



Full wwPDB EM Validation Report ⓘ

Sep 20, 2026 – 11:22 pm BST

PDB ID : 9QET / pdb_00009qet
EMDB ID : EMD-53092
Title : Human pre-60S - State 1B
Authors : Thoms, M.; Denk, T.; Beckmann, R.
Deposited on : 2025-03-11
Resolution : 3.13 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

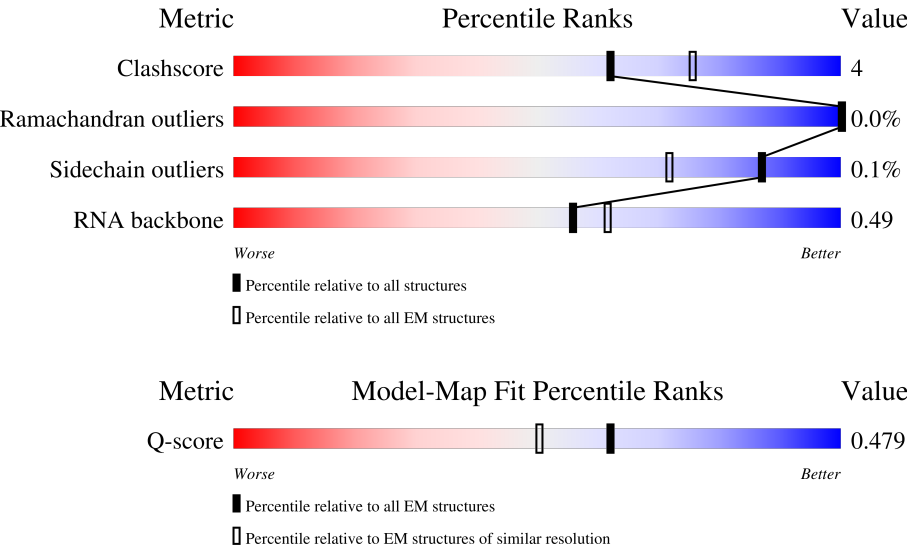
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.13 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.



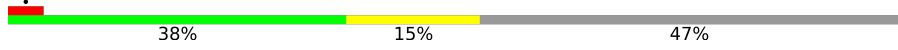
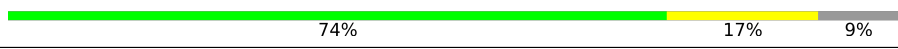
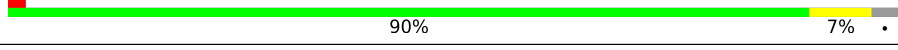
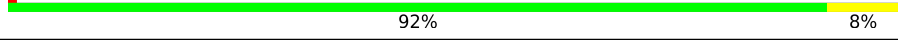
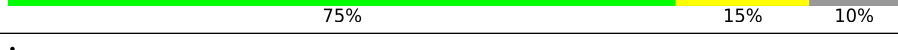
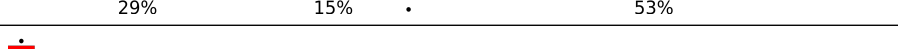
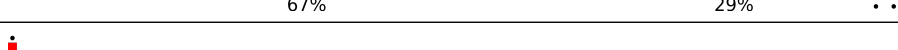
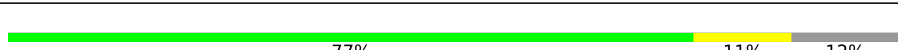
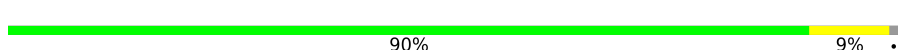
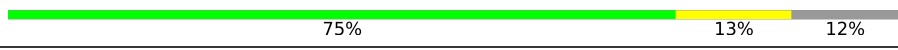
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14478 (2.63 - 3.63)

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	CA	245	
2	CB	731	
3	CC	549	

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Mol	Chain	Length	Quality of chain
4	CD	634	
5	CE	129	
6	CF	239	
7	CG	485	
8	CH	260	
9	CI	163	
10	CJ	306	
11	CK	365	
12	L5	5070	
13	L7	121	
14	L8	157	
15	LB	403	
16	LC	427	
17	LD	297	
18	LE	288	
19	LF	248	
20	LG	266	
21	LH	192	
22	LJ	178	
23	LL	211	
24	LM	215	
25	LN	204	
26	LO	203	
27	LP	184	
28	LQ	188	

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Mol	Chain	Length	Quality of chain
29	LS	176	
30	LT	160	
31	LV	140	
32	LY	145	
33	La	148	
34	Ld	125	
35	Le	135	
36	Lf	110	
37	Lh	123	
38	Li	105	
39	Lr	137	
40	Lt	165	
41	Lz	217	

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 114018 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	CA	245	Total	C	N	O	S	0	0
			1860	1153	319	375	13		

- Molecule 2 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	CB	448	Total	C	N	O	S	0	0
			3506	2220	631	644	11		

- Molecule 3 is a protein called Guanine nucleotide-binding protein-like 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CC	80	Total	C	N	O	S	0	0
			594	369	126	96	3		

- Molecule 4 is a protein called GTP-binding protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CD	460	Total	C	N	O	S	0	0
			3735	2374	660	684	17		

- Molecule 5 is a protein called Protein LLP homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CE	68	Total	C	N	O	S	0	0
			537	333	115	87	2		

- Molecule 6 is a protein called mRNA turnover protein 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CF	218	Total	C	N	O	S	0	0
			1775	1131	312	321	11		

- Molecule 7 is a protein called Notchless protein homolog 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CG	471	Total	C	N	O	S	0	0
			3449	2149	641	648	11		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CG	85	ALA	GLU	engineered mutation	UNP Q9NVX2

- Molecule 8 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CH	259	Total	C	N	O	S	0	0
			2066	1315	389	353	9		

- Molecule 9 is a protein called Probable ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CI	115	Total	C	N	O	S	0	0
			987	628	192	157	10		

- Molecule 10 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CJ	275	Total	C	N	O	S	0	0
			2176	1393	381	391	11		

- Molecule 11 is a protein called Ribosome biogenesis regulatory protein homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
11	CK	195	Total	C	N	O	0	0
			1545	968	304	273		

- Molecule 12 is a RNA chain called 28S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L5	2371	Total	C	N	O	P	0	0
			50823	22627	9311	16515	2370		

- Molecule 13 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L7	120	Total	C	N	O	P	0	0
			2561	1141	456	844	120		

- Molecule 14 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L8	115	Total	C	N	O	P	0	0
			2450	1095	440	801	114		

- Molecule 15 is a protein called 60S ribosomal protein L3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LB	381	Total	C	N	O	S	0	0
			3054	1942	568	531	13		

- Molecule 16 is a protein called 60S ribosomal protein L4.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LC	328	Total	C	N	O	S	0	0
			2628	1664	518	433	13		

- Molecule 17 is a protein called 60S ribosomal protein L5.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LD	230	Total	C	N	O	S	0	0
			1879	1192	338	336	13		

- Molecule 18 is a protein called Large ribosomal subunit protein eL6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LE	208	Total	C	N	O	S	0	0
			1673	1081	315	273	4		

- Molecule 19 is a protein called Large ribosomal subunit protein uL30.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LF	219	Total	C	N	O	S	0	0
			1790	1148	341	292	9		

- Molecule 20 is a protein called 60S ribosomal protein L7a.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LG	170	Total	C	N	O	S	0	0
			1376	872	268	232	4		

- Molecule 21 is a protein called 60S ribosomal protein L9.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LH	190	Total	C	N	O	S	0	0
			1510	950	282	272	6		

- Molecule 22 is a protein called 60S ribosomal protein L11.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LJ	170	Total	C	N	O	S	0	0
			1335	845	245	239	6		

- Molecule 23 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LL	180	Total	C	N	O	S	0	0
			1440	902	299	236	3		

- Molecule 24 is a protein called 60S ribosomal protein L14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LM	135	Total	C	N	O	S	0	0
			1105	707	213	178	7		

- Molecule 25 is a protein called 60S ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LN	179	Total	C	N	O	S	0	0
			1516	955	319	238	4		

- Molecule 26 is a protein called 60S ribosomal protein L13a.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LO	201	Total	C	N	O	S	0	0
			1642	1058	320	259	5		

- Molecule 27 is a protein called 60S ribosomal protein L17.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LP	136	Total	C	N	O	S	0	0
			1089	683	206	193	7		

- Molecule 28 is a protein called 60S ribosomal protein L18.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LQ	151	Total	C	N	O	S	0	0
			1223	768	247	203	5		

- Molecule 29 is a protein called 60S ribosomal protein L18a.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LS	176	Total	C	N	O	S	0	0
			1457	927	283	236	11		

- Molecule 30 is a protein called 60S ribosomal protein L21.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LT	127	Total	C	N	O	S	0	0
			994	630	190	172	2		

- Molecule 31 is a protein called 60S ribosomal protein L23.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LV	137	Total	C	N	O	S	0	0
			1019	639	196	179	5		

- Molecule 32 is a protein called 60S ribosomal protein L26.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LY	132	Total	C	N	O	S	0	0
			1092	686	219	184	3		

- Molecule 33 is a protein called 60S ribosomal protein L27a.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	La	105	Total	C	N	O	S	0	0
			823	524	160	136	3		

- Molecule 34 is a protein called 60S ribosomal protein L31.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	Ld	93	Total	C	N	O	0	0
			613	390	121	102		

- Molecule 35 is a protein called 60S ribosomal protein L32.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	Le	128	Total	C	N	O	S	0	0
			1053	667	216	165	5		

- Molecule 36 is a protein called 60S ribosomal protein L35a.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	Lf	109	Total	C	N	O	S	0	0
			872	552	173	144	3		

- Molecule 37 is a protein called 60S ribosomal protein L35.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	Lh	104	Total	C	N	O	S	0	0
			666	407	139	119	1		

- Molecule 38 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Li	104	Total	C	N	O	S	0	0
			839	524	178	132	5		

- Molecule 39 is a protein called 60S ribosomal protein L28.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	Lr	123	Total	C	N	O	S	0	0
			984	611	205	164	4		

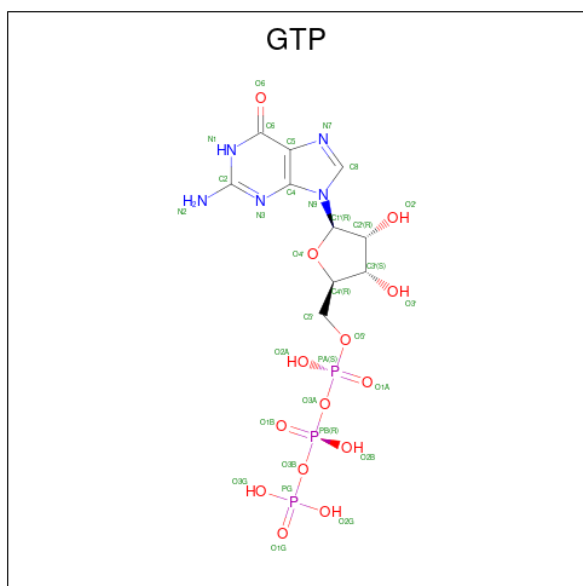
- Molecule 40 is a protein called Large ribosomal subunit protein uL11.

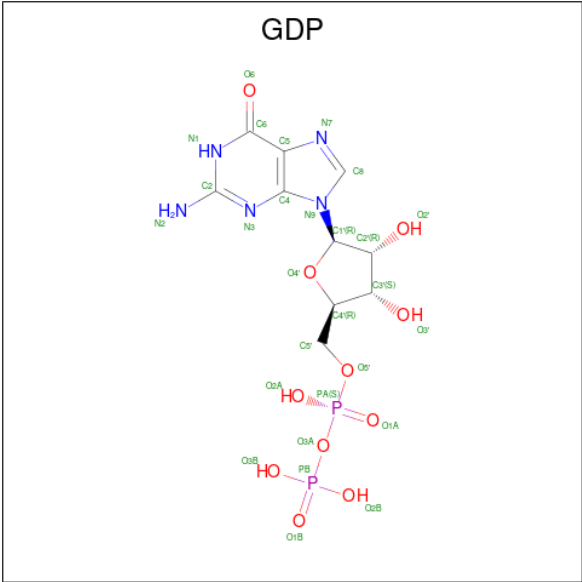
Mol	Chain	Residues	Atoms					AltConf	Trace
40	Lt	159	Total	C	N	O	S	0	0
			1186	736	223	223	4		

- Molecule 41 is a protein called 60S ribosomal protein L10a.

Mol	Chain	Residues	Atoms				AltConf	Trace
41	Lz	208	Total	C	N	O	0	0
			1033	616	208	209		

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).





Mol	Chain	Residues	Atoms					AltConf
44	CD	1	Total	C	N	O	P	0
			28	10	5	11	2	

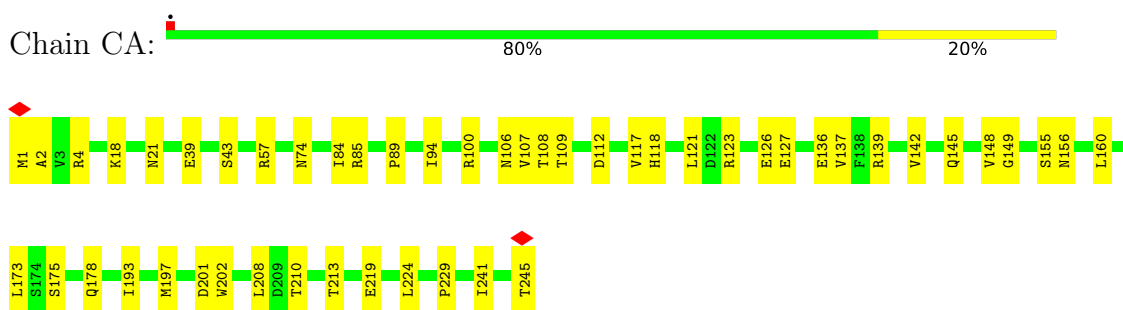
- Molecule 45 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
45	CI	1	Total	Zn	0
			1	1	

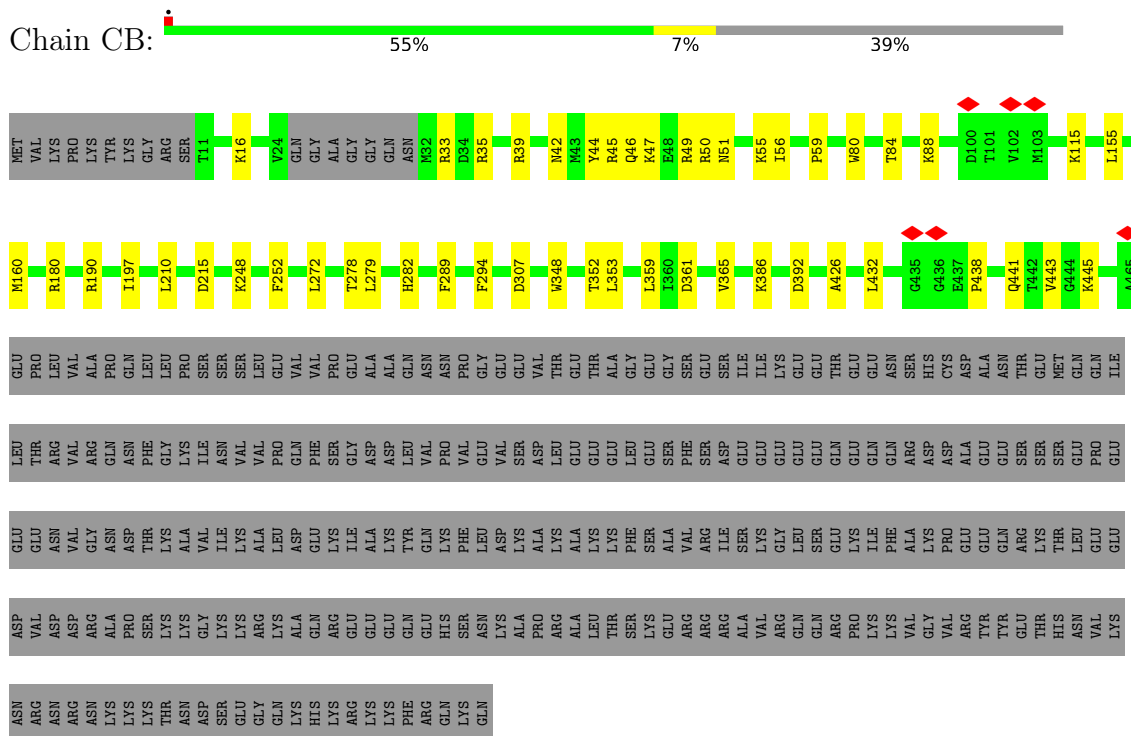
3 Residue-property plots

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

- Molecule 1: Eukaryotic translation initiation factor 6

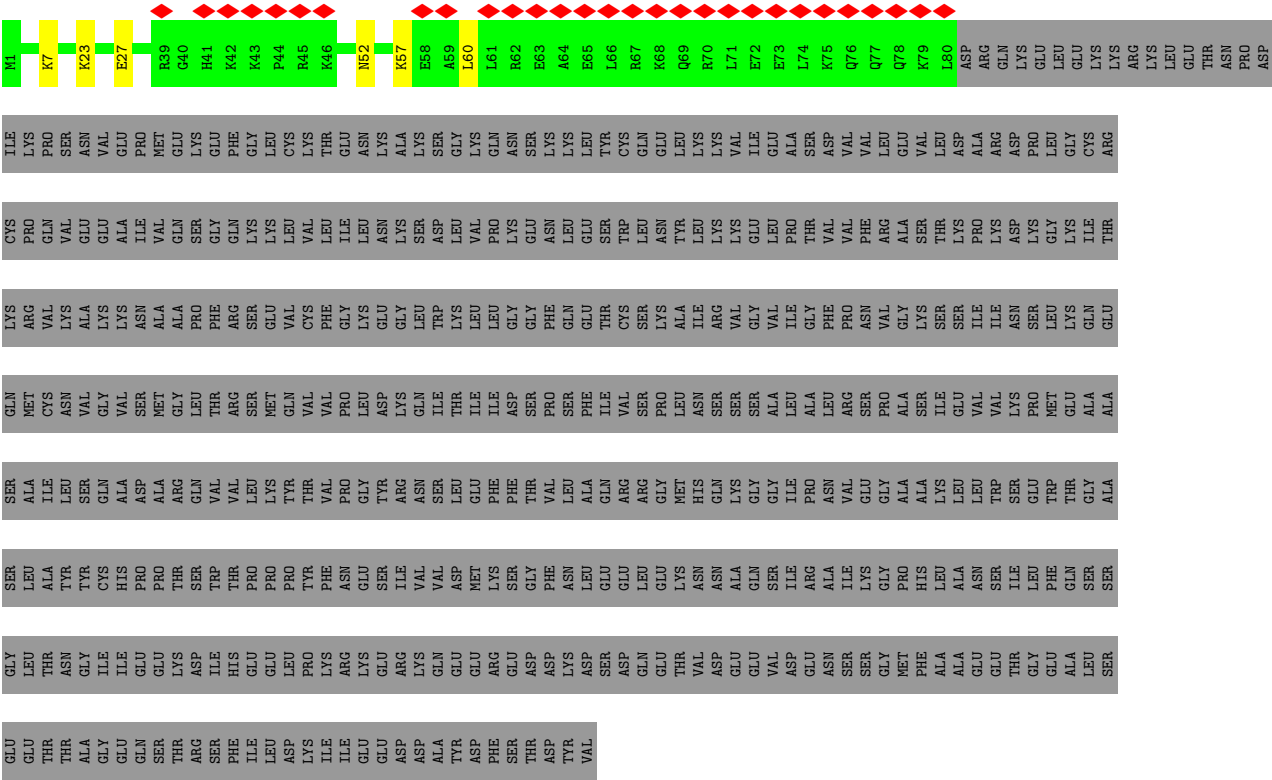


- Molecule 2: Nucleolar GTP-binding protein 2

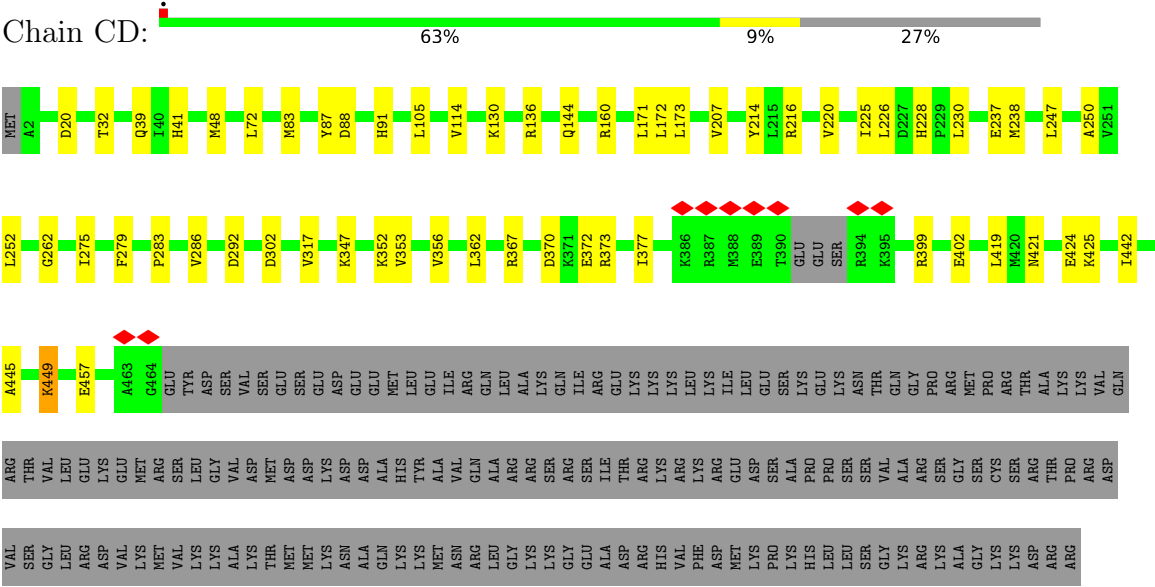


- Molecule 3: Guanine nucleotide-binding protein-like 3

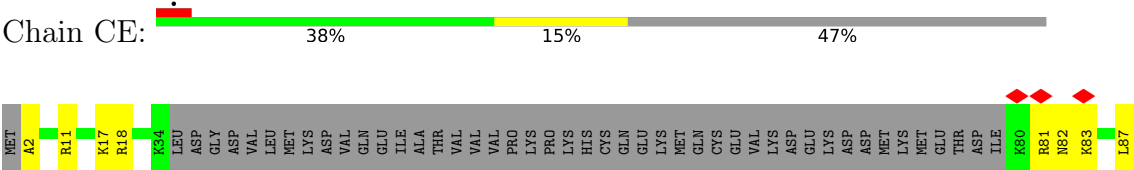


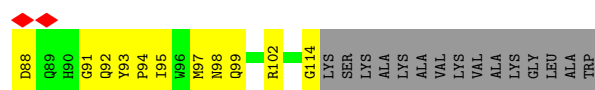


• Molecule 4: GTP-binding protein 4



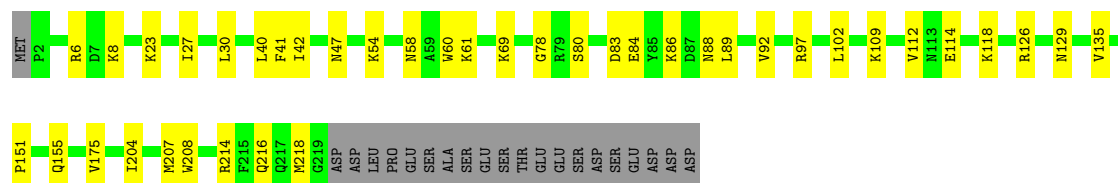
• Molecule 5: Protein LLP homolog





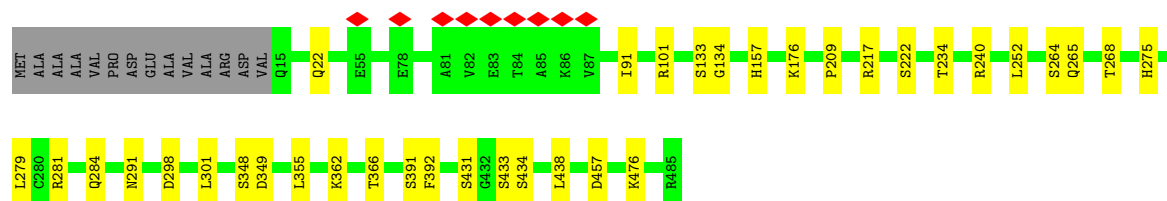
- Molecule 6: mRNA turnover protein 4 homolog

Chain CF: 74% 17% 9%



- Molecule 7: Notchless protein homolog 1

Chain CG: 90% 7% .



