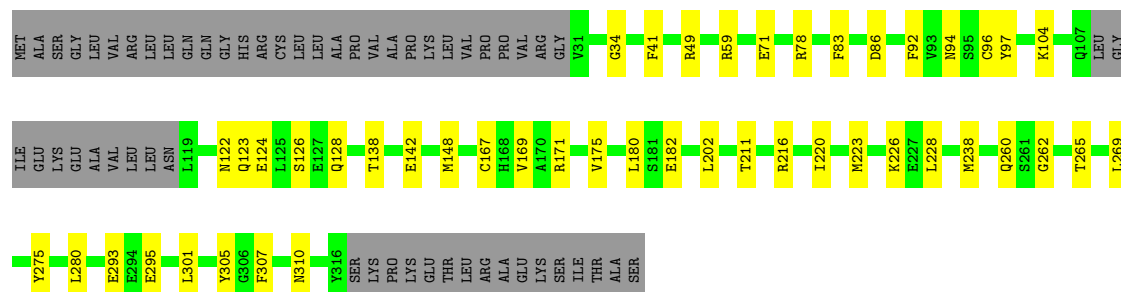
- Molecule 33: 39S ribosomal protein L42, mitochondrial



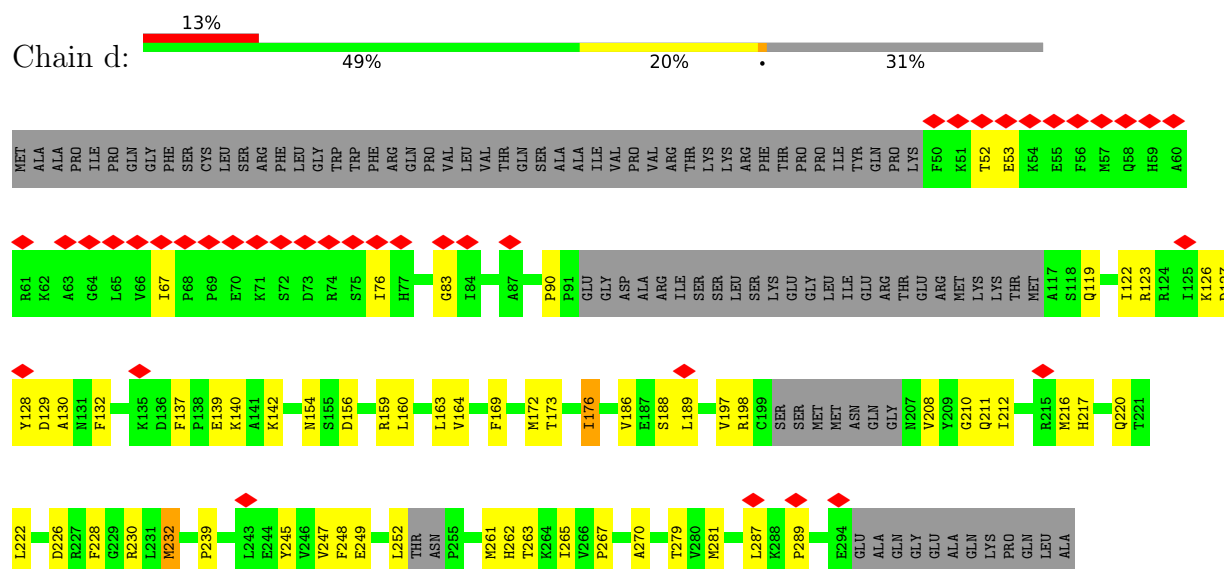
- Molecule 34: 39S ribosomal protein L43, mitochondrial



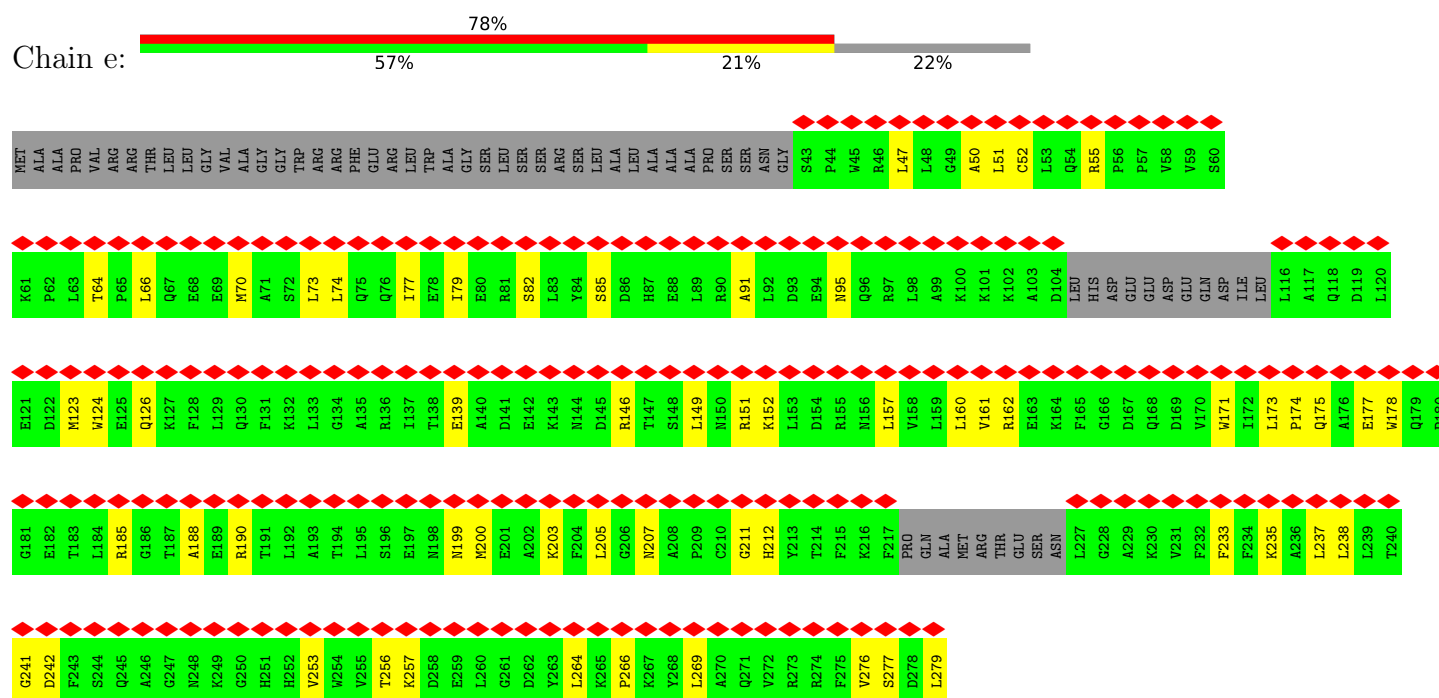
- Molecule 35: 39S ribosomal protein L44, mitochondrial



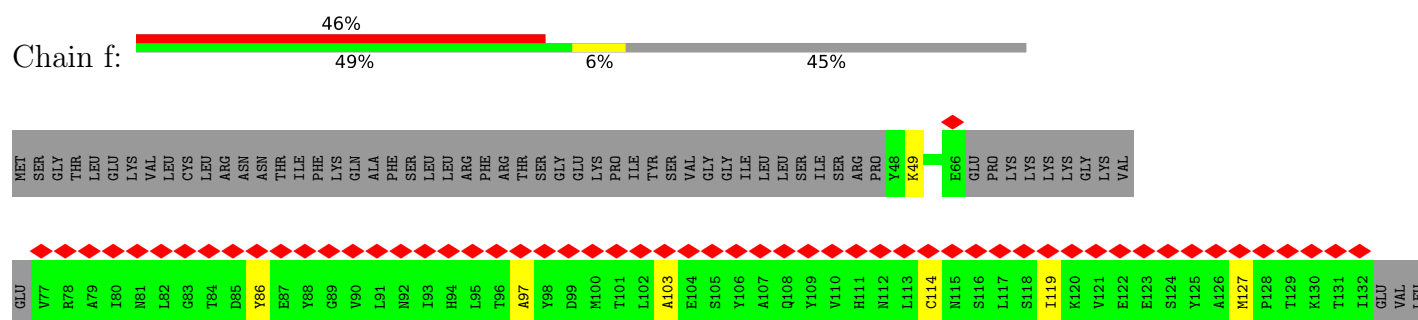
- Molecule 36: 39S ribosomal protein L45, mitochondrial



- Molecule 37: 39S ribosomal protein L46, mitochondrial

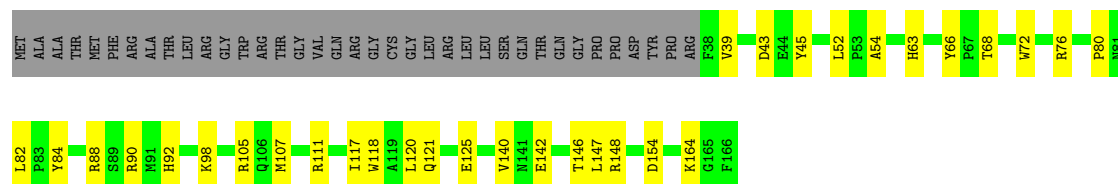


- Molecule 38: 39S ribosomal protein L48, mitochondrial

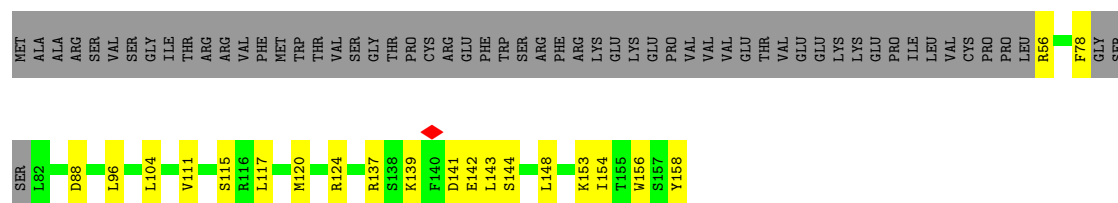




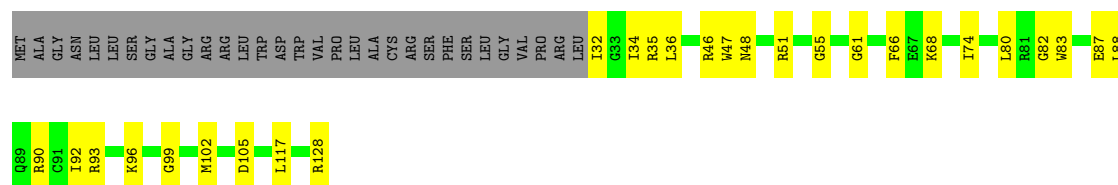
- Molecule 39: 39S ribosomal protein L49, mitochondrial



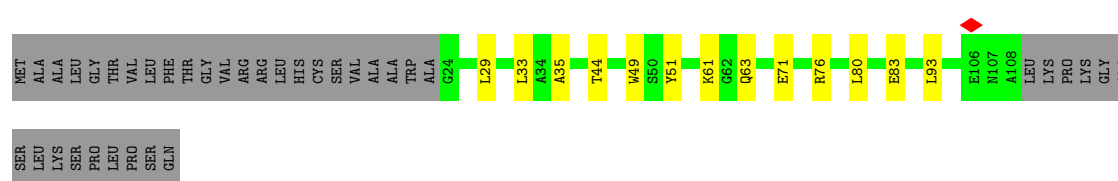
- Molecule 40: 39S ribosomal protein L50, mitochondrial



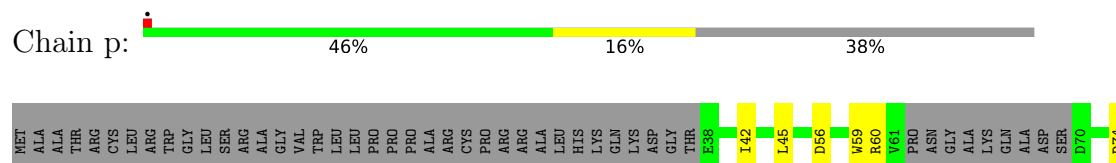
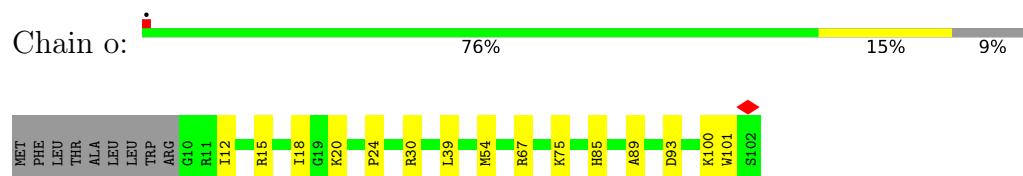
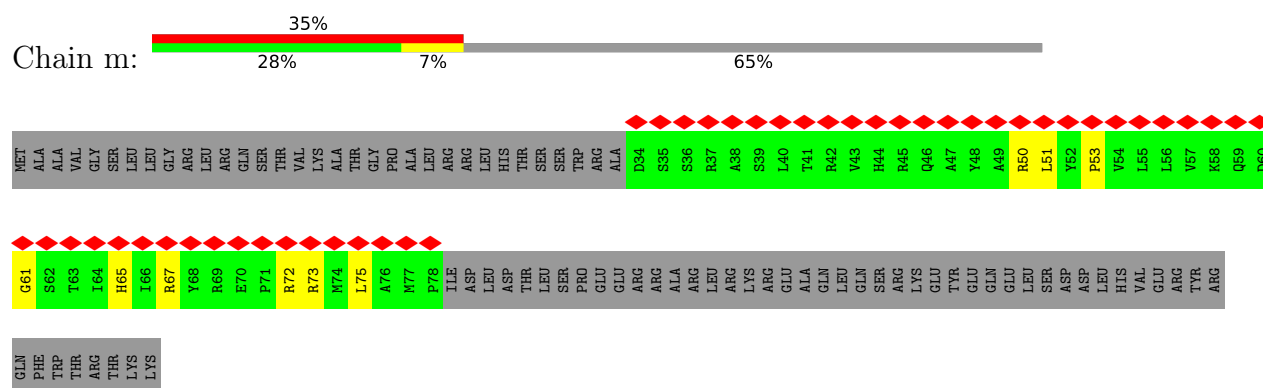
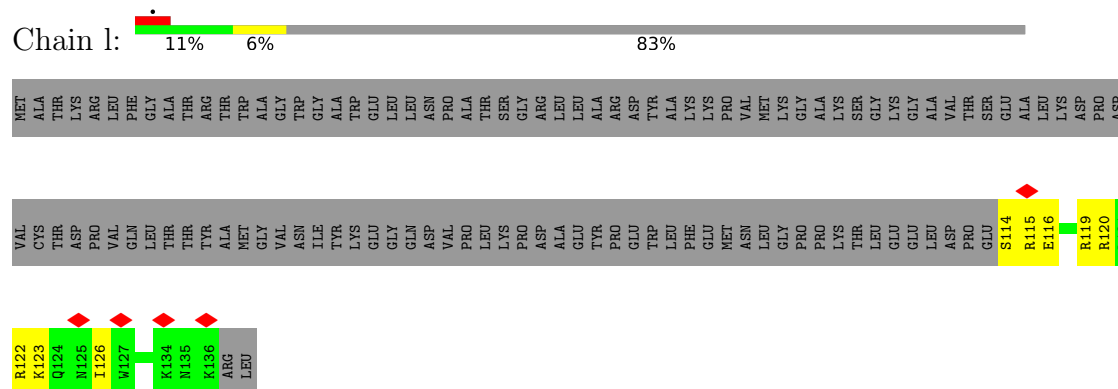
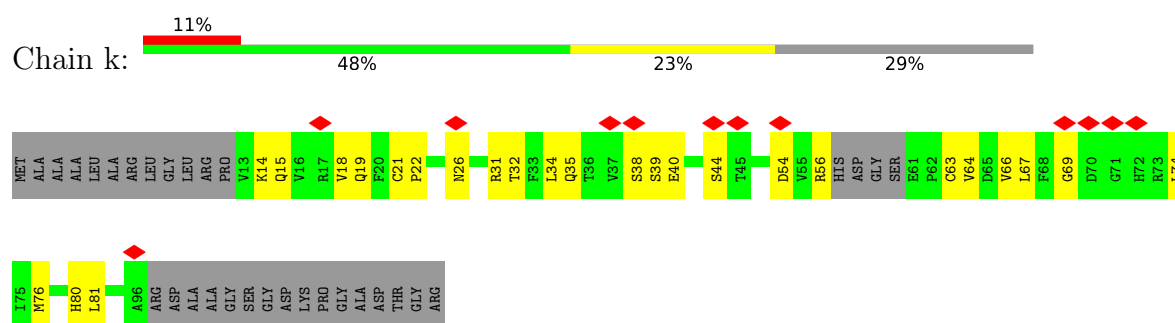
- Molecule 41: 39S ribosomal protein L51, mitochondrial



- Molecule 42: 39S ribosomal protein L52, mitochondrial



- Molecule 43: 39S ribosomal protein L53, mitochondrial

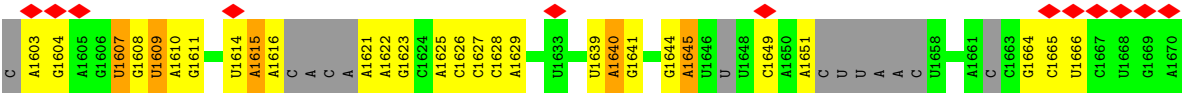




U1444	A1360	U1266	A1191	A	C1048	A959	C870	A781	A700	A623	C540	A472	C322
U1445	G1366	A1270	U1194	A	G1049	U960	C871	A782	U701	A624	U541	G475	A323
C1446	C1447	G1271	C	U	A961	G962	C872	G783	U702	C625	U541	A476	A324
U1448	G1370	G1272	A	A	A1053	A963	C873	G784	A703	U626	A544	G477	A325
C1449	U1371	G1273	C	C	G1054	U964	C874	U785	C704	A627	A544	A402	A403
C1450	U1372	C1284	C	C	A1055	G965	U875	U786	C705	U628	A546	A404	C330
C1451	U1379	U1285	A	A	C1056	U968	C876	A789	A711	G629	C547	U480	C331
G1453	U1286	U1286	A	A	C1057	U969	C879	A790	A712	G630	C548	A483	G332
A1458	A1382	G1287	A1122	A1122	C1058	A971	A880	A792	C716	G634	C	A484	C408
A1459	A1383	G1289	C1124	C1123	U1059	G972	C887	A793	U717	U635	A	A485	C409
A1460	G1384	C1293	U1125	G973	U1061	G973	A888	A799	U718	A639	C	U487	U410
G1461	U1385	C1292	G1126	A974	G1062	G975	U889	G808	C719	G640	U	U488	U411
G1462	A1293	A1293	C1127	G975	C1066	U983	C890	A810	A720	U641	C	A490	G412
A1463	U1294	A	A	U	U1067	U984	G891	A811	C723	U642	C	A491	U413
C1464	U1295	C	C	C	U1068	U985	G900	A812	A724	A643	A	A492	A415
A1465	U1296	U	U	U	U1069	C982	G901	C814	A725	A644	A558	C493	U343
A1466	A1301	A	A	A	A1070	C983	G904	U815	C726	A645	A559	C494	A344
U1470	U1402	A1304	U1134	A1135	U1073	U984	U905	U816	A728	G647	U563	C496	G345
A1471	C1403	A1304	U1136	U1137	U1074	U986	A	C817	A731	A651	C564	A497	U347
A1472	U1404	G1307	U1138	U1139	A1075	U990	C	C818	A732	C652	U563	U498	G348
A1473	C1407	U1308	C1143	U1143	U1077	U991	C	C819	G733	A653	A567	U499	U350
A1475	G1408	U1308	G1144	G1144	A1078	A998	U910	C820	U734	U654	A568	U501	G352
G1476	G1410	U1308	C1151	C1151	U1079	A999	C	C821	C735	U654	A569	A502	C355
U1480	A1411	C1312	C1154	C1154	U1080	A1002	U911	C822	A736	C661	C570	G504	A356
C1485	U1412	C1313	G1155	G1155	G1081	G1005	C913	C831	U737	C662	A571	U504	U429
A1486	G1413	U1316	U1156	U1156	C1082	A1006	C914	C832	U738	G663	U572	A508	G437
C1487	A1414	C1317	C1156	C1156	U1083	A1007	G915	C837	U739	C664	A573	A509	A438
A1488	U1416	A1320	G1161	G1161	U1088	A1008	U916	C838	U740	A605	U574	A510	A361
G1491	C1417	U1321	U1162	U1162	U1089	A1012	G917	C841	C744	A668	C577	A511	A440
C1492	U1418	G1322	A1163	A1163	A1090	C1013	A920	A842	U745	U672	A588	G512	A363
C1498	G1421	U1324	C1164	C1164	C	C1014	A921	C843	U746	G675	A591	G515	U365
C1499	U1422	G1325	U1165	U1165	U	U1015	G922	C844	C747	U678	C592	C516	U367
G1500	U1422	G1326	C1166	C1166	A	G1016	G923	U845	A748	C679	C593	C517	U368
C1501	C1423	C1334	U1167	U1167	C	C1017	U924	G849	G751	A680	A594	C519	A369
C1502	U1426	A1335	A1168	A1168	A	C1018	U924	C850	U752	U681	G599	C520	G370
G1503	U1427	A1335	C1169	C1169	A	A1024	U929	A851	C756	U	A	A521	U371
U1504	U1428	C1338	G1174	G1174	A	G1025	A930	U852	A	A	A	A522	A374
A1507	C1429	C1339	A1175	A1175	C	A1026	A931	C853	A	A	A	U523	A381
U1510	U1430	G1340	G1176	G1176	C	G1027	U932	A854	A762	A	A	U524	A392
U1511	A1431	A1341	C1177	C1177	C	C1028	C933	C855	C763	A	C	A525	U393
U1512	U1432	G1346	U1178	U1178	A	C1029	U936	C856	A764	C	A	A526	U394
U1513	U1434	C1347	G1179	G1179	C	G1030	U937	A857	U772	A	A	G527	U395
C1514	U1438	C1351	U1180	U1180	A	U1031	U937	G858	U773	C	C	A528	C389
U1518	A	U1356	A1181	A1181	G	U1035	U948	U859	A774	U	U	A529	A462
C1519	A	U1357	G1185	G1185	C	A1036	A949	U861	A775	A	U	A530	A463
A1520	A	U1358	U1184	U1184	C	A1037	A953	G866	A776	A693	U	A531	A464
A1521	A	U1359	G1189	G1189	C	C1038	C954	G867	A777	C694	U	A532	A465
			A1189	A1189	C	A1039	C955	G868	G778	U695	A	U534	C391
			U1189	U1189	C	C1039	C956	G869	G779	A621	U	U535	A394
			A1265	A1265	A	G1042	C957	A869	A780	C536	U	A537	A395
													C397



● Molecule 55: mitochondrial Val tRNA



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	28807	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	1.178	Depositor
Minimum map value	-0.747	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	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, PNS, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	D	0.53	0/1879	0.81	0/2527
2	E	0.85	1/2465 (0.0%)	0.90	6/3344 (0.2%)
3	F	0.97	2/2071 (0.1%)	0.87	1/2817 (0.0%)
4	H	0.59	0/798	0.92	2/1073 (0.2%)
5	I	0.47	0/1308	0.78	2/1761 (0.1%)
6	J	0.19	0/1077	0.51	0/1452
7	K	0.89	0/1495	0.85	4/2029 (0.2%)
8	L	0.77	0/904	0.87	1/1218 (0.1%)
9	M	0.93	0/2359	0.89	2/3185 (0.1%)
10	N	0.74	1/1697 (0.1%)	0.79	0/2281
11	O	0.75	0/1269	0.92	3/1708 (0.2%)
12	P	0.56	1/1173 (0.1%)	0.84	1/1588 (0.1%)
13	Q	0.68	0/1846	0.83	0/2487
14	R	1.00	0/1174	0.96	2/1572 (0.1%)
15	S	0.93	0/1276	0.93	1/1729 (0.1%)
16	T	0.94	2/1335 (0.1%)	1.07	4/1796 (0.2%)
17	U	0.74	1/1183 (0.1%)	0.82	2/1600 (0.1%)
18	V	0.32	0/1616	0.65	1/2189 (0.0%)
19	W	0.91	0/881	0.87	2/1188 (0.2%)
20	X	0.61	0/2090	0.85	4/2825 (0.1%)
21	Y	0.68	0/1552	0.69	1/2079 (0.0%)
22	Z	0.85	0/1003	0.86	0/1354
23	0	0.81	0/895	0.90	1/1201 (0.1%)
24	1	0.33	0/438	0.73	0/583
25	2	1.03	0/357	0.85	0/475
26	3	1.08	0/852	0.89	0/1136
27	4	0.65	0/329	0.71	0/435
28	5	0.41	0/3250	0.70	2/4429 (0.0%)
29	6	0.51	0/2726	0.73	2/3715 (0.1%)
30	7	0.49	0/2391	0.72	0/3234
31	8	0.22	0/855	0.57	1/1152 (0.1%)
32	9	0.68	0/972	0.85	2/1306 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	a	0.70	0/630	0.72	0/852
34	b	0.85	0/1202	0.94	2/1626 (0.1%)
35	c	0.63	0/2264	0.73	0/3059
36	d	0.34	0/1790	0.73	2/2423 (0.1%)
37	e	0.18	0/1797	0.53	0/2422
38	f	0.35	0/931	0.59	1/1259 (0.1%)
39	g	0.81	0/1102	0.80	0/1503
40	h	0.43	0/847	0.63	0/1150
41	i	1.11	1/849 (0.1%)	0.92	0/1135
42	j	0.65	0/698	0.75	0/940
43	k	0.25	0/635	0.65	0/855
44	l	0.25	0/226	0.67	0/299
45	m	0.18	0/379	0.49	0/510
46	o	0.90	0/807	0.95	0/1083
47	p	0.42	0/1071	0.65	0/1433
48	q	0.45	0/1413	0.71	0/1906
49	r	0.72	0/1238	0.80	3/1676 (0.2%)
50	s	0.62	0/3114	0.74	0/4225
51	u	0.40	0/949	0.75	0/1281
52	v	0.30	0/597	0.76	0/796
53	w	0.25	0/647	0.72	0/871
54	A	0.89	0/34974	0.71	5/54421 (0.0%)
55	B	0.20	0/1328	0.35	0/2056
All	All	0.75	9/105004 (0.0%)	0.76	60/149249 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
2	E	0	1
5	I	0	1
9	M	0	2
12	P	0	1
13	Q	0	1
15	S	0	1
16	T	0	1
18	V	0	1
23	0	0	1
26	3	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
32	9	0	1
35	c	0	1
36	d	0	3
50	s	0	1
All	All	0	18

