



Full wwPDB EM Validation Report ⓘ

Mar 29, 2026 – 04:32 PM UTC

PDB ID : 8XT3 / pdb_00008xt3
EMDB ID : EMD-38635
Title : Cryo-EM structure of the human 39S mitoribosome with 10uM Tigecycline
Authors : Li, X.; Wang, M.; Cheng, J.
Deposited on : 2024-01-10
Resolution : 3.10 Å (reported)
Based on initial model : 7A5I

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:

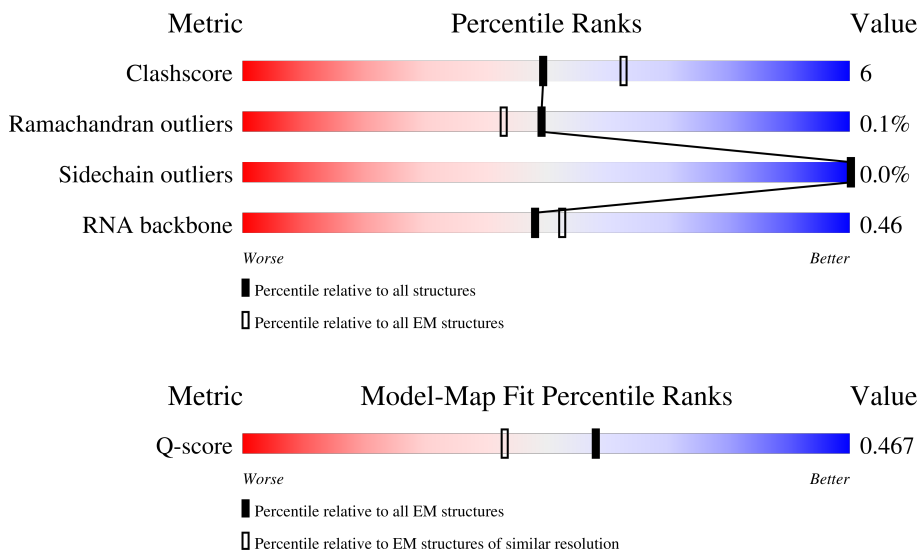
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.10 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	14724 (2.60 - 3.60)

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	L1	1559	61% (green), 31% (yellow), 8% (orange), 0% (red), 0% (grey)
2	L2	69	39% (green), 36% (yellow), 6% (orange), 19% (grey)
3	LB	305	70% (green), 8% (yellow), 22% (grey)

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Mol	Chain	Length	Quality of chain
4	LC	348	70% 17% 13%
5	LD	311	68% 12% 20%
6	LI	267	27% 9% 64%
7	LJ	261	40% 17% 39%
8	LK	192	5% 72% 19% 9%
9	LM	178	84% 15%
10	LN	145	72% 8% 21%
11	LO	296	85% 11%
12	LP	251	77% 11% 12%
13	LQ	175	74% 13% 13%
14	LR	179	61% 19% 18%
15	LS	292	68% 7% 25%
16	LT	149	81% 13% 6%
17	LU	205	63% 15% 22%
18	LV	212	67% 11% 22%
19	LW	153	5% 81% 12% 7%
20	LX	216	9% 75% 19% 6%
21	La	148	61% 14% 25%
22	Lb	256	83% 12% 5%
23	Lu	250	63% 7% 30%
24	Ld	161	58% 16% 25%
25	Lf	188	49% 8% 43%
26	Lg	65	72% 8% 20%
27	Lh	92	42% 8% 50%
28	Li	188	42% 9% 49%

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Mol	Chain	Length	Quality of chain
29	Lj	103	
30	Lk	423	
31	Ll	380	
32	Lm	338	
33	Ln	206	
34	Lo	137	
35	Lp	142	
36	Lq	215	
37	Lr	332	
38	Ls	306	
39	Lt	279	
40	Lv	212	
41	Lw	166	
42	Lx	158	
43	Ly	128	
44	Lz	123	
45	L3	112	
46	L4	138	
47	L5	128	
48	L6	102	
49	L7	206	
50	L8	222	
51	SR	196	
52	Sf	439	

2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 100095 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 16s rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	L1	1500	31847	14290	5750	10307	1500	0	0

- Molecule 2 is a RNA chain called Val tRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	L2	56	1191	534	214	387	56	0	0

- Molecule 3 is a protein called Large ribosomal subunit protein uL2m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	LB	237	1851	1151	375	316	9	0	0

- Molecule 4 is a protein called Large ribosomal subunit protein uL3m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	LC	304	2393	1538	415	429	11	0	0

- Molecule 5 is a protein called Large ribosomal subunit protein uL4m.

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

- Molecule 6 is a protein called Large ribosomal subunit protein bL9m.

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

- Molecule 7 is a protein called Large ribosomal subunit protein uL10m.

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

- Molecule 8 is a protein called Large ribosomal subunit protein uL11m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	LK	175	1330	847	237	244	2	0	0

- Molecule 9 is a protein called Large ribosomal subunit protein uL13m.

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

- Molecule 10 is a protein called Large ribosomal subunit protein uL14m.

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

- Molecule 11 is a protein called Large ribosomal subunit protein uL15m.

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

- Molecule 12 is a protein called Large ribosomal subunit protein uL16m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	LP	221	1779	1138	325	306	10	0	0

- Molecule 13 is a protein called Large ribosomal subunit protein bL17m.

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

- Molecule 14 is a protein called Mitochondrial ribosomal protein L18, isoform CRA_b.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	LR	146	1189	743	226	215	5	0	0

- Molecule 15 is a protein called Large ribosomal subunit protein bL19m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	LS	219	1822	1168	322	323	9	0	0

- Molecule 16 is a protein called Large ribosomal subunit protein bL20m.

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

- Molecule 17 is a protein called Large ribosomal subunit protein bL21m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	LU	160	1284	829	226	225	4	0	0

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

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

- Molecule 19 is a protein called Large ribosomal subunit protein uL23m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	LW	143	1188	752	224	208	4	0	0

- Molecule 20 is a protein called Large ribosomal subunit protein uL24m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	LX	202	1652	1053	294	297	8	0	0

- Molecule 21 is a protein called Large ribosomal subunit protein bL27m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	La	111	871	558	164	146	3	0	0

- Molecule 22 is a protein called Large ribosomal subunit protein bL28m.

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

- Molecule 23 is a protein called Large ribosomal subunit protein uL29m.

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

- Molecule 24 is a protein called Large ribosomal subunit protein uL30m.

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

- Molecule 25 is a protein called Large ribosomal subunit protein bL32m.

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

- Molecule 26 is a protein called Large ribosomal subunit protein bL33m.

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

- Molecule 27 is a protein called Large ribosomal subunit protein bL34m.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Lh	46	376	233	83	59	1	0	0

- Molecule 28 is a protein called Large ribosomal subunit protein bL35m.

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

- Molecule 29 is a protein called Large ribosomal subunit protein bL36m.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lj	38	Total	C	N	O	S	0	0
			341	217	72	48	4		

- Molecule 30 is a protein called Large ribosomal subunit protein mL37.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Lk	394	Total	C	N	O	S	0	0
			3210	2073	560	566	11		

- Molecule 31 is a protein called Large ribosomal subunit protein mL38.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Ll	354	Total	C	N	O	S	0	0
			2947	1881	525	532	9		

- Molecule 32 is a protein called Large ribosomal subunit protein mL39.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Lm	293	Total	C	N	O	S	0	0
			2382	1525	404	435	18		

- Molecule 33 is a protein called Large ribosomal subunit protein mL40.

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

- Molecule 34 is a protein called Large ribosomal subunit protein mL41.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	Lo	124	Total	C	N	O	S	0	0
			997	644	170	181	2		

- Molecule 35 is a protein called Large ribosomal subunit protein mL42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	Lp	97	815	514	147	149	5	0	0

- Molecule 36 is a protein called Large ribosomal subunit protein mL43.

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

- Molecule 37 is a protein called Large ribosomal subunit protein mL44.

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

- Molecule 38 is a protein called Large ribosomal subunit protein mL45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
38	Ls	214	1754	1117	304	320	13	0	0

- Molecule 39 is a protein called Large ribosomal subunit protein mL46.

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

- Molecule 40 is a protein called Large ribosomal subunit protein mL48.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
40	Lv	131	1039	663	169	203	4	0	0

- Molecule 41 is a protein called Large ribosomal subunit protein mL49.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
41	Lw	132	1097	710	191	194	2	0	0

- Molecule 42 is a protein called Large ribosomal subunit protein mL50.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
42	Lx	110	895	568	156	168	3	0	0

- Molecule 43 is a protein called Large ribosomal subunit protein mL51.

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

- Molecule 44 is a protein called 39S ribosomal protein L52, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
44	Lz	92	732	454	142	134	2	0	0

- Molecule 45 is a protein called Large ribosomal subunit protein mL53.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
45	L3	96	743	462	143	133	5	0	0

- Molecule 46 is a protein called Large ribosomal subunit protein mL54.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
46	L4	83	703	446	124	130	3	0	0

- Molecule 47 is a protein called Large ribosomal subunit protein mL55.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
47	L5	45	372	232	76	62	2	0	0

- Molecule 48 is a protein called Large ribosomal subunit protein mL63.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
48	L6	94	797	501	165	128	3	0	0

- Molecule 49 is a protein called Large ribosomal subunit protein mL62.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
49	L7	127	1058	661	201	192	4	0	0

- Molecule 50 is a protein called Large ribosomal subunit protein mL64.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
50	L8	128	1076	671	208	192	5	0	0

- Molecule 51 is a protein called Large ribosomal subunit protein mL66.

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

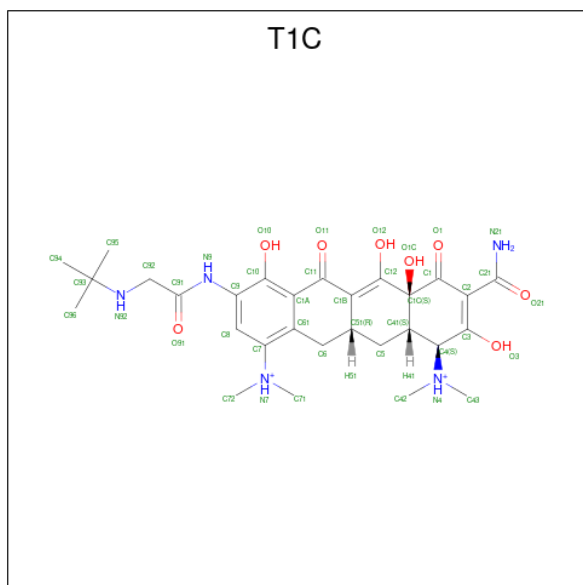
- Molecule 52 is a protein called Large ribosomal subunit protein mL65.

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

- Molecule 53 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
53	L1	91	Total	Mg	0
			91	91	
53	LB	1	Total	Mg	0
			1	1	
53	La	1	Total	Mg	0
			1	1	
53	Lw	1	Total	Mg	0
			1	1	
53	L6	1	Total	Mg	0
			1	1	

- Molecule 54 is TIGECYCLINE (CCD ID: T1C) (formula: C₂₉H₄₁N₅O₈) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
54	L1	1	42	29	5	8	0

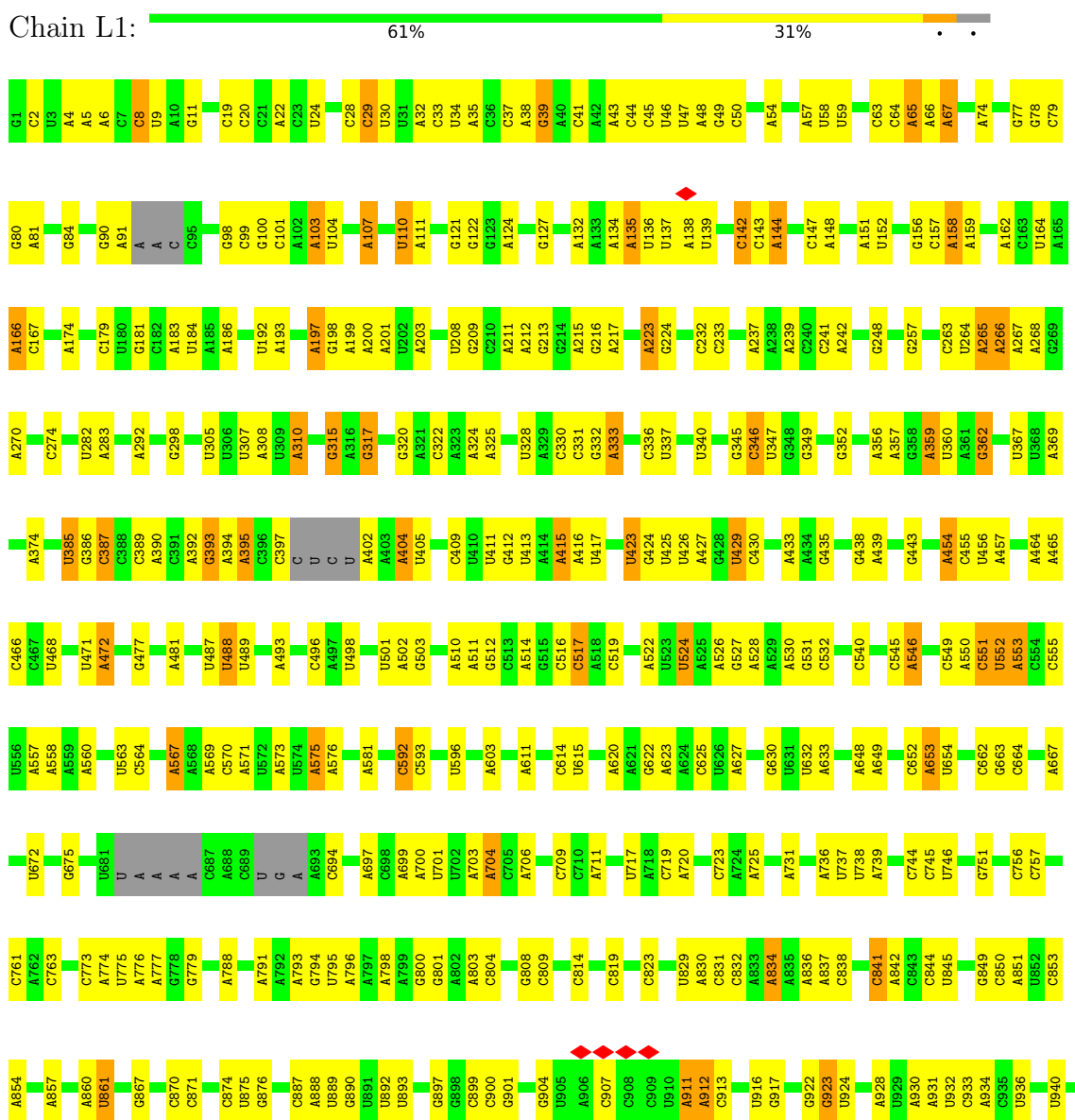
- Molecule 55 is ZINC ION (CCD ID: ZN) (formula: Zn).

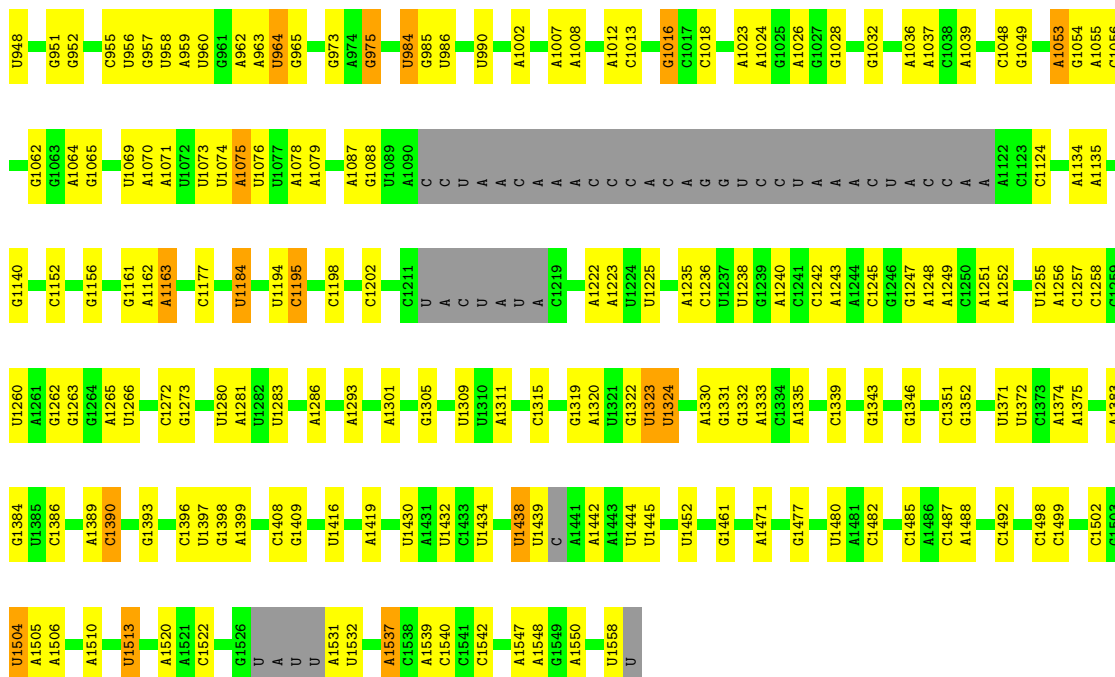
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
55	Lf	1	1	1	0
55	Lj	1	1	1	0
55	SR	1	1	1	0

3 Residue-property plots [i](#)

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: 16s rRNA

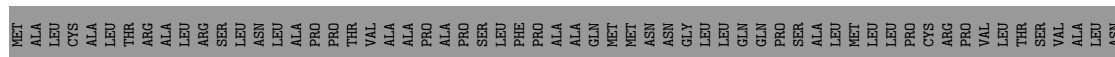




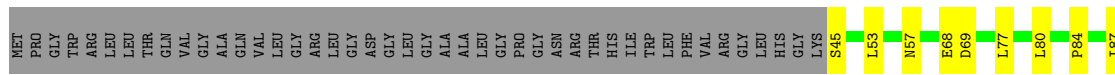
• Molecule 2: Val tRNA

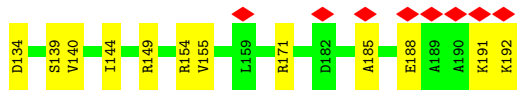


• Molecule 3: Large ribosomal subunit protein uL2m

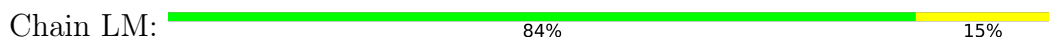


• Molecule 4: Large ribosomal subunit protein uL3m

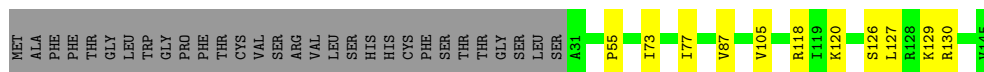




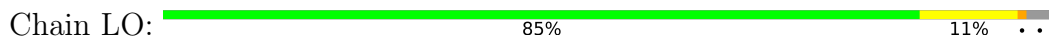
• Molecule 9: Large ribosomal subunit protein uL13m



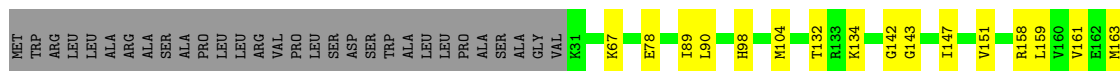
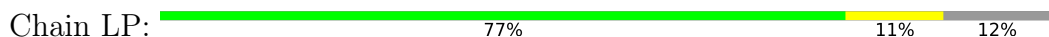
• Molecule 10: Large ribosomal subunit protein uL14m



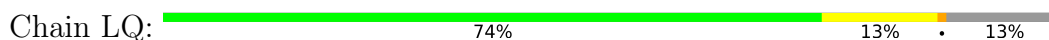
• Molecule 11: Large ribosomal subunit protein uL15m



• Molecule 12: Large ribosomal subunit protein uL16m

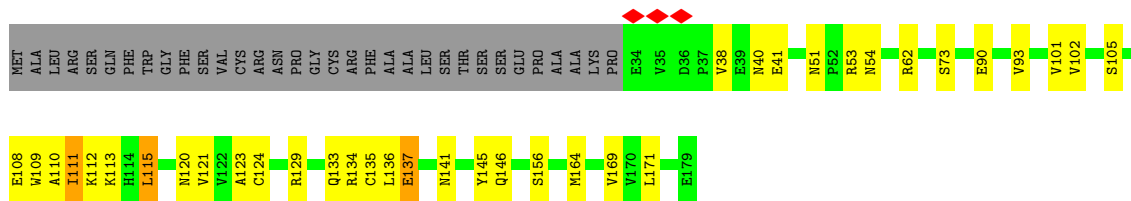


• Molecule 13: Large ribosomal subunit protein bL17m

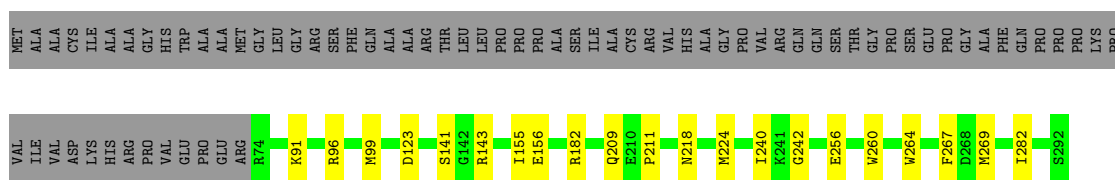


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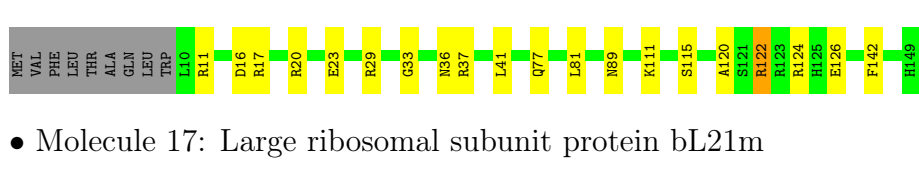
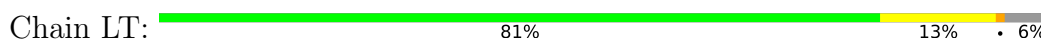
• Molecule 14: Mitochondrial ribosomal protein L18, isoform CRA_b



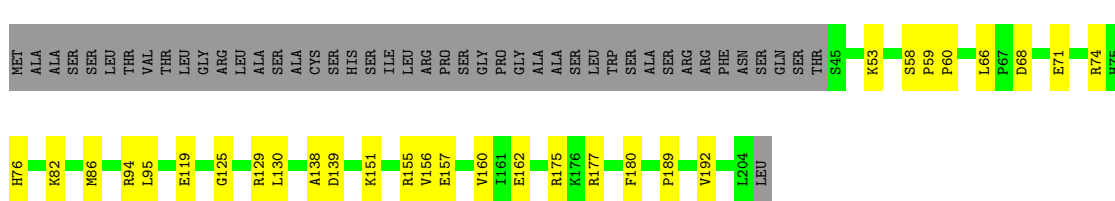
• Molecule 15: Large ribosomal subunit protein bL19m



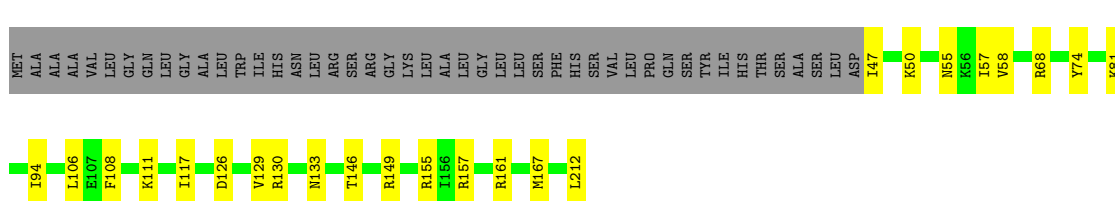
• Molecule 16: Large ribosomal subunit protein bL20m



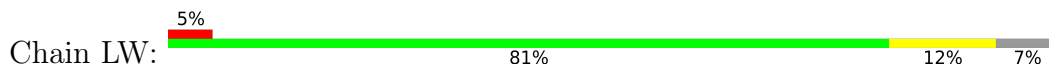
• Molecule 17: Large ribosomal subunit protein bL21m



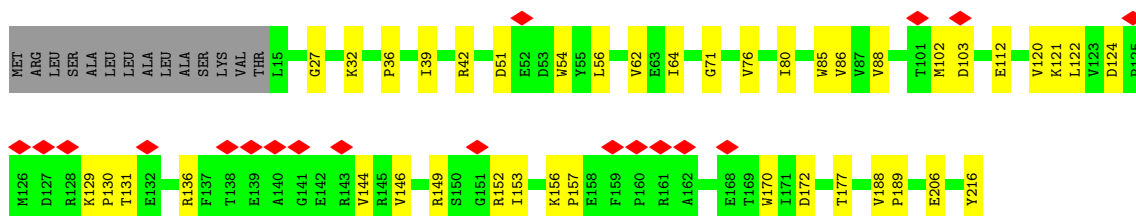
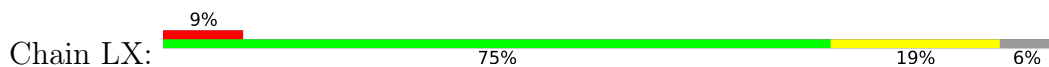
• Molecule 18: 39S ribosomal protein L22, mitochondrial



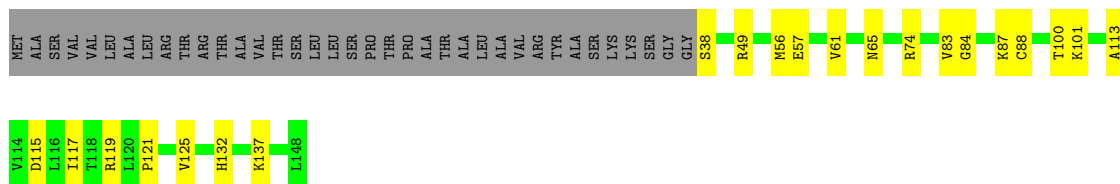
• Molecule 19: Large ribosomal subunit protein uL23m