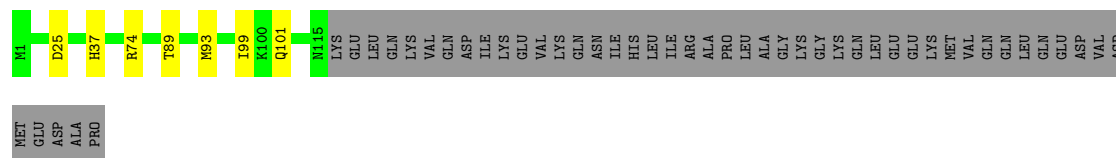
- Molecule 8: Ribosome biogenesis protein NSA2 homolog

Chain CH: 92% 8%



- Molecule 9: Probable ribosome biogenesis protein RLP24

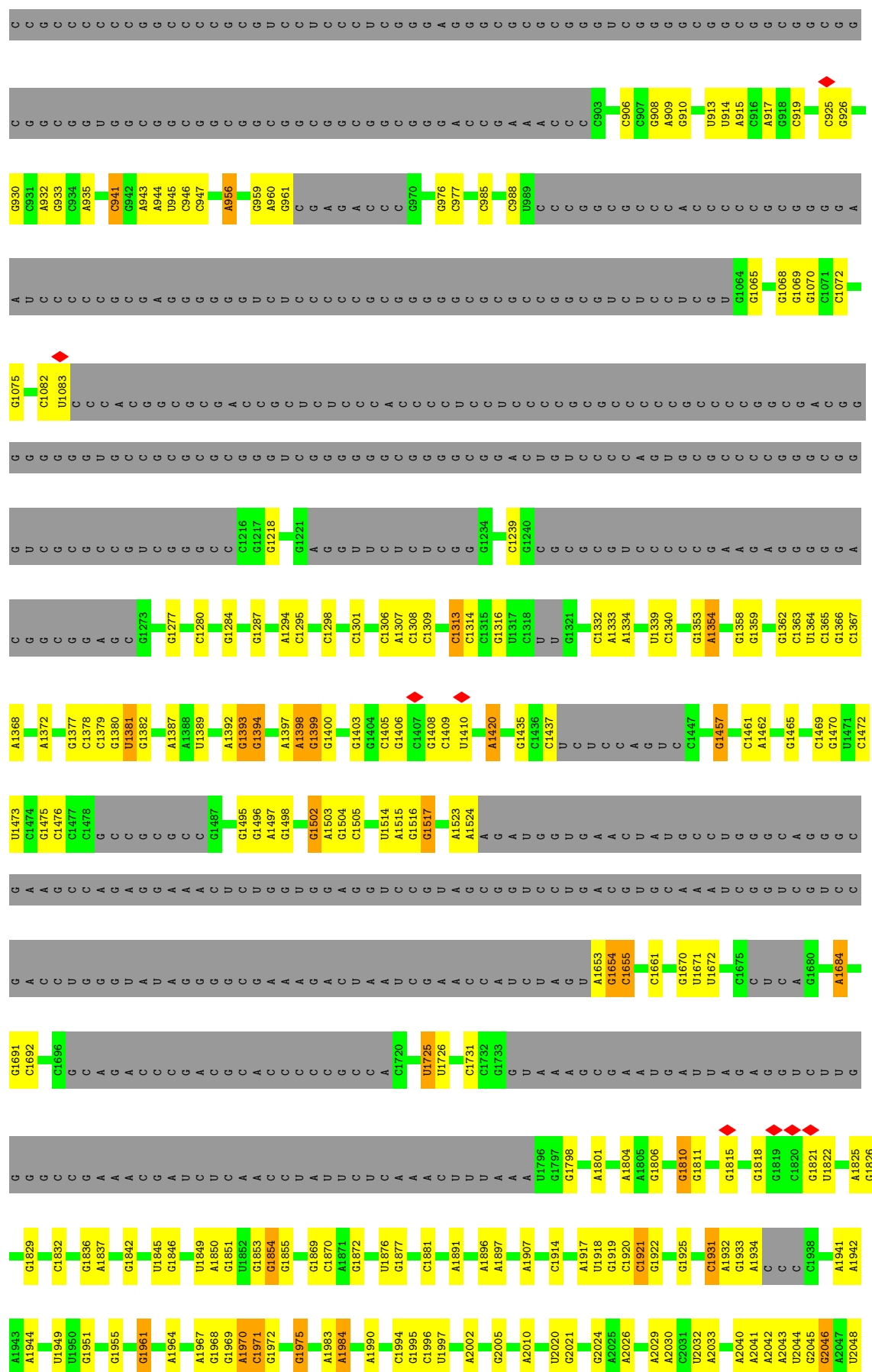
Chain CI: 66% . 29%



- Molecule 10: Ribosome production factor 2 homolog

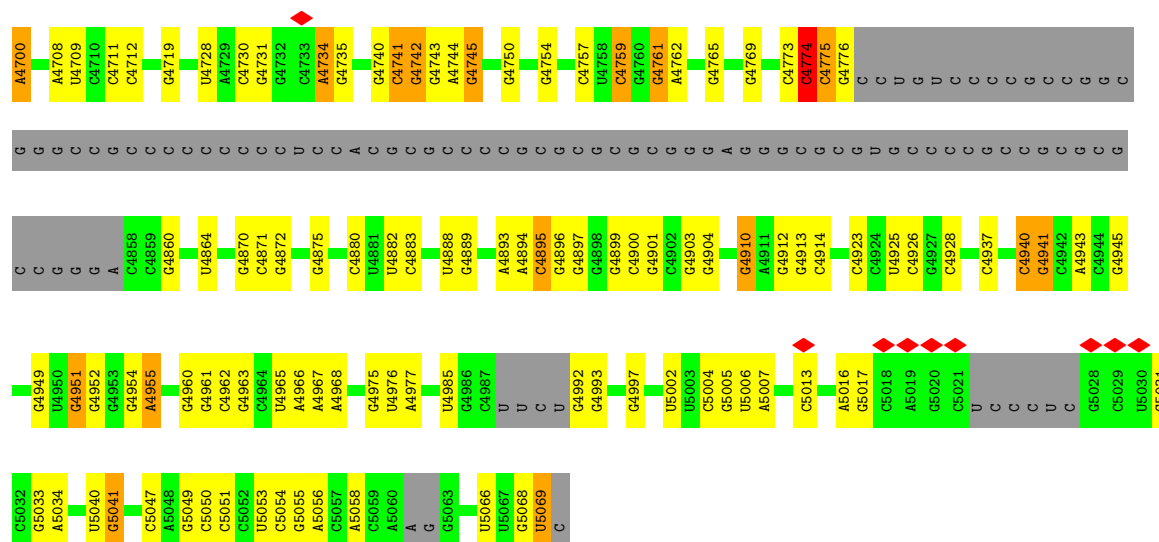
Chain CJ: 75% 15% 10%





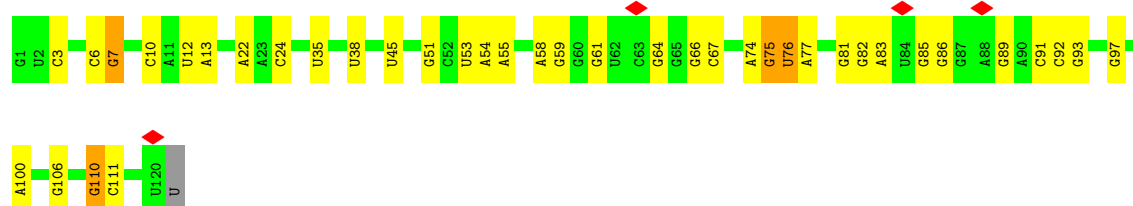


G4604	U4512	G4330	U4229	A	G	C3977	A	A3896	U
A4605	A4513	G4331	U4232	C	A	C	C	A	U
G4606	A4518	C4335	A4233	C	G	C3909	C	C	G
A4607	C4519	A4336	G4237	G	C	C3911	G	G	C
G4617	U4521	G4337	C4237	C	C	G	G	A	G
C4618	G	A	G4238	U	G	G	G	A	U
U4619	A	U	A4239	A4164	C	G	G	U	C
U4620	G4524	U	A4240	G4165	C	C	C	U	C
G4623	C4525	C4341	C4243	G4166	C	G	G	C	C
U4632	U4526	U4344	G4249	G4167	C	C	C	U	C
G4633	G4527	G4347	G4250	G4168	C	C	C	A	C
U4634	G4528	A	A4251	A4170	C	C	C	U	C
A4635	U	C	G4254	C4171	C	C	C	A	C
U4636	U	C4350	G4257	G4172	C	C	C	U	C
G4637	U	U4354	C4258	G4173	C	C	C	A	C
U4641	A	U4354	C4259	G4180	C	C	C	A	C
U4642	G4534	U4361	C4260	U4181	C	C	C	A	C
G4643	C4536	C4365	C4261	G4182	C	C	C	A	C
U4644	U	G4368	U4265	G4183	C	C	C	A	C
C4645	C4539	G4371	G4266	U4184	C	C	C	A	C
U4646	U4540	U	A4267	G4185	C	C	C	A	C
G4647	G4541	G	A4268	A4186	C	C	C	A	C
A4648	A4544	U	A4271	U4190	C	C	C	A	C
U4649	C4545	U	G4272	A	C	C	C	A	C
G4650	A4546	C	A4273	C	C	C	C	A	C
A4651	C4547	A	A4276	U	C	C	C	A	C
C4652	A4548	G	A4277	G4195	C	C	C	A	C
U4653	U4552	U	A4278	C4199	C	C	C	A	C
C4654	A4553	A	G4279	G4200	C	C	C	A	C
A4655	G4554	A	G4280	G4201	C	C	C	A	C
U	U	A4381	A4282	U4202	C	C	C	A	C
A	U	G4382	U4287	C4203	C	C	C	A	C
G4658	U4558	A4385	C4288	C4204	C	C	C	A	C
C4662	A4559	C4389	U4289	A4205	C	C	C	A	C
G4663	C4560	A4390	G4291	U4210	C	C	C	A	C
A4664	C4561	G4391	A4292	C	C	C	C	A	C
C4670	G4567	G4392	U4293	A	C	C	C	A	C
C4671	A4568	C4393	U4294	A	C	C	C	A	C
A4672	U4569	U	U4295	C	C	C	C	A	C
G4678	U4572	A	U4296	G	C	C	C	A	C
U4682	G4573	A	G4297	U	C	C	C	A	C
U4683	U4574	C	A4304	A	C	C	C	A	C
A4684	G4575	U	G4305	A	C	C	C	A	C
A4691	U4580	G4400	U4306	C	C	C	C	A	C
A4692	C4593	G4401	A4307	G4222	C	C	C	A	C
C4693	U4597	U4404	C4308	C4223	C	C	C	A	C
G4694	U4598	G4405	G4309	A4224	C	C	C	A	C
C4695	U4599	U4406	C4316	G4225	C	C	C	A	C
U4699		G4407	G4316	G4226	C	C	C	A	C
		G4408		G4228	C	C	C	A	C



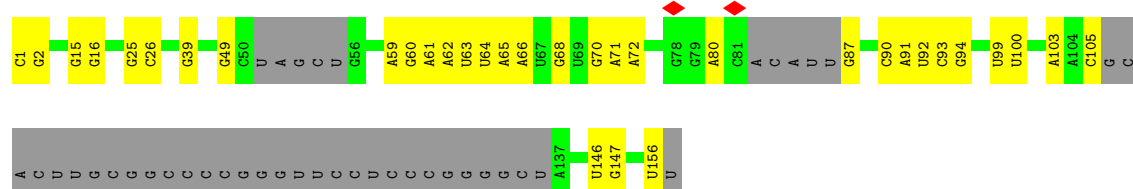
• Molecule 13: 5S rRNA

Chain L7: 67% 29%



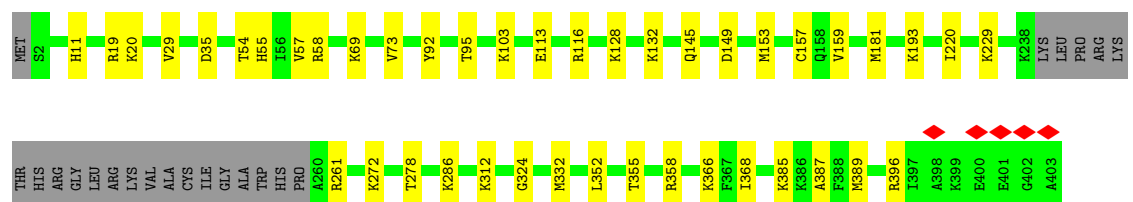
• Molecule 14: 5.8S rRNA

Chain L8: 52% 22% 27%

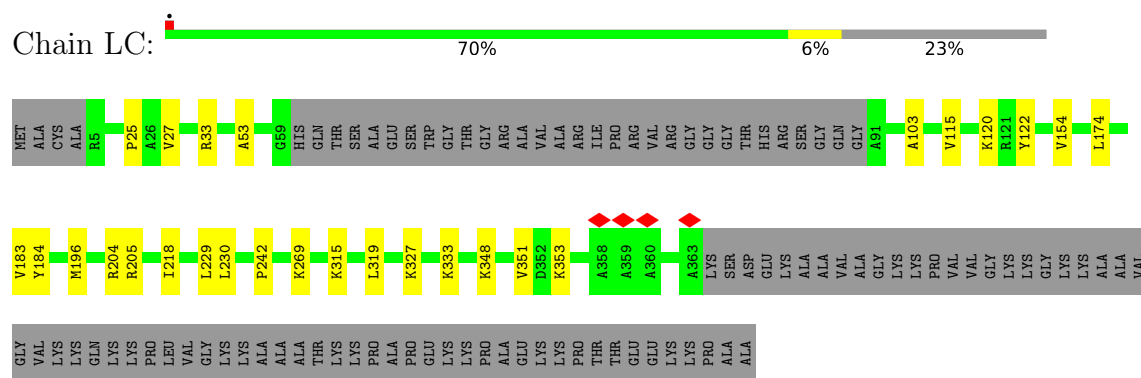


• Molecule 15: 60S ribosomal protein L3

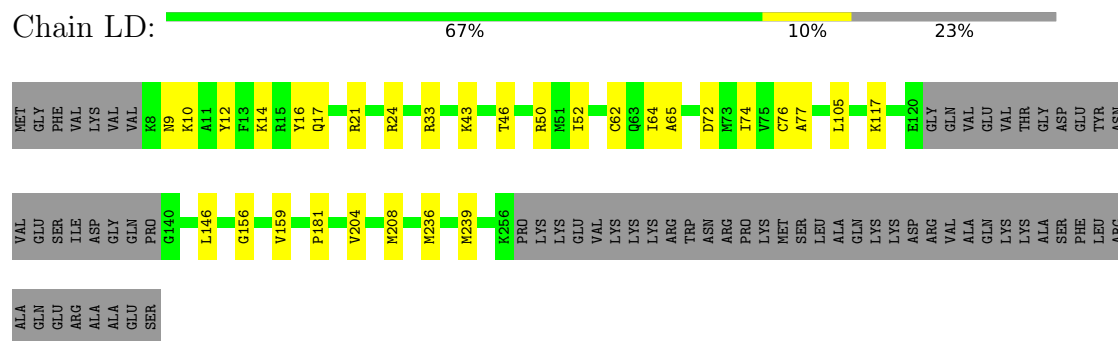
Chain LB: 84% 11% 5%



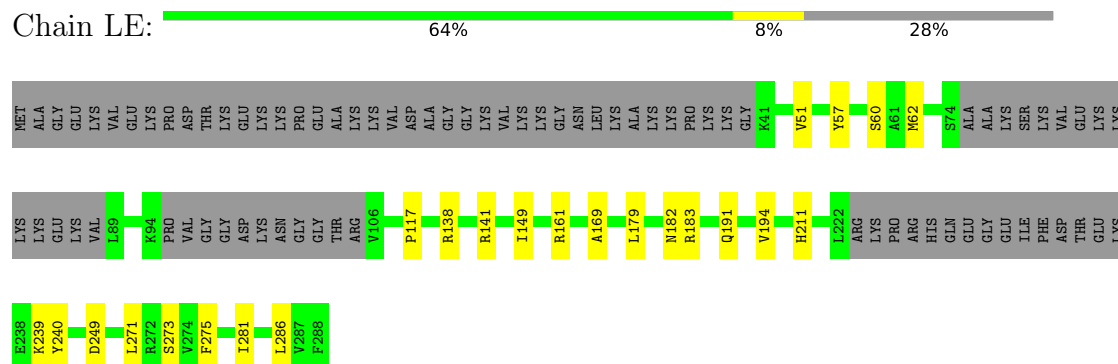
• Molecule 16: 60S ribosomal protein L4



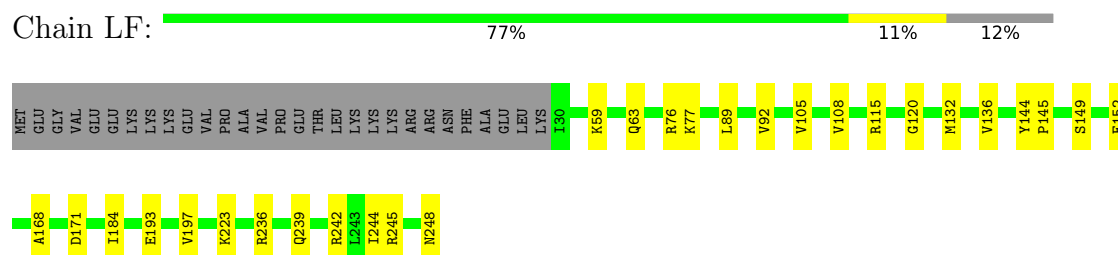
• Molecule 17: 60S ribosomal protein L5



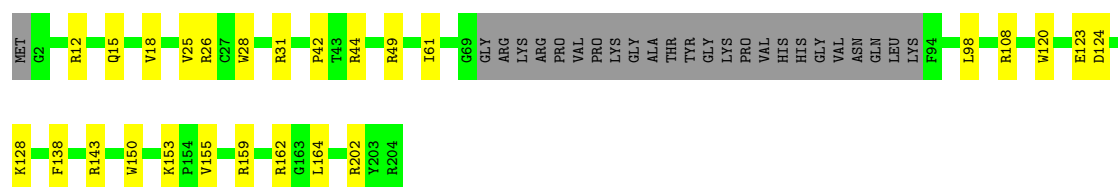
• Molecule 18: Large ribosomal subunit protein eL6



• Molecule 19: Large ribosomal subunit protein uL30



• Molecule 20: 60S ribosomal protein L7a



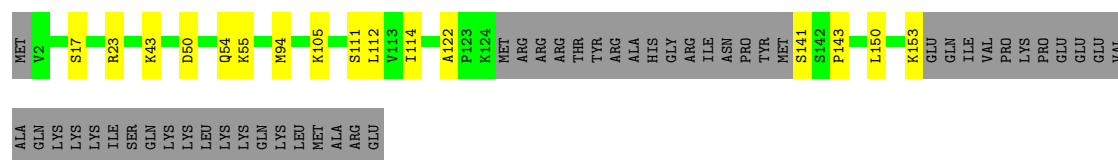
- Molecule 26: 60S ribosomal protein L13a

Chain LO: 87% 12% .