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	189	PRO	CG-CD	-10.64	1.14	1.50
10	N	151	VAL	C-N	7.95	1.48	1.33
41	i	68	LYS	C-N	-7.66	1.12	1.33
16	T	189	PRO	CB-CG	-7.53	1.11	1.49
3	F	194	GLU	C-N	-7.22	1.24	1.32
3	F	145	LEU	CG-CD2	-5.46	1.34	1.52
2	E	206	VAL	CB-CG1	-5.36	1.34	1.52
17	U	43	ARG	CA-CB	-5.32	1.39	1.53
12	P	173	ARG	C-N	-5.09	1.23	1.33

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	189	PRO	N-CD-CG	-17.70	76.64	103.20
20	X	36	ARG	CA-C-N	15.92	143.49	121.20
20	X	36	ARG	C-N-CA	15.92	143.49	121.20
16	T	189	PRO	CB-CG-CD	14.53	152.60	106.10
16	T	189	PRO	CA-CB-CG	-13.31	79.21	104.50
49	r	99	MET	CA-C-N	9.37	133.41	120.39
49	r	99	MET	C-N-CA	9.37	133.41	120.39
34	b	5	GLY	CA-C-N	9.10	134.51	120.68
34	b	5	GLY	C-N-CA	9.10	134.51	120.68
18	V	108	MET	CB-CG-SD	-7.50	90.21	112.70
16	T	189	PRO	CA-N-CD	-7.37	101.68	112.00
7	K	101	VAL	N-CA-C	-7.32	106.76	113.71
5	I	100	GLN	CA-CB-CG	6.59	127.28	114.10
3	F	86	VAL	N-CA-C	-6.53	107.50	113.71
38	f	172	GLU	N-CA-CB	6.50	119.78	110.16
9	M	137	GLY	CA-C-N	6.45	131.59	123.14
9	M	137	GLY	C-N-CA	6.45	131.59	123.14
28	5	74	ILE	CA-C-N	6.41	139.59	120.69
28	5	74	ILE	C-N-CA	6.41	139.59	120.69
2	E	327	GLU	CA-C-N	6.25	131.02	121.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	327	GLU	C-N-CA	6.25	131.02	121.03
21	Y	111	MET	CB-CG-SD	-6.08	94.46	112.70
4	H	65	ALA	CA-C-N	-5.92	116.53	122.63
4	H	65	ALA	C-N-CA	-5.92	116.53	122.63
31	8	97	LYS	CA-CB-CG	5.88	125.86	114.10
11	O	123	ILE	N-CA-CB	5.84	119.19	111.25
23	0	88	GLU	CA-CB-CG	-5.79	102.52	114.10
11	O	49	VAL	CA-C-N	-5.78	111.50	121.66
11	O	49	VAL	C-N-CA	-5.78	111.50	121.66
15	S	112	ASP	N-CA-C	5.77	115.72	108.45
29	6	187	VAL	CA-C-N	5.75	129.75	122.16
29	6	187	VAL	C-N-CA	5.75	129.75	122.16
49	r	192	TRP	CA-CB-CG	5.64	124.33	113.60
19	W	147	MET	CB-CG-SD	5.62	129.57	112.70
2	E	233	GLN	CA-C-N	-5.62	110.81	121.54
2	E	233	GLN	C-N-CA	-5.62	110.81	121.54
20	X	196	ILE	N-CA-C	-5.50	104.68	109.19
20	X	196	ILE	CB-CA-C	5.41	114.64	109.33
54	A	383	U	N1-C1'-C2'	5.38	120.07	112.00
7	K	125	LEU	CD1-CG-CD2	-5.37	98.99	110.80
19	W	143	LYS	N-CA-CB	5.34	119.85	111.20
2	E	313	ASN	CA-C-N	5.33	128.06	120.49
2	E	313	ASN	C-N-CA	5.33	128.06	120.49
32	9	69	LYS	CA-CB-CG	5.33	124.76	114.10
36	d	176	ILE	CB-CA-C	-5.33	104.60	111.20
54	A	1061	U	N3-C4-O4	-5.30	103.49	119.40
17	U	24	PHE	N-CA-C	5.30	118.45	109.76
7	K	25	MET	CA-CB-CG	5.30	124.69	114.10
54	A	495	C	C2'-C3'-O3'	5.29	117.44	109.50
32	9	41	ILE	N-CA-C	-5.28	108.69	113.71
7	K	25	MET	CB-CG-SD	5.27	128.52	112.70
14	R	40	ARG	CA-C-N	5.19	127.19	120.44
14	R	40	ARG	C-N-CA	5.19	127.19	120.44
54	A	1430	U	N3-C4-O4	-5.18	103.86	119.40
54	A	704	A	P-O3'-C3'	5.16	127.94	120.20
5	I	84	ARG	CB-CG-CD	5.11	123.05	111.30
8	L	129	LYS	CB-CA-C	-5.07	102.23	110.85
36	d	216	MET	CA-CB-CG	5.04	124.17	114.10
17	U	47	GLU	CA-CB-CG	-5.02	104.06	114.10
12	P	61	VAL	N-CA-C	-5.01	108.95	113.71

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
23	0	106	ASN	Peptide
26	3	182	ASP	Peptide
32	9	68	PHE	Peptide
1	D	206	TYR	Peptide
2	E	344	SER	Peptide
5	I	101	ASN	Peptide
9	M	46	GLY	Peptide
9	M	60	GLY	Peptide
12	P	58	LEU	Peptide
13	Q	226	PRO	Peptide
15	S	101	PHE	Peptide
16	T	85	ASP	Peptide
18	V	94	HIS	Peptide
35	c	122	ASN	Peptide
36	d	172	MET	Peptide
36	d	186	VAL	Peptide
36	d	232	MET	Peptide
50	s	270	LYS	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1842	0	1896	46	0
2	E	2396	0	2402	40	0
3	F	2013	0	2044	48	0
4	H	784	0	832	19	0
5	I	1283	0	1369	47	0
6	J	1061	0	1141	16	0
7	K	1451	0	1448	25	0
8	L	889	0	941	24	0
9	M	2305	0	2378	62	0
10	N	1654	0	1681	22	0
11	O	1245	0	1283	28	0
12	P	1148	0	1148	32	0
13	Q	1805	0	1841	32	0
14	R	1153	0	1214	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
15	S	1251	0	1322	36	0
16	T	1305	0	1352	18	0
17	U	1154	0	1154	31	0
18	V	1575	0	1583	29	0
19	W	859	0	888	25	0
20	X	2035	0	2054	42	0
21	Y	1517	0	1561	29	0
22	Z	978	0	1030	17	0
23	0	880	0	902	26	0
24	1	433	0	475	22	0
25	2	351	0	375	5	0
26	3	831	0	883	12	0
27	4	322	0	346	9	0
28	5	3156	0	3138	68	0
29	6	2640	0	2464	61	0
30	7	2334	0	2343	53	0
31	8	836	0	844	18	0
32	9	947	0	949	31	0
33	a	611	0	595	13	0
34	b	1178	0	1180	36	0
35	c	2217	0	2220	35	0
36	d	1741	0	1727	46	0
37	e	1762	0	1767	42	0
38	f	915	0	917	8	0
39	g	1067	0	1056	22	0
40	h	827	0	806	17	0
41	i	827	0	856	23	0
42	j	684	0	673	11	0
43	k	627	0	636	20	0
44	l	221	0	227	8	0
45	m	372	0	387	6	0
46	o	786	0	791	15	0
47	p	1058	0	1083	29	0
48	q	1379	0	1359	16	0
49	r	1203	0	1219	27	0
50	s	3036	0	3022	43	0
51	u	927	0	921	38	0
52	v	588	0	604	21	0
53	w	638	0	636	21	0
54	A	31265	0	15866	337	0
55	B	1191	0	607	20	0
56	0	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
56	r	1	0	0	0	0
57	A	1	0	0	0	0
57	g	1	0	0	0	0
58	v	21	0	21	1	0
All	All	99578	0	84457	1480	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 8.

