



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 02:00 PM UTC

PDB ID : 8PV2 / pdb_00008pv2
EMDB ID : EMD-17951
Title : Chaetomium thermophilum pre-60S State 10 - pre-5S rotation with Ytm1-Erb1
Authors : Thoms, M.; Cheng, J.; Denk, T.; Berninghausen, O.; Beckmann, R.
Deposited on : 2023-07-17
Resolution : 2.63 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

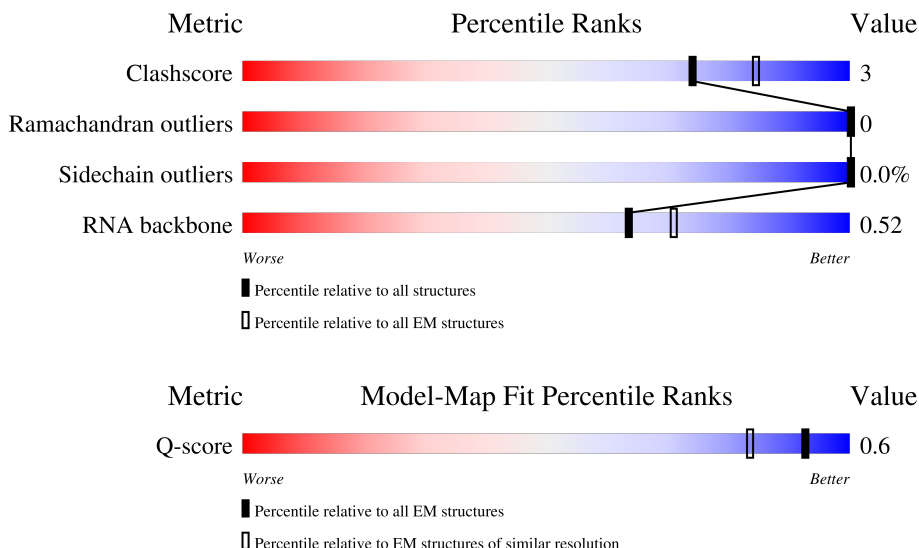
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.63 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.



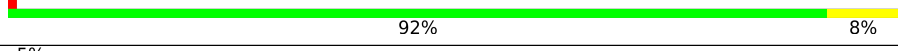
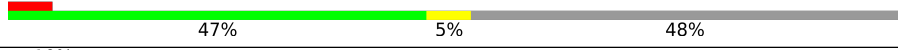
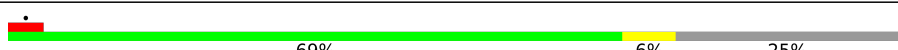
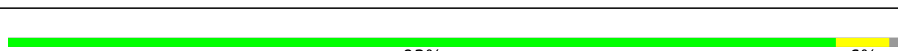
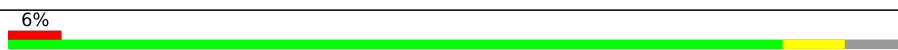
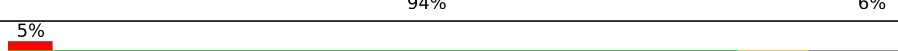
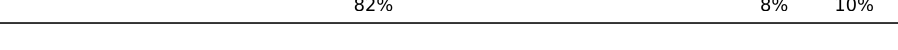
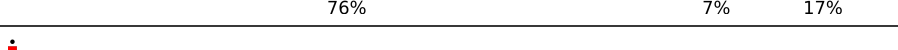
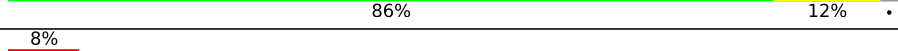
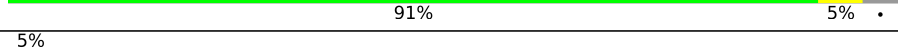
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	8888 (2.13 - 3.13)

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	C1	3338	
2	C2	156	
3	C4	119	

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Mol	Chain	Length	Quality of chain
4	CF	270	
5	CH	661	
6	CK	261	
7	CL	558	
8	CN	246	
9	CO	120	
10	CQ	225	
11	Cb	117	
12	Cd	627	
13	Cf	350	
14	Cg	202	
15	Ch	517	
16	Cz	123	
17	LA	254	
18	LB	392	
19	LC	365	
20	LD	304	
21	LE	200	
22	CM	249	
22	LF	249	
23	LG	262	
24	LH	229	
25	LJ	173	
26	LK	165	
27	LL	213	

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Mol	Chain	Length	Quality of chain
28	LM	142	
29	LN	203	
30	LO	204	
31	LP	187	
32	LQ	213	
33	LR	2898	
34	LS	174	
35	LT	160	
36	LU	127	
37	LV	139	
38	LX	156	
39	LY	138	
40	LZ	135	
41	La	149	
42	Lc	108	
43	Ld	120	
44	Le	131	
45	Lf	109	
46	Lg	119	
47	Lh	935	
48	Li	110	
49	Lj	95	
50	Lk	94	
51	Ll	51	
52	Lp	92	

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Mol	Chain	Length	Quality of chain
53	Lq	147	6% 86% 8%
54	CC	801	28% 52% 20%
55	CD	495	16% 63% 21%
56	CJ	679	28% 80% 12%

2 Entry composition [i](#)

There are 60 unique types of molecules in this entry. The entry contains 155881 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called 26S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	3056	Total	C	N	O	P	0	0
			65414	29219	11840	21299	3056		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C1	3338	C	-	insertion	GB XR_002966752

- Molecule 2 is a RNA chain called 5.8S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	153	Total	C	N	O	P	0	0
			3259	1457	581	1068	153		

- Molecule 3 is a RNA chain called 5S rRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C4	119	Total	C	N	O	P	0	0
			2536	1131	453	833	119		

- Molecule 4 is a protein called Large ribosomal subunit protein uL10.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CF	245	Total	C	N	O	S	0	0
			1934	1215	350	360	9		

- Molecule 5 is a protein called Nucleolar GTP-binding protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CH	627	Total	C	N	O	S	0	0
			5036	3167	914	936	19		

- Molecule 6 is a protein called Ribosome biogenesis protein NSA2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CK	237	Total	C	N	O	S	0	0
			1903	1198	368	333	4		

- Molecule 7 is a protein called Putative GTP binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CL	79	Total	C	N	O	S	0	0
			622	389	125	108			

- Molecule 8 is a protein called Eukaryotic translation initiation factor 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CN	246	Total	C	N	O	S	0	0
			1853	1156	322	368	7		

- Molecule 9 is a protein called DUF2423 domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CO	62	Total	C	N	O	S	0	0
			468	290	94	82	2		

- Molecule 10 is a protein called Ribosome biogenesis protein RLP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CQ	183	Total	C	N	O	S	0	0
			1480	925	304	241	10		

- Molecule 11 is a protein called Zinc finger domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Cb	101	Total	C	N	O	S	0	0
			830	517	161	148	4		

- Molecule 12 is a protein called Nucleolar GTP-binding protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Cd	462	Total	C	N	O	S	0	0
			3691	2350	671	659	11		

- Molecule 13 is a protein called Ribosome production factor 2 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Cf	285	Total	C	N	O	S	0	0
			2282	1443	417	401	21		

- Molecule 14 is a protein called Ribosome biogenesis regulatory protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	Cg	188	Total	C	N	O	S	0	0
			1478	924	283	270	1		

- Molecule 15 is a protein called Ribosome assembly protein 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	Ch	485	Total	C	N	O	S	1	0
			3812	2396	696	710	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Ch	117	ASP	GLU	insertion	UNP G0SC29

- Molecule 16 is a protein called rRNA-processing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Cz	101	Total	C	N	O	S	0	0
			869	541	180	144	4		

- Molecule 17 is a protein called 60S ribosomal protein L2-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LA	191	Total	C	N	O	S	0	0
			1454	917	278	256	3		

- Molecule 18 is a protein called 60S ribosomal protein L3-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LB	389	Total	C	N	O	S	0	0
			3104	1973	579	539	13		

- Molecule 19 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LC	363	Total	C	N	O	S	0	0
			2751	1737	527	478	9		

- Molecule 20 is a protein called 60S ribosomal protein l5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LD	286	Total	C	N	O	S	0	0
			2266	1434	407	422	3		

- Molecule 21 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LE	191	Total	C	N	O	S	0	0
			1477	944	267	263	3		

- Molecule 22 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LF	248	Total	C	N	O	S	0	0
			2023	1297	377	346	3		
22	CM	134	Total	C	N	O		0	0
			685	414	137	134			

- Molecule 23 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	LG	235	Total	C	N	O	S	0	0
			1889	1210	350	324	5		

- Molecule 24 is a protein called 60S ribosomal protein l9-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LH	190	Total	C	N	O	S	0	0
			1495	949	268	272	6		

- Molecule 25 is a protein called Putative ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	LJ	169	Total	C	N	O	S	0	0
			1357	850	266	235	6		

- Molecule 26 is a protein called 60S ribosomal protein L12-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	LK	158	Total	C	N	O	S	0	0
			1184	743	215	224	2		

- Molecule 27 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	LL	203	Total	C	N	O	S	0	0
			1587	989	325	271	2		

- Molecule 28 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	LM	141	Total	C	N	O	S	0	0
			1126	714	216	195	1		

- Molecule 29 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	LN	202	Total	C	N	O	S	0	0
			1704	1062	360	278	4		

- Molecule 30 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	LO	203	Total	C	N	O	S	0	0
			1611	1034	305	267	5		

- Molecule 31 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	LP	171	Total	C	N	O	S	0	0
			1343	834	274	232	3		

- Molecule 32 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	LQ	150	Total	C	N	O	S	0	0
			1200	759	239	200	2		

- Molecule 33 is a protein called Ribosomal protein L19.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	LR	155	Total	C	N	O	S	0	0
			1241	772	262	203	4		

- Molecule 34 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	LS	174	Total	C	N	O	S	0	0
			1426	917	266	238	5		

- Molecule 35 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	LT	129	Total	C	N	O	S	0	0
			1027	651	195	179	2		

- Molecule 36 is a protein called 60S ribosomal protein L22-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	LU	105	Total	C	N	O	S	0	0
			846	548	146	151	1		

- Molecule 37 is a protein called 60S ribosomal protein l23-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	LV	135	Total	C	N	O	S	0	0
			991	630	184	170	7		

- Molecule 38 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
38	LX	122	Total	C	N	O	0	0
			967	620	175	172		

- Molecule 39 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	LY	133	Total	C	N	O	S	0	0
			1056	658	213	183	2		

- Molecule 40 is a protein called 60S ribosomal protein L27.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	LZ	135	Total	C	N	O	S	0	0
			1112	713	207	188	4		

- Molecule 41 is a protein called 60S ribosomal protein L28-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	La	108	Total	C	N	O	S	0	0
			872	556	168	147	1		

- Molecule 42 is a protein called 60S ribosomal protein l30-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
42	Lc	95	Total	C	N	O	S	0	0
			705	449	122	129	5		

- Molecule 43 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
43	Ld	110	Total	C	N	O	S	0	0
			875	555	171	148	1		

- Molecule 44 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
44	Le	126	Total	C	N	O	S	0	0
			1017	640	208	163	6		

- Molecule 45 is a protein called 60S ribosomal protein l33-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
45	Lf	108	Total	C	N	O	S	0	0
			862	546	171	144	1		

- Molecule 46 is a protein called Ribosomal protein l34-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
46	Lg	118	Total	C	N	O	S	0	0
			914	567	186	157	4		

- Molecule 47 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
47	Lh	115	Total	C	N	O	0	0
			951	605	189	157		

- Molecule 48 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
48	Li	101	Total	C	N	O	S	0	0
			827	509	181	136	1		

- Molecule 49 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
49	Lj	88	Total	C	N	O	S	0	0
			698	427	154	112	5		

- Molecule 50 is a protein called 60S ribosomal protein L38-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
50	Lk	76	Total	C	N	O	S	0	0
			632	400	121	109	2		

- Molecule 51 is a protein called Ribosomal protein eL39.