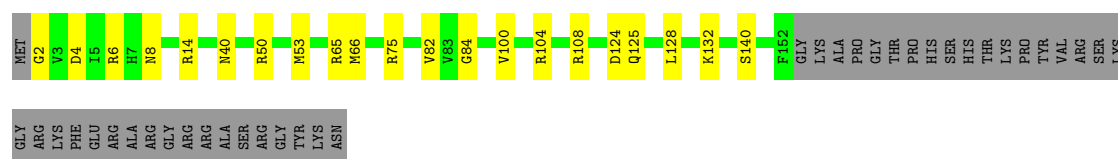
- Molecule 27: 60S ribosomal protein L17

Chain LP: 65% 9% 26%



- Molecule 28: 60S ribosomal protein L18

Chain LQ: 69% 11% 20%



- Molecule 29: 60S ribosomal protein L18a

Chain LS: 88% 12%



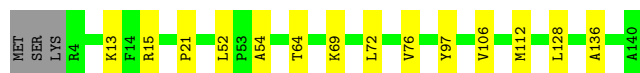
- Molecule 30: 60S ribosomal protein L21

Chain LT: 74% 6% 21%



- Molecule 31: 60S ribosomal protein L23

Chain LV:  88% 10%



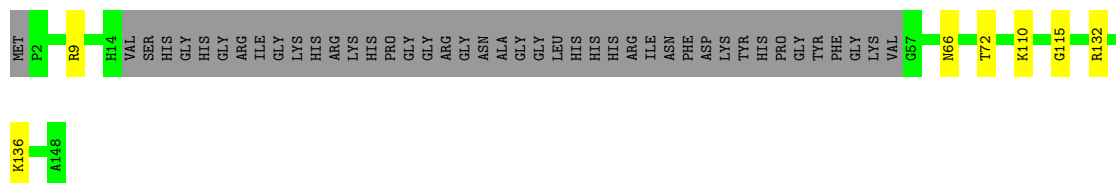
- Molecule 32: 60S ribosomal protein L26

Chain LY:  74% 17% 9%



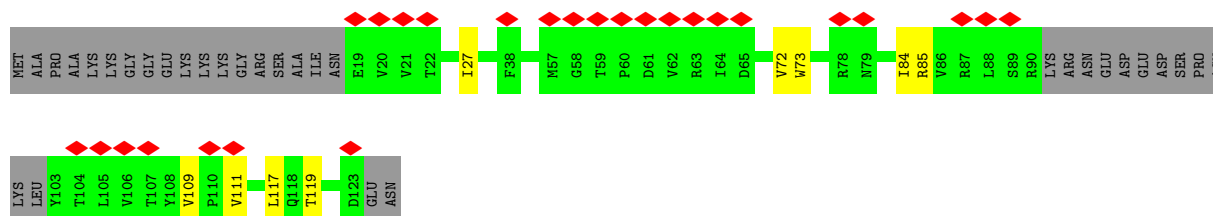
- Molecule 33: 60S ribosomal protein L27a

Chain La:  66% 5% 29%



- Molecule 34: 60S ribosomal protein L31

Chain Ld:  21% 67% 7% 26%



- Molecule 35: 60S ribosomal protein L32

Chain Le:  88% 7% 5%

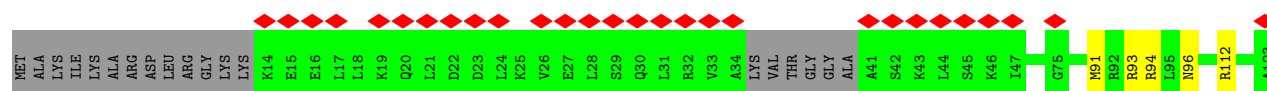
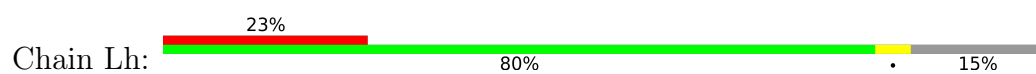


- Molecule 36: 60S ribosomal protein L35a

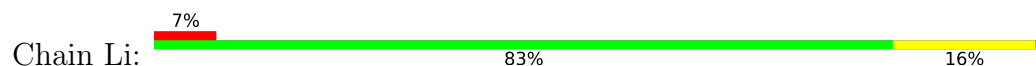
Chain Lf:  91% 8%



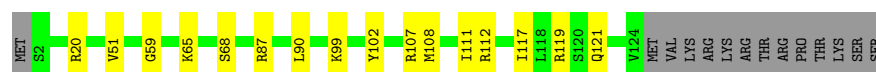
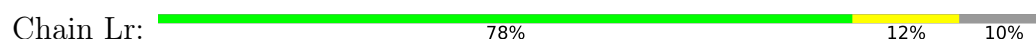
- Molecule 37: 60S ribosomal protein L35



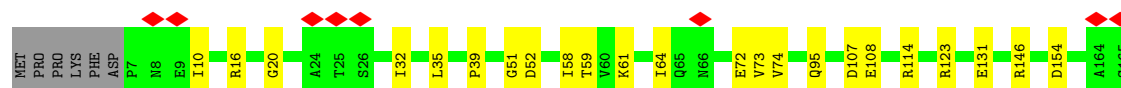
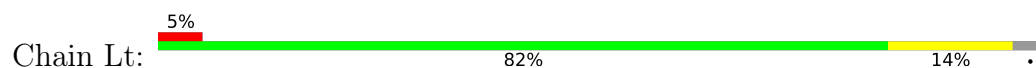
- Molecule 38: 60S ribosomal protein L36



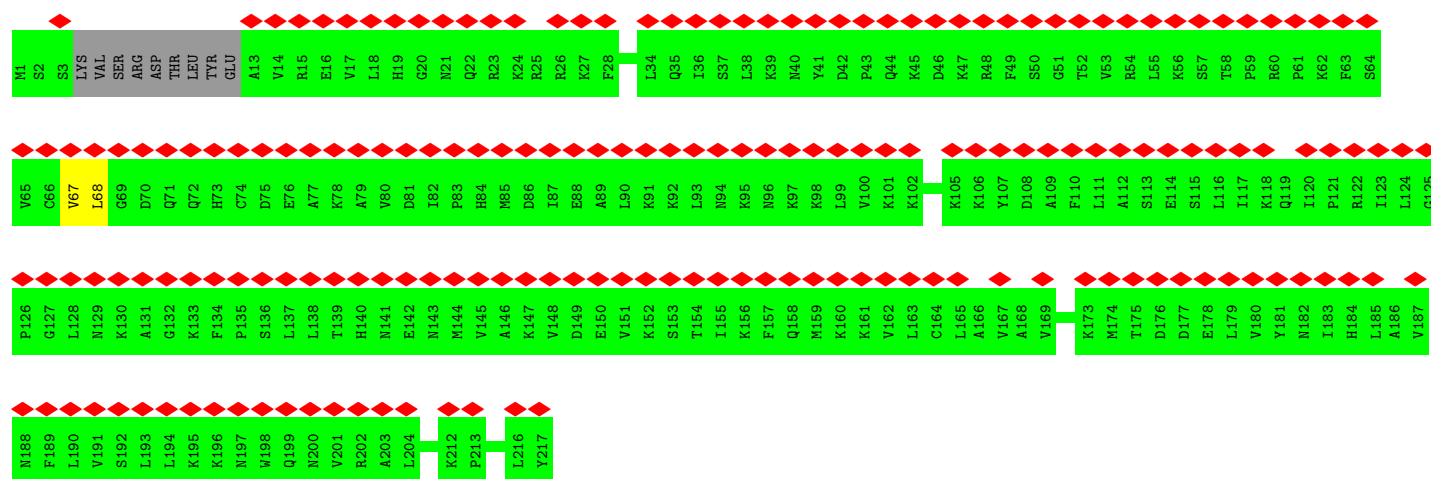
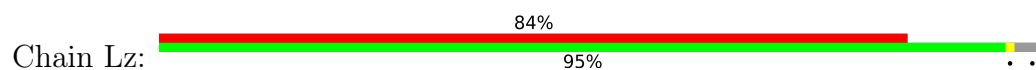
- Molecule 39: 60S ribosomal protein L28



- Molecule 40: Large ribosomal subunit protein uL11



- Molecule 41: 60S ribosomal protein L10a



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	41515	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	43.6	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	4.738	Depositor
Minimum map value	0.000	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.090	Depositor
Recommended contour level	0.334	Depositor
Map size ($\text{\AA}$)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	CA	0.19	0/1885	0.47	0/2564
2	CB	0.18	0/3579	0.42	0/4846
3	CC	0.18	0/602	0.40	0/800
4	CD	0.21	0/3808	0.49	1/5145 (0.0%)
5	CE	0.21	0/543	0.50	0/718
6	CF	0.17	0/1810	0.43	0/2425
7	CG	0.19	0/3526	0.43	0/4799
8	CH	0.18	0/2106	0.35	0/2820
9	CI	0.22	0/1008	0.55	0/1333
10	CJ	0.16	0/2218	0.40	0/2983
11	CK	0.17	0/1577	0.42	0/2141
12	L5	0.17	0/56814	0.32	1/88545 (0.0%)
13	L7	0.16	0/2861	0.29	0/4459
14	L8	0.16	0/2736	0.31	0/4256
15	LB	0.18	0/3115	0.35	0/4167
16	LC	0.19	0/2676	0.38	0/3593
17	LD	0.19	0/1916	0.41	0/2566
18	LE	0.18	0/1705	0.41	0/2290
19	LF	0.19	0/1824	0.42	0/2437
20	LG	0.20	0/1398	0.47	0/1885
21	LH	0.16	0/1529	0.36	0/2058
22	LJ	0.20	0/1358	0.52	1/1820 (0.1%)
23	LL	0.19	0/1464	0.42	0/1960
24	LM	0.20	0/1127	0.43	0/1508
25	LN	0.20	0/1554	0.41	0/2078
26	LO	0.19	0/1674	0.36	0/2241
27	LP	0.16	0/1110	0.41	0/1489
28	LQ	0.19	0/1239	0.44	0/1658
29	LS	0.18	0/1497	0.40	0/2009
30	LT	0.16	0/1015	0.43	0/1365
31	LV	0.18	0/1033	0.45	0/1383
32	LY	0.18	0/1109	0.49	0/1477

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
33	La	0.17	0/837	0.34	0/1118
34	Ld	0.15	0/624	0.41	0/856
35	Le	0.19	0/1071	0.40	0/1429
36	Lf	0.18	0/891	0.29	0/1194
37	Lh	0.12	0/670	0.31	0/907
38	Li	0.23	0/850	0.63	1/1125 (0.1%)
39	Lr	0.20	0/999	0.42	0/1340
40	Lt	0.18	0/1202	0.49	2/1622 (0.1%)
41	Lz	0.16	0/1031	0.50	0/1434
All	All	0.18	0/121591	0.37	6/176843 (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
32	LY	0	1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	Lt	114	ARG	CA-C-N	-6.29	111.00	122.38
40	Lt	114	ARG	C-N-CA	-6.29	111.00	122.38
4	CD	449	LYS	CA-CB-CG	6.20	126.50	114.10
22	LJ	81	GLU	N-CA-CB	5.15	118.26	110.28
38	Li	88	GLU	N-CA-CB	5.09	118.70	110.40
12	L5	4774	C	P-O3'-C3'	5.02	127.73	120.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
32	LY	83	GLU	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	CA	1860	0	1835	35	0
2	CB	3506	0	3476	34	0
3	CC	594	0	584	5	0
4	CD	3735	0	3746	48	0
5	CE	537	0	549	17	0
6	CF	1775	0	1813	24	0
7	CG	3449	0	3178	20	0
8	CH	2066	0	2168	15	0
9	CI	987	0	1029	7	0
10	CJ	2176	0	2200	31	0
11	CK	1545	0	1525	15	0
12	L5	50823	0	25729	396	0
13	L7	2561	0	1295	19	0
14	L8	2450	0	1245	9	0
15	LB	3054	0	3161	31	0
16	LC	2628	0	2801	20	0
17	LD	1879	0	1887	19	0
18	LE	1673	0	1803	16	0
19	LF	1790	0	1873	21	0
20	LG	1376	0	1468	15	0
21	LH	1510	0	1579	12	0
22	LJ	1335	0	1345	10	0
23	LL	1440	0	1549	21	0
24	LM	1105	0	1156	8	0
25	LN	1516	0	1550	19	0
26	LO	1642	0	1779	20	0
27	LP	1089	0	1115	11	0
28	LQ	1223	0	1330	16	0
29	LS	1457	0	1491	14	0
30	LT	994	0	996	6	0
31	LV	1019	0	1079	10	0
32	LY	1092	0	1167	17	0
33	La	823	0	879	6	0
34	Ld	613	0	493	6	0
35	Le	1053	0	1147	8	0
36	Lf	872	0	901	6	0
37	Lh	666	0	516	4	0
38	Li	839	0	910	11	0
39	Lr	984	0	1048	13	0
40	Lt	1186	0	1226	14	0
41	Lz	1033	0	456	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
42	CB	32	0	12	0	0
43	CB	1	0	0	0	0
43	CD	1	0	0	0	0
44	CD	28	0	12	0	0
45	CI	1	0	0	0	0
All	All	114018	0	87101	837	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 4.