All (1480) 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	1.46	1.16
2:E:106:MET:HA	2:E:119:VAL:O	1.46	1.15
30:7:106:ALA:HA	30:7:126:LYS:O	1.42	1.15
54:A:1289:G:N2	54:A:1295:A:H62	1.52	1.07
36:d:197:VAL:HA	36:d:211:GLN:O	1.55	1.04
54:A:304:A:N6	54:A:825:U:H3	1.57	1.02
54:A:662:C:N4	54:A:772:U:H3	1.60	0.98
9:M:94:LYS:O	9:M:138:VAL:HA	1.67	0.94
54:A:1289:G:H21	54:A:1295:A:H62	0.97	0.93
54:A:360:U:O4	54:A:454:A:C6	2.25	0.89
43:k:19:GLN:HA	43:k:54:ASP:O	1.70	0.89
54:A:1289:G:H21	54:A:1295:A:N6	1.72	0.86
54:A:360:U:C4	54:A:454:A:N1	2.45	0.85
55:B:1607:U:H3	55:B:1664:G:H1	0.86	0.85
54:A:360:U:O4	54:A:454:A:N1	2.12	0.82
36:d:139:GLU:O	36:d:142:LYS:HB3	1.79	0.81
35:c:260:GLN:HA	35:c:269:LEU:O	1.80	0.81
32:9:113:ASN:N	32:9:113:ASN:HD22	1.77	0.81
16:T:133:ASN:ND2	36:d:232:MET:SD	2.53	0.80
50:s:243:ILE:HG22	50:s:245:LYS:H	1.46	0.80
54:A:77:G:N2	54:A:80:G:O2'	2.15	0.80
54:A:662:C:H42	54:A:772:U:H3	0.80	0.78
19:W:49:ARG:HD3	19:W:71:ARG:HH21	1.46	0.78
22:Z:76:ARG:NH2	54:A:470:G:N3	2.33	0.77
28:5:290:THR:HA	28:5:343:GLN:O	1.86	0.76
19:W:71:ARG:HH22	54:A:1156:G:H5''	1.49	0.76
54:A:1518:U:N3	54:A:1521:A:N6	2.35	0.75
24:1:47:ASP:O	24:1:51:LYS:HA	1.87	0.74
20:X:96:LYS:O	54:A:58:U:O2'	2.06	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:121:LYS:HE3	18:V:130:PRO:HB2	1.69	0.74
17:U:71:ARG:HD2	54:A:701:U:H2'	1.70	0.73
51:u:151:CYS:HB3	51:u:154:ASP:HB2	1.69	0.73
7:K:73:GLU:OE2	49:r:149:ARG:NH2	2.21	0.72
7:K:124:ARG:NH1	33:a:117:PHE:O	2.22	0.72
54:A:360:U:O4	54:A:453:C:N4	2.22	0.72
17:U:11:ARG:NH2	18:V:212:LYS:O	2.23	0.72
54:A:162:A:N6	54:A:167:C:OP2	2.22	0.72
3:F:281:ARG:NH2	9:M:128:THR:OG1	2.24	0.71
19:W:101:LYS:NZ	54:A:394:A:OP1	2.23	0.71
14:R:40:ARG:HG2	54:A:626:U:H4'	1.70	0.71
30:7:106:ALA:CA	30:7:126:LYS:O	2.32	0.70
34:b:29:LEU:HA	34:b:76:VAL:O	1.91	0.70
33:a:77:ARG:NH2	35:c:293:GLU:OE1	2.24	0.70
3:F:117:ARG:NH1	54:A:235:C:OP1	2.25	0.70
4:H:120:ARG:NH2	20:X:136:ASP:OD1	2.24	0.70
16:T:111:LYS:NZ	54:A:1002:A:OP1	2.24	0.70
54:A:199:A:O2'	54:A:200:A:N7	2.24	0.69
14:R:33:GLY:O	14:R:36:ASN:ND2	2.26	0.69
54:A:408:C:O2'	54:A:409:C:O2	2.08	0.69
8:L:104:ASN:ND2	13:Q:158:GLN:OE1	2.24	0.69
9:M:222:TYR:HE2	9:M:262:PRO:HB3	1.57	0.69
15:S:104:ARG:NH1	54:A:477:G:OP1	2.25	0.69
8:L:123:ILE:HD12	8:L:141:ALA:HB2	1.75	0.69
34:b:78:GLU:HG2	34:b:84:VAL:HG22	1.74	0.69
46:o:89:ALA:O	46:o:93:ASP:HB2	1.93	0.69
34:b:48:GLU:OE1	46:o:101:TRP:NE1	2.26	0.68
54:A:48:A:N3	54:A:241:C:O2'	2.25	0.68
30:7:203:THR:HG22	30:7:280:VAL:H	1.57	0.68
14:R:54:THR:HG21	15:S:172:MET:H	1.58	0.68
28:5:147:ILE:HG23	28:5:191:GLN:HE21	1.57	0.68
35:c:148:MET:HG2	35:c:305:TYR:HB3	1.75	0.68
54:A:1518:U:C4	54:A:1521:A:N6	2.62	0.68
5:I:161:VAL:HA	5:I:164:MET:HE2	1.75	0.68
29:6:235:TRP:HE3	29:6:237:LEU:HD13	1.59	0.68
37:e:124:TRP:HB3	45:m:73:ARG:HG3	1.76	0.68
43:k:34:LEU:HA	43:k:38:SER:HB2	1.74	0.68
18:V:42:ARG:NH2	54:A:128:A:N3	2.41	0.68
54:A:1067:U:O2'	54:A:1414:A:N3	2.27	0.68
2:E:107:MET:HE3	2:E:121:LEU:HD21	1.76	0.68
54:A:523:U:C4	54:A:526:A:N1	2.62	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:63:GLN:HG2	3:F:81:ASP:HB3	1.76	0.67
19:W:145:VAL:HG21	29:6:343:GLU:HB3	1.75	0.67
50:s:336:THR:HA	50:s:339:GLN:HE21	1.56	0.67
1:D:105:ARG:NH2	54:A:733:G:OP2	2.27	0.67
54:A:304:A:N6	54:A:825:U:N3	2.27	0.67
54:A:304:A:H62	54:A:825:U:H3	0.75	0.67
12:P:52:ASN:HB3	12:P:55:ASN:HB2	1.76	0.67
29:6:216:LEU:O	29:6:236:LEU:HA	1.94	0.67
30:7:167:VAL:HG23	30:7:235:TYR:HB3	1.77	0.67
5:I:35:ARG:NH2	54:A:440:A:OP1	2.27	0.67
32:9:54:LYS:NZ	54:A:745:C:O3'	2.28	0.67
54:A:1339:C:H5	54:A:1360:A:H61	1.43	0.66
20:X:177:HIS:O	20:X:184:ARG:NH1	2.28	0.66
24:1:16:ILE:HA	24:1:64:SER:HA	1.75	0.66
24:1:16:ILE:HD13	24:1:61:LYS:HE2	1.77	0.66
6:J:108:VAL:HG21	6:J:154:ARG:HG2	1.77	0.66
18:V:23:MET:HE1	54:A:132:A:H4'	1.77	0.66
22:Z:101:LYS:HE3	42:j:80:LEU:HD22	1.77	0.66
53:w:100:VAL:HB	53:w:142:GLN:HB3	1.76	0.66
32:9:53:ILE:HG22	32:9:55:GLU:H	1.61	0.66
49:r:41:THR:O	49:r:47:THR:HA	1.95	0.66
29:6:356:ARG:NH2	54:A:420:A:OP1	2.29	0.65
5:I:188:ARG:HH21	43:k:22:PRO:HG3	1.60	0.65
54:A:1491:G:H1'	54:A:1492:C:H2'	1.78	0.65
8:L:87:VAL:HG11	8:L:123:ILE:HG12	1.79	0.65
28:5:80:ARG:NH1	28:5:82:TYR:OH	2.29	0.65
29:6:56:ARG:NH2	55:B:1625:A:OP1	2.29	0.65
52:v:10:LEU:HD22	53:w:116:VAL:HG21	1.78	0.65
8:L:49:SER:HB3	8:L:78:LYS:HZ1	1.60	0.65
41:i:46:ARG:NH2	54:A:609:U:OP2	2.29	0.65
54:A:15:C:N3	54:A:96:U:O4	2.29	0.65
51:u:158:LYS:HG2	51:u:160:GLU:HG2	1.78	0.65
54:A:953:A:C6	54:A:954:C:N4	2.65	0.65
1:D:194:ASN:OD1	1:D:243:THR:OG1	2.14	0.65
15:S:118:ASN:C	15:S:118:ASN:HD22	2.04	0.65
22:Z:71:ARG:NH1	22:Z:92:GLU:O	2.29	0.65
49:r:93:ILE:HD11	49:r:119:VAL:HG21	1.79	0.65
29:6:214:TRP:HA	29:6:273:PHE:O	1.96	0.65
54:A:1078:A:H2'	54:A:1079:A:H8	1.62	0.65
18:V:96:ARG:O	18:V:108:MET:HA	1.97	0.64
44:l:122:ARG:NH2	54:A:544:A:O2'	2.30	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:c:275:TYR:HA	35:c:280:LEU:HA	1.80	0.64
43:k:80:HIS:O	49:r:36:ARG:NH1	2.30	0.64
30:7:107:LEU:HB2	30:7:126:LYS:HB2	1.80	0.64
54:A:530:A:H2'	54:A:531:G:H8	1.62	0.64
26:3:113:ARG:NH2	54:A:80:G:OP2	2.31	0.64
54:A:197:A:H62	54:A:625:C:H5	1.46	0.64
12:P:54:ARG:NH2	12:P:57:GLU:OE1	2.30	0.64
32:9:22:THR:HG23	32:9:24:LYS:H	1.63	0.64
54:A:1078:A:H2'	54:A:1079:A:C8	2.33	0.64
54:A:1289:G:C2	54:A:1295:A:N6	2.65	0.63
5:I:119:HIS:HD2	5:I:121:ILE:HB	1.61	0.63
5:I:140:TYR:HB3	5:I:143:LEU:HB2	1.80	0.63
29:6:175:VAL:HB	29:6:187:VAL:HB	1.80	0.63
52:v:46:GLU:H	52:v:51:ARG:HH21	1.46	0.63
9:M:180:ASP:HB2	9:M:183:SER:H	1.64	0.63
1:D:129:VAL:CA	1:D:139:ILE:O	2.36	0.63
54:A:610:C:N3	54:A:615:U:O4	2.32	0.63
12:P:58:LEU:HD23	47:p:177:ARG:HH21	1.62	0.63
51:u:111:VAL:HG12	51:u:125:VAL:HG22	1.80	0.63
9:M:59:ARG:NH2	54:A:347:U:OP2	2.31	0.62
54:A:717:U:O2'	54:A:736:A:N6	2.32	0.62
12:P:57:GLU:O	47:p:177:ARG:NH2	2.33	0.62
39:g:80:PRO:HB2	39:g:82:LEU:HD13	1.79	0.62
24:1:47:ASP:O	24:1:51:LYS:CA	2.47	0.62
36:d:197:VAL:CA	36:d:211:GLN:O	2.40	0.62
54:A:1446:C:H42	54:A:1470:A:H61	1.46	0.62
9:M:71:GLN:OE1	54:A:364:A:O2'	2.18	0.62
16:T:212:LEU:HA	34:b:119:PHE:HE2	1.62	0.62
51:u:135:LEU:HD22	51:u:179:LEU:HB3	1.80	0.62
8:L:58:ILE:HD11	8:L:76:ALA:HB2	1.81	0.62
11:O:64:LYS:NZ	11:O:97:TYR:O	2.32	0.62
12:P:42:GLU:HA	29:6:337:MET:HE1	1.81	0.62
36:d:119:GLN:OE1	36:d:123:ARG:NH1	2.33	0.62
54:A:1340:G:N2	54:A:1502:C:OP2	2.33	0.62
1:D:259:LYS:NZ	54:A:269:G:OP2	2.29	0.62
17:U:71:ARG:NH2	17:U:96:TYR:OH	2.32	0.62
54:A:1341:A:O2'	54:A:1503:G:N2	2.31	0.62
2:E:69:ASP:OD2	2:E:154:ARG:NH1	2.32	0.62
11:O:110:ILE:HD11	11:O:122:VAL:HG23	1.82	0.62
13:Q:139:GLN:HB3	13:Q:150:ILE:HG22	1.82	0.62
14:R:57:ARG:NH2	15:S:170:ILE:O	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:126:LYS:NZ	36:d:132:PHE:O	2.32	0.62
54:A:257:G:O6	54:A:307:U:O2	2.17	0.62
7:K:52:ASP:O	16:T:206:ARG:NH1	2.31	0.62
28:5:343:GLN:HG3	28:5:417:LEU:HD22	1.79	0.62
21:Y:70:ASP:OD2	21:Y:72:LYS:NZ	2.30	0.61
45:m:51:LEU:HB3	45:m:67:ARG:HB3	1.82	0.61
54:A:304:A:N6	54:A:825:U:C4	2.67	0.61
55:B:1609:U:O2	55:B:1616:A:N6	2.33	0.61
54:A:130:G:N1	54:A:133:A:OP2	2.30	0.61
55:B:1628:C:N4	55:B:1640:A:N1	2.48	0.61
12:P:66:ARG:NH2	54:A:1204:A:O2'	2.34	0.61
50:s:152:GLN:HA	50:s:156:TYR:HB2	1.80	0.61
51:u:196:LEU:HD12	51:u:199:TYR:HB2	1.82	0.61
9:M:202:LYS:NZ	9:M:296:SER:O	2.33	0.61
15:S:127:ARG:NH2	15:S:157:GLU:OE1	2.31	0.61
54:A:360:U:C4	54:A:428:G:O6	2.53	0.61
9:M:119:THR:HG22	9:M:123:ASN:HD21	1.65	0.61
29:6:72:ARG:NH1	29:6:76:GLU:OE2	2.33	0.61
26:3:183:ARG:NH1	29:6:355:LYS:O	2.34	0.61
13:Q:84:ARG:O	54:A:1487:C:O2'	2.19	0.61
52:v:23:LEU:O	52:v:28:ARG:NH1	2.34	0.61
4:H:103:GLU:HG2	4:H:104:ASN:H	1.65	0.61
9:M:277:MET:SD	39:g:45:TYR:OH	2.59	0.61
21:Y:91:ARG:NH1	21:Y:148:GLU:OE1	2.33	0.61
47:p:75:ARG:NH1	47:p:109:GLU:OE1	2.34	0.61
29:6:44:ASN:O	29:6:47:ARG:NH1	2.34	0.61
31:8:165:ASP:OD2	37:e:185:ARG:NH1	2.33	0.61
37:e:211:GLY:O	37:e:233:PHE:HB2	2.01	0.61
27:4:68:ASN:HD21	54:A:1356:U:H5'	1.66	0.60
34:b:37:GLY:H	34:b:44:ARG:HH12	1.48	0.60
4:H:131:TYR:HD2	20:X:139:TYR:HA	1.65	0.60
43:k:76:MET:HE2	43:k:81:LEU:HD22	1.84	0.60
50:s:295:GLY:N	50:s:339:GLN:OE1	2.34	0.60
5:I:116:LEU:HD12	5:I:121:ILE:HG21	1.82	0.60
28:5:110:ARG:NH1	54:A:737:U:O2'	2.33	0.60
53:w:133:ILE:O	53:w:137:LYS:NZ	2.35	0.60
1:D:135:ARG:NH2	54:A:858:G:OP1	2.34	0.60
14:R:32:ARG:O	14:R:35:LYS:NZ	2.35	0.60
28:5:80:ARG:HH12	54:A:37:C:H5	1.49	0.60
2:E:260:LYS:NZ	54:A:1550:A:OP1	2.34	0.60
7:K:108:ILE:HD13	7:K:125:LEU:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:P:102:VAL:HG12	12:P:103:VAL:HG23	1.82	0.60
14:R:78:GLU:OE2	34:b:135:ASN:ND2	2.30	0.60
37:e:146:ARG:HA	37:e:151:ARG:HD2	1.84	0.60
54:A:871:C:H2'	54:A:872:G:H8	1.65	0.60
8:L:39:ARG:HH21	13:Q:158:GLN:HE21	1.50	0.60
8:L:46:LEU:O	8:L:78:LYS:NZ	2.33	0.60
50:s:249:GLU:HA	50:s:356:VAL:HG21	1.83	0.60
1:D:68:SER:HA	28:5:38:THR:HG21	1.82	0.60
36:d:245:TYR:HB2	36:d:265:ILE:HB	1.84	0.60
54:A:200:A:H2'	54:A:232:C:H41	1.66	0.60
54:A:1408:C:H2'	54:A:1409:G:H8	1.66	0.60
50:s:405:ILE:HG12	50:s:410:VAL:HG12	1.83	0.59
2:E:208:ALA:HB2	2:E:297:VAL:HG23	1.85	0.59
42:j:44:THR:O	42:j:63:GLN:NE2	2.35	0.59
5:I:100:GLN:HE21	5:I:100:GLN:HA	1.67	0.59
9:M:98:LEU:HD21	9:M:167:ILE:HD11	1.83	0.59
13:Q:221:LYS:NZ	13:Q:241:LYS:O	2.35	0.59
54:A:49:G:N2	54:A:339:G:O2'	2.35	0.59
3:F:160:SER:OG	41:i:83:TRP:O	2.14	0.59
34:b:31:PHE:HA	34:b:74:ARG:O	2.02	0.59
46:o:20:LYS:NZ	54:A:441:C:O2'	2.36	0.59
54:A:1518:U:H3	54:A:1521:A:N6	2.00	0.59
5:I:117:ARG:NH1	6:J:133:GLN:OE1	2.35	0.59
11:O:25:ARG:NH2	11:O:51:GLU:OE1	2.28	0.59
12:P:169:GLY:O	47:p:184:ASN:ND2	2.35	0.59
36:d:197:VAL:HG12	36:d:212:ILE:HG12	1.85	0.59
11:O:75:MET:HE2	13:Q:269:MET:HG3	1.85	0.59
15:S:115:LEU:HB2	34:b:11:LEU:HD11	1.84	0.59
4:H:86:THR:HG23	4:H:89:ARG:HE	1.68	0.59
12:P:44:VAL:HG13	29:6:225:LEU:HB2	1.84	0.59
55:B:1622:A:H2'	55:B:1623:G:H8	1.68	0.59
31:8:150:LEU:HB2	37:e:212:HIS:HE1	1.68	0.59
7:K:119:ARG:NH2	54:A:1035:U:OP2	2.27	0.59
11:O:131:PRO:HD2	23:0:134:THR:HG22	1.83	0.59
27:4:79:CYS:SG	27:4:98:HIS:ND1	2.75	0.59
46:o:15:ARG:HB3	46:o:18:ILE:HG12	1.85	0.59
13:Q:182:ARG:HG2	13:Q:187:LEU:HD21	1.85	0.59
54:A:292:A:OP2	54:A:831:C:N4	2.36	0.59
54:A:359:A:N6	54:A:455:C:OP1	2.36	0.59
33:a:66:ASP:HB3	35:c:280:LEU:HD21	1.83	0.58
46:o:24:PRO:HG2	49:r:169:TRP:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:75:GLU:HG3	3:F:210:ARG:HH21	1.68	0.58
28:5:251:HIS:O	28:5:371:LYS:NZ	2.36	0.58
43:k:64:VAL:HG22	43:k:76:MET:HB3	1.84	0.58
39:g:105:ARG:HH11	54:A:381:A:H5'	1.68	0.58
29:6:227:GLU:HG3	29:6:229:ASP:H	1.69	0.58
9:M:150:ALA:H	9:M:170:ASN:HD22	1.51	0.58
13:Q:116:ILE:HD13	13:Q:178:LYS:HD3	1.85	0.58
17:U:30:ARG:NH1	21:Y:118:GLU:OE2	2.32	0.58
29:6:66:GLN:O	29:6:75:ARG:NH2	2.37	0.58
31:8:160:GLU:OE1	37:e:207:ASN:ND2	2.34	0.58
37:e:55:ARG:HD3	37:e:157:LEU:HD13	1.84	0.58
45:m:53:PRO:HB2	45:m:65:HIS:HD2	1.68	0.58
5:I:62:PRO:HA	5:I:65:LEU:HD13	1.84	0.58
26:3:179:LYS:O	29:6:370:ARG:NH2	2.37	0.58
51:u:102:ARG:NH2	52:v:25:TYR:O	2.37	0.58
22:Z:98:GLN:OE1	42:j:76:ARG:NH2	2.37	0.58
43:k:18:VAL:HG11	43:k:34:LEU:HD21	1.86	0.58
17:U:24:PHE:HB2	17:U:45:PRO:HG3	1.86	0.58
33:a:141:ASP:OD2	34:b:117:LYS:NZ	2.37	0.58
9:M:37:GLU:OE2	54:A:623:A:N6	2.24	0.58
14:R:11:ARG:HH22	54:A:606:C:H1'	1.68	0.58
30:7:113:TRP:HE1	30:7:117:LYS:HB3	1.69	0.58
36:d:90:PRO:HB3	36:d:245:TYR:HE2	1.69	0.58
36:d:226:ASP:HB3	36:d:228:PHE:H	1.68	0.58
54:A:1450:C:H42	54:A:1466:A:H61	1.52	0.58
20:X:19:GLY:O	20:X:22:SER:OG	2.21	0.57
24:1:47:ASP:O	24:1:51:LYS:N	2.36	0.57
54:A:77:G:OP2	54:A:79:C:N4	2.36	0.57
1:D:113:ARG:O	1:D:147:ARG:NH1	2.37	0.57
7:K:26:GLN:NE2	7:K:147:GLN:OE1	2.37	0.57
12:P:137:LEU:HD11	47:p:184:ASN:HB3	1.85	0.57
37:e:55:ARG:NH1	37:e:149:LEU:O	2.37	0.57
41:i:99:GLY:HA2	41:i:102:MET:HG3	1.86	0.57
44:l:115:ARG:NH2	44:l:116:GLU:OE1	2.37	0.57
25:2:88:LYS:HB3	32:9:18:MET:HE1	1.85	0.57
12:P:113:LYS:NZ	55:B:1621:A:OP2	2.37	0.57
21:Y:88:GLN:NE2	32:9:83:GLU:HA	2.19	0.57
28:5:343:GLN:HB3	28:5:356:VAL:HG23	1.86	0.57
30:7:163:MET:HB2	30:7:186:ASP:HB3	1.85	0.57
2:E:221:ARG:NH2	54:A:1438:U:OP2	2.35	0.57
49:r:149:ARG:HD3	49:r:152:THR:HG21	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:146:ASP:HB2	47:p:143:GLN:HE21	1.68	0.57
11:O:11:HIS:O	54:A:1488:A:O2'	2.19	0.57
15:S:139:ASP:OD1	35:c:310:ASN:ND2	2.38	0.57
28:5:126:THR:HG22	28:5:372:ASN:HB2	1.86	0.57
39:g:121:GLN:NE2	39:g:125:GLU:OE1	2.37	0.57
43:k:15:GLN:HB3	43:k:67:LEU:HB2	1.87	0.57
44:l:122:ARG:HH12	54:A:525:A:H4'	1.69	0.57
15:S:152:ASP:OD1	15:S:152:ASP:N	2.34	0.57
28:5:408:PRO:HG2	28:5:412:ARG:HH12	1.69	0.57
4:H:87:LYS:NZ	54:A:1125:U:O2	2.38	0.57
17:U:36:PRO:HB2	17:U:39:THR:HG23	1.86	0.57
17:U:80:ARG:NH2	17:U:84:ASN:O	2.37	0.57
19:W:100:THR:OG1	19:W:132:HIS:NE2	2.38	0.57
28:5:289:HIS:ND1	28:5:290:THR:OG1	2.34	0.57
20:X:4:HIS:NE2	21:Y:214:GLU:OE2	2.32	0.57
38:f:114:CYS:HA	38:f:119:ILE:HD12	1.85	0.57
13:Q:102:ARG:HH21	13:Q:169:PRO:HA	1.69	0.57
54:A:269:G:H5'	54:A:270:A:H5''	1.87	0.57
54:A:512:G:H1'	54:A:529:A:H2'	1.86	0.57
54:A:879:C:H4'	54:A:880:A:H5'	1.86	0.57
9:M:17:ARG:NH1	40:h:115:SER:O	2.38	0.56
13:Q:121:THR:HG22	13:Q:171:VAL:HA	1.87	0.56
23:0:90:ASN:OD1	23:0:93:ARG:NH1	2.25	0.56
23:0:129:LYS:HG2	36:d:289:PRO:HB3	1.86	0.56
23:0:155:GLU:OE1	23:0:172:LYS:NZ	2.38	0.56
28:5:174:GLU:HA	28:5:296:LYS:HB2	1.86	0.56
28:5:213:TRP:HB3	28:5:322:LEU:HD11	1.87	0.56
35:c:92:PHE:HE1	35:c:175:VAL:HG13	1.69	0.56
45:m:72:ARG:HH21	45:m:75:LEU:HD11	1.70	0.56
50:s:225:ARG:NH1	54:A:779:G:OP2	2.29	0.56
51:u:121:THR:OG1	51:u:174:SER:O	2.21	0.56
54:A:214:G:N3	54:A:225:C:O2'	2.36	0.56
21:Y:69:ASP:OD1	21:Y:69:ASP:N	2.38	0.56
23:0:119:LYS:O	23:0:120:HIS:ND1	2.39	0.56
36:d:247:VAL:O	36:d:262:HIS:N	2.31	0.56
50:s:185:VAL:HG13	50:s:195:LEU:HD23	1.86	0.56
11:O:10:SER:HB2	11:O:13:ARG:HG3	1.87	0.56
17:U:76:SER:HB2	54:A:672:U:H5''	1.88	0.56
18:V:79:VAL:HG22	18:V:86:VAL:HG22	1.86	0.56
18:V:185:ARG:HA	21:Y:92:ASN:HB3	1.86	0.56
41:i:32:ILE:HD11	54:A:143:C:H2'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:L:49:SER:HB3	8:L:78:LYS:NZ	2.20	0.56
28:5:293:LEU:O	28:5:346:GLY:HA2	2.06	0.56
54:A:117:G:N2	54:A:120:A:OP2	2.34	0.56
54:A:1408:C:H2'	54:A:1409:G:C8	2.40	0.56
7:K:25:MET:O	7:K:149:ARG:NH1	2.38	0.56
29:6:367:ASP:OD1	29:6:370:ARG:NH1	2.38	0.56
10:N:123:ARG:NH2	10:N:162:GLU:OE1	2.37	0.56
11:O:48:ARG:NH2	54:A:784:G:OP1	2.38	0.56
11:O:129:CYS:SG	23:0:156:THR:OG1	2.63	0.56
22:Z:101:LYS:NZ	42:j:83:GLU:OE1	2.38	0.56
31:8:129:ARG:NH1	55:B:1627:C:OP1	2.39	0.56
43:k:18:VAL:HG23	43:k:64:VAL:HG12	1.88	0.56
47:p:104:HIS:HA	47:p:132:GLU:HA	1.88	0.56
9:M:133:LYS:HG2	26:3:168:ARG:NH2	2.21	0.56
12:P:61:VAL:HG11	29:6:344:PHE:CE2	2.41	0.56
43:k:14:LYS:HD3	43:k:69:GLY:H	1.71	0.56
48:q:125:MET:HA	48:q:128:MET:HB2	1.86	0.56
49:r:110:GLU:OE1	49:r:113:ARG:NH2	2.38	0.56
54:A:140:A:H2'	54:A:141:A:H8	1.69	0.56
5:I:125:VAL:HG22	54:A:524:U:H3	1.70	0.55
16:T:109:ASN:HD21	23:0:101:ILE:HG21	1.69	0.55
30:7:99:TYR:O	30:7:103:SER:OG	2.18	0.55
55:B:1607:U:O4	55:B:1664:G:O6	2.24	0.55
2:E:266:ARG:NH1	54:A:1476:G:O3'	2.40	0.55
19:W:67:ILE:HG21	19:W:131:VAL:HG11	1.89	0.55
37:e:279:LEU:HD11	38:f:176:SER:HB2	1.87	0.55
14:R:128:PHE:O	14:R:132:LEU:N	2.39	0.55
18:V:25:PRO:HG2	18:V:28:SER:HB3	1.88	0.55
18:V:122:LEU:HD21	18:V:154:ILE:HG21	1.88	0.55
28:5:380:GLN:HB3	28:5:410:THR:HG22	1.89	0.55
32:9:31:ARG:NH1	54:A:751:G:O2'	2.39	0.55
34:b:80:LEU:HD11	35:c:78:ARG:HD3	1.89	0.55
51:u:108:ASP:HB3	51:u:128:SER:HB3	1.87	0.55
3:F:107:LYS:HG2	41:i:74:ILE:HG22	1.89	0.55
3:F:221:LEU:HD13	3:F:264:PRO:HB2	1.89	0.55
5:I:148:VAL:O	43:k:31:ARG:NH2	2.40	0.55
22:Z:65:LYS:HG3	22:Z:66:LEU:HG	1.89	0.55
23:0:144:GLN:OE1	23:0:173:ARG:NH1	2.39	0.55
30:7:81:MET:HE1	30:7:91:CYS:HA	1.88	0.55
51:u:108:ASP:OD2	51:u:185:ARG:NH1	2.33	0.55
1:D:202:ARG:NH2	54:A:851:A:OP2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:252:TRP:O	2:E:255:THR:OG1	2.25	0.55
3:F:220:ASP:OD1	3:F:221:LEU:N	2.39	0.55
30:7:64:LYS:NZ	30:7:82:ASN:OD1	2.39	0.55
23:0:90:ASN:O	23:0:94:ARG:HG2	2.06	0.55
27:4:68:ASN:OD1	27:4:101:ARG:NH1	2.39	0.55
29:6:198:ALA:O	29:6:254:TYR:OH	2.24	0.55
5:I:164:MET:HA	5:I:167:ILE:HG12	1.89	0.55
24:1:20:MET:HB3	24:1:30:PHE:O	2.07	0.55
28:5:93:LEU:HB3	28:5:270:ILE:HD11	1.88	0.55
43:k:32:THR:HA	43:k:35:GLN:HG2	1.89	0.55
2:E:298:LYS:NZ	54:A:1534:C:OP1	2.40	0.55
3:F:211:ARG:HH22	40:h:56:ARG:HG2	1.72	0.55
28:5:125:LYS:HA	28:5:253:LEU:HD21	1.88	0.55
54:A:1176:G:N2	54:A:1225:U:O2	2.34	0.55
5:I:128:ASN:ND2	5:I:149:GLY:O	2.40	0.54
15:S:103:SER:O	15:S:103:SER:OG	2.25	0.54
30:7:262:ASP:OD1	30:7:263:VAL:N	2.40	0.54
34:b:4:ARG:NH1	54:A:160:G:N7	2.54	0.54
54:A:50:C:O2'	54:A:340:U:O4	2.21	0.54
51:u:149:LEU:HD23	51:u:150:LYS:HB2	1.89	0.54
10:N:224:LEU:HD11	46:o:39:LEU:HG	1.89	0.54
11:O:79:TRP:NE1	13:Q:267:PHE:O	2.25	0.54
18:V:95:TYR:HB3	18:V:108:MET:HE1	1.88	0.54
8:L:102:SER:OG	8:L:104:ASN:OD1	2.24	0.54
9:M:77:ARG:NH2	54:A:1247:G:O6	2.40	0.54
27:4:69:LYS:NZ	54:A:1284:C:OP2	2.41	0.54
12:P:51:ARG:NH2	29:6:160:ASP:OD1	2.40	0.54
13:Q:152:ARG:HG3	13:Q:161:GLU:HG2	1.90	0.54
22:Z:71:ARG:NH2	54:A:470:G:OP2	2.41	0.54
6:J:111:LEU:HG	6:J:154:ARG:HB2	1.90	0.54
54:A:360:U:N3	54:A:428:G:C6	2.75	0.54
55:B:1622:A:H2'	55:B:1623:G:C8	2.42	0.54
1:D:105:ARG:HH21	1:D:130:ARG:NH2	2.05	0.54
3:F:126:LYS:NZ	54:A:237:A:OP1	2.30	0.54
18:V:29:VAL:HG21	36:d:67:ILE:HG12	1.89	0.54
23:0:86:THR:HG21	54:A:1013:C:H5'	1.90	0.54
23:0:110:CYS:SG	23:0:112:GLU:HB2	2.48	0.54
24:1:20:MET:HG3	24:1:56:PHE:HD2	1.71	0.54
5:I:121:ILE:HD11	5:I:154:LEU:HB3	1.89	0.54
9:M:94:LYS:NZ	9:M:135:ASP:OD2	2.39	0.54
10:N:205:ARG:NH2	10:N:249:LYS:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:6:234:HIS:ND1	29:6:255:LEU:O	2.39	0.54
54:A:495:C:O2'	54:A:496:C:O5'	2.24	0.54
22:Z:88:MET:SD	54:A:412:G:N2	2.68	0.54
54:A:1137:U:H2'	54:A:1138:U:C6	2.43	0.54
5:I:52:GLU:O	10:N:211:ASN:ND2	2.41	0.54
9:M:51:ARG:HH12	9:M:60:GLY:HA2	1.73	0.54
14:R:112:THR:OG1	34:b:127:GLN:NE2	2.37	0.54
14:R:119:LEU:HD11	33:a:58:ILE:HD13	1.88	0.54
3:F:167:MET:SD	3:F:279:ARG:NH2	2.81	0.53
18:V:20:ARG:NH2	18:V:42:ARG:O	2.41	0.53
28:5:139:LEU:O	28:5:145:ASN:ND2	2.41	0.53
28:5:198:LEU:HD21	28:5:419:LEU:HD13	1.90	0.53
29:6:219:THR:O	29:6:268:LEU:HA	2.07	0.53
27:4:77:LYS:NZ	54:A:541:U:O3'	2.36	0.53
28:5:50:TYR:CE2	28:5:57:PRO:HG3	2.44	0.53
34:b:26:LEU:HD22	34:b:105:ALA:HA	1.88	0.53
35:c:123:GLN:OE1	35:c:126:SER:OG	2.26	0.53
39:g:154:ASP:OD1	39:g:154:ASP:N	2.40	0.53
40:h:139:LYS:HD3	40:h:142:GLU:HB3	1.90	0.53
50:s:188:LEU:HD12	50:s:426:LEU:HD21	1.90	0.53
54:A:403:A:H62	54:A:1162:A:H2	1.56	0.53
3:F:218:LEU:HD23	3:F:260:VAL:HB	1.91	0.53
10:N:127:PRO:HA	10:N:152:THR:HG23	1.88	0.53
13:Q:96:ARG:NE	13:Q:285:GLU:OE1	2.36	0.53
3:F:49:ARG:NH1	3:F:270:GLU:OE2	2.31	0.53
17:U:21:ARG:NH2	32:9:137:ARG:O	2.41	0.53
32:9:113:ASN:O	32:9:116:LYS:NZ	2.42	0.53
38:f:127:MET:HB2	38:f:154:GLU:HB2	1.91	0.53
50:s:310:ARG:HH21	54:A:747:C:P	2.30	0.53
5:I:80:ARG:HA	5:I:83:ARG:HG2	1.89	0.53
6:J:69:LYS:HB3	6:J:81:LYS:HB3	1.91	0.53
7:K:59:ILE:HB	7:K:127:LEU:HD23	1.89	0.53
7:K:90:VAL:HG11	7:K:98:ARG:HH21	1.74	0.53
14:R:112:THR:HG23	15:S:142:THR:HG21	1.91	0.53
18:V:55:TYR:O	18:V:145:ARG:NH2	2.42	0.53
21:Y:90:LEU:HD12	21:Y:142:LEU:HD13	1.91	0.53
29:6:175:VAL:HG22	29:6:204:VAL:HG12	1.90	0.53
53:w:90:TYR:HD2	53:w:93:ILE:HG12	1.73	0.53
11:O:33:LEU:HD21	11:O:59:LEU:HD13	1.90	0.53
18:V:66:GLU:OE1	18:V:119:GLN:NE2	2.42	0.53
35:c:94:ASN:ND2	35:c:180:LEU:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:p:186:GLU:HG2	47:p:189:ARG:HH22	1.71	0.53
52:v:51:ARG:HA	58:v:101:PNS:H422	1.90	0.53
54:A:501:U:H4'	54:A:502:A:H3'	1.89	0.53
54:A:1240:A:H2'	54:A:1242:C:H5''	1.90	0.53
54:A:1338:C:O2'	54:A:1381:A:N3	2.38	0.53
12:P:131:VAL:O	12:P:135:ARG:HG2	2.08	0.53
49:r:105:THR:HG23	49:r:107:LEU:HD23	1.89	0.53
54:A:844:C:H2'	54:A:845:U:H6	1.74	0.53
6:J:125:ALA:HB2	6:J:140:VAL:HG21	1.91	0.53
12:P:44:VAL:HG21	29:6:340:PRO:HB3	1.91	0.53
32:9:20:LYS:O	32:9:25:ARG:NH2	2.42	0.53
39:g:118:TRP:NE1	39:g:142:GLU:OE1	2.34	0.53
49:r:158:SER:O	49:r:158:SER:OG	2.23	0.53
50:s:51:MET:O	50:s:62:ARG:NH1	2.35	0.53
54:A:523:U:O4	54:A:526:A:C6	2.60	0.53
8:L:136:LYS:HZ3	51:u:167:TRP:HB3	1.73	0.53
13:Q:275:THR:O	13:Q:275:THR:OG1	2.23	0.53
20:X:112:ARG:NH2	54:A:1085:A:O3'	2.42	0.53
3:F:200:PRO:HB3	3:F:237:LEU:HD11	1.90	0.52
17:U:66:ALA:HB2	17:U:100:ALA:HB2	1.91	0.52
24:1:43:LEU:O	24:1:55:LEU:HA	2.09	0.52
50:s:228:ASP:OD1	50:s:228:ASP:N	2.40	0.52
1:D:111:ARG:NH2	1:D:179:GLY:O	2.42	0.52
6:J:25:ARG:HA	6:J:65:PRO:HA	1.89	0.52
12:P:85:ARG:HG2	12:P:120:ARG:HH12	1.74	0.52
39:g:107:MET:SD	39:g:148:ARG:NH1	2.77	0.52
29:6:218:LEU:O	29:6:233:LEU:HA	2.08	0.52
29:6:239:ASN:OD1	29:6:275:GLN:NE2	2.40	0.52
35:c:124:GLU:OE2	35:c:128:GLN:NE2	2.42	0.52
54:A:496:C:H2'	54:A:497:A:C8	2.44	0.52
18:V:47:GLU:OE2	18:V:117:HIS:NE2	2.40	0.52
20:X:116:SER:O	20:X:120:ASP:N	2.43	0.52
2:E:235:LYS:O	2:E:239:ARG:NH2	2.41	0.52
5:I:80:ARG:HB2	5:I:84:ARG:NH1	2.24	0.52
9:M:118:LEU:HD21	9:M:129:ILE:HD11	1.92	0.52
21:Y:162:ARG:HH22	54:A:23:C:H6	1.56	0.52
54:A:629:U:H5''	54:A:630:G:H5''	1.91	0.52
21:Y:103:TYR:HE2	32:9:62:VAL:HG22	1.74	0.52
39:g:111:ARG:HG3	39:g:146:THR:HG22	1.92	0.52
36:d:123:ARG:HH21	36:d:126:LYS:HG3	1.75	0.52
47:p:56:ASP:HB3	47:p:60:ARG:HE	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
49:r:70:CYS:HB2	49:r:107:LEU:HD13	1.91	0.52
51:u:113:GLN:HB3	52:v:68:ARG:HG2	1.91	0.52
54:A:517:C:H2'	54:A:518:A:C8	2.44	0.52
1:D:228:LEU:HD21	1:D:234:MET:HE2	1.92	0.52
6:J:113:THR:HA	6:J:156:VAL:HB	1.91	0.52
9:M:154:ILE:HD12	9:M:167:ILE:HD13	1.92	0.52
28:5:125:LYS:HB2	28:5:215:ARG:HH12	1.74	0.52
29:6:173:LEU:HD12	29:6:272:LEU:HD22	1.91	0.52
34:b:38:ALA:O	34:b:41:ARG:HB2	2.10	0.52
35:c:228:LEU:HB2	35:c:307:PHE:CD2	2.45	0.52
29:6:364:ARG:NE	54:A:1189:A:OP2	2.42	0.52
32:9:17:ARG:HH21	54:A:119:A:H5''	1.74	0.52
33:a:62:HIS:O	33:a:62:HIS:ND1	2.39	0.52
53:w:123:GLU:HG2	53:w:130:ILE:HD12	1.92	0.52
13:Q:87:THR:OG1	13:Q:88:ASP:N	2.43	0.51
30:7:59:THR:HG22	30:7:84:ASN:HD21	1.74	0.51
49:r:86:VAL:O	49:r:90:SER:CB	2.58	0.51
54:A:867:G:O2'	54:A:964:U:OP2	2.24	0.51
54:A:1024:A:C6	54:A:1315:C:H1'	2.45	0.51
20:X:92:ALA:HB3	20:X:98:SER:HB3	1.92	0.51
37:e:257:LYS:NZ	37:e:277:SER:O	2.42	0.51
54:A:1070:A:N7	54:A:1252:A:C2	2.78	0.51
54:A:1081:G:H2'	54:A:1082:C:C6	2.45	0.51
1:D:263:ASN:ND2	54:A:841:C:O5'	2.43	0.51
20:X:79:LEU:HD21	20:X:145:ILE:HD11	1.91	0.51
54:A:820:C:O2'	54:A:931:A:OP1	2.24	0.51
1:D:199:GLU:HB2	1:D:202:ARG:HB2	1.93	0.51
2:E:198:PHE:O	2:E:199:ARG:HD2	2.10	0.51
9:M:247:ILE:HG22	9:M:253:PHE:HD1	1.75	0.51
16:T:69:ARG:NH1	36:d:228:PHE:O	2.43	0.51
28:5:229:ARG:NH2	28:5:231:SER:OG	2.43	0.51
36:d:159:ARG:O	36:d:163:LEU:HB2	2.10	0.51
37:e:146:ARG:HB3	37:e:253:VAL:HG13	1.91	0.51
53:w:79:ILE:HG12	53:w:126:PHE:HZ	1.76	0.51
1:D:146:SER:HA	28:5:263:ILE:HD13	1.93	0.51