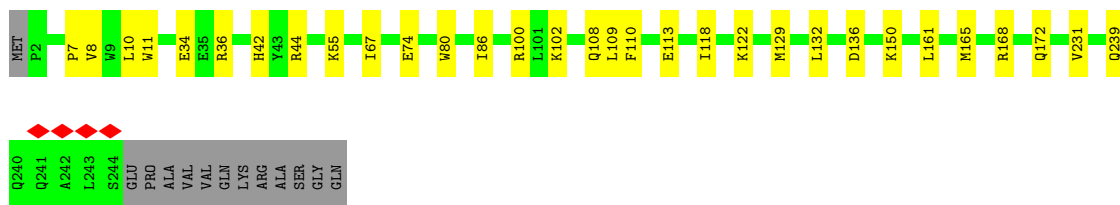
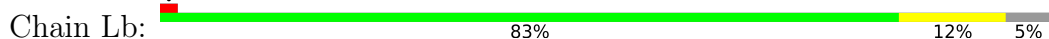
• Molecule 20: Large ribosomal subunit protein uL24m



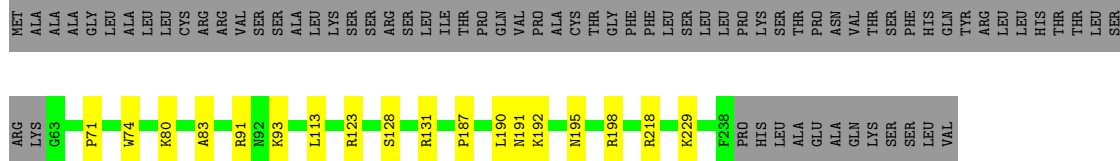
• Molecule 21: Large ribosomal subunit protein bL27m



• Molecule 22: Large ribosomal subunit protein bL28m



• Molecule 23: Large ribosomal subunit protein uL29m




• Molecule 24: Large ribosomal subunit protein uL30m

Chain Lj:  30% 7% 63%

MET ALA ALA ASN LEU PHE LE ARG LYS MET VAL ASN PRO LEU LEU TYR LEU SER ARG HIS THR VAL LYS PRO ARG ALA LEU SER THR PHE LEU PHE GLY SER ILE ARG GLY ALA ALA PRO VAL ALA VAL ARG SER LEU SER PRO HIS LEU

LEU PRO ALA LEU LEU F66 V71 C76 Y90 K93 H98 K99 K103

- Molecule 30: Large ribosomal subunit protein mL37

Chain Lk:  78% 15% 7%

MET ALA LEU ALA SER PRO ALA ARG ARG ALA ALA ALA GLY SER GLN LEU GLY LEU GLY PHE GLY ALA PRO ARG ARG GLY A30 F60 V67 R80 L113 L121 K125 T126 K127 L128 L132 L137 S138 L139 V140 H146 I147 E152 L155

H160 H164 Q165 R173 E174 T175 V179 I185 Q186 L187 K194 R201 I202 C203 T208 A211 T212 R215 L219 R229 L230 S231 T232 R242 E246 I270 Y271 D272 V273 K274 H275 D276 P288 H289 T290 L291 Y292 P301 L309 R310 A311 K312 M313

L322 Q343 F354 L355 V356 N367 K371 N372 V376 Q384 R395 V404 A416 L417 A423

- Molecule 31: Large ribosomal subunit protein mL38


Chain Ll:  72% 21% 7%

MET ALA ALA PRO TRP ARG ALA ALA CYS CYS ARG ARG TRP ARG GLY PHE SER THR SER ALA VAL LEU GLY R27 D39 L45 L48 E49 K50 E64 A67 H69 T73 Y74 R75 K85 I88 R99 R114 E120 R124 L132

E138 T142 K148 Y155 G156 L161 L173 H174 V175 A176 Y177 A178 V179 D183 L184 M185 P186 V187 Y188 G189 G190 P195 A198 P202 E203 V204 E207 E210 G211 S212 L213 V214 L217 D229 L233 H234 W235 L236 L237 I240 A246 T251

L255 P256 F270 L272 F273 K274 Q275 D276 S288 F298 R299 F303 Y304 Q308 M311 F312 P313 F318 A319 W323 V327 I330 F331 H332 Q333 L334 L335 D336 M337 R338 E339 P352 R364 Y369 P375 Y380

- Molecule 32: Large ribosomal subunit protein mL39

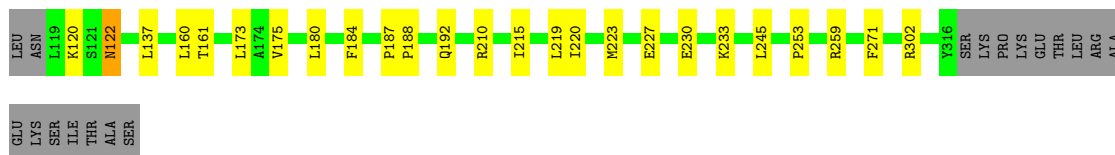
Chain Lm:  73% 13% 13%

MET GLU ALA LEU ALA MET GLY SER ARG ALA LEU ARG LEU LEU TRP VAL ALA PRO GLY GLY ILE THR SER ALA SER Q34 L40 F41 E42 M43 R44 E51 R64 T73 Y80 M81 S86 Y99 L107 V108 D109 P112 H113

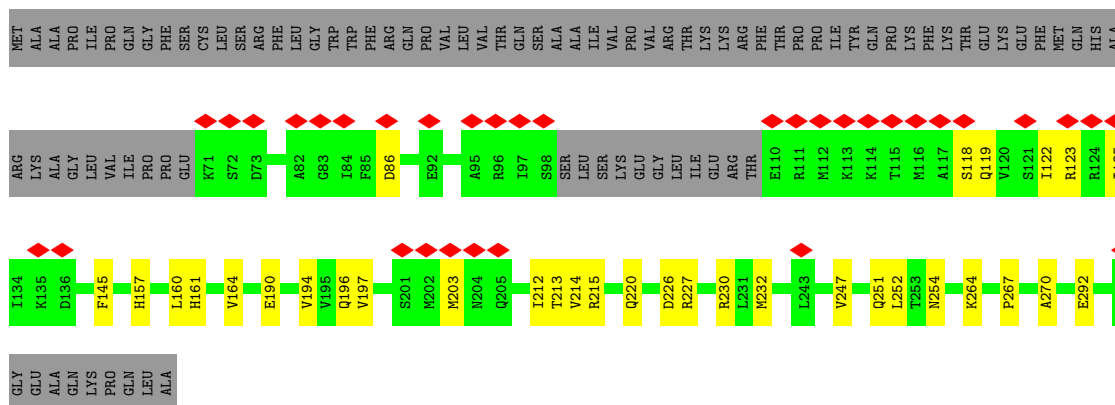
D114 K117 K121 I125 N139 Y142 A157 F158 V174 F179 C180 L189 N198 V221 E228 N247 I251 R256 I261 P267 L268 L269 L274 C275 F276 S281 R285 R296 F297 Q298 S301 V304 R307 A308 H309 R321

E326 ASP GLN SER LYS ALA THR LEU GLU CYS THR SER THR

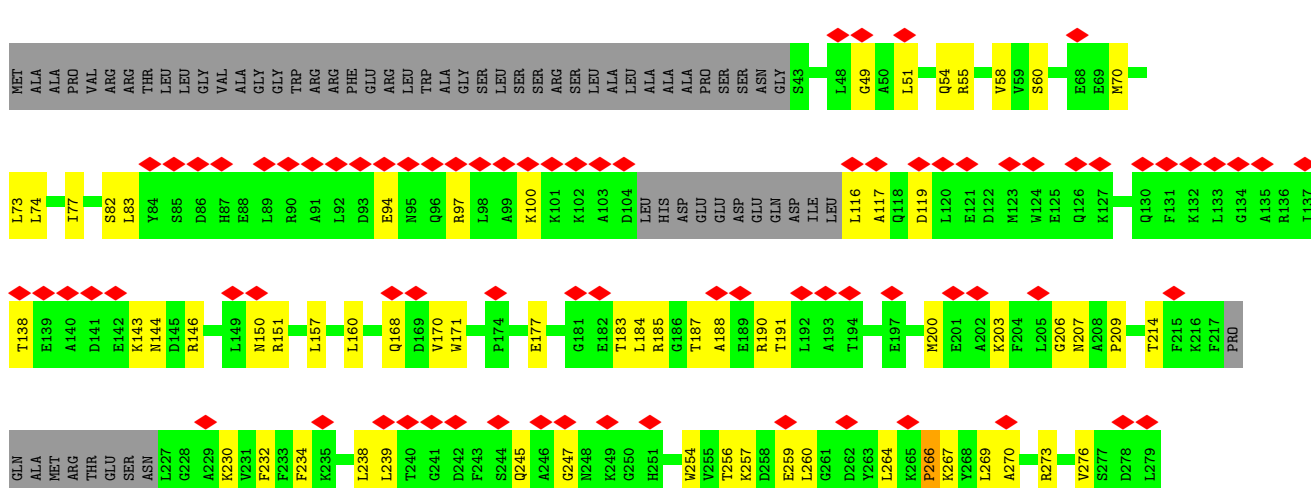
- Molecule 33: Large ribosomal subunit protein mL40



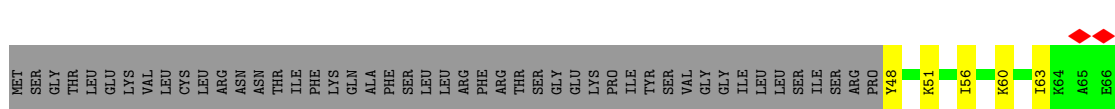
• Molecule 38: Large ribosomal subunit protein mL45

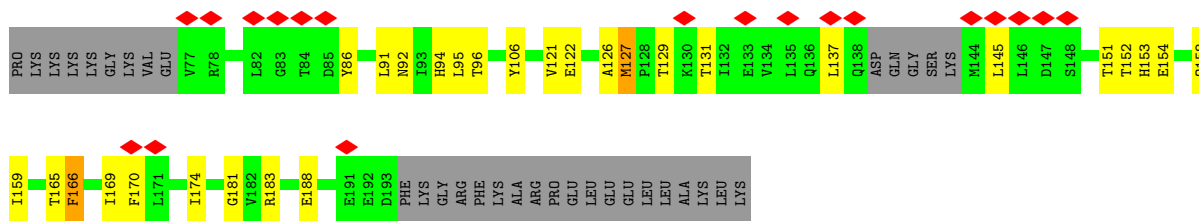


• Molecule 39: Large ribosomal subunit protein mL46

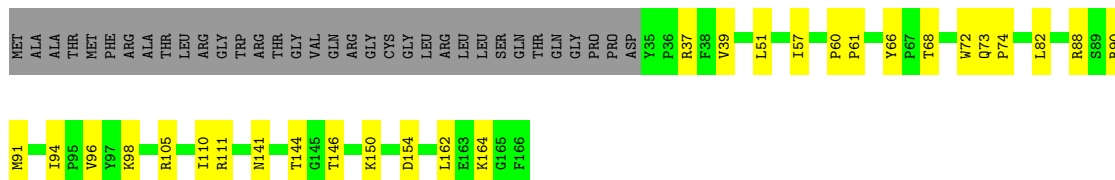


• Molecule 40: Large ribosomal subunit protein mL48

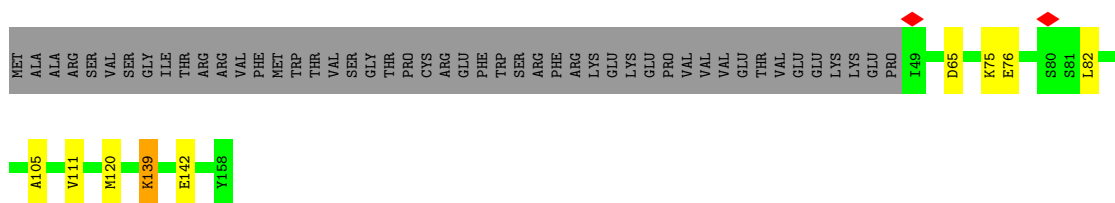




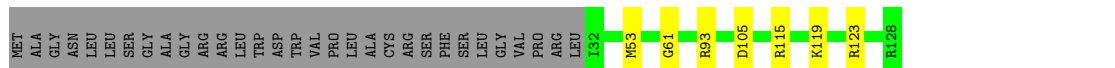
- Molecule 41: Large ribosomal subunit protein mL49



- Molecule 42: Large ribosomal subunit protein mL50



- Molecule 43: Large ribosomal subunit protein mL51



- Molecule 44: 39S ribosomal protein L52, mitochondrial



- Molecule 45: Large ribosomal subunit protein mL53



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	52961	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; Relion	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.068	Depositor
Minimum map value	-0.018	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	446.88, 446.88, 446.88	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.064, 1.064, 1.064	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: T1C, MG, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	L1	0.17	0/35628	0.38	0/55448
2	L2	0.14	0/1328	0.30	0/2056
3	LB	0.20	0/1888	0.48	2/2538 (0.1%)
4	LC	0.23	0/2462	0.56	3/3340 (0.1%)
5	LD	0.24	0/2071	0.51	0/2817
6	LI	0.28	0/798	0.71	3/1073 (0.3%)
7	LJ	0.49	0/1308	1.06	11/1761 (0.6%)
8	LK	0.28	0/1348	0.61	0/1813
9	LM	0.27	0/1495	0.57	0/2029
10	LN	0.19	0/904	0.45	0/1218
11	LO	0.24	0/2359	0.53	1/3185 (0.0%)
12	LP	0.20	0/1826	0.46	0/2458
13	LQ	0.27	0/1269	0.54	0/1708
14	LR	0.38	1/1215 (0.1%)	0.76	8/1645 (0.5%)
15	LS	0.26	0/1863	0.56	0/2509
16	LT	0.29	0/1174	0.50	0/1572
17	LU	0.24	0/1311	0.54	0/1778
18	LV	0.34	1/1402 (0.1%)	0.53	1/1886 (0.1%)
19	LW	0.21	0/1217	0.52	0/1644
20	LX	0.25	0/1697	0.57	2/2302 (0.1%)
21	La	0.23	0/893	0.46	0/1204
22	Lb	0.24	0/2090	0.55	2/2825 (0.1%)
23	Lu	0.24	0/1552	0.48	0/2079
24	Ld	0.25	0/1003	0.57	0/1354
25	Lf	0.22	0/895	0.47	0/1201
26	Lg	0.25	0/438	0.59	0/583
27	Lh	0.23	0/382	0.47	0/507
28	Li	0.25	0/852	0.51	0/1136
29	Lj	0.20	0/349	0.42	0/461
30	Lk	0.21	0/3305	0.47	0/4502
31	Ll	0.27	0/3042	0.61	0/4140
32	Lm	0.28	0/2439	0.56	3/3299 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	Ln	0.31	0/855	0.69	0/1152
34	Lo	0.21	0/1025	0.52	0/1379
35	Lp	0.21	0/839	0.53	0/1136
36	Lq	0.21	0/1202	0.50	0/1626
37	Lr	0.25	0/2264	0.54	3/3059 (0.1%)
38	Ls	0.31	0/1800	0.58	1/2436 (0.0%)
39	Lt	0.24	0/1797	0.61	0/2422
40	Lv	0.26	0/1055	0.71	4/1427 (0.3%)
41	Lw	0.32	0/1134	0.61	0/1547
42	Lx	0.34	0/918	0.68	2/1249 (0.2%)
43	Ly	0.23	0/849	0.47	0/1135
44	Lz	0.28	0/747	0.68	0/1005
45	L3	0.35	0/754	0.67	1/1017 (0.1%)
46	L4	0.39	0/722	0.82	3/978 (0.3%)
47	L5	0.23	0/379	0.59	0/510
48	L6	0.32	0/818	0.57	0/1097
49	L7	0.20	0/1071	0.51	0/1433
50	L8	0.23	0/1107	0.48	0/1498
51	SR	0.24	0/1238	0.52	0/1676
52	Sf	0.22	0/3114	0.46	0/4225
All	All	0.23	2/105491 (0.0%)	0.51	50/150078 (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
6	LI	0	1
7	LJ	0	2
8	LK	0	2
11	LO	0	1
13	LQ	0	1
16	LT	0	1
18	LV	0	1
22	Lb	0	1
31	Ll	0	1
37	Lr	0	1
40	Lv	0	2
46	L4	0	1
52	Sf	0	1
All	All	0	16

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	LV	58	VAL	C-N	8.20	1.46	1.33
14	LR	115	LEU	CG-CD1	-7.66	1.27	1.52

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	LR	111	ILE	N-CA-C	-10.26	103.59	111.90
14	LR	111	ILE	CB-CA-C	8.92	119.87	111.30
38	Ls	123	ARG	CB-CG-CD	8.38	130.57	111.30
37	Lr	102	GLU	N-CA-CB	7.98	121.97	110.16
7	LJ	168	LEU	CB-CG-CD2	-7.77	87.38	110.70
7	LJ	112	MET	CA-CB-CG	7.66	129.41	114.10
14	LR	115	LEU	CD1-CG-CD2	-7.33	94.67	110.80
7	LJ	115	GLN	N-CA-CB	6.30	119.48	110.16
46	L4	110	LEU	CB-CG-CD2	-6.26	91.92	110.70
42	Lx	139	LYS	CD-CE-NZ	-6.25	91.89	111.90
14	LR	111	ILE	CG1-CB-CG2	-6.24	91.97	110.70
40	Lv	126	ALA	CA-C-N	6.17	136.74	122.31
40	Lv	126	ALA	C-N-CA	6.17	136.74	122.31
40	Lv	166	PHE	CB-CA-C	6.16	118.59	109.29
7	LJ	159	PRO	CA-C-N	-6.06	113.39	122.24
7	LJ	159	PRO	C-N-CA	-6.06	113.39	122.24
40	Lv	166	PHE	N-CA-CB	-6.06	101.42	111.06
14	LR	137	GLU	CA-CB-CG	6.01	126.13	114.10
46	L4	134	LYS	CA-C-N	-5.93	113.47	121.71
46	L4	134	LYS	C-N-CA	-5.93	113.47	121.71
14	LR	136	LEU	CA-C-N	5.91	132.83	121.54
14	LR	136	LEU	C-N-CA	5.91	132.83	121.54
22	Lb	55	LYS	N-CA-C	-5.89	106.01	113.43
14	LR	137	GLU	N-CA-CB	-5.80	100.68	110.49
7	LJ	111	LEU	CA-CB-CG	5.76	136.47	116.30
7	LJ	163	GLU	CA-C-N	-5.75	112.97	120.44
7	LJ	163	GLU	C-N-CA	-5.75	112.97	120.44
18	LV	161	ARG	CB-CA-C	-5.71	109.97	116.54
22	Lb	239	GLN	N-CA-CB	5.64	119.76	110.39
6	LI	141	GLU	N-CA-CB	5.56	119.62	110.39
32	Lm	81	MET	CB-CG-SD	5.55	129.35	112.70
37	Lr	101	GLU	CA-C-N	-5.53	112.44	120.29
37	Lr	101	GLU	C-N-CA	-5.53	112.44	120.29
20	LX	112	GLU	CA-C-N	5.48	132.65	121.48
20	LX	112	GLU	C-N-CA	5.48	132.65	121.48
4	LC	126	ASP	CA-C-N	-5.38	114.13	122.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	LC	126	ASP	C-N-CA	-5.38	114.13	122.09
32	Lm	42	GLU	N-CA-CB	5.35	119.28	110.39
45	L3	11	ARG	CA-CB-CG	5.32	124.73	114.10
7	LJ	160	LYS	CA-C-O	5.31	130.54	122.20
7	LJ	168	LEU	CB-CG-CD1	5.30	126.61	110.70
7	LJ	95	MET	CG-SD-CE	-5.29	89.26	100.90
4	LC	77	LEU	CA-C-O	-5.27	112.97	120.51
11	LO	255	MET	CB-CG-SD	5.22	128.36	112.70
3	LB	227	GLN	CA-C-N	5.19	128.57	120.68
3	LB	227	GLN	C-N-CA	5.19	128.57	120.68
42	Lx	76	GLU	N-CA-CB	5.18	118.84	110.40
6	LI	87	LYS	CA-C-N	5.12	131.33	121.54
6	LI	87	LYS	C-N-CA	5.12	131.33	121.54
32	Lm	228	GLU	N-CA-CB	5.03	118.74	110.39

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
46	L4	89	ASP	Peptide
6	LI	69	ARG	Sidechain
7	LJ	159	PRO	Peptide
7	LJ	169	ARG	Sidechain
8	LK	57	THR	Peptide
8	LK	60	ILE	Peptide
11	LO	39	ARG	Sidechain
13	LQ	110	ILE	Peptide
16	LT	122	ARG	Sidechain
18	LV	129	VAL	Peptide
22	Lb	172	GLN	Peptide
31	Ll	288	SER	Peptide
37	Lr	122	ASN	Peptide
40	Lv	127	MET	Peptide
40	Lv	165	THR	Peptide
52	Sf	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	L1	31847	0	16178	214	0
2	L2	1191	0	607	13	0
3	LB	1851	0	1909	15	0
4	LC	2393	0	2398	46	0
5	LD	2013	0	2044	25	0
6	LI	784	0	832	20	0
7	LJ	1283	0	1370	39	0
8	LK	1330	0	1407	27	0
9	LM	1451	0	1448	25	0
10	LN	889	0	941	8	0
11	LO	2305	0	2378	25	0
12	LP	1779	0	1808	17	0
13	LQ	1245	0	1283	19	0
14	LR	1189	0	1180	31	0
15	LS	1822	0	1859	19	0
16	LT	1153	0	1214	17	0
17	LU	1284	0	1354	21	0
18	LV	1368	0	1410	21	0
19	LW	1188	0	1180	14	0
20	LX	1652	0	1658	28	0
21	La	871	0	898	17	0
22	Lb	2035	0	2054	20	0
23	Lu	1517	0	1561	16	0
24	Ld	978	0	1030	18	0
25	Lf	880	0	902	11	0
26	Lg	433	0	475	4	0
27	Lh	376	0	406	7	0
28	Li	831	0	883	14	0
29	Lj	341	0	361	6	0
30	Lk	3210	0	3206	44	0
31	Ll	2947	0	2841	60	0
32	Lm	2382	0	2393	28	0
33	Ln	836	0	844	20	0
34	Lo	997	0	987	23	0
35	Lp	815	0	792	14	0
36	Lq	1178	0	1180	21	0
37	Lr	2217	0	2220	24	0
38	Ls	1754	0	1732	25	0
39	Lt	1762	0	1767	40	0
40	Lv	1039	0	1044	31	0
41	Lw	1097	0	1085	21	0
42	Lx	895	0	881	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
43	Ly	827	0	857	6	0
44	Lz	732	0	730	7	0
45	L3	743	0	758	21	0
46	L4	703	0	693	14	0
47	L5	372	0	387	11	0
48	L6	797	0	804	17	0
49	L7	1058	0	1083	12	0
50	L8	1076	0	1049	14	0
51	SR	1203	0	1219	23	0
52	Sf	3036	0	3022	38	0
53	L1	91	0	0	0	0
53	L6	1	0	0	0	0
53	LB	1	0	0	0	0
53	La	1	0	0	0	0
53	Lw	1	0	0	0	0
54	L1	42	0	38	4	0
55	Lf	1	0	0	0	0
55	Lj	1	0	0	0	0
55	SR	1	0	0	0	0
All	All	100095	0	84640	1044	0