All (837) 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)
12:L5:3860:A:H61	12:L5:4560:C:N4	1.62	0.96
12:L5:2845:A:H61	12:L5:3843:C:H42	1.08	0.93
12:L5:4745:G:H1	12:L5:4955:A:N6	1.66	0.92
12:L5:4745:G:H1	12:L5:4955:A:H61	0.92	0.89
12:L5:3930:U:H3	12:L5:4180:G:H1	1.16	0.88
12:L5:4295:U:H3	12:L5:4316:G:H1	0.88	0.85
12:L5:4534:G:H1	12:L5:4552:U:H3	1.19	0.85
12:L5:2845:A:H61	12:L5:3843:C:N4	1.81	0.79
12:L5:2845:A:N6	12:L5:3843:C:H42	1.82	0.78
12:L5:4993:G:H1	12:L5:5058:A:H2	1.33	0.75
12:L5:3860:A:N6	12:L5:4560:C:N4	2.35	0.73
10:CJ:164:ILE:O	10:CJ:168:ARG:HB2	1.89	0.73
1:CA:123:ARG:HH21	1:CA:127:GLU:HG3	1.56	0.71
12:L5:4997:G:H1	12:L5:5053:U:H3	1.38	0.71
2:CB:80:TRP:HB3	8:CH:259:LEU:HD13	1.73	0.71
12:L5:432:U:H3	12:L5:3887:C:H42	1.37	0.71
23:LL:63:THR:HG22	23:LL:65:ARG:H	1.55	0.70
12:L5:1362:G:OP1	23:LL:39:ARG:NH2	2.24	0.69
12:L5:3955:G:C2	12:L5:3966:A:N7	2.61	0.68
12:L5:3967:G:N1	12:L5:4055:U:N3	2.41	0.67
2:CB:197:ILE:HD11	2:CB:386:LYS:HB3	1.76	0.67
15:LB:92:TYR:HB2	15:LB:159:VAL:HB	1.76	0.67
12:L5:1684:A:H62	12:L5:1853:G:H8	1.43	0.67
26:LO:85:ARG:HG3	26:LO:99:LEU:HD11	1.76	0.66
12:L5:4344:U:H3	12:L5:4368:G:H1	1.42	0.66
12:L5:4910:G:H4'	15:LB:95:THR:HG22	1.76	0.66
29:LS:19:THR:HG22	29:LS:21:LYS:H	1.61	0.66
12:L5:1353:G:N7	28:LQ:104:ARG:NH2	2.43	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:CB:155:LEU:HD22	4:CD:230:LEU:HD21	1.78	0.65
11:CK:148:ARG:NH2	12:L5:4199:C:OP2	2.30	0.64
28:LQ:82:VAL:HG12	28:LQ:84:GLY:H	1.61	0.64
5:CE:92:GLN:NE2	12:L5:4962:C:O2	2.31	0.64
13:L7:51:G:H21	22:LJ:12:MET:HE1	1.62	0.63
12:L5:4993:G:O6	12:L5:5058:A:N1	2.31	0.63
6:CF:109:LYS:HG3	6:CF:218:MET:HE1	1.80	0.63
20:LG:67:ARG:HH12	25:LN:25:VAL:HB	1.64	0.63
7:CG:279:LEU:HD23	40:Lt:95:GLN:HG2	1.80	0.63
7:CG:291:ASN:ND2	7:CG:349:ASP:OD1	2.30	0.63
38:Li:68:ARG:HA	38:Li:71:LYS:HG2	1.80	0.62
6:CF:42:ILE:HD11	6:CF:92:VAL:HG13	1.81	0.62
33:La:132:ARG:HE	33:La:136:LYS:HE3	1.64	0.62
12:L5:3955:G:N2	12:L5:3966:A:C5	2.67	0.62
4:CD:275:ILE:HG13	4:CD:279:PHE:HE1	1.65	0.62
11:CK:178:LYS:HE3	12:L5:4199:C:H5''	1.80	0.62
12:L5:1951:G:O2'	29:LS:95:ARG:NH2	2.33	0.62
4:CD:347:LYS:HE2	4:CD:352:LYS:HE2	1.81	0.61
12:L5:4623:G:OP1	15:LB:19:ARG:NH2	2.34	0.61
2:CB:51:ASN:HD21	2:CB:55:LYS:HE3	1.66	0.61
6:CF:114:GLU:OE1	6:CF:118:LYS:NZ	2.34	0.61
2:CB:16:LYS:NZ	12:L5:3924:C:OP1	2.34	0.61
2:CB:352:THR:HG23	12:L5:4539:U:H5''	1.82	0.61
1:CA:106:ASN:ND2	31:LV:136:ALA:O	2.33	0.61
1:CA:245:THR:HB	4:CD:347:LYS:HE3	1.81	0.61
15:LB:153:MET:O	15:LB:157:CYS:HB2	2.01	0.61
12:L5:3955:G:C2	12:L5:3966:A:C8	2.89	0.61
23:LL:130:LYS:NZ	23:LL:132:SER:OG	2.34	0.61
12:L5:1972:G:N2	40:Lt:131:GLU:OE1	2.35	0.60
20:LG:106:THR:OG1	20:LG:109:GLU:OE1	2.18	0.60
33:La:115:GLY:O	33:La:136:LYS:NZ	2.35	0.60
12:L5:109:G:OP2	23:LL:74:ARG:NH2	2.34	0.60
12:L5:3860:A:N6	12:L5:4560:C:C4	2.68	0.60
12:L5:1316:G:OP1	35:Le:43:ASN:ND2	2.34	0.59
5:CE:18:ARG:HH21	15:LB:352:LEU:HD13	1.66	0.59
12:L5:1398:A:OP2	12:L5:1420:A:N6	2.36	0.59
12:L5:4078:C:O2'	12:L5:4173:G:N2	2.36	0.59
21:LH:93:ARG:HG3	21:LH:182:SER:HB2	1.85	0.59
12:L5:264:C:O2	37:Lh:112:ARG:NH2	2.35	0.59
19:LF:105:VAL:HG13	19:LF:136:VAL:HG12	1.84	0.59
7:CG:281:ARG:HB2	7:CG:362:LYS:HE2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:LO:34:VAL:HG22	26:LO:103:LYS:HB2	1.85	0.59
40:Lt:10:ILE:HA	40:Lt:64:ILE:O	2.03	0.59
12:L5:2263:A:H5''	39:Lr:108:MET:HG3	1.85	0.59
12:L5:3955:G:N2	12:L5:3966:A:C4	2.71	0.59
10:CJ:79:GLU:HA	10:CJ:108:MET:HE1	1.85	0.58
12:L5:1853:G:OP2	12:L5:1853:G:N2	2.33	0.58
12:L5:67:C:OP2	12:L5:312:G:N2	2.35	0.58
12:L5:458:C:OP1	39:Lr:87:ARG:NH2	2.36	0.58
12:L5:1372:A:OP1	25:LN:202:ARG:NH2	2.34	0.58
4:CD:144:GLN:NE2	12:L5:4437:U:O4	2.36	0.58
12:L5:4618:G:H5''	31:LV:15:ARG:HB2	1.85	0.58
25:LN:31:ARG:NH2	25:LN:124:ASP:OD2	2.37	0.58
4:CD:367:ARG:NH2	4:CD:372:GLU:OE2	2.37	0.58
12:L5:432:U:H3	12:L5:3887:C:N4	2.02	0.58
12:L5:215:C:OP1	12:L5:219:G:N2	2.37	0.58
3:CC:52:ASN:ND2	12:L5:1955:G:OP2	2.37	0.58
1:CA:74:ASN:OD1	9:CI:74:ARG:NH1	2.37	0.57
5:CE:11:ARG:NH2	12:L5:4678:G:N7	2.52	0.57
12:L5:4691:A:H5'	21:LH:71:ARG:HH11	1.69	0.57
16:LC:33:ARG:HG3	16:LC:122:TYR:HE2	1.68	0.57
12:L5:3959:U:O2	12:L5:3960:A:N6	2.38	0.57
12:L5:4897:G:OP1	24:LM:128:LYS:NZ	2.37	0.57
18:LE:141:ARG:NH2	18:LE:191:GLN:O	2.38	0.57
25:LN:150:TRP:HA	25:LN:153:LYS:HE2	1.87	0.57
13:L7:7:G:OP1	17:LD:33:ARG:NH1	2.37	0.57
4:CD:88:ASP:HB3	4:CD:91:HIS:HB2	1.87	0.57
10:CJ:64:LYS:NZ	13:L7:10:C:OP1	2.38	0.57
12:L5:4712:C:OP1	26:LO:74:ARG:NH2	2.38	0.57
4:CD:83:MET:O	4:CD:87:TYR:HB2	2.05	0.57
12:L5:679:C:H2'	12:L5:680:G:H8	1.70	0.57
12:L5:2335:C:H2'	12:L5:2336:G:H8	1.69	0.57
12:L5:1377:G:H21	12:L5:1380:G:H5'	1.69	0.57
12:L5:4534:G:N2	12:L5:4552:U:O2	2.33	0.57
12:L5:6:C:H5''	20:LG:197:LYS:HB3	1.87	0.56
1:CA:109:THR:HB	1:CA:149:GLY:HA2	1.86	0.56
39:Lr:107:ARG:HE	39:Lr:108:MET:HG2	1.69	0.56
5:CE:99:GLN:HA	5:CE:102:ARG:HG2	1.86	0.56
12:L5:1457:G:O2'	28:LQ:75:ARG:NH2	2.37	0.56
12:L5:3961:G:N2	12:L5:3964:U:O3'	2.38	0.56
12:L5:4040:C:H5'	12:L5:4045:G:H22	1.71	0.56
8:CH:2:PRO:HG3	12:L5:4604:G:H4'	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:CK:107:ARG:HD3	11:CK:108:PRO:HD2	1.87	0.56
12:L5:4072:C:H2'	12:L5:4073:A:H8	1.70	0.56
12:L5:1907:A:H4'	19:LF:223:LYS:HE3	1.88	0.56
12:L5:4759:C:O2	26:LO:165:LYS:NZ	2.37	0.56
29:LS:81:TRP:HE1	29:LS:92:ASN:HD22	1.54	0.56
32:LY:31:SER:HA	32:LY:48:PRO:HA	1.87	0.56
12:L5:3929:G:H1	12:L5:4181:U:H3	1.54	0.55
18:LE:161:ARG:NH1	18:LE:273:SER:OG	2.39	0.55
12:L5:4617:G:OP2	15:LB:358:ARG:NH2	2.38	0.55
15:LB:57:VAL:HG22	15:LB:73:VAL:HG22	1.88	0.55
12:L5:667:A:H5''	12:L5:668:C:H5''	1.87	0.55
12:L5:3967:G:N2	12:L5:4055:U:O2	2.40	0.55
12:L5:3967:G:O6	12:L5:4055:U:O4	2.24	0.55
15:LB:35:ASP:OD2	15:LB:193:LYS:NZ	2.34	0.55
26:LO:62:MET:HE3	26:LO:69:GLY:HA2	1.88	0.55
17:LD:43:LYS:HE2	17:LD:46:THR:HG21	1.88	0.55
1:CA:136:GLU:OE2	4:CD:373:ARG:NH2	2.36	0.55
4:CD:457:GLU:HG2	9:CI:99:ILE:HD12	1.89	0.55
5:CE:83:LYS:NZ	12:L5:4904:G:OP1	2.37	0.55
12:L5:4670:C:O2'	12:L5:4672:A:OP2	2.25	0.55
4:CD:399:ARG:NH2	12:L5:4597:U:O2'	2.40	0.55
8:CH:17:ARG:NH1	21:LH:175:PHE:O	2.39	0.55
9:CI:37:HIS:NE2	31:LV:97:TYR:OH	2.32	0.55
12:L5:4204:C:H5''	22:LJ:64:ARG:HD3	1.89	0.55
12:L5:4407:G:H2'	12:L5:4408:G:C8	2.41	0.55
16:LC:218:ILE:HA	16:LC:229:LEU:HD13	1.89	0.55
24:LM:55:MET:O	29:LS:157:ARG:NH2	2.40	0.55
35:Le:85:LEU:HD21	35:Le:115:ALA:HB2	1.88	0.55
2:CB:282:HIS:HB3	2:CB:289:PHE:HB3	1.88	0.55
12:L5:3955:G:C2	12:L5:3966:A:C5	2.94	0.55
36:Lf:43:LEU:O	36:Lf:109:ARG:NH2	2.39	0.55
12:L5:317:A:H2'	12:L5:318:A:H8	1.71	0.55
12:L5:4620:U:OP2	12:L5:4670:C:N4	2.40	0.55
12:L5:3976:C:N4	12:L5:4035:G:OP2	2.40	0.54
20:LG:152:ALA:HA	20:LG:205:THR:HG22	1.89	0.54
2:CB:155:LEU:HD21	4:CD:238:MET:HE2	1.89	0.54
12:L5:2062:C:O2'	29:LS:111:ARG:NH2	2.40	0.54
19:LF:115:ARG:NH1	28:LQ:4:ASP:O	2.39	0.54
39:Lr:90:LEU:HD22	39:Lr:111:ILE:HG23	1.89	0.54
1:CA:219:GLU:HA	1:CA:224:LEU:HD13	1.89	0.54
5:CE:2:ALA:N	12:L5:4593:C:OP2	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:LF:236:ARG:HG2	19:LF:239:GLN:HB2	1.90	0.54
35:Le:84:GLU:OE2	39:Lr:20:ARG:NH1	2.37	0.54
1:CA:4:ARG:HB3	1:CA:208:LEU:HD23	1.89	0.54
12:L5:1853:G:H5''	12:L5:1854:G:H5'	1.88	0.54
26:LO:58:LEU:HD11	26:LO:145:VAL:HG13	1.90	0.54
12:L5:73:A:OP1	23:LL:106:SER:OG	2.26	0.54
12:L5:1354:A:OP1	28:LQ:108:ARG:NH2	2.41	0.54
12:L5:3839:G:N2	12:L5:3843:C:O2'	2.41	0.54
12:L5:4769:G:H5''	26:LO:176:ARG:HD3	1.89	0.54
12:L5:3971:G:N2	12:L5:3973:G:N3	2.56	0.54
28:LQ:50:ARG:HH12	28:LQ:140:SER:HB2	1.72	0.54
20:LG:165:GLU:OE2	25:LN:26:ARG:NH2	2.41	0.54
12:L5:19:G:OP2	37:Lh:93:ARG:NH2	2.36	0.53
14:L8:72:A:H61	14:L8:80:A:H62	1.56	0.53
23:LL:91:ALA:HB1	23:LL:96:ILE:HB	1.91	0.53
12:L5:300:A:H2'	12:L5:301:G:H8	1.74	0.53
12:L5:1801:A:O2'	30:LT:102:ARG:NH2	2.41	0.53
12:L5:4910:G:N2	26:LO:106:ASP:O	2.42	0.53
17:LD:65:ALA:HB2	17:LD:74:ILE:HD13	1.89	0.53
16:LC:204:ARG:NH1	16:LC:205:ARG:O	2.40	0.53
6:CF:47:ASN:ND2	6:CF:129:ASN:OD1	2.42	0.53
18:LE:239:LYS:NZ	18:LE:240:TYR:O	2.41	0.53
1:CA:155:SER:OG	1:CA:156:ASN:N	2.41	0.53
1:CA:175:SER:O	1:CA:178:GLN:NE2	2.40	0.53
7:CG:157:HIS:CE1	7:CG:176:LYS:HD3	2.44	0.53
10:CJ:104:VAL:HG22	10:CJ:118:GLU:HG2	1.90	0.53
12:L5:318:A:H2'	12:L5:319:A:H8	1.74	0.53
12:L5:1932:A:OP2	26:LO:49:ARG:NH2	2.42	0.53
24:LM:11:ARG:NH1	24:LM:58:THR:O	2.40	0.53
40:Lt:20:GLY:HA2	40:Lt:51:GLY:HA2	1.90	0.53
4:CD:39:GLN:OE1	4:CD:41:HIS:NE2	2.40	0.53
12:L5:307:A:N3	12:L5:310:G:O2'	2.39	0.53
26:LO:128:ARG:NH1	29:LS:162:GLN:OE1	2.39	0.53
40:Lt:61:LYS:HB3	40:Lt:72:GLU:HG2	1.90	0.53
12:L5:3946:G:H2'	12:L5:3947:A:H8	1.74	0.53
12:L5:4527:G:OP2	12:L5:4527:G:N2	2.35	0.53
2:CB:348:TRP:HA	2:CB:361:ASP:O	2.09	0.53
4:CD:445:ALA:O	4:CD:449:LYS:HB3	2.09	0.53
7:CG:355:LEU:HB3	7:CG:366:THR:HG22	1.91	0.53
10:CJ:211:ARG:NH1	10:CJ:213:GLU:OE2	2.42	0.53
12:L5:4075:U:H1'	12:L5:4076:G:H2'	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L5:152:U:OP1	25:LN:49:ARG:NH1	2.38	0.52
12:L5:4258:C:H5'	22:LJ:68:ILE:HD11	1.91	0.52
4:CD:421:ASN:HB2	4:CD:424:GLU:HB2	1.91	0.52
10:CJ:207:CYS:SG	10:CJ:208:ARG:N	2.83	0.52
12:L5:74:G:H5''	23:LL:59:VAL:HB	1.91	0.52
31:LV:106:VAL:HA	31:LV:112:MET:HA	1.91	0.52
1:CA:1:MET:HE3	1:CA:2:ALA:H	1.73	0.52
7:CG:433:SER:OG	7:CG:434:SER:N	2.43	0.52
32:LY:70:VAL:HA	32:LY:82:ILE:HG22	1.92	0.52
12:L5:3955:G:N3	12:L5:3966:A:N7	2.57	0.52
18:LE:141:ARG:NH1	36:Lf:110:ILE:O	2.42	0.52
27:LP:112:LEU:HD12	27:LP:150:LEU:HB3	1.91	0.52
12:L5:404:U:O2'	32:LY:87:ARG:NH2	2.41	0.52
12:L5:1364:U:OP2	23:LL:36:ARG:NH2	2.42	0.52
2:CB:115:LYS:NZ	12:L5:4308:C:O2	2.40	0.52
12:L5:4641:U:H3	12:L5:4658:G:H1	1.58	0.52
12:L5:1332:C:H2'	12:L5:1333:A:H8	1.73	0.52
12:L5:1523:A:H62	12:L5:1653:A:H1'	1.74	0.52
12:L5:1845:U:H2'	12:L5:1846:G:H8	1.74	0.52
12:L5:4672:A:OP1	31:LV:15:ARG:NH2	2.42	0.52
13:L7:85:G:H2'	13:L7:86:G:H8	1.75	0.52
20:LG:94:GLN:HA	20:LG:97:LYS:HG2	1.92	0.52
5:CE:82:ASN:ND2	12:L5:4903:G:OP1	2.43	0.52
12:L5:4449:A:N6	12:L5:4502:C:O2'	2.43	0.52
15:LB:220:ILE:HG12	15:LB:278:THR:HG23	1.91	0.52
1:CA:241:ILE:O	1:CA:245:THR:OG1	2.23	0.52
2:CB:33:ARG:NH2	12:L5:4541:G:O2'	2.43	0.52
12:L5:1984:A:N7	12:L5:2010:A:O2'	2.43	0.52
18:LE:138:ARG:NE	18:LE:169:ALA:O	2.41	0.52
6:CF:41:PHE:HD2	6:CF:204:ILE:HG21	1.73	0.51
12:L5:5066:U:OP1	27:LP:43:LYS:NZ	2.43	0.51
28:LQ:50:ARG:HA	28:LQ:53:MET:HG3	1.91	0.51
1:CA:108:THR:HG23	1:CA:117:VAL:HG12	1.91	0.51
7:CG:240:ARG:NH1	7:CG:275:HIS:O	2.43	0.51
16:LC:327:LYS:NZ	19:LF:171:ASP:OD1	2.37	0.51
34:Ld:27:ILE:HB	34:Ld:84:ILE:HG22	1.92	0.51
12:L5:3855:C:O2'	27:LP:54:GLN:NE2	2.44	0.51
25:LN:138:PHE:HA	25:LN:143:ARG:HD2	1.92	0.51
12:L5:4265:U:OP1	17:LD:12:TYR:OH	2.28	0.51
19:LF:149:SER:OG	19:LF:245:ARG:NH1	2.44	0.51
4:CD:216:ARG:HH22	12:L5:4607:A:H5'	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:Le:85:LEU:HD22	35:Le:111:ILE:HG23	1.91	0.51
8:CH:105:MET:SD	8:CH:231:THR:OG1	2.69	0.51
10:CJ:139:THR:HB	10:CJ:182:TYR:HE1	1.76	0.51
12:L5:280:G:O6	25:LN:15:GLN:NE2	2.32	0.51
12:L5:308:G:O6	25:LN:12:ARG:NH1	2.44	0.51
12:L5:5051:C:H4'	15:LB:324:GLY:HA2	1.93	0.51
39:Lr:59:GLY:O	39:Lr:121:GLN:NE2	2.34	0.51
3:CC:52:ASN:OD1	3:CC:57:LYS:NZ	2.36	0.51
12:L5:1394:G:OP1	23:LL:186:ARG:NH1	2.44	0.51
12:L5:5016:A:N6	12:L5:5033:G:O2'	2.33	0.51
4:CD:207:VAL:O	8:CH:3:GLN:NE2	2.39	0.51
12:L5:1389:U:OP1	12:L5:1496:G:O2'	2.29	0.51
6:CF:126:ARG:NH2	12:L5:1967:A:O2'	2.43	0.50
12:L5:1975:G:O2'	40:Lt:16:ARG:NH1	2.44	0.50
12:L5:3944:G:H2'	12:L5:3945:A:C8	2.46	0.50
12:L5:3969:G:O2'	12:L5:4054:C:N4	2.40	0.50
7:CG:133:SER:OG	7:CG:134:GLY:N	2.45	0.50
11:CK:141:ARG:HB2	11:CK:149:ALA:HB2	1.92	0.50
12:L5:3930:U:O4	12:L5:4180:G:O6	2.30	0.50
31:LV:13:LYS:HD3	31:LV:128:LEU:HD22	1.93	0.50
32:LY:10:ASP:HB3	32:LY:13:LYS:HB2	1.94	0.50
10:CJ:22:ARG:NH2	10:CJ:84:LYS:O	2.44	0.50
12:L5:2297:G:H4'	16:LC:242:PRO:HB2	1.93	0.50
25:LN:44:ARG:NH1	25:LN:120:TRP:O	2.43	0.50
29:LS:71:SER:O	29:LS:76:LYS:NZ	2.42	0.50
6:CF:207:MET:HE3	6:CF:216:GLN:HE21	1.76	0.50
15:LB:261:ARG:HE	26:LO:64:THR:HG21	1.77	0.50
17:LD:50:ARG:NH2	17:LD:72:ASP:OD2	2.44	0.50
40:Lt:146:ARG:NH1	40:Lt:154:ASP:OD2	2.44	0.50
12:L5:102:G:HO2'	12:L5:1381:U:HO2'	1.60	0.50
12:L5:659:G:H2'	12:L5:660:A:H8	1.76	0.50
7:CG:431:SER:O	7:CG:438:LEU:HA	2.12	0.50
10:CJ:212:ILE:HD13	11:CK:73:ILE:HG13	1.93	0.50
12:L5:151:G:OP1	25:LN:49:ARG:NH2	2.45	0.50
17:LD:62:CYS:HB3	17:LD:105:LEU:HD22	1.93	0.50
29:LS:83:ARG:HB2	29:LS:127:MET:HE2	1.93	0.50
4:CD:172:LEU:HD21	4:CD:247:LEU:HD12	1.93	0.49
8:CH:103:SER:O	8:CH:108:GLN:NE2	2.45	0.49
12:L5:691:C:H2'	12:L5:692:A:C8	2.48	0.49
4:CD:419:LEU:HD12	4:CD:425:LYS:HA	1.94	0.49
12:L5:1363:C:H3'	23:LL:36:ARG:HH12	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L5:4559:A:O2'	12:L5:4561:C:OP2	2.30	0.49
14:L8:26:C:O2'	16:LC:53:ALA:O	2.30	0.49
15:LB:113:GLU:HA	15:LB:116:ARG:HD2	1.94	0.49
6:CF:80:SER:HB3	6:CF:83:ASP:HB2	1.94	0.49
7:CG:391:SER:OG	7:CG:392:PHE:N	2.45	0.49
12:L5:4238:G:H2'	12:L5:4239:A:H8	1.77	0.49
12:L5:4295:U:O4	12:L5:4316:G:O6	2.30	0.49
12:L5:1654:G:H5''	12:L5:1655:C:H5	1.77	0.49
12:L5:5068:G:N2	12:L5:5069:U:O4	2.36	0.49
2:CB:44:TYR:OH	8:CH:166:LYS:O	2.26	0.49
10:CJ:119:LEU:HD13	10:CJ:223:LEU:HD13	1.94	0.49
10:CJ:234:ASP:OD2	10:CJ:235:LEU:N	2.46	0.49
11:CK:73:ILE:HG23	11:CK:77:TRP:CZ3	2.48	0.49
12:L5:137:G:H2'	12:L5:138:G:H8	1.76	0.49
12:L5:1406:G:H2'	12:L5:1409:C:H41	1.78	0.49
14:L8:90:C:H2'	14:L8:91:A:C8	2.48	0.49
12:L5:417:G:OP1	12:L5:2329:U:O2'	2.30	0.49
12:L5:4992:G:H2'	12:L5:4993:G:C8	2.48	0.49
4:CD:262:GLY:HA2	40:Lt:39:PRO:HB2	1.95	0.49
5:CE:17:LYS:HD2	15:LB:355:THR:HB	1.95	0.49
6:CF:214:ARG:HH11	6:CF:216:GLN:HG2	1.77	0.49
12:L5:499:G:H2'	12:L5:504:G:H22	1.77	0.49
37:Lh:91:MET:HG2	37:Lh:94:ARG:HE	1.78	0.49
12:L5:3878:C:OP2	12:L5:4518:A:N6	2.45	0.49
12:L5:4266:G:O2'	12:L5:4268:A:N7	2.43	0.49
26:LO:193:THR:HG22	26:LO:197:LYS:HE2	1.95	0.49
1:CA:4:ARG:NH1	1:CA:210:THR:O	2.46	0.49
12:L5:4061:G:H3'	12:L5:4062:A:H8	1.78	0.49
12:L5:4893:A:OP1	26:LO:188:LYS:NZ	2.46	0.49
12:L5:4992:G:H2'	12:L5:4993:G:H8	1.78	0.49
40:Lt:52:ASP:N	40:Lt:52:ASP:OD1	2.44	0.49
1:CA:142:VAL:HG22	1:CA:173:LEU:HD21	1.95	0.48
12:L5:1798:G:O2'	30:LT:60:LYS:NZ	2.46	0.48
20:LG:155:VAL:O	20:LG:181:TYR:HA	2.13	0.48
21:LH:92:MET:HG2	21:LH:181:VAL:HA	1.94	0.48
12:L5:468:U:H1'	12:L5:686:A:H61	1.78	0.48
12:L5:730:G:OP2	19:LF:76:ARG:NH1	2.46	0.48
12:L5:1850:A:H2'	12:L5:1851:G:C8	2.48	0.48
21:LH:18:ILE:HG12	21:LH:27:VAL:HG22	1.95	0.48
1:CA:21:ASN:ND2	1:CA:112:ASP:OD2	2.47	0.48
12:L5:947:C:H5''	18:LE:51:VAL:HG11	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:LE:179:LEU:HD12	18:LE:183:ARG:HA	1.96	0.48
10:CJ:11:LYS:HB2	12:L5:4271:A:H5''	1.95	0.48
12:L5:956:A:H1'	12:L5:2076:G:H5''	1.96	0.48
12:L5:1461:C:H2'	12:L5:1462:A:H8	1.79	0.48
12:L5:4761:G:H2'	12:L5:4762:A:H8	1.79	0.48
40:Lt:32:ILE:HD12	40:Lt:35:LEU:HD12	1.95	0.48
10:CJ:221:LEU:HD23	10:CJ:223:LEU:HD21	1.95	0.48
12:L5:62:A:N3	12:L5:77:U:O2'	2.38	0.48
12:L5:1692:C:H5''	28:LQ:53:MET:SD	2.54	0.48
12:L5:3935:C:H2'	12:L5:3936:A:C8	2.48	0.48
7:CG:348:SER:OG	7:CG:349:ASP:N	2.47	0.48
12:L5:2843:U:O2'	12:L5:4632:U:OP1	2.31	0.48
2:CB:279:LEU:HD21	2:CB:294:PHE:HD1	1.79	0.48
5:CE:93:TYR:HD2	5:CE:102:ARG:HB2	1.76	0.48
12:L5:102:G:O2'	12:L5:1381:U:O2'	2.29	0.48
12:L5:5040:U:OP2	15:LB:396:ARG:NH2	2.46	0.48
13:L7:85:G:H2'	13:L7:86:G:C8	2.49	0.48
14:L8:70:G:H22	14:L8:87:G:H1'	1.77	0.48
5:CE:98:ASN:OD1	5:CE:99:GLN:N	2.45	0.48
12:L5:308:G:OP2	12:L5:308:G:N2	2.30	0.48
12:L5:4774:C:O2'	12:L5:4775:C:O5'	2.31	0.48
21:LH:12:ILE:HG12	21:LH:18:ILE:HD12	1.94	0.48
32:LY:1:MET:HE3	32:LY:2:LYS:H	1.79	0.48
41:Lz:67:VAL:HA	41:Lz:68:LEU:HA	1.57	0.48
6:CF:97:ARG:NH1	6:CF:97:ARG:HA	2.28	0.48
22:LJ:94:LEU:O	22:LJ:174:ILE:HA	2.14	0.48
5:CE:81:ARG:HH12	5:CE:94:PRO:HD3	1.79	0.48
7:CG:217:ARG:NH2	7:CG:234:THR:OG1	2.47	0.48
13:L7:3:C:OP1	13:L7:58:A:O2'	2.24	0.48
32:LY:59:ARG:HB2	32:LY:103:LYS:HD2	1.96	0.48
4:CD:48:MET:HE2	4:CD:114:VAL:HG13	1.95	0.47
7:CG:268:THR:HG22	7:CG:284:GLN:HG2	1.95	0.47
12:L5:695:G:H3'	12:L5:696:C:H4'	1.95	0.47
12:L5:5041:G:N1	15:LB:389:MET:O	2.46	0.47
17:LD:10:LYS:O	17:LD:14:LYS:NZ	2.47	0.47
1:CA:100:ARG:NH2	9:CI:25:ASP:O	2.48	0.47
11:CK:73:ILE:HD12	11:CK:77:TRP:HZ3	1.79	0.47
12:L5:257:C:H2'	12:L5:258:G:H8	1.78	0.47
12:L5:1332:C:H2'	12:L5:1333:A:C8	2.48	0.47
4:CD:172:LEU:HD23	4:CD:220:VAL:HB	1.96	0.47
4:CD:442:ILE:HD13	9:CI:89:THR:HG21	1.94	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L5:1914:C:H4'	26:LO:89:PRO:HD3	1.96	0.47
12:L5:1961:G:N2	12:L5:2024:G:O2'	2.47	0.47
12:L5:3938:G:N2	12:L5:4171:C:OP2	2.44	0.47
21:LH:120:GLU:OE1	21:LH:124:ARG:NH1	2.35	0.47
12:L5:5005:G:N2	12:L5:5041:G:O2'	2.48	0.47
7:CG:101:ARG:NH2	17:LD:117:LYS:O	2.45	0.47
12:L5:2083:C:OP2	28:LQ:14:ARG:NH2	2.47	0.47
17:LD:156:GLY:HA2	17:LD:181:PRO:HG3	1.96	0.47
39:Lr:65:LYS:O	39:Lr:102:TYR:OH	2.28	0.47
40:Lt:59:THR:HB	40:Lt:74:VAL:HB	1.96	0.47
19:LF:184:ILE:HD11	19:LF:193:GLU:HG2	1.97	0.47
4:CD:160:ARG:NH1	8:CH:5:GLU:OE1	2.47	0.47
10:CJ:232:SER:OG	10:CJ:234:ASP:OD2	2.32	0.47
12:L5:158:A:N1	12:L5:276:C:O2'	2.41	0.47
12:L5:941:C:OP2	19:LF:242:ARG:NH1	2.47	0.47
12:L5:4894:A:H5''	12:L5:4895:C:H3'	1.95	0.47
20:LG:88:ASP:OD1	20:LG:89:ARG:N	2.42	0.47
21:LH:92:MET:HE2	21:LH:179:ILE:HG22	1.97	0.47
22:LJ:120:ASP:HB3	22:LJ:123:ILE:HG12	1.97	0.47
12:L5:3935:C:H2'	12:L5:3936:A:H8	1.80	0.47
12:L5:4541:G:N2	12:L5:4544:A:OP2	2.40	0.47
30:LT:75:VAL:HG22	30:LT:88:ARG:HG3	1.97	0.47
32:LY:114:ASP:OD1	32:LY:115:ARG:N	2.48	0.47
2:CB:88:LYS:HE2	8:CH:235:LYS:HE3	1.95	0.47
12:L5:4940:C:H5'	12:L5:4941:G:H5''	1.96	0.47
16:LC:348:LYS:HA	16:LC:351:VAL:HG12	1.96	0.47
19:LF:108:VAL:HG13	19:LF:132:MET:HE3	1.97	0.47
22:LJ:136:ARG:NH1	22:LJ:156:ARG:O	2.48	0.47
12:L5:1239:C:H5	18:LE:60:SER:HB2	1.80	0.47
19:LF:244:ILE:O	19:LF:248:ASN:HB2	2.15	0.47
33:La:72:THR:HG22	33:La:110:LYS:HB3	1.97	0.47
4:CD:20:ASP:OD1	12:L5:4405:G:N2	2.46	0.46
10:CJ:149:ASP:HA	10:CJ:152:VAL:HG22	1.97	0.46
12:L5:5006:U:H4'	12:L5:5007:A:H5'	1.96	0.46
21:LH:23:ARG:NH1	21:LH:41:ILE:O	2.49	0.46
2:CB:272:LEU:HB2	2:CB:278:THR:HG21	1.98	0.46
12:L5:703:G:H2'	12:L5:704:C:H4'	1.96	0.46
12:L5:3860:A:N6	12:L5:4560:C:H42	2.11	0.46
16:LC:183:VAL:HG22	16:LC:204:ARG:HB3	1.98	0.46
17:LD:204:VAL:O	17:LD:208:MET:HG3	2.16	0.46
29:LS:173:ASN:ND2	29:LS:175:PHE:O	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
34:Ld:109:VAL:HG12	34:Ld:111:VAL:H	1.77	0.46
2:CB:215:ASP:HA	2:CB:248:LYS:HZ3	1.79	0.46
10:CJ:120:GLY:O	10:CJ:223:LEU:HA	2.15	0.46
12:L5:194:C:O2	32:LY:121:ARG:NH2	2.48	0.46
12:L5:4734:A:H2'	12:L5:4735:G:C8	2.50	0.46
12:L5:4743:G:H2'	12:L5:4744:A:C8	2.50	0.46
15:LB:286:LYS:HB3	15:LB:332:MET:HE3	1.96	0.46
18:LE:161:ARG:HE	18:LE:275:PHE:HB2	1.80	0.46
24:LM:115:ALA:HB1	26:LO:192:TYR:HB3	1.96	0.46
28:LQ:124:ASP:OD2	28:LQ:125:GLN:N	2.49	0.46
12:L5:318:A:H2'	12:L5:319:A:C8	2.51	0.46
12:L5:3933:G:H2'	12:L5:3934:G:C8	2.50	0.46
12:L5:5016:A:H3'	12:L5:5017:G:H8	1.81	0.46
27:LP:122:ALA:HB3	27:LP:143:PRO:HG2	1.97	0.46
38:Li:65:LYS:HE3	38:Li:68:ARG:HH21	1.81	0.46
1:CA:155:SER:OG	1:CA:201:ASP:OD1	2.33	0.46
3:CC:23:LYS:O	3:CC:27:GLU:HG3	2.16	0.46
10:CJ:177:LEU:HD12	11:CK:77:TRP:CE2	2.50	0.46
12:L5:4223:C:H2'	12:L5:4224:A:C8	2.51	0.46
12:L5:4962:C:H2'	12:L5:4963:G:H8	1.80	0.46
24:LM:50:MET:HE3	24:LM:50:MET:HB2	1.90	0.46
28:LQ:66:MET:HE1	28:LQ:100:VAL:HB	1.97	0.46
29:LS:99:ASP:OD1	29:LS:100:LEU:N	2.44	0.46
3:CC:7:LYS:HA	12:L5:1931:C:H1'	1.98	0.46
4:CD:32:THR:OG1	12:L5:4464:A:N7	2.43	0.46
11:CK:144:TRP:HA	11:CK:148:ARG:HG3	1.98	0.46
12:L5:382:G:N1	12:L5:385:A:OP2	2.38	0.46
25:LN:120:TRP:HZ2	25:LN:123:GLU:HG2	1.80	0.46
29:LS:154:LEU:HB3	29:LS:157:ARG:HD3	1.97	0.46
4:CD:88:ASP:OD2	4:CD:91:HIS:ND1	2.31	0.46
7:CG:22:GLN:O	7:CG:91:ILE:HA	2.16	0.46
12:L5:82:U:HO2'	12:L5:1382:G:HO2'	1.62	0.46
12:L5:1308:C:OP1	26:LO:93:LYS:NZ	2.44	0.46
13:L7:12:U:OP2	13:L7:67:C:O2'	2.32	0.46
15:LB:103:LYS:HB3	15:LB:153:MET:HE2	1.96	0.46
18:LE:191:GLN:HA	18:LE:194:VAL:HG22	1.98	0.46
2:CB:180:ARG:NH1	12:L5:4441:A:N3	2.59	0.46
12:L5:3897:G:N2	12:L5:3898:G:O6	2.48	0.46
12:L5:4223:C:H2'	12:L5:4224:A:H8	1.81	0.46
12:L5:4238:G:H2'	12:L5:4239:A:C8	2.51	0.46
12:L5:4239:A:H2'	12:L5:4240:G:C8	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L5:4965:U:H4'	12:L5:4966:A:H5'	1.98	0.46
13:L7:82:G:H2'	13:L7:83:A:C8	2.51	0.46
19:LF:92:VAL:O	19:LF:120:GLY:HA2	2.15	0.46
25:LN:98:LEU:HD12	25:LN:128:LYS:HD2	1.96	0.46
9:CI:101:GLN:NE2	15:LB:387:ALA:O	2.48	0.46
10:CJ:214:LEU:O	11:CK:62:GLN:NE2	2.49	0.46
12:L5:189:G:H2'	12:L5:190:G:H8	1.81	0.46
12:L5:268:G:H2'	12:L5:269:G:H8	1.81	0.46
12:L5:460:C:H2'	12:L5:461:G:H8	1.80	0.46
12:L5:4071:U:H2'	12:L5:4072:C:C6	2.51	0.46
13:L7:75:G:H4'	13:L7:76:U:H5'	1.98	0.46
17:LD:236:MET:HG2	17:LD:239:MET:HE2	1.98	0.46
23:LL:70:VAL:HG22	23:LL:159:ASN:ND2	2.31	0.46
35:Le:35:TRP:O	35:Le:36:ARG:NH1	2.48	0.46
4:CD:130:LYS:NZ	12:L5:4405:G:OP2	2.43	0.45
6:CF:23:LYS:O	6:CF:27:ILE:HG12	2.16	0.45
11:CK:131:LEU:HD22	11:CK:140:TRP:HB3	1.98	0.45
19:LF:149:SER:HB3	19:LF:244:ILE:HG21	1.98	0.45
6:CF:40:LEU:HD21	6:CF:102:LEU:HD22	1.98	0.45
12:L5:1933:G:H2'	12:L5:1934:A:C8	2.52	0.45
20:LG:61:ILE:HD12	20:LG:64:GLN:HE21	1.81	0.45
6:CF:54:LYS:NZ	12:L5:1996:C:O2	2.46	0.45
12:L5:505:G:O6	12:L5:654:C:N4	2.50	0.45
12:L5:513:U:O2'	12:L5:515:C:N4	2.42	0.45
12:L5:2361:G:O2'	12:L5:3859:G:O6	2.28	0.45
10:CJ:75:GLN:HG2	10:CJ:113:VAL:HG21	1.98	0.45
12:L5:254:G:H2'	12:L5:255:C:O4'	2.17	0.45
10:CJ:141:PRO:HB3	10:CJ:182:TYR:CE2	2.52	0.45
12:L5:1514:U:H2'	12:L5:1515:A:C8	2.51	0.45
12:L5:4166:G:H2'	12:L5:4167:G:C8	2.50	0.45
17:LD:146:LEU:HD21	17:LD:159:VAL:HG12	1.99	0.45
2:CB:392:ASP:OD1	2:CB:392:ASP:N	2.47	0.45
5:CE:95:ILE:HD11	15:LB:132:LYS:HE3	1.99	0.45
12:L5:1333:A:H2'	12:L5:1334:A:C8	2.52	0.45
1:CA:160:LEU:HD22	1:CA:193:ILE:HG21	1.99	0.45
12:L5:197:A:N1	12:L5:225:G:O2'	2.41	0.45
12:L5:3932:U:H2'	12:L5:3933:G:C8	2.52	0.45
15:LB:69:LYS:HA	15:LB:69:LYS:HD3	1.74	0.45
19:LF:89:LEU:HG	19:LF:145:PRO:HG2	1.99	0.45
2:CB:50:ARG:HH12	12:L5:3911:C:H4'	1.81	0.45
4:CD:302:ASP:N	4:CD:302:ASP:OD1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:367:ARG:NH2	4:CD:370:ASP:O	2.50	0.45
8:CH:136:ILE:HD11	8:CH:149:MET:HE3	1.97	0.45
12:L5:908:G:H2'	12:L5:909:A:H8	1.82	0.45
12:L5:1333:A:H2'	12:L5:1334:A:H8	1.82	0.45
14:L8:72:A:N6	14:L8:80:A:H62	2.15	0.45
18:LE:117:PRO:O	39:Lr:112:ARG:NH1	2.40	0.45
21:LH:115:ARG:HG2	21:LH:123:ILE:HG12	1.98	0.45
31:LV:69:LYS:HB2	31:LV:72:LEU:HD12	1.99	0.45
4:CD:72:LEU:HD23	4:CD:72:LEU:HA	1.87	0.45
6:CF:86:LYS:H	6:CF:89:LEU:HD12	1.81	0.45
12:L5:456:C:H2'	12:L5:457:G:C8	2.52	0.45
23:LL:116:ARG:NH2	23:LL:155:MET:O	2.46	0.45
32:LY:124:LYS:HA	32:LY:127:GLN:HG3	1.99	0.45
2:CB:426:ALA:HB2	2:CB:443:VAL:HG21	1.99	0.44
4:CD:353:VAL:HA	4:CD:356:VAL:HB	1.98	0.44
7:CG:209:PRO:HB3	7:CG:301:LEU:HD22	1.99	0.44
12:L5:170:C:H42	12:L5:266:C:H42	1.63	0.44
12:L5:226:G:OP2	32:LY:1:MET:N	2.46	0.44
12:L5:1503:A:H4'	12:L5:1504:G:H5'	1.99	0.44
6:CF:151:PRO:O	6:CF:155:GLN:HG2	2.18	0.44
12:L5:511:C:H5''	23:LL:165:LYS:HD2	2.00	0.44
12:L5:976:G:O2'	16:LC:333:LYS:NZ	2.39	0.44
12:L5:3955:G:O2'	12:L5:3966:A:N6	2.40	0.44
12:L5:3956:G:O5'	12:L5:3966:A:N6	2.50	0.44
12:L5:4064:C:H2'	12:L5:4065:G:C8	2.52	0.44
12:L5:5002:U:OP2	15:LB:385:LYS:NZ	2.37	0.44
15:LB:312:LYS:NZ	15:LB:368:ILE:O	2.42	0.44
1:CA:85:ARG:NH2	1:CA:89:PRO:O	2.50	0.44
2:CB:353:LEU:HD22	2:CB:359:LEU:HD11	1.99	0.44
12:L5:457:G:OP1	39:Lr:119:ARG:NH2	2.50	0.44
12:L5:4572:U:OP1	14:L8:1:C:N4	2.51	0.44
24:LM:94:LYS:HG2	26:LO:203:VAL:HG21	1.99	0.44
26:LO:65:ASN:OD1	26:LO:67:SER:OG	2.35	0.44
1:CA:84:ILE:HG22	1:CA:94:ILE:HD13	1.98	0.44
12:L5:443:G:O3'	36:Lf:54:LYS:NZ	2.46	0.44
12:L5:4966:A:H5''	15:LB:128:LYS:HG3	1.99	0.44
27:LP:17:SER:OG	27:LP:94:MET:SD	2.75	0.44
6:CF:78:GLY:HA3	6:CF:84:GLU:HA	1.99	0.44
12:L5:690:C:OP1	39:Lr:87:ARG:NH1	2.47	0.44
12:L5:742:G:H2'	12:L5:743:G:H8	1.82	0.44
12:L5:1308:C:H2'	12:L5:1309:C:C6	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L5:1849:U:H2'	12:L5:1850:A:C8	2.53	0.44
12:L5:2345:G:N7	33:La:9:ARG:NH2	2.65	0.44
20:LG:80:ILE:HD11	25:LN:18:VAL:HG23	1.99	0.44
32:LY:117:LYS:HA	32:LY:120:GLU:HG3	1.99	0.44
10:CJ:192:LYS:HG2	10:CJ:224:VAL:HG22	1.99	0.44
12:L5:3842:C:H1'	31:LV:52:LEU:HD12	1.99	0.44
12:L5:4043:G:N2	12:L5:4045:G:N3	2.64	0.44
16:LC:25:PRO:HB2	16:LC:27:VAL:HG22	1.98	0.44
36:Lf:56:ASN:OD1	36:Lf:66:LYS:NZ	2.47	0.44
12:L5:725:G:H2'	12:L5:726:G:H8	1.83	0.44
12:L5:1306:C:H2'	12:L5:1307:A:H8	1.81	0.44
12:L5:1921:C:O2'	29:LS:160:ARG:NH2	2.48	0.44
12:L5:3938:G:H5'	12:L5:4170:A:H2	1.83	0.44
12:L5:4081:G:H2'	12:L5:4082:G:C8	2.53	0.44
12:L5:4167:G:H2'	12:L5:4168:G:C8	2.53	0.44
22:LJ:114:ASP:OD1	22:LJ:114:ASP:N	2.50	0.44
30:LT:127:GLN:NE2	30:LT:129:LYS:O	2.40	0.44
2:CB:47:LYS:HB3	2:CB:49:ARG:HH12	1.83	0.44
4:CD:347:LYS:HA	4:CD:347:LYS:HD2	1.72	0.44
12:L5:706:C:HO2'	12:L5:1298:C:HO2'	1.62	0.44
12:L5:2322:G:OP1	35:Le:36:ARG:NH2	2.48	0.44
13:L7:110:G:H2'	13:L7:111:C:C6	2.53	0.44
19:LF:145:PRO:O	19:LF:149:SER:HB2	2.18	0.44
12:L5:3886:G:OP1	26:LO:85:ARG:NH2	2.50	0.44
12:L5:3933:G:H2'	12:L5:3934:G:H8	1.81	0.44
12:L5:3955:G:H22	12:L5:3966:A:H3'	1.82	0.43
12:L5:4072:C:H2'	12:L5:4073:A:C8	2.51	0.43
12:L5:909:A:H2'	12:L5:910:G:H8	1.81	0.43
12:L5:4166:G:H2'	12:L5:4167:G:H8	1.83	0.43
12:L5:4204:C:H2'	12:L5:4205:A:C8	2.53	0.43
23:LL:65:ARG:HD3	33:La:66:ASN:HD22	1.83	0.43
27:LP:114:ILE:HD13	27:LP:150:LEU:HD21	1.99	0.43
29:LS:70:LYS:HD3	29:LS:70:LYS:HA	1.76	0.43
34:Ld:72:VAL:HG13	34:Ld:73:TRP:HD1	1.83	0.43
2:CB:56:ILE:HD12	2:CB:59:PRO:HB3	1.99	0.43
4:CD:171:LEU:HA	4:CD:250:ALA:O	2.18	0.43
6:CF:135:VAL:HG23	6:CF:175:VAL:HB	1.99	0.43
11:CK:73:ILE:HG23	11:CK:77:TRP:CE3	2.53	0.43
12:L5:86:U:H2'	12:L5:87:A:H8	1.83	0.43
12:L5:3871:A:H2'	12:L5:3872:A:C8	2.52	0.43
12:L5:4954:G:H2'	12:L5:4955:A:C8	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L5:4975:G:O2'	12:L5:4977:A:N6	2.45	0.43
23:LL:150:LEU:HD23	23:LL:154:VAL:HG22	2.00	0.43
1:CA:126:GLU:HG3	1:CA:137:VAL:HG11	1.99	0.43
2:CB:307:ASP:OD1	2:CB:307:ASP:N	2.49	0.43
12:L5:365:U:H2'	12:L5:366:A:H8	1.83	0.43
12:L5:4067:U:H2'	12:L5:4068:U:C6	2.53	0.43
13:L7:76:U:H2'	13:L7:77:A:C8	2.53	0.43
38:Li:37:THR:HA	38:Li:40:VAL:HG12	2.01	0.43
38:Li:94:LEU:HA	38:Li:97:MET:HG3	1.99	0.43
40:Lt:58:ILE:HD12	40:Lt:73:VAL:HG13	2.00	0.43
1:CA:107:VAL:HB	1:CA:118:HIS:HB2	2.00	0.43
6:CF:60:TRP:HH2	6:CF:112:VAL:HG22	1.83	0.43
12:L5:490:C:N4	12:L5:491:G:O6	2.50	0.43
12:L5:679:C:H2'	12:L5:680:G:C8	2.50	0.43
12:L5:4967:A:H2'	12:L5:4968:A:C8	2.53	0.43
27:LP:23:ARG:NH2	27:LP:141:SER:OG	2.50	0.43
28:LQ:128:LEU:HD23	28:LQ:128:LEU:HA	1.91	0.43
2:CB:84:THR:O	12:L5:4295:U:O2'	2.36	0.43
6:CF:61:LYS:O	40:Lt:123:ARG:NH1	2.51	0.43
12:L5:1399:G:H2'	12:L5:1400:G:H8	1.84	0.43
1:CA:39:GLU:HA	1:CA:43:SER:HB2	2.01	0.43
4:CD:173:LEU:HD23	4:CD:252:LEU:HB2	2.00	0.43
7:CG:457:ASP:HB3	7:CG:476:LYS:HB3	2.00	0.43
12:L5:230:G:OP1	32:LY:15:ARG:NH1	2.44	0.43
12:L5:307:A:OP1	38:Li:86:LYS:NZ	2.52	0.43
12:L5:1896:A:OP1	19:LF:223:LYS:NZ	2.47	0.43
12:L5:2072:C:OP1	28:LQ:2:GLY:N	2.51	0.43
15:LB:229:LYS:HG3	15:LB:272:LYS:HD3	2.01	0.43
2:CB:190:ARG:NH1	12:L5:4507:A:OP1	2.52	0.43
10:CJ:175:ILE:HB	11:CK:92:LEU:HD11	2.01	0.43
12:L5:502:C:H3'	12:L5:503:C:H3'	2.00	0.43
12:L5:506:C:H2'	12:L5:507:G:H8	1.84	0.43
12:L5:2020:U:H2'	12:L5:2021:G:H8	1.84	0.43
12:L5:4389:C:H2'	12:L5:4390:A:C8	2.54	0.43
13:L7:6:C:H4'	17:LD:52:ILE:HD13	2.01	0.43
18:LE:161:ARG:O	18:LE:182:ASN:ND2	2.51	0.43
19:LF:59:LYS:O	19:LF:63:GLN:HG3	2.19	0.43
5:CE:93:TYR:CD2	5:CE:102:ARG:HB2	2.53	0.43
7:CG:298:ASP:N	7:CG:298:ASP:OD1	2.51	0.43
10:CJ:40:ASN:OD1	10:CJ:40:ASN:N	2.51	0.43
10:CJ:193:ILE:HG23	10:CJ:223:LEU:HB2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:LB:58:ARG:HA	15:LB:366:LYS:HG3	2.00	0.43
4:CD:216:ARG:NH2	12:L5:4606:G:O2'	2.52	0.43
10:CJ:35:LEU:HD12	10:CJ:53:TYR:HB2	2.00	0.43
12:L5:4662:C:O2'	12:L5:5004:C:OP1	2.35	0.43
12:L5:4761:G:H2'	12:L5:4762:A:C8	2.54	0.43
13:L7:35:U:O2	13:L7:45:U:O2'	2.35	0.43
16:LC:115:VAL:HB	16:LC:120:LYS:HE3	2.00	0.43
17:LD:64:ILE:HG13	17:LD:105:LEU:HD21	2.00	0.43
20:LG:191:GLY:HA2	20:LG:194:VAL:HG22	2.01	0.43
38:Li:90:LEU:HA	38:Li:93:VAL:HG22	2.00	0.43
1:CA:202:TRP:HB3	4:CD:377:ILE:HD12	2.01	0.42
4:CD:226:LEU:HB2	4:CD:228:HIS:CE1	2.54	0.42
5:CE:87:LEU:HD11	5:CE:91:GLY:HA2	2.01	0.42
12:L5:3932:U:H2'	12:L5:3933:G:H8	1.84	0.42
12:L5:4043:G:OP1	12:L5:4045:G:N2	2.51	0.42
12:L5:4728:U:OP1	15:LB:132:LYS:NZ	2.50	0.42
15:LB:54:THR:OG1	15:LB:55:HIS:N	2.52	0.42
2:CB:160:MET:HB2	2:CB:160:MET:HE2	1.76	0.42
12:L5:14:C:H2'	12:L5:15:A:H8	1.84	0.42
12:L5:436:C:H2'	12:L5:437:G:H8	1.84	0.42
12:L5:4467:A:O2'	12:L5:4510:A:N3	2.43	0.42
12:L5:5056:A:O2'	34:Ld:119:THR:O	2.35	0.42
13:L7:92:C:H2'	13:L7:93:G:H8	1.84	0.42
19:LF:77:LYS:HE3	19:LF:77:LYS:HB2	1.78	0.42
20:LG:66:GLN:HG3	25:LN:28:TRP:HH2	1.84	0.42
29:LS:120:ARG:O	29:LS:124:ILE:HG12	2.18	0.42
1:CA:229:PRO:HB2	4:CD:362:LEU:HD21	2.00	0.42
2:CB:46:GLN:HE21	8:CH:146:TRP:HA	1.85	0.42
12:L5:4458:C:OP1	15:LB:11:HIS:NE2	2.52	0.42
15:LB:20:LYS:HE3	15:LB:20:LYS:HB2	1.87	0.42
15:LB:145:GLN:NE2	15:LB:149:ASP:OD2	2.52	0.42
38:Li:59:GLU:HA	38:Li:62:LYS:HD3	2.01	0.42
12:L5:137:G:OP1	37:Lh:96:ASN:ND2	2.52	0.42
12:L5:1068:G:H2'	12:L5:1069:G:C8	2.54	0.42
12:L5:1725:U:H2'	12:L5:1726:U:H6	1.84	0.42
12:L5:3871:A:H2'	12:L5:3872:A:H8	1.84	0.42
12:L5:4239:A:H2'	12:L5:4240:G:H8	1.84	0.42
12:L5:4742:G:H2'	12:L5:4743:G:H8	1.83	0.42
13:L7:58:A:H2'	13:L7:59:G:H8	1.84	0.42
25:LN:42:PRO:HD3	25:LN:61:ILE:HG13	2.00	0.42
27:LP:111:SER:O	27:LP:111:SER:OG	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CD:292:ASP:OD1	4:CD:292:ASP:N	2.51	0.42
12:L5:189:G:H2'	12:L5:190:G:C8	2.54	0.42
12:L5:299:C:H2'	12:L5:300:A:H8	1.84	0.42
12:L5:419:A:N3	12:L5:1332:C:O2'	2.51	0.42
12:L5:710:G:H2'	12:L5:711:A:C8	2.55	0.42
12:L5:4260:U:H2'	12:L5:4261:C:C6	2.54	0.42
20:LG:157:ILE:HA	20:LG:201:THR:HG22	2.02	0.42
21:LH:44:GLU:HG3	24:LM:2:VAL:HG12	2.01	0.42
31:LV:21:PRO:HA	31:LV:54:ALA:HA	2.01	0.42
1:CA:197:MET:HE2	1:CA:197:MET:HB3	1.78	0.42
12:L5:669:C:H5'	39:Lr:68:SER:HB2	2.01	0.42
12:L5:4260:U:H2'	12:L5:4261:C:H6	1.85	0.42
12:L5:4951:G:H2'	12:L5:4952:G:H8	1.83	0.42
17:LD:9:ASN:H	17:LD:12:TYR:HB3	1.84	0.42
39:Lr:51:VAL:HG12	39:Lr:117:ILE:HD12	2.01	0.42
2:CB:35:ARG:NH2	2:CB:39:ARG:HH12	2.18	0.42
12:L5:163:A:H2'	12:L5:164:G:H8	1.85	0.42
12:L5:1876:U:H2'	12:L5:1877:G:C8	2.55	0.42
12:L5:3964:U:O2'	12:L5:3966:A:O4'	2.36	0.42
12:L5:4643:G:H2'	12:L5:4644:G:C8	2.54	0.42
12:L5:4711:C:O2'	26:LO:145:VAL:O	2.33	0.42
16:LC:315:LYS:HD2	19:LF:168:ALA:HB1	2.00	0.42
4:CD:225:ILE:HA	4:CD:237:GLU:HG2	2.01	0.42
4:CD:347:LYS:NZ	4:CD:353:VAL:HG23	2.34	0.42
4:CD:399:ARG:NH1	4:CD:402:GLU:OE1	2.53	0.42
5:CE:114:GLY:HA2	12:L5:4741:C:H5	1.85	0.42
8:CH:98:ARG:HG2	8:CH:100:LYS:HB2	2.02	0.42
10:CJ:63:TYR:HH	10:CJ:85:SER:HG	1.65	0.42
12:L5:753:C:H41	12:L5:910:G:H1	1.66	0.42
12:L5:1517:G:H22	16:LC:103:ALA:HA	1.85	0.42
12:L5:4168:G:H3'	12:L5:4169:G:H8	1.85	0.42
12:L5:4743:G:H2'	12:L5:4744:A:H8	1.84	0.42
12:L5:4896:G:H2'	12:L5:4897:G:H8	1.84	0.42
23:LL:117:LEU:HD23	23:LL:117:LEU:HA	1.93	0.42
32:LY:111:LEU:HB3	32:LY:116:LYS:HE3	2.00	0.42
34:Ld:85:ARG:HH11	34:Ld:117:LEU:HD13	1.84	0.42
16:LC:154:VAL:HG11	16:LC:174:LEU:HD11	2.02	0.42
30:LT:114:GLN:HG2	30:LT:117:LYS:HZ3	1.85	0.42
12:L5:1475:G:N2	12:L5:1476:C:N3	2.67	0.42
12:L5:4496:A:H61	12:L5:4504:C:H42	1.67	0.42
12:L5:4642:U:H2'	12:L5:4643:G:C8	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:LL:58:ILE:HD12	23:LL:116:ARG:HD2	2.01	0.42
23:LL:80:GLU:OE2	23:LL:104:ASN:ND2	2.52	0.42
12:L5:181:C:H42	12:L5:255:C:H42	1.68	0.41
12:L5:226:G:N7	16:LC:184:TYR:OH	2.50	0.41
12:L5:1461:C:H2'	12:L5:1462:A:C8	2.55	0.41
12:L5:1970:A:H5'	12:L5:1971:C:H5'	2.01	0.41
12:L5:4165:C:H2'	12:L5:4166:G:C8	2.55	0.41
20:LG:75:LYS:HD2	20:LG:75:LYS:HA	1.88	0.41
23:LL:158:ARG:HA	23:LL:158:ARG:HD3	1.82	0.41
1:CA:112:ASP:OD2	1:CA:156:ASN:ND2	2.36	0.41
2:CB:441:GLN:O	2:CB:445:LYS:HG2	2.20	0.41
4:CD:250:ALA:HA	4:CD:283:PRO:HG2	2.01	0.41
12:L5:299:C:H2'	12:L5:300:A:C8	2.56	0.41
12:L5:1504:G:H2'	12:L5:1505:C:C6	2.55	0.41
12:L5:3961:G:H1'	12:L5:3965:A:N1	2.34	0.41
12:L5:3961:G:O2'	12:L5:3965:A:OP1	2.38	0.41
12:L5:4699:U:H1'	12:L5:4700:A:H5''	2.00	0.41
14:L8:91:A:H2'	14:L8:92:U:C6	2.55	0.41
14:L8:146:U:H2'	14:L8:147:G:H8	1.85	0.41
28:LQ:40:ASN:OD1	28:LQ:132:LYS:NZ	2.50	0.41
3:CC:60:LEU:HD21	30:LT:154:ILE:HD11	2.01	0.41
12:L5:162:A:H2'	12:L5:163:A:H8	1.84	0.41
12:L5:418:A:N7	14:L8:15:G:N2	2.67	0.41
12:L5:504:G:O2'	12:L5:505:G:O4'	2.38	0.41
12:L5:4079:C:H1'	12:L5:4172:A:N1	2.35	0.41
32:LY:103:LYS:HD3	32:LY:103:LYS:HA	1.89	0.41
38:Li:58:MET:HE2	38:Li:58:MET:HB3	1.87	0.41
4:CD:136:ARG:NH2	12:L5:4435:U:O2'	2.54	0.41
12:L5:654:C:H4'	16:LC:269:LYS:HB2	2.03	0.41
12:L5:1313:C:OP1	35:Le:44:ARG:NH2	2.52	0.41
13:L7:55:A:H4'	22:LJ:155:HIS:HB2	2.02	0.41
18:LE:211:HIS:NE2	18:LE:249:ASP:OD2	2.50	0.41
25:LN:155:VAL:O	25:LN:162:ARG:NH2	2.52	0.41
27:LP:50:ASP:HB3	27:LP:55:LYS:HB2	2.01	0.41
2:CB:252:PHE:O	2:CB:278:THR:HA	2.20	0.41
2:CB:432:LEU:HA	2:CB:438:PRO:HA	2.03	0.41
11:CK:32:LEU:HD22	11:CK:41:ALA:HB1	2.01	0.41
12:L5:54:G:H4'	25:LN:108:ARG:HH12	1.85	0.41
12:L5:75:G:O6	23:LL:103:ARG:NH1	2.53	0.41
12:L5:1339:U:H2'	12:L5:1340:C:C6	2.55	0.41
12:L5:4745:G:N2	12:L5:4955:A:N1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LH:53:LYS:HA	21:LH:53:LYS:HD3	1.72	0.41
22:LJ:18:ARG:HG3	22:LJ:135:GLY:HA3	2.01	0.41
38:Li:76:ARG:HD3	38:Li:76:ARG:HA	1.88	0.41
1:CA:57:ARG:HE	1:CA:57:ARG:HB2	1.73	0.41
5:CE:81:ARG:HH21	5:CE:88:ASP:HB3	1.86	0.41
12:L5:691:C:H2'	12:L5:692:A:H8	1.84	0.41
12:L5:4265:U:N3	17:LD:17:GLN:O	2.53	0.41
12:L5:4775:C:O4'	12:L5:4860:G:N2	2.53	0.41
17:LD:12:TYR:O	17:LD:16:TYR:HB2	2.20	0.41
4:CD:286:VAL:HB	4:CD:317:VAL:HG22	2.03	0.41
8:CH:102:LEU:HD11	8:CH:188:LEU:HD21	2.01	0.41
11:CK:69:THR:O	11:CK:73:ILE:HG12	2.20	0.41
12:L5:190:G:H2'	12:L5:191:G:H8	1.85	0.41
12:L5:352:G:C6	16:LC:196:MET:HE2	2.56	0.41
12:L5:506:C:H2'	12:L5:507:G:C8	2.55	0.41
12:L5:1368:A:H1'	32:LY:1:MET:HE2	2.03	0.41
12:L5:1398:A:H5''	33:La:132:ARG:HH12	1.86	0.41
12:L5:1725:U:H2'	12:L5:1726:U:C6	2.55	0.41
12:L5:2045:G:N2	12:L5:2046:G:N7	2.68	0.41
12:L5:4076:G:H21	38:Li:68:ARG:NH2	2.18	0.41
13:L7:13:A:OP2	13:L7:66:G:N2	2.47	0.41
19:LF:144:TYR:HA	19:LF:145:PRO:HD3	1.84	0.41
1:CA:117:VAL:HB	1:CA:121:LEU:HD22	2.01	0.41
1:CA:213:THR:OG1	4:CD:214:TYR:O	2.37	0.41
10:CJ:151:ASP:O	10:CJ:157:ARG:NH1	2.53	0.41
12:L5:462:G:H2'	12:L5:463:A:C8	2.55	0.41
12:L5:475:G:H2'	12:L5:476:G:H8	1.86	0.41
12:L5:1399:G:H2'	12:L5:1400:G:C8	2.55	0.41
12:L5:2325:C:OP1	35:Le:101:HIS:ND1	2.54	0.41
12:L5:4225:G:H2'	12:L5:4226:G:H8	1.86	0.41
12:L5:4293:U:O3'	12:L5:4330:G:O2'	2.33	0.41
12:L5:4742:G:H2'	12:L5:4743:G:C8	2.56	0.41
28:LQ:6:ARG:HH21	28:LQ:8:ASN:ND2	2.19	0.41
7:CG:222:SER:HB3	7:CG:252:LEU:HD22	2.02	0.41
7:CG:264:SER:OG	7:CG:265:GLN:N	2.54	0.41
8:CH:41:LYS:NZ	12:L5:1931:C:OP1	2.51	0.41
10:CJ:164:ILE:O	10:CJ:168:ARG:CB	2.66	0.41
12:L5:1392:A:H2'	12:L5:1393:G:C8	2.55	0.41
12:L5:1469:C:H2'	12:L5:1470:G:H8	1.86	0.41
12:L5:1502:G:OP1	28:LQ:65:ARG:NH1	2.54	0.41
12:L5:1653:A:H2'	12:L5:1655:C:C4	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L5:1825:A:H2'	12:L5:1826:G:C8	2.56	0.41
12:L5:4296:U:H2'	12:L5:4297:G:C8	2.56	0.41
12:L5:4654:C:H2'	12:L5:4655:A:C8	2.55	0.41
16:LC:319:LEU:HD13	19:LF:152:GLU:HG3	2.03	0.41
17:LD:21:ARG:HG3	17:LD:24:ARG:HH21	1.86	0.41
18:LE:281:ILE:HG23	18:LE:286:LEU:HD21	2.03	0.41
22:LJ:120:ASP:OD2	22:LJ:122:SER:OG	2.28	0.41
23:LL:56:ARG:NH1	23:LL:74:ARG:O	2.54	0.41
27:LP:111:SER:HG	27:LP:153:LYS:H	1.69	0.41
31:LV:64:THR:HG22	31:LV:76:VAL:HG22	2.03	0.41
2:CB:210:LEU:HD22	2:CB:365:VAL:HG11	2.03	0.41
9:CI:93:MET:HE2	9:CI:93:MET:HB3	1.88	0.41
12:L5:257:C:H2'	12:L5:258:G:C8	2.56	0.41
12:L5:710:G:H2'	12:L5:711:A:H8	1.86	0.41
12:L5:4077:A:N1	12:L5:4171:C:N4	2.68	0.41
12:L5:4287:G:H2'	12:L5:4288:C:C6	2.56	0.41
18:LE:149:ILE:HD13	18:LE:271:LEU:HD21	2.02	0.41
40:Lt:107:ASP:OD1	40:Lt:108:GLU:N	2.53	0.41
8:CH:141:ARG:HB3	8:CH:143:LYS:NZ	2.36	0.40
10:CJ:140:LYS:NZ	10:CJ:170:PRO:O	2.46	0.40
10:CJ:149:ASP:HB3	10:CJ:156:TYR:CD2	2.56	0.40
12:L5:162:A:H2'	12:L5:163:A:C8	2.55	0.40
12:L5:919:C:OP1	24:LM:69:HIS:ND1	2.36	0.40
12:L5:2032:U:H2'	12:L5:2033:A:H8	1.85	0.40
12:L5:4492:U:H5''	12:L5:4493:U:H5'	2.02	0.40
12:L5:4633:G:N2	12:L5:4664:A:OP2	2.42	0.40
13:L7:81:G:H2'	13:L7:82:G:H8	1.86	0.40
16:LC:230:LEU:HD23	16:LC:230:LEU:HA	1.97	0.40
20:LG:228:ASP:OD1	20:LG:228:ASP:N	2.54	0.40
1:CA:142:VAL:HG23	1:CA:148:VAL:HG12	2.04	0.40
6:CF:88:ASN:HB2	6:CF:208:TRP:HE1	1.86	0.40
12:L5:131:C:H2'	12:L5:132:G:C8	2.56	0.40
12:L5:229:G:H5''	32:LY:11:ARG:HG3	2.02	0.40
12:L5:4185:G:H2'	12:L5:4186:A:C8	2.56	0.40
13:L7:81:G:H2'	13:L7:82:G:C8	2.56	0.40
17:LD:76:CYS:SG	17:LD:77:ALA:N	2.94	0.40
18:LE:57:TYR:HD1	18:LE:62:MET:HE2	1.85	0.40
32:LY:26:ARG:O	32:LY:30:MET:HG3	2.21	0.40
36:Lf:14:TYR:OH	36:Lf:92:LEU:O	2.31	0.40
1:CA:126:GLU:OE1	1:CA:139:ARG:NH2	2.48	0.40
6:CF:69:LYS:HE3	6:CF:69:LYS:HB2	1.93	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L5:456:C:H2'	12:L5:457:G:H8	1.87	0.40
12:L5:930:G:OP1	16:LC:353:LYS:NZ	2.43	0.40
12:L5:1810:G:H2'	12:L5:1811:G:C8	2.57	0.40
12:L5:1994:C:H2'	12:L5:1995:G:H8	1.85	0.40
12:L5:3952:A:H1'	12:L5:3953:G:C8	2.56	0.40
12:L5:4079:C:H2'	12:L5:4080:C:C6	2.56	0.40
27:LP:105:LYS:HE3	27:LP:105:LYS:HB3	1.94	0.40
1:CA:18:LYS:HE2	1:CA:18:LYS:HB2	1.89	0.40
4:CD:105:LEU:HD21	12:L5:4436:U:H5'	2.03	0.40
6:CF:6:ARG:NH1	12:L5:1964:A:O3'	2.52	0.40
12:L5:267:G:H2'	12:L5:268:G:H8	1.87	0.40
12:L5:475:G:H2'	12:L5:476:G:C8	2.57	0.40
12:L5:709:C:OP1	36:Lf:89:ARG:NH2	2.55	0.40
12:L5:2032:U:H2'	12:L5:2033:A:C8	2.56	0.40
12:L5:3955:G:H1	12:L5:3966:A:H5''	1.87	0.40
15:LB:181:MET:HE3	15:LB:181:MET:HB2	2.01	0.40
25:LN:159:ARG:HB3	25:LN:164:LEU:HB2	2.03	0.40
34:Ld:85:ARG:NH1	34:Ld:117:LEU:HB3	2.36	0.40
39:Lr:99:LYS:HA	39:Lr:99:LYS:HD3	1.90	0.40
1:CA:100:ARG:HA	1:CA:100:ARG:HH11	1.86	0.40
2:CB:42:ASN:OD1	2:CB:45:ARG:NH1	2.55	0.40
5:CE:94:PRO:HD2	5:CE:97:MET:SD	2.61	0.40
6:CF:8:LYS:NZ	12:L5:1964:A:OP1	2.41	0.40
6:CF:30:LEU:HD23	6:CF:30:LEU:HA	1.87	0.40
10:CJ:247:LYS:HA	10:CJ:248:PRO:HD3	1.97	0.40
12:L5:153:G:H2'	12:L5:154:G:H8	1.85	0.40
12:L5:1810:G:H2'	12:L5:1811:G:H8	1.85	0.40
12:L5:2029:A:H2'	12:L5:2030:A:C8	2.56	0.40
12:L5:4993:G:C6	12:L5:5058:A:N1	2.90	0.40
38:Li:77:VAL:HG23	38:Li:79:THR:H	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	CA	243/245 (99%)	234 (96%)	9 (4%)	0	100	100
2	CB	444/731 (61%)	437 (98%)	7 (2%)	0	100	100
3	CC	78/549 (14%)	76 (97%)	2 (3%)	0	100	100
4	CD	456/634 (72%)	452 (99%)	4 (1%)	0	100	100
5	CE	64/129 (50%)	63 (98%)	1 (2%)	0	100	100
6	CF	216/239 (90%)	212 (98%)	4 (2%)	0	100	100
7	CG	469/485 (97%)	454 (97%)	15 (3%)	0	100	100
8	CH	257/260 (99%)	252 (98%)	5 (2%)	0	100	100
9	CI	113/163 (69%)	110 (97%)	3 (3%)	0	100	100
10	CJ	273/306 (89%)	268 (98%)	5 (2%)	0	100	100
11	CK	193/365 (53%)	186 (96%)	7 (4%)	0	100	100
15	LB	377/403 (94%)	369 (98%)	7 (2%)	1 (0%)	36	64
16	LC	324/427 (76%)	322 (99%)	2 (1%)	0	100	100
17	LD	226/297 (76%)	217 (96%)	9 (4%)	0	100	100
18	LE	200/288 (69%)	194 (97%)	6 (3%)	0	100	100
19	LF	217/248 (88%)	210 (97%)	6 (3%)	1 (0%)	24	54
20	LG	166/266 (62%)	166 (100%)	0	0	100	100
21	LH	188/192 (98%)	183 (97%)	5 (3%)	0	100	100
22	LJ	168/178 (94%)	164 (98%)	4 (2%)	0	100	100
23	LL	178/211 (84%)	176 (99%)	2 (1%)	0	100	100
24	LM	133/215 (62%)	130 (98%)	3 (2%)	0	100	100
25	LN	175/204 (86%)	173 (99%)	2 (1%)	0	100	100
26	LO	199/203 (98%)	197 (99%)	2 (1%)	0	100	100
27	LP	132/184 (72%)	129 (98%)	3 (2%)	0	100	100
28	LQ	149/188 (79%)	148 (99%)	1 (1%)	0	100	100
29	LS	174/176 (99%)	172 (99%)	2 (1%)	0	100	100
30	LT	125/160 (78%)	123 (98%)	2 (2%)	0	100	100
31	LV	135/140 (96%)	133 (98%)	2 (2%)	0	100	100
32	LY	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
33	La	101/148 (68%)	101 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
34	Ld	89/125 (71%)	88 (99%)	1 (1%)	0	100	100
35	Le	126/135 (93%)	124 (98%)	2 (2%)	0	100	100
36	Lf	107/110 (97%)	107 (100%)	0	0	100	100
37	Lh	100/123 (81%)	100 (100%)	0	0	100	100
38	Li	102/105 (97%)	100 (98%)	2 (2%)	0	100	100
39	Lr	121/137 (88%)	117 (97%)	4 (3%)	0	100	100
40	Lt	157/165 (95%)	153 (98%)	4 (2%)	0	100	100
41	Lz	204/217 (94%)	179 (88%)	25 (12%)	0	100	100
All	All	7309/9496 (77%)	7148 (98%)	159 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
15	LB	29	VAL
19	LF	197	VAL