9:M:69:GLY:O	54:A:370:G:N2	2.43	0.51
29:6:268:LEU:O	29:6:318:PHE:HA	2.11	0.51
54:A:89:U:O2'	54:A:218:G:O6	2.25	0.51
54:A:280:U:H2'	54:A:281:C:C6	2.46	0.51
10:N:144:LYS:HE2	54:A:437:G:H5''	1.91	0.51
12:P:85:ARG:HB3	12:P:120:ARG:HH22	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:272:ASP:OD1	28:5:272:ASP:N	2.43	0.51
28:5:307:ASP:OD2	28:5:310:ARG:NH2	2.43	0.51
53:w:82:ARG:NH1	53:w:125:GLU:OE2	2.43	0.51
14:R:48:ARG:NH2	54:A:174:A:OP2	2.44	0.51
2:E:106:MET:CA	2:E:119:VAL:O	2.38	0.51
5:I:104:LEU:HD21	5:I:174:LEU:HD22	1.92	0.51
34:b:36:ASP:HA	46:o:100:LYS:HG2	1.92	0.51
15:S:204:LEU:HD22	33:a:52:THR:HG21	1.93	0.51
16:T:68:ARG:NH1	36:d:230:ARG:HD2	2.26	0.51
37:e:266:PRO:HD2	37:e:269:LEU:HB2	1.93	0.51
54:A:1178:A:H2'	54:A:1179:G:H8	1.75	0.51
3:F:83:HIS:CD2	3:F:84:PRO:HD2	2.46	0.51
8:L:119:ILE:HG21	8:L:123:ILE:HD11	1.93	0.51
54:A:156:G:H4'	54:A:158:A:C2	2.46	0.51
55:B:1628:C:H2'	55:B:1629:A:H8	1.76	0.51
3:F:234:THR:O	48:q:25:TYR:N	2.45	0.50
7:K:12:ALA:HA	35:c:269:LEU:HD11	1.92	0.50
12:P:171:VAL:HG12	12:P:173:ARG:H	1.75	0.50
20:X:143:PHE:O	20:X:147:LYS:HB2	2.11	0.50
26:3:131:LYS:O	26:3:136:LYS:NZ	2.44	0.50
28:5:365:ASP:OD1	28:5:365:ASP:N	2.41	0.50
34:b:30:SER:HB2	34:b:76:VAL:HB	1.92	0.50
43:k:40:GLU:O	43:k:44:SER:N	2.43	0.50
4:H:123:LEU:O	4:H:128:LEU:N	2.44	0.50
17:U:30:ARG:O	21:Y:121:ARG:NH1	2.41	0.50
22:Z:103:ILE:HG22	46:o:54:MET:HG3	1.93	0.50
27:4:67:LYS:NZ	54:A:1296:U:OP2	2.44	0.50
31:8:160:GLU:O	37:e:207:ASN:ND2	2.44	0.50
31:8:179:THR:OG1	45:m:61:GLY:O	2.28	0.50
1:D:86:ASP:OD2	1:D:92:ARG:HB2	2.11	0.50
29:6:216:LEU:HA	29:6:271:LEU:O	2.12	0.50
29:6:332:HIS:CD2	47:p:129:ARG:HG3	2.47	0.50
34:b:4:ARG:HG2	54:A:161:G:OP2	2.11	0.50
7:K:74:GLN:HG2	49:r:162:ILE:HG13	1.92	0.50
10:N:105:MET:HE3	10:N:183:LEU:HD21	1.92	0.50
29:6:39:ASP:N	29:6:39:ASP:OD1	2.44	0.50
47:p:74:ASP:OD1	47:p:74:ASP:N	2.39	0.50
48:q:48:PRO:HD2	48:q:51:GLN:OE1	2.12	0.50
50:s:86:MET:SD	54:A:772:U:O2'	2.67	0.50
50:s:365:LYS:NZ	50:s:402:TYR:O	2.43	0.50
51:u:96:MET:O	51:u:99:SER:OG	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:w:93:ILE:HG22	53:w:110:LEU:HD21	1.93	0.50
54:A:1058:C:H2'	54:A:1059:U:H6	1.77	0.50
4:H:108:ARG:NH2	4:H:143:GLU:OE2	2.45	0.50
9:M:97:SER:HA	9:M:141:VAL:HB	1.93	0.50
11:O:108:LEU:HD12	11:O:133:LEU:HD13	1.93	0.50
29:6:235:TRP:CE3	29:6:237:LEU:HD13	2.43	0.50
37:e:50:ALA:HB2	37:e:175:GLN:HG2	1.92	0.50
37:e:64:THR:HG22	37:e:66:LEU:H	1.77	0.50
37:e:199:ASN:HB3	37:e:242:ASP:HB2	1.92	0.50
47:p:100:GLU:OE1	47:p:102:ARG:NH2	2.44	0.50
53:w:119:ILE:HA	53:w:122:MET:SD	2.51	0.50
18:V:170:TRP:HE1	32:9:75:SER:HB2	1.76	0.50
28:5:229:ARG:HG3	28:5:291:LEU:HD13	1.93	0.50
30:7:216:PHE:CE1	30:7:257:ILE:HG12	2.47	0.50
51:u:183:GLU:HA	51:u:186:GLU:HG2	1.92	0.50
54:A:15:C:C4	54:A:96:U:O4	2.63	0.50
54:A:112:G:N2	54:A:124:A:OP2	2.34	0.50
54:A:190:A:O2'	54:A:1012:A:OP1	2.27	0.50
3:F:249:ASN:HD22	41:i:55:GLY:C	2.19	0.50
11:O:74:ARG:NH1	11:O:77:ASP:OD2	2.45	0.50
18:V:147:SER:OG	18:V:150:SER:O	2.28	0.50
19:W:143:LYS:NZ	29:6:345:VAL:HG21	2.26	0.50
29:6:234:HIS:HA	29:6:296:ARG:HH22	1.77	0.50
36:d:173:THR:HA	36:d:176:ILE:HG12	1.94	0.50
50:s:214:GLU:HA	50:s:228:ASP:HA	1.94	0.50
54:A:1394:A:H2'	54:A:1431:A:N6	2.26	0.50
37:e:70:MET:HA	37:e:73:LEU:HG	1.94	0.50
53:w:138:LEU:HD13	53:w:144:ILE:HG12	1.93	0.50
54:A:973:G:O2'	54:A:975:G:OP2	2.25	0.50
54:A:1154:C:O2'	54:A:1223:A:O2'	2.24	0.50
1:D:248:SER:OG	1:D:249:ASN:N	2.45	0.50
12:P:156:ASP:HA	12:P:159:LYS:HG3	1.94	0.50
13:Q:196:GLU:HA	13:Q:199:THR:HG22	1.92	0.50
54:A:416:A:H2'	54:A:417:U:C6	2.47	0.50
54:A:727:C:H3'	54:A:728:A:H8	1.76	0.50
3:F:137:ARG:NH1	54:A:1262:G:OP1	2.36	0.49
4:H:54:VAL:HG21	20:X:105:TRP:HB3	1.93	0.49
20:X:3:LEU:HD23	41:i:102:MET:HA	1.94	0.49
26:3:100:ARG:NH1	54:A:62:C:OP1	2.45	0.49
35:c:167:CYS:SG	35:c:171:ARG:NH2	2.78	0.49
54:A:519:C:H5'	54:A:520:C:H5'	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:A:962:A:O2'	54:A:965:G:N3	2.40	0.49
12:P:44:VAL:HG22	29:6:225:LEU:HD13	1.94	0.49
12:P:130:ARG:NH2	29:6:130:VAL:O	2.41	0.49
31:8:171:PHE:HE1	37:e:203:LYS:HG2	1.77	0.49
49:r:94:ARG:NH2	54:A:1511:U:OP1	2.45	0.49
54:A:1048:C:H2'	54:A:1321:U:H4'	1.93	0.49
2:E:68:GLU:OE2	30:7:315:LYS:NZ	2.33	0.49
15:S:112:ASP:O	15:S:194:ARG:HA	2.11	0.49
37:e:51:LEU:HD12	37:e:188:ALA:HB1	1.93	0.49
47:p:110:TRP:H	47:p:110:TRP:CD1	2.30	0.49
54:A:1015:U:O2'	54:A:1434:U:H5'	2.12	0.49
54:A:640:G:O2'	54:A:1005:G:O6	2.30	0.49
54:A:1292:C:N4	54:A:1346:G:N2	2.60	0.49
3:F:241:ASN:OD1	3:F:256:HIS:NE2	2.30	0.49
5:I:128:ASN:HA	5:I:131:LEU:HB3	1.94	0.49
19:W:61:VAL:HG13	19:W:65:ASN:HB2	1.94	0.49
30:7:269:ILE:HG22	30:7:271:ARG:H	1.77	0.49
53:w:111:ASP:HB3	53:w:114:ASP:H	1.77	0.49
54:A:81:A:C5	54:A:82:U:H1'	2.46	0.49
2:E:334:ASP:HB3	2:E:337:VAL:HG13	1.94	0.49
5:I:187:SER:O	5:I:191:PHE:N	2.40	0.49
21:Y:88:GLN:HE21	32:9:83:GLU:HA	1.76	0.49
26:3:118:HIS:CD2	26:3:169:ARG:HD2	2.47	0.49
32:9:113:ASN:N	32:9:113:ASN:ND2	2.50	0.49
34:b:28:ARG:NH2	35:c:71:GLU:OE2	2.45	0.49
53:w:101:ASN:OD1	53:w:142:GLN:NE2	2.45	0.49
1:D:293:LYS:NZ	54:A:850:C:OP2	2.43	0.49
15:S:107:LYS:HE3	16:T:212:LEU:HD22	1.95	0.49
24:1:25:GLY:H	48:q:121:ILE:HD12	1.78	0.49
35:c:59:ARG:NH2	35:c:182:GLU:O	2.45	0.49
3:F:266:VAL:O	3:F:270:GLU:HG3	2.12	0.49
8:L:70:GLY:O	8:L:130:ARG:NH2	2.45	0.49
9:M:56:GLU:OE1	9:M:63:PRO:HD3	2.12	0.49
20:X:176:LEU:HD13	20:X:188:TYR:HE2	1.78	0.49
30:7:281:SER:OG	30:7:320:SER:O	2.29	0.49
30:7:320:SER:O	30:7:320:SER:OG	2.31	0.49
34:b:141:ARG:NH2	34:b:149:GLN:O	2.35	0.49
5:I:33:VAL:HG13	10:N:244:LYS:HB3	1.95	0.49
5:I:145:PRO:O	43:k:26:ASN:ND2	2.35	0.49
9:M:35:LYS:HE3	54:A:230:A:H1'	1.94	0.49
11:O:32:LEU:HB3	11:O:52:MET:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:d:188:SER:OG	36:d:217:HIS:O	2.30	0.49
53:w:148:ILE:HA	53:w:151:LYS:HE3	1.95	0.49
11:O:80:LEU:HD23	11:O:85:LEU:HB2	1.95	0.49
28:5:229:ARG:HH22	28:5:279:PHE:HE2	1.61	0.49
29:6:162:PHE:HB3	29:6:165:ALA:HB3	1.93	0.49
31:8:121:TRP:CD1	37:e:70:MET:HE1	2.47	0.49
54:A:495:C:H2'	54:A:496:C:C2	2.48	0.49
7:K:67:PHE:HB3	7:K:71:LYS:HB2	1.94	0.48
20:X:116:SER:O	20:X:120:ASP:HA	2.13	0.48
28:5:145:ASN:HA	28:5:194:LYS:HZ1	1.77	0.48
2:E:96:ARG:NH2	2:E:197:HIS:O	2.36	0.48
15:S:118:ASN:C	15:S:118:ASN:ND2	2.71	0.48
22:Z:100:HIS:HB3	22:Z:106:VAL:HG11	1.95	0.48
28:5:50:TYR:HE2	28:5:57:PRO:HG3	1.78	0.48
30:7:79:PHE:HB3	30:7:81:MET:HE3	1.95	0.48
37:e:85:SER:HB2	45:m:50:ARG:H	1.78	0.48
37:e:200:MET:HE2	37:e:238:LEU:HD22	1.93	0.48
54:A:916:U:H2'	54:A:917:G:C8	2.47	0.48
5:I:47:LEU:HD12	10:N:226:ILE:HG12	1.95	0.48
18:V:74:GLY:HA3	18:V:91:LEU:HD13	1.95	0.48
37:e:177:GLU:O	37:e:190:ARG:NH2	2.46	0.48
49:r:123:HIS:HB3	54:A:1521:A:H4'	1.95	0.48
51:u:118:MET:HE3	51:u:118:MET:HB2	1.76	0.48
54:A:642:A:H2'	54:A:643:A:O4'	2.14	0.48
17:U:8:PRO:HD3	32:9:136:LEU:HD21	1.94	0.48
19:W:72:HIS:O	19:W:74:ARG:N	2.45	0.48
29:6:365:TYR:HA	29:6:368:ARG:HD3	1.94	0.48
39:g:63:HIS:HB2	39:g:66:TYR:CZ	2.48	0.48
17:U:44:ILE:HD11	17:U:53:LEU:HD13	1.95	0.48
23:O:125:TYR:OH	36:d:287:LEU:O	2.23	0.48
28:5:223:ARG:NH1	54:A:740:U:OP1	2.43	0.48
32:9:42:GLY:HA3	32:9:51:VAL:O	2.13	0.48
35:c:262:GLY:O	35:c:265:THR:OG1	2.27	0.48
36:d:210:GLY:O	36:d:249:GLU:HA	2.13	0.48
49:r:86:VAL:O	49:r:90:SER:HB2	2.13	0.48
51:u:110:CYS:HA	52:v:26:THR:HG23	1.96	0.48
54:A:390:A:N6	54:A:409:C:N3	2.61	0.48
54:A:485:A:H2'	54:A:486:A:O4'	2.14	0.48
54:A:1411:A:H2'	54:A:1412:G:H8	1.78	0.48
3:F:231:VAL:HG13	48:q:26:ARG:HD2	1.94	0.48
19:W:49:ARG:HD3	19:W:71:ARG:NH2	2.24	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:g:39:VAL:HG21	48:q:72:PRO:HB2	1.96	0.48
54:A:140:A:H2'	54:A:141:A:C8	2.47	0.48
54:A:230:A:H2'	54:A:231:C:H5''	1.95	0.48
17:U:28:LEU:HA	17:U:42:PHE:HA	1.96	0.48
36:d:127:ASP:N	36:d:127:ASP:OD1	2.46	0.48
50:s:362:THR:OG1	50:s:363:ASP:N	2.47	0.48
4:H:85:ASP:OD1	54:A:1126:G:O2'	2.26	0.48
10:N:198:MET:HA	10:N:201:ASP:HB2	1.94	0.48
49:r:92:PHE:CE1	49:r:107:LEU:HD21	2.48	0.48
50:s:336:THR:HA	50:s:339:GLN:NE2	2.27	0.48
54:A:187:U:H2'	54:A:188:G:C8	2.49	0.48
54:A:212:A:N1	54:A:221:A:O2'	2.38	0.48
54:A:283:A:O2'	54:A:793:A:OP1	2.31	0.48
54:A:1359:A:H4'	54:A:1360:A:C8	2.48	0.48
2:E:301:ASP:N	2:E:301:ASP:OD2	2.45	0.48
5:I:133:PRO:O	5:I:137:ASP:HB2	2.14	0.48
9:M:62:ARG:HB2	41:i:128:ARG:HH11	1.78	0.48
21:Y:230:LYS:NZ	54:A:10:A:OP2	2.46	0.48
24:l:42:THR:HG22	24:l:57:VAL:HG22	1.96	0.48
34:b:27:GLN:O	34:b:61:VAL:HA	2.13	0.48
54:A:455:C:H42	54:A:470:G:H22	1.62	0.48
28:5:204:VAL:O	28:5:228:ALA:HA	2.14	0.48
30:7:198:ASN:O	30:7:201:SER:OG	2.27	0.48
51:u:92:PHE:HA	51:u:96:MET:HG3	1.96	0.48
52:v:54:GLN:HG2	52:v:57:LYS:HE2	1.96	0.48
1:D:146:SER:HB3	28:5:262:ILE:HG13	1.95	0.47
1:D:197:GLU:HA	1:D:204:ALA:HA	1.96	0.47
3:F:160:SER:HB3	41:i:80:LEU:HD13	1.95	0.47
9:M:17:ARG:HH11	40:h:115:SER:HB2	1.79	0.47
36:d:198:ARG:HB2	36:d:211:GLN:HB3	1.94	0.47
44:l:114:SER:OG	44:l:115:ARG:N	2.46	0.47
46:o:30:ARG:HH12	54:A:484:A:H5'	1.78	0.47
54:A:223:A:H4'	54:A:224:G:H5'	1.96	0.47
54:A:923:G:N2	54:A:962:A:OP2	2.33	0.47
10:N:191:SER:OG	10:N:192:ARG:N	2.46	0.47
15:S:178:LYS:HD3	15:S:178:LYS:HA	1.66	0.47
19:W:143:LYS:HZ2	29:6:345:VAL:HG21	1.79	0.47
28:5:358:GLN:HB3	28:5:373:LEU:HB2	1.95	0.47
30:7:271:ARG:HB3	30:7:273:SER:H	1.79	0.47
40:h:120:MET:HE2	40:h:120:MET:HB3	1.82	0.47
54:A:484:A:O2'	54:A:485:A:H5'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:A:512:G:N3	54:A:529:A:O2'	2.45	0.47
54:A:1129:U:H2'	54:A:1130:U:C6	2.48	0.47
3:F:206:LEU:HD21	3:F:210:ARG:HH11	1.78	0.47
8:L:129:LYS:HE2	8:L:129:LYS:HB2	1.64	0.47
9:M:130:GLN:HA	9:M:131:PRO:HD3	1.78	0.47
12:P:169:GLY:HA2	47:p:187:ARG:HH11	1.79	0.47
15:S:133:VAL:HG11	15:S:154:VAL:HG11	1.95	0.47
15:S:136:VAL:HG21	15:S:154:VAL:HG21	1.96	0.47
20:X:89:GLN:HA	20:X:102:LYS:HA	1.96	0.47
34:b:9:ARG:HB3	34:b:113:ILE:HD11	1.95	0.47
52:v:14:ARG:HH22	53:w:116:VAL:HG13	1.79	0.47
54:A:49:G:H2'	54:A:50:C:H6	1.80	0.47
54:A:1057:C:H2'	54:A:1058:C:C6	2.49	0.47
2:E:79:PRO:HD2	2:E:322:ASP:HB2	1.97	0.47
12:P:134:GLN:HE22	29:6:136:ARG:HG2	1.78	0.47
19:W:63:ALA:O	54:A:1190:G:O2'	2.25	0.47
28:5:246:GLU:HA	28:5:249:LYS:NZ	2.29	0.47
32:9:16:ASP:OD1	32:9:17:ARG:N	2.47	0.47
32:9:28:ARG:N	54:A:668:A:OP1	2.47	0.47
51:u:125:VAL:HB	51:u:177:ILE:HG22	1.96	0.47
54:A:314:A:H8	54:A:317:G:N2	2.12	0.47
54:A:1411:A:H2'	54:A:1412:G:C8	2.49	0.47
11:O:57:GLU:OE1	11:O:105:THR:OG1	2.31	0.47
21:Y:128:SER:OG	21:Y:131:ARG:NE	2.44	0.47
29:6:233:LEU:HB3	29:6:298:PHE:CE1	2.48	0.47
49:r:92:PHE:HE1	49:r:107:LEU:HD21	1.79	0.47
51:u:144:LYS:HE2	51:u:144:LYS:HB3	1.79	0.47
54:A:1178:A:H2'	54:A:1179:G:C8	2.49	0.47
30:7:218:THR:HG23	30:7:255:HIS:CE1	2.50	0.47
31:8:101:ARG:NH2	37:e:82:SER:OG	2.33	0.47
44:l:119:ARG:HG2	44:l:123:LYS:HE3	1.96	0.47
50:s:150:LEU:HD23	50:s:410:VAL:HG11	1.97	0.47
54:A:1289:G:N2	54:A:1295:A:N6	2.36	0.47
3:F:168:LYS:NZ	39:g:90:ARG:HH22	2.13	0.47
4:H:123:LEU:HA	4:H:128:LEU:HB2	1.97	0.47
9:M:45:ARG:NH1	54:A:599:G:O6	2.36	0.47
11:O:26:ILE:HD12	13:Q:264:TRP:CD1	2.50	0.47
17:U:49:THR:HG22	32:9:38:ALA:HB1	1.97	0.47
18:V:72:LYS:HG3	18:V:91:LEU:HD21	1.96	0.47
19:W:62:HIS:HA	19:W:94:GLU:HG2	1.96	0.47
22:Z:35:LYS:HB3	54:A:449:U:H1'	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:193:LEU:HD12	50:s:190:PRO:HA	1.97	0.47
30:7:52:LYS:HG2	30:7:219:LEU:HD21	1.97	0.47
31:8:101:ARG:NH1	37:e:79:ILE:O	2.47	0.47
34:b:118:PRO:HD2	34:b:119:PHE:CE1	2.50	0.47
35:c:41:PHE:HE2	41:i:36:LEU:HD13	1.78	0.47
54:A:314:A:H8	54:A:317:G:H21	1.63	0.47
54:A:455:C:N4	54:A:470:G:H22	2.13	0.47
54:A:1447:C:H2'	54:A:1448:U:C6	2.50	0.47
2:E:52:HIS:CE1	30:7:305:HIS:O	2.68	0.47
8:L:109:GLU:HG3	8:L:115:VAL:HG22	1.95	0.47
14:R:126:GLU:HA	15:S:66:LEU:HD11	1.97	0.47
29:6:183:ASP:N	29:6:183:ASP:OD1	2.46	0.47
40:h:139:LYS:HG3	40:h:143:LEU:HD23	1.96	0.47
52:v:47:ASP:OD2	52:v:47:ASP:N	2.46	0.47
4:H:98:LEU:HD22	4:H:102:VAL:HG21	1.97	0.47
13:Q:120:THR:HA	13:Q:131:SER:O	2.15	0.47
13:Q:154:VAL:HG23	13:Q:158:GLN:C	2.40	0.47
17:U:61:TYR:HE2	21:Y:67:PHE:CZ	2.33	0.47
20:X:56:ASN:N	20:X:56:ASN:OD1	2.47	0.47
28:5:63:LYS:HD3	28:5:65:HIS:CE1	2.50	0.47
30:7:94:HIS:NE2	36:d:279:THR:OG1	2.34	0.47
50:s:166:TYR:HA	54:A:746:U:H3	1.79	0.47
2:E:81:LYS:NZ	2:E:322:ASP:OD1	2.47	0.47
5:I:80:ARG:HB2	5:I:84:ARG:HH12	1.80	0.47
5:I:168:LEU:HD11	5:I:174:LEU:HD23	1.96	0.47
9:M:94:LYS:N	9:M:137:GLY:O	2.48	0.47
19:W:95:GLY:HA3	19:W:134:VAL:O	2.15	0.47
32:9:23:SER:OG	32:9:23:SER:O	2.32	0.47
43:k:39:SER:OG	43:k:40:GLU:N	2.48	0.47
46:o:30:ARG:NH1	54:A:484:A:OP2	2.45	0.47
2:E:318:THR:OG1	2:E:319:TYR:N	2.48	0.46
5:I:115:GLN:HE22	5:I:167:ILE:HD12	1.79	0.46
10:N:101:HIS:HA	10:N:104:MET:HE3	1.96	0.46
11:O:53:ARG:HH11	11:O:107:MET:HE3	1.79	0.46
12:P:41:ASN:HD21	29:6:293:LEU:HD23	1.81	0.46
13:Q:277:LYS:H	13:Q:277:LYS:HD2	1.80	0.46
35:c:148:MET:HE2	35:c:148:MET:HB3	1.83	0.46
54:A:980:C:H2'	54:A:981:A:C8	2.50	0.46
8:L:118:ARG:HH12	51:u:189:GLU:HG2	1.80	0.46
15:S:97:ALA:HA	15:S:135:LEU:O	2.15	0.46
18:V:72:LYS:NZ	18:V:73:GLN:O	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:X:121:LYS:HE2	28:5:51:GLU:HG2	1.97	0.46
31:8:150:LEU:HB2	37:e:212:HIS:CE1	2.49	0.46
35:c:138:THR:O	35:c:142:GLU:HG2	2.15	0.46
43:k:19:GLN:HE21	43:k:63:CYS:HB3	1.79	0.46
2:E:275:ARG:O	2:E:284:TYR:HB2	2.14	0.46
9:M:133:LYS:HZ3	54:A:219:C:H5'	1.80	0.46
11:O:58:LYS:HD2	13:Q:269:MET:HB3	1.97	0.46
35:c:216:ARG:HA	35:c:220:ILE:HD12	1.97	0.46
37:e:160:LEU:HD11	37:e:264:LEU:HD11	1.96	0.46
40:h:137:ARG:HE	40:h:141:ASP:C	2.21	0.46
41:i:93:ARG:HH22	54:A:68:U:H5'	1.80	0.46
54:A:1511:U:OP2	54:A:1512:A:O2'	2.24	0.46
6:J:18:GLY:N	6:J:72:VAL:O	2.47	0.46
9:M:96:LEU:HD21	9:M:101:LEU:HB2	1.97	0.46
17:U:52:ASP:O	17:U:56:TYR:HB2	2.15	0.46
19:W:148:LEU:HD23	29:6:341:VAL:HG21	1.96	0.46
23:O:93:ARG:NH2	54:A:640:G:OP2	2.48	0.46
31:8:120:LYS:HA	31:8:120:LYS:HD3	1.72	0.46
36:d:137:PHE:HA	36:d:140:LYS:HE3	1.97	0.46
37:e:91:ALA:O	37:e:95:ASN:ND2	2.36	0.46
55:B:1639:U:H2'	55:B:1640:A:C8	2.51	0.46
3:F:59:ARG:NH1	3:F:88:ALA:O	2.46	0.46
3:F:92:ARG:NH2	54:A:208:U:O3'	2.49	0.46
21:Y:86:THR:OG1	21:Y:89:GLN:NE2	2.45	0.46
29:6:230:ALA:HB2	29:6:299:ARG:HE	1.80	0.46
32:9:96:VAL:HG12	32:9:100:ILE:HG12	1.97	0.46
36:d:262:HIS:CD2	36:d:263:THR:HG23	2.50	0.46
42:j:29:LEU:HD21	42:j:35:ALA:HB2	1.97	0.46
52:v:12:LEU:HD21	52:v:59:LEU:HD23	1.97	0.46
1:D:92:ARG:HD2	54:A:854:A:C2	2.51	0.46
5:I:95:MET:HA	5:I:181:ILE:HA	1.97	0.46
22:Z:135:SER:HA	42:j:71:GLU:OE2	2.16	0.46
30:7:193:MET:HE1	30:7:285:ASN:HD21	1.80	0.46
54:A:184:U:O2'	54:A:186:A:OP1	2.20	0.46
54:A:454:A:H5'	54:A:455:C:O5'	2.16	0.46
54:A:472:A:C8	54:A:591:C:H5''	2.50	0.46
1:D:253:ASN:ND2	54:A:861:U:O4'	2.45	0.46
9:M:19:LEU:HD23	9:M:19:LEU:HA	1.73	0.46
9:M:185:ASP:OD1	54:A:218:G:N2	2.49	0.46
10:N:139:ARG:HA	54:A:1312:C:H5''	1.97	0.46
14:R:11:ARG:HB2	54:A:622:G:C8	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:1:35:ASN:OD1	24:1:38:ARG:NH1	2.45	0.46
54:A:640:G:N2	54:A:641:U:O4	2.27	0.46
54:A:1384:G:H2'	54:A:1385:U:C6	2.50	0.46
2:E:104:LEU:HB2	2:E:121:LEU:HB2	1.98	0.46
5:I:44:ARG:O	5:I:48:MET:HG2	2.16	0.46
9:M:142:GLU:OE2	9:M:160:SER:OG	2.29	0.46
11:O:106:ARG:O	11:O:123:ILE:HA	2.16	0.46
12:P:157:SER:OG	55:B:1640:A:OP1	2.31	0.46
17:U:19:VAL:HG23	32:9:58:PRO:HB3	1.97	0.46
24:1:20:MET:O	24:1:29:CYS:HA	2.16	0.46
34:b:15:LEU:HD11	35:c:169:VAL:HA	1.98	0.46
36:d:267:PRO:HG2	36:d:270:ALA:HB2	1.97	0.46
39:g:140:VAL:HG22	46:o:85:HIS:ND1	2.31	0.46
53:w:114:ASP:HA	53:w:117:GLU:HG3	1.98	0.46
1:D:184:LEU:HA	1:D:187:LEU:HD13	1.97	0.46
9:M:296:SER:HA	47:p:42:ILE:HD13	1.98	0.46
11:O:120:MET:HE3	11:O:120:MET:HB3	1.73	0.46
21:Y:83:ALA:N	32:9:74:VAL:O	2.48	0.46
25:2:59:LYS:NZ	54:A:311:G:OP2	2.44	0.46
28:5:85:PRO:HG3	54:A:743:C:H4'	1.98	0.46
50:s:345:PHE:CD1	50:s:351:VAL:HA	2.51	0.46
51:u:106:ALA:HB2	51:u:138:MET:HE1	1.98	0.46
54:A:79:C:OP2	54:A:1229:C:O2'	2.34	0.46
3:F:76:ARG:NH1	40:h:111:VAL:HG21	2.31	0.46
13:Q:225:LYS:O	13:Q:229:TRP:NE1	2.34	0.46
27:4:92:CYS:HG	27:4:98:HIS:CE1	2.34	0.46
30:7:46:ASP:O	30:7:50:LYS:HG2	2.16	0.46
39:g:120:LEU:HD22	39:g:147:LEU:HD13	1.98	0.46
51:u:95:ASP:OD1	51:u:96:MET:N	2.49	0.46
53:w:141:PRO:HA	53:w:144:ILE:HD12	1.97	0.46
14:R:17:ARG:NH2	54:A:195:C:OP2	2.48	0.45
20:X:116:SER:O	20:X:120:ASP:CA	2.64	0.45
26:3:168:ARG:NH2	54:A:220:C:OP2	2.49	0.45
34:b:35:ARG:O	34:b:44:ARG:NH1	2.49	0.45
43:k:39:SER:OG	43:k:40:GLU:OE1	2.34	0.45
43:k:66:VAL:HB	43:k:74:LEU:HB2	1.97	0.45
1:D:107:ILE:HD11	1:D:139:ILE:HG21	1.98	0.45
4:H:72:ARG:HH22	26:3:100:ARG:NH2	2.14	0.45
7:K:5:SER:HB2	7:K:8:PRO:HD2	1.97	0.45
8:L:37:ARG:HH22	8:L:56:ARG:HD2	1.80	0.45
16:T:190:LYS:O	33:a:108:MET:HE1	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:5:356:VAL:HG12	28:5:375:TRP:HB2	1.99	0.45
41:i:61:GLY:HA3	54:A:216:G:H1	1.82	0.45
50:s:184:LEU:HA	50:s:184:LEU:HD23	1.80	0.45
1:D:85:ARG:NH2	54:A:252:C:O2'	2.50	0.45
12:P:85:ARG:HD2	12:P:158:MET:HE2	1.97	0.45
13:Q:282:ILE:O	13:Q:286:ILE:HG12	2.16	0.45
15:S:175:ARG:HB2	15:S:180:PHE:HB3	1.97	0.45
17:U:64:PRO:HB2	17:U:100:ALA:HB3	1.98	0.45
29:6:240:ILE:HG12	29:6:248:GLY:HA3	1.98	0.45
49:r:93:ILE:HD13	49:r:93:ILE:HA	1.76	0.45
50:s:115:LEU:HB2	50:s:394:TRP:CD1	2.50	0.45
54:A:324:A:H61	54:A:1066:C:H4'	1.80	0.45
54:A:920:A:H2'	54:A:921:A:C8	2.51	0.45
54:A:1288:A:N6	54:A:1293:A:O2'	2.49	0.45
7:K:133:ILE:HB	7:K:138:LEU:HD21	1.98	0.45
13:Q:118:ARG:HA	13:Q:133:PHE:O	2.17	0.45
14:R:20:ARG:O	14:R:23:GLU:HB2	2.17	0.45
17:U:46:MET:HE1	17:U:72:VAL:HG13	1.97	0.45
19:W:125:VAL:O	29:6:37:ASN:ND2	2.48	0.45
28:5:158:ILE:O	28:5:162:ARG:HB3	2.15	0.45
29:6:280:ASP:OD1	29:6:280:ASP:N	2.48	0.45
37:e:203:LYS:N	37:e:237:LEU:O	2.48	0.45
49:r:168:ARG:HG2	49:r:171:ARG:HH11	1.82	0.45
50:s:228:ASP:O	50:s:230:ARG:NH1	2.49	0.45
51:u:127:VAL:HG23	51:u:179:LEU:HA	1.98	0.45
52:v:9:VAL:HG12	52:v:55:LEU:HD13	1.99	0.45
3:F:86:VAL:HG13	3:F:87:PHE:CD2	2.52	0.45
4:H:72:ARG:HH22	26:3:100:ARG:HH22	1.65	0.45
5:I:100:GLN:HE21	5:I:100:GLN:CA	2.29	0.45
8:L:51:TYR:CZ	8:L:78:LYS:HA	2.51	0.45
28:5:107:PHE:HB3	28:5:222:VAL:HG12	1.98	0.45
34:b:26:LEU:HD21	34:b:29:LEU:HD11	1.97	0.45
39:g:43:ASP:OD2	39:g:43:ASP:N	2.49	0.45
50:s:198:ALA:HB2	50:s:243:ILE:HG13	1.98	0.45
54:A:1167:A:H2'	54:A:1168:A:C8	2.52	0.45
3:F:291:SER:HB3	39:g:54:ALA:HA	1.99	0.45
5:I:36:HIS:ND1	5:I:37:ARG:O	2.49	0.45
17:U:61:TYR:OH	21:Y:110:ASN:ND2	2.26	0.45
19:W:76:HIS:HB2	19:W:130:PHE:CD1	2.51	0.45
28:5:223:ARG:NH2	54:A:739:A:O3'	2.50	0.45
28:5:297:ALA:HB3	28:5:303:ARG:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:7:143:TRP:CE2	30:7:179:PHE:HB3	2.52	0.45
32:9:24:LYS:NZ	54:A:752:U:OP2	2.50	0.45
35:c:202:LEU:HD21	35:c:211:THR:HA	1.98	0.45
36:d:129:ASP:OD1	36:d:130:ALA:N	2.50	0.45
39:g:88:ARG:NH1	39:g:92:HIS:O	2.49	0.45
48:q:112:GLN:HA	48:q:115:ARG:HG2	1.99	0.45
7:K:69:GLY:HA2	49:r:152:THR:HG22	1.99	0.45
9:M:287:ASP:HB3	9:M:290:LEU:HD12	1.98	0.45
11:O:14:VAL:HG21	54:A:1487:C:C4	2.52	0.45
17:U:16:GLN:HE21	32:9:59:GLU:HG3	1.81	0.45
17:U:80:ARG:NH2	17:U:84:ASN:OD1	2.50	0.45
19:W:76:HIS:HB2	19:W:130:PHE:CE1	2.52	0.45
37:e:52:CYS:HB3	37:e:235:LYS:HD2	1.98	0.45
37:e:139:GLU:HG2	37:e:152:LYS:HA	1.99	0.45
50:s:373:GLN:HB3	50:s:392:ILE:HB	1.99	0.45
52:v:31:TYR:O	52:v:35:ILE:HD12	2.16	0.45
5:I:132:LYS:HA	5:I:135:LEU:HD12	1.98	0.45
12:P:172:LEU:HD23	12:P:172:LEU:HA	1.84	0.45
22:Z:73:LYS:HB3	22:Z:116:LEU:HA	1.98	0.45
28:5:122:TRP:HA	28:5:253:LEU:HD23	1.99	0.45
37:e:161:VAL:HG23	37:e:174:PRO:HG3	1.99	0.45
42:j:61:LYS:NZ	54:A:588:A:OP1	2.41	0.45
44:l:123:LYS:HA	44:l:126:ILE:HG22	1.98	0.45
54:A:362:G:O2'	54:A:1195:C:O2	2.28	0.45
54:A:523:U:O4	54:A:526:A:N1	2.49	0.45
54:A:1025:G:OP1	54:A:1271:G:O2'	2.32	0.45
5:I:31:LYS:O	5:I:38:ARG:NH1	2.48	0.45
19:W:147:MET:C	29:6:338:ARG:HH21	2.24	0.45
26:3:173:VAL:HG23	26:3:174:ASP:H	1.80	0.45
28:5:244:GLU:O	28:5:248:THR:HG23	2.17	0.45
39:g:76:ARG:NH2	39:g:164:LYS:O	2.50	0.45
54:A:1292:C:H42	54:A:1346:G:N2	2.14	0.45
3:F:291:SER:HA	39:g:52:LEU:HD23	1.99	0.45
9:M:46:GLY:HA2	9:M:49:CYS:HA	1.99	0.45
12:P:105:ALA:C	12:P:128:ILE:HD11	2.42	0.45
13:Q:83:ARG:HG3	13:Q:143:ARG:HG3	1.99	0.45
14:R:94:GLN:HE21	42:j:33:LEU:HD11	1.81	0.45
41:i:88:LEU:O	41:i:92:ILE:HG13	2.17	0.45
48:q:116:GLU:HA	48:q:119:GLN:HG3	1.99	0.45
50:s:222:ARG:HH21	54:A:664:C:H5'	1.82	0.45
2:E:177:LYS:HB3	2:E:298:LYS:HD2	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:26:ALA:HB1	6:J:57:THR:HG23	1.99	0.44
31:8:133:ARG:HH12	55:B:1626:C:H4'	1.81	0.44
33:a:71:HIS:ND1	34:b:138:THR:OG1	2.45	0.44
36:d:169:PHE:O	36:d:173:THR:OG1	2.34	0.44
37:e:52:CYS:HB2	37:e:173:LEU:HD21	1.99	0.44
40:h:153:LYS:HA	40:h:153:LYS:HD3	1.81	0.44
41:i:92:ILE:HG22	41:i:96:LYS:HE3	1.99	0.44
47:p:175:LEU:HD23	47:p:179:ARG:HG3	1.99	0.44
51:u:97:MET:HG2	51:u:100:LEU:HD12	1.98	0.44
54:A:109:A:O2'	54:A:110:U:H5''	2.17	0.44
55:B:1621:A:H61	55:B:1645:A:H3'	1.82	0.44
5:I:61:HIS:HB2	49:r:78:LYS:HZ1	1.82	0.44
8:L:39:ARG:HH21	13:Q:158:GLN:NE2	2.14	0.44
9:M:169:LYS:HD3	47:p:144:PHE:HZ	1.82	0.44
28:5:31:TYR:HD1	54:A:851:A:C6	2.35	0.44
28:5:300:ARG:NH2	54:A:725:A:OP2	2.49	0.44
50:s:153:GLU:OE1	50:s:153:GLU:N	2.50	0.44
51:u:199:TYR:HE1	52:v:60:VAL:HG21	1.82	0.44
4:H:84:GLU:OE1	20:X:44:ARG:NH2	2.40	0.44
10:N:228:LYS:HD3	22:Z:78:ARG:NH2	2.31	0.44
15:S:126:GLU:OE1	42:j:51:TYR:HE1	2.01	0.44
20:X:168:ARG:HH21	28:5:53:PRO:HB2	1.81	0.44
21:Y:69:ASP:HA	21:Y:111:MET:HE3	1.98	0.44
28:5:145:ASN:HA	28:5:194:LYS:NZ	2.32	0.44
34:b:35:ARG:HG3	40:h:158:TYR:CE2	2.51	0.44
54:A:785:U:H2'	54:A:786:U:C6	2.53	0.44
54:A:789:A:N6	54:A:998:A:O2'	2.50	0.44
3:F:110:SER:O	3:F:110:SER:OG	2.33	0.44
15:S:163:LYS:HB2	34:b:106:ASP:HB3	1.99	0.44
20:X:55:LYS:HB3	20:X:55:LYS:HE2	1.77	0.44
23:O:137:ILE:O	23:O:141:ILE:HG12	2.17	0.44
29:6:233:LEU:HB3	29:6:298:PHE:HE1	1.83	0.44
31:8:164:ARG:HH12	38:f:86:TYR:C	2.25	0.44
41:i:105:ASP:OD1	41:i:105:ASP:N	2.48	0.44
51:u:192:LYS:O	51:u:196:LEU:N	2.49	0.44
3:F:103:GLN:HE22	3:F:250:VAL:H	1.66	0.44
9:M:45:ARG:NH2	54:A:599:G:N7	2.51	0.44
11:O:130:LEU:HD23	11:O:130:LEU:HA	1.81	0.44
22:Z:148:GLN:HB3	22:Z:150:HIS:CE1	2.53	0.44
47:p:186:GLU:HA	47:p:189:ARG:NH1	2.32	0.44
53:w:85:TYR:HA	53:w:88:LYS:HG2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:A:1347:C:O2'	54:A:1351:C:N4	2.44	0.44
1:D:155:GLU:OE1	1:D:250:VAL:HB	2.18	0.44
3:F:86:VAL:HG23	3:F:175:LYS:HG2	1.99	0.44
3:F:280:TYR:OH	9:M:109:ARG:HD2	2.17	0.44
6:J:47:ASN:OD1	6:J:48:GLN:N	2.51	0.44
7:K:8:PRO:HG2	35:c:295:GLU:HG3	2.00	0.44
16:T:108:PHE:HB3	23:0:118:GLN:HE21	1.81	0.44
25:2:52:GLU:OE1	54:A:249:C:H1'	2.18	0.44
47:p:186:GLU:HG2	47:p:189:ARG:NH2	2.33	0.44
54:A:1520:A:H2'	54:A:1521:A:H8	1.82	0.44
2:E:170:LEU:HD23	2:E:170:LEU:HA	1.84	0.44
7:K:36:SER:O	7:K:40:GLN:HG3	2.18	0.44
16:T:51:TRP:CD1	16:T:76:CYS:HB3	2.53	0.44
17:U:26:ILE:HG21	17:U:26:ILE:HD13	1.81	0.44
19:W:55:LYS:HE2	19:W:61:VAL:HG22	2.00	0.44
54:A:1447:C:H2'	54:A:1448:U:H6	1.82	0.44
11:O:38:ARG:HG3	11:O:85:LEU:HD21	2.00	0.44