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

All (1044) 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)
9:LM:81:THR:O	9:LM:86:GLY:HA3	1.60	1.01
29:Lj:76:CYS:SG	29:Lj:98:HIS:CE1	2.65	0.90
38:Ls:160:LEU:O	38:Ls:164:VAL:HB	1.72	0.90
46:L4:110:LEU:HD13	46:L4:117:TYR:HA	1.56	0.87
46:L4:132:LEU:O	46:L4:136:LYS:HB2	1.76	0.85
45:L3:12:PRO:O	45:L3:69:GLY:N	2.16	0.77
7:LJ:163:GLU:HA	7:LJ:166:ARG:HG2	1.66	0.77
2:L2:1609:U:O2	2:L2:1616:A:N6	2.19	0.75
30:Lk:126:THR:HG22	30:Lk:372:ASN:HB2	1.70	0.74
18:LV:133:ASN:ND2	38:Ls:232:MET:SD	2.62	0.73
31:Ll:187:VAL:HG23	31:Ll:319:PHE:HB3	1.71	0.72
10:LN:120:LYS:HE3	15:LS:156:GLU:HG2	1.71	0.71
13:LQ:88:LYS:O	13:LQ:92:VAL:HB	1.91	0.71
2:L2:1607:U:H3	2:L2:1664:G:H1	1.39	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Lv:127:MET:HB2	40:Lv:154:GLU:HB3	1.74	0.70
10:LN:55:PRO:HB3	10:LN:77:ILE:HG12	1.74	0.70
20:LX:121:LYS:HD2	20:LX:130:PRO:HB2	1.73	0.69
27:Lh:72:THR:HG23	27:Lh:75:GLY:H	1.56	0.69
42:Lx:75:LYS:HZ2	42:Lx:82:LEU:HB3	1.56	0.69
31:Ll:175:VAL:HG22	31:Ll:204:VAL:HG13	1.73	0.69
1:L1:1343:G:HO2'	29:Lj:66:PHE:N	1.90	0.69
18:LV:55:ASN:ND2	18:LV:74:TYR:O	2.26	0.68
21:La:101:LYS:HD3	40:Lv:56:ILE:HG21	1.74	0.68
7:LJ:161:VAL:HA	7:LJ:164:MET:HE2	1.76	0.68
6:LI:53:THR:N	6:LI:86:THR:HG1	1.91	0.68
30:Lk:272:ASP:OD2	30:Lk:274:LYS:NZ	2.27	0.67
7:LJ:134:PHE:O	7:LJ:138:SER:HB2	1.93	0.67
1:L1:393:G:N2	21:La:56:MET:SD	2.67	0.67
31:Ll:212:SER:HB2	31:Ll:274:LYS:HE2	1.75	0.67
17:LU:125:GLY:N	17:LU:160:VAL:O	2.27	0.67
21:La:125:VAL:HG11	31:Ll:64:GLU:HG2	1.77	0.66
39:Lt:74:LEU:HD22	47:L5:42:ARG:HB3	1.76	0.66
40:Lv:92:ASN:OD1	40:Lv:158:GLN:NE2	2.28	0.66
40:Lv:60:LYS:HA	40:Lv:63:ILE:HG22	1.77	0.66
40:Lv:129:THR:HA	40:Lv:152:THR:O	1.96	0.66
31:Ll:214:TRP:HB2	31:Ll:240:ILE:HB	1.78	0.66
1:L1:438:G:N7	12:LP:67:LYS:NZ	2.43	0.65
1:L1:211:A:OP2	41:Lw:111:ARG:NH2	2.30	0.65
31:Ll:179:VAL:O	31:Ll:183:ASP:HB3	1.96	0.65
1:L1:433:A:HO2'	24:Ld:35:LYS:N	1.93	0.65
16:LT:111:LYS:NZ	17:LU:139:ASP:OD1	2.30	0.65
48:L6:44:GLU:OE2	48:L6:48:TRP:NE1	2.26	0.65
37:Lr:215:ILE:HG23	37:Lr:219:LEU:HD12	1.79	0.65
39:Lt:151:ARG:NH1	39:Lt:254:TRP:O	2.28	0.65
46:L4:105:LYS:HZ3	46:L4:110:LEU:HA	1.61	0.65
45:L3:13:VAL:HA	45:L3:68:PHE:HA	1.77	0.65
4:LC:57:ASN:HD22	13:LQ:146:ASN:HD22	1.45	0.64
12:LP:90:LEU:HD13	12:LP:159:LEU:HD23	1.79	0.64
28:Li:175:ASP:HB3	28:Li:178:GLN:HG2	1.80	0.64
1:L1:197:A:H62	1:L1:625:C:H5	1.43	0.64
1:L1:861:U:O4	3:LB:246:ARG:NH2	2.31	0.64
35:Lp:44:ASN:ND2	36:Lq:135:ASN:OD1	2.31	0.64
45:L3:64:VAL:HB	45:L3:76:MET:HB2	1.79	0.64
1:L1:394:A:OP1	21:La:101:LYS:NZ	2.31	0.64
20:LX:27:GLY:HA2	20:LX:32:LYS:HE3	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
52:Sf:227:ASP:OD1	52:Sf:230:ARG:NH2	2.31	0.63
1:L1:875:U:H5''	1:L1:876:G:H5'	1.79	0.63
12:LP:218:ILE:HG23	12:LP:223:MET:HB2	1.80	0.63
20:LX:177:THR:HG22	34:Lo:71:LYS:H	1.64	0.63
52:Sf:201:ASP:OD2	52:Sf:242:ARG:NH1	2.32	0.63
30:Lk:201:ARG:HG2	30:Lk:232:THR:HG22	1.81	0.63
47:L5:57:VAL:HG12	47:L5:63:THR:HG22	1.81	0.63
45:L3:15:GLN:HG3	45:L3:67:LEU:HB2	1.81	0.62
29:Lj:76:CYS:SG	29:Lj:98:HIS:HE1	2.16	0.62
39:Lt:177:GLU:O	39:Lt:190:ARG:NH2	2.33	0.62
40:Lv:96:THR:HB	40:Lv:154:GLU:HG2	1.80	0.62
14:LR:133:GLN:O	14:LR:137:GLU:HB2	2.00	0.62
14:LR:38:VAL:HB	14:LR:41:GLU:HG3	1.81	0.62
32:Lm:247:ASN:ND2	32:Lm:251:ILE:O	2.32	0.62
45:L3:14:LYS:NZ	45:L3:68:PHE:O	2.29	0.62
33:Ln:113:ARG:O	33:Ln:117:LEU:HB2	2.00	0.61
8:LK:86:THR:HG23	8:LK:89:TYR:H	1.64	0.61
39:Lt:143:LYS:HG3	39:Lt:144:ASN:H	1.64	0.61
46:L4:76:ASN:ND2	46:L4:80:GLU:O	2.33	0.61
1:L1:725:A:OP1	30:Lk:173:ARG:NH1	2.32	0.61
36:Lq:35:ARG:HG3	48:L6:101:TRP:HB2	1.83	0.61
1:L1:320:G:OP1	3:LB:269:ARG:NH1	2.29	0.61
51:SR:166:GLY:O	51:SR:171:ARG:NH1	2.34	0.61
2:L2:1621:A:OP2	14:LR:112:LYS:NZ	2.33	0.61
18:LV:68:ARG:O	38:Ls:230:ARG:HD3	2.00	0.61
52:Sf:319:GLN:HA	52:Sf:322:VAL:HB	1.82	0.61
6:LI:115:LYS:O	6:LI:118:LEU:O	2.19	0.61
12:LP:134:LYS:NZ	12:LP:143:GLY:O	2.34	0.61
14:LR:62:ARG:NH2	21:La:137:LYS:O	2.34	0.61
39:Lt:273:ARG:HA	39:Lt:276:VAL:HG12	1.82	0.61
1:L1:142:C:OP1	18:LV:50:LYS:NZ	2.33	0.60
7:LJ:188:ARG:HD2	45:L3:55:VAL:HG13	1.82	0.60
19:LW:27:GLN:HG2	23:Lu:113:LEU:HB3	1.83	0.60
1:L1:393:G:H1'	21:La:57:GLU:HG3	1.83	0.60
4:LC:129:VAL:O	4:LC:190:GLY:N	2.34	0.60
20:LX:64:ILE:O	20:LX:71:GLY:N	2.33	0.60
31:LI:157:LEU:O	31:LI:161:LEU:N	2.34	0.60
6:LI:98:LEU:HB2	6:LI:110:ASP:HB2	1.82	0.60
52:Sf:152:GLN:HA	52:Sf:156:TYR:HB2	1.83	0.60
1:L1:746:U:H4'	34:Lo:52:GLN:HB3	1.83	0.60
20:LX:124:ASP:HB2	20:LX:152:ARG:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:LC:69:ASP:OD1	4:LC:154:ARG:NH1	2.35	0.60
5:LD:282:PRO:O	5:LD:290:TYR:OH	2.19	0.60
1:L1:719:C:H5''	30:Lk:301:PRO:HB3	1.83	0.60
1:L1:901:G:H1	1:L1:916:U:H3	1.50	0.60
14:LR:124:CYS:SG	14:LR:156:SER:OG	2.58	0.60
38:Ls:86:ASP:O	38:Ls:196:GLN:NE2	2.35	0.60
4:LC:127:CYS:HB2	4:LC:193:LEU:O	2.02	0.60
7:LJ:47:LEU:HD22	12:LP:226:ILE:HG12	1.84	0.60
31:Ll:173:LEU:HD13	31:Ll:272:LEU:HD22	1.83	0.60
4:LC:129:VAL:HB	4:LC:191:THR:HG22	1.83	0.60
35:Lp:104:GLU:HG2	35:Lp:107:PRO:HD2	1.81	0.60
17:LU:53:LYS:NZ	17:LU:58:SER:OG	2.35	0.60
19:LW:64:PRO:HB2	19:LW:100:ALA:HB3	1.84	0.60
21:La:100:THR:OG1	21:La:132:HIS:NE2	2.35	0.60
12:LP:98:HIS:HB3	12:LP:151:VAL:HG12	1.84	0.59
39:Lt:200:MET:HE1	39:Lt:238:LEU:HG	1.84	0.59
4:LC:68:GLU:OE1	4:LC:154:ARG:NH2	2.35	0.59
5:LD:175:LYS:HG2	5:LD:273:LEU:HD13	1.83	0.59
8:LK:73:LYS:O	8:LK:76:ARG:N	2.35	0.59
39:Lt:264:LEU:HD22	39:Lt:269:LEU:HB3	1.83	0.59
6:LI:115:LYS:O	6:LI:118:LEU:C	2.46	0.59
16:LT:33:GLY:O	16:LT:36:ASN:ND2	2.36	0.59
52:Sf:239:ASN:HB2	52:Sf:299:PHE:HB2	1.83	0.59
1:L1:110:U:O2'	19:LW:83:ARG:NH2	2.33	0.59
4:LC:45:SER:O	32:Lm:307:ARG:NH2	2.35	0.59
28:Li:146:GLU:OE1	31:Ll:364:ARG:NH1	2.36	0.59
1:L1:107:A:N6	1:L1:110:U:OP2	2.32	0.59
1:L1:706:A:O2'	34:Lo:28:ARG:NH1	2.32	0.59
39:Lt:51:LEU:HD11	39:Lt:188:ALA:HA	1.84	0.59
3:LB:228:LEU:O	3:LB:231:LYS:N	2.35	0.59
36:Lq:79:TYR:HB2	36:Lq:83:ALA:HB3	1.84	0.59
52:Sf:242:ARG:NH2	52:Sf:290:ASP:OD2	2.35	0.59
1:L1:37:C:O2	30:Lk:80:ARG:NH2	2.35	0.59
1:L1:667:A:H5''	34:Lo:28:ARG:HE	1.68	0.59
7:LJ:62:PRO:HA	7:LJ:65:LEU:HB2	1.85	0.59
13:LQ:52:MET:HE1	13:LQ:123:ILE:HG21	1.84	0.59
31:Ll:202:PRO:HD2	31:Ll:235:TRP:HZ3	1.68	0.59
39:Lt:49:GLY:HA2	39:Lt:232:PHE:HB3	1.85	0.59
1:L1:77:G:OP2	1:L1:79:C:N4	2.35	0.59
1:L1:216:G:H1	43:Ly:61:GLY:HA3	1.68	0.59
38:Ls:197:VAL:HG22	38:Ls:212:ILE:HG12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LJ:162:LYS:HB3	7:LJ:166:ARG:HH12	1.67	0.58
19:LW:18:ARG:NH2	20:LX:206:GLU:OE1	2.36	0.58
23:Lu:93:LYS:HE2	34:Lo:70:LEU:HD11	1.84	0.58
31:Ll:67:ALA:O	31:Ll:75:ARG:NH2	2.35	0.58
14:LR:53:ARG:NH1	31:Ll:155:TYR:OH	2.36	0.58
7:LJ:136:GLU:HA	7:LJ:141:GLN:HG2	1.84	0.58
19:LW:29:VAL:HG23	19:LW:41:GLN:HB3	1.85	0.58
15:LS:182:ARG:HD2	15:LS:218:ASN:HB3	1.83	0.58
32:Lm:179:PHE:O	32:Lm:298:GLN:HA	2.04	0.58
4:LC:248:ILE:HG22	4:LC:250:ARG:HG2	1.85	0.58
48:L6:10:GLY:HA3	51:SR:167:PRO:HG3	1.86	0.58
20:LX:80:ILE:HB	20:LX:85:TRP:HB2	1.85	0.58
31:Ll:177:TYR:O	31:Ll:184:LEU:HA	2.04	0.58
1:L1:8:C:O2	20:LX:42:ARG:NH1	2.35	0.58
8:LK:109:ALA:O	8:LK:171:ARG:NH1	2.37	0.58
52:Sf:185:VAL:HG23	52:Sf:195:LEU:HD13	1.85	0.58
5:LD:103:GLN:HE22	5:LD:249:ASN:HB2	1.69	0.58
11:LO:252:LEU:HD13	11:LO:255:MET:HE3	1.85	0.58
20:LX:76:VAL:HG12	20:LX:88:VAL:HG22	1.85	0.58
30:Lk:229:ARG:NH1	30:Lk:231:SER:OG	2.37	0.57
32:Lm:157:ALA:O	35:Lp:93:LYS:NZ	2.35	0.57
1:L1:488:U:OP1	51:SR:182:ARG:NH2	2.37	0.57
7:LJ:166:ARG:HA	7:LJ:169:ARG:HG2	1.85	0.57
21:La:84:GLY:O	21:La:87:LYS:N	2.36	0.57
1:L1:867:G:O2'	1:L1:964:U:OP2	2.22	0.57
1:L1:402:A:OP2	31:Ll:27:ARG:N	2.37	0.57
1:L1:575:A:H2'	51:SR:189:ARG:HE	1.68	0.57
51:SR:90:SER:HA	51:SR:93:ILE:HG12	1.87	0.57
5:LD:234:THR:O	50:L8:25:TYR:N	2.37	0.57
10:LN:129:LYS:NZ	15:LS:123:ASP:OD1	2.37	0.57
32:Lm:73:THR:HG1	32:Lm:99:TYR:HH	1.52	0.57
6:Ll:84:GLU:OE1	22:Lb:44:ARG:NH1	2.37	0.57
1:L1:551:C:O2'	1:L1:553:A:N6	2.38	0.57
37:Lr:259:ARG:HB2	37:Lr:271:PHE:HB2	1.87	0.57
1:L1:973:G:O2'	1:L1:975:G:OP2	2.23	0.57
3:LB:194:ASN:ND2	3:LB:245:GLY:O	2.37	0.57
52:Sf:92:MET:HE2	52:Sf:276:ARG:HE	1.70	0.57
4:LC:307:TYR:HA	4:LC:310:LEU:HD13	1.86	0.57
5:LD:70:ARG:HA	5:LD:196:PRO:HD3	1.87	0.57
46:L4:76:ASN:HD22	46:L4:82:GLN:H	1.53	0.57
1:L1:201:A:N3	28:Li:104:ARG:NH2	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Ld:82:GLU:OE1	24:Ld:115:HIS:NE2	2.29	0.56
39:Lt:94:GLU:HG3	39:Lt:116:LEU:HD12	1.87	0.56
49:L7:111:ILE:O	49:L7:116:ARG:NH2	2.38	0.56
1:L1:144:A:N3	1:L1:192:U:O2'	2.35	0.56
1:L1:1184:U:H4'	28:Li:138:PRO:HG2	1.87	0.56
7:LJ:47:LEU:HA	48:L6:35:MET:HE1	1.87	0.56
8:LK:71:LEU:HB2	8:LK:79:GLU:HB2	1.86	0.56
9:LM:67:PHE:HB3	9:LM:71:LYS:HB2	1.87	0.56
19:LW:16:GLN:HG2	34:Lo:55:GLU:HA	1.86	0.56
20:LX:124:ASP:OD2	20:LX:152:ARG:NH1	2.38	0.56
30:Lk:146:HIS:O	30:Lk:194:LYS:NZ	2.38	0.56
45:L3:11:ARG:HD3	45:L3:12:PRO:HD3	1.86	0.56
1:L1:738:U:H2'	1:L1:739:A:H8	1.71	0.56
37:Lr:160:LEU:HD21	37:Lr:223:MET:HB2	1.87	0.56
38:Ls:119:GLN:HA	38:Ls:122:ILE:HB	1.88	0.56
52:Sf:257:VAL:HG23	52:Sf:390:LYS:HE3	1.87	0.56
52:Sf:81:ARG:O	52:Sf:85:LYS:HB3	2.06	0.56
1:L1:652:C:H4'	1:L1:653:A:H5''	1.87	0.56
5:LD:186:ASP:OD2	11:LO:21:ARG:NH1	2.38	0.56
1:L1:1070:A:H2'	1:L1:1071:A:C8	2.41	0.56
7:LJ:160:LYS:HG2	7:LJ:163:GLU:OE1	2.04	0.56
17:LU:95:LEU:HD23	17:LU:138:ALA:HB2	1.88	0.56
9:LM:20:LEU:HD22	9:LM:141:LEU:HD13	1.88	0.56
14:LR:111:ILE:HG22	14:LR:115:LEU:HD11	1.88	0.56
20:LX:131:THR:HG22	20:LX:149:ARG:HD2	1.87	0.56
1:L1:179:C:OP2	11:LO:53:HIS:NE2	2.39	0.56
4:LC:234:THR:O	4:LC:236:THR:N	2.39	0.56
14:LR:51:ASN:HB3	14:LR:54:ASN:HB2	1.87	0.56
14:LR:164:MET:HE3	14:LR:169:VAL:HG21	1.86	0.56
1:L1:791:A:H4'	4:LC:235:LYS:HB3	1.88	0.56
5:LD:59:ARG:HE	5:LD:84:PRO:HB2	1.71	0.56
23:Lu:83:ALA:HB3	34:Lo:74:VAL:HB	1.88	0.56
39:Lt:54:GLN:HA	39:Lt:157:LEU:O	2.05	0.55
1:L1:385:U:H2'	1:L1:386:G:H8	1.71	0.55
17:LU:94:ARG:HG3	36:Lq:126:ILE:HG12	1.87	0.55
2:L2:1642:G:H2'	2:L2:1643:A:C8	2.42	0.55
6:LI:146:LEU:HD23	6:LI:147:ARG:HG2	1.87	0.55
30:Lk:276:ASP:OD1	52:Sf:158:ARG:NH1	2.40	0.55
40:Lv:129:THR:HG1	40:Lv:153:HIS:HD1	1.54	0.55
1:L1:603:A:O2'	16:LT:16:ASP:OD2	2.24	0.55
4:LC:109:LEU:HD21	4:LC:337:VAL:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:LD:49:ARG:NH1	5:LD:81:ASP:O	2.37	0.55
37:Lr:80:GLN:O	37:Lr:210:ARG:NH2	2.39	0.55
18:LV:157:ARG:HB2	18:LV:167:MET:HG3	1.87	0.55
32:Lm:189:LEU:O	32:Lm:295:ARG:NH2	2.40	0.55
40:Lv:137:LEU:HB2	40:Lv:145:LEU:HG	1.89	0.55
52:Sf:369:PHE:HB3	52:Sf:424:PHE:HE2	1.70	0.55
6:LI:107:VAL:N	6:LI:110:ASP:OD2	2.38	0.55
8:LK:154:ARG:NH1	8:LK:155:VAL:O	2.39	0.55
13:LQ:110:ILE:O	13:LQ:120:MET:HB2	2.07	0.55
40:Lv:131:THR:HG22	40:Lv:151:THR:HG22	1.89	0.55
51:SR:38:VAL:HA	51:SR:50:GLU:O	2.07	0.55
1:L1:411:U:H2'	1:L1:412:G:C8	2.42	0.55
6:LI:115:LYS:HB3	6:LI:118:LEU:HB3	1.89	0.55
23:Lu:187:PRO:HD2	23:Lu:190:LEU:HD12	1.87	0.55
25:Lf:110:CYS:HB2	25:Lf:117:LYS:HD2	1.89	0.55
31:Ll:235:TRP:NE1	31:Ll:237:LEU:HB2	2.22	0.55
52:Sf:369:PHE:HB3	52:Sf:424:PHE:CE2	2.42	0.55
1:L1:652:C:OP1	25:Lf:139:ARG:NH2	2.40	0.55
41:Lw:68:THR:OG1	41:Lw:72:TRP:N	2.40	0.55
1:L1:1070:A:N3	1:L1:1251:A:O2'	2.37	0.54
38:Ls:126:LYS:NZ	38:Ls:132:PHE:O	2.32	0.54
52:Sf:300:HIS:HB2	52:Sf:361:ILE:HG12	1.89	0.54
1:L1:911:A:O2'	1:L1:912:A:N7	2.36	0.54
21:La:115:ASP:OD1	21:La:119:ARG:NH1	2.39	0.54
28:Li:172:TYR:HB2	28:Li:175:ASP:HB2	1.89	0.54
47:L5:72:ARG:NE	47:L5:74:MET:O	2.39	0.54
4:LC:104:LEU:HG	15:LS:91:LYS:HB2	1.90	0.54
13:LQ:43:GLU:OE1	25:Lf:127:TYR:OH	2.24	0.54
45:L3:63:CYS:SG	45:L3:64:VAL:N	2.80	0.54
50:L8:40:PRO:HG3	50:L8:51:GLN:HB3	1.88	0.54
1:L1:122:G:N7	27:Lh:87:ARG:NH2	2.47	0.54
12:LP:191:SER:H	12:LP:194:THR:HG1	1.56	0.54
14:LR:109:TRP:CD1	14:LR:113:LYS:HZ2	2.26	0.54
40:Lv:92:ASN:HB3	40:Lv:94:HIS:CE1	2.43	0.54
1:L1:132:A:C6	1:L1:135:A:C6	2.95	0.54
14:LR:73:SER:O	14:LR:146:GLN:NE2	2.41	0.54
20:LX:170:TRP:CZ3	23:Lu:80:LYS:HE3	2.43	0.54
39:Lt:183:THR:HG22	39:Lt:185:ARG:H	1.72	0.54
5:LD:167:MET:SD	5:LD:276:GLN:NE2	2.73	0.54
16:LT:77:GLN:NE2	16:LT:81:LEU:O	2.40	0.54
32:Lm:276:PHE:HB2	32:Lm:304:VAL:HG22	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LX:54:TRP:NE1	20:LX:56:LEU:O	2.41	0.53
31:Ll:187:VAL:HG11	31:Ll:270:PHE:CE2	2.43	0.53
39:Lt:74:LEU:HD23	39:Lt:77:ILE:HD11	1.89	0.53
1:L1:148:A:HO2'	18:LV:146:THR:HG1	1.55	0.53
31:Ll:332:HIS:O	49:L7:129:ARG:NH2	2.41	0.53
6:LI:98:LEU:O	6:LI:109:GLY:N	2.42	0.53
8:LK:49:PHE:CE1	8:LK:80:ILE:HG12	2.44	0.53
1:L1:395:A:OP1	40:Lv:48:TYR:N	2.42	0.53
6:LI:58:ARG:HH21	22:Lb:67:ILE:HD13	1.73	0.53
33:Ln:139:MET:HE1	40:Lv:169:ILE:HG12	1.91	0.53
38:Ls:194:VAL:HA	38:Ls:214:VAL:HG22	1.89	0.53
4:LC:208:ALA:HB2	4:LC:297:VAL:HG12	1.90	0.53
13:LQ:108:LEU:HD13	25:Lf:122:LEU:HD21	1.89	0.53
14:LR:137:GLU:OE2	31:Ll:188:TYR:HB3	2.09	0.53
1:L1:468:U:O2'	1:L1:481:A:N3	2.39	0.53
27:Lh:88:LYS:HE3	34:Lo:18:MET:HE3	1.90	0.53
33:Ln:109:GLU:OE1	33:Ln:113:ARG:NH1	2.42	0.53
1:L1:429:U:H2'	1:L1:430:C:C6	2.44	0.53
2:L2:1609:U:C2	2:L2:1616:A:N6	2.77	0.53
30:Lk:215:ARG:NH2	30:Lk:367:ASN:OD1	2.41	0.53
39:Lt:82:SER:OG	39:Lt:83:LEU:N	2.41	0.53
50:L8:127:LYS:HG2	50:L8:131:MET:HE2	1.91	0.53
1:L1:841:C:H3'	1:L1:842:A:H8	1.74	0.53
1:L1:1263:G:N2	1:L1:1266:U:O2	2.40	0.53
9:LM:178:LEU:HD13	51:SR:35:PHE:HE2	1.74	0.53
13:LQ:45:PRO:HG2	13:LQ:48:ARG:HH11	1.74	0.53
32:Lm:114:ASP:HB2	32:Lm:117:LYS:HB2	1.91	0.53
37:Lr:230:GLU:O	37:Lr:233:LYS:NZ	2.42	0.53
38:Ls:125:ILE:HG23	38:Ls:252:LEU:HD11	1.89	0.53
1:L1:197:A:N1	1:L1:349:G:O2'	2.40	0.53
52:Sf:63:ILE:HD13	52:Sf:66:TRP:HE1	1.74	0.53
1:L1:570:C:H5'	9:LM:29:GLY:HA3	1.91	0.52
4:LC:213:LYS:HG3	4:LC:261:MET:HE3	1.91	0.52
20:LX:102:MET:HG3	20:LX:103:ASP:H	1.74	0.52
31:Ll:308:GLN:OE1	44:Lz:110:LYS:N	2.34	0.52
1:L1:265:A:O2'	1:L1:266:A:O5'	2.27	0.52
4:LC:234:THR:HG22	4:LC:235:LYS:H	1.73	0.52
20:LX:129:LYS:HG2	20:LX:130:PRO:HD2	1.90	0.52
33:Ln:160:GLU:O	39:Lt:207:ASN:ND2	2.42	0.52
51:SR:124:ARG:NH1	51:SR:153:ARG:O	2.42	0.52
52:Sf:316:CYS:HB3	52:Sf:319:GLN:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:283:A:O2'	1:L1:793:A:OP1	2.27	0.52
9:LM:25:MET:O	9:LM:149:ARG:NH1	2.42	0.52
1:L1:237:A:N3	1:L1:1260:U:O2'	2.40	0.52
34:Lo:86:LEU:HD21	34:Lo:91:LEU:HD12	1.91	0.52
39:Lt:160:LEU:HG	39:Lt:171:TRP:HB3	1.91	0.52
40:Lv:121:VAL:HG22	40:Lv:159:ILE:HG22	1.92	0.52
50:L8:137:GLN:HA	50:L8:140:ARG:HG2	1.92	0.52
1:L1:1537:A:N1	4:LC:165:TYR:OH	2.34	0.52
9:LM:20:LEU:HB2	9:LM:141:LEU:HD22	1.90	0.52
14:LR:129:ARG:HD2	31:Ll:132:LEU:HD21	1.91	0.52
16:LT:122:ARG:HE	17:LU:66:LEU:HD22	1.75	0.52
20:LX:76:VAL:HA	20:LX:88:VAL:HA	1.91	0.52
32:Lm:180:CYS:HA	32:Lm:297:PHE:O	2.09	0.52
13:LQ:26:ILE:HG13	15:LS:264:TRP:HD1	1.75	0.52
48:L6:68:ARG:O	48:L6:72:GLU:HG2	2.10	0.52
30:Lk:354:PHE:HB3	30:Lk:417:LEU:HD11	1.91	0.52
31:Ll:85:LYS:HZ1	31:Ll:88:ILE:HG23	1.74	0.52
10:LN:126:SER:HA	10:LN:129:LYS:HD3	1.92	0.52
19:LW:37:GLU:HB3	19:LW:104:THR:HG23	1.92	0.52
47:L5:54:VAL:HG21	47:L5:68:TYR:HB3	1.92	0.52
6:LI:53:THR:N	6:LI:86:THR:OG1	2.43	0.52
47:L5:51:LEU:HB3	47:L5:67:ARG:HB3	1.91	0.52
52:Sf:73:ALA:O	52:Sf:79:LYS:NZ	2.43	0.52
1:L1:307:U:H2'	1:L1:308:A:H8	1.75	0.52
39:Lt:138:THR:OG1	39:Lt:150:ASN:O	2.26	0.52
46:L4:107:LEU:HA	46:L4:110:LEU:HD12	1.91	0.52
17:LU:130:LEU:HB2	17:LU:156:VAL:HB	1.92	0.51
52:Sf:191:HIS:O	52:Sf:428:ARG:NH2	2.37	0.51
7:LJ:190:GLY:O	7:LJ:194:TYR:HD2	1.93	0.51
17:LU:119:GLU:HG2	17:LU:189:PRO:HB2	1.93	0.51
52:Sf:90:LYS:NZ	52:Sf:232:GLN:OE1	2.42	0.51
36:Lq:85:ARG:NH2	36:Lq:87:GLU:OE2	2.44	0.51
1:L1:84:G:N7	28:Li:105:LYS:NZ	2.51	0.51
1:L1:98:G:O6	23:Lu:229:LYS:NZ	2.36	0.51
7:LJ:148:VAL:O	45:L3:31:ARG:NH1	2.44	0.51
24:Ld:68:ILE:HD11	24:Ld:122:LEU:HD13	1.92	0.51
50:L8:147:GLN:HA	50:L8:150:LYS:HG2	1.91	0.51
1:L1:2:C:O2'	18:LV:149:ARG:O	2.26	0.51
1:L1:28:C:O2'	1:L1:32:A:N3	2.38	0.51
25:Lf:118:GLN:HB2	25:Lf:121:VAL:HG22	1.92	0.51
37:Lr:220:ILE:HG23	37:Lr:223:MET:HE2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:Lv:95:LEU:HD21	40:Lv:106:TYR:HB3	1.93	0.51
1:L1:517:C:O3'	8:LK:106:LYS:NZ	2.44	0.51
24:Ld:43:GLU:O	24:Ld:47:GLN:HG2	2.11	0.51
1:L1:487:U:OP1	51:SR:182:ARG:NH1	2.43	0.51
1:L1:829:U:OP2	1:L1:834:A:N6	2.34	0.51
24:Ld:134:MET:HG3	44:Lz:71:GLU:HG3	1.93	0.51
28:Li:106:THR:HG23	28:Li:162:THR:HA	1.92	0.51
7:LJ:97:ALA:HB3	7:LJ:154:LEU:HB2	1.93	0.51
7:LJ:189:GLN:HA	7:LJ:192:ILE:HG12	1.93	0.51
13:LQ:141:HIS:O	13:LQ:147:GLN:NE2	2.40	0.51
41:Lw:73:GLN:O	41:Lw:88:ARG:NH1	2.35	0.51
1:L1:346:C:OP2	11:LO:59:ARG:NH1	2.44	0.51
9:LM:25:MET:SD	51:SR:148:ASN:ND2	2.84	0.51
10:LN:87:VAL:HG12	10:LN:127:LEU:HD11	1.93	0.51
31:Ll:45:LEU:HD23	31:Ll:48:LEU:HD12	1.93	0.51
1:L1:333:A:OP2	1:L1:1064:A:O2'	2.28	0.50
11:LO:31:PRO:HG2	48:L6:86:ARG:HH12	1.76	0.50
32:Lm:256:ARG:HD3	32:Lm:261:ILE:HG12	1.93	0.50
3:LB:235:GLN:HB3	3:LB:294:SER:HA	1.93	0.50
30:Lk:60:PHE:HB3	30:Lk:67:VAL:HG12	1.92	0.50
31:Ll:179:VAL:HG23	31:Ll:183:ASP:HB3	1.92	0.50
1:L1:667:A:OP1	34:Lo:28:ARG:NH2	2.45	0.50
9:LM:168:ARG:NH1	9:LM:170:TRP:O	2.43	0.50
18:LV:133:ASN:ND2	38:Ls:226:ASP:OD2	2.36	0.50
31:Ll:233:LEU:HD12	31:Ll:298:PHE:CD1	2.46	0.50
42:Lx:97:LYS:NZ	42:Lx:120:MET:O	2.42	0.50
8:LK:48:GLN:NE2	8:LK:52:GLU:OE2	2.44	0.50
9:LM:71:LYS:HG2	51:SR:174:MET:HE3	1.93	0.50
11:LO:142:GLU:HB2	11:LO:162:LEU:HD23	1.92	0.50
13:LQ:26:ILE:HG13	15:LS:264:TRP:CD1	2.45	0.50
19:LW:1:MET:HE1	34:Lo:39:LYS:HB2	1.92	0.50
30:Lk:211:ALA:HB1	30:Lk:322:LEU:HD22	1.93	0.50
40:Lv:106:TYR:OH	40:Lv:174:ILE:O	2.30	0.50
1:L1:164:U:OP2	36:Lq:116:ARG:NH1	2.42	0.50
1:L1:704:A:N6	52:Sf:272:PRO:O	2.40	0.50
36:Lq:44:ARG:NH2	48:L6:99:LYS:O	2.43	0.50
15:LS:209:GLN:HE21	15:LS:211:PRO:HG3	1.76	0.50
49:L7:44:SER:OG	49:L7:46:ASP:OD1	2.24	0.50
1:L1:849:G:N7	3:LB:230:SER:OG	2.40	0.50
3:LB:201:GLY:O	30:Lk:30:ALA:N	2.45	0.50
14:LR:110:ALA:HB3	14:LR:111:ILE:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:59:U:OP2	22:Lb:100:ARG:NH1	2.44	0.50
1:L1:423:U:O2	1:L1:596:U:O2'	2.30	0.50
1:L1:1283:U:H5''	29:Lj:71:VAL:HG22	1.94	0.50
3:LB:110:LEU:HD22	30:Lk:30:ALA:HB2	1.93	0.50
31:Ll:73:THR:HG22	31:Ll:75:ARG:H	1.76	0.50
37:Lr:92:PHE:HE1	37:Lr:175:VAL:HG13	1.76	0.50
4:LC:111:THR:O	4:LC:114:GLY:N	2.44	0.50
12:LP:142:GLY:O	21:La:38:SER:OG	2.30	0.50
30:Lk:309:LEU:O	30:Lk:313:MET:HG3	2.12	0.50
33:Ln:113:ARG:O	33:Ln:117:LEU:CB	2.60	0.50
1:L1:39:G:H4'	23:Lu:192:LYS:HG2	1.94	0.49
12:LP:132:THR:HG22	12:LP:147:ILE:HA	1.94	0.49
13:LQ:20:LEU:H	13:LQ:24:SER:HB2	1.76	0.49
15:LS:96:ARG:HA	15:LS:99:MET:HG3	1.93	0.49
22:Lb:118:ILE:O	22:Lb:168:ARG:NH1	2.44	0.49
36:Lq:133:PHE:CG	37:Lr:259:ARG:HD2	2.47	0.49
1:L1:8:C:N4	1:L1:103:A:OP2	2.37	0.49
1:L1:340:U:OP2	43:Ly:115:ARG:NH1	2.45	0.49
17:LU:175:ARG:HB2	17:LU:180:PHE:HB3	1.94	0.49
30:Lk:343:GLN:HG2	30:Lk:356:VAL:HG22	1.94	0.49
41:Lw:66:TYR:CE2	41:Lw:74:PRO:HD3	2.47	0.49
4:LC:102:LEU:HD12	4:LC:150:LYS:HD2	1.95	0.49
12:LP:78:GLU:OE2	12:LP:158:ARG:NH1	2.45	0.49
31:Ll:256:PRO:HG2	31:Ll:330:ILE:HD12	1.93	0.49
37:Lr:227:GLU:OE2	37:Lr:302:ARG:HD3	2.13	0.49
42:Lx:75:LYS:HA	42:Lx:75:LYS:HE3	1.94	0.49
1:L1:29:C:N4	23:Lu:198:ARG:O	2.44	0.49
1:L1:472:A:O2'	1:L1:592:C:OP1	2.24	0.49
17:LU:68:ASP:N	17:LU:68:ASP:OD1	2.44	0.49
19:LW:150:TRP:CH2	38:Ls:264:LYS:HE3	2.47	0.49
30:Lk:165:GLN:HE21	30:Lk:179:VAL:HG11	1.78	0.49
33:Ln:160:GLU:HA	33:Ln:163:LYS:HG2	1.95	0.49
34:Lo:16:ASP:OD1	34:Lo:25:ARG:NH2	2.46	0.49
47:L5:58:LYS:HG2	47:L5:62:SER:HB2	1.94	0.49
1:L1:1152:C:O2'	1:L1:1245:C:OP2	2.26	0.49
1:L1:1393:G:O2'	1:L1:1396:C:OP2	2.22	0.49
19:LW:36:PRO:HD3	52:Sf:270:LYS:HB3	1.94	0.49
31:Ll:299:ARG:H	31:Ll:303:PHE:HE2	1.59	0.49
33:Ln:168:LEU:HD21	39:Lt:206:GLY:HA2	1.93	0.49
36:Lq:36:ASP:HA	48:L6:100:LYS:HG2	1.94	0.49
8:LK:52:GLU:HB3	8:LK:56:ARG:HE	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:LR:109:TRP:CD1	14:LR:113:LYS:HG3	2.48	0.49
25:Lf:129:LYS:NZ	38:Ls:292:GLU:OE2	2.33	0.49
32:Lm:64:LYS:HD2	32:Lm:80:VAL:HG12	1.95	0.49
1:L1:725:A:O2'	30:Lk:384:GLN:NE2	2.43	0.49
22:Lb:34:GLU:OE1	22:Lb:36:ARG:HG2	2.12	0.49
30:Lk:384:GLN:N	30:Lk:404:VAL:O	2.46	0.49
52:Sf:306:LEU:HD13	52:Sf:323:VAL:HG21	1.95	0.49
1:L1:1332:G:H2'	1:L1:1333:A:H8	1.77	0.49
4:LC:109:LEU:HD13	4:LC:119:VAL:HG11	1.95	0.49
11:LO:115:PRO:HD3	11:LO:255:MET:HG2	1.95	0.49
1:L1:362:G:O2'	1:L1:1195:C:O2	2.26	0.49
30:Lk:121:LEU:HD21	30:Lk:128:LEU:HB2	1.95	0.49
36:Lq:25:GLN:HA	36:Lq:80:LEU:HD12	1.95	0.49
48:L6:15:ARG:HB3	48:L6:18:ILE:HG12	1.94	0.49
52:Sf:240:GLN:NE2	52:Sf:284:VAL:O	2.45	0.49
7:LJ:193:ASN:O	7:LJ:197:LEU:HB2	2.12	0.48
8:LK:113:THR:HG23	8:LK:115:LYS:H	1.78	0.48
8:LK:114:LEU:HA	8:LK:117:VAL:HG12	1.94	0.48
17:LU:82:LYS:O	17:LU:86:MET:HG3	2.13	0.48
33:Ln:177:HIS:O	39:Lt:60:SER:N	2.43	0.48
1:L1:389:C:O2'	1:L1:409:C:N4	2.42	0.48
1:L1:405:U:O2'	1:L1:1163:A:N7	2.40	0.48
1:L1:788:A:O2'	4:LC:215:PHE:O	2.25	0.48
1:L1:1007:A:H2'	1:L1:1008:A:C8	2.48	0.48
24:Ld:71:ARG:NH1	24:Ld:73:LYS:O	2.45	0.48
39:Lt:168:GLN:HB3	39:Lt:170:VAL:HG22	1.96	0.48
40:Lv:122:GLU:HB2	40:Lv:158:GLN:HG3	1.94	0.48
52:Sf:207:HIS:ND1	52:Sf:234:ASP:OD1	2.38	0.48
1:L1:315:G:OP1	1:L1:317:G:O2'	2.29	0.48
1:L1:928:A:H3'	1:L1:955:C:H42	1.77	0.48
9:LM:135:GLU:O	9:LM:139:LYS:HG3	2.13	0.48
9:LM:168:ARG:HA	51:SR:91:GLN:HE22	1.78	0.48
1:L1:74:A:OP2	28:Li:108:LYS:NZ	2.42	0.48
1:L1:90:G:OP2	50:L8:59:LYS:NZ	2.38	0.48
3:LB:126:VAL:HA	3:LB:142:VAL:HG12	1.96	0.48
31:Ll:64:GLU:O	31:Ll:69:HIS:NE2	2.46	0.48
4:LC:218:VAL:HG13	4:LC:258:PRO:HD3	1.95	0.48
4:LC:221:ARG:HA	4:LC:261:MET:SD	2.53	0.48
6:LI:120:ARG:NH1	22:Lb:136:ASP:OD2	2.47	0.48
31:Ll:375:PRO:O	49:L7:141:ARG:NH2	2.47	0.48
43:Ly:53:MET:HE3	43:Ly:53:MET:HB3	1.74	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L3:18:VAL:HG12	45:L3:64:VAL:HG22	1.95	0.48
4:LC:221:ARG:HG3	4:LC:261:MET:HB2	1.95	0.48
5:LD:230:ILE:O	5:LD:234:THR:OG1	2.31	0.48
19:LW:143:ARG:HG2	32:Lm:80:VAL:HG21	1.96	0.48
26:Lg:55:LEU:H	50:L8:128:MET:HE3	1.78	0.48
1:L1:844:C:H2'	1:L1:845:U:H6	1.79	0.48
1:L1:1074:U:O2'	1:L1:1076:U:O4	2.30	0.48
4:LC:80:LEU:HA	4:LC:84:PRO:HG3	1.96	0.48
32:Lm:44:ARG:HB3	32:Lm:261:ILE:HD12	1.96	0.48
36:Lq:16:HIS:HB3	36:Lq:19:LEU:HD12	1.95	0.48
36:Lq:37:GLY:O	36:Lq:44:ARG:NH1	2.44	0.48
45:L3:17:ARG:HH22	45:L3:19:GLN:HB2	1.78	0.48
1:L1:292:A:OP2	1:L1:831:C:N4	2.46	0.48
1:L1:103:A:OP1	37:Lr:31:VAL:N	2.47	0.48
1:L1:622:G:C8	16:LT:11:ARG:HG2	2.49	0.48
1:L1:1398:G:OP2	1:L1:1398:G:N2	2.40	0.48
1:L1:1482:C:OP1	15:LS:141:SER:OG	2.31	0.48
11:LO:286:THR:HB	41:Lw:37:ARG:HB2	1.96	0.48
13:LQ:84:ASP:OD2	25:Lf:149:PHE:HA	2.14	0.48
1:L1:795:U:H2'	1:L1:796:A:C8	2.49	0.48
1:L1:1272:C:H2'	1:L1:1273:G:H8	1.79	0.48
36:Lq:136:LYS:O	37:Lr:259:ARG:NH2	2.46	0.48
37:Lr:59:ARG:HH21	37:Lr:184:PHE:HB2	1.79	0.48
38:Ls:131:ASN:OD1	38:Ls:133:LYS:NZ	2.45	0.48
4:LC:87:ILE:HG23	4:LC:317:PRO:HG2	1.96	0.47
8:LK:47:ASN:OD1	8:LK:48:GLN:N	2.47	0.47
20:LX:62:VAL:HG12	20:LX:122:LEU:HD23	1.95	0.47
30:Lk:212:THR:HG21	30:Lk:273:VAL:HG13	1.96	0.47
34:Lo:53:ILE:HB	34:Lo:56:MET:HB2	1.96	0.47
40:Lv:96:THR:HG22	40:Lv:183:ARG:HB3	1.95	0.47
41:Lw:144:THR:O	41:Lw:146:THR:N	2.46	0.47
1:L1:697:A:N3	23:Lu:123:ARG:NH2	2.63	0.47
1:L1:1156:G:OP1	21:La:49:ARG:NH1	2.37	0.47
6:LI:134:PRO:HA	6:LI:137:LYS:HG2	1.96	0.47
7:LJ:80:ARG:HB3	7:LJ:84:ARG:NH1	2.29	0.47
14:LR:101:VAL:HG12	14:LR:102:VAL:HG23	1.96	0.47
31:Ll:323:TRP:NE1	31:Ll:339:GLU:OE2	2.46	0.47
8:LK:188:GLU:HB3	8:LK:192:LYS:HE3	1.95	0.47
32:Lm:51:GLU:HG2	32:Lm:221:VAL:HG23	1.96	0.47
4:LC:275:ARG:HB3	4:LC:284:TYR:HB2	1.95	0.47
5:LD:241:ASN:OD1	5:LD:256:HIS:NE2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Ll:190:GLY:N	31:Ll:318:PHE:O	2.48	0.47
34:Lo:90:GLN:O	34:Lo:94:GLU:HG2	2.14	0.47
45:L3:91:ALA:O	45:L3:95:ARG:HG3	2.14	0.47
1:L1:457:A:H4'	1:L1:581:A:C5	2.50	0.47
1:L1:1002:A:OP1	18:LV:111:LYS:NZ	2.37	0.47
9:LM:138:LEU:HD23	9:LM:141:LEU:HD12	1.95	0.47
9:LM:178:LEU:HD12	51:SR:100:LEU:HD21	1.95	0.47
14:LR:90:GLU:HG2	14:LR:105:SER:HB3	1.96	0.47
24:Ld:46:PHE:CZ	24:Ld:111:LYS:HG2	2.50	0.47
40:Lv:181:GLY:HA3	47:L5:64:ILE:HD11	1.95	0.47
9:LM:168:ARG:HA	51:SR:91:GLN:NE2	2.30	0.47
23:Lu:198:ARG:NH1	27:Lh:70:LEU:O	2.47	0.47
31:Ll:217:LEU:HD13	31:Ll:236:LEU:HD13	1.96	0.47
32:Lm:158:PHE:C	35:Lp:93:LYS:HZ1	2.23	0.47
1:L1:611:A:H5''	36:Lq:36:ASP:HB3	1.97	0.47
1:L1:819:C:O2'	1:L1:951:G:OP1	2.30	0.47
1:L1:1397:U:OP1	4:LC:234:THR:OG1	2.24	0.47
1:L1:1408:C:H2'	1:L1:1409:G:C8	2.50	0.47
2:L2:1621:A:O5'	31:Ll:99:ARG:NH2	2.48	0.47
4:LC:96:ARG:NH2	4:LC:197:HIS:O	2.41	0.47
5:LD:181:LYS:NZ	5:LD:253:MET:O	2.42	0.47
11:LO:237:ALA:HB2	11:LO:244:LEU:HD13	1.95	0.47
14:LR:141:ASN:OD1	49:L7:184:ASN:ND2	2.32	0.47
21:La:121:PRO:HA	31:Ll:50:LYS:HD3	1.96	0.47
24:Ld:71:ARG:HD3	24:Ld:86:ILE:HD12	1.97	0.47
32:Lm:142:TYR:HH	32:Lm:301:SER:HG	1.60	0.47
33:Ln:173:LYS:NZ	33:Ln:174:GLU:O	2.44	0.47
40:Lv:170:PHE:O	40:Lv:174:ILE:HG12	2.14	0.47
45:L3:27:VAL:O	45:L3:31:ARG:HG3	2.14	0.47
46:L4:122:ARG:O	46:L4:126:ILE:HG12	2.14	0.47
7:LJ:86:ILE:HA	7:LJ:89:VAL:HG22	1.97	0.47
18:LV:94:ILE:HD13	18:LV:106:LEU:HD11	1.96	0.47
22:Lb:7:PRO:HD2	22:Lb:10:LEU:HD12	1.96	0.47
14:LR:133:GLN:O	14:LR:137:GLU:CB	2.63	0.47
23:Lu:191:ASN:O	23:Lu:195:ASN:ND2	2.48	0.47
39:Lt:55:ARG:HG2	39:Lt:238:LEU:HD22	1.96	0.47
31:Ll:236:LEU:O	31:Ll:251:THR:OG1	2.31	0.47
41:Lw:141:ASN:HB3	41:Lw:146:THR:HG22	1.97	0.47
1:L1:560:A:H62	1:L1:1305:G:H21	1.63	0.46
1:L1:751:G:H5''	34:Lo:24:LYS:HG2	1.96	0.46
4:LC:202:GLN:NE2	4:LC:301:ASP:OD1	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:LT:29:ARG:HA	16:LT:29:ARG:HD3	1.75	0.46
17:LU:129:ARG:NH2	17:LU:151:LYS:O	2.48	0.46