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	CA	213/213 (100%)	212 (100%)	1 (0%)	81	82
2	CB	374/654 (57%)	374 (100%)	0	100	100
3	CC	51/485 (10%)	51 (100%)	0	100	100
4	CD	406/574 (71%)	406 (100%)	0	100	100
5	CE	50/115 (44%)	50 (100%)	0	100	100
6	CF	194/214 (91%)	193 (100%)	1 (0%)	81	82
7	CG	327/403 (81%)	327 (100%)	0	100	100
8	CH	217/228 (95%)	217 (100%)	0	100	100
9	CI	106/149 (71%)	106 (100%)	0	100	100
10	CJ	234/279 (84%)	234 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	CK	151/300 (50%)	151 (100%)	0	100	100
15	LB	327/349 (94%)	327 (100%)	0	100	100
16	LC	276/348 (79%)	276 (100%)	0	100	100
17	LD	193/250 (77%)	193 (100%)	0	100	100
18	LE	183/252 (73%)	183 (100%)	0	100	100
19	LF	182/215 (85%)	182 (100%)	0	100	100
20	LG	147/223 (66%)	147 (100%)	0	100	100
21	LH	167/171 (98%)	167 (100%)	0	100	100
22	LJ	137/149 (92%)	137 (100%)	0	100	100
23	LL	148/177 (84%)	147 (99%)	1 (1%)	76	79
24	LM	113/161 (70%)	113 (100%)	0	100	100
25	LN	152/172 (88%)	152 (100%)	0	100	100
26	LO	171/174 (98%)	171 (100%)	0	100	100
27	LP	119/163 (73%)	119 (100%)	0	100	100
28	LQ	136/165 (82%)	136 (100%)	0	100	100
29	LS	156/157 (99%)	156 (100%)	0	100	100
30	LT	101/140 (72%)	101 (100%)	0	100	100
31	LV	104/107 (97%)	104 (100%)	0	100	100
32	LY	121/135 (90%)	121 (100%)	0	100	100
33	La	87/121 (72%)	87 (100%)	0	100	100
34	Ld	39/110 (36%)	39 (100%)	0	100	100
35	Le	114/121 (94%)	114 (100%)	0	100	100
36	Lf	87/89 (98%)	87 (100%)	0	100	100
37	Lh	36/110 (33%)	36 (100%)	0	100	100
38	Li	85/89 (96%)	85 (100%)	0	100	100
39	Lr	106/121 (88%)	106 (100%)	0	100	100
40	Lt	127/137 (93%)	127 (100%)	0	100	100
All	All	5937/8020 (74%)	5934 (100%)	3 (0%)	87	89