28:5:73:PRO:HG2	28:5:75:PHE:CE1	2.53	0.44
34:b:28:ARG:NE	34:b:78:GLU:OE1	2.39	0.44
35:c:238:MET:HE1	35:c:293:GLU:HG2	2.00	0.44
36:d:52:THR:OG1	36:d:53:GLU:N	2.51	0.44
38:f:97:ALA:HB3	38:f:103:ALA:HB2	1.99	0.44
47:p:113:GLU:HA	47:p:116:ARG:HB2	2.00	0.44
54:A:1219:C:N4	54:A:1220:U:O4	2.50	0.44
6:J:66:LEU:HB3	6:J:82:ILE:HD11	1.99	0.44
16:T:53:LYS:HB2	16:T:53:LYS:HE3	1.84	0.44
24:1:42:THR:O	48:q:135:TRP:NE1	2.43	0.44
30:7:37:PRO:HA	30:7:40:LEU:HB2	1.99	0.44
30:7:51:GLU:OE1	30:7:54:ARG:NE	2.51	0.44
30:7:133:CYS:SG	30:7:134:ASP:N	2.91	0.44
47:p:118:LYS:HB2	47:p:161:ALA:HB1	1.99	0.44
54:A:842:A:O2'	54:A:871:C:OP1	2.27	0.44
25:2:85:LYS:HE2	54:A:123:G:O6	2.18	0.43
28:5:257:TYR:CD2	28:5:258:PRO:HA	2.52	0.43
29:6:175:VAL:HG21	29:6:270:PHE:HD2	1.83	0.43
30:7:166:LEU:HD23	30:7:181:TYR:HE1	1.83	0.43
34:b:26:LEU:HD23	34:b:61:VAL:HG11	2.00	0.43
54:A:1503:G:H2'	54:A:1504:U:O4'	2.17	0.43
54:A:1520:A:H2'	54:A:1521:A:C8	2.52	0.43
4:H:98:LEU:HD13	4:H:102:VAL:HB	2.00	0.43
17:U:65:VAL:HG13	17:U:97:VAL:HG13	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:V:22:GLY:HA2	18:V:85:TRP:HZ3	1.83	0.43
20:X:8:VAL:HG21	21:Y:210:ARG:NH1	2.33	0.43
20:X:118:ILE:HD11	20:X:191:TYR:CD2	2.53	0.43
25:2:53:TYR:CZ	25:2:55:PRO:HB3	2.53	0.43
32:9:33:ARG:HE	32:9:33:ARG:HB2	1.63	0.43
33:a:105:GLU:O	33:a:108:MET:HB3	2.18	0.43
54:A:360:U:C4	54:A:454:A:C6	2.99	0.43
54:A:1058:C:H2'	54:A:1059:U:C6	2.53	0.43
14:R:79:HIS:ND1	33:a:44:ASN:O	2.45	0.43
34:b:27:GLN:HE21	34:b:80:LEU:HA	1.83	0.43
43:k:63:CYS:HA	43:k:76:MET:O	2.17	0.43
46:o:67:ARG:NH2	54:A:412:G:N7	2.47	0.43
49:r:150:TYR:OH	54:A:571:A:OP1	2.28	0.43
50:s:357:SER:OG	50:s:358:GLN:N	2.51	0.43
55:B:1615:A:H2'	55:B:1616:A:C8	2.53	0.43
1:D:130:ARG:N	1:D:139:ILE:O	2.51	0.43
9:M:119:THR:HG22	9:M:123:ASN:ND2	2.29	0.43
14:R:128:PHE:CE2	54:A:574:U:H2'	2.52	0.43
15:S:165:GLU:HB3	15:S:187:THR:HG22	2.00	0.43
16:T:105:GLN:NE2	23:0:104:LYS:O	2.37	0.43
17:U:44:ILE:HD13	17:U:44:ILE:HA	1.79	0.43
23:0:106:ASN:OD1	54:A:1542:C:O2'	2.25	0.43
24:1:20:MET:CB	24:1:30:PHE:O	2.66	0.43
37:e:162:ARG:HD3	37:e:171:TRP:HE3	1.83	0.43
48:q:113:LYS:HB3	48:q:113:LYS:HE3	1.70	0.43
6:J:128:GLU:HA	6:J:133:GLN:HE21	1.83	0.43
8:L:64:ASN:N	8:L:64:ASN:OD1	2.50	0.43
15:S:122:LEU:O	15:S:163:LYS:NZ	2.47	0.43
18:V:124:ASP:HB2	18:V:127:ASP:HB2	2.00	0.43
28:5:127:LYS:HB3	28:5:373:LEU:HD13	1.99	0.43
30:7:150:MET:HB2	30:7:278:TYR:OH	2.18	0.43
35:c:220:ILE:HG23	35:c:223:MET:HE3	2.01	0.43
36:d:156:ASP:HB3	36:d:159:ARG:NH2	2.34	0.43
3:F:282:PRO:HB3	3:F:286:PHE:CZ	2.54	0.43
12:P:128:ILE:HA	12:P:128:ILE:HD12	1.85	0.43
16:T:133:ASN:HD22	36:d:226:ASP:CG	2.26	0.43
23:0:102:LYS:HA	23:0:102:LYS:HD2	1.84	0.43
28:5:341:VAL:HA	28:5:357:PHE:O	2.18	0.43
30:7:117:LYS:HE3	30:7:220:GLU:HB2	2.00	0.43
43:k:21:CYS:SG	43:k:56:ARG:NE	2.91	0.43
54:A:47:U:H2'	54:A:48:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:A:634:G:H2'	54:A:635:U:O4'	2.18	0.43
54:A:1055:A:H62	54:A:1320:A:H61	1.67	0.43
15:S:122:LEU:HD21	42:j:49:TRP:CH2	2.53	0.43
20:X:157:PHE:HE1	28:5:52:ILE:HD11	1.84	0.43
23:0:169:ASP:HA	23:0:172:LYS:HG3	2.01	0.43
28:5:111:CYS:SG	28:5:266:HIS:ND1	2.91	0.43
54:A:446:C:O2'	54:A:1167:A:N3	2.43	0.43
9:M:229:PHE:HE2	9:M:259:ARG:HH12	1.65	0.43
13:Q:120:THR:HG22	13:Q:132:GLN:HB3	2.00	0.43
19:W:70:GLN:HG3	19:W:72:HIS:O	2.19	0.43
20:X:230:TYR:HB3	32:9:92:PHE:CD2	2.54	0.43
28:5:281:GLU:OE2	28:5:281:GLU:N	2.51	0.43
28:5:391:VAL:HG13	28:5:398:VAL:HB	2.01	0.43
30:7:218:THR:HG23	30:7:255:HIS:HE1	1.84	0.43
44:l:115:ARG:NH1	54:A:522:A:OP1	2.50	0.43
47:p:75:ARG:HG2	47:p:110:TRP:HE1	1.84	0.43
54:A:1370:G:H1'	54:A:1399:A:N3	2.34	0.43
2:E:65:VAL:HG21	2:E:155:PHE:CZ	2.53	0.43
2:E:296:LEU:HD23	2:E:296:LEU:HA	1.85	0.43
9:M:205:LEU:HG	9:M:263:ARG:NH1	2.34	0.43
13:Q:224:MET:HG3	13:Q:243:ILE:HG23	2.00	0.43
18:V:49:ILE:HG21	18:V:54:TRP:HE3	1.83	0.43
24:1:17:LEU:HA	24:1:32:THR:O	2.18	0.43
28:5:125:LYS:HE2	28:5:371:LYS:HG2	2.01	0.43
30:7:160:ASP:OD1	30:7:160:ASP:N	2.52	0.43
30:7:276:PHE:HD2	30:7:277:GLN:HG3	1.84	0.43
31:8:121:TRP:HZ3	55:B:1628:C:H4'	1.84	0.43
36:d:160:LEU:O	36:d:164:VAL:HG12	2.19	0.43
54:A:461:A:OP1	54:A:463:A:N6	2.43	0.43
54:A:1074:U:O2'	54:A:1075:A:O5'	2.31	0.43
1:D:181:ALA:HB2	1:D:243:THR:HG22	2.01	0.43
1:D:231:LYS:HE3	1:D:231:LYS:HB2	1.89	0.43
5:I:181:ILE:O	5:I:184:THR:OG1	2.24	0.43
7:K:21:LEU:HD23	7:K:59:ILE:HG12	2.01	0.43
10:N:104:MET:HE3	10:N:104:MET:HB3	1.83	0.43
10:N:188:LYS:NZ	10:N:198:MET:SD	2.80	0.43
10:N:218:ILE:HA	10:N:223:MET:HG3	2.00	0.43
15:S:99:VAL:HG22	15:S:133:VAL:HG22	2.01	0.43
15:S:142:THR:HG23	33:a:62:HIS:NE2	2.34	0.43
24:1:18:VAL:O	24:1:31:ASN:HA	2.19	0.43
30:7:107:LEU:HD23	30:7:107:LEU:HA	1.91	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:8:121:TRP:CZ3	55:B:1628:C:H4'	2.54	0.43
36:d:119:GLN:HA	36:d:122:ILE:HD12	2.01	0.43
51:u:101:LEU:HD13	51:u:127:VAL:HG11	2.00	0.43
52:v:14:ARG:NH2	53:w:116:VAL:HG13	2.34	0.43
18:V:54:TRP:HE1	18:V:79:VAL:HG11	1.84	0.42
24:1:25:GLY:H	48:q:121:ILE:HG23	1.82	0.42
28:5:79:ASP:OD2	28:5:79:ASP:N	2.49	0.42
28:5:305:GLN:HB2	28:5:308:GLN:OE1	2.18	0.42
37:e:205:LEU:HD22	38:f:171:LEU:HD11	2.01	0.42
52:v:31:TYR:O	52:v:34:SER:OG	2.24	0.42
3:F:165:LEU:HB2	3:F:170:ARG:HD3	2.01	0.42
6:J:31:PRO:HB2	6:J:34:PRO:HG2	2.00	0.42
9:M:233:ARG:HB3	9:M:244:LEU:HD11	1.99	0.42
17:U:137:ARG:HG2	18:V:104:TYR:CD1	2.54	0.42
18:V:179:VAL:HG21	32:9:77:LEU:HD12	2.01	0.42
20:X:110:PHE:O	20:X:126:THR:HA	2.19	0.42
20:X:161:LEU:O	20:X:165:MET:HG2	2.19	0.42
21:Y:185:VAL:HG21	54:A:37:C:C4	2.55	0.42
23:O:138:ARG:NH1	54:A:651:A:OP1	2.51	0.42
36:d:83:GLY:O	36:d:262:HIS:NE2	2.52	0.42
40:h:78:PHE:HE1	40:h:96:LEU:HB3	1.83	0.42
51:u:118:MET:O	51:u:120:TYR:N	2.50	0.42
51:u:197:ARG:HG2	52:v:66:LEU:HD13	2.01	0.42
54:A:72:G:O2'	54:A:84:G:O6	2.26	0.42
1:D:202:ARG:HE	1:D:205:GLN:HE22	1.68	0.42
1:D:207:ILE:H	1:D:207:ILE:HG13	1.54	0.42
2:E:145:LEU:HD23	2:E:145:LEU:HA	1.78	0.42
2:E:204:VAL:HG12	2:E:206:VAL:HG23	2.01	0.42
2:E:222:TRP:CD1	2:E:256:LYS:HB3	2.54	0.42
3:F:287:SER:HB3	41:i:66:PHE:O	2.19	0.42
9:M:44:ARG:HD3	9:M:45:ARG:HD2	2.01	0.42
15:S:201:ALA:HA	15:S:202:PRO:HD3	1.87	0.42
16:T:72:GLU:HG2	16:T:179:VAL:HG22	2.00	0.42
20:X:53:ASN:OD1	20:X:53:ASN:N	2.49	0.42
21:Y:86:THR:HG1	21:Y:89:GLN:HE21	1.63	0.42
28:5:91:PRO:HB3	28:5:95:GLU:HB3	2.01	0.42
29:6:224:HIS:CD2	29:6:226:LEU:H	2.37	0.42
44:l:120:ARG:NH2	54:A:520:C:OP1	2.51	0.42
50:s:92:MET:SD	50:s:276:ARG:HD3	2.60	0.42
54:A:1357:U:O4	54:A:1358:A:N6	2.52	0.42
1:D:113:ARG:HG3	1:D:147:ARG:NH1	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:257:MET:SD	54:A:1042:G:N2	2.93	0.42
10:N:202:GLN:O	10:N:206:GLU:HG3	2.19	0.42
11:O:122:VAL:HG11	11:O:133:LEU:HD11	2.02	0.42
28:5:230:LEU:HB2	28:5:292:TYR:HE2	1.83	0.42
30:7:102:LYS:HB3	30:7:102:LYS:HE2	1.81	0.42
30:7:216:PHE:HE1	30:7:257:ILE:HG12	1.83	0.42
35:c:34:GLY:HA3	54:A:605:U:H5''	2.01	0.42
35:c:96:CYS:SG	35:c:182:GLU:HG2	2.60	0.42
50:s:242:ARG:HA	50:s:295:GLY:HA2	2.01	0.42
50:s:271:LEU:HD12	50:s:272:PRO:HD2	2.01	0.42
53:w:139:MET:HE2	53:w:139:MET:HB3	1.98	0.42
54:A:1200:G:H8	54:A:1200:G:H5''	1.85	0.42
5:I:167:ILE:HG13	5:I:168:LEU:HD22	2.00	0.42
9:M:84:ASN:ND2	26:3:111:ILE:O	2.47	0.42
28:5:113:LEU:HD22	28:5:119:GLN:HG2	2.01	0.42
35:c:226:LYS:HE3	35:c:226:LYS:HB3	1.75	0.42
47:p:78:ILE:HG12	47:p:101:VAL:HG22	2.02	0.42
50:s:66:TRP:O	50:s:69:THR:OG1	2.29	0.42
51:u:199:TYR:CE1	52:v:60:VAL:HG21	2.54	0.42
5:I:99:CYS:HB3	5:I:152:MET:HE3	2.02	0.42
5:I:119:HIS:ND1	5:I:160:LYS:HE3	2.34	0.42
8:L:128:ARG:NH2	51:u:120:TYR:O	2.53	0.42
9:M:59:ARG:NH1	54:A:346:C:OP2	2.52	0.42
16:T:109:ASN:HD21	23:0:101:ILE:HD13	1.84	0.42
18:V:41:ARG:NH2	54:A:130:G:N7	2.59	0.42
24:1:16:ILE:HD11	24:1:36:ARG:HA	2.01	0.42
38:f:163:SER:O	38:f:167:ALA:N	2.40	0.42
50:s:78:GLU:O	50:s:82:ILE:HG12	2.20	0.42
52:v:20:GLY:O	52:v:28:ARG:NH2	2.53	0.42
54:A:844:C:H2'	54:A:845:U:C6	2.52	0.42
3:F:280:TYR:CD1	9:M:125:ARG:HD2	2.55	0.42
4:H:64:LEU:H	4:H:64:LEU:HD23	1.85	0.42
6:J:145:ILE:HG23	6:J:155:VAL:HG21	2.02	0.42
27:4:95:HIS:HB2	27:4:98:HIS:CE1	2.54	0.42
29:6:175:VAL:HG21	29:6:270:PHE:CD2	2.55	0.42
34:b:44:ARG:O	34:b:48:GLU:HG3	2.19	0.42
35:c:49:ARG:NE	54:A:141:A:N1	2.67	0.42
54:A:1007:A:H2'	54:A:1008:A:C8	2.55	0.42
4:H:131:TYR:CD2	20:X:139:TYR:HA	2.52	0.42
4:H:138:LYS:HA	4:H:141:GLU:CD	2.44	0.42
15:S:167:TRP:H	15:S:167:TRP:CD1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:65:ASN:ND2	54:A:1191:A:H4'	2.35	0.42
19:W:73:PHE:CE2	19:W:87:LYS:HD3	2.55	0.42
20:X:7:PRO:HD2	20:X:10:LEU:HD13	2.01	0.42
21:Y:234:LEU:HD23	21:Y:234:LEU:HA	1.78	0.42
23:O:156:THR:HG22	23:O:173:ARG:HG2	2.02	0.42
30:7:175:ILE:H	30:7:175:ILE:HD12	1.85	0.42
35:c:104:LYS:HA	35:c:104:LYS:HD3	1.76	0.42
37:e:123:MET:HA	37:e:126:GLN:HG2	2.02	0.42
47:p:45:LEU:HD23	47:p:45:LEU:HA	1.89	0.42
47:p:132:GLU:N	47:p:132:GLU:OE1	2.53	0.42
52:v:6:ARG:HH12	52:v:10:LEU:HD11	1.84	0.42
54:A:742:A:H2'	54:A:743:C:C6	2.55	0.42
1:D:211:GLY:H	1:D:247:VAL:HG13	1.85	0.42
7:K:39:LEU:HD11	7:K:125:LEU:HD12	2.01	0.42
12:P:49:THR:HG21	29:6:228:PRO:HB3	2.02	0.42
16:T:68:ARG:HH11	36:d:230:ARG:HH11	1.68	0.42
30:7:276:PHE:CD2	30:7:277:GLN:HG3	2.55	0.42
36:d:248:PHE:HA	36:d:261:MET:HA	2.02	0.42
51:u:158:LYS:NZ	54:A:1448:U:O2'	2.36	0.42
51:u:166:ASP:OD1	51:u:167:TRP:N	2.48	0.42
54:A:901:G:H1	54:A:916:U:H3	1.67	0.42
2:E:103:LYS:NZ	2:E:291:GLY:O	2.52	0.42
2:E:295:CYS:SG	2:E:296:LEU:N	2.93	0.42
3:F:108:ARG:HG2	3:F:161:TYR:CD1	2.55	0.42
4:H:79:VAL:HG11	20:X:91:TYR:CE2	2.55	0.42
9:M:212:PRO:HD3	48:q:103:LEU:HD11	2.02	0.42
28:5:236:LEU:HD21	28:5:289:HIS:HD2	1.85	0.42
48:q:88:GLU:HA	48:q:91:GLU:HG3	2.00	0.42
54:A:201:A:C5	54:A:232:C:N4	2.88	0.42
2:E:221:ARG:HA	2:E:261:MET:SD	2.59	0.41
3:F:137:ARG:H	3:F:137:ARG:HG2	1.54	0.41
5:I:98:VAL:HG13	5:I:177:LEU:HB2	2.02	0.41
5:I:125:VAL:HG22	54:A:524:U:N3	2.34	0.41
9:M:176:THR:HG22	9:M:214:TYR:HE1	1.85	0.41
16:T:117:ILE:HD13	16:T:117:ILE:HG21	1.83	0.41
20:X:121:LYS:HB3	20:X:121:LYS:HE3	1.72	0.41
20:X:124:THR:O	20:X:124:THR:OG1	2.36	0.41
20:X:189:ASP:HA	20:X:192:LYS:HB3	2.00	0.41
27:4:68:ASN:HD21	54:A:1356:U:C5'	2.30	0.41
29:6:218:LEU:HB3	29:6:234:HIS:HB2	2.02	0.41
33:a:104:GLU:HB3	33:a:105:GLU:H	1.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:e:152:LYS:HZ3	37:e:256:THR:HG21	1.85	0.41
40:h:88:ASP:OD1	40:h:124:ARG:NH2	2.53	0.41
54:A:564:C:HO2'	54:A:1018:C:HO2'	1.56	0.41
5:I:99:CYS:HB2	5:I:154:LEU:HD11	2.01	0.41
9:M:94:LYS:HB2	9:M:129:ILE:HG22	2.01	0.41
9:M:189:LYS:HE3	9:M:189:LYS:HB2	1.83	0.41
10:N:183:LEU:HD23	10:N:183:LEU:HA	1.83	0.41
17:U:126:LEU:HD11	36:d:76:ILE:HD12	2.01	0.41
19:W:148:LEU:O	29:6:338:ARG:NH2	2.53	0.41
23:0:117:LYS:HG3	23:0:118:GLN:O	2.20	0.41
28:5:210:SER:OG	28:5:274:LYS:NZ	2.48	0.41
29:6:219:THR:HA	29:6:232:TYR:O	2.20	0.41
29:6:255:LEU:HD23	29:6:255:LEU:HA	1.91	0.41
30:7:149:MET:HE1	30:7:275:CYS:SG	2.60	0.41
50:s:103:ASP:OD1	50:s:325:ARG:HD2	2.20	0.41
54:A:53:A:H3'	54:A:54:A:H4'	2.02	0.41
1:D:126:VAL:HG13	1:D:140:ALA:HB1	2.01	0.41
1:D:164:LEU:O	1:D:180:ASP:HB2	2.21	0.41
2:E:248:ILE:HG22	2:E:250:ARG:HG2	2.01	0.41
3:F:262:THR:O	3:F:265:THR:OG1	2.34	0.41
7:K:63:ARG:NH1	7:K:130:ASP:OD1	2.36	0.41
9:M:104:LEU:HA	9:M:104:LEU:HD23	1.87	0.41
20:X:147:LYS:HB3	20:X:147:LYS:HE2	1.83	0.41
20:X:208:LEU:O	20:X:212:ILE:HG12	2.19	0.41
30:7:36:SER:HB2	30:7:39:GLU:OE1	2.19	0.41
41:i:74:ILE:HD11	41:i:82:GLY:N	2.35	0.41
41:i:87:GLU:HG2	41:i:117:LEU:HD11	2.03	0.41
46:o:12:ILE:HD13	46:o:12:ILE:HA	1.89	0.41
50:s:150:LEU:HD21	50:s:402:TYR:CD1	2.55	0.41
54:A:960:U:H2'	54:A:961:G:C8	2.55	0.41
54:A:1473:U:O4	54:A:1474:A:N6	2.53	0.41
15:S:169:ARG:NH2	54:A:475:G:OP1	2.53	0.41
20:X:176:LEU:HD13	20:X:188:TYR:CE2	2.56	0.41
21:Y:99:HIS:ND1	32:9:63:PRO:HG3	2.35	0.41
22:Z:78:ARG:O	22:Z:83:LYS:NZ	2.53	0.41
34:b:2:THR:HG21	54:A:160:G:H5''	2.02	0.41
39:g:68:THR:HG22	39:g:72:TRP:O	2.20	0.41
46:o:30:ARG:NH1	54:A:483:A:H2'	2.35	0.41
50:s:51:MET:SD	50:s:61:ARG:HG2	2.59	0.41
1:D:61:ALA:O	1:D:63:PHE:N	2.53	0.41
1:D:105:ARG:HH21	1:D:130:ARG:HH22	1.66	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:198:PHE:C	2:E:199:ARG:HD2	2.44	0.41
3:F:234:THR:OG1	3:F:242:LEU:HD23	2.21	0.41
9:M:182:ARG:O	9:M:186:ILE:HD12	2.20	0.41
10:N:81:GLU:CD	10:N:199:ARG:HH12	2.29	0.41
17:U:134:ARG:HA	17:U:137:ARG:HG3	2.03	0.41
47:p:128:ASN:OD1	47:p:129:ARG:N	2.45	0.41
49:r:71:PRO:HA	49:r:74:ARG:HE	1.84	0.41
54:A:191:U:H2'	54:A:192:U:C6	2.54	0.41
54:A:544:A:H2'	54:A:545:C:C6	2.55	0.41
54:A:1204:A:H2'	54:A:1205:A:O4'	2.21	0.41
1:D:274:ARG:HB2	54:A:322:C:C4	2.56	0.41
5:I:56:PRO:HG3	10:N:208:ASN:HB3	2.02	0.41
5:I:123:MET:SD	5:I:123:MET:N	2.94	0.41
8:L:136:LYS:NZ	51:u:167:TRP:HB3	2.36	0.41
9:M:98:LEU:HA	9:M:98:LEU:HD23	1.77	0.41
12:P:169:GLY:HA2	47:p:187:ARG:NH1	2.35	0.41
20:X:227:PHE:CE1	32:9:119:PHE:HB2	2.55	0.41
21:Y:171:ASP:OD2	21:Y:175:ARG:NH1	2.44	0.41
30:7:146:CYS:HB3	30:7:179:PHE:CZ	2.56	0.41
30:7:302:LEU:HD23	30:7:302:LEU:HA	1.88	0.41
35:c:86:ASP:N	35:c:86:ASP:OD1	2.53	0.41
35:c:96:CYS:SG	35:c:97:TYR:N	2.94	0.41
37:e:47:LEU:HB3	37:e:178:TRP:CE2	2.56	0.41
37:e:200:MET:HA	37:e:241:GLY:HA2	2.02	0.41
51:u:150:LYS:HG3	51:u:151:CYS:H	1.85	0.41
54:A:912:A:OP2	54:A:913:C:N4	2.54	0.41
2:E:101:ALA:O	2:E:297:VAL:HG12	2.21	0.41
7:K:144:GLU:OE1	34:b:146:ARG:NH2	2.54	0.41
9:M:32:GLY:O	54:A:206:U:O2'	2.32	0.41
10:N:94:GLY:HA2	10:N:154:VAL:O	2.21	0.41
15:S:175:ARG:HH21	54:A:592:C:H1'	1.86	0.41
20:X:113:GLU:OE2	20:X:124:THR:HG22	2.21	0.41
21:Y:78:LYS:HE3	21:Y:78:LYS:HB2	1.86	0.41
24:1:16:ILE:O	24:1:33:LYS:HA	2.20	0.41
30:7:67:VAL:HG11	30:7:119:LEU:HD13	2.03	0.41
30:7:315:LYS:HA	30:7:315:LYS:HD3	1.83	0.41
36:d:220:GLN:O	36:d:239:PRO:HA	2.21	0.41
47:p:123:HIS:CG	47:p:157:MET:HE2	2.55	0.41
50:s:250:PHE:CE2	50:s:371:CYS:HB3	2.56	0.41
52:v:40:ARG:HH21	53:w:113:LEU:HD21	1.84	0.41
54:A:711:A:H2'	54:A:712:A:C8	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:A:817:A:H2'	54:A:818:C:O4'	2.21	0.41
54:A:929:U:OP2	54:A:955:C:N4	2.54	0.41
54:A:1228:U:H2'	54:A:1229:C:O4'	2.21	0.41
54:A:1359:A:H4'	54:A:1360:A:H8	1.85	0.41
55:B:1665:C:H2'	55:B:1666:U:C6	2.56	0.41
1:D:198:SER:HB2	1:D:206:TYR:HE2	1.86	0.41
1:D:200:PRO:HG2	1:D:237:LEU:HD23	2.01	0.41
3:F:216:VAL:HG22	3:F:258:THR:OG1	2.19	0.41
5:I:119:HIS:CE1	5:I:158:GLU:HG2	2.56	0.41
7:K:107:ALA:O	7:K:111:MET:HG2	2.21	0.41
11:O:52:MET:HE3	11:O:52:MET:HB3	1.53	0.41
20:X:102:LYS:HE2	20:X:102:LYS:HB3	1.83	0.41
22:Z:38:ARG:NH1	54:A:405:U:OP1	2.47	0.41
35:c:83:PHE:CE2	35:c:202:LEU:HB2	2.56	0.41
35:c:301:LEU:HD23	35:c:301:LEU:HA	1.81	0.41
37:e:162:ARG:HD3	37:e:171:TRP:CE3	2.56	0.41
39:g:98:LYS:HD2	39:g:154:ASP:OD2	2.21	0.41
41:i:48:ASN:HB3	41:i:51:ARG:H	1.86	0.41
48:q:50:TRP:CZ2	54:A:91:A:H2'	2.56	0.41
50:s:273:LEU:HD12	50:s:273:LEU:HA	1.93	0.41
54:A:1198:C:H2'	54:A:1199:A:O4'	2.21	0.41
1:D:113:ARG:HG3	1:D:147:ARG:HH12	1.86	0.41
3:F:159:THR:HG22	41:i:90:ARG:CZ	2.51	0.41
6:J:84:GLN:HE22	6:J:124:LYS:HG3	1.86	0.41
9:M:56:GLU:HG2	54:A:345:G:H5'	2.03	0.41
9:M:68:GLU:CD	9:M:73:PRO:HA	2.46	0.41
14:R:65:ARG:HH21	14:R:99:ARG:CZ	2.34	0.41
17:U:111:PHE:HZ	21:Y:127:PRO:HD3	1.86	0.41
18:V:21:TYR:HB2	18:V:83:ARG:HD3	2.01	0.41
23:O:167:GLU:HA	23:O:170:GLN:HG2	2.03	0.41
24:1:16:ILE:HD11	24:1:36:ARG:HG2	2.02	0.41
29:6:27:ARG:N	54:A:402:A:H5''	2.35	0.41
29:6:216:LEU:HD22	29:6:235:TRP:CZ3	2.56	0.41
31:8:139:MET:HE3	31:8:143:GLN:HE21	1.86	0.41
34:b:27:GLN:NE2	34:b:80:LEU:HD23	2.35	0.41
34:b:77:ALA:HB2	34:b:104:LEU:HD23	2.03	0.41
36:d:128:TYR:CZ	36:d:208:VAL:HG21	2.56	0.41
37:e:74:LEU:HA	37:e:77:ILE:HG12	2.03	0.41
39:g:117:ILE:HD13	39:g:142:GLU:HA	2.02	0.41
41:i:35:ARG:HA	54:A:6:A:H4'	2.01	0.41
48:q:94:PRO:HG2	48:q:99:MET:HE3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
50:s:332:LEU:HD13	50:s:372:TYR:HB2	2.03	0.41
51:u:159:ILE:HG23	51:u:168:LEU:HD21	2.02	0.41
53:w:124:ASP:N	53:w:124:ASP:OD1	2.53	0.41
54:A:49:G:H2'	54:A:50:C:C6	2.56	0.41
54:A:1458:A:O2'	54:A:1459:A:O4'	2.38	0.41
1:D:91:ILE:HG21	1:D:91:ILE:HD13	1.83	0.41
6:J:39:LEU:HB3	6:J:44:VAL:HG21	2.02	0.41
11:O:149:LEU:HA	11:O:149:LEU:HD23	1.86	0.41
15:S:128:ILE:HG21	15:S:128:ILE:HD13	1.77	0.41
18:V:181:ASP:HA	18:V:184:GLU:OE2	2.21	0.41
19:W:90:TYR:CZ	54:A:1203:A:H4'	2.55	0.41
24:l:15:ASN:OD1	24:l:35:ASN:ND2	2.53	0.41
30:7:281:SER:N	30:7:298:GLN:O	2.52	0.41
36:d:198:ARG:HA	36:d:198:ARG:HD3	1.93	0.41
38:f:49:LYS:HB2	54:A:1162:A:C8	2.56	0.41
50:s:276:ARG:HD3	50:s:276:ARG:HH21	1.63	0.41
54:A:200:A:O2'	54:A:201:A:O5'	2.37	0.41
54:A:455:C:H5'	54:A:593:C:O2'	2.21	0.41
54:A:889:U:H4'	54:A:890:G:O5'	2.21	0.41
54:A:1054:G:H2'	54:A:1318:C:O2'	2.21	0.41
2:E:48:TRP:CD1	2:E:50:ASP:H	2.39	0.40
5:I:47:LEU:O	5:I:51:THR:OG1	2.33	0.40
8:L:144:PHE:CE1	51:u:120:TYR:HB2	2.56	0.40
9:M:154:ILE:HG22	9:M:156:VAL:HG13	2.02	0.40
12:P:120:ARG:HD2	12:P:120:ARG:HA	1.87	0.40
14:R:102:LEU:HD23	14:R:102:LEU:HA	1.81	0.40
15:S:85:GLU:HA	15:S:88:VAL:HG22	2.03	0.40
23:0:87:ILE:O	23:0:91:ARG:HB2	2.20	0.40
37:e:235:LYS:HZ3	37:e:276:VAL:HG22	1.86	0.40
42:j:93:LEU:HD23	42:j:93:LEU:HA	1.92	0.40
49:r:35:PHE:N	49:r:56:THR:HG22	2.36	0.40
49:r:73:CYS:SG	49:r:78:LYS:HE3	2.61	0.40
49:r:133:PRO:HG3	54:A:1521:A:N3	2.36	0.40
54:A:1077:U:H2'	54:A:1078:A:H5'	2.03	0.40
1:D:95:GLY:HA2	1:D:269:ARG:HB2	2.03	0.40
2:E:130:LEU:O	2:E:189:PRO:HB3	2.21	0.40
3:F:58:HIS:CD2	3:F:58:HIS:H	2.40	0.40
5:I:176:LEU:O	5:I:188:ARG:NH1	2.54	0.40
13:Q:100:LEU:HD21	13:Q:286:ILE:HD13	2.03	0.40
15:S:100:HIS:ND1	15:S:100:HIS:O	2.54	0.40
40:h:104:LEU:HD23	40:h:104:LEU:HA	1.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:h:154:ILE:HG22	40:h:156:TRP:NE1	2.36	0.40
41:i:32:ILE:HG22	41:i:34:ILE:H	1.85	0.40
50:s:308:ARG:HB2	50:s:320:ILE:HD13	2.03	0.40
54:A:409:C:H3'	54:A:410:U:O2	2.21	0.40
54:A:1460:A:C5	54:A:1461:G:H1'	2.56	0.40
3:F:142:ARG:NH2	54:A:124:A:OP1	2.41	0.40
3:F:255:LYS:HE3	41:i:47:TRP:CZ3	2.55	0.40
5:I:111:LEU:O	5:I:115:GLN:HG3	2.21	0.40
7:K:48:HIS:HB3	7:K:51:SER:HB3	2.03	0.40
8:L:140:ILE:HD13	8:L:140:ILE:HG21	1.86	0.40
9:M:115:PRO:HG2	9:M:267:PHE:CZ	2.55	0.40
11:O:116:ASP:OD2	54:A:783:G:O2'	2.30	0.40
15:S:158:ALA:HB2	15:S:195:ILE:HG12	2.02	0.40
20:X:119:LEU:HD22	28:5:53:PRO:HD2	2.03	0.40
29:6:221:LEU:HD13	29:6:231:GLU:HG2	2.03	0.40
30:7:79:PHE:HD1	36:d:281:MET:HG2	1.87	0.40
31:8:133:ARG:NH1	55:B:1626:C:H4'	2.36	0.40
36:d:128:TYR:HB2	36:d:252:LEU:HD23	2.02	0.40
36:d:189:LEU:HD12	36:d:217:HIS:HE2	1.85	0.40
40:h:137:ARG:HH21	40:h:142:GLU:HA	1.86	0.40
40:h:144:SER:HA	40:h:148:LEU:HD11	2.04	0.40
50:s:332:LEU:HD21	50:s:359:ALA:HB2	2.03	0.40
55:B:1603:A:H2'	55:B:1604:G:C8	2.57	0.40
1:D:112:PHE:CZ	1:D:167:ASN:HB2	2.57	0.40
2:E:94:SER:OG	2:E:184:ASN:OD1	2.23	0.40
2:E:129:VAL:O	2:E:190:GLY:N	2.54	0.40
3:F:96:LEU:HA	3:F:96:LEU:HD23	1.88	0.40
13:Q:101:GLU:HG2	13:Q:104:LYS:HD2	2.03	0.40
13:Q:190:LEU:HD23	13:Q:190:LEU:HA	1.86	0.40
21:Y:175:ARG:HE	21:Y:175:ARG:HB2	1.69	0.40
24:1:25:GLY:N	48:q:121:ILE:HD12	2.37	0.40
30:7:162:TYR:CD2	30:7:189:LEU:HD11	2.57	0.40
36:d:154:ASN:ND2	36:d:159:ARG:HH12	2.20	0.40
54:A:304:A:H8	54:A:304:A:H2'	1.71	0.40
54:A:370:G:H2'	54:A:371:U:O4'	2.20	0.40
54:A:1074:U:H1'	54:A:1075:A:H8	1.86	0.40
1:D:66:TRP:HZ2	54:A:857:A:H5''	1.86	0.40
1:D:130:ARG:HB3	1:D:139:ILE:HG13	2.03	0.40
7:K:171:THR:HG22	49:r:59:GLU:H	1.85	0.40
7:K:177:ARG:NH1	54:A:1513:U:O2	2.54	0.40
8:L:113:ASN:OD1	8:L:136:LYS:NZ	2.38	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:M:257:CYS:HA	47:p:59:TRP:CH2	2.56	0.40
13:Q:154:VAL:HA	13:Q:159:GLY:HA2	2.03	0.40
15:S:122:LEU:HD23	15:S:122:LEU:HA	1.78	0.40
17:U:151:PHE:HD1	36:d:222:LEU:HD11	1.86	0.40
21:Y:171:ASP:OD1	21:Y:171:ASP:N	2.52	0.40
23:O:138:ARG:HB3	54:A:651:A:N3	2.36	0.40
30:7:52:LYS:HE2	30:7:52:LYS:HB3	1.85	0.40
30:7:113:TRP:NE1	30:7:117:LYS:HB3	2.36	0.40
30:7:130:PHE:HD2	30:7:305:HIS:HD2	1.68	0.40
39:g:84:TYR:CD1	39:g:120:LEU:HD12	2.57	0.40
40:h:117:LEU:HD12	40:h:117:LEU:HA	1.77	0.40
46:o:75:LYS:HG3	54:A:384:U:C5	2.56	0.40
51:u:145:MET:O	51:u:149:LEU:HB2	2.21	0.40
54:A:48:A:H2'	54:A:49:G:O4'	2.21	0.40
54:A:510:A:O2'	54:A:536:C:O3'	2.39	0.40
54:A:1464:C:H6	54:A:1464:C:H2'	1.73	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	234/305 (77%)	209 (89%)	23 (10%)	2 (1%)	14	47
2	E	302/348 (87%)	272 (90%)	30 (10%)	0	100	100
3	F	248/311 (80%)	231 (93%)	17 (7%)	0	100	100
4	H	93/267 (35%)	89 (96%)	4 (4%)	0	100	100
5	I	154/261 (59%)	141 (92%)	13 (8%)	0	100	100
6	J	138/192 (72%)	128 (93%)	10 (7%)	0	100	100
7	K	175/178 (98%)	164 (94%)	11 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	L	113/145 (78%)	105 (93%)	8 (7%)	0	100	100
9	M	285/296 (96%)	269 (94%)	16 (6%)	0	100	100
10	N	203/251 (81%)	189 (93%)	14 (7%)	0	100	100
11	O	150/175 (86%)	143 (95%)	7 (5%)	0	100	100
12	P	139/180 (77%)	129 (93%)	10 (7%)	0	100	100
13	Q	215/292 (74%)	200 (93%)	15 (7%)	0	100	100
14	R	138/149 (93%)	130 (94%)	8 (6%)	0	100	100
15	S	154/205 (75%)	142 (92%)	12 (8%)	0	100	100
16	T	155/206 (75%)	150 (97%)	5 (3%)	0	100	100
17	U	135/153 (88%)	125 (93%)	10 (7%)	0	100	100
18	V	188/216 (87%)	180 (96%)	8 (4%)	0	100	100
19	W	107/148 (72%)	99 (92%)	8 (8%)	0	100	100
20	X	241/256 (94%)	229 (95%)	12 (5%)	0	100	100
21	Y	174/250 (70%)	169 (97%)	5 (3%)	0	100	100
22	Z	118/161 (73%)	106 (90%)	12 (10%)	0	100	100
23	0	106/188 (56%)	99 (93%)	7 (7%)	0	100	100
24	1	50/65 (77%)	46 (92%)	4 (8%)	0	100	100
25	2	41/92 (45%)	40 (98%)	1 (2%)	0	100	100
26	3	93/188 (50%)	87 (94%)	6 (6%)	0	100	100
27	4	34/103 (33%)	33 (97%)	1 (3%)	0	100	100
28	5	383/423 (90%)	353 (92%)	30 (8%)	0	100	100
29	6	316/380 (83%)	296 (94%)	20 (6%)	0	100	100
30	7	285/338 (84%)	263 (92%)	22 (8%)	0	100	100
31	8	97/206 (47%)	91 (94%)	6 (6%)	0	100	100
32	9	113/137 (82%)	107 (95%)	6 (5%)	0	100	100
33	a	69/142 (49%)	67 (97%)	2 (3%)	0	100	100
34	b	146/215 (68%)	128 (88%)	18 (12%)	0	100	100
35	c	271/332 (82%)	254 (94%)	17 (6%)	0	100	100
36	d	203/306 (66%)	187 (92%)	16 (8%)	0	100	100
37	e	211/279 (76%)	194 (92%)	17 (8%)	0	100	100
38	f	110/212 (52%)	102 (93%)	8 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
39	g	127/166 (76%)	116 (91%)	11 (9%)	0	100	100
40	h	96/158 (61%)	93 (97%)	3 (3%)	0	100	100
41	i	95/128 (74%)	87 (92%)	8 (8%)	0	100	100
42	j	83/123 (68%)	80 (96%)	3 (4%)	0	100	100
43	k	76/112 (68%)	72 (95%)	4 (5%)	0	100	100
44	l	21/138 (15%)	21 (100%)	0	0	100	100
45	m	43/128 (34%)	37 (86%)	6 (14%)	0	100	100
46	o	91/102 (89%)	83 (91%)	8 (9%)	0	100	100
47	p	119/206 (58%)	114 (96%)	5 (4%)	0	100	100
48	q	162/222 (73%)	156 (96%)	6 (4%)	0	100	100
49	r	140/196 (71%)	131 (94%)	9 (6%)	0	100	100
50	s	366/439 (83%)	349 (95%)	17 (5%)	0	100	100
51	u	109/234 (47%)	99 (91%)	10 (9%)	0	100	100
52	v	67/70 (96%)	67 (100%)	0	0	100	100
53	w	77/156 (49%)	71 (92%)	6 (8%)	0	100	100
All	All	8059/11129 (72%)	7522 (93%)	535 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	271	ASN
1	D	207	ILE