31:Ll:176:ALA:HA	31:Ll:185:MET:O	2.15	0.46
31:Ll:195:PRO:HA	31:Ll:198:ALA:HB3	1.96	0.46
52:Sf:111:LYS:HG3	52:Sf:212:ARG:HH21	1.80	0.46
13:LQ:110:ILE:HG13	13:LQ:120:MET:HB3	1.97	0.46
16:LT:89:ASN:ND2	16:LT:120:ALA:O	2.35	0.46
40:Lv:166:PHE:CD1	40:Lv:169:ILE:HD12	2.50	0.46
1:L1:307:U:H2'	1:L1:308:A:C8	2.51	0.46
1:L1:564:C:O2'	1:L1:1018:C:O2'	2.26	0.46
1:L1:795:U:H4'	15:LS:260:TRP:HH2	1.79	0.46
4:LC:128:HIS:HA	4:LC:191:THR:O	2.15	0.46
31:Ll:217:LEU:O	31:Ll:270:PHE:HA	2.16	0.46
37:Lr:93:VAL:HG22	37:Lr:180:LEU:HD12	1.97	0.46
20:LX:36:PRO:HD2	20:LX:39:ILE:HB	1.97	0.46
20:LX:156:LYS:NZ	20:LX:157:PRO:O	2.43	0.46
33:Ln:125:LYS:HA	33:Ln:128:GLU:HG2	1.98	0.46
33:Ln:177:HIS:N	39:Lt:58:VAL:O	2.49	0.46
34:Lo:99:ALA:HA	34:Lo:102:LYS:HE3	1.97	0.46
37:Lr:91:ALA:O	37:Lr:122:ASN:ND2	2.47	0.46
47:L5:58:LYS:HE2	47:L5:60:ASP:HB3	1.97	0.46
1:L1:265:A:O2'	1:L1:266:A:O4'	2.29	0.46
3:LB:140:ALA:HB2	3:LB:153:ALA:HB2	1.96	0.46
1:L1:192:U:H2'	1:L1:193:A:C8	2.50	0.46
16:LT:16:ASP:OD1	16:LT:16:ASP:N	2.45	0.46
30:Lk:147:ILE:HD13	30:Lk:187:LEU:HG	1.97	0.46
1:L1:79:C:O2'	11:LO:80:LYS:NZ	2.49	0.46
1:L1:1202:C:O2'	21:La:88:CYS:SG	2.73	0.46
28:Li:162:THR:OG1	28:Li:167:LYS:NZ	2.48	0.46
34:Lo:46:SER:OG	34:Lo:47:GLY:N	2.43	0.46
41:Lw:90:ARG:HB3	41:Lw:91:MET:HE2	1.98	0.46
1:L1:706:A:HO2'	34:Lo:28:ARG:HH11	1.60	0.46
1:L1:1198:C:OP1	28:Li:124:ARG:NH2	2.49	0.46
39:Lt:184:LEU:HB3	39:Lt:234:PHE:HZ	1.78	0.46
40:Lv:129:THR:OG1	40:Lv:153:HIS:ND1	2.44	0.46
46:L4:76:ASN:ND2	46:L4:82:GLN:H	2.13	0.46
1:L1:524:U:C2	7:LJ:125:VAL:HG11	2.50	0.46
1:L1:842:A:O2'	1:L1:871:C:OP1	2.27	0.46
7:LJ:93:ASN:HD21	7:LJ:155:VAL:HB	1.81	0.46
22:Lb:132:LEU:HD23	22:Lb:132:LEU:HA	1.83	0.46
22:Lb:161:LEU:O	22:Lb:165:MET:HG3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:Li:101:LYS:HB3	28:Li:103:LYS:HD3	1.97	0.46
37:Lr:245:LEU:HD12	37:Lr:253:PRO:HD3	1.97	0.46
39:Lt:94:GLU:HA	39:Lt:97:ARG:HG2	1.98	0.46
48:L6:12:ILE:HG13	48:L6:23:ARG:HB2	1.97	0.46
1:L1:1301:A:O2'	12:LP:182:LYS:O	2.33	0.45
7:LJ:134:PHE:O	7:LJ:138:SER:CB	2.62	0.45
25:Lf:159:LEU:HD11	25:Lf:174:ILE:HD12	1.98	0.45
35:Lp:69:TYR:O	35:Lp:72:THR:OG1	2.32	0.45
48:L6:65:VAL:O	48:L6:69:GLU:HG3	2.16	0.45
49:L7:106:ALA:HA	49:L7:116:ARG:HD3	1.98	0.45
51:SR:37:GLU:O	51:SR:51:GLY:HA2	2.16	0.45
1:L1:424:G:H2'	1:L1:425:U:H6	1.81	0.45
6:LI:98:LEU:HD11	6:LI:105:VAL:HG12	1.98	0.45
24:Ld:86:ILE:HG12	24:Ld:113:VAL:HG21	1.98	0.45
1:L1:4:A:N7	18:LV:47:ILE:N	2.65	0.45
1:L1:416:A:H2'	1:L1:417:U:C6	2.52	0.45
1:L1:603:A:N1	1:L1:623:A:O2'	2.48	0.45
1:L1:893:U:O2	1:L1:897:G:C6	2.70	0.45
11:LO:207:PRO:HD2	11:LO:210:LEU:HB2	1.98	0.45
1:L1:648:A:H2'	1:L1:649:A:C8	2.51	0.45
11:LO:190:PRO:HB2	41:Lw:51:LEU:HD21	1.99	0.45
47:L5:57:VAL:HA	47:L5:62:SER:O	2.17	0.45
51:SR:58:LYS:HE3	51:SR:58:LYS:HB2	1.82	0.45
1:L1:223:A:H4'	1:L1:224:G:H5'	1.99	0.45
18:LV:68:ARG:HE	38:Ls:230:ARG:HD2	1.81	0.45
37:Lr:161:THR:O	37:Lr:192:GLN:NE2	2.49	0.45
38:Ls:196:GLN:HB3	38:Ls:213:THR:HB	1.97	0.45
38:Ls:251:GLN:NE2	38:Ls:254:ASN:HB2	2.32	0.45
1:L1:1238:U:H4'	26:Lg:62:ILE:HG21	1.99	0.45
23:Lu:128:SER:OG	23:Lu:131:ARG:NE	2.33	0.45
27:Lh:58:ILE:HG22	34:Lo:30:PHE:CZ	2.52	0.45
28:Li:108:LYS:HA	28:Li:108:LYS:HD3	1.77	0.45
30:Lk:113:LEU:HD12	30:Lk:311:ALA:HB1	1.99	0.45
31:Ll:138:GLU:O	31:Ll:142:THR:HG22	2.17	0.45
33:Ln:146:ALA:HB1	39:Lt:209:PRO:HB2	1.99	0.45
41:Lw:98:LYS:HB2	41:Lw:98:LYS:HE2	1.80	0.45
42:Lx:105:ALA:HB1	42:Lx:111:VAL:HG22	1.99	0.45
47:L5:58:LYS:O	47:L5:61:GLY:N	2.36	0.45
1:L1:940:U:H3	1:L1:952:G:H1	1.65	0.45
8:LK:130:PHE:O	8:LK:133:GLN:O	2.35	0.45
14:LR:134:ARG:O	14:LR:137:GLU:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Ld:100:HIS:HB3	24:Ld:106:VAL:HG11	1.99	0.45
30:Lk:203:CYS:O	52:Sf:179:GLN:NE2	2.35	0.45
38:Ls:213:THR:HG23	38:Ls:247:VAL:HG22	1.99	0.45
39:Lt:146:ARG:NH2	39:Lt:259:GLU:HG3	2.32	0.45
51:SR:99:MET:HE3	51:SR:99:MET:HB3	1.88	0.45
1:L1:209:G:OP1	5:LD:92:ARG:NH1	2.43	0.45
32:Lm:40:LEU:HA	32:Lm:43:MET:HG3	1.98	0.45
1:L1:359:A:O2'	1:L1:454:A:N6	2.50	0.45
1:L1:404:A:O2'	24:Ld:37:THR:HG21	2.17	0.45
1:L1:663:G:H2'	1:L1:664:C:C6	2.52	0.45
1:L1:800:G:N2	1:L1:803:A:N6	2.65	0.45
1:L1:1280:U:H2'	1:L1:1281:A:H8	1.81	0.45
4:LC:236:THR:HG22	4:LC:239:ARG:HD3	1.99	0.45
6:LI:55:ILE:HD13	22:Lb:44:ARG:HD3	1.98	0.45
11:LO:197:GLY:HA3	50:L8:62:ALA:HB2	1.98	0.45
20:LX:216:TYR:HE1	23:Lu:191:ASN:HD22	1.65	0.45
50:L8:112:GLN:OE1	50:L8:115:ARG:NH2	2.46	0.45
52:Sf:66:TRP:O	52:Sf:69:THR:OG1	2.27	0.45
52:Sf:85:LYS:HE3	52:Sf:86:MET:HE2	1.98	0.45
1:L1:310:A:H5'	27:Lh:58:ILE:HD11	1.99	0.45
1:L1:761:C:OP2	1:L1:763:C:N4	2.35	0.45
3:LB:235:GLN:HB2	3:LB:292:MET:HE2	1.99	0.45
22:Lb:110:PHE:CD2	22:Lb:129:MET:HE3	2.52	0.45
37:Lr:120:LYS:HA	37:Lr:120:LYS:HD2	1.85	0.45
47:L5:55:LEU:HA	47:L5:64:ILE:O	2.17	0.45
5:LD:195:LEU:HB2	5:LD:229:SER:HB3	1.99	0.44
14:LR:109:TRP:HA	14:LR:112:LYS:HD3	1.99	0.44
16:LT:33:GLY:O	16:LT:37:ARG:NH1	2.50	0.44
31:Ll:275:GLN:HG2	31:Ll:311:MET:HB3	1.98	0.44
45:L3:20:PHE:HZ	45:L3:31:ARG:HA	1.82	0.44
1:L1:99:C:N3	5:LD:104:LYS:NZ	2.65	0.44
1:L1:181:G:H2'	1:L1:1023:A:N7	2.32	0.44
8:LK:113:THR:HG22	8:LK:116:HIS:ND1	2.32	0.44
11:LO:249:LYS:HE3	11:LO:249:LYS:HB2	1.88	0.44
14:LR:121:VAL:HG12	14:LR:156:SER:HB2	1.98	0.44
20:LX:170:TRP:NE1	20:LX:172:ASP:OD1	2.51	0.44
40:Lv:96:THR:OG1	40:Lv:153:HIS:O	2.33	0.44
1:L1:65:A:H5''	6:LI:69:ARG:NH2	2.33	0.44
1:L1:545:C:H3'	1:L1:546:A:H8	1.83	0.44
5:LD:99:VAL:HG21	5:LD:173:GLY:HA3	1.98	0.44
32:Lm:109:ASP:OD2	32:Lm:121:LYS:NZ	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ln:164:ARG:HB3	40:Lv:86:TYR:HB3	1.98	0.44
41:Lw:94:ILE:HD11	41:Lw:162:LEU:HG	1.99	0.44
1:L1:328:U:H1'	27:Lh:52:GLU:HG3	1.98	0.44
3:LB:157:MET:HE3	3:LB:157:MET:HB2	1.92	0.44
3:LB:176:ALA:HB1	3:LB:244:VAL:HG11	2.00	0.44
32:Lm:269:ILE:HD12	32:Lm:274:ILE:HB	1.99	0.44
42:Lx:139:LYS:HZ3	48:L6:101:TRP:CD1	2.35	0.44
52:Sf:63:ILE:HA	52:Sf:66:TRP:CD1	2.52	0.44
1:L1:48:A:OP2	6:LI:75:ARG:NH2	2.50	0.44
1:L1:166:A:C8	35:Lp:134:LYS:HG3	2.52	0.44
1:L1:263:C:O3'	30:Lk:395:ARG:NH2	2.48	0.44
4:LC:217:GLY:HA2	4:LC:258:PRO:HB3	2.00	0.44
5:LD:181:LYS:HD3	5:LD:181:LYS:HA	1.82	0.44
8:LK:140:VAL:O	8:LK:144:ILE:HG12	2.18	0.44
11:LO:184:LEU:HA	11:LO:187:VAL:HG12	1.99	0.44
38:Ls:190:GLU:OE2	38:Ls:215:ARG:NH2	2.47	0.44
52:Sf:212:ARG:HD3	52:Sf:379:LEU:HB3	2.00	0.44
1:L1:397:C:H5'	40:Lv:60:LYS:HD2	1.99	0.44
1:L1:439:A:H61	1:L1:1311:A:H2	1.66	0.44
7:LJ:95:MET:HE1	7:LJ:121:ILE:CD1	2.47	0.44
16:LT:89:ASN:HD21	16:LT:124:ARG:HB2	1.83	0.44
17:LU:155:ARG:NH2	17:LU:157:GLU:OE2	2.49	0.44
17:LU:162:GLU:HB3	17:LU:192:VAL:HB	1.98	0.44
30:Lk:132:LEU:HB2	30:Lk:137:LEU:HD21	1.99	0.44
35:Lp:107:PRO:HA	35:Lp:110:GLU:HG2	2.00	0.44
46:L4:105:LYS:HZ3	46:L4:110:LEU:HD23	1.82	0.44
9:LM:28:PRO:HG2	9:LM:67:PHE:HE1	1.81	0.44
23:Lu:71:PRO:HA	23:Lu:74:TRP:CD2	2.53	0.44
49:L7:110:TRP:CD1	49:L7:110:TRP:H	2.35	0.44
51:SR:39:VAL:O	51:SR:49:ILE:HA	2.18	0.44
1:L1:1504:U:H2'	1:L1:1505:A:C8	2.53	0.44
2:L2:1626:C:O2'	33:Ln:133:ARG:NH2	2.48	0.44
8:LK:60:ILE:N	46:L4:77:ILE:O	2.44	0.44
9:LM:151:ILE:HD13	9:LM:151:ILE:HA	1.83	0.44
13:LQ:79:TRP:NE1	15:LS:267:PHE:O	2.46	0.44
32:Lm:112:PRO:HB2	32:Lm:267:PRO:HG3	1.99	0.44
45:L3:78:GLY:HA2	45:L3:81:LEU:HB2	1.98	0.44
1:L1:156:G:H4'	1:L1:158:A:C2	2.53	0.44
4:LC:252:TRP:O	4:LC:255:THR:OG1	2.30	0.44
30:Lk:140:VAL:HB	30:Lk:416:ALA:HB2	1.99	0.44
30:Lk:152:GLU:HA	30:Lk:155:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:Lk:232:THR:HG23	30:Lk:289:HIS:HB2	1.98	0.44
31:Ll:352:PRO:O	31:Ll:369:TYR:OH	2.35	0.44
38:Ls:118:SER:HA	38:Ls:197:VAL:O	2.18	0.44
38:Ls:157:HIS:O	38:Ls:161:HIS:ND1	2.51	0.44
52:Sf:381:THR:O	52:Sf:385:GLN:HG2	2.18	0.44
4:LC:141:LYS:HE3	4:LC:141:LYS:HB3	1.84	0.43
7:LJ:95:MET:HG2	7:LJ:181:ILE:CD1	2.48	0.43
30:Lk:229:ARG:HH21	30:Lk:288:PRO:HG3	1.82	0.43
44:Lz:93:LEU:O	44:Lz:97:LYS:HG2	2.17	0.43
45:L3:20:PHE:CE2	45:L3:31:ARG:HG2	2.52	0.43
52:Sf:318:ASP:OD1	52:Sf:318:ASP:N	2.51	0.43
1:L1:282:U:H2'	1:L1:283:A:C8	2.53	0.43
4:LC:217:GLY:O	4:LC:221:ARG:HB2	2.18	0.43
12:LP:104:MET:HE3	12:LP:104:MET:HB3	1.85	0.43
16:LT:115:SER:OG	35:Lp:60:CYS:SG	2.76	0.43
23:Lu:91:ARG:NH1	34:Lo:83:GLU:OE2	2.50	0.43
30:Lk:128:LEU:HD11	30:Lk:376:VAL:HB	1.99	0.43
32:Lm:73:THR:OG1	32:Lm:99:TYR:OH	2.23	0.43
32:Lm:139:ASN:HB3	32:Lm:174:VAL:HG21	2.00	0.43
32:Lm:198:ASN:HD22	35:Lp:92:LEU:HD22	1.83	0.43
35:Lp:67:ILE:HG23	36:Lq:138:THR:HG21	2.00	0.43
38:Ls:267:PRO:HG2	38:Ls:270:ALA:HB2	1.99	0.43
1:L1:801:G:O2'	1:L1:984:U:O4	2.32	0.43
7:LJ:126:PHE:HA	7:LJ:127:PRO:HD3	1.91	0.43
16:LT:20:ARG:O	16:LT:23:GLU:HG3	2.17	0.43
29:Lj:90:VAL:O	29:Lj:99:LYS:HA	2.18	0.43
30:Lk:139:LEU:HD11	30:Lk:423:ALA:HB3	2.01	0.43
30:Lk:165:GLN:HE22	30:Lk:175:THR:HB	1.83	0.43
38:Ls:251:GLN:HE21	38:Ls:254:ASN:HB2	1.83	0.43
40:Lv:92:ASN:CB	40:Lv:94:HIS:CE1	3.01	0.43
10:LN:127:LEU:HA	10:LN:130:ARG:HG2	2.00	0.43
1:L1:386:G:H2'	1:L1:387:C:H6	1.82	0.43
1:L1:899:C:H2'	1:L1:923:G:H5''	2.01	0.43
2:L2:1643:A:OP1	31:Ll:114:ARG:NH2	2.38	0.43
11:LO:79:PRO:HD3	28:Li:127:ALA:HA	2.00	0.43
22:Lb:108:GLN:HG2	22:Lb:110:PHE:CE2	2.53	0.43
39:Lt:203:LYS:HB2	39:Lt:239:LEU:HD11	2.01	0.43
33:Ln:114:ARG:HE	39:Lt:73:LEU:HD11	1.83	0.43
42:Lx:139:LYS:HG3	42:Lx:142:GLU:OE1	2.18	0.43
45:L3:74:LEU:HG	45:L3:76:MET:HE3	2.00	0.43
1:L1:1339:C:O2'	1:L1:1445:U:OP1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:LN:118:ARG:HA	10:LN:118:ARG:HD3	1.85	0.43
15:LS:256:GLU:O	15:LS:260:TRP:HD1	2.02	0.43
24:Ld:37:THR:HG22	24:Ld:38:ARG:H	1.84	0.43
26:Lg:46:TYR:HA	26:Lg:53:ARG:HA	1.99	0.43
31:Ll:120:GLU:HG2	31:Ll:124:ARG:HH11	1.82	0.43
32:Lm:281:SER:HB2	32:Lm:321:ARG:HG2	2.01	0.43
39:Lt:256:THR:O	39:Lt:260:LEU:HB2	2.18	0.43
41:Lw:82:LEU:HD13	41:Lw:164:LYS:HE3	1.99	0.43
1:L1:625:C:OP2	16:LT:17:ARG:NH1	2.52	0.43
1:L1:739:A:O2'	30:Lk:270:ILE:O	2.37	0.43
7:LJ:168:LEU:HD21	7:LJ:176:LEU:HB2	2.01	0.43
21:La:61:VAL:HG13	21:La:65:ASN:HB2	2.00	0.43
37:Lr:137:LEU:HD11	37:Lr:219:LEU:HD13	2.00	0.43
39:Lt:119:ASP:OD1	39:Lt:119:ASP:N	2.51	0.43
48:L6:71:PHE:CE2	48:L6:75:LYS:HD2	2.54	0.43
1:L1:1070:A:H2'	1:L1:1071:A:H8	1.84	0.43
1:L1:1323:U:O4	54:L1:1691:T1C:H953	2.18	0.43
1:L1:1504:U:H2'	1:L1:1505:A:H8	1.84	0.43
10:LN:73:ILE:HD11	10:LN:105:VAL:HG21	2.01	0.43
11:LO:286:THR:OG1	41:Lw:39:VAL:HG23	2.19	0.43
15:LS:240:ILE:HG22	15:LS:242:GLY:H	1.84	0.43
22:Lb:74:GLU:OE1	22:Lb:74:GLU:N	2.51	0.43
30:Lk:185:ILE:HD11	30:Lk:292:TYR:CZ	2.54	0.43
1:L1:567:A:OP1	51:SR:171:ARG:NH2	2.39	0.43
1:L1:623:A:N6	11:LO:37:GLU:OE2	2.32	0.43
9:LM:25:MET:HB2	9:LM:151:ILE:HD11	2.00	0.43
9:LM:59:ILE:HB	9:LM:127:LEU:HD23	2.01	0.43
18:LV:126:ASP:O	18:LV:130:ARG:HB2	2.19	0.43
39:Lt:266:PRO:HB2	39:Lt:267:LYS:H	1.54	0.43
49:L7:174:LYS:HD3	49:L7:174:LYS:HA	1.73	0.43
1:L1:192:U:H2'	1:L1:193:A:H8	1.83	0.42
8:LK:155:VAL:HB	46:L4:101:LEU:HD11	2.01	0.42
9:LM:80:HIS:HA	9:LM:86:GLY:O	2.18	0.42
15:LS:224:MET:HE3	15:LS:224:MET:HB3	1.88	0.42
17:LU:125:GLY:CA	17:LU:160:VAL:O	2.67	0.42
20:LX:86:VAL:HG21	20:LX:120:VAL:HG21	2.01	0.42
22:Lb:42:HIS:CG	22:Lb:86:ILE:HD11	2.54	0.42
22:Lb:231:VAL:HG21	34:Lo:114:LEU:HD21	2.01	0.42
31:Ll:304:TYR:CE2	31:Ll:313:PRO:HD3	2.54	0.42
31:Ll:331:PHE:CD2	31:Ll:339:GLU:HG3	2.54	0.42
39:Lt:116:LEU:HG	39:Lt:117:ALA:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
45:L3:19:GLN:HA	45:L3:54:ASP:HB3	2.01	0.42
1:L1:198:G:N7	11:LO:51:ARG:NH1	2.64	0.42
1:L1:575:A:C4	51:SR:189:ARG:HG2	2.54	0.42
1:L1:1513:U:H3	9:LM:177:ARG:H	1.66	0.42
7:LJ:46:LYS:HG2	48:L6:27:VAL:HG13	2.01	0.42
31:Ll:186:PRO:HD3	49:L7:191:LYS:HE3	2.01	0.42
1:L1:395:A:H5'	21:La:74:ARG:HE	1.83	0.42
7:LJ:174:LEU:HD12	7:LJ:174:LEU:HA	1.76	0.42
13:LQ:131:PRO:HB3	25:Lf:184:TRP:HZ3	1.84	0.42
18:LV:212:LEU:HA	36:Lq:119:PHE:HE1	1.83	0.42
19:LW:44:ILE:HD11	19:LW:93:LYS:HD2	2.01	0.42
31:Ll:229:ASP:CG	31:Ll:299:ARG:HH12	2.26	0.42
33:Ln:172:GLU:OE2	40:Lv:183:ARG:NH1	2.52	0.42
34:Lo:103:ASP:OD2	34:Lo:117:TYR:OH	2.37	0.42
37:Lr:187:PRO:HA	37:Lr:188:PRO:HD3	1.93	0.42
40:Lv:166:PHE:CE2	40:Lv:170:PHE:HE2	2.38	0.42
1:L1:1280:U:H2'	1:L1:1281:A:C8	2.54	0.42
1:L1:1408:C:H2'	1:L1:1409:G:H8	1.84	0.42
6:LI:58:ARG:HA	6:LI:80:TYR:HA	2.00	0.42
6:LI:98:LEU:HD23	6:LI:129:ALA:HB2	2.00	0.42
8:LK:55:GLU:HA	8:LK:58:LYS:HE2	2.00	0.42
9:LM:158:TYR:HD1	9:LM:162:GLU:HG3	1.85	0.42
13:LQ:62:TYR:HE2	15:LS:269:MET:HG2	1.84	0.42
36:Lq:30:SER:O	36:Lq:75:VAL:HA	2.20	0.42
39:Lt:188:ALA:O	39:Lt:191:THR:OG1	2.32	0.42
39:Lt:257:LYS:HE3	39:Lt:273:ARG:HB2	2.00	0.42
46:L4:92:TYR:HA	46:L4:93:PRO:HD3	1.92	0.42
4:LC:97:VAL:O	4:LC:197:HIS:NE2	2.51	0.42
7:LJ:116:LEU:O	7:LJ:121:ILE:HG22	2.20	0.42
14:LR:38:VAL:HG12	14:LR:40:ASN:H	1.84	0.42
16:LT:122:ARG:NH1	16:LT:142:PHE:HE2	2.18	0.42
25:Lf:133:GLU:O	25:Lf:137:ILE:HG12	2.19	0.42
31:Ll:178:ALA:HA	31:Ll:184:LEU:HG	2.02	0.42
36:Lq:72:VAL:HG13	36:Lq:90:HIS:HB2	2.01	0.42
1:L1:67:A:HO2'	43:Ly:93:ARG:HH22	1.65	0.42
1:L1:152:U:O2	1:L1:1037:A:O2'	2.37	0.42
1:L1:415:A:H2'	1:L1:416:A:C8	2.55	0.42
1:L1:892:U:O2'	3:LB:284:ARG:O	2.36	0.42
4:LC:155:PHE:HA	32:Lm:309:HIS:CE1	2.54	0.42
7:LJ:44:ARG:NH1	12:LP:234:ASP:OD2	2.31	0.42
21:La:113:ALA:O	21:La:117:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:Lr:51:LEU:HD23	37:Lr:51:LEU:HA	1.88	0.42
38:Ls:203:MET:SD	38:Ls:203:MET:N	2.90	0.42
1:L1:592:C:O2'	17:LU:175:ARG:NH2	2.53	0.42
1:L1:1134:A:H2'	1:L1:1135:A:C8	2.55	0.42
5:LD:262:THR:O	5:LD:265:THR:OG1	2.30	0.42
12:LP:89:ILE:HB	12:LP:161:VAL:HG22	2.02	0.42
12:LP:163:MET:HE2	12:LP:163:MET:HB3	1.82	0.42
19:LW:89:LYS:HA	19:LW:90:PRO:HD3	1.94	0.42
22:Lb:8:VAL:O	22:Lb:11:TRP:HB2	2.20	0.42
30:Lk:208:THR:O	52:Sf:160:ARG:NH2	2.53	0.42
30:Lk:219:LEU:HD12	30:Lk:219:LEU:HA	1.85	0.42
35:Lp:136:LEU:HD23	35:Lp:136:LEU:HA	1.91	0.42
37:Lr:79:LEU:HD21	37:Lr:173:LEU:HD22	2.01	0.42
41:Lw:96:VAL:HG22	41:Lw:110:ILE:HG12	2.01	0.42
49:L7:185:ARG:HB3	49:L7:189:ARG:HH22	1.85	0.42
52:Sf:201:ASP:HB2	52:Sf:240:GLN:HB3	2.01	0.42
1:L1:1016:G:H5'	1:L1:1434:U:H4'	2.01	0.42
1:L1:1074:U:O2	1:L1:1075:A:N6	2.51	0.42
54:L1:1691:T1C:H961	54:L1:1691:T1C:H921	1.73	0.42
2:L2:1603:A:N6	2:L2:1669:G:O6	2.53	0.42
2:L2:1611:G:N2	2:L2:1625:A:H1'	2.34	0.42
5:LD:59:ARG:HH21	5:LD:84:PRO:HB2	1.85	0.42
15:LS:143:ARG:HD3	15:LS:143:ARG:HA	1.80	0.42
36:Lq:19:LEU:HA	36:Lq:19:LEU:HD23	1.82	0.42
39:Lt:260:LEU:HG	39:Lt:264:LEU:HD12	2.01	0.42
41:Lw:144:THR:O	41:Lw:144:THR:OG1	2.36	0.42
42:Lx:139:LYS:O	42:Lx:139:LYS:HG2	2.19	0.42
1:L1:356:A:H2'	1:L1:357:A:C8	2.55	0.42
5:LD:113:LYS:HG3	5:LD:157:GLY:H	1.85	0.42
8:LK:113:THR:HG21	8:LK:115:LYS:HE2	2.01	0.42
11:LO:256:LEU:HD23	11:LO:256:LEU:HA	1.92	0.42
12:LP:205:ARG:NH2	12:LP:249:LYS:O	2.52	0.42
13:LQ:77:ASP:O	13:LQ:83:LYS:NZ	2.52	0.42
14:LR:110:ALA:HA	31:Ll:138:GLU:OE2	2.19	0.42
15:LS:96:ARG:HH11	15:LS:282:ILE:HG12	1.84	0.42
18:LV:57:ILE:O	38:Ls:227:ARG:NE	2.52	0.42
31:Ll:45:LEU:HD23	31:Ll:45:LEU:HA	1.91	0.42
50:L8:28:ARG:HH22	50:L8:31:PRO:HG3	1.84	0.42
1:L1:148:A:O2'	18:LV:146:THR:OG1	2.27	0.42
1:L1:1078:A:H2'	1:L1:1079:A:H8	1.85	0.42
1:L1:1324:U:H5''	1:L1:1390:C:N4	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L1:1330:A:H2'	1:L1:1331:G:C8	2.55	0.42
2:L2:1664:G:H2'	2:L2:1665:C:C6	2.55	0.42
3:LB:111:ARG:NH2	3:LB:165:ASN:OD1	2.42	0.42
7:LJ:115:GLN:HE21	7:LJ:167:ILE:CG2	2.33	0.42
12:LP:170:GLU:HA	12:LP:173:GLN:HB3	2.01	0.42
31:Ll:233:LEU:HD11	31:Ll:236:LEU:HB2	2.02	0.42
31:Ll:255:LEU:HD12	31:Ll:255:LEU:HA	1.92	0.42
32:Lm:142:TYR:OH	32:Lm:301:SER:OG	2.34	0.42
35:Lp:75:ILE:HD12	35:Lp:75:ILE:HA	1.95	0.42
37:Lr:86:ASP:OD1	37:Lr:87:LEU:N	2.53	0.42
41:Lw:105:ARG:NH2	48:L6:83:PRO:HD3	2.35	0.42
42:Lx:65:ASP:OD1	42:Lx:65:ASP:N	2.50	0.42
44:Lz:65:ARG:O	44:Lz:69:GLU:HG3	2.20	0.42
51:SR:40:GLU:HG2	51:SR:49:ILE:HG22	2.01	0.42
1:L1:49:G:H2'	1:L1:50:C:H6	1.85	0.41
7:LJ:121:ILE:HD11	7:LJ:154:LEU:HB3	2.02	0.41
26:Lg:60:LYS:HD2	26:Lg:60:LYS:HA	1.82	0.41
52:Sf:105:TRP:CG	52:Sf:271:LEU:HD13	2.54	0.41
1:L1:35:A:C8	34:Lo:39:LYS:HD2	2.55	0.41
5:LD:191:ASP:OD1	5:LD:192:SER:N	2.53	0.41
22:Lb:80:TRP:CE2	22:Lb:109:LEU:HD11	2.55	0.41
29:Lj:93:LYS:HB2	29:Lj:93:LYS:HE2	1.81	0.41
40:Lv:51:LYS:HD3	40:Lv:51:LYS:HA	1.87	0.41
2:L2:1603:A:H2'	2:L2:1604:G:C8	2.56	0.41
14:LR:93:VAL:HG21	14:LR:135:CYS:SG	2.61	0.41
14:LR:145:TYR:HB2	14:LR:171:LEU:HD12	2.02	0.41
21:La:83:VAL:HA	21:La:88:CYS:O	2.21	0.41
24:Ld:99:VAL:HG21	44:Lz:77:VAL:HG22	2.02	0.41
39:Lt:187:THR:HA	39:Lt:190:ARG:HG2	2.01	0.41
9:LM:177:ARG:HE	51:SR:38:VAL:HG22	1.84	0.41
24:Ld:101:LYS:HE3	44:Lz:80:LEU:HG	2.01	0.41
30:Lk:125:LYS:HG2	30:Lk:371:LYS:HG3	2.03	0.41
32:Lm:81:MET:HE2	32:Lm:86:SER:HB3	2.01	0.41
38:Ls:145:PHE:HE1	38:Ls:220:GLN:HE22	1.69	0.41
39:Lt:214:THR:HB	39:Lt:230:LYS:HD2	2.02	0.41
40:Lv:91:LEU:HD13	40:Lv:188:GLU:HA	2.03	0.41
40:Lv:95:LEU:HD11	40:Lv:106:TYR:HD2	1.85	0.41
51:SR:35:PHE:HB3	51:SR:36:ARG:H	1.75	0.41
1:L1:1075:A:O2'	22:Lb:102:LYS:O	2.24	0.41
8:LK:130:PHE:O	8:LK:133:GLN:C	2.63	0.41
18:LV:108:PHE:HE2	25:Lf:116:LEU:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:LX:144:VAL:HG13	20:LX:153:ILE:HG23	2.02	0.41
35:Lp:93:LYS:HA	35:Lp:93:LYS:HD3	1.81	0.41
43:Ly:119:LYS:O	43:Ly:123:ARG:HB2	2.20	0.41
50:L8:37:PRO:HG3	50:L8:68:SER:HA	2.03	0.41
1:L1:183:A:OP2	17:LU:177:ARG:NH1	2.42	0.41
1:L1:466:C:OP2	24:Ld:77:ARG:NH2	2.50	0.41
2:L2:1626:C:O2	33:Ln:129:ARG:NH1	2.51	0.41
4:LC:127:CYS:HB3	4:LC:193:LEU:HB2	2.01	0.41
5:LD:280:TYR:HE1	41:Lw:57:ILE:HA	1.86	0.41
11:LO:47:ARG:HB3	11:LO:48:LYS:H	1.65	0.41
14:LR:120:ASN:O	14:LR:123:ALA:HB3	2.21	0.41
15:LS:155:ILE:HG22	15:LS:156:GLU:OE1	2.20	0.41
17:LU:71:GLU:OE1	17:LU:74:ARG:NH2	2.54	0.41
18:LV:94:ILE:HD11	18:LV:117:ILE:HG21	2.02	0.41
24:Ld:123:LYS:HB2	24:Ld:144:GLU:HG2	2.03	0.41
36:Lq:133:PHE:HD1	36:Lq:136:LYS:HD2	1.84	0.41
52:Sf:332:LEU:HD13	52:Sf:372:TYR:HB2	2.02	0.41
1:L1:717:U:O2'	1:L1:736:A:N7	2.52	0.41
5:LD:49:ARG:HG3	5:LD:263:LEU:HD22	2.02	0.41
13:LQ:52:MET:HE3	13:LQ:52:MET:HB3	1.71	0.41
15:LS:96:ARG:NH1	15:LS:282:ILE:HG12	2.35	0.41
18:LV:126:ASP:OD2	18:LV:130:ARG:NH1	2.54	0.41
20:LX:51:ASP:OD1	20:LX:51:ASP:N	2.54	0.41
39:Lt:97:ARG:HA	39:Lt:100:LYS:HE2	2.02	0.41
45:L3:20:PHE:HB2	45:L3:55:VAL:HA	2.01	0.41
1:L1:1012:A:H4'	16:LT:41:LEU:HD13	2.02	0.41
1:L1:1374:A:H2'	1:L1:1375:A:C8	2.55	0.41
4:LC:165:TYR:HB3	4:LC:170:LEU:O	2.21	0.41
11:LO:28:LYS:HB2	48:L6:94:HIS:CD2	2.56	0.41
20:LX:136:ARG:HD2	20:LX:146:VAL:HG21	2.03	0.41
31:Ll:39:ASP:OD1	31:Ll:39:ASP:N	2.53	0.41
31:Ll:148:LYS:HB2	31:Ll:148:LYS:HE3	1.85	0.41
45:L3:16:VAL:HG22	45:L3:66:VAL:HG22	2.03	0.41
1:L1:264:U:P	30:Lk:395:ARG:HH22	2.44	0.41
1:L1:552:U:H2'	1:L1:553:A:N3	2.36	0.41
1:L1:800:G:N2	1:L1:803:A:C6	2.89	0.41
1:L1:804:C:O2	4:LC:231:HIS:NE2	2.48	0.41
1:L1:916:U:H2'	1:L1:917:G:H8	1.85	0.41
4:LC:322:ASP:OD1	4:LC:322:ASP:N	2.51	0.41
5:LD:224:GLU:OE2	50:L8:32:ARG:NH1	2.37	0.41
7:LJ:83:ARG:HA	7:LJ:86:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:LJ:95:MET:HE1	7:LJ:121:ILE:HD12	2.03	0.41
7:LJ:115:GLN:HE21	7:LJ:167:ILE:HG21	1.86	0.41
8:LK:149:ARG:NH1	46:L4:102:GLY:O	2.54	0.41
9:LM:19:TYR:CD1	9:LM:145:LEU:HD11	2.56	0.41
11:LO:30:ASN:O	11:LO:33:SER:OG	2.29	0.41
11:LO:182:ARG:O	11:LO:186:ILE:HG12	2.21	0.41
14:LR:108:GLU:HG3	14:LR:110:ALA:H	1.86	0.41
17:LU:76:HIS:ND1	35:Lp:50:ALA:HA	2.36	0.41
18:LV:155:ARG:O	18:LV:167:MET:N	2.47	0.41
23:Lu:218:ARG:NH2	43:Ly:105:ASP:OD1	2.54	0.41
30:Lk:185:ILE:HD13	30:Lk:185:ILE:HA	1.82	0.41
30:Lk:290:THR:HA	30:Lk:343:GLN:O	2.20	0.41
31:Ll:327:VAL:HG12	31:Ll:331:PHE:HE2	1.86	0.41
31:Ll:330:ILE:HG13	31:Ll:334:LEU:HD22	2.03	0.41
31:Ll:335:LEU:HD22	31:Ll:337:MET:HB2	2.03	0.41
41:Lw:154:ASP:OD1	41:Lw:154:ASP:N	2.54	0.41
46:L4:105:LYS:NZ	46:L4:110:LEU:HD23	2.35	0.41
49:L7:81:CYS:SG	49:L7:98:LYS:HB3	2.61	0.41
52:Sf:142:LEU:HD13	52:Sf:422:VAL:HG21	2.02	0.41
52:Sf:160:ARG:HA	52:Sf:160:ARG:HD3	1.71	0.41
1:L1:241:C:H2'	1:L1:242:A:C8	2.56	0.41
1:L1:522:A:H4'	8:LK:139:SER:HB3	2.02	0.41
4:LC:332:LEU:HD23	4:LC:332:LEU:HA	1.97	0.41
9:LM:156:ASP:OD1	9:LM:156:ASP:N	2.49	0.41
31:Ll:190:GLY:HA2	31:Ll:319:PHE:HA	2.03	0.41
37:Lr:137:LEU:HD23	37:Lr:137:LEU:HA	1.93	0.41
1:L1:347:U:O2'	1:L1:1053:A:N1	2.50	0.40
1:L1:1064:A:H2'	1:L1:1065:G:H8	1.85	0.40
1:L1:1323:U:C4	54:L1:1691:T1C:H953	2.55	0.40
7:LJ:108:ASP:HA	7:LJ:111:LEU:HG	2.03	0.40
18:LV:81:LYS:HA	18:LV:81:LYS:HD2	1.82	0.40
20:LX:131:THR:HA	20:LX:149:ARG:HH11	1.87	0.40
20:LX:188:VAL:HA	20:LX:189:PRO:HD3	1.88	0.40
22:Lb:150:LYS:HB3	22:Lb:150:LYS:HE3	1.91	0.40
31:Ll:233:LEU:HD11	31:Ll:236:LEU:HD22	2.03	0.40
1:L1:916:U:H2'	1:L1:917:G:C8	2.56	0.40
5:LD:220:ASP:O	5:LD:245:ALA:N	2.54	0.40
7:LJ:93:ASN:ND2	7:LJ:155:VAL:HB	2.36	0.40
7:LJ:104:LEU:N	45:L3:40:GLU:OE2	2.55	0.40
14:LR:134:ARG:HA	14:LR:137:GLU:HB3	2.03	0.40
30:Lk:160:HIS:HA	30:Lk:164:TRP:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:Ln:119:LYS:HE3	33:Ln:119:LYS:HB3	1.82	0.40
33:Ln:126:GLN:O	33:Ln:129:ARG:HG2	2.21	0.40
41:Lw:68:THR:HG1	41:Lw:72:TRP:N	2.19	0.40
50:L8:112:GLN:NE2	50:L8:115:ARG:HH12	2.19	0.40
1:L1:336:C:H2'	1:L1:337:U:C6	2.56	0.40
1:L1:703:A:OP1	19:LW:50:ARG:NH2	2.42	0.40
1:L1:1064:A:H2'	1:L1:1065:G:C8	2.56	0.40
54:L1:1691:T1C:H432	54:L1:1691:T1C:H41	1.75	0.40
4:LC:53:LEU:HA	13:LQ:146:ASN:HD21	1.86	0.40
7:LJ:186:LEU:HA	7:LJ:186:LEU:HD23	1.92	0.40
8:LK:134:ASP:OD1	8:LK:134:ASP:N	2.54	0.40
8:LK:188:GLU:HA	8:LK:191:LYS:HD2	2.04	0.40
17:LU:53:LYS:HD2	17:LU:53:LYS:HA	1.91	0.40
20:LX:156:LYS:HE3	20:LX:156:LYS:HB3	1.89	0.40
30:Lk:242:ARG:O	30:Lk:246:GLU:HG2	2.20	0.40
36:Lq:26:LEU:HD22	36:Lq:105:ALA:HA	2.04	0.40
39:Lt:245:GLN:NE2	39:Lt:247:GLY:O	2.54	0.40
41:Lw:60:PRO:HA	41:Lw:61:PRO:HD3	1.91	0.40
41:Lw:150:LYS:NZ	48:L6:79:THR:O	2.44	0.40
1:L1:632:U:H2'	1:L1:633:A:C8	2.57	0.40
1:L1:738:U:H2'	1:L1:739:A:C8	2.52	0.40
1:L1:1078:A:H2'	1:L1:1079:A:C8	2.55	0.40
1:L1:1438:U:OP2	4:LC:221:ARG:NH2	2.42	0.40
1:L1:1531:A:H2'	1:L1:1532:U:O4'	2.22	0.40
6:LI:109:GLY:HA2	6:LI:140:PHE:CD2	2.57	0.40
7:LJ:82:LEU:HA	7:LJ:85:GLU:OE1	2.21	0.40
8:LK:55:GLU:O	8:LK:58:LYS:HG2	2.21	0.40
8:LK:185:ALA:HA	8:LK:188:GLU:OE1	2.21	0.40
11:LO:177:ALA:HA	11:LO:222:TYR:CD1	2.56	0.40
14:LR:111:ILE:HG22	14:LR:115:LEU:CD1	2.50	0.40
16:LT:122:ARG:O	16:LT:126:GLU:HG3	2.21	0.40
17:LU:59:PRO:HA	17:LU:60:PRO:HD3	1.95	0.40
22:Lb:113:GLU:OE2	22:Lb:122:LYS:HB3	2.20	0.40
31:Ll:184:LEU:HB2	49:L7:191:LYS:NZ	2.36	0.40
33:Ln:117:LEU:HD21	39:Lt:70:MET:HE1	2.03	0.40
37:Lr:60:ARG:HA	37:Lr:60:ARG:HD2	1.90	0.40
50:L8:30:PRO:HA	50:L8:31:PRO:HD3	1.96	0.40
1:L1:80:G:H2'	1:L1:81:A:C8	2.56	0.40
1:L1:1255:U:O2'	1:L1:1257:C:OP1	2.34	0.40
4:LC:202:GLN:O	4:LC:272:LYS:HA	2.21	0.40
14:LR:134:ARG:C	14:LR:137:GLU:HB3	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Ld:65:LYS:HG3	44:Lz:84:MET:HE1	2.03	0.40
24:Ld:150:HIS:HB3	24:Ld:152:LYS:HE2	2.03	0.40
28:Li:187:LYS:HD3	28:Li:187:LYS:HA	1.80	0.40
32:Lm:107:LEU:O	32:Lm:125:ILE:HA	2.22	0.40
40:Lv:122:GLU:N	40:Lv:158:GLN:O	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	LB	235/305 (77%)	228 (97%)	7 (3%)	0	100	100
4	LC	302/348 (87%)	281 (93%)	21 (7%)	0	100	100
5	LD	248/311 (80%)	237 (96%)	11 (4%)	0	100	100
6	LI	93/267 (35%)	88 (95%)	5 (5%)	0	100	100
7	LJ	154/261 (59%)	138 (90%)	16 (10%)	0	100	100
8	LK	173/192 (90%)	165 (95%)	8 (5%)	0	100	100
9	LM	175/178 (98%)	164 (94%)	10 (6%)	1 (1%)	21	52
10	LN	113/145 (78%)	107 (95%)	6 (5%)	0	100	100
11	LO	285/296 (96%)	270 (95%)	15 (5%)	0	100	100
12	LP	219/251 (87%)	216 (99%)	3 (1%)	0	100	100
13	LQ	150/175 (86%)	141 (94%)	8 (5%)	1 (1%)	18	49
14	LR	144/179 (80%)	140 (97%)	4 (3%)	0	100	100
15	LS	217/292 (74%)	202 (93%)	15 (7%)	0	100	100
16	LT	138/149 (93%)	134 (97%)	4 (3%)	0	100	100
17	LU	158/205 (77%)	148 (94%)	10 (6%)	0	100	100
18	LV	164/212 (77%)	157 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	LW	139/153 (91%)	138 (99%)	1 (1%)	0	100	100
20	LX	200/216 (93%)	189 (94%)	11 (6%)	0	100	100
21	La	109/148 (74%)	106 (97%)	3 (3%)	0	100	100
22	Lb	241/256 (94%)	233 (97%)	8 (3%)	0	100	100
23	Lu	174/250 (70%)	172 (99%)	2 (1%)	0	100	100
24	Ld	118/161 (73%)	113 (96%)	5 (4%)	0	100	100
25	Lf	106/188 (56%)	101 (95%)	5 (5%)	0	100	100
26	Lg	50/65 (77%)	50 (100%)	0	0	100	100
27	Lh	44/92 (48%)	43 (98%)	1 (2%)	0	100	100
28	Li	93/188 (50%)	91 (98%)	2 (2%)	0	100	100
29	Lj	36/103 (35%)	36 (100%)	0	0	100	100
30	Lk	392/423 (93%)	382 (97%)	10 (3%)	0	100	100
31	Ll	352/380 (93%)	330 (94%)	22 (6%)	0	100	100
32	Lm	291/338 (86%)	279 (96%)	12 (4%)	0	100	100
33	Ln	97/206 (47%)	88 (91%)	9 (9%)	0	100	100
34	Lo	122/137 (89%)	118 (97%)	4 (3%)	0	100	100
35	Lp	93/142 (66%)	90 (97%)	3 (3%)	0	100	100
36	Lq	146/215 (68%)	135 (92%)	11 (8%)	0	100	100
37	Lr	271/332 (82%)	266 (98%)	5 (2%)	0	100	100
38	Ls	210/306 (69%)	202 (96%)	8 (4%)	0	100	100
39	Lt	211/279 (76%)	187 (89%)	22 (10%)	2 (1%)	14	44
40	Lv	125/212 (59%)	119 (95%)	6 (5%)	0	100	100
41	Lw	130/166 (78%)	123 (95%)	7 (5%)	0	100	100
42	Lx	108/158 (68%)	104 (96%)	4 (4%)	0	100	100
43	Ly	95/128 (74%)	91 (96%)	4 (4%)	0	100	100
44	Lz	90/123 (73%)	83 (92%)	7 (8%)	0	100	100
45	L3	94/112 (84%)	90 (96%)	4 (4%)	0	100	100
46	L4	81/138 (59%)	74 (91%)	7 (9%)	0	100	100
47	L5	43/128 (34%)	40 (93%)	3 (7%)	0	100	100
48	L6	92/102 (90%)	89 (97%)	3 (3%)	0	100	100
49	L7	119/206 (58%)	116 (98%)	3 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
50	L8	126/222 (57%)	123 (98%)	3 (2%)	0	100	100
51	SR	140/196 (71%)	137 (98%)	3 (2%)	0	100	100
52	Sf	366/439 (83%)	354 (97%)	11 (3%)	1 (0%)	36	67
All	All	8072/10674 (76%)	7708 (96%)	359 (4%)	5 (0%)	49	78