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	CA	145	GLN

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Mol	Chain	Res	Type
6	CF	58	ASN
23	LL	159	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
2	CB	51	ASN
2	CB	83	ASN
2	CB	194	GLN
2	CB	282	HIS
2	CB	383	GLN
4	CD	64	GLN
4	CD	84	ASN
4	CD	354	ASN
6	CF	70	ASN
6	CF	113	ASN
6	CF	216	GLN
7	CG	323	GLN
7	CG	334	ASN
7	CG	376	ASN
8	CH	108	GLN
8	CH	232	GLN
9	CI	24	ASN
9	CI	110	ASN
10	CJ	256	HIS
15	LB	289	GLN
16	LC	38	ASN
16	LC	212	ASN
16	LC	329	ASN
17	LD	17	GLN
17	LD	39	GLN
17	LD	111	ASN
17	LD	225	GLN
18	LE	47	ASN
19	LF	56	HIS
19	LF	119	ASN
19	LF	239	GLN
21	LH	39	ASN
21	LH	98	HIS
22	LJ	46	GLN
22	LJ	98	ASN
23	LL	159	ASN

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Mol	Chain	Res	Type
24	LM	131	GLN
26	LO	167	HIS
27	LP	54	GLN
28	LQ	45	GLN
29	LS	108	GLN
30	LT	58	HIS
32	LY	20	ASN
32	LY	65	GLN
32	LY	96	HIS
33	La	60	HIS
34	Ld	28	ASN
34	Ld	79	ASN
34	Ld	118	GLN
35	Le	23	HIS
35	Le	117	GLN
35	Le	126	ASN
36	Lf	20	ASN
36	Lf	21	GLN
39	Lr	23	GLN
39	Lr	31	ASN
40	Lt	68	GLN
40	Lt	142	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
12	L5	2327/5070 (45%)	532 (22%)	13 (0%)
13	L7	119/121 (98%)	17 (14%)	1 (0%)
14	L8	111/157 (70%)	22 (19%)	0
All	All	2557/5348 (47%)	571 (22%)	14 (0%)

All (571) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
12	L5	13	U
12	L5	56	A
12	L5	59	A
12	L5	64	A
12	L5	65	A
12	L5	66	A
12	L5	69	A

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Mol	Chain	Res	Type
12	L5	71	C
12	L5	72	C
12	L5	92	C
12	L5	93	G
12	L5	108	A
12	L5	109	G
12	L5	110	C
12	L5	119	G
12	L5	120	A
12	L5	121	A
12	L5	122	U
12	L5	140	G
12	L5	142	G
12	L5	143	C
12	L5	152	U
12	L5	157	U
12	L5	159	C
12	L5	165	A
12	L5	170	C
12	L5	180	C
12	L5	183	C
12	L5	184	U
12	L5	185	C
12	L5	192	G
12	L5	193	G
12	L5	195	C
12	L5	200	U
12	L5	201	C
12	L5	209	U
12	L5	212	A
12	L5	217	C
12	L5	218	A
12	L5	219	G
12	L5	220	C
12	L5	232	G
12	L5	233	U
12	L5	234	G
12	L5	235	A
12	L5	237	G
12	L5	246	G
12	L5	252	C
12	L5	255	C

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Mol	Chain	Res	Type
12	L5	256	G
12	L5	266	C
12	L5	267	G
12	L5	279	A
12	L5	280	G
12	L5	306	A
12	L5	310	G
12	L5	315	G
12	L5	317	A
12	L5	318	A
12	L5	340	C
12	L5	349	A
12	L5	350	C
12	L5	362	A
12	L5	363	A
12	L5	371	A
12	L5	373	G
12	L5	380	U
12	L5	387	G
12	L5	398	A
12	L5	399	G
12	L5	407	A
12	L5	408	A
12	L5	409	G
12	L5	410	A
12	L5	413	G
12	L5	414	C
12	L5	432	U
12	L5	440	U
12	L5	449	C
12	L5	450	G
12	L5	452	A
12	L5	454	U
12	L5	465	G
12	L5	468	U
12	L5	469	C
12	L5	484	U
12	L5	485	C
12	L5	486	C
12	L5	489	C
12	L5	494	U
12	L5	497	G

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Mol	Chain	Res	Type
12	L5	498	C
12	L5	499	G
12	L5	500	G
12	L5	502	C
12	L5	503	C
12	L5	504	G
12	L5	505	G
12	L5	509	A
12	L5	510	U
12	L5	511	C
12	L5	512	U
12	L5	513	U
12	L5	514	U
12	L5	515	C
12	L5	518	G
12	L5	643	C
12	L5	656	C
12	L5	657	C
12	L5	659	G
12	L5	665	C
12	L5	666	G
12	L5	667	A
12	L5	668	C
12	L5	669	C
12	L5	672	C
12	L5	673	C
12	L5	686	A
12	L5	688	U
12	L5	696	C
12	L5	697	G
12	L5	700	G
12	L5	703	G
12	L5	704	C
12	L5	706	C
12	L5	725	G
12	L5	731	G
12	L5	739	G
12	L5	740	G
12	L5	742	G
12	L5	749	G
12	L5	753	C
12	L5	758	G

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Mol	Chain	Res	Type
12	L5	759	G
12	L5	760	G
12	L5	906	C
12	L5	913	U
12	L5	914	U
12	L5	915	A
12	L5	917	A
12	L5	925	C
12	L5	926	G
12	L5	932	A
12	L5	933	G
12	L5	935	A
12	L5	941	C
12	L5	943	A
12	L5	944	A
12	L5	945	U
12	L5	946	C
12	L5	956	A
12	L5	959	G
12	L5	960	A
12	L5	961	G
12	L5	977	C
12	L5	985	C
12	L5	988	C
12	L5	1065	G
12	L5	1070	G
12	L5	1072	C
12	L5	1075	G
12	L5	1082	C
12	L5	1083	U
12	L5	1218	G
12	L5	1277	G
12	L5	1280	C
12	L5	1284	G
12	L5	1287	G
12	L5	1294	A
12	L5	1295	C
12	L5	1301	C
12	L5	1313	C
12	L5	1314	C
12	L5	1354	A
12	L5	1358	G

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Mol	Chain	Res	Type
12	L5	1359	G
12	L5	1365	C
12	L5	1366	G
12	L5	1367	C
12	L5	1378	C
12	L5	1379	C
12	L5	1381	U
12	L5	1387	A
12	L5	1393	G
12	L5	1394	G
12	L5	1397	A
12	L5	1398	A
12	L5	1399	G
12	L5	1403	G
12	L5	1405	C
12	L5	1408	G
12	L5	1410	U
12	L5	1420	A
12	L5	1435	G
12	L5	1437	C
12	L5	1457	G
12	L5	1465	G
12	L5	1472	C
12	L5	1473	U
12	L5	1495	G
12	L5	1497	A
12	L5	1498	G
12	L5	1502	G
12	L5	1516	G
12	L5	1517	G
12	L5	1524	A
12	L5	1654	G
12	L5	1655	C
12	L5	1661	C
12	L5	1670	G
12	L5	1671	U
12	L5	1672	U
12	L5	1684	A
12	L5	1691	G
12	L5	1725	U
12	L5	1731	C
12	L5	1804	A