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	190/245 (78%)	190 (100%)	0	100	100
2	E	259/290 (89%)	259 (100%)	0	100	100
3	F	217/262 (83%)	217 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	140 (99%)	1 (1%)	76	78
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	4	35/89 (39%)	35 (100%)	0	100	100
28	5	348/368 (95%)	348 (100%)	0	100	100
29	6	265/332 (80%)	265 (100%)	0	100	100
30	7	263/303 (87%)	263 (100%)	0	100	100
31	8	91/190 (48%)	91 (100%)	0	100	100
32	9	99/112 (88%)	98 (99%)	1 (1%)	68	75
33	a	69/133 (52%)	69 (100%)	0	100	100
34	b	130/186 (70%)	130 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
35	c	241/288 (84%)	241 (100%)	0	100	100
36	d	193/274 (70%)	193 (100%)	0	100	100
37	e	188/236 (80%)	188 (100%)	0	100	100
38	f	101/188 (54%)	101 (100%)	0	100	100
39	g	119/148 (80%)	119 (100%)	0	100	100
40	h	95/148 (64%)	95 (100%)	0	100	100
41	i	86/110 (78%)	86 (100%)	0	100	100
42	j	68/97 (70%)	68 (100%)	0	100	100
43	k	71/90 (79%)	71 (100%)	0	100	100
44	l	23/116 (20%)	23 (100%)	0	100	100
45	m	40/113 (35%)	40 (100%)	0	100	100
46	o	79/87 (91%)	79 (100%)	0	100	100
47	p	117/181 (65%)	117 (100%)	0	100	100
48	q	141/178 (79%)	141 (100%)	0	100	100
49	r	133/169 (79%)	133 (100%)	0	100	100
50	s	326/381 (86%)	326 (100%)	0	100	100
51	u	105/200 (52%)	105 (100%)	0	100	100
52	v	59/60 (98%)	59 (100%)	0	100	100
53	w	73/136 (54%)	73 (100%)	0	100	100
All	All	7239/9609 (75%)	7237 (100%)	2 (0%)	100	100