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
39	Lt	266	PRO
39	Lt	270	ALA
9	LM	154	ARG
52	Sf	260	GLU
13	LQ	111	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	LB	191/245 (78%)	191 (100%)	0	100	100
4	LC	258/290 (89%)	258 (100%)	0	100	100
5	LD	217/262 (83%)	217 (100%)	0	100	100
6	LI	86/228 (38%)	86 (100%)	0	100	100
7	LJ	145/232 (62%)	145 (100%)	0	100	100
8	LK	138/150 (92%)	138 (100%)	0	100	100
9	LM	155/156 (99%)	155 (100%)	0	100	100
10	LN	98/124 (79%)	98 (100%)	0	100	100
11	LO	245/249 (98%)	244 (100%)	1 (0%)	84	86
12	LP	188/211 (89%)	188 (100%)	0	100	100
13	LQ	133/150 (89%)	133 (100%)	0	100	100
14	LR	128/154 (83%)	128 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
15	LS	201/256 (78%)	201 (100%)	0	100	100
16	LT	118/126 (94%)	118 (100%)	0	100	100
17	LU	145/180 (81%)	145 (100%)	0	100	100
18	LV	146/182 (80%)	146 (100%)	0	100	100
19	LW	128/135 (95%)	128 (100%)	0	100	100
20	LX	180/191 (94%)	180 (100%)	0	100	100
21	La	91/119 (76%)	91 (100%)	0	100	100
22	Lb	219/229 (96%)	219 (100%)	0	100	100
23	Lu	159/223 (71%)	159 (100%)	0	100	100
24	Ld	111/147 (76%)	111 (100%)	0	100	100
25	Lf	97/164 (59%)	97 (100%)	0	100	100
26	Lg	49/60 (82%)	49 (100%)	0	100	100
27	Lh	40/72 (56%)	40 (100%)	0	100	100
28	Li	88/166 (53%)	88 (100%)	0	100	100
29	Lj	37/89 (42%)	37 (100%)	0	100	100
30	Lk	353/368 (96%)	353 (100%)	0	100	100
31	Ll	313/332 (94%)	313 (100%)	0	100	100
32	Lm	269/303 (89%)	269 (100%)	0	100	100
33	Ln	91/190 (48%)	91 (100%)	0	100	100
34	Lo	104/112 (93%)	104 (100%)	0	100	100
35	Lp	93/133 (70%)	93 (100%)	0	100	100
36	Lq	130/186 (70%)	130 (100%)	0	100	100
37	Lr	241/288 (84%)	241 (100%)	0	100	100
38	Ls	196/274 (72%)	196 (100%)	0	100	100
39	Lt	188/236 (80%)	188 (100%)	0	100	100
40	Lv	117/188 (62%)	117 (100%)	0	100	100
41	Lw	122/148 (82%)	122 (100%)	0	100	100
42	Lx	104/148 (70%)	104 (100%)	0	100	100
43	Ly	86/110 (78%)	86 (100%)	0	100	100
44	Lz	73/97 (75%)	73 (100%)	0	100	100
45	L3	81/90 (90%)	81 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
46	L4	78/116 (67%)	78 (100%)	0	100	100
47	L5	40/113 (35%)	40 (100%)	0	100	100
48	L6	80/87 (92%)	80 (100%)	0	100	100
49	L7	117/181 (65%)	117 (100%)	0	100	100
50	L8	110/178 (62%)	110 (100%)	0	100	100
51	SR	133/169 (79%)	133 (100%)	0	100	100
52	Sf	326/381 (86%)	326 (100%)	0	100	100
All	All	7236/9218 (78%)	7235 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	LO	30	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (77) such sidechains are listed below:

Mol	Chain	Res	Type
3	LB	276	HIS
4	LC	52	HIS
4	LC	72	GLN
4	LC	313	ASN
5	LD	103	GLN
5	LD	105	ASN
5	LD	249	ASN
6	LI	121	ASN
6	LI	136	ASN
7	LJ	141	GLN
7	LJ	151	ASN
8	LK	48	GLN
8	LK	126	GLN
8	LK	168	GLN
9	LM	9	GLN
9	LM	64	HIS
9	LM	89	GLN
9	LM	160	GLN
10	LN	59	HIS
11	LO	30	ASN
13	LQ	11	HIS

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Mol	Chain	Res	Type
13	LQ	146	ASN
14	LR	96	GLN
14	LR	120	ASN
14	LR	161	GLN
16	LT	77	GLN
17	LU	100	HIS
19	LW	82	HIS
19	LW	103	GLN
20	LX	73	GLN
21	La	62	HIS
21	La	72	HIS
22	Lb	15	GLN
22	Lb	93	ASN
22	Lb	237	GLN
23	Lu	122	GLN
23	Lu	189	HIS
24	Ld	98	GLN
24	Ld	148	GLN
25	Lf	140	GLN
26	Lg	31	ASN
27	Lh	57	ASN
30	Lk	150	GLN
30	Lk	160	HIS
30	Lk	221	GLN
30	Lk	269	ASN
30	Lk	302	HIS
30	Lk	420	HIS
31	Ll	163	HIS
31	Ll	333	GLN
32	Lm	69	HIS
32	Lm	111	GLN
33	Ln	144	GLN
36	Lq	58	ASN
36	Lq	129	GLN
37	Lr	69	HIS
37	Lr	73	GLN
37	Lr	94	ASN
37	Lr	134	GLN
37	Lr	139	GLN
37	Lr	168	HIS
38	Ls	251	GLN
40	Lv	61	HIS

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Mol	Chain	Res	Type
40	Lv	94	HIS
40	Lv	138	GLN
40	Lv	158	GLN
41	Lw	92	HIS
45	L3	46	ASN
46	L4	76	ASN
49	L7	104	HIS
49	L7	146	ASN
50	L8	60	GLN
51	SR	79	HIS
51	SR	146	GLN
52	Sf	373	GLN
52	Sf	375	ASN
52	Sf	420	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	L1	1491/1559 (95%)	351 (23%)	16 (1%)
2	L2	51/69 (73%)	19 (37%)	0
All	All	1542/1628 (94%)	370 (23%)	16 (1%)

All (370) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	L1	5	A
1	L1	6	A
1	L1	8	C
1	L1	9	U
1	L1	11	G
1	L1	19	C
1	L1	20	C
1	L1	22	A
1	L1	24	U
1	L1	29	C
1	L1	30	U
1	L1	34	U
1	L1	38	A
1	L1	39	G
1	L1	41	C
1	L1	43	A

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Mol	Chain	Res	Type
1	L1	44	C
1	L1	45	C
1	L1	46	U
1	L1	47	U
1	L1	54	A
1	L1	57	A
1	L1	58	U
1	L1	63	C
1	L1	64	C
1	L1	65	A
1	L1	66	A
1	L1	67	A
1	L1	78	G
1	L1	91	A
1	L1	100	G
1	L1	101	C
1	L1	103	A
1	L1	104	U
1	L1	107	A
1	L1	110	U
1	L1	111	A
1	L1	121	G
1	L1	124	A
1	L1	127	G
1	L1	134	A
1	L1	135	A
1	L1	136	U
1	L1	137	U
1	L1	138	A
1	L1	139	U
1	L1	142	C
1	L1	143	C
1	L1	144	A
1	L1	147	C
1	L1	151	A
1	L1	157	C
1	L1	158	A
1	L1	159	A
1	L1	162	A
1	L1	166	A
1	L1	167	C
1	L1	174	A

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Mol	Chain	Res	Type
1	L1	184	U
1	L1	186	A
1	L1	197	A
1	L1	199	A
1	L1	200	A
1	L1	203	A
1	L1	208	U
1	L1	212	A
1	L1	213	G
1	L1	215	A
1	L1	217	A
1	L1	223	A
1	L1	232	C
1	L1	233	C
1	L1	239	A
1	L1	248	G
1	L1	257	G
1	L1	265	A
1	L1	266	A
1	L1	267	A
1	L1	268	A
1	L1	270	A
1	L1	274	C
1	L1	298	G
1	L1	305	U
1	L1	310	A
1	L1	315	G
1	L1	317	G
1	L1	322	C
1	L1	324	A
1	L1	325	A
1	L1	330	C
1	L1	331	C
1	L1	332	G
1	L1	333	A
1	L1	345	G
1	L1	346	C
1	L1	352	G
1	L1	359	A
1	L1	360	U
1	L1	362	G
1	L1	367	U

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Mol	Chain	Res	Type
1	L1	369	A
1	L1	374	A
1	L1	385	U
1	L1	387	C
1	L1	390	A
1	L1	392	A
1	L1	393	G
1	L1	395	A
1	L1	404	A
1	L1	413	U
1	L1	415	A
1	L1	423	U
1	L1	426	U
1	L1	427	A
1	L1	429	U
1	L1	435	G
1	L1	443	G
1	L1	454	A
1	L1	455	C
1	L1	456	U
1	L1	464	A
1	L1	465	A
1	L1	471	U
1	L1	472	A
1	L1	477	G
1	L1	488	U
1	L1	489	U
1	L1	493	A
1	L1	496	C
1	L1	498	U
1	L1	501	U
1	L1	502	A
1	L1	503	G
1	L1	510	A
1	L1	511	A
1	L1	512	G
1	L1	514	A
1	L1	517	C
1	L1	519	C
1	L1	524	U
1	L1	526	A
1	L1	527	G

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Mol	Chain	Res	Type
1	L1	528	A
1	L1	530	A
1	L1	531	G
1	L1	532	C
1	L1	540	C
1	L1	546	A
1	L1	549	C
1	L1	550	A
1	L1	551	C
1	L1	552	U
1	L1	553	A
1	L1	555	C
1	L1	557	A
1	L1	558	A
1	L1	563	U
1	L1	567	A
1	L1	569	A
1	L1	571	A
1	L1	573	A
1	L1	575	A
1	L1	576	A
1	L1	592	C
1	L1	593	C
1	L1	614	C
1	L1	615	U
1	L1	620	A
1	L1	627	A
1	L1	630	G
1	L1	653	A
1	L1	654	U
1	L1	662	C
1	L1	672	U
1	L1	675	G
1	L1	694	C
1	L1	699	A
1	L1	700	A
1	L1	701	U
1	L1	704	A
1	L1	709	C
1	L1	711	A
1	L1	720	A
1	L1	723	C

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Mol	Chain	Res	Type
1	L1	731	A
1	L1	737	U
1	L1	744	C
1	L1	745	C
1	L1	756	C
1	L1	757	C
1	L1	773	C
1	L1	774	A
1	L1	775	U
1	L1	776	A
1	L1	777	A
1	L1	779	G
1	L1	794	G
1	L1	798	A
1	L1	808	G
1	L1	809	C
1	L1	814	C
1	L1	823	C
1	L1	830	A
1	L1	832	C
1	L1	834	A
1	L1	836	A
1	L1	837	A
1	L1	838	C
1	L1	841	C
1	L1	850	C
1	L1	851	A
1	L1	853	C
1	L1	854	A
1	L1	857	A
1	L1	860	A
1	L1	861	U
1	L1	870	C
1	L1	874	C
1	L1	887	C
1	L1	888	A
1	L1	889	U
1	L1	890	G
1	L1	900	C
1	L1	904	G
1	L1	907	C
1	L1	911	A