Mol	Chain	Residues	Atoms				AltConf	Trace
51	Ll	50	Total	C	N	O	0	0
			436	275	97	64		

- Molecule 52 is a protein called 60S ribosomal protein L43-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
52	Lp	91	Total	C	N	O	S	0	0
			698	430	138	124	6		

- Molecule 53 is a protein called Putative 60S ribosomal protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
53	Lq	139	Total	C	N	O	0	0
			1073	672	213	188		

- Molecule 54 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
54	CC	499	Total	C	N	O	S	0	0
			3890	2492	697	691	10		

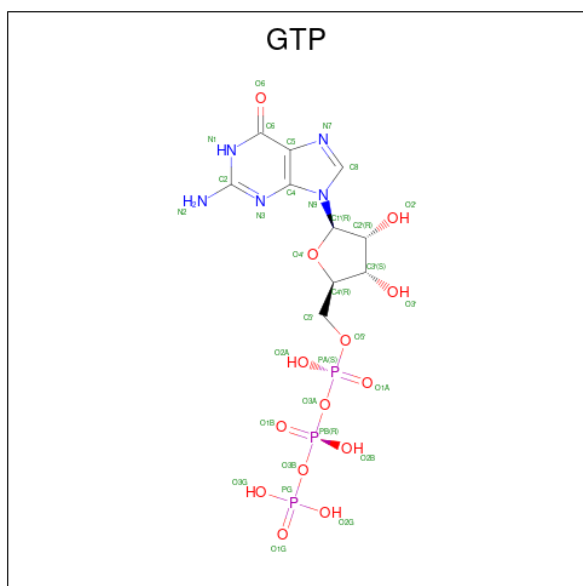
- Molecule 55 is a protein called Ribosome biogenesis protein YTM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
55	CD	453	Total	C	N	O	S	0	0
			3390	2126	598	660	6		

- Molecule 56 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
56	CJ	493	Total	C	N	O	S	0	0
			3577	2274	659	633	11		

- Molecule 57 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					AltConf
57	CH	1	Total	C	N	O	P	0
			32	10	5	14	3	
57	Cd	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 58 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
58	CH	1	Total 1	Mg 1	0
58	Cd	2	Total 2	Mg 2	0

- Molecule 59 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
59	CQ	1	Total 1	Zn 1	0
59	Cb	1	Total 1	Zn 1	0
59	Lg	1	Total 1	Zn 1	0
59	Lj	1	Total 1	Zn 1	0
59	Lp	1	Total 1	Zn 1	0

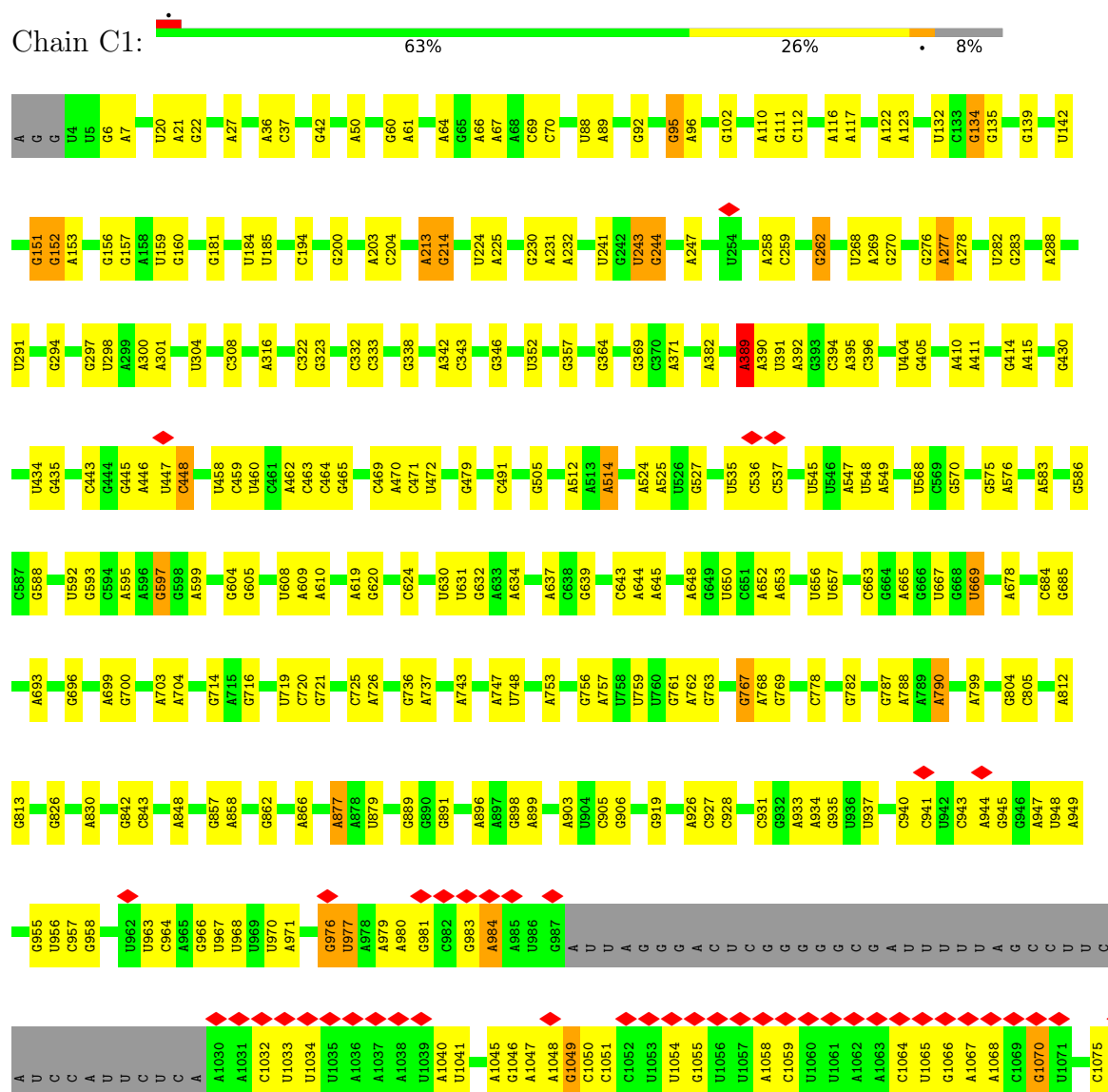
- Molecule 60 is water.

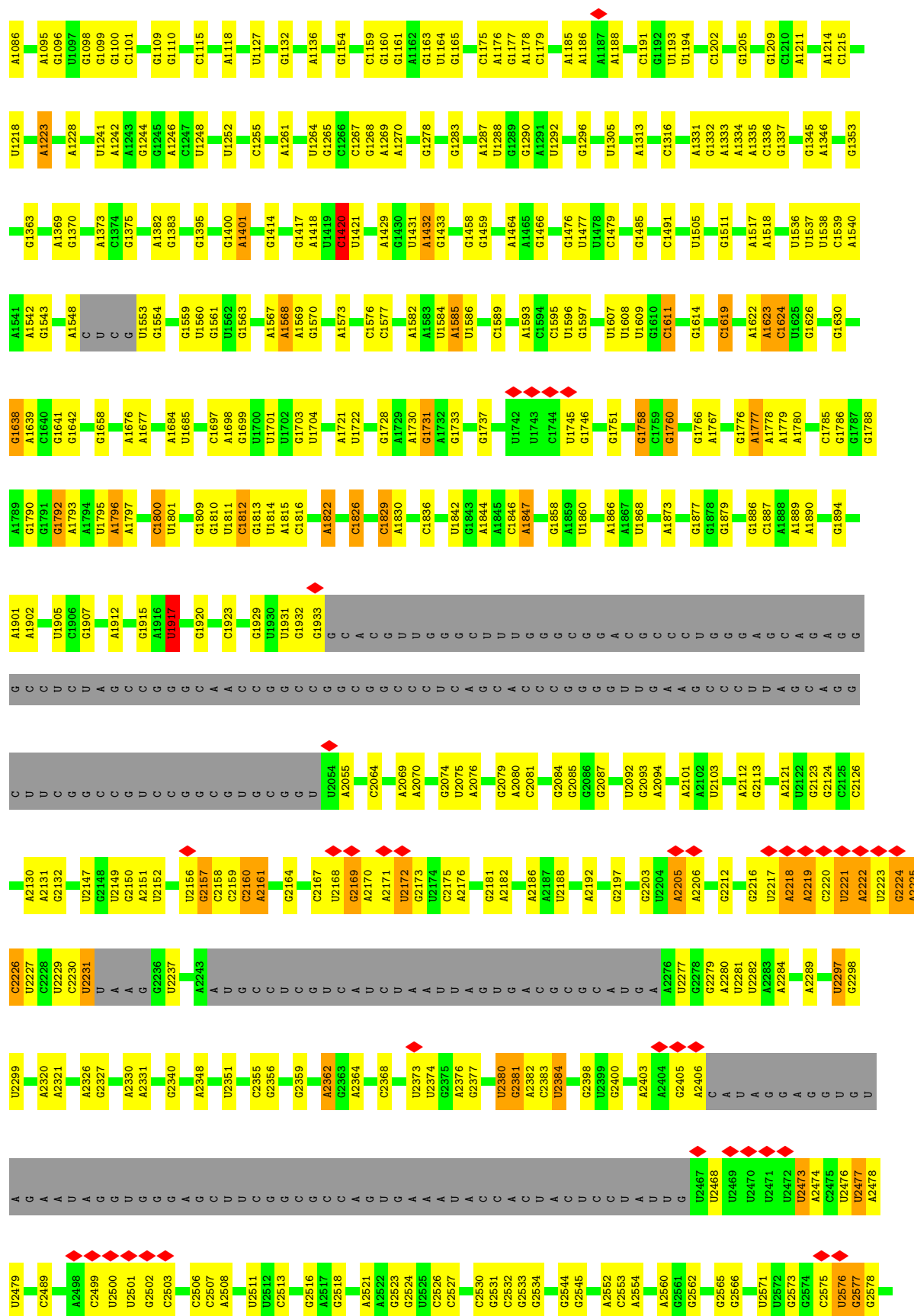
Mol	Chain	Residues	Atoms		AltConf
60	CH	1	Total 1	O 1	0
60	Cd	2	Total 2	O 2	0

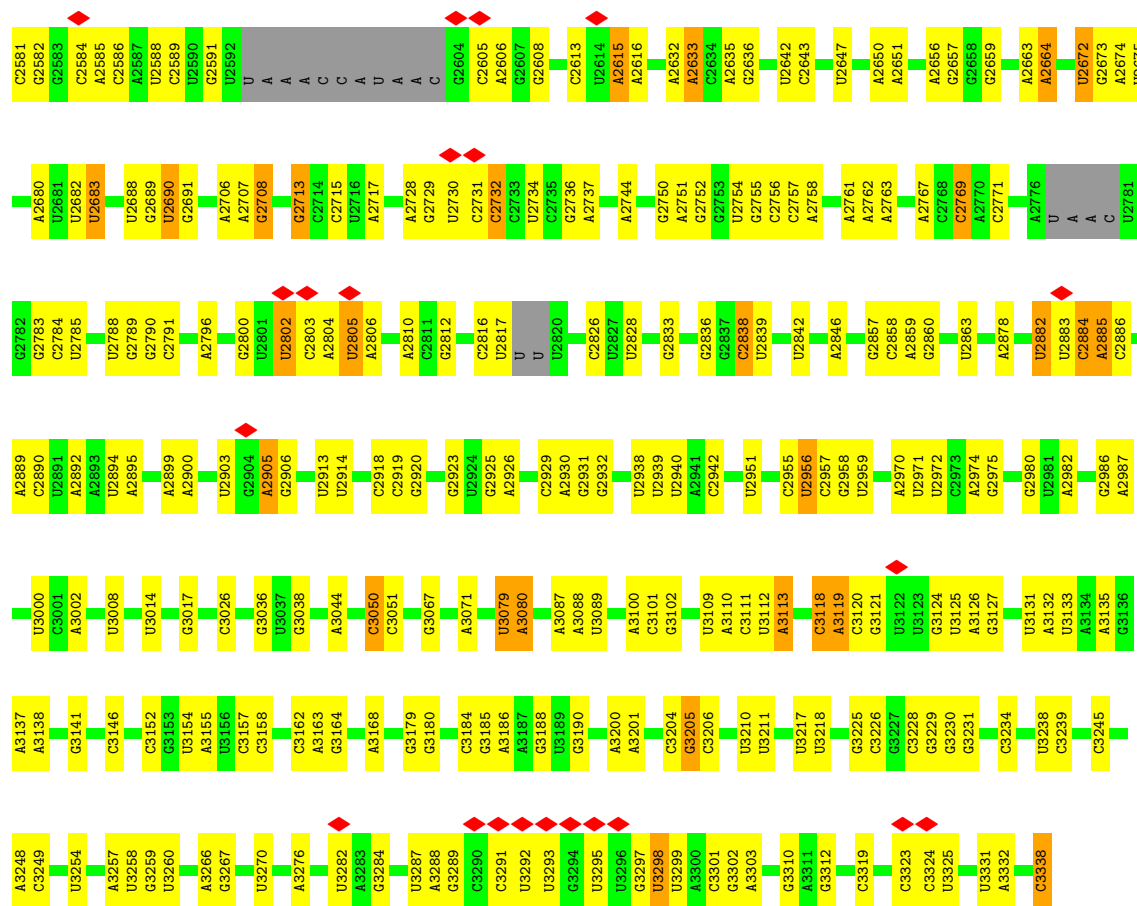
3 Residue-property plots

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.