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
15	S	118	ASN
32	9	113	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (71) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	252	HIS
1	D	276	HIS
2	E	115	GLN
2	E	280	HIS

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Mol	Chain	Res	Type
3	F	208	HIS
3	F	228	GLN
5	I	61	HIS
5	I	189	GLN
5	I	193	ASN
7	K	9	GLN
7	K	160	GLN
8	L	48	ASN
8	L	80	GLN
9	M	102	GLN
9	M	123	ASN
10	N	202	GLN
11	O	109	GLN
12	P	87	GLN
12	P	147	GLN
13	Q	172	GLN
13	Q	237	ASN
14	R	22	GLN
14	R	36	ASN
16	T	133	ASN
16	T	210	HIS
17	U	16	GLN
17	U	55	ASN
18	V	92	ASN
19	W	80	HIS
19	W	107	HIS
20	X	94	ASN
20	X	108	GLN
21	Y	73	ASN
22	Z	150	HIS
23	0	115	HIS
23	0	170	GLN
28	5	65	HIS
28	5	94	HIS
28	5	165	GLN
28	5	186	GLN
28	5	191	GLN
28	5	214	ASN
28	5	372	ASN
29	6	277	GLN
29	6	292	GLN
30	7	232	HIS

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Mol	Chain	Res	Type
30	7	247	ASN
34	b	24	GLN
34	b	66	ASN
35	c	65	ASN
35	c	310	ASN
36	d	196	GLN
36	d	274	GLN
37	e	67	GLN
37	e	212	HIS
38	f	115	ASN
40	h	151	ASN
43	k	19	GLN
45	m	65	HIS
47	p	143	GLN
47	p	152	GLN
48	q	81	GLN
49	r	96	HIS
50	s	319	GLN
50	s	358	GLN
50	s	373	GLN
50	s	375	ASN
50	s	427	ASN
51	u	113	GLN
53	w	80	GLN
53	w	142	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
54	A	1460/1559 (93%)	490 (33%)	35 (2%)
55	B	51/69 (73%)	13 (25%)	1 (1%)
All	All	1511/1628 (92%)	503 (33%)	36 (2%)

All (503) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
54	A	4	A
54	A	6	A
54	A	8	C
54	A	9	U
54	A	11	G

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Mol	Chain	Res	Type
54	A	19	C
54	A	23	C
54	A	24	U
54	A	29	C
54	A	30	U
54	A	34	U
54	A	38	A
54	A	39	G
54	A	43	A
54	A	44	C
54	A	45	C
54	A	46	U
54	A	47	U
54	A	54	A
54	A	57	A
54	A	58	U
54	A	61	A
54	A	62	C
54	A	71	A
54	A	78	G
54	A	80	G
54	A	81	A
54	A	90	G
54	A	100	G
54	A	107	A
54	A	110	U
54	A	111	A
54	A	116	C
54	A	121	G
54	A	122	G
54	A	124	A
54	A	125	A
54	A	133	A
54	A	134	A
54	A	135	A
54	A	136	U
54	A	137	U
54	A	138	A
54	A	139	U
54	A	140	A
54	A	142	C
54	A	147	C

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Mol	Chain	Res	Type
54	A	150	A
54	A	153	A
54	A	154	U
54	A	157	C
54	A	158	A
54	A	159	A
54	A	162	A
54	A	166	A
54	A	169	C
54	A	170	C
54	A	174	A
54	A	177	U
54	A	179	C
54	A	184	U
54	A	185	A
54	A	186	A
54	A	197	A
54	A	198	G
54	A	199	A
54	A	200	A
54	A	201	A
54	A	202	U
54	A	203	A
54	A	204	A
54	A	208	U
54	A	212	A
54	A	213	G
54	A	216	G
54	A	217	A
54	A	218	G
54	A	222	A
54	A	223	A
54	A	230	A
54	A	231	C
54	A	232	C
54	A	233	C
54	A	245	C
54	A	248	G
54	A	257	G
54	A	264	U
54	A	265	A
54	A	269	G

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Mol	Chain	Res	Type
54	A	270	A
54	A	274	C
54	A	278	C
54	A	281	C
54	A	286	U
54	A	287	A
54	A	288	G
54	A	296	G
54	A	298	G
54	A	304	A
54	A	305	U
54	A	315	G
54	A	316	A
54	A	317	G
54	A	319	C
54	A	321	A
54	A	322	C
54	A	323	A
54	A	324	A
54	A	325	A
54	A	329	A
54	A	330	C
54	A	332	G
54	A	336	C
54	A	342	A
54	A	343	U
54	A	345	G
54	A	346	C
54	A	349	G
54	A	351	U
54	A	352	G
54	A	355	C
54	A	356	A
54	A	359	A
54	A	361	A
54	A	362	G
54	A	363	A
54	A	366	C
54	A	367	U
54	A	368	U
54	A	369	A
54	A	371	U

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Mol	Chain	Res	Type
54	A	374	A
54	A	383	U
54	A	385	U
54	A	389	C
54	A	391	C
54	A	395	A
54	A	404	A
54	A	408	C
54	A	409	C
54	A	410	U
54	A	413	U
54	A	415	A
54	A	422	C
54	A	423	U
54	A	426	U
54	A	427	A
54	A	428	G
54	A	429	U
54	A	439	A
54	A	443	G
54	A	447	U
54	A	454	A
54	A	456	U
54	A	457	A
54	A	459	G
54	A	461	A
54	A	462	A
54	A	464	A
54	A	465	A
54	A	466	C
54	A	471	U
54	A	472	A
54	A	477	G
54	A	480	U
54	A	484	A
54	A	487	U
54	A	488	U
54	A	489	U
54	A	490	A
54	A	493	A
54	A	495	C
54	A	496	C

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Mol	Chain	Res	Type
54	A	498	U
54	A	499	A
54	A	501	U
54	A	502	A
54	A	503	G
54	A	504	G
54	A	510	A
54	A	511	A
54	A	512	G
54	A	513	C
54	A	514	A
54	A	516	C
54	A	517	C
54	A	520	C
54	A	522	A
54	A	523	U
54	A	524	U
54	A	525	A
54	A	527	G
54	A	528	A
54	A	530	A
54	A	532	C
54	A	534	U
54	A	540	C
54	A	541	U
54	A	546	A
54	A	560	A
54	A	563	U
54	A	564	C
54	A	567	A
54	A	569	A
54	A	571	A
54	A	572	U
54	A	573	A
54	A	575	A
54	A	576	A
54	A	577	C
54	A	592	C
54	A	593	C
54	A	594	A
54	A	610	C
54	A	611	A

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Mol	Chain	Res	Type
54	A	612	C
54	A	615	U
54	A	620	A
54	A	625	C
54	A	627	A
54	A	629	U
54	A	630	G
54	A	631	U
54	A	635	U
54	A	639	A
54	A	645	A
54	A	647	G
54	A	651	A
54	A	652	C
54	A	654	U
54	A	661	C
54	A	664	C
54	A	665	A
54	A	672	U
54	A	675	G
54	A	678	A
54	A	679	G
54	A	694	C
54	A	695	U
54	A	699	A
54	A	700	A
54	A	701	U
54	A	702	U
54	A	704	A
54	A	705	C
54	A	711	A
54	A	716	C
54	A	717	U
54	A	718	A
54	A	720	A
54	A	723	C
54	A	726	C
54	A	731	A
54	A	734	U
54	A	735	C
54	A	737	U
54	A	744	C

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Mol	Chain	Res	Type
54	A	746	U
54	A	748	A
54	A	756	C
54	A	762	A
54	A	764	A
54	A	774	A
54	A	776	A
54	A	777	A
54	A	781	A
54	A	792	A
54	A	808	G
54	A	810	A
54	A	811	A
54	A	813	U
54	A	814	C
54	A	815	U
54	A	818	C
54	A	823	C
54	A	832	C
54	A	837	A
54	A	838	C
54	A	841	C
54	A	849	G
54	A	850	C
54	A	851	A
54	A	852	U
54	A	853	C
54	A	854	A
54	A	856	C
54	A	857	A
54	A	860	A
54	A	861	U
54	A	866	G
54	A	869	A
54	A	870	C
54	A	874	C
54	A	876	G
54	A	887	C
54	A	888	A
54	A	889	U
54	A	890	G
54	A	893	U

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Mol	Chain	Res	Type
54	A	900	C
54	A	904	G
54	A	911	A
54	A	913	C
54	A	920	A
54	A	922	G
54	A	923	G
54	A	924	U
54	A	929	U
54	A	930	A
54	A	931	A
54	A	933	C
54	A	936	U
54	A	937	U
54	A	948	U
54	A	949	A
54	A	954	C
54	A	956	U
54	A	957	G
54	A	958	U
54	A	959	A
54	A	960	U
54	A	962	A
54	A	963	A
54	A	964	U
54	A	965	G
54	A	968	U
54	A	971	A
54	A	975	G
54	A	984	U
54	A	986	U
54	A	990	U
54	A	991	U
54	A	1013	C
54	A	1014	C
54	A	1016	G
54	A	1024	A
54	A	1025	G
54	A	1026	A
54	A	1028	G
54	A	1030	G
54	A	1031	G

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Mol	Chain	Res	Type
54	A	1036	A
54	A	1037	A
54	A	1039	A
54	A	1048	C
54	A	1049	G
54	A	1053	A
54	A	1054	G
54	A	1055	A
54	A	1060	A
54	A	1062	G
54	A	1069	U
54	A	1070	A
54	A	1073	U
54	A	1075	A
54	A	1078	A
54	A	1080	U
54	A	1086	C
54	A	1087	A
54	A	1088	G
54	A	1124	C
54	A	1128	A
54	A	1134	A
54	A	1136	U
54	A	1139	C
54	A	1140	G
54	A	1143	U
54	A	1144	G
54	A	1151	C
54	A	1161	G
54	A	1162	A
54	A	1163	A
54	A	1164	C
54	A	1165	C
54	A	1168	A
54	A	1169	C
54	A	1174	G
54	A	1177	C
54	A	1181	A
54	A	1184	U
54	A	1185	G
54	A	1189	A
54	A	1191	A

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Mol	Chain	Res	Type
54	A	1194	U
54	A	1195	C
54	A	1200	G
54	A	1202	C
54	A	1220	U
54	A	1222	A
54	A	1223	A
54	A	1226	G
54	A	1231	A
54	A	1236	C
54	A	1240	A
54	A	1243	A
54	A	1246	G
54	A	1247	G
54	A	1248	A
54	A	1249	A
54	A	1256	A
54	A	1258	C
54	A	1262	G
54	A	1264	G
54	A	1265	A
54	A	1266	U
54	A	1270	A
54	A	1273	G
54	A	1285	U
54	A	1286	A
54	A	1288	A
54	A	1293	A
54	A	1301	A
54	A	1304	A
54	A	1307	G
54	A	1308	U
54	A	1314	A
54	A	1316	C
54	A	1319	G
54	A	1320	A
54	A	1323	U
54	A	1324	U
54	A	1326	G
54	A	1334	C
54	A	1335	A
54	A	1346	G

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Mol	Chain	Res	Type
54	A	1351	C
54	A	1359	A
54	A	1360	A
54	A	1366	G
54	A	1370	G
54	A	1371	U
54	A	1372	U
54	A	1379	U
54	A	1381	A
54	A	1383	A
54	A	1384	G
54	A	1395	U
54	A	1396	C
54	A	1399	A
54	A	1402	U
54	A	1403	C
54	A	1404	A
54	A	1407	C
54	A	1408	C
54	A	1410	G
54	A	1411	A
54	A	1416	U
54	A	1417	C
54	A	1418	C
54	A	1419	A
54	A	1420	G
54	A	1423	C
54	A	1426	U
54	A	1428	U
54	A	1430	U
54	A	1432	U
54	A	1438	U
54	A	1439	U
54	A	1444	U
54	A	1452	U
54	A	1453	G
54	A	1458	A
54	A	1459	A
54	A	1461	G
54	A	1466	A
54	A	1471	A
54	A	1480	U

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Mol	Chain	Res	Type
54	A	1485	C
54	A	1486	A
54	A	1487	C
54	A	1488	A
54	A	1492	C
54	A	1498	C
54	A	1499	C
54	A	1501	C
54	A	1502	C
54	A	1507	A
54	A	1510	A
54	A	1511	U
54	A	1513	U
54	A	1514	C
54	A	1519	C
54	A	1520	A
54	A	1526	G
54	A	1532	U
54	A	1537	A
54	A	1543	A
54	A	1547	A
54	A	1548	A
54	A	1553	A
55	B	1607	U
55	B	1608	G
55	B	1609	U
55	B	1610	A
55	B	1611	G
55	B	1614	U
55	B	1615	A
55	B	1640	A
55	B	1641	G
55	B	1644	G
55	B	1645	A
55	B	1649	C
55	B	1651	A

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
54	A	33	C
54	A	57	A

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Mol	Chain	Res	Type
54	A	135	A
54	A	136	U
54	A	137	U
54	A	139	U
54	A	153	A
54	A	200	A
54	A	201	A
54	A	286	U
54	A	324	A
54	A	351	U
54	A	427	A
54	A	461	A
54	A	495	C
54	A	502	A
54	A	516	C
54	A	604	A
54	A	704	A
54	A	837	A
54	A	860	A
54	A	888	A
54	A	889	U
54	A	936	U
54	A	958	U
54	A	983	C
54	A	990	U
54	A	1074	U
54	A	1235	A
54	A	1319	G
54	A	1371	U
54	A	1422	U
54	A	1443	A
54	A	1531	A
54	A	1536	C
55	B	1607	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 4 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
58	PNS	v	101	-	14,20,21	2.20	4 (28%)	18,26,29	1.14	1 (5%)

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

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
58	v	101	PNS	C34-N36	5.18	1.45	1.33
58	v	101	PNS	C39-N41	5.15	1.45	1.33
58	v	101	PNS	O35-C34	-2.29	1.19	1.23
58	v	101	PNS	O40-C39	-2.12	1.19	1.23

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
58	v	101	PNS	C37-C38-C39	-2.25	108.65	112.39

There are no chirality outliers.

All (11) torsion outliers are listed below:

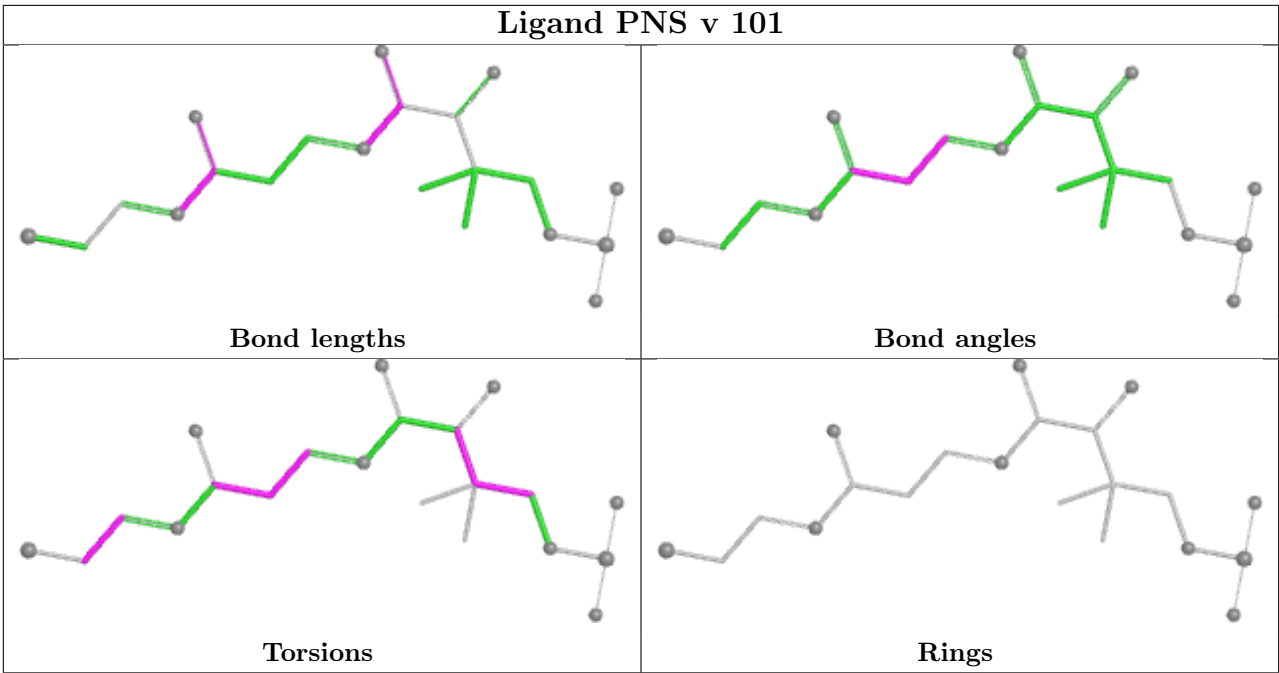
Mol	Chain	Res	Type	Atoms
58	v	101	PNS	C28-C29-C32-O33
58	v	101	PNS	C31-C29-C32-O33
58	v	101	PNS	N41-C42-C43-S44
58	v	101	PNS	C30-C29-C32-O33
58	v	101	PNS	N36-C37-C38-C39
58	v	101	PNS	C31-C29-C32-C34
58	v	101	PNS	O27-C28-C29-C30
58	v	101	PNS	O27-C28-C29-C31
58	v	101	PNS	C28-C29-C32-C34
58	v	101	PNS	C37-C38-C39-O40
58	v	101	PNS	C37-C38-C39-N41

There are no ring outliers.

1 monomer is involved in 1 short contact:

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

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
41	i	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	68:LYS	C	69:HIS	N	1.12

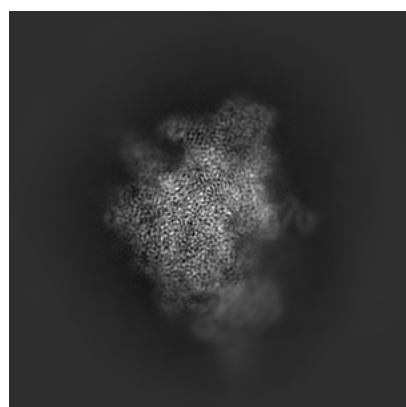
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-12927. These allow visual inspection of the internal detail of the map and identification of artifacts.

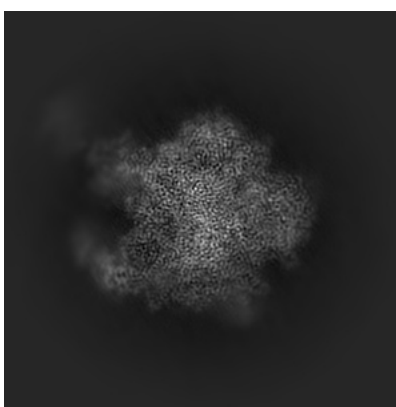
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

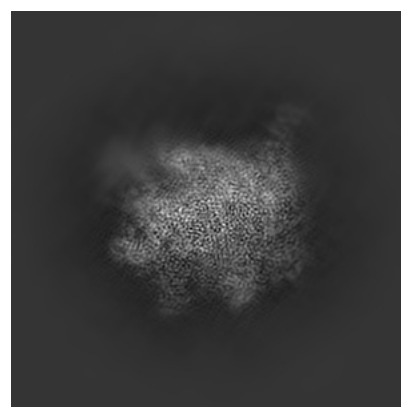
6.1.1 Primary map



X



Y

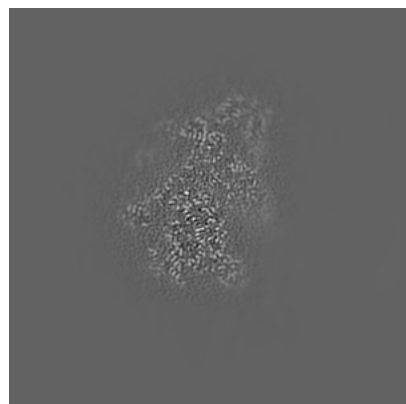


Z

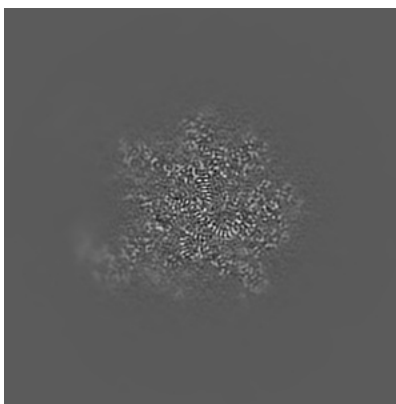
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

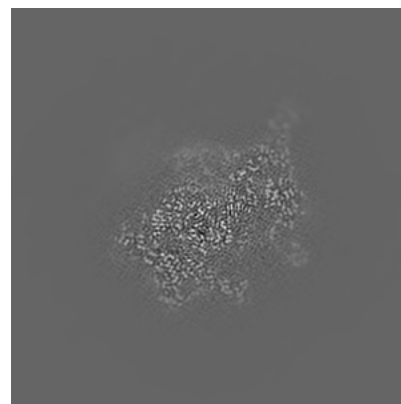
6.2.1 Primary map



X Index: 180



Y Index: 180

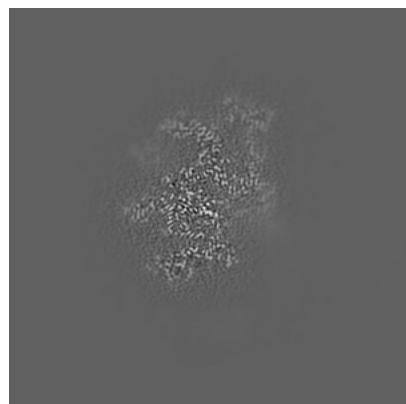


Z Index: 180

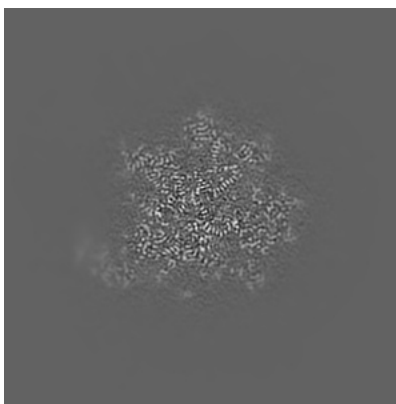
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

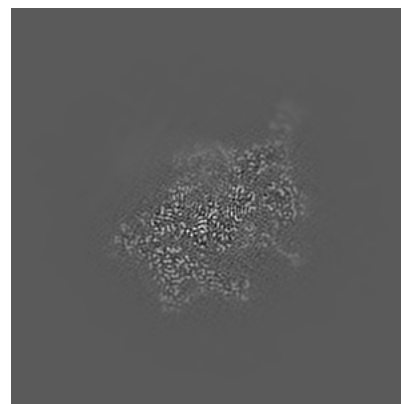
6.3.1 Primary map



X Index: 172



Y Index: 174

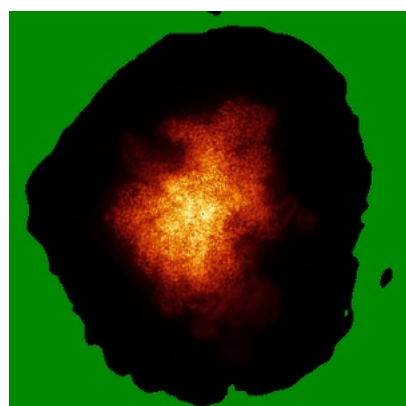


Z Index: 178

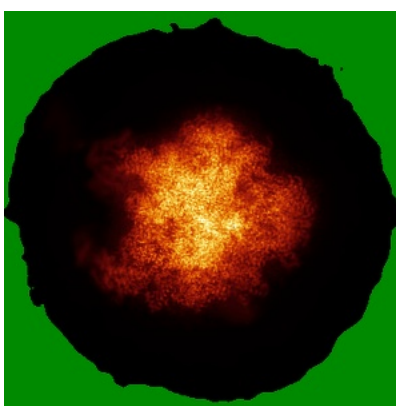
The images above show the largest variance slices of the map in three orthogonal directions.