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Mol	Chain	Res	Type
1	L1	912	A
1	L1	913	C
1	L1	922	G
1	L1	923	G
1	L1	924	U
1	L1	930	A
1	L1	931	A
1	L1	932	U
1	L1	933	C
1	L1	934	A
1	L1	936	U
1	L1	948	U
1	L1	956	U
1	L1	957	G
1	L1	958	U
1	L1	959	A
1	L1	960	U
1	L1	962	A
1	L1	963	A
1	L1	964	U
1	L1	965	G
1	L1	975	G
1	L1	984	U
1	L1	985	G
1	L1	986	U
1	L1	990	U
1	L1	1013	C
1	L1	1016	G
1	L1	1024	A
1	L1	1026	A
1	L1	1028	G
1	L1	1032	G
1	L1	1036	A
1	L1	1039	A
1	L1	1048	C
1	L1	1049	G
1	L1	1053	A
1	L1	1054	G
1	L1	1055	A
1	L1	1056	C
1	L1	1062	G
1	L1	1069	U

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Mol	Chain	Res	Type
1	L1	1073	U
1	L1	1075	A
1	L1	1087	A
1	L1	1088	G
1	L1	1124	C
1	L1	1140	G
1	L1	1161	G
1	L1	1162	A
1	L1	1163	A
1	L1	1177	C
1	L1	1184	U
1	L1	1194	U
1	L1	1195	C
1	L1	1222	A
1	L1	1223	A
1	L1	1225	U
1	L1	1236	C
1	L1	1240	A
1	L1	1242	C
1	L1	1243	A
1	L1	1247	G
1	L1	1248	A
1	L1	1249	A
1	L1	1252	A
1	L1	1256	A
1	L1	1258	C
1	L1	1262	G
1	L1	1265	A
1	L1	1286	A
1	L1	1293	A
1	L1	1309	U
1	L1	1315	C
1	L1	1319	G
1	L1	1320	A
1	L1	1322	G
1	L1	1323	U
1	L1	1324	U
1	L1	1335	A
1	L1	1346	G
1	L1	1351	C
1	L1	1352	G
1	L1	1371	U

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Mol	Chain	Res	Type
1	L1	1372	U
1	L1	1383	A
1	L1	1384	G
1	L1	1386	C
1	L1	1389	A
1	L1	1390	C
1	L1	1399	A
1	L1	1416	U
1	L1	1419	A
1	L1	1430	U
1	L1	1432	U
1	L1	1438	U
1	L1	1439	U
1	L1	1442	A
1	L1	1444	U
1	L1	1452	U
1	L1	1461	G
1	L1	1471	A
1	L1	1477	G
1	L1	1480	U
1	L1	1485	C
1	L1	1487	C
1	L1	1488	A
1	L1	1492	C
1	L1	1498	C
1	L1	1499	C
1	L1	1502	C
1	L1	1504	U
1	L1	1506	A
1	L1	1510	A
1	L1	1513	U
1	L1	1520	A
1	L1	1522	C
1	L1	1537	A
1	L1	1539	A
1	L1	1540	C
1	L1	1542	C
1	L1	1547	A
1	L1	1548	A
1	L1	1550	A
1	L1	1558	U
2	L2	1605	A

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Mol	Chain	Res	Type
2	L2	1608	G
2	L2	1609	U
2	L2	1610	A
2	L2	1611	G
2	L2	1613	U
2	L2	1614	U
2	L2	1615	A
2	L2	1625	A
2	L2	1628	C
2	L2	1629	A
2	L2	1630	A
2	L2	1640	A
2	L2	1641	G
2	L2	1644	G
2	L2	1650	A
2	L2	1651	A
2	L2	1669	G
2	L2	1670	A

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	L1	33	C
1	L1	63	C
1	L1	135	A
1	L1	136	U
1	L1	137	U
1	L1	267	A
1	L1	516	C
1	L1	551	C
1	L1	575	A
1	L1	837	A
1	L1	860	A
1	L1	889	U
1	L1	930	A
1	L1	1235	A
1	L1	1319	G
1	L1	1371	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 99 ligands modelled in this entry, 98 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
54	T1C	L1	1691	53	45,45,45	1.14	4 (8%)	56,72,72	1.05	5 (8%)

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
54	T1C	L1	1691	53	-	11/22/80/80	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
54	L1	1691	T1C	C21-N21	5.00	1.47	1.33
54	L1	1691	T1C	C4-N4	2.33	1.52	1.47
54	L1	1691	T1C	O11-C11	2.25	1.28	1.23
54	L1	1691	T1C	C7-N7	2.14	1.48	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	L1	1691	T1C	C1-C1C-C12	3.14	113.56	109.88
54	L1	1691	T1C	C11-C1B-C12	2.95	121.13	118.80
54	L1	1691	T1C	O1C-C1C-C12	-2.74	105.77	110.14
54	L1	1691	T1C	C1C-C41-C4	2.70	115.32	111.64
54	L1	1691	T1C	C1C-C1-C2	2.13	119.14	115.75

There are no chirality outliers.

All (11) torsion outliers are listed below:

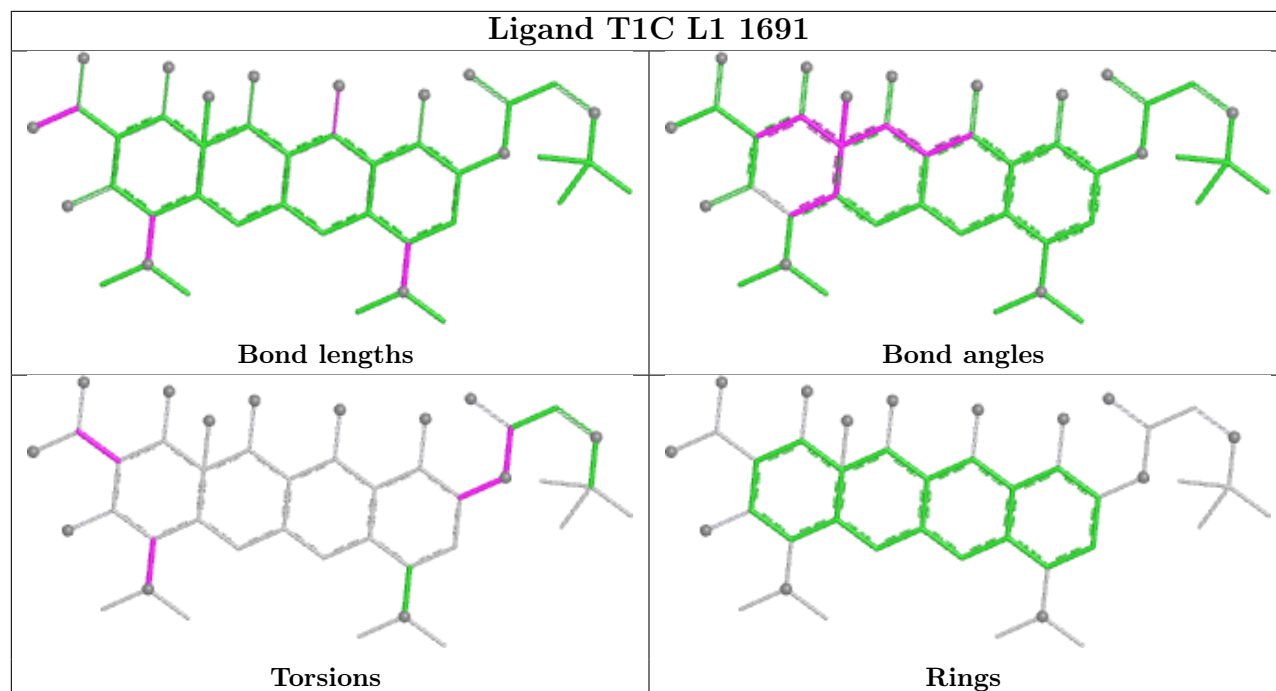
Mol	Chain	Res	Type	Atoms
54	L1	1691	T1C	C92-C91-N9-C9
54	L1	1691	T1C	C41-C4-N4-C43
54	L1	1691	T1C	C3-C4-N4-C43
54	L1	1691	T1C	C3-C4-N4-C42
54	L1	1691	T1C	C3-C2-C21-O21
54	L1	1691	T1C	C3-C2-C21-N21
54	L1	1691	T1C	C1-C2-C21-O21
54	L1	1691	T1C	O91-C91-N9-C9
54	L1	1691	T1C	C41-C4-N4-C42
54	L1	1691	T1C	C1-C2-C21-N21
54	L1	1691	T1C	C10-C9-N9-C91

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
54	L1	1691	T1C	4	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

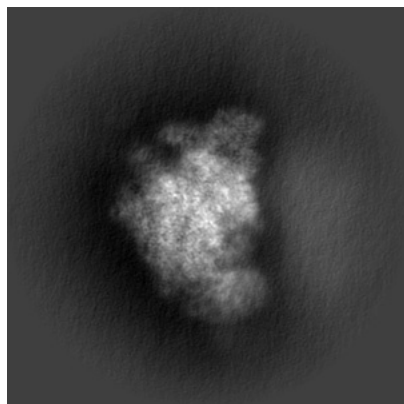
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38635. These allow visual inspection of the internal detail of the map and identification of artifacts.

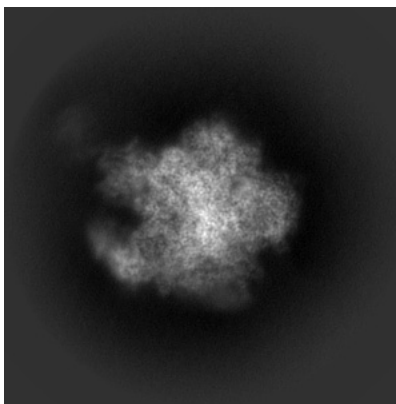
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

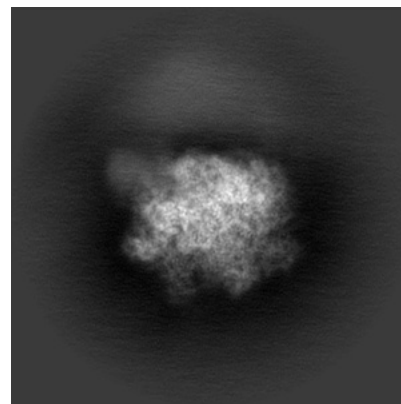
6.1.1 Primary map



X

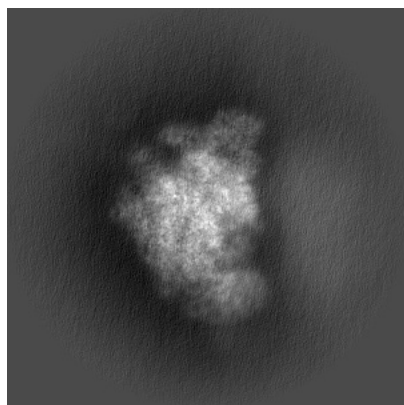


Y

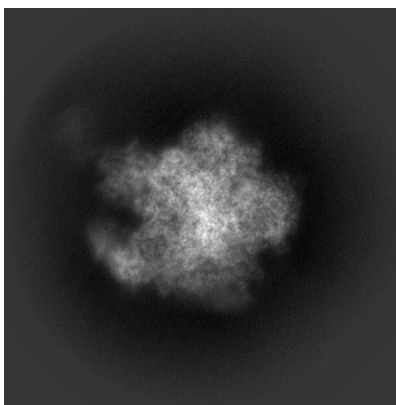


Z

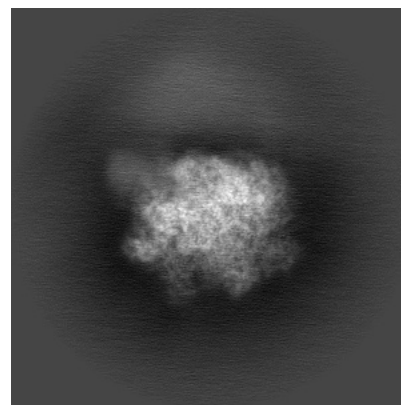
6.1.2 Raw map



X



Y

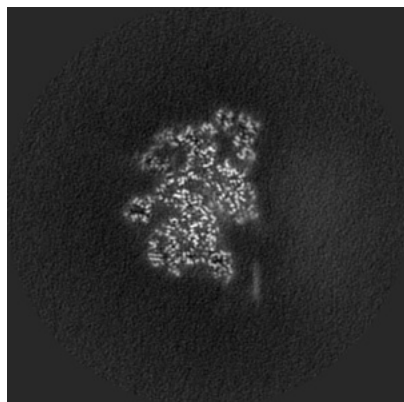


Z

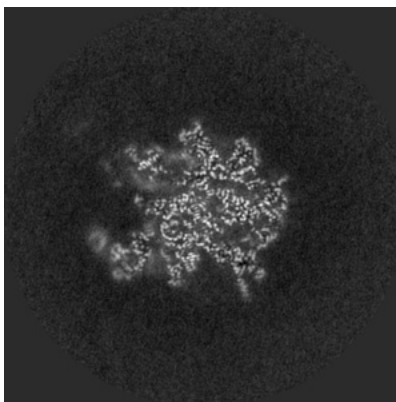
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

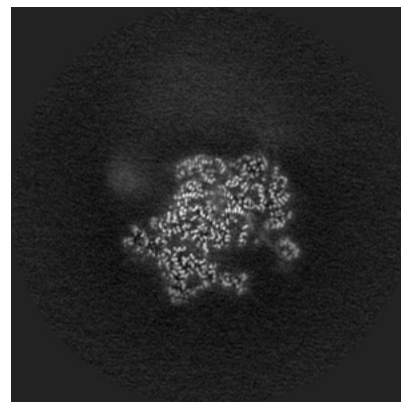
6.2.1 Primary map



X Index: 210

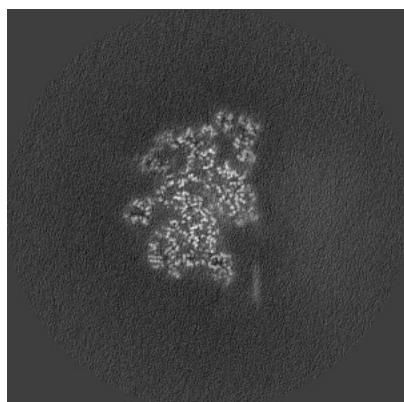


Y Index: 210

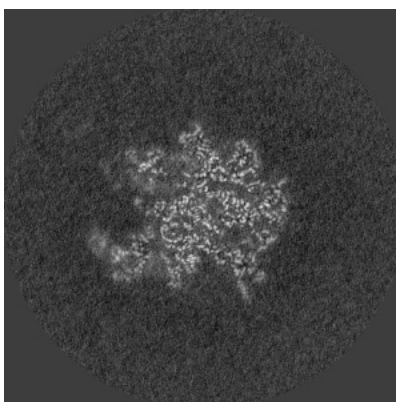


Z Index: 210

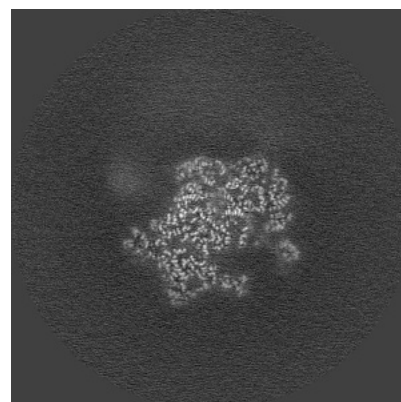
6.2.2 Raw map



X Index: 210



Y Index: 210

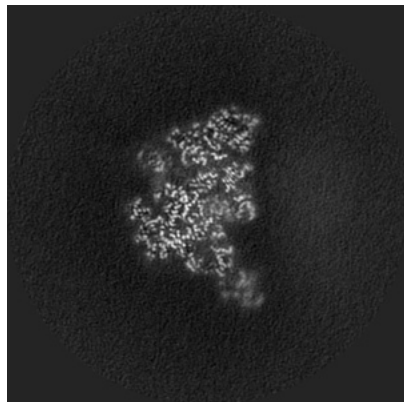


Z Index: 210

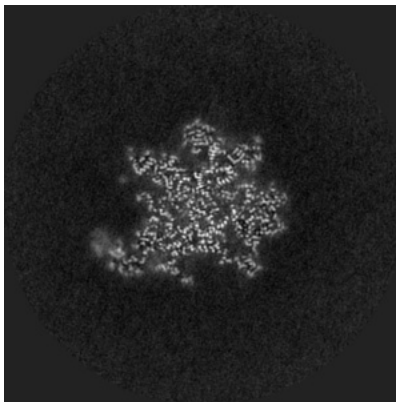
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

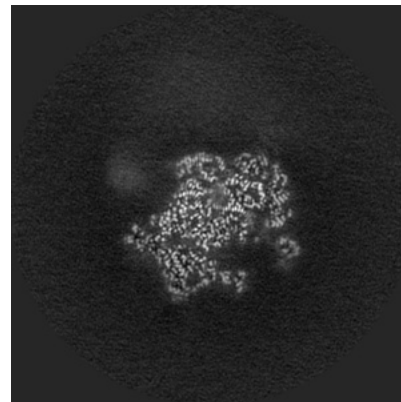
6.3.1 Primary map



X Index: 221

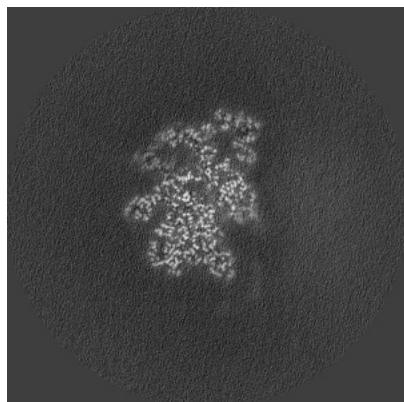


Y Index: 201

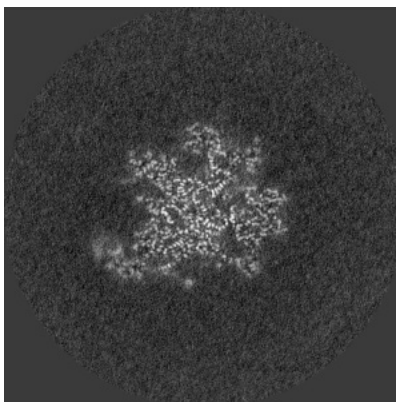


Z Index: 211

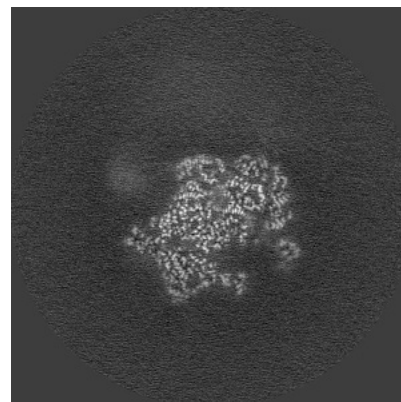
6.3.2 Raw map



X Index: 208



Y Index: 199

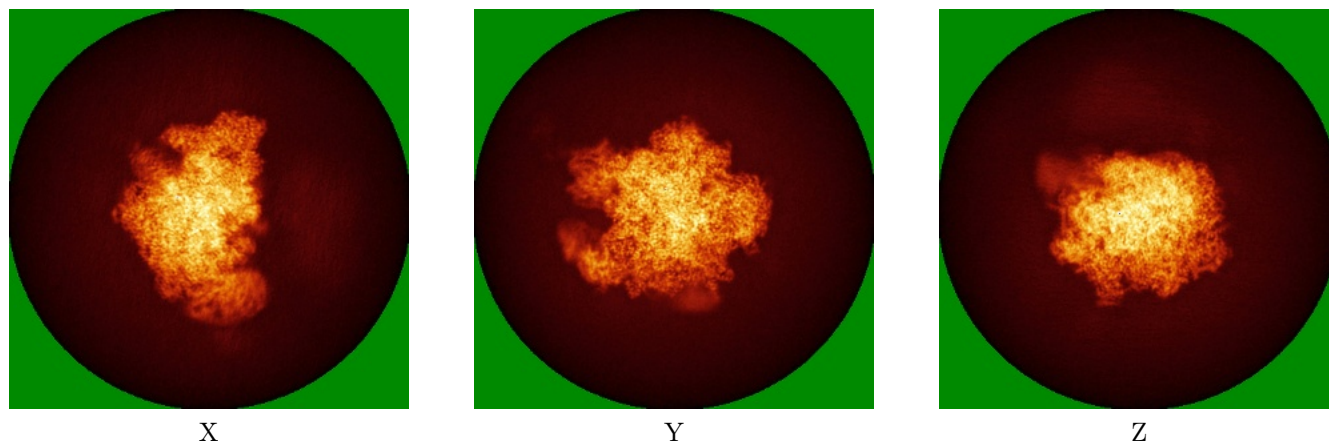


Z Index: 211

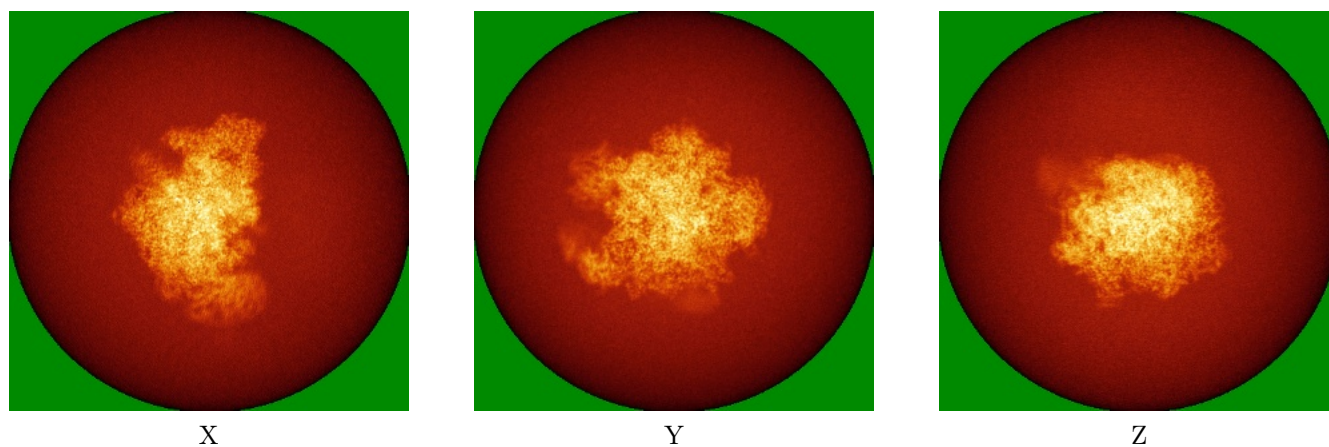
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



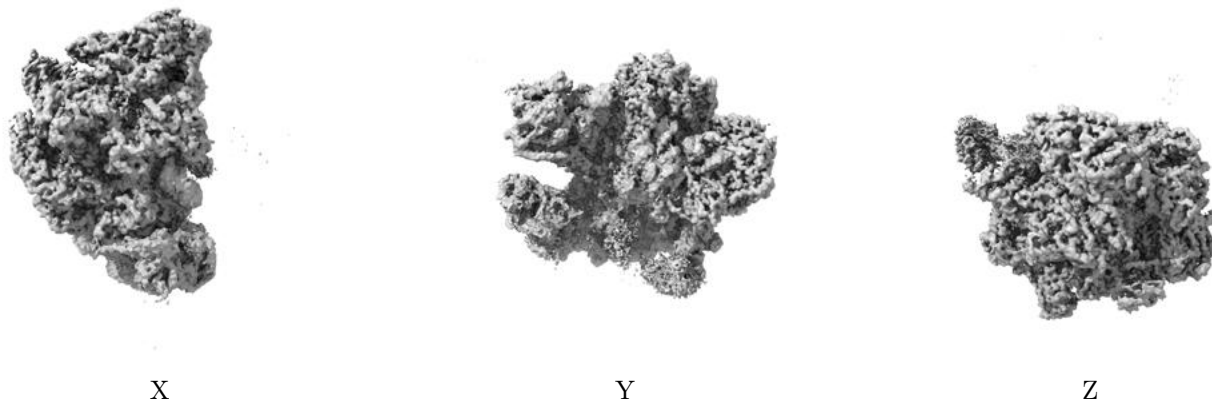
6.4.2 Raw map



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.