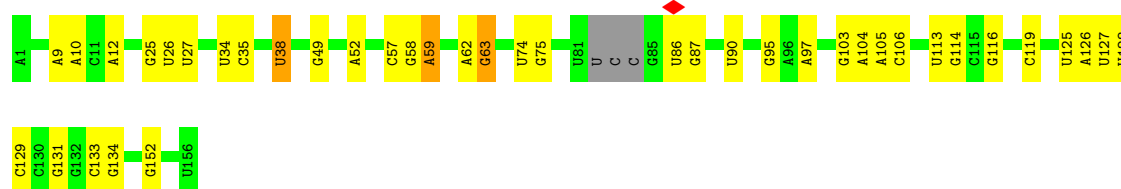
• Molecule 1: 26S rRNA







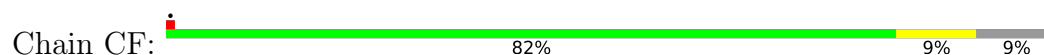
• Molecule 2: 5.8S rRNA

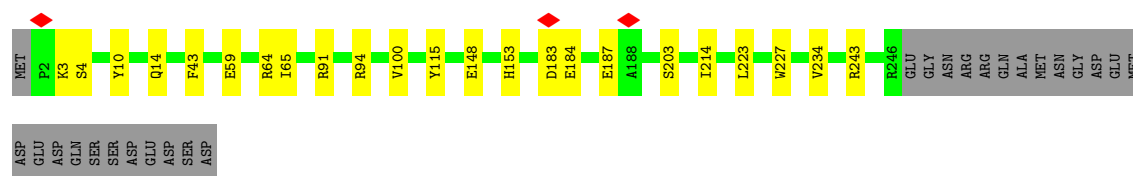


• Molecule 3: 5S rRNA

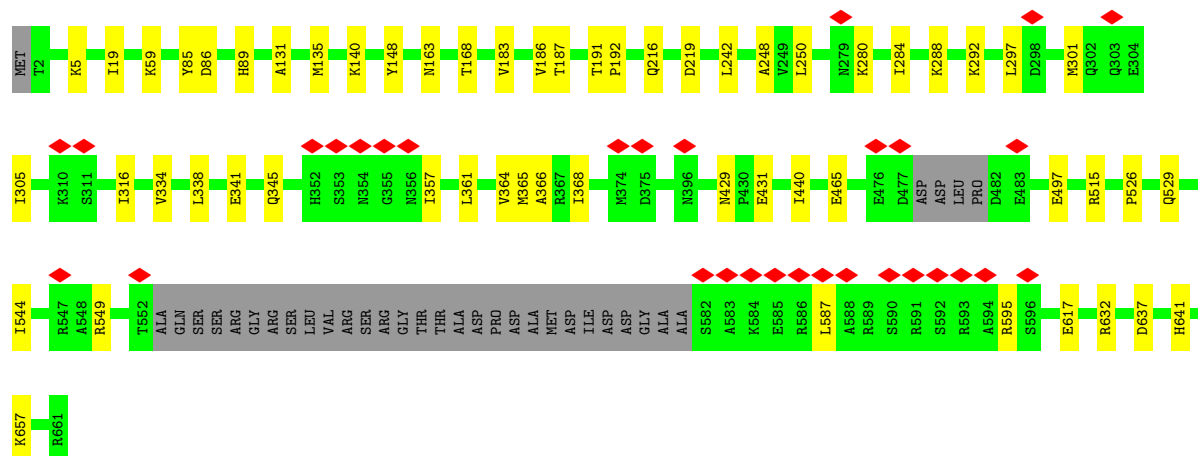
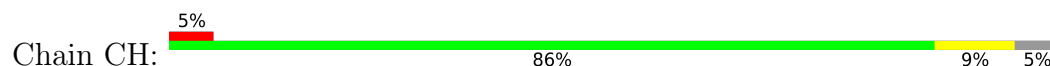


• Molecule 4: Large ribosomal subunit protein uL10

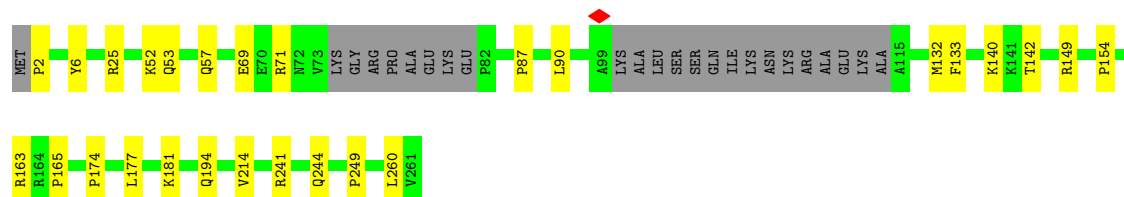
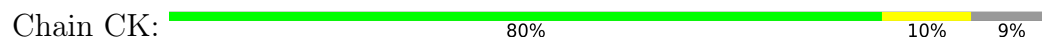




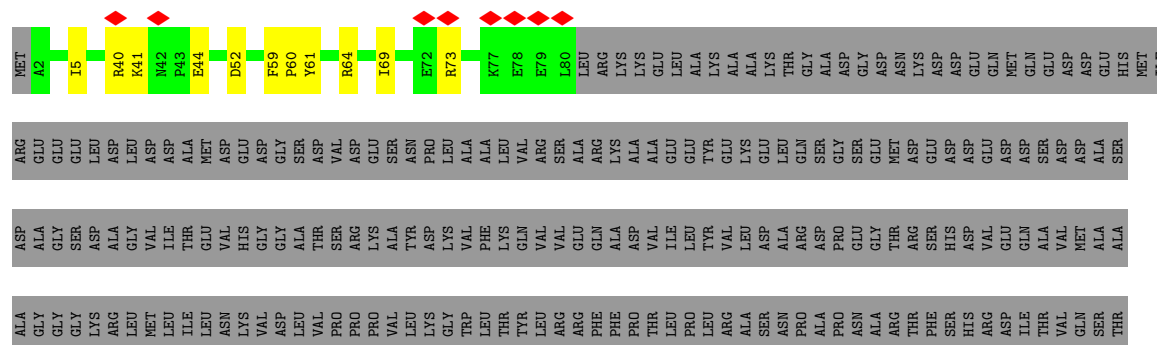
- Molecule 5: Nucleolar GTP-binding protein 1

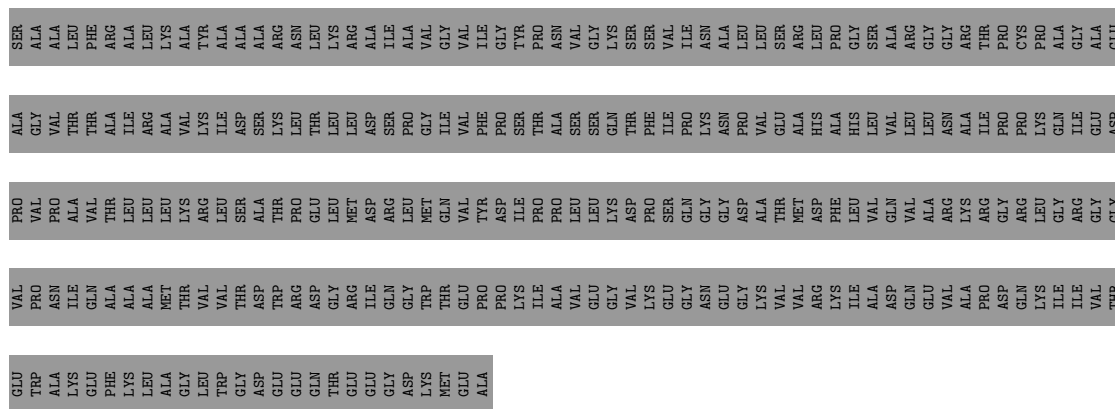


- Molecule 6: Ribosome biogenesis protein NSA2 homolog

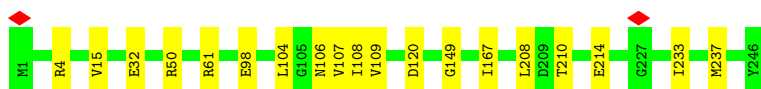


- Molecule 7: Putative GTP binding protein

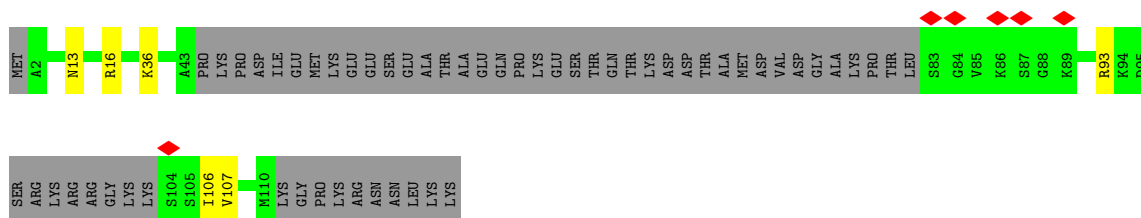




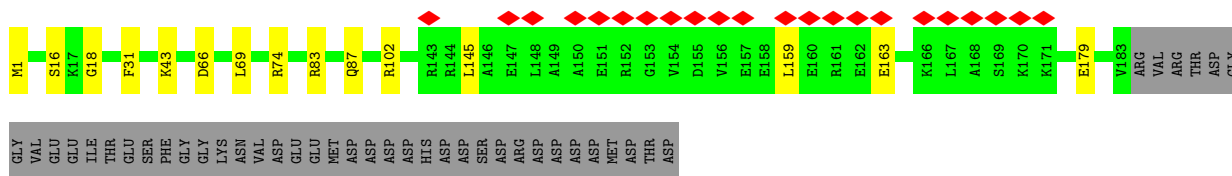
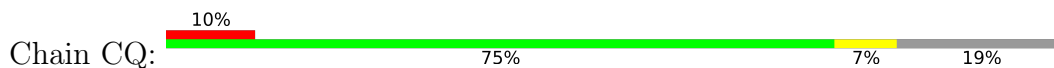
- Molecule 8: Eukaryotic translation initiation factor 6



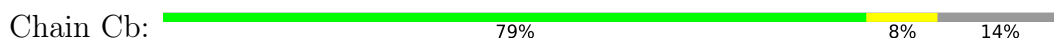
- Molecule 9: DUF2423 domain-containing protein