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Mol	Chain	Res	Type
12	L5	1806	G
12	L5	1810	G
12	L5	1815	G
12	L5	1818	G
12	L5	1821	G
12	L5	1822	U
12	L5	1829	G
12	L5	1832	C
12	L5	1836	G
12	L5	1837	A
12	L5	1842	G
12	L5	1854	G
12	L5	1855	G
12	L5	1869	G
12	L5	1870	C
12	L5	1872	G
12	L5	1881	C
12	L5	1891	A
12	L5	1897	A
12	L5	1917	A
12	L5	1918	U
12	L5	1919	G
12	L5	1920	C
12	L5	1921	C
12	L5	1922	G
12	L5	1925	G
12	L5	1931	C
12	L5	1941	A
12	L5	1942	A
12	L5	1944	A
12	L5	1949	U
12	L5	1961	G
12	L5	1968	G
12	L5	1969	G
12	L5	1970	A
12	L5	1971	C
12	L5	1975	G
12	L5	1983	A
12	L5	1984	A
12	L5	1990	A
12	L5	1997	U
12	L5	2002	A

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Mol	Chain	Res	Type
12	L5	2005	G
12	L5	2026	A
12	L5	2040	A
12	L5	2041	A
12	L5	2042	A
12	L5	2043	A
12	L5	2044	U
12	L5	2046	G
12	L5	2048	U
12	L5	2052	G
12	L5	2055	G
12	L5	2056	G
12	L5	2069	A
12	L5	2071	A
12	L5	2084	C
12	L5	2085	G
12	L5	2091	C
12	L5	2289	C
12	L5	2300	A
12	L5	2301	G
12	L5	2306	G
12	L5	2313	A
12	L5	2316	G
12	L5	2331	G
12	L5	2332	A
12	L5	2333	G
12	L5	2348	G
12	L5	2351	C
12	L5	2357	G
12	L5	2360	A
12	L5	2362	U
12	L5	2833	A
12	L5	2835	A
12	L5	2837	U
12	L5	2841	G
12	L5	2855	G
12	L5	3839	G
12	L5	3840	U
12	L5	3849	A
12	L5	3850	C
12	L5	3851	U
12	L5	3852	A

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Mol	Chain	Res	Type
12	L5	3853	U
12	L5	3855	C
12	L5	3865	A
12	L5	3867	A
12	L5	3869	C
12	L5	3872	A
12	L5	3873	G
12	L5	3875	G
12	L5	3877	A
12	L5	3879	G
12	L5	3892	U
12	L5	3916	G
12	L5	3922	G
12	L5	3931	C
12	L5	3939	G
12	L5	3942	A
12	L5	3943	A
12	L5	3944	G
12	L5	3949	A
12	L5	3950	U
12	L5	3952	A
12	L5	3953	G
12	L5	3955	G
12	L5	3956	G
12	L5	3958	G
12	L5	3959	U
12	L5	3961	G
12	L5	3962	A
12	L5	3963	A
12	L5	3964	U
12	L5	3965	A
12	L5	3966	A
12	L5	3967	G
12	L5	3969	G
12	L5	3970	G
12	L5	3971	G
12	L5	3973	G
12	L5	3974	G
12	L5	3977	C
12	L5	4036	G
12	L5	4038	C
12	L5	4039	G

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Mol	Chain	Res	Type
12	L5	4041	C
12	L5	4042	G
12	L5	4043	G
12	L5	4045	G
12	L5	4046	A
12	L5	4048	A
12	L5	4049	U
12	L5	4051	C
12	L5	4052	C
12	L5	4053	A
12	L5	4054	C
12	L5	4055	U
12	L5	4056	A
12	L5	4057	C
12	L5	4058	U
12	L5	4059	C
12	L5	4064	C
12	L5	4065	G
12	L5	4069	U
12	L5	4070	U
12	L5	4071	U
12	L5	4076	G
12	L5	4081	G
12	L5	4165	C
12	L5	4170	A
12	L5	4171	C
12	L5	4180	G
12	L5	4183	G
12	L5	4184	G
12	L5	4185	G
12	L5	4200	G
12	L5	4201	G
12	L5	4203	A
12	L5	4228	G
12	L5	4229	U
12	L5	4232	U
12	L5	4233	A
12	L5	4237	C
12	L5	4243	C
12	L5	4249	G
12	L5	4251	A
12	L5	4254	G

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Mol	Chain	Res	Type
12	L5	4257	A
12	L5	4268	A
12	L5	4272	G
12	L5	4274	A
12	L5	4275	G
12	L5	4276	G
12	L5	4277	G
12	L5	4282	A
12	L5	4290	U
12	L5	4291	G
12	L5	4293	U
12	L5	4294	C
12	L5	4297	G
12	L5	4304	A
12	L5	4305	G
12	L5	4306	U
12	L5	4307	A
12	L5	4308	C
12	L5	4309	G
12	L5	4331	G
12	L5	4335	C
12	L5	4347	G
12	L5	4354	U
12	L5	4361	U
12	L5	4365	C
12	L5	4368	G
12	L5	4382	G
12	L5	4385	A
12	L5	4392	G
12	L5	4393	G
12	L5	4401	G
12	L5	4404	U
12	L5	4426	C
12	L5	4428	A
12	L5	4432	C
12	L5	4437	U
12	L5	4440	G
12	L5	4446	U
12	L5	4464	A
12	L5	4465	U
12	L5	4471	U
12	L5	4475	G

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Mol	Chain	Res	Type
12	L5	4476	C
12	L5	4477	A
12	L5	4498	U
12	L5	4499	G
12	L5	4503	A
12	L5	4512	U
12	L5	4513	A
12	L5	4518	A
12	L5	4519	C
12	L5	4520	G
12	L5	4524	G
12	L5	4526	U
12	L5	4527	G
12	L5	4536	C
12	L5	4545	G
12	L5	4547	C
12	L5	4548	A
12	L5	4553	A
12	L5	4560	C
12	L5	4567	G
12	L5	4569	U
12	L5	4573	G
12	L5	4575	G
12	L5	4590	A
12	L5	4598	C
12	L5	4599	A
12	L5	4617	G
12	L5	4634	U
12	L5	4636	U
12	L5	4637	G
12	L5	4642	U
12	L5	4647	G
12	L5	4652	G
12	L5	4670	C
12	L5	4672	A
12	L5	4678	G
12	L5	4682	U
12	L5	4684	A
12	L5	4692	A
12	L5	4693	C
12	L5	4694	G
12	L5	4695	C

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Mol	Chain	Res	Type
12	L5	4700	A
12	L5	4708	A
12	L5	4709	U
12	L5	4719	G
12	L5	4730	C
12	L5	4731	G
12	L5	4734	A
12	L5	4740	G
12	L5	4741	C
12	L5	4742	G
12	L5	4745	G
12	L5	4750	G
12	L5	4754	G
12	L5	4757	C
12	L5	4759	C
12	L5	4761	G
12	L5	4765	G
12	L5	4773	C
12	L5	4775	C
12	L5	4776	G
12	L5	4864	U
12	L5	4870	G
12	L5	4871	C
12	L5	4872	G
12	L5	4875	G
12	L5	4880	C
12	L5	4882	U
12	L5	4883	C
12	L5	4888	U
12	L5	4889	G
12	L5	4895	C
12	L5	4899	G
12	L5	4900	C
12	L5	4901	G
12	L5	4910	G
12	L5	4912	G
12	L5	4914	C
12	L5	4923	C
12	L5	4925	U
12	L5	4926	C
12	L5	4928	C
12	L5	4937	C

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Mol	Chain	Res	Type
12	L5	4940	C
12	L5	4941	G
12	L5	4943	A
12	L5	4945	G
12	L5	4949	G
12	L5	4951	G
12	L5	4955	A
12	L5	4960	G
12	L5	4961	G
12	L5	4976	U
12	L5	4985	U
12	L5	5013	C
12	L5	5031	G
12	L5	5034	A
12	L5	5041	G
12	L5	5047	C
12	L5	5049	G
12	L5	5050	C
12	L5	5054	C
12	L5	5055	G
12	L5	5069	U
13	L7	7	G
13	L7	22	A
13	L7	24	C
13	L7	38	U
13	L7	53	U
13	L7	54	A
13	L7	61	G
13	L7	64	G
13	L7	74	A
13	L7	75	G
13	L7	76	U
13	L7	89	G
13	L7	91	C
13	L7	97	G
13	L7	100	A
13	L7	106	G
13	L7	110	G
14	L8	2	G
14	L8	16	G
14	L8	25	G
14	L8	39	G

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Mol	Chain	Res	Type
14	L8	49	G
14	L8	59	A
14	L8	60	G
14	L8	61	A
14	L8	62	A
14	L8	63	U
14	L8	64	U
14	L8	65	A
14	L8	66	A
14	L8	68	G
14	L8	71	A
14	L8	93	C
14	L8	94	G
14	L8	99	U
14	L8	100	U
14	L8	103	A
14	L8	105	C
14	L8	156	U

All (14) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
12	L5	317	A
12	L5	406	C
12	L5	493	G
12	L5	914	U
12	L5	1082	C
12	L5	2854	G
12	L5	4305	G
12	L5	4392	G
12	L5	4498	U
12	L5	4597	U
12	L5	4699	U
12	L5	4774	C
12	L5	4913	G
13	L7	74	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	$\# Z > 2$
42	GTP	CB	1001	43	30,34,34	0.85	1 (3%)	46,54,54	1.70	11 (23%)
44	GDP	CD	702	43	28,30,30	1.15	3 (10%)	44,47,47	1.82	7 (15%)

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
42	GTP	CB	1001	43	-	6/22/38/38	0/3/3/3
44	GDP	CD	702	43	-	5/16/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
44	CD	702	GDP	C5-C4	3.01	1.47	1.38
44	CD	702	GDP	C6-N1	-2.48	1.34	1.38
44	CD	702	GDP	C5-N7	-2.20	1.34	1.39
42	CB	1001	GTP	C2-N3	2.19	1.38	1.33

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	CD	702	GDP	C5-C4-N3	-6.03	118.68	128.46
42	CB	1001	GTP	C5-C4-N3	-5.04	120.29	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
44	CD	702	GDP	C2-N3-C4	4.79	120.84	112.30
44	CD	702	GDP	N9-C4-N3	4.54	135.06	125.94
42	CB	1001	GTP	C2-N3-C4	4.48	120.29	112.30
44	CD	702	GDP	PA-O3A-PB	-3.47	120.90	132.83
42	CB	1001	GTP	N9-C4-N3	3.26	132.49	125.94
42	CB	1001	GTP	PA-O3A-PB	-3.09	122.21	132.83
44	CD	702	GDP	C6-C5-N7	3.09	136.00	130.25
42	CB	1001	GTP	C2-N1-C6	-2.99	119.65	125.10
42	CB	1001	GTP	PB-O3B-PG	-2.67	123.67	132.83
42	CB	1001	GTP	N9-C8-N7	-2.66	108.39	113.39
42	CB	1001	GTP	C5-C6-N1	2.57	119.70	113.19
44	CD	702	GDP	C4-C5-N7	-2.53	106.71	110.72
42	CB	1001	GTP	C8-N7-C5	2.51	108.79	104.24
42	CB	1001	GTP	O6-C6-C5	-2.41	120.20	126.60
44	CD	702	GDP	O6-C6-C5	-2.16	120.86	126.60
42	CB	1001	GTP	C3'-C2'-C1'	2.05	105.33	101.43

There are no chirality outliers.

All (11) torsion outliers are listed below:

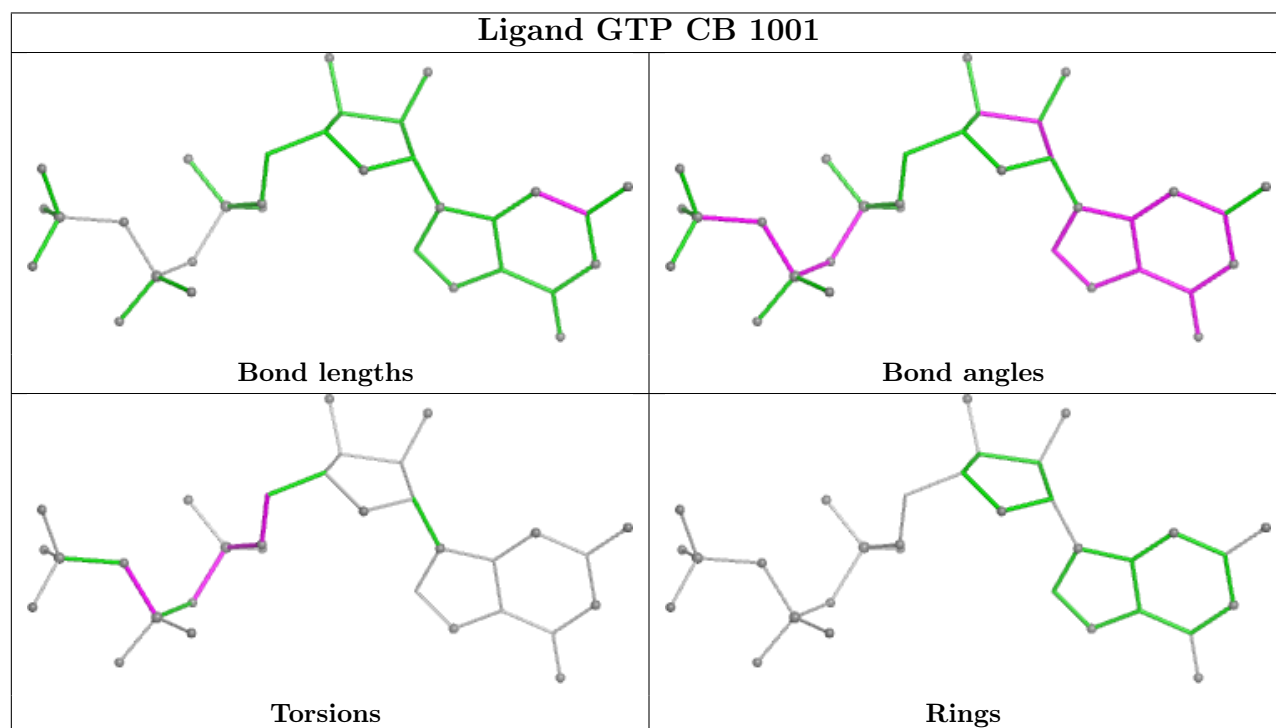
Mol	Chain	Res	Type	Atoms
42	CB	1001	GTP	PB-O3A-PA-O5'
42	CB	1001	GTP	C5'-O5'-PA-O3A
42	CB	1001	GTP	C5'-O5'-PA-O1A
42	CB	1001	GTP	C5'-O5'-PA-O2A
44	CD	702	GDP	C5'-O5'-PA-O3A
44	CD	702	GDP	C5'-O5'-PA-O1A
44	CD	702	GDP	C5'-O5'-PA-O2A
44	CD	702	GDP	O4'-C4'-C5'-O5'
44	CD	702	GDP	C3'-C4'-C5'-O5'
42	CB	1001	GTP	PG-O3B-PB-O1B
42	CB	1001	GTP	C4'-C5'-O5'-PA

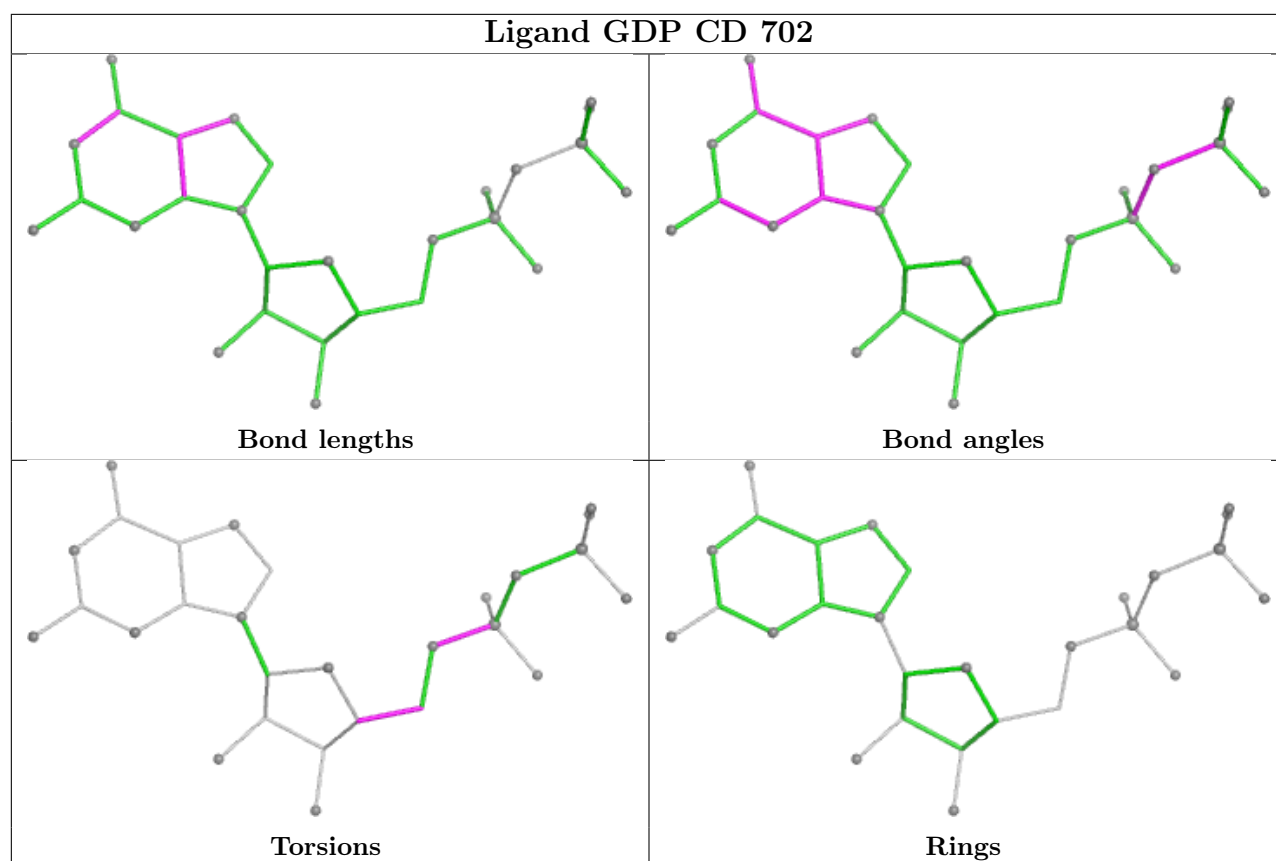
There are no ring outliers.

No monomer is involved in short contacts.

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.

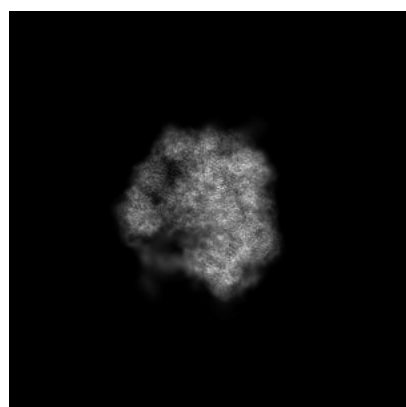
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-53092. These allow visual inspection of the internal detail of the map and identification of artifacts.

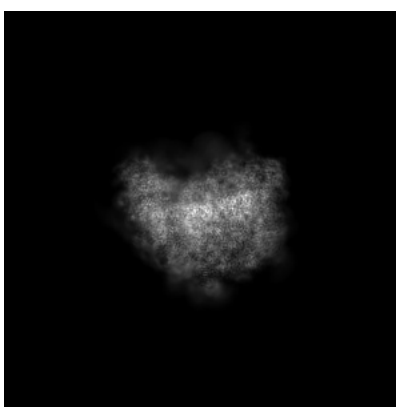
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

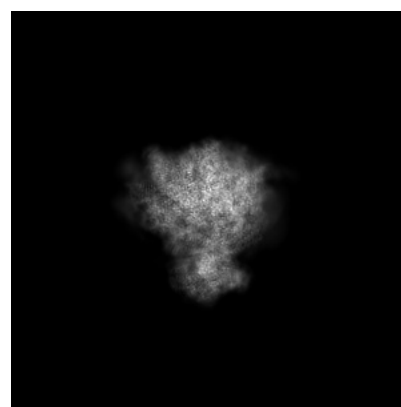
6.1.1 Primary map



X



Y

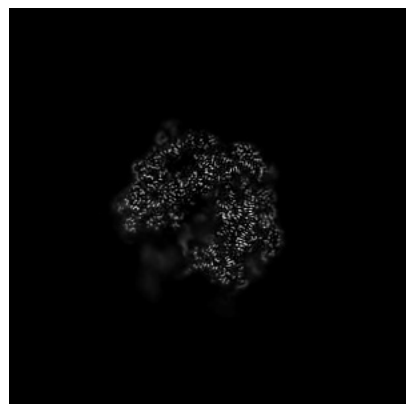


Z

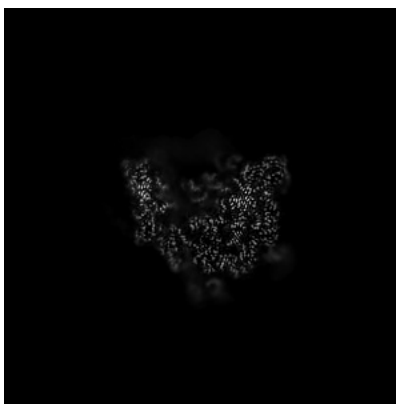
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

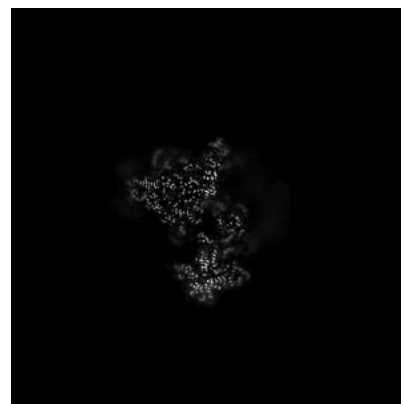
6.2.1 Primary map



X Index: 250



Y Index: 250

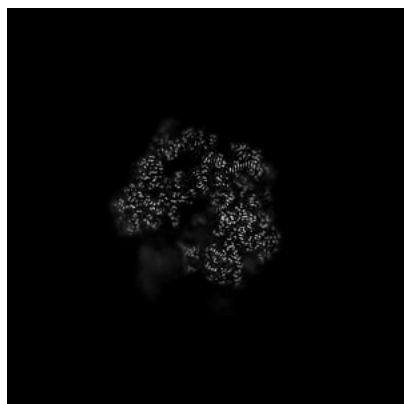


Z Index: 250

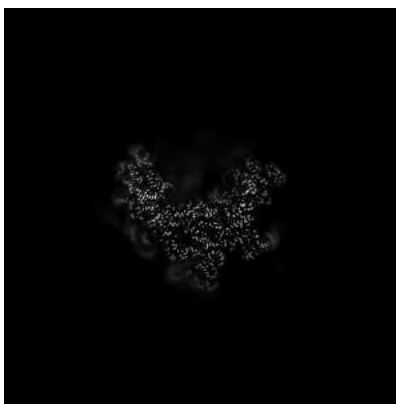
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

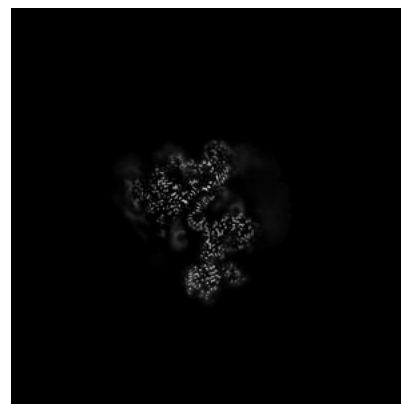
6.3.1 Primary map



X Index: 246



Y Index: 274

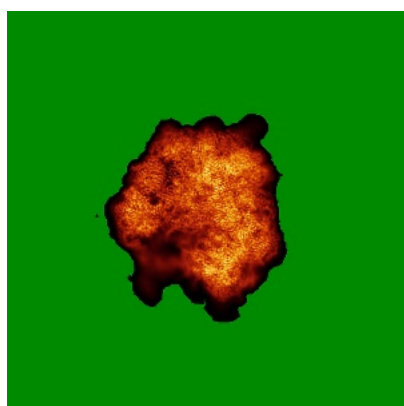


Z Index: 258

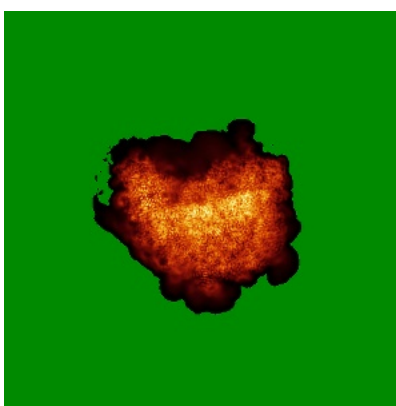
The images above show the largest variance slices of the map in three orthogonal directions.