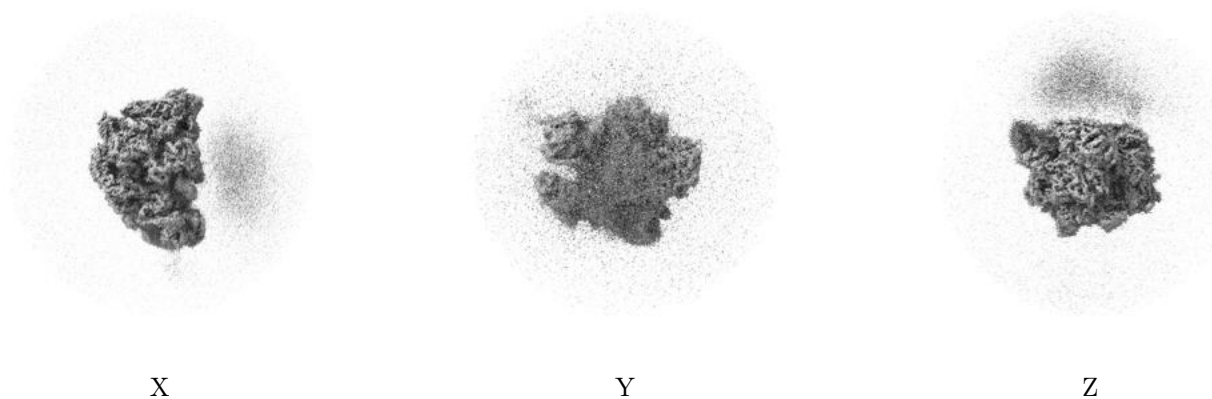
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



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

6.5.2 Raw map



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

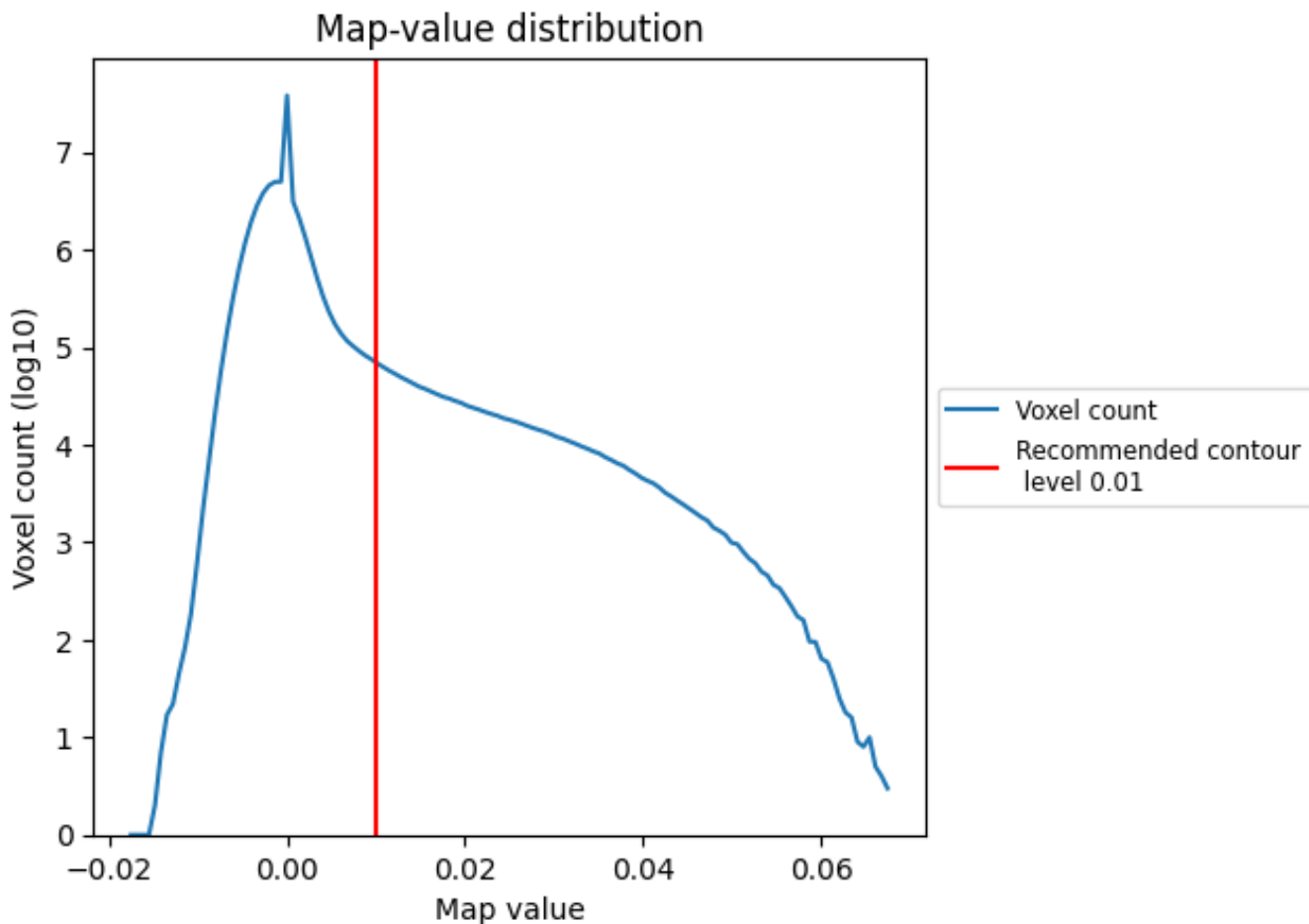
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

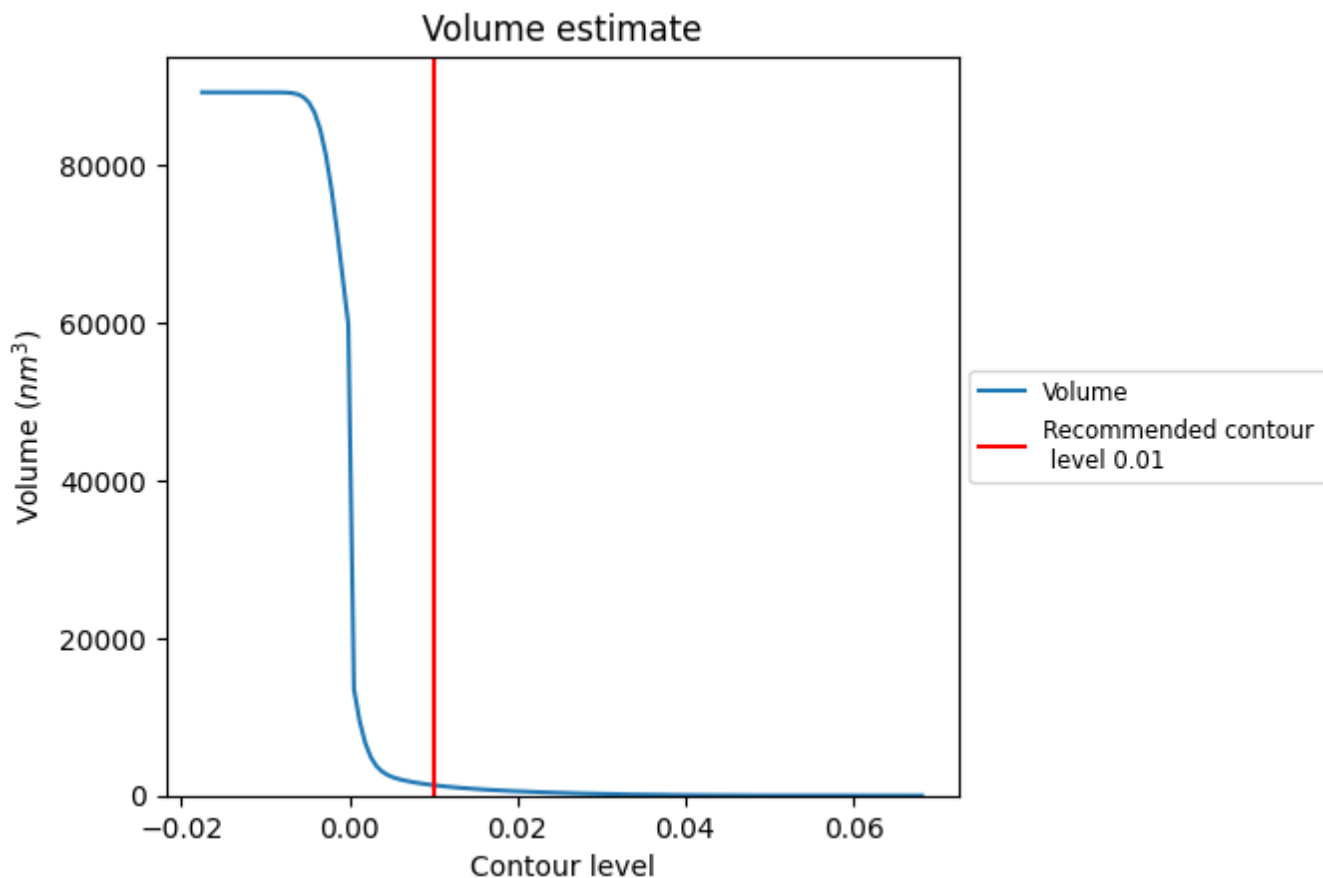
This section contains the results of statistical analysis of the map.

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.

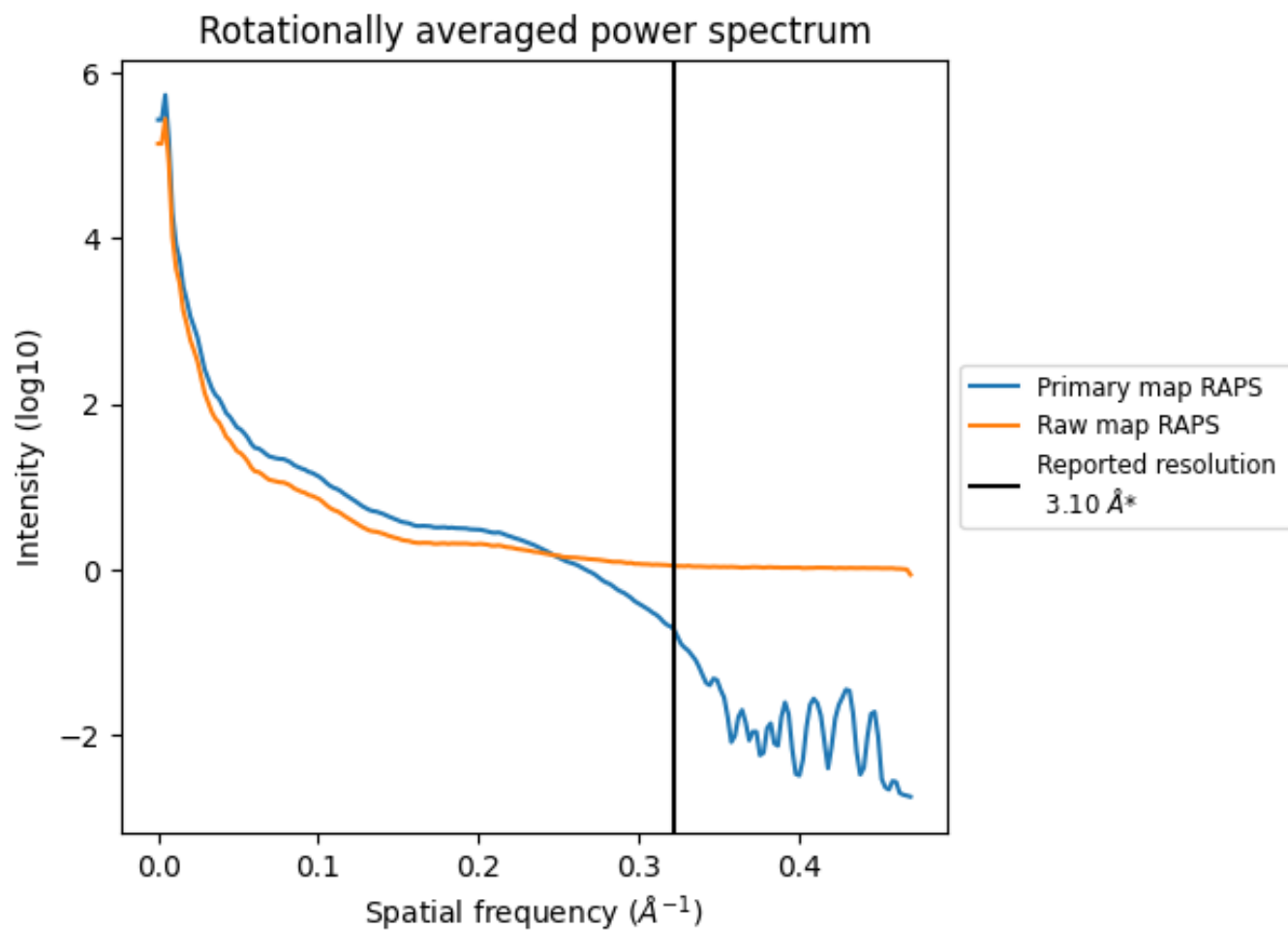
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1320 nm^3 ; this corresponds to an approximate mass of 1193 kDa.

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

7.3 Rotationally averaged power spectrum i

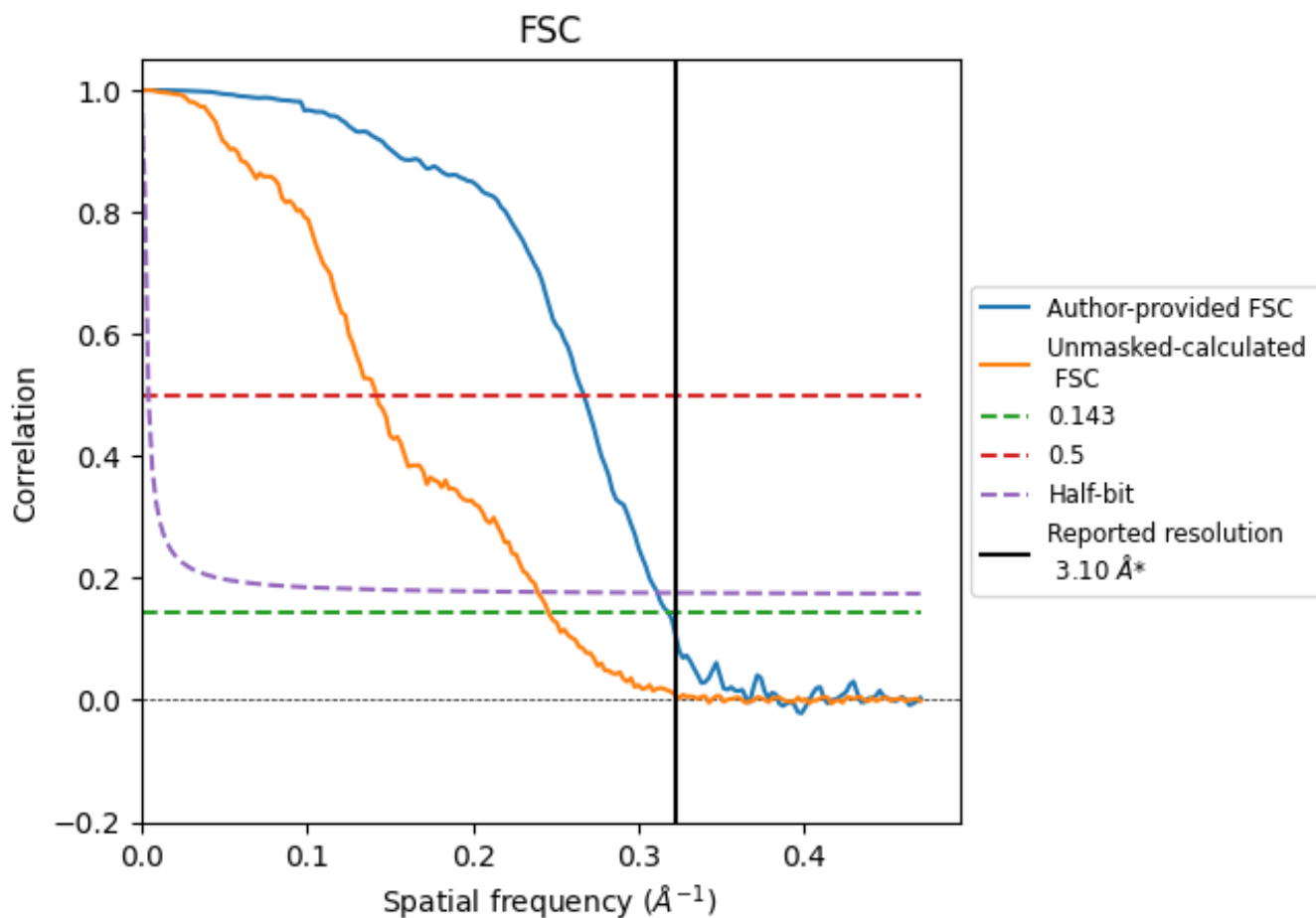


*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

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 0.323 Å⁻¹

8.2 Resolution estimates [i](#)

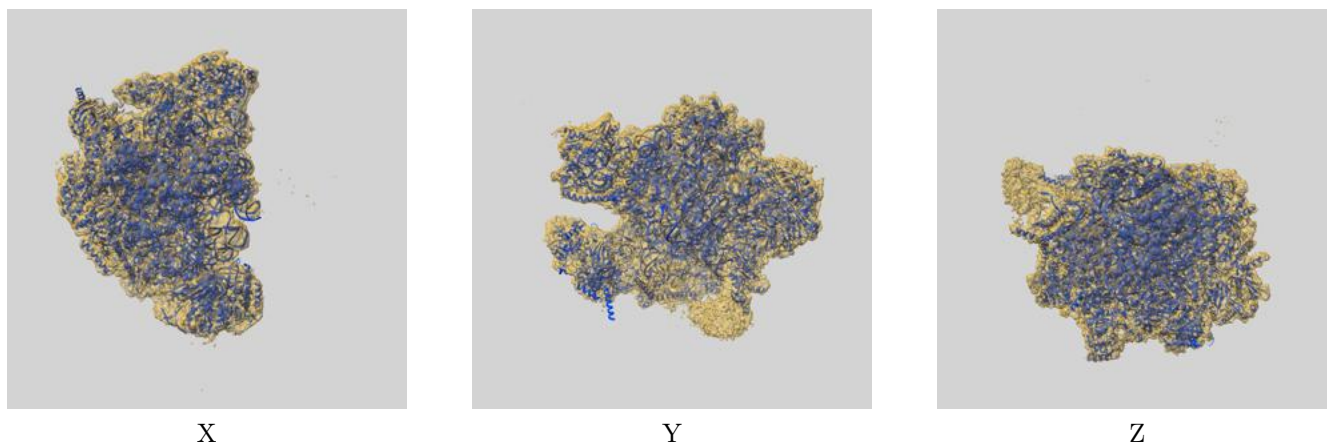
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.14	3.75	3.21
Unmasked-calculated*	4.07	7.05	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.07 differs from the reported value 3.1 by more than 10 %

9 Map-model fit [i](#)

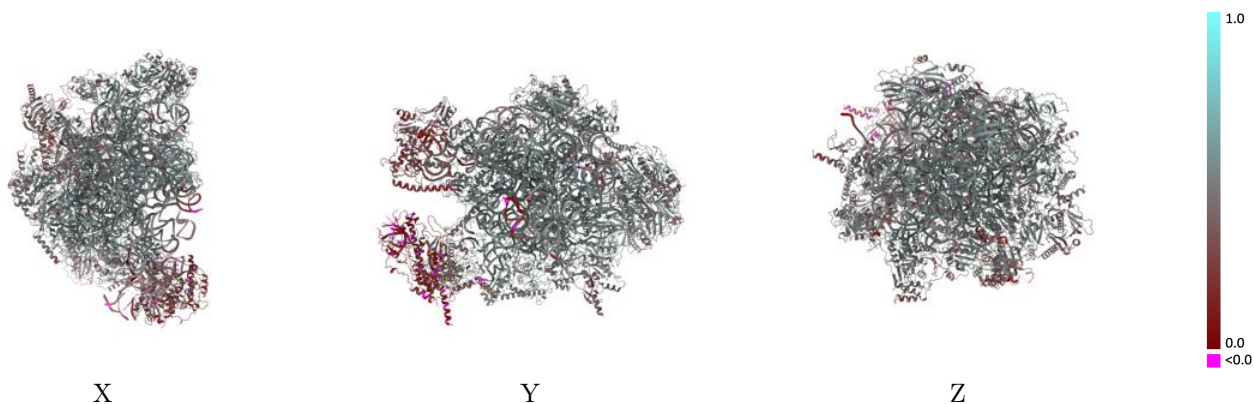
This section contains information regarding the fit between EMDB map EMD-38635 and PDB model 8XT3. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



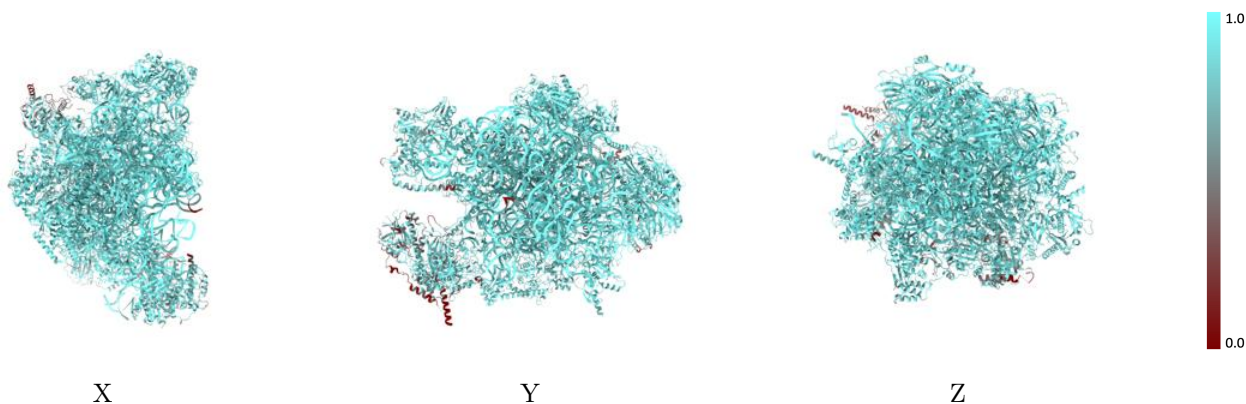
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



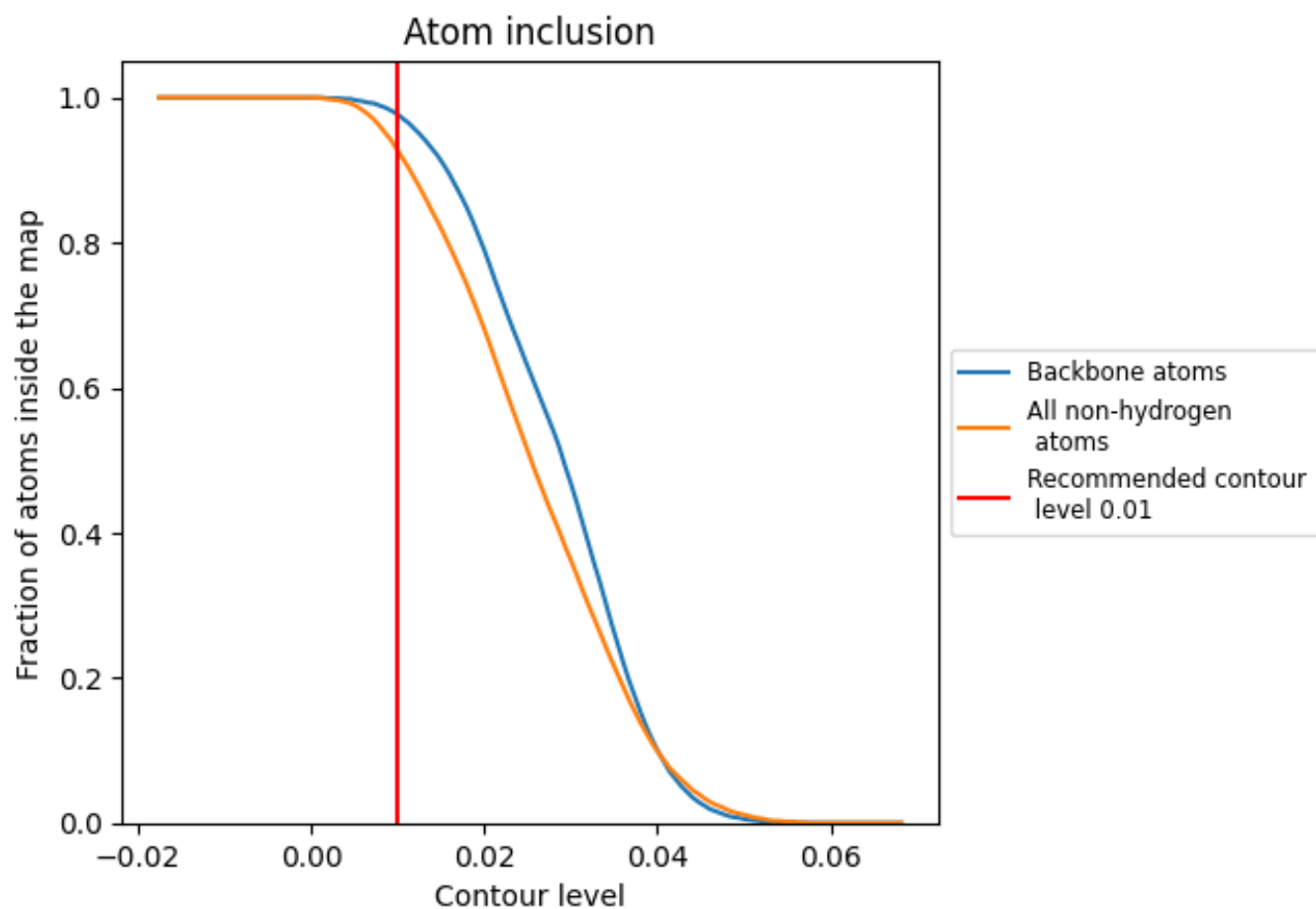
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary





































The table lists the average atom inclusion at the recommended contour level (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9270	 0.4670
L1	 0.9910	 0.5010
L2	 0.9400	 0.2700
L3	 0.9000	 0.3830
L4	 0.7920	 0.3100
L5	 0.6770	 0.1810
L6	 0.9660	 0.5210
L7	 0.8980	 0.4400
L8	 0.8570	 0.4210
LB	 0.9510	 0.5170
LC	 0.9610	 0.5080
LD	 0.9580	 0.5200
LI	 0.9250	 0.4440
LJ	 0.8680	 0.3660
LK	 0.7680	 0.2450
LM	 0.9680	 0.5130
LN	 0.9450	 0.4990
LO	 0.9450	 0.5090
LP	 0.9490	 0.5000
LQ	 0.9600	 0.5040
LR	 0.9390	 0.4520
LS	 0.9180	 0.4830
LT	 0.9600	 0.5140
LU	 0.9440	 0.5130
LV	 0.9420	 0.5160
LW	 0.8930	 0.4820
LX	 0.7550	 0.4280
La	 0.9860	 0.5350
Lb	 0.9030	 0.4780
Ld	 0.9430	 0.5170
Lf	 0.9340	 0.4980
Lg	 0.9500	 0.4880
Lh	 0.9830	 0.5380
Li	 0.9800	 0.5410
Lj	 0.9820	 0.5350



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Chain	Atom inclusion	Q-score
Lk	 0.9230	 0.4830
Ll	 0.9070	 0.4050
Lm	 0.8920	 0.4280
Ln	 0.5910	 0.1870
Lo	 0.8840	 0.4740
Lp	 0.9130	 0.4750
Lq	 0.9620	 0.5190
Lr	 0.9170	 0.4750
Ls	 0.6910	 0.3970
Lt	 0.5210	 0.1400
Lu	 0.9360	 0.4910
Lv	 0.6810	 0.2410
Lw	 0.9560	 0.4950
Lx	 0.8340	 0.4250
Ly	 0.9760	 0.5250
Lz	 0.9220	 0.4730
SR	 0.9730	 0.5060
Sf	 0.9460	 0.5000