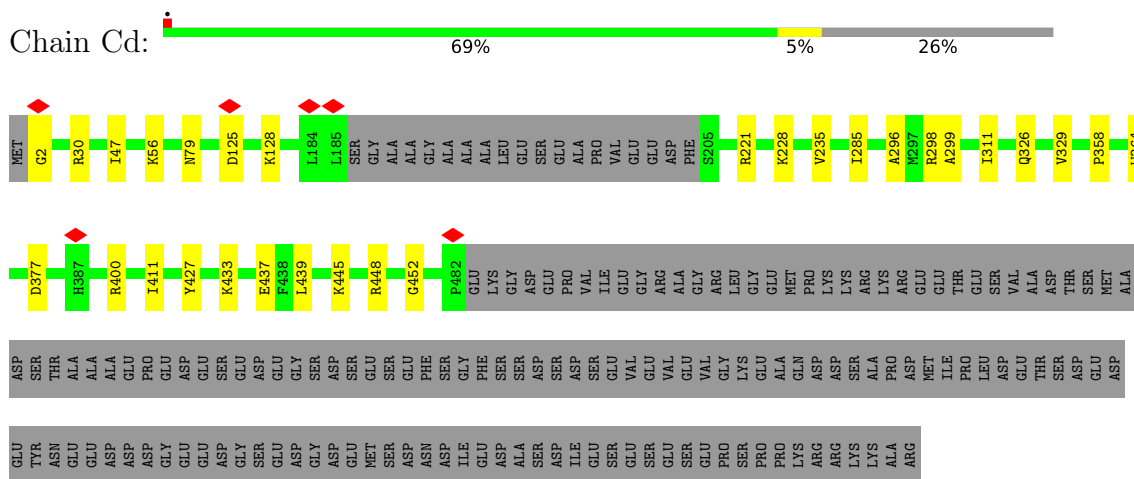
- Molecule 10: Ribosome biogenesis protein RLP24



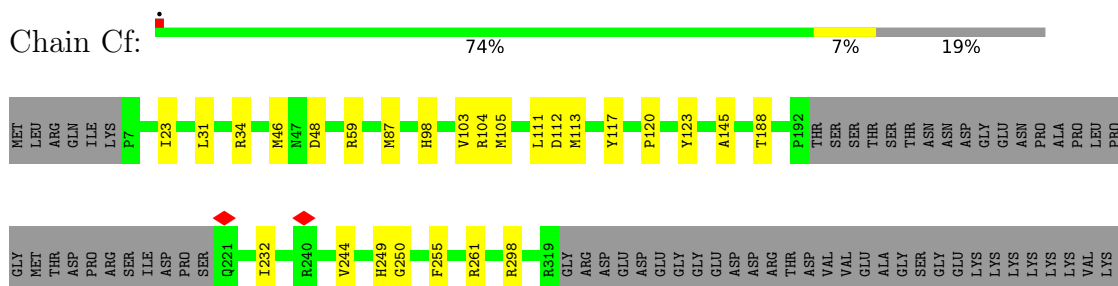
- Molecule 11: Zinc finger domain-containing protein



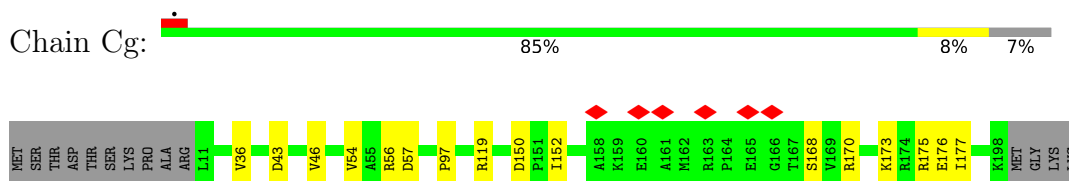
- Molecule 12: Nucleolar GTP-binding protein 2



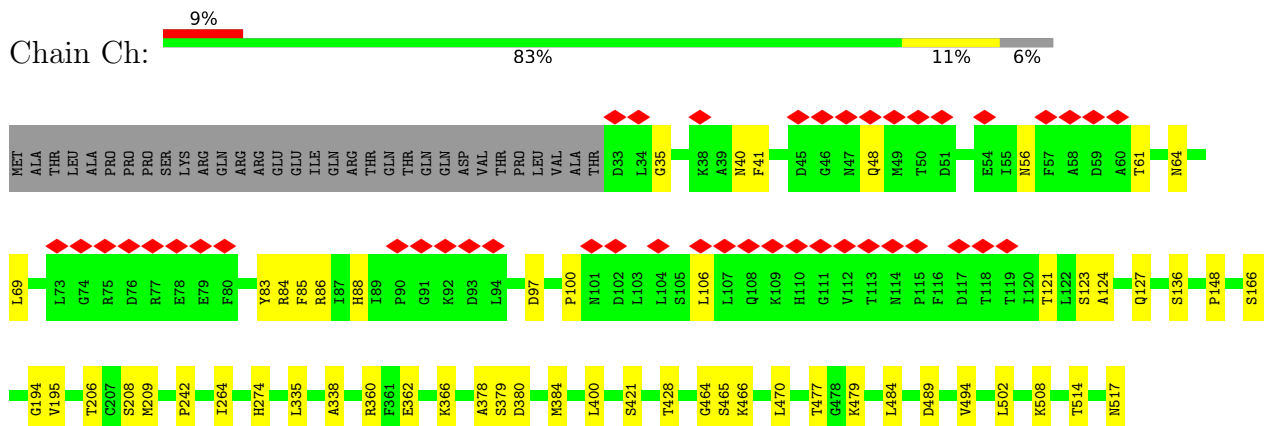
- Molecule 13: Ribosome production factor 2 homolog



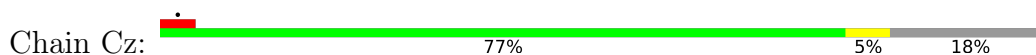
- Molecule 14: Ribosome biogenesis regulatory protein



- Molecule 15: Ribosome assembly protein 4

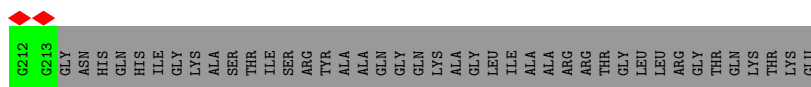
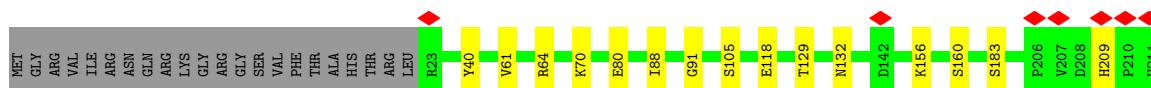


- Molecule 16: rRNA-processing protein





- Molecule 17: 60S ribosomal protein L2-like protein



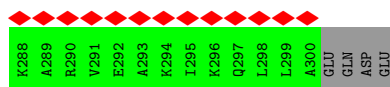
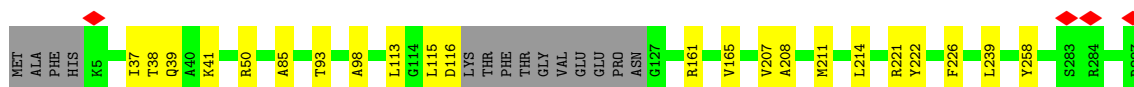
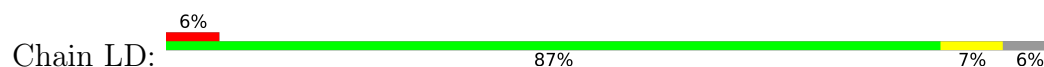
- Molecule 18: 60S ribosomal protein L3-like protein



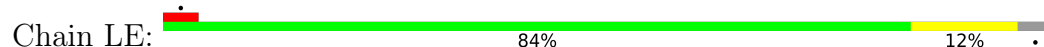
- Molecule 19: 60S ribosomal protein L4-like protein



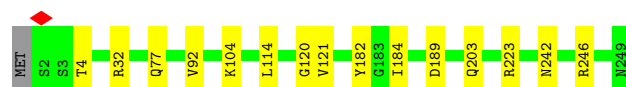
- Molecule 20: 60S ribosomal protein L5-like protein



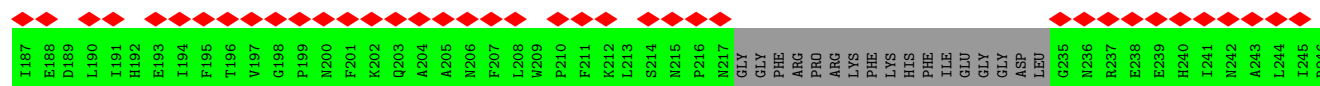
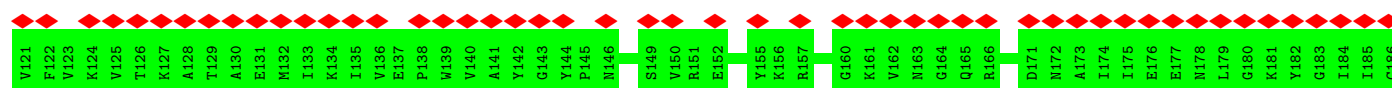
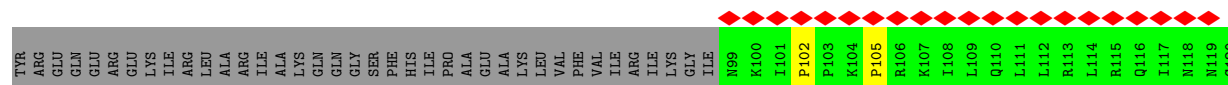
- Molecule 21: 60S ribosomal protein L6



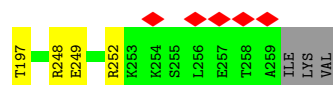
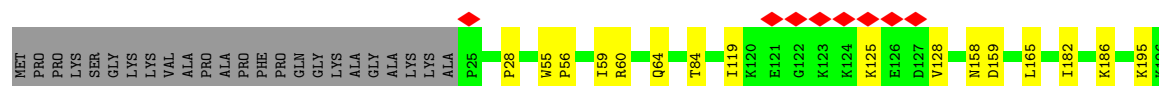
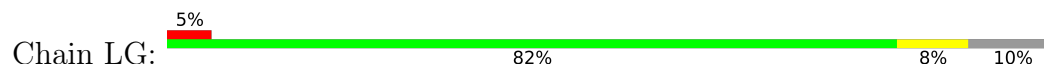
- Molecule 22: 60S ribosomal protein l7-like protein



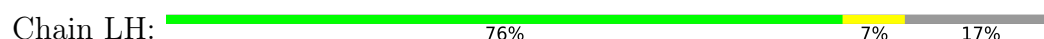
- Molecule 22: 60S ribosomal protein 17-like protein

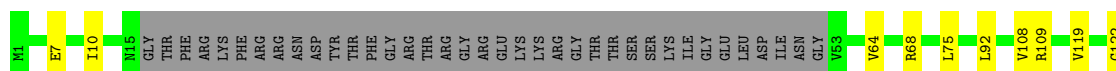


- Molecule 23: 60S ribosomal protein L8

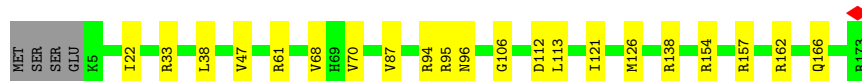


- Molecule 24: 60S ribosomal protein 19-like protein

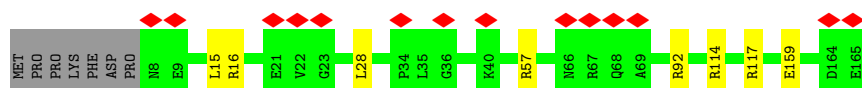




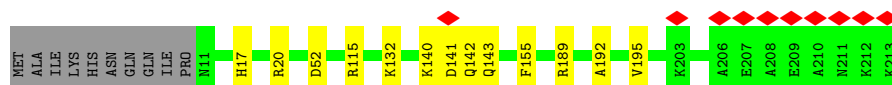
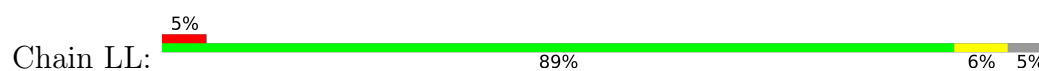
- Molecule 25: Putative ribosomal protein



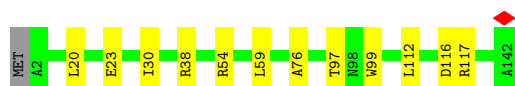
- Molecule 26: 60S ribosomal protein L12-like protein