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

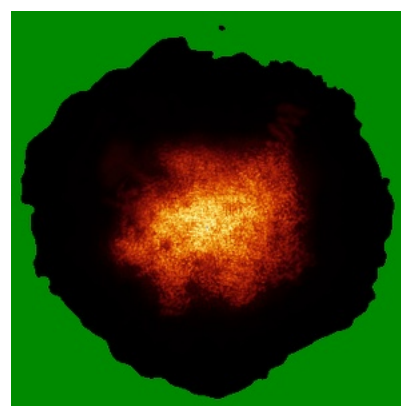
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

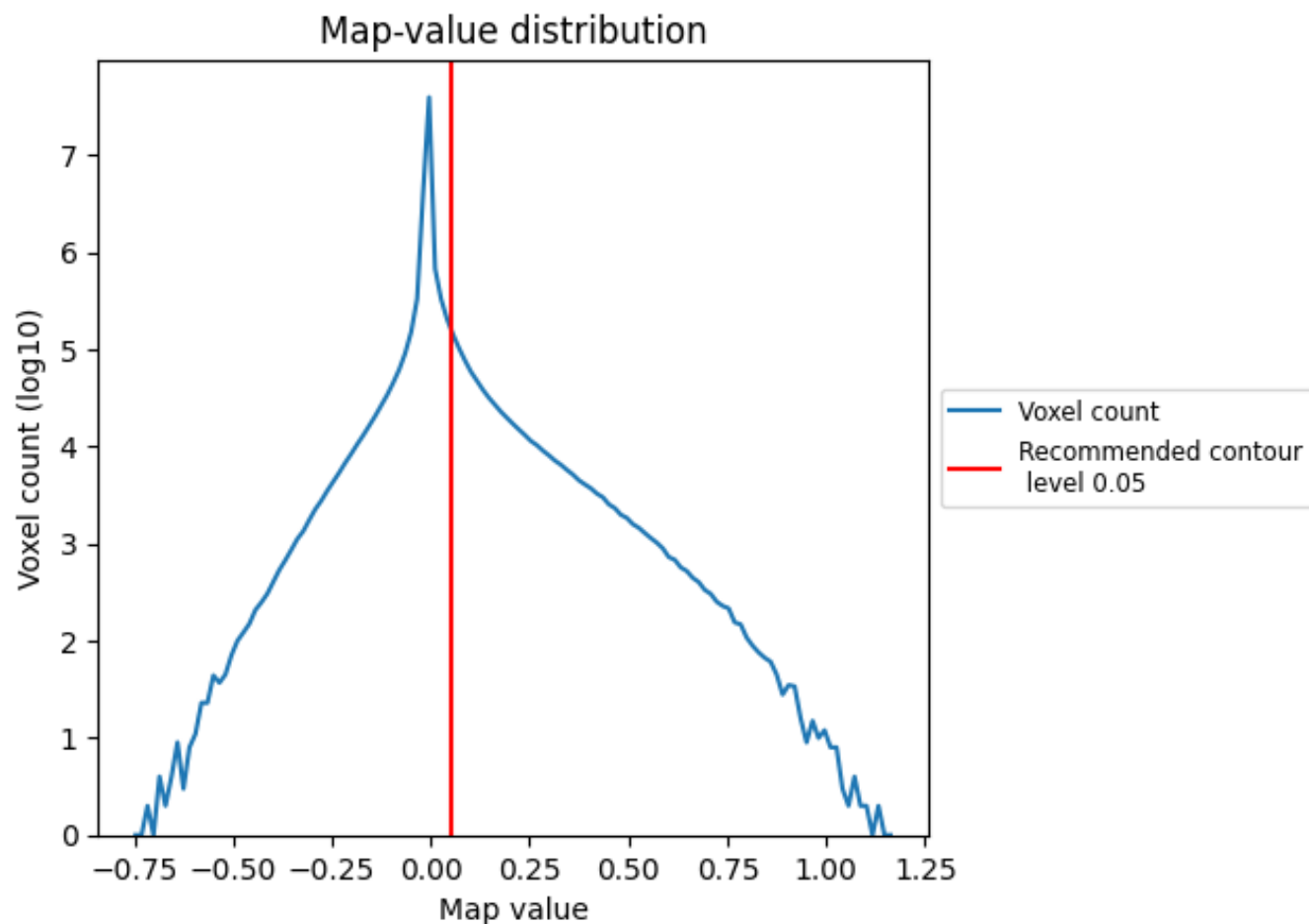
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

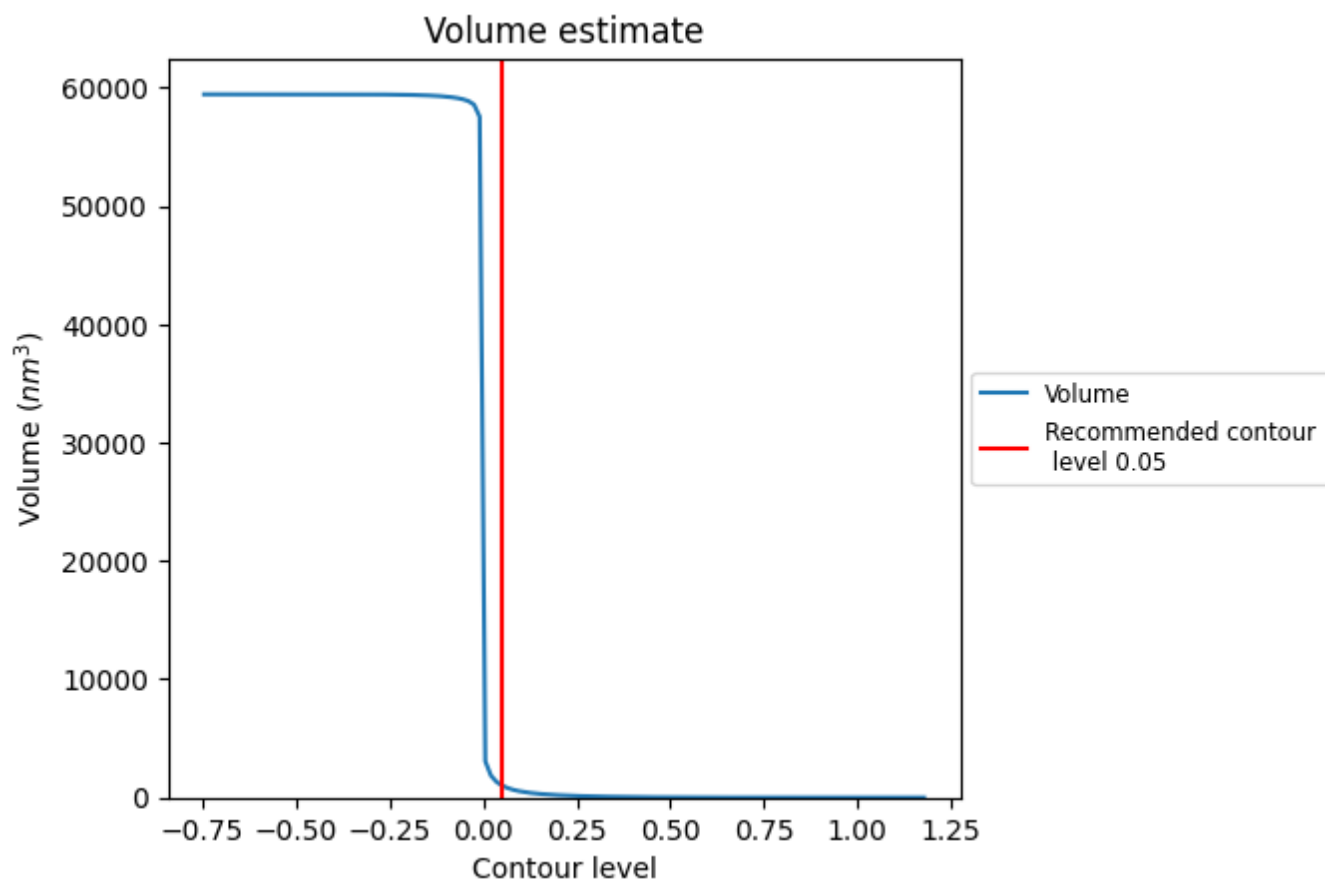
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

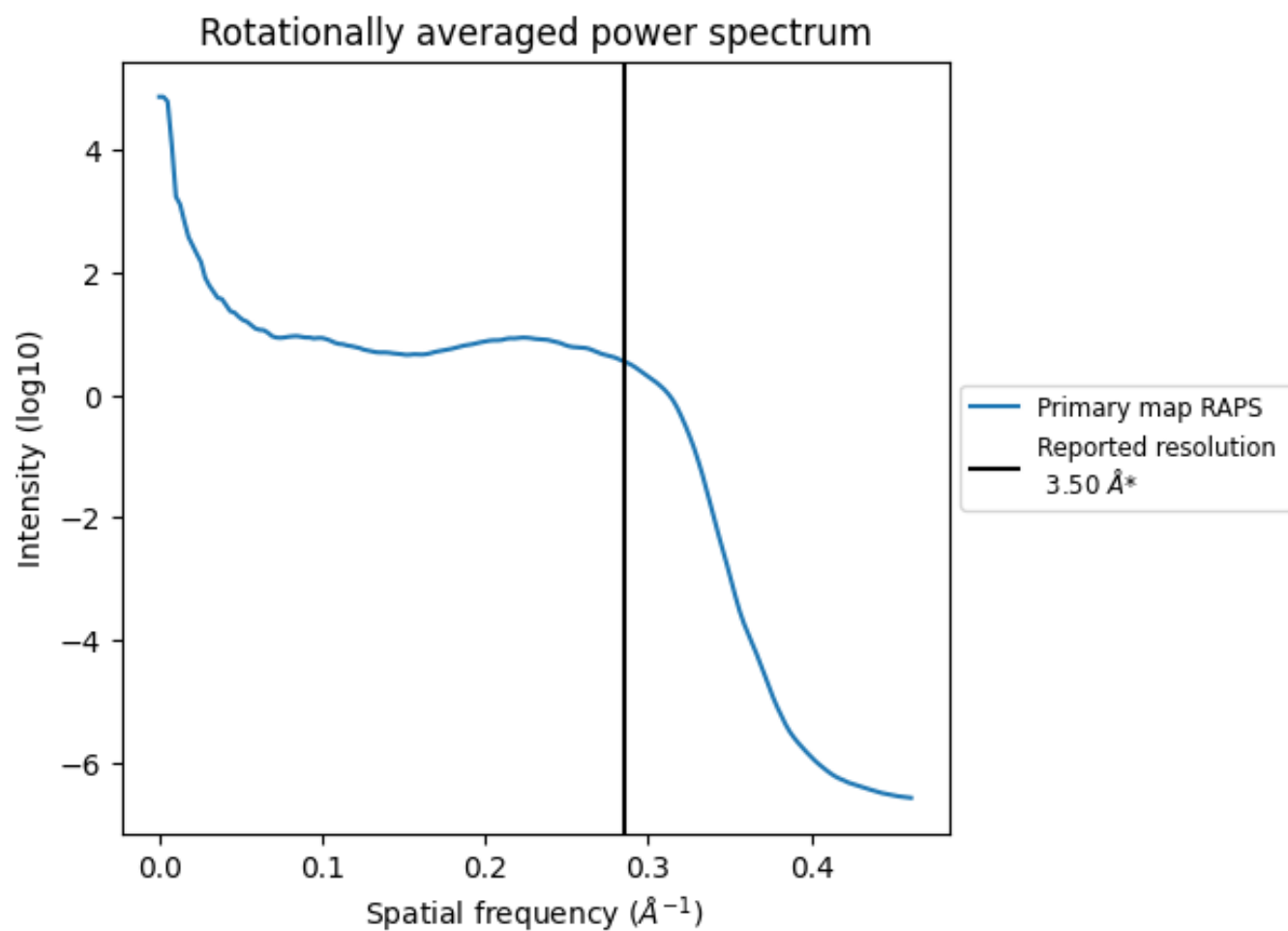
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1014 nm^3 ; this corresponds to an approximate mass of 916 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

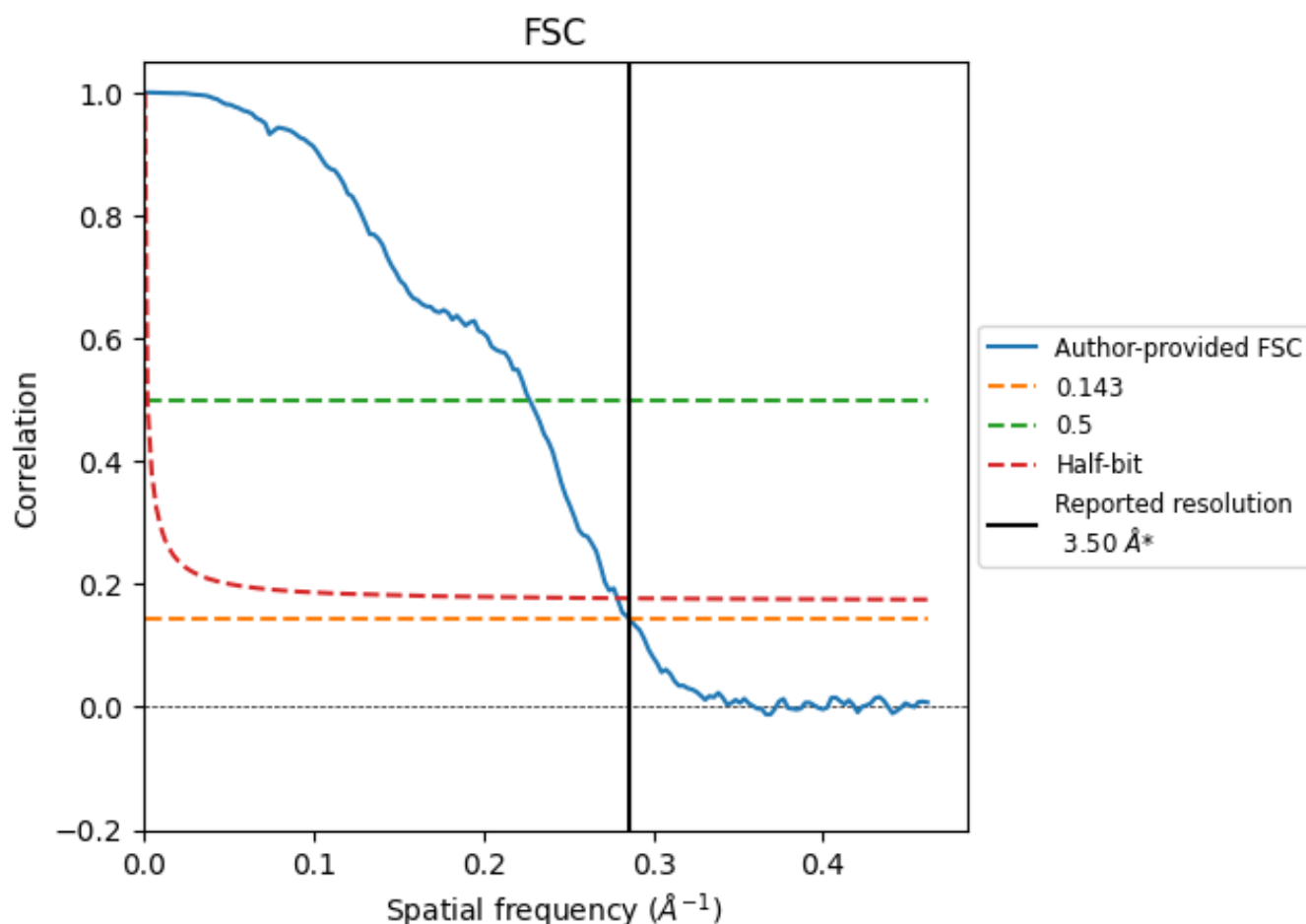


*Reported resolution corresponds to spatial frequency of 0.286 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



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

8.2 Resolution estimates [i](#)

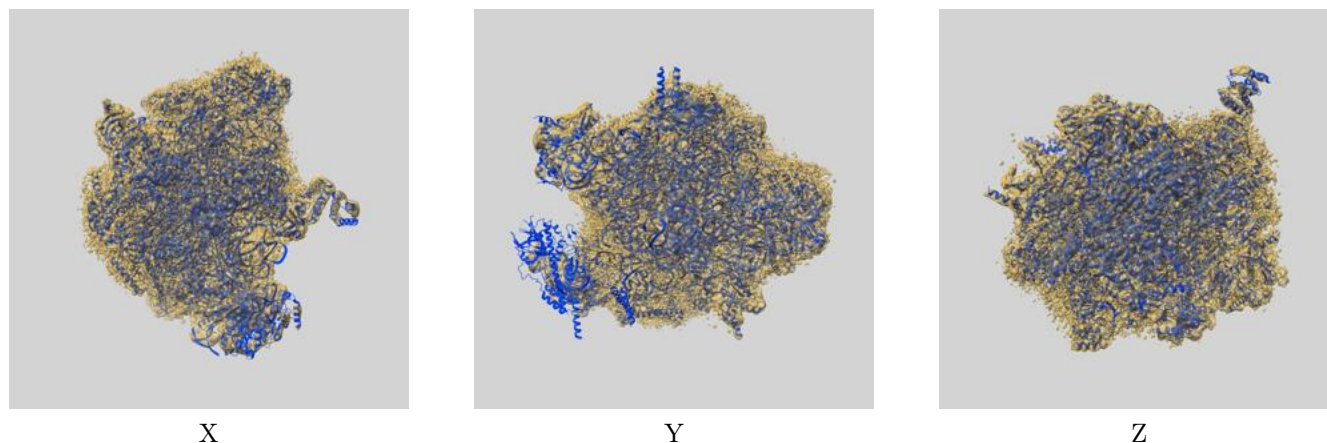
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.50	-	-
Author-provided FSC curve	3.50	4.40	3.59
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

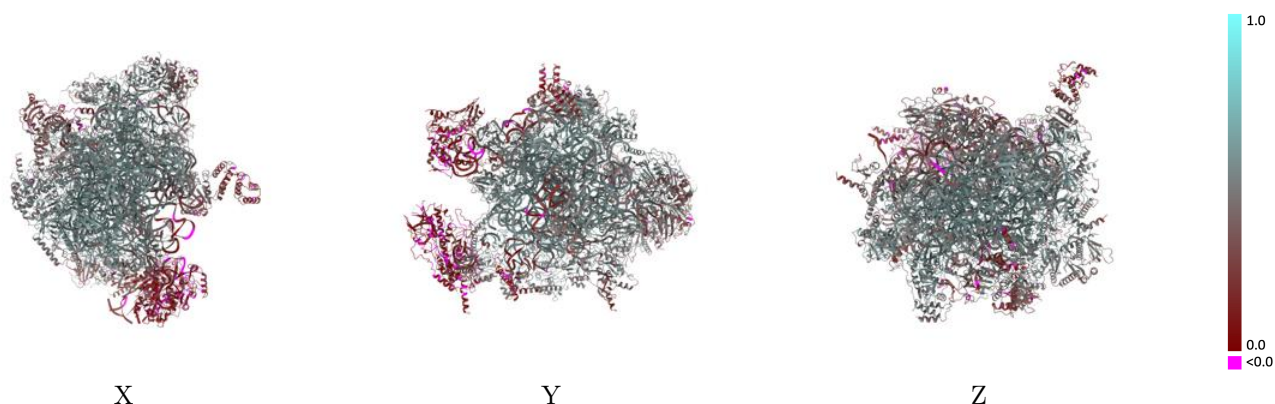
This section contains information regarding the fit between EMDB map EMD-12927 and PDB model 7OIE. Per-residue inclusion information can be found in section [3](#) on page [15](#).

9.1 Map-model overlay [i](#)



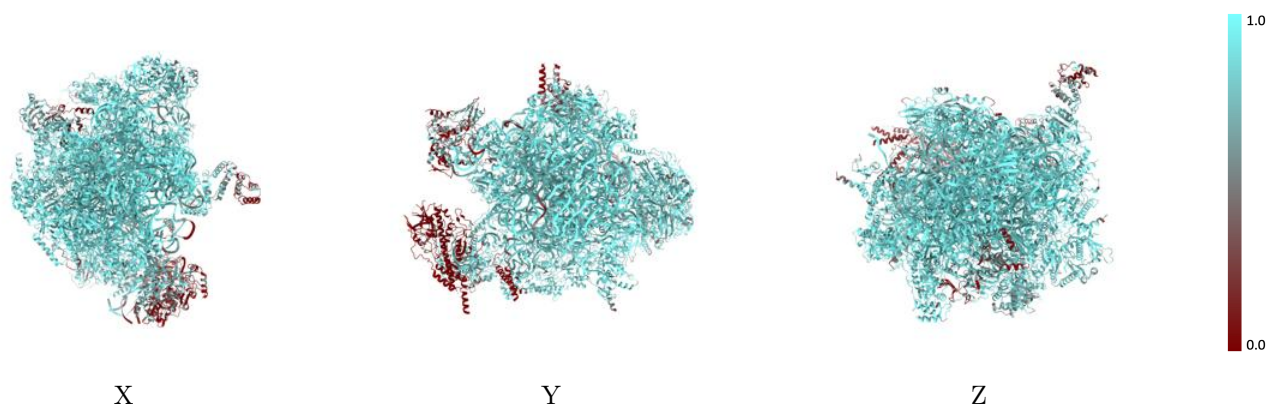
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



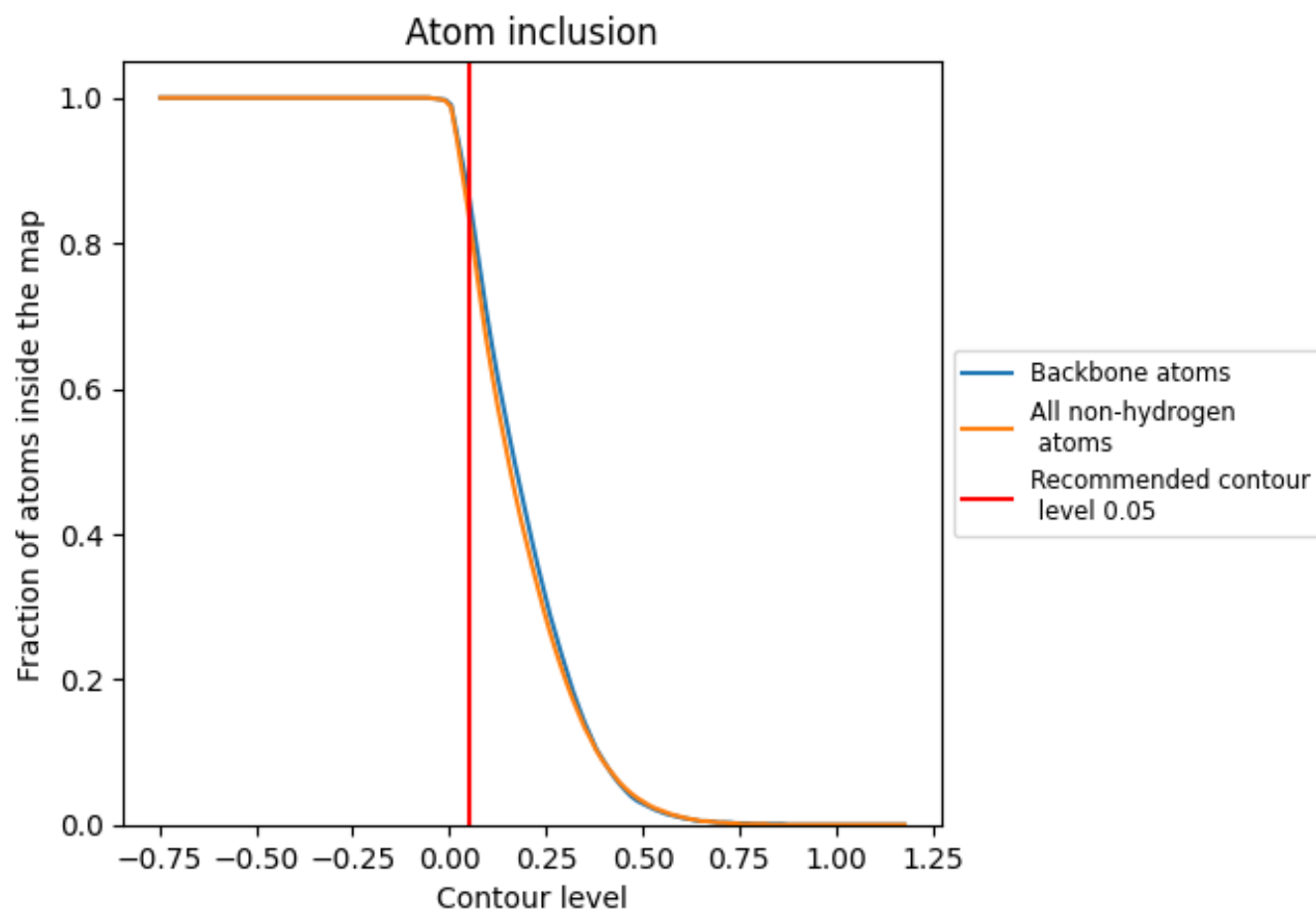
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 87% of all backbone atoms, 84% 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	 0.8420	 0.4580
0	 0.9190	 0.5100
1	 0.6880	 0.2760
2	 0.9760	 0.5900
3	 0.9700	 0.5920
4	 0.9380	 0.5160
5	 0.8110	 0.4020
6	 0.8330	 0.4010
7	 0.8610	 0.4520
8	 0.0060	 0.0970
9	 0.8950	 0.4840
A	 0.9350	 0.4980
B	 0.6950	 0.2100
D	 0.9280	 0.4980
E	 0.9380	 0.5370
F	 0.9490	 0.5560
H	 0.8070	 0.4370
I	 0.5280	 0.2330
J	 0.1480	 0.1010
K	 0.9510	 0.5480
L	 0.9270	 0.5260
M	 0.9480	 0.5510
N	 0.9300	 0.5260
O	 0.9280	 0.5350
P	 0.9060	 0.4620
Q	 0.9220	 0.5140
R	 0.8940	 0.5360
S	 0.9250	 0.5410
T	 0.9490	 0.5500
U	 0.8580	 0.4790
V	 0.5080	 0.3040
W	 0.9360	 0.5440
X	 0.9030	 0.5040
Y	 0.9160	 0.5170
Z	 0.9030	 0.5320



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Chain	Atom inclusion	Q-score
a	 0.9540	 0.5360
b	 0.9530	 0.5460
c	 0.9160	 0.5060
d	 0.6300	 0.3030
e	 0.0000	 0.0820
f	 0.1550	 0.1700
g	 0.9500	 0.5420
h	 0.8790	 0.4450
i	 0.9740	 0.5760
j	 0.8960	 0.4980
k	 0.6570	 0.2270
l	 0.6120	 0.1990
m	 0.0000	 0.0590
o	 0.9440	 0.5590
p	 0.8800	 0.4630
q	 0.5580	 0.3330
r	 0.9160	 0.5050
s	 0.9110	 0.4960
u	 0.8450	 0.4080
v	 0.6020	 0.2620
w	 0.2310	 0.1690