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

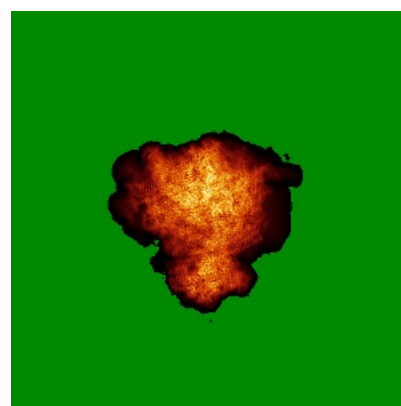
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.334. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

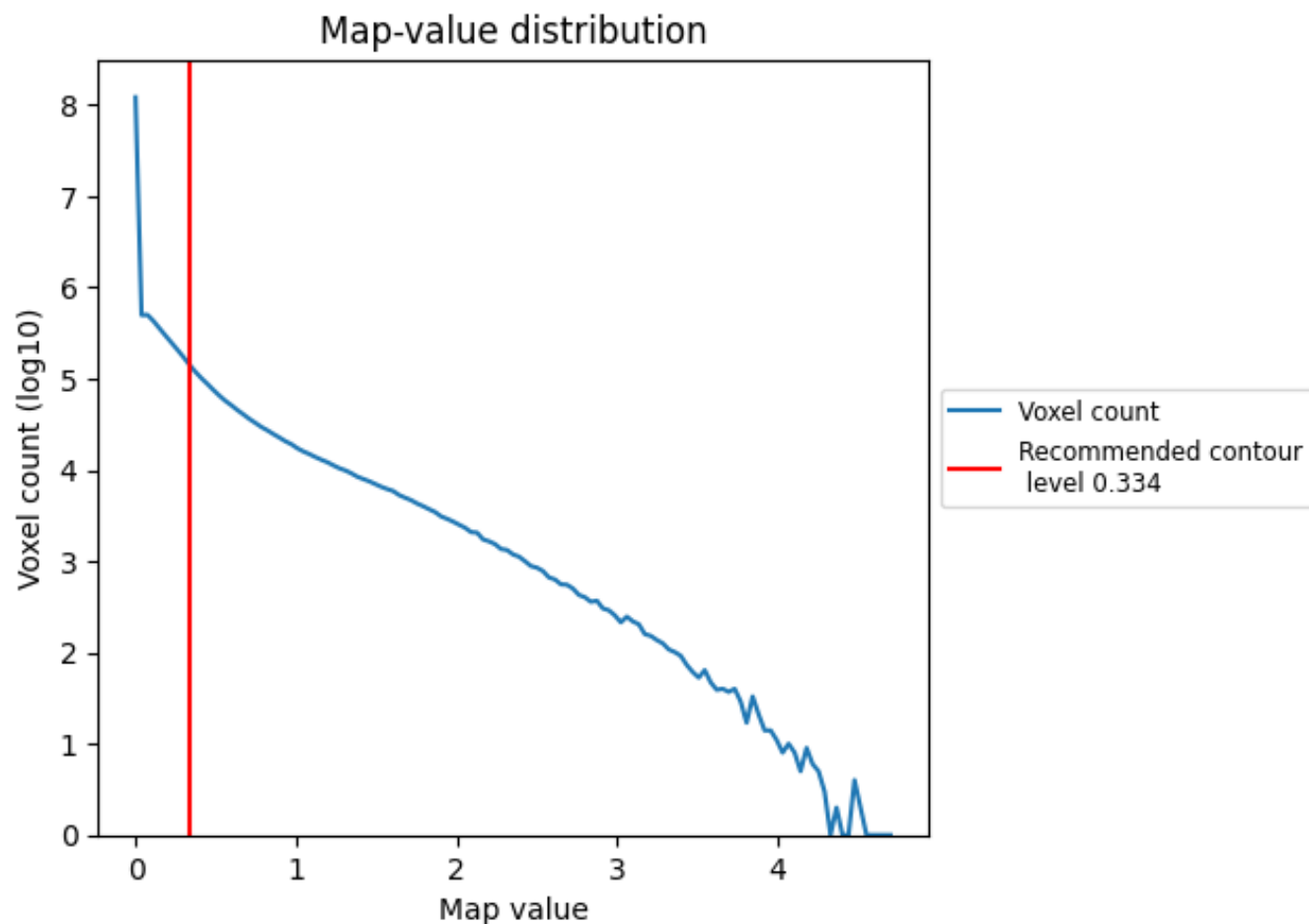
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

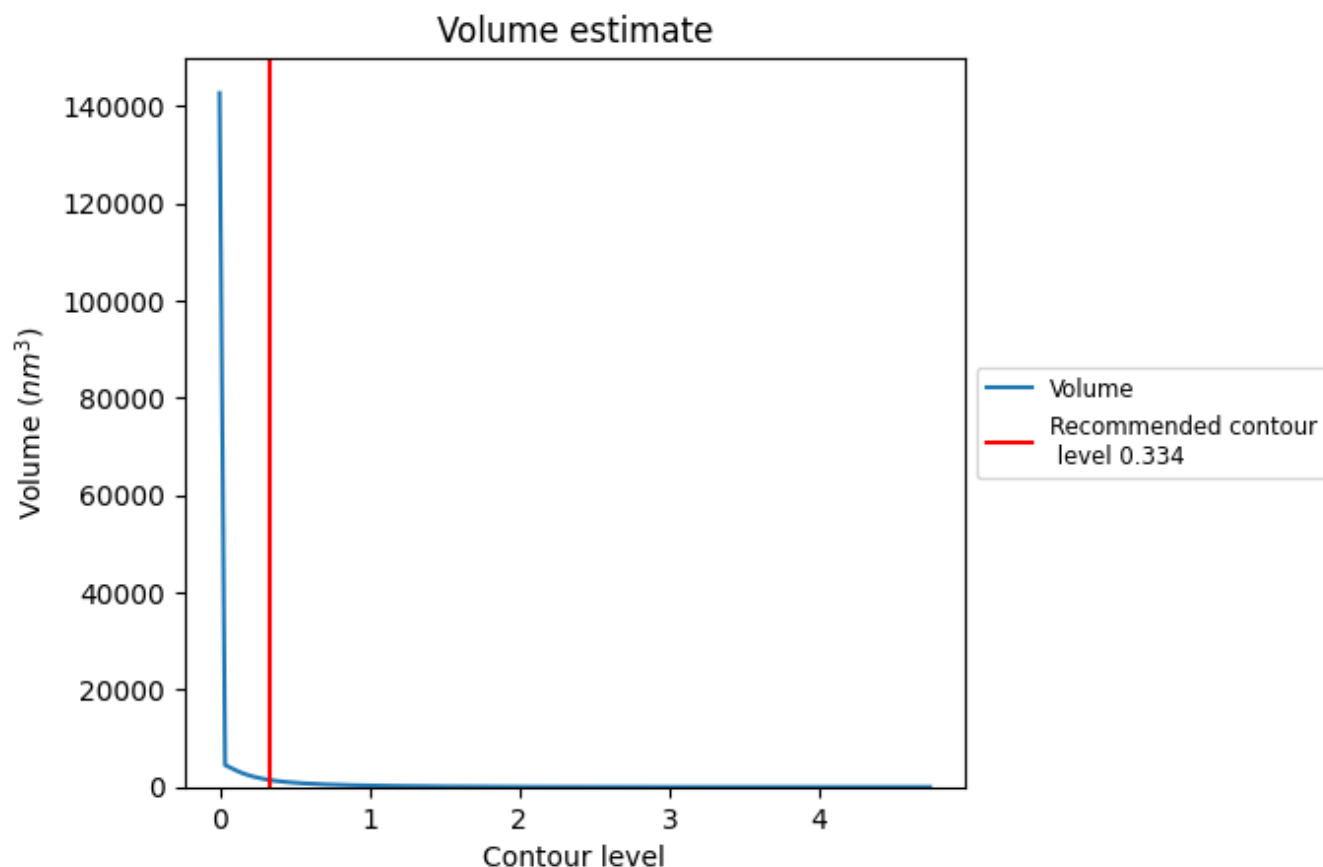
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

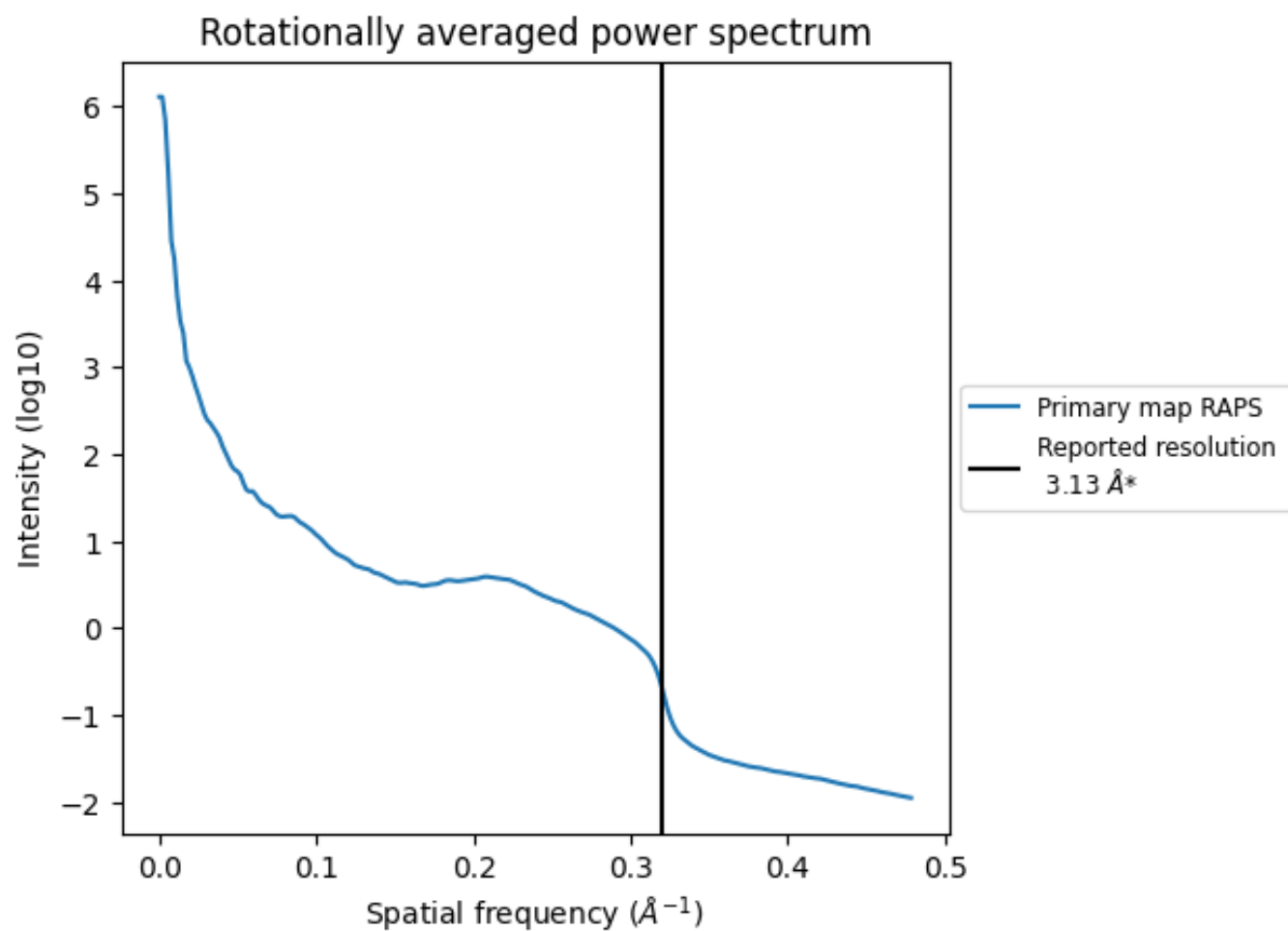
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1428 nm^3 ; this corresponds to an approximate mass of 1290 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.319 Å⁻¹

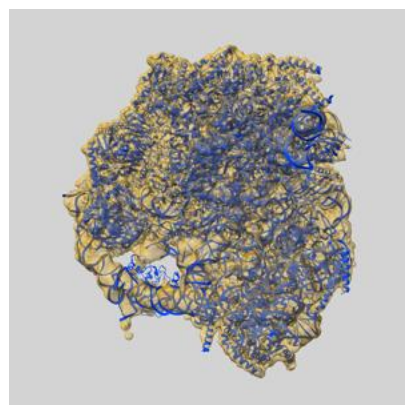
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

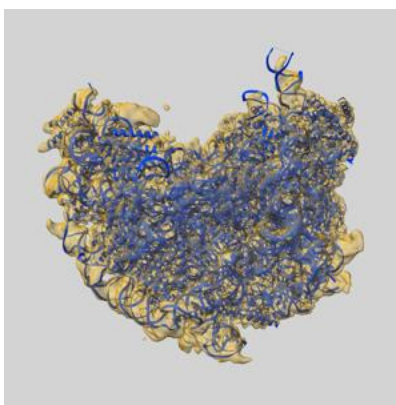
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-53092 and PDB model 9QET. Per-residue inclusion information can be found in section 3 on page 13.

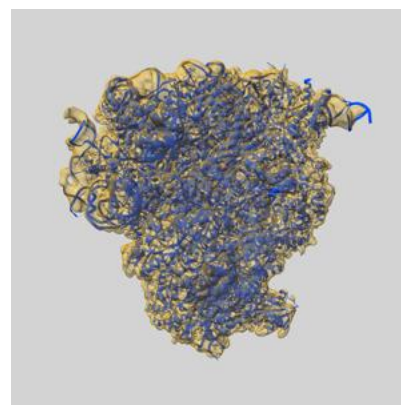
9.1 Map-model overlay [i](#)



X



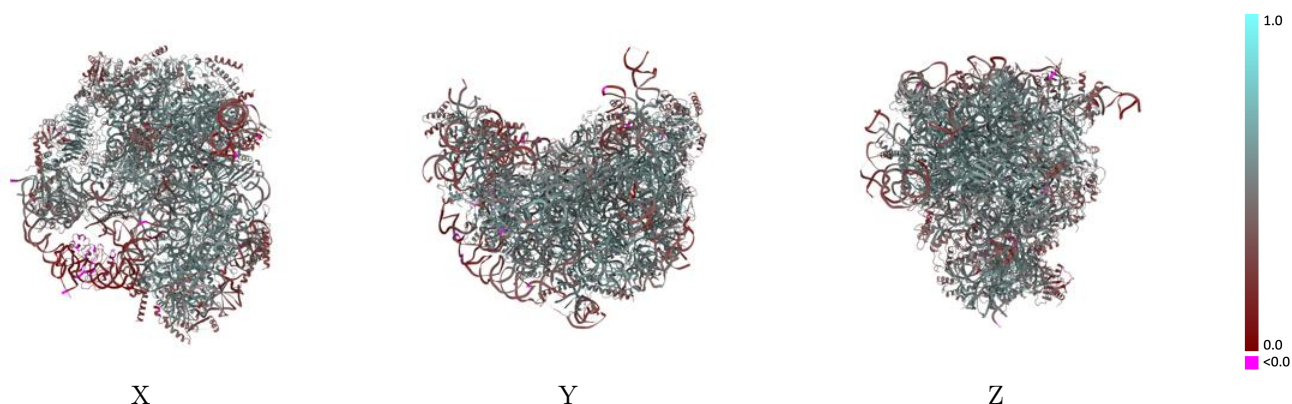
Y



Z

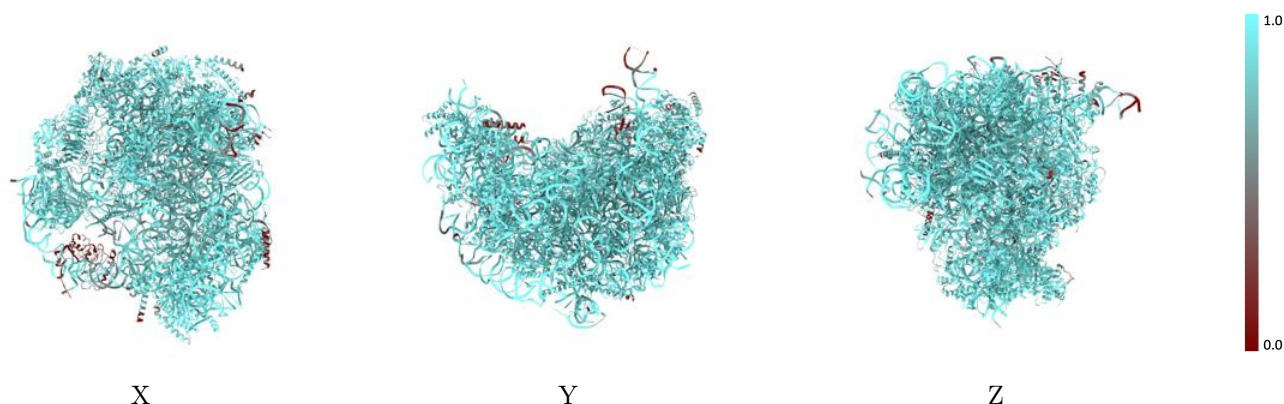
The images above show the 3D surface view of the map at the recommended contour level 0.334 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



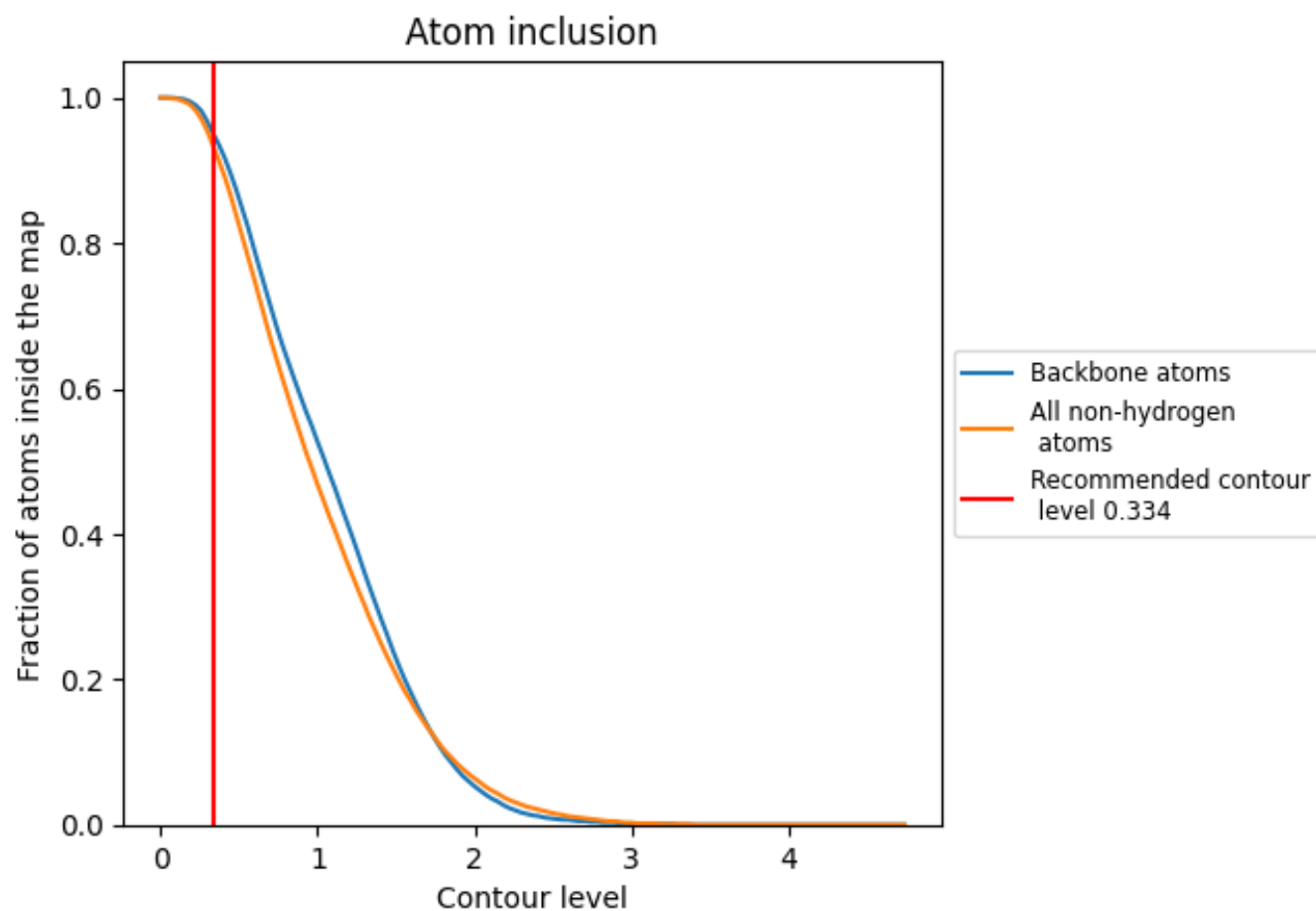
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.334).

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% 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 (0.334) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9340	 0.4790
CA	 0.9230	 0.4960
CB	 0.9070	 0.4720
CC	 0.6410	 0.4400
CD	 0.9120	 0.4910
CE	 0.8070	 0.4110
CF	 0.9030	 0.4490
CG	 0.9680	 0.5260
CH	 0.9510	 0.5610
CI	 0.9310	 0.4930
CJ	 0.9410	 0.4700
CK	 0.8740	 0.4110
L5	 0.9550	 0.4620
L7	 0.9620	 0.4200
L8	 0.9230	 0.4380
LB	 0.9550	 0.5600
LC	 0.9690	 0.5600
LD	 0.9670	 0.5280
LE	 0.9450	 0.5100
LF	 0.9510	 0.5600
LG	 0.9150	 0.4080
LH	 0.9540	 0.5520
LJ	 0.9180	 0.4330
LL	 0.9620	 0.5280
LM	 0.9620	 0.5530
LN	 0.9910	 0.5730
LO	 0.9690	 0.5700
LP	 0.9250	 0.5110
LQ	 0.9460	 0.5430
LS	 0.9480	 0.5590
LT	 0.8460	 0.4320
LV	 0.9570	 0.5430
LY	 0.9510	 0.4920
La	 0.9710	 0.5400
Ld	 0.6670	 0.3240



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Chain	Atom inclusion	Q-score
Le	 0.9700	 0.5800
Lf	 0.9830	 0.6080
Lh	 0.7690	 0.4070
Li	 0.8860	 0.4380
Lr	 0.9700	 0.5530
Lt	 0.8570	 0.3620
Lz	 0.1390	 0.0640