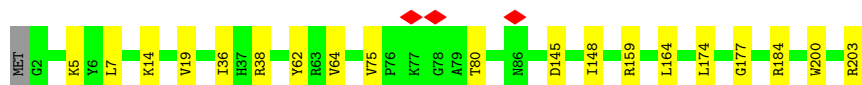
- Molecule 27: 60S ribosomal protein L13



- Molecule 28: 60S ribosomal protein L14-like protein



- Molecule 29: Ribosomal protein L15

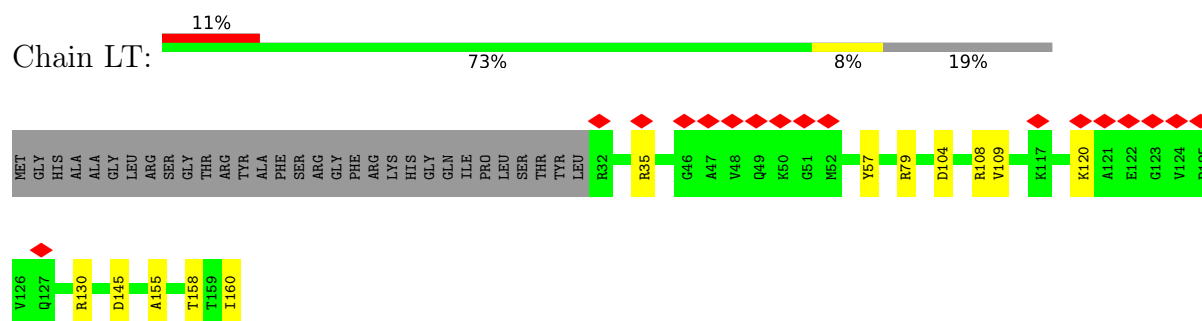


- Molecule 30: 60S ribosomal protein L16-like protein

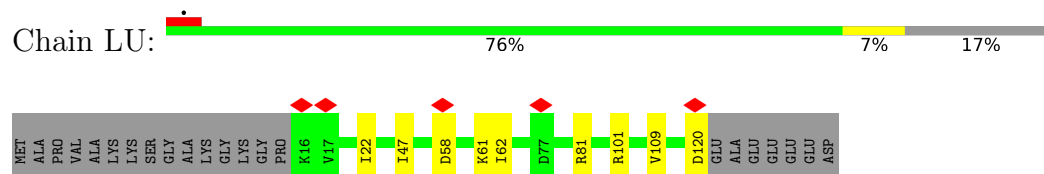




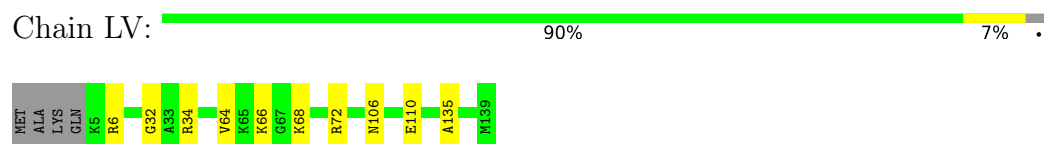
- Molecule 35: 60S ribosomal protein l21-like protein



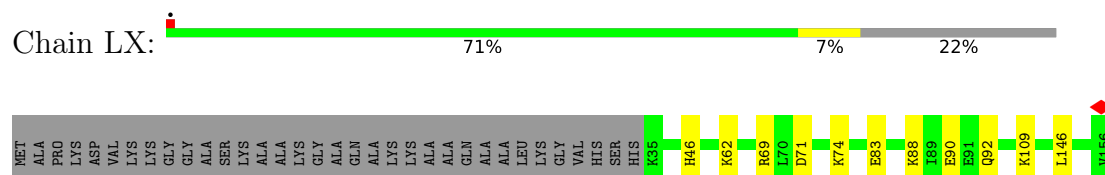
- Molecule 36: 60S ribosomal protein L22-like protein



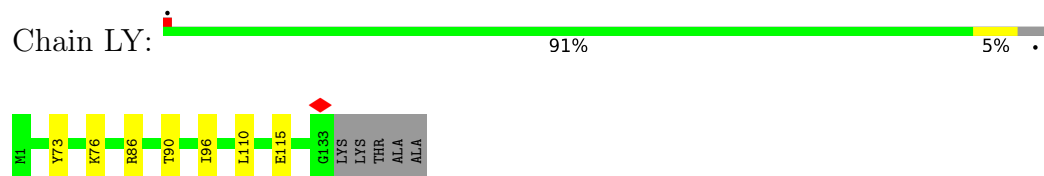
- Molecule 37: 60S ribosomal protein l23-like protein



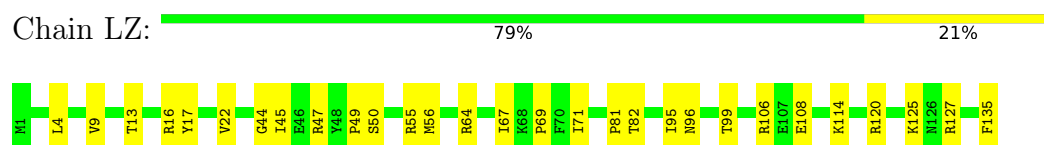
- Molecule 38: 60S ribosomal protein L25-like protein



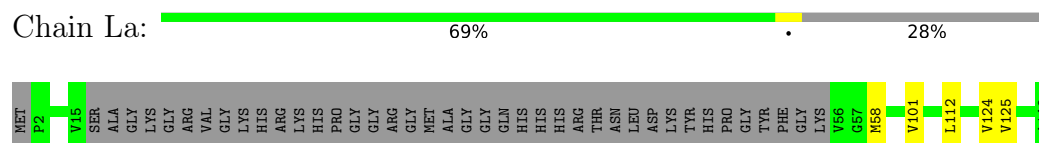
- Molecule 39: 60S ribosomal protein L26-like protein



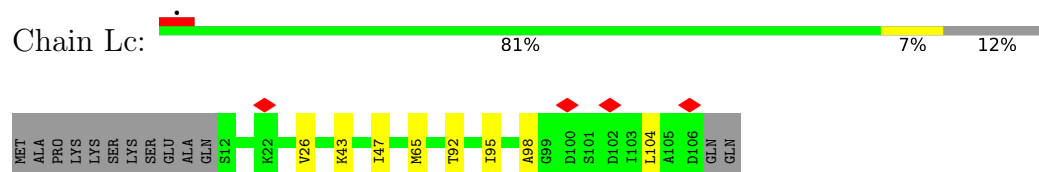
- Molecule 40: 60S ribosomal protein L27



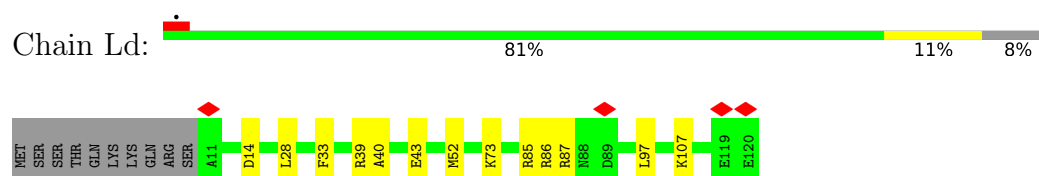
- Molecule 41: 60S ribosomal protein L28-like protein



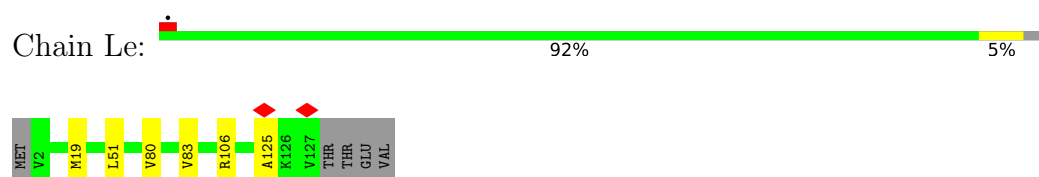
- Molecule 42: 60S ribosomal protein l30-like protein



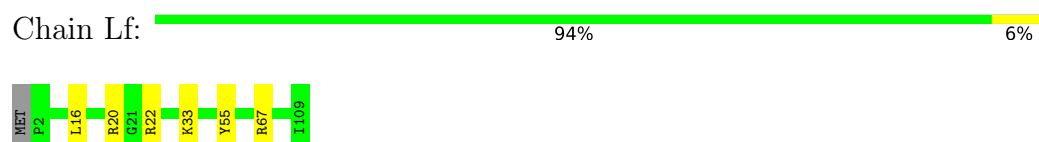
- Molecule 43: Putative 60S ribosomal protein



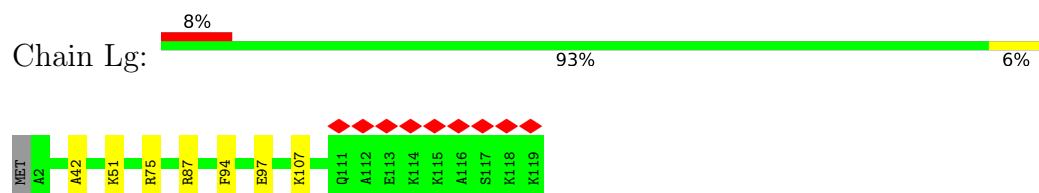
- Molecule 44: 60S ribosomal protein L32-like protein



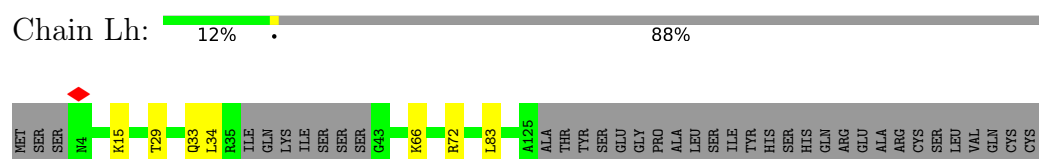
- Molecule 45: 60S ribosomal protein l33-like protein



- Molecule 46: Ribosomal protein l34-like protein

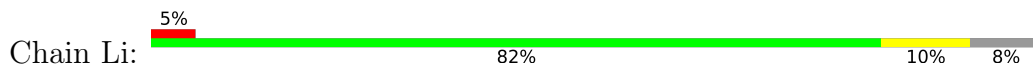


- Molecule 47: dolichyl-diphosphooligosaccharide--protein glycotransferase

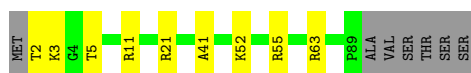
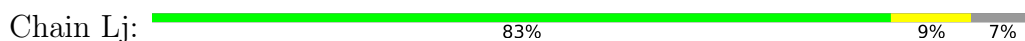


[illegible]

- Molecule 48: 60S ribosomal protein L36

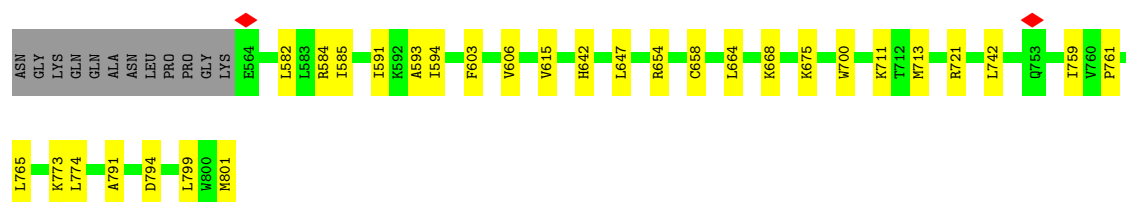


- Molecule 49: Ribosomal protein L37

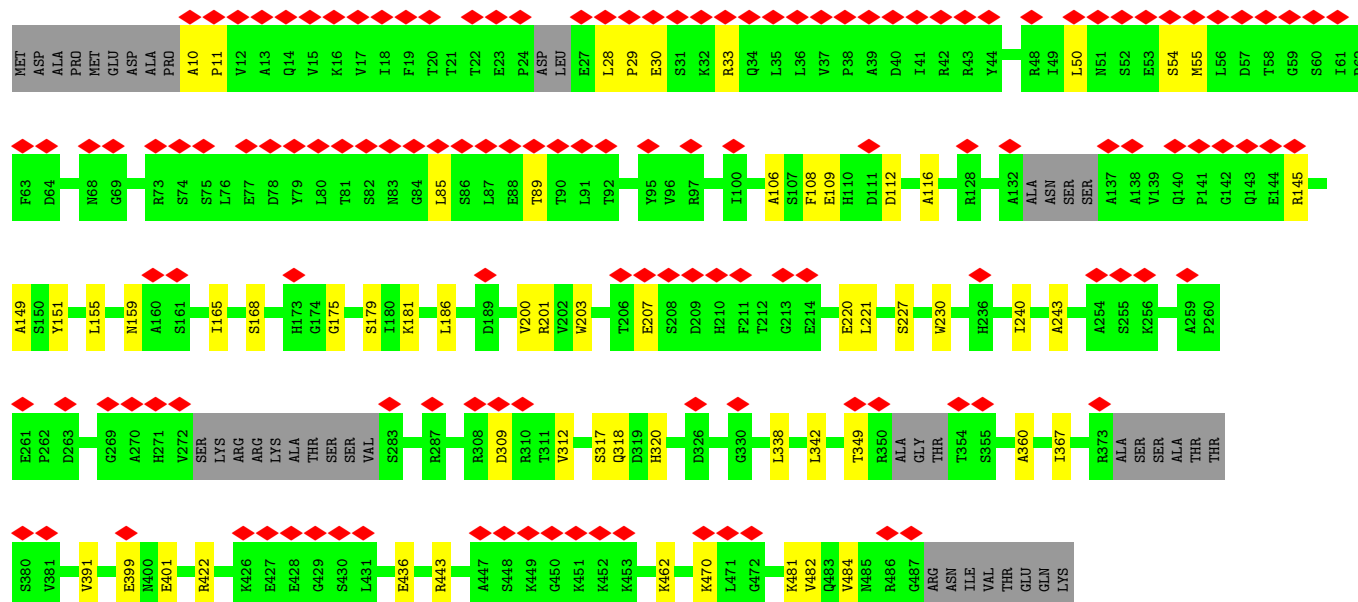
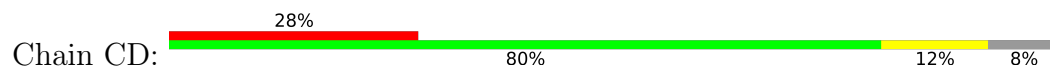


- Molecule 50: 60S ribosomal protein L38-like protein

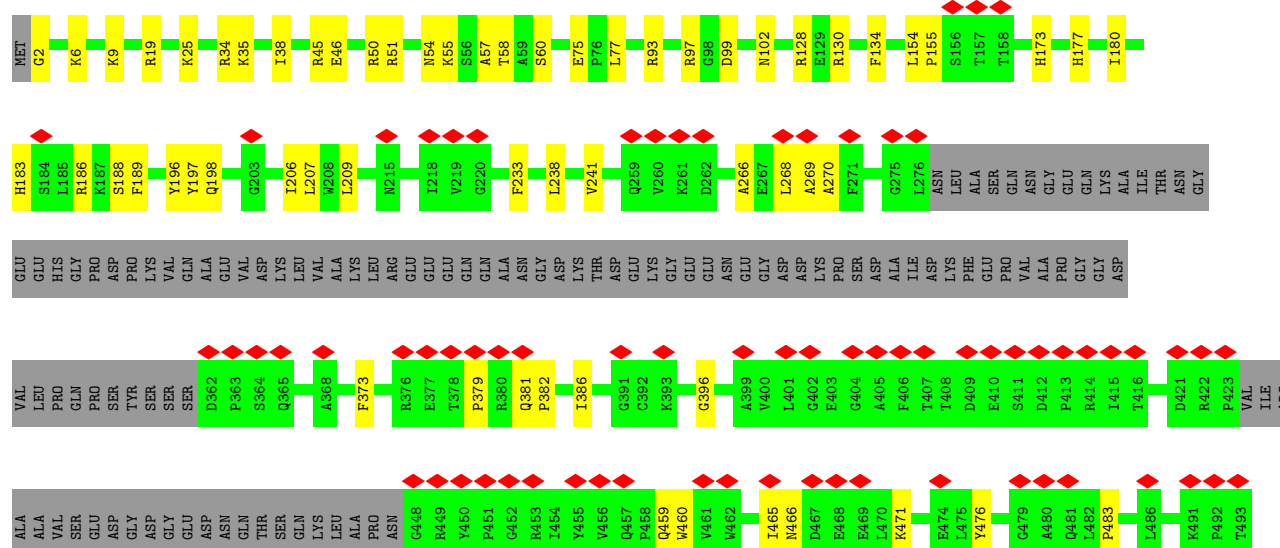


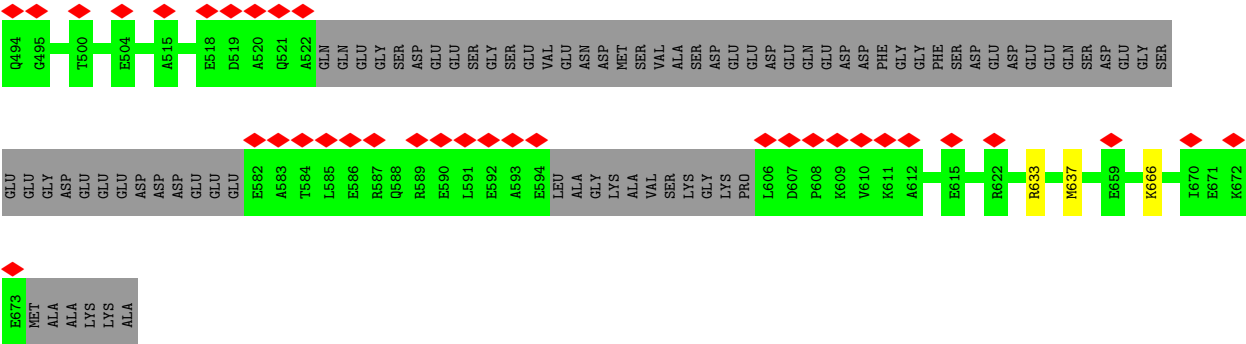


• Molecule 55: Ribosome biogenesis protein YTM1



• Molecule 56: Pescadillo homolog





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	66943	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	45.6	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	8.046	Depositor
Minimum map value	0.000	Depositor
Average map value	0.018	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.7	Depositor
Map size (Å)	522.5, 522.5, 522.5	wwPDB
Map dimensions	500, 500, 500	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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: GTP, OMC, ZN, A2M, MG, OMU, OMG

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	C1	0.26	0/72351	0.35	0/112799
2	C2	0.25	0/3643	0.33	0/5672
3	C4	0.24	0/2833	0.34	0/4414
4	CF	0.19	0/1972	0.39	0/2660
5	CH	0.22	0/5120	0.43	1/6895 (0.0%)
6	CK	0.23	0/1939	0.39	0/2608
7	CL	0.19	0/631	0.37	0/843
8	CN	0.24	0/1878	0.50	0/2555
9	CO	0.23	0/470	0.39	0/619
10	CQ	0.24	0/1504	0.46	0/2000
11	Cb	0.22	0/845	0.49	0/1128
12	Cd	0.22	0/3770	0.41	0/5082
13	Cf	0.23	0/2326	0.41	0/3113
14	Cg	0.20	0/1508	0.37	0/2051
15	Ch	0.26	0/3914	0.50	0/5319
16	Cz	0.18	0/877	0.33	0/1148
17	LA	0.23	0/1488	0.45	0/2009
18	LB	0.25	0/3172	0.46	0/4260
19	LC	0.21	0/2808	0.39	0/3785
20	LD	0.24	0/2308	0.39	0/3105
21	LE	0.20	0/1504	0.43	0/2027
22	CM	0.15	0/692	0.34	0/966
22	LF	0.25	0/2061	0.47	0/2765
23	LG	0.23	0/1918	0.48	0/2565
24	LH	0.22	0/1515	0.42	0/2037
25	LJ	0.20	0/1379	0.44	0/1844
26	LK	0.21	0/1198	0.45	0/1611
27	LL	0.20	0/1614	0.37	0/2168
28	LM	0.24	0/1145	0.39	0/1539
29	LN	0.23	0/1741	0.42	0/2332
30	LO	0.24	0/1645	0.42	0/2205
31	LP	0.24	0/1364	0.44	0/1835

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	LQ	0.20	0/1218	0.41	0/1639
33	LR	0.22	0/1260	0.39	0/1683
34	LS	0.23	0/1461	0.41	0/1966
35	LT	0.20	0/1046	0.47	0/1409
36	LU	0.22	0/859	0.47	0/1151
37	LV	0.22	0/1009	0.39	0/1357
38	LX	0.24	0/983	0.48	0/1327
39	LY	0.20	0/1070	0.47	0/1432
40	LZ	0.26	0/1135	0.52	0/1519
41	La	0.19	0/892	0.34	0/1200
42	Lc	0.22	0/714	0.41	0/960
43	Ld	0.23	0/889	0.41	0/1192
44	Le	0.23	0/1035	0.43	0/1379
45	Lf	0.24	0/883	0.39	0/1187
46	Lg	0.25	0/927	0.44	0/1244
47	Lh	0.20	0/961	0.37	0/1277
48	Li	0.18	0/834	0.42	0/1099
49	Lj	0.26	0/712	0.52	0/944
50	Lk	0.26	0/640	0.58	0/850
51	Ll	0.22	0/446	0.36	0/593
52	Lp	0.25	0/706	0.56	0/940
53	Lq	0.20	0/1091	0.42	0/1468
54	CC	0.22	0/4005	0.51	2/5466 (0.0%)
55	CD	0.18	0/3464	0.49	0/4720
56	CJ	0.21	0/3651	0.47	0/4951
All	All	0.24	0/165024	0.40	3/238912 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
54	CC	375	PRO	CA-C-N	5.65	132.33	121.54
54	CC	375	PRO	C-N-CA	5.65	132.33	121.54
5	CH	617	GLU	N-CA-CB	5.40	118.66	110.28

There are no chirality outliers.

There are no planarity outliers.

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	C1	65414	0	33003	346	0
2	C2	3259	0	1647	18	0
3	C4	2536	0	1286	13	0
4	CF	1934	0	1945	14	0
5	CH	5036	0	5106	36	0
6	CK	1903	0	1990	19	0
7	CL	622	0	641	8	0
8	CN	1853	0	1852	13	0
9	CO	468	0	503	4	0
10	CQ	1480	0	1523	13	0
11	Cb	830	0	838	7	0
12	Cd	3691	0	3817	22	0
13	Cf	2282	0	2347	16	0
14	Cg	1478	0	1517	10	0
15	Ch	3812	0	3715	32	0
16	Cz	869	0	956	6	0
17	LA	1454	0	1490	10	0
18	LB	3104	0	3221	24	0
19	LC	2751	0	2875	18	0
20	LD	2266	0	2219	14	0
21	LE	1477	0	1567	15	0
22	CM	685	0	355	1	0
22	LF	2023	0	2132	12	0
23	LG	1889	0	2043	14	0
24	LH	1495	0	1573	9	0
25	LJ	1357	0	1385	17	0
26	LK	1184	0	1249	5	0
27	LL	1587	0	1655	10	0
28	LM	1126	0	1198	9	0
29	LN	1704	0	1767	13	0
30	LO	1611	0	1702	14	0
31	LP	1343	0	1369	10	0
32	LQ	1200	0	1296	12	0
33	LR	1241	0	1298	11	0
34	LS	1426	0	1481	14	0
35	LT	1027	0	1076	13	0
36	LU	846	0	883	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	LV	991	0	1044	6	0
38	LX	967	0	1041	12	0
39	LY	1056	0	1143	6	0
40	LZ	1112	0	1181	23	0
41	La	872	0	903	3	0
42	Lc	705	0	751	5	0
43	Ld	875	0	918	8	0
44	Le	1017	0	1092	4	0
45	Lf	862	0	891	3	0
46	Lg	914	0	960	6	0
47	Lh	951	0	1057	5	0
48	Li	827	0	906	9	0
49	Lj	698	0	726	8	0
50	Lk	632	0	693	8	0
51	Ll	436	0	473	2	0
52	Lp	698	0	737	4	0
53	Lq	1073	0	1130	8	0
54	CC	3890	0	3803	54	0
55	CD	3390	0	3306	34	0
56	CJ	3577	0	3265	47	0
57	CH	32	0	12	1	0
57	Cd	32	0	12	0	0
58	CH	1	0	0	0	0
58	Cd	2	0	0	0	0
59	CQ	1	0	0	0	0
59	Cb	1	0	0	0	0
59	Lg	1	0	0	0	0
59	Lj	1	0	0	0	0
59	Lp	1	0	0	0	0
60	CH	1	0	0	0	0
60	Cd	2	0	0	0	0
All	All	155881	0	122564	876	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 3.

All (876) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3289:G:H1	1:C1:3298:U:H3	1.23	0.84
54:CC:408:MET:O	54:CC:412:LEU:HB2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2101:A:HO2'	49:Lj:2:THR:N	1.82	0.78
1:C1:1809:G:HO2'	56:CJ:2:GLY:N	1.83	0.77
1:C1:1054:U:H3	1:C1:1070:G:H1	0.86	0.75
1:C1:1431:U:H2'	1:C1:1432:A2M:H8	1.75	0.69
12:Cd:285:ILE:HD11	12:Cd:296:ALA:HB2	1.75	0.68
14:Cg:43:ASP:HB3	14:Cg:46:VAL:HG22	1.75	0.68
12:Cd:364:TRP:HA	12:Cd:377:ASP:O	1.93	0.68
38:LX:88:LYS:O	38:LX:92:GLN:HB2	1.92	0.68
47:Lh:15:LYS:O	47:Lh:66:LYS:NZ	2.27	0.68
23:LG:28:PRO:O	40:LZ:127:ARG:NH2	2.27	0.67
1:C1:949:A:H62	1:C1:1098:G:H8	1.43	0.66
1:C1:2400:G:H1	1:C1:2473:U:H3	1.43	0.66
1:C1:7:A:H5''	56:CJ:93:ARG:HG3	1.78	0.66
54:CC:362:PRO:HD3	54:CC:384:PRO:HB2	1.76	0.66
54:CC:510:THR:O	54:CC:539:SER:OG	2.12	0.66
1:C1:1548:A:OP2	56:CJ:19:ARG:NH2	2.29	0.65
1:C1:3270:U:H5''	18:LB:309:MET:HE2	1.78	0.65
20:LD:85:ALA:HB2	20:LD:258:TYR:HB2	1.78	0.65
54:CC:459:VAL:HG12	54:CC:470:THR:HG22	1.79	0.64
8:CN:109:VAL:HB	8:CN:149:GLY:HA2	1.80	0.64
15:Ch:100:PRO:HG3	15:Ch:106:LEU:HD22	1.79	0.64
1:C1:2899:A:H2'	18:LB:256:TRP:HB3	1.79	0.64
1:C1:1420:OMC:HM22	1:C1:1421:U:H5'	1.78	0.64
15:Ch:384:MET:HB2	15:Ch:400:LEU:HB2	1.80	0.64
1:C1:1459:G:OP2	5:CH:515:ARG:NH1	2.30	0.63
1:C1:1842:U:OP1	33:LR:70:ARG:NH2	2.31	0.63
17:LA:105:SER:HB3	17:LA:160:SER:HB3	1.79	0.63
31:LP:125:GLN:HB3	31:LP:141:SER:HB2	1.81	0.63
1:C1:2788:U:O4	6:CK:52:LYS:NZ	2.31	0.63
25:LJ:162:ARG:O	25:LJ:166:GLN:NE2	2.32	0.63
55:CD:28:LEU:HD12	55:CD:29:PRO:HD2	1.81	0.63
40:LZ:50:SER:HB2	40:LZ:64:ARG:HB3	1.81	0.63
18:LB:331:GLY:HA3	18:LB:337:MET:HE1	1.80	0.63
15:Ch:41:PHE:HD2	15:Ch:69:LEU:HD13	1.63	0.63
56:CJ:51:ARG:NH1	56:CJ:55:LYS:O	2.31	0.63
19:LC:185:VAL:HG11	19:LC:231:GLY:HA3	1.79	0.62
15:Ch:84:ARG:NH1	15:Ch:97:ASP:OD1	2.33	0.62
49:Lj:21:ARG:NH2	49:Lj:41:ALA:O	2.27	0.62
1:C1:984:A:N1	1:C1:1033:U:O2'	2.33	0.62
9:CO:13:ASN:OD1	9:CO:16:ARG:NH2	2.32	0.62
1:C1:1193:U:H5	4:CF:3:LYS:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1619:C:OP2	46:Lg:75:ARG:NH1	2.29	0.62
56:CJ:154:LEU:HD12	56:CJ:155:PRO:HD2	1.81	0.62
1:C1:2380:OMU:HM22	1:C1:2381:G:H3'	1.82	0.61
1:C1:1614:G:N7	40:LZ:16:ARG:NH1	2.49	0.61
5:CH:465:GLU:OE2	10:CQ:102:ARG:NH2	2.34	0.61
10:CQ:145:LEU:HD22	10:CQ:159:LEU:HB3	1.83	0.61
1:C1:64:A:H5''	29:LN:174:LEU:HD13	1.83	0.61
1:C1:1810:G:N7	56:CJ:2:GLY:N	2.49	0.60
1:C1:2405:G:H1	1:C1:2468:U:H3	1.49	0.60
1:C1:1373:A:N6	1:C1:1401:A:O2'	2.34	0.60
2:C2:12:A:OP1	31:LP:3:ARG:NH1	2.35	0.60
1:C1:1795:U:H4'	1:C1:1796:A:H5''	1.83	0.60
54:CC:446:GLN:HG3	54:CC:801:MET:HB2	1.84	0.60
1:C1:2087:G:O2'	12:Cd:448:ARG:NH1	2.34	0.60
1:C1:2586:C:O3'	25:LJ:61:ARG:NH2	2.35	0.60
5:CH:366:ALA:HA	8:CN:167:ILE:HD11	1.84	0.60
15:Ch:264:ILE:HD12	15:Ch:274:HIS:HB2	1.84	0.60
1:C1:2767:A:N6	1:C1:2913:U:O2'	2.35	0.60
5:CH:248:ALA:HB2	5:CH:338:LEU:HD21	1.84	0.60
15:Ch:470:LEU:HB2	15:Ch:484:LEU:HB2	1.82	0.60
1:C1:1067:A:O2'	35:LT:35:ARG:NH2	2.35	0.60
1:C1:1826:C:OP1	1:C1:1829:C:N4	2.34	0.60
13:Cf:31:LEU:HB3	13:Cf:87:MET:HG3	1.82	0.60
54:CC:742:LEU:HB2	54:CC:765:LEU:HB2	1.84	0.60
56:CJ:6:LYS:HB2	56:CJ:9:LYS:HD3	1.84	0.60
1:C1:1553:U:O4	56:CJ:35:LYS:NZ	2.34	0.59
54:CC:700:TRP:HB3	54:CC:711:LYS:HB2	1.84	0.59
39:LY:86:ARG:HB3	39:LY:96:ILE:HD11	1.83	0.59
56:CJ:173:HIS:O	56:CJ:177:HIS:ND1	2.32	0.59
40:LZ:49:PRO:HD3	40:LZ:67:ILE:HG12	1.84	0.59
12:Cd:427:TYR:O	12:Cd:445:LYS:NZ	2.35	0.59
1:C1:2859:A:N7	5:CH:5:LYS:NZ	2.51	0.59
27:LL:115:ARG:NH2	27:LL:155:PHE:O	2.36	0.59
1:C1:948:U:H2'	1:C1:949:A:H8	1.68	0.59
1:C1:2477:U:OP2	1:C1:2545:G:N2	2.35	0.59
54:CC:713:MET:HE1	54:CC:759:ILE:HG21	1.85	0.59
55:CD:54:SER:OG	55:CD:55:MET:SD	2.61	0.59
15:Ch:489:ASP:HB3	15:Ch:508:LYS:HB3	1.84	0.59
54:CC:447:THR:HB	54:CC:799:LEU:HB3	1.84	0.59
6:CK:163:ARG:HH22	12:Cd:228:LYS:HG2	1.69	0.58
15:Ch:195:VAL:HG12	15:Ch:206:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:CH:242:LEU:O	5:CH:280:LYS:NZ	2.36	0.58
36:LU:47:ILE:HD12	36:LU:62:ILE:HD11	1.86	0.58
56:CJ:460:TRP:NE1	56:CJ:471:LYS:O	2.35	0.58
8:CN:106:ASN:ND2	37:LV:135:ALA:O	2.34	0.57
1:C1:69:C:OP2	1:C1:294:G:N2	2.37	0.57
19:LC:36:VAL:HG21	19:LC:251:LEU:HD21	1.86	0.57
2:C2:52:A:OP1	51:Ll:21:ARG:NH1	2.36	0.57
27:LL:140:LYS:HA	27:LL:143:GLN:HG3	1.85	0.57
40:LZ:16:ARG:NH2	40:LZ:17:TYR:OH	2.38	0.57
54:CC:593:ALA:HB3	54:CC:606:VAL:HB	1.85	0.57
1:C1:3204:C:H2'	1:C1:3205:G:H8	1.68	0.57
3:C4:44:C:OP2	25:LJ:138:ARG:NH2	2.38	0.57
40:LZ:9:VAL:O	40:LZ:82:THR:OG1	2.22	0.57
1:C1:1912:A:N1	12:Cd:448:ARG:NH2	2.52	0.57
1:C1:2789:G:H2'	1:C1:2790:G:C8	2.40	0.57
6:CK:165:PRO:HG2	12:Cd:326:GLN:NE2	2.19	0.57
1:C1:2532:C:H5'	40:LZ:56:MET:HA	1.86	0.57
1:C1:2878:A:H61	1:C1:2886:C:H42	1.53	0.57
39:LY:110:LEU:HD11	39:LY:115:GLU:HG3	1.87	0.57
3:C4:88:G:N2	3:C4:91:A:OP2	2.35	0.57
50:Lk:8:ILE:HG22	50:Lk:47:LEU:HD21	1.86	0.57
1:C1:1641:G:H2'	1:C1:1642:G:C8	2.39	0.56
1:C1:1920:G:H21	1:C1:3303:A:H8	1.53	0.56
1:C1:2562:G:HO2'	12:Cd:2:GLY:N	2.03	0.56
18:LB:84:MET:O	18:LB:203:PRO:HA	2.05	0.56
55:CD:200:VAL:HB	55:CD:221:LEU:HB2	1.87	0.56
5:CH:497:GLU:HG3	43:Ld:107:LYS:HD2	1.87	0.56
1:C1:1611:C:OP2	40:LZ:47:ARG:NH2	2.39	0.56
17:LA:80:GLU:HG3	52:Lp:66:GLY:HA2	1.88	0.56
28:LM:54:ARG:HG2	34:LS:70:LEU:HD22	1.86	0.56
1:C1:2708:G:OP2	20:LD:41:LYS:NZ	2.38	0.56
37:LV:32:GLY:HA3	37:LV:68:LYS:HD3	1.88	0.56
56:CJ:386:ILE:HD11	56:CJ:465:ILE:HG12	1.86	0.56
1:C1:243:U:O4	27:LL:132:LYS:NZ	2.36	0.56
1:C1:262:G:H5''	29:LN:14:LYS:HE2	1.87	0.56
3:C4:53:U:O2'	3:C4:55:A:N7	2.39	0.56
8:CN:120:ASP:OD1	11:Cb:30:ARG:NH2	2.38	0.56
24:LH:68:ARG:NH1	24:LH:188:ASN:OD1	2.39	0.56
25:LJ:112:ASP:OD2	25:LJ:112:ASP:N	2.39	0.56
1:C1:346:G:O6	49:Lj:55:ARG:NH2	2.38	0.56
15:Ch:338:ALA:O	15:Ch:360:ARG:NH1	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:LN:177:GLY:O	29:LN:184:ARG:NH1	2.39	0.56
55:CD:159:ASN:HB3	55:CD:165:ILE:HD11	1.86	0.56
1:C1:639:G:O2'	1:C1:1418:A:OP1	2.24	0.56
1:C1:1305:U:O2'	34:LS:1:MET:SD	2.64	0.56
56:CJ:134:PHE:HE1	56:CJ:241:VAL:HG23	1.71	0.56
23:LG:165:LEU:HA	29:LN:7:LEU:HD11	1.86	0.55
7:CL:5:ILE:HD13	30:LO:49:PHE:HB2	1.89	0.55
15:Ch:61:THR:OG1	15:Ch:64:ASN:OD1	2.24	0.55
55:CD:201:ARG:NH2	55:CD:220:GLU:OE2	2.39	0.55
1:C1:2932:G:N7	6:CK:140:LYS:NZ	2.48	0.55
1:C1:1045:A:O2'	35:LT:108:ARG:NH2	2.39	0.55
1:C1:1154:G:OP2	22:LF:223:ARG:NH1	2.39	0.55
1:C1:1559:G:N2	1:C1:1559:G:OP2	2.39	0.55
1:C1:3109:U:H3	1:C1:3338:C:H42	1.55	0.55
6:CK:181:LYS:HE3	6:CK:194:GLN:HG2	1.87	0.55
41:La:112:LEU:HD22	41:La:125:VAL:HG11	1.89	0.55
1:C1:1081:A:OP2	35:LT:130:ARG:NH1	2.40	0.55
8:CN:32:GLU:OE1	8:CN:50:ARG:NH1	2.40	0.55
18:LB:136:LYS:HA	18:LB:139:GLU:HG2	1.89	0.55
5:CH:526:PRO:HB2	5:CH:529:GLN:HG3	1.89	0.55
23:LG:249:GLU:OE1	23:LG:252:ARG:NH2	2.40	0.55
55:CD:85:LEU:HD22	55:CD:89:THR:HG21	1.89	0.55
56:CJ:58:THR:HG22	56:CJ:60:SER:H	1.71	0.55
30:LO:52:LYS:NZ	30:LO:146:GLU:OE1	2.34	0.54
37:LV:64:VAL:O	37:LV:72:ARG:NH1	2.39	0.54
43:Ld:28:LEU:HD11	43:Ld:40:ALA:HB2	1.89	0.54
1:C1:2079:G:OP1	1:C1:2081:C:N4	2.40	0.54
1:C1:2231:U:O4	13:Cf:298:ARG:NH1	2.41	0.54
20:LD:37:ILE:HG13	20:LD:38:THR:HG23	1.89	0.54
54:CC:494:ASN:HB3	54:CC:497:GLU:HB2	1.89	0.54
16:Cz:80:ILE:HG12	16:Cz:84:LYS:HE3	1.89	0.54
21:LE:24:ALA:O	53:Lq:88:ARG:NH1	2.39	0.54
54:CC:606:VAL:HG22	54:CC:615:VAL:HG22	1.88	0.54
53:Lq:9:ILE:HG22	53:Lq:47:VAL:HG22	1.90	0.54
28:LM:54:ARG:NH2	28:LM:76:ALA:O	2.35	0.54
7:CL:73:ARG:HH22	16:Cz:72:LYS:HD2	1.72	0.54
55:CD:108:PHE:HB2	55:CD:482:VAL:HB	1.89	0.54
1:C1:1698:A:H4'	33:LR:117:LYS:HD2	1.90	0.54
1:C1:2591:G:H21	1:C1:2605:C:H41	1.55	0.54
15:Ch:35:GLY:O	15:Ch:56:ASN:ND2	2.40	0.54
1:C1:1559:G:O6	38:LX:46:HIS:NE2	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1737:G:OP1	36:LU:101:ARG:NH2	2.33	0.53
5:CH:86:ASP:OD2	5:CH:89:HIS:ND1	2.39	0.53
39:LY:73:TYR:HE2	39:LY:76:LYS:HG3	1.72	0.53
50:Lk:14:ILE:HA	50:Lk:17:ARG:HD3	1.90	0.53
1:C1:1095:A:H2'	1:C1:1096:G:C8	2.43	0.53
1:C1:1812:OMC:H2'	1:C1:1813:G:H8	1.72	0.53
2:C2:59:A:N7	38:LX:69:ARG:NH2	2.56	0.53
12:Cd:433:LYS:NZ	12:Cd:437:GLU:OE1	2.41	0.53
25:LJ:33:ARG:HD2	25:LJ:121:ILE:HA	1.89	0.53
29:LN:159:ARG:HB3	29:LN:164:LEU:HB2	1.90	0.53
1:C1:1264:U:H2'	1:C1:1265:G:H8	1.74	0.53
10:CQ:179:GLU:OE1	43:Ld:86:ARG:NH1	2.40	0.53
28:LM:97:THR:HG22	28:LM:99:TRP:H	1.73	0.53
36:LU:58:ASP:O	36:LU:61:LYS:NZ	2.41	0.53
1:C1:3000:U:OP2	1:C1:3050:C:N4	2.42	0.53
1:C1:1077:U:O2'	1:C1:1078:U:O2	2.26	0.53
1:C1:2632:A:OP2	25:LJ:95:ARG:NH1	2.42	0.53
1:C1:2769:C:OP2	1:C1:2914:U:O2'	2.25	0.53
25:LJ:87:VAL:HG21	25:LJ:113:LEU:HD23	1.89	0.53
54:CC:761:PRO:O	56:CJ:633:ARG:NH1	2.39	0.53
1:C1:2516:G:N1	46:Lg:97:GLU:OE1	2.35	0.53
1:C1:2892:A:OP2	37:LV:6:ARG:NH1	2.40	0.53
5:CH:183:VAL:HG21	5:CH:219:ASP:HB2	1.90	0.53
15:Ch:83:TYR:HD2	15:Ch:124:ALA:HB1	1.73	0.53
28:LM:59:LEU:O	34:LS:155:ARG:NH2	2.40	0.53
1:C1:1160:G:OP2	30:LO:96:ARG:NH2	2.42	0.53
13:Cf:145:ALA:HB3	13:Cf:188:THR:HG22	1.91	0.53
1:C1:2511:U:OP1	46:Lg:107:LYS:NZ	2.42	0.53
8:CN:4:ARG:NH1	8:CN:210:THR:O	2.41	0.53
54:CC:521:ILE:HD13	54:CC:603:PHE:HE2	1.74	0.53
1:C1:1630:G:H5'	17:LA:70:LYS:HG3	1.90	0.53
1:C1:3008:U:O2'	10:CQ:16:SER:O	2.26	0.53
3:C4:86:C:N4	3:C4:87:G:O6	2.42	0.53
29:LN:145:ASP:HB3	29:LN:148:ILE:HG22	1.91	0.53
40:LZ:96:ASN:H	40:LZ:99:THR:HB	1.74	0.53
1:C1:2362:A:H5'	1:C1:2905:A:H61	1.74	0.53
23:LG:55:TRP:O	23:LG:60:ARG:NH1	2.41	0.53
9:CO:36:LYS:HE2	18:LB:208:THR:HG22	1.90	0.52
54:CC:367:ARG:HH21	54:CC:385:THR:HG22	1.75	0.52
56:CJ:54:ASN:HB3	56:CJ:57:ALA:HB2	1.90	0.52
1:C1:2708:G:O3'	20:LD:39:GLN:NE2	2.35	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:CQ:145:LEU:HD11	10:CQ:163:GLU:HG3	1.91	0.52
30:LO:13:LYS:O	34:LS:169:ARG:NH2	2.36	0.52
40:LZ:13:THR:HB	46:Lg:87:ARG:HG3	1.90	0.52
4:CF:59:GLU:OE1	4:CF:115:TYR:OH	2.26	0.52
5:CH:292:LYS:HE2	5:CH:297:LEU:HD12	1.91	0.52
55:CD:230:TRP:HB3	55:CD:243:ALA:HB3	1.91	0.52
1:C1:259:C:OP1	29:LN:5:LYS:NZ	2.42	0.52
1:C1:643:C:H2'	1:C1:644:A:H8	1.74	0.52
1:C1:877:A:O2'	1:C1:879:U:OP2	2.28	0.52
2:C2:26:U:O2'	19:LC:52:ALA:O	2.26	0.52
19:LC:287:LEU:HD11	32:LQ:60:LEU:HB2	1.92	0.52
1:C1:352:U:OP1	49:Lj:11:ARG:NH2	2.42	0.52
1:C1:976:G:H4'	1:C1:977:U:H5'	1.92	0.52
2:C2:126:A:O2'	2:C2:128:U:OP2	2.26	0.52
5:CH:632:ARG:HB3	5:CH:637:ASP:HB3	1.91	0.52
1:C1:1067:A:H2'	1:C1:1068:A:C8	2.45	0.52
1:C1:1814:U:OP2	51:Ll:10:LYS:NZ	2.42	0.52
1:C1:2842:U:OP1	18:LB:10:ARG:NH1	2.42	0.52
14:Cg:152:ILE:HD13	35:LT:57:TYR:HB2	1.92	0.52
1:C1:1779:A:H2'	1:C1:1780:A:C8	2.45	0.52
1:C1:967:U:H2'	1:C1:968:U:H6	1.74	0.52
1:C1:2064:C:OP2	33:LR:71:ARG:NH1	2.43	0.52
23:LG:125:LYS:HA	23:LG:128:VAL:HG12	1.92	0.52
1:C1:1316:C:OP1	32:LQ:31:GLY:N	2.43	0.51
5:CH:85:TYR:O	5:CH:148:TYR:OH	2.28	0.51
25:LJ:38:LEU:HD13	25:LJ:70:VAL:HG23	1.91	0.51
1:C1:300:A:H2'	1:C1:301:A:C8	2.46	0.51
1:C1:1054:U:O2	1:C1:1070:G:N2	2.37	0.51
1:C1:2516:G:O2'	40:LZ:135:PHE:OXT	2.28	0.51
15:Ch:208:SER:OG	15:Ch:209:MET:N	2.44	0.51
48:Li:99:LEU:HA	48:Li:102:ILE:HG12	1.92	0.51
54:CC:359:GLU:HA	56:CJ:666:LYS:HE2	1.93	0.51
1:C1:643:C:H2'	1:C1:644:A:C8	2.46	0.51
21:LE:139:GLU:HG3	21:LE:152:LYS:HE2	1.93	0.51
1:C1:726:A:OP1	32:LQ:94:ARG:NH1	2.42	0.51
1:C1:1758:G:O2'	1:C1:1760:G:OP2	2.28	0.51
1:C1:2074:G:C6	11:Cb:76:ARG:HD3	2.46	0.51
1:C1:1244:G:O2'	1:C1:1261:A:N1	2.41	0.51
1:C1:1701:U:O2'	1:C1:1703:G:N7	2.42	0.51
7:CL:40:ARG:HG3	7:CL:41:LYS:HD2	1.92	0.51
1:C1:663:C:O2'	1:C1:667:U:OP1	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1626:G:O2'	1:C1:1788:G:N2	2.33	0.51
29:LN:36:ILE:HG12	29:LN:64:VAL:HG23	1.93	0.51
53:Lq:11:GLU:HA	53:Lq:14:ARG:HD2	1.93	0.51
15:Ch:477:THR:HG22	15:Ch:479:LYS:HG3	1.93	0.51
1:C1:2581:C:H5''	14:Cg:177:ILE:HG23	1.92	0.50
1:C1:2860:G:O2'	1:C1:2982:A:N1	2.42	0.50
17:LA:118:GLU:OE2	17:LA:156:LYS:NZ	2.42	0.50
54:CC:432:LEU:HD21	56:CJ:637:MET:HG3	1.93	0.50
56:CJ:373:PHE:HA	56:CJ:396:GLY:O	2.11	0.50
2:C2:58:G:O6	49:Lj:63:ARG:NH1	2.42	0.50
8:CN:210:THR:HG23	8:CN:214:GLU:HG3	1.92	0.50
35:LT:104:ASP:OD1	35:LT:108:ARG:NH1	2.42	0.50
1:C1:2802:U:H3'	16:Cz:76:ARG:HH22	1.76	0.50
55:CD:342:LEU:HD23	55:CD:360:ALA:HB1	1.93	0.50
20:LD:98:ALA:HB1	20:LD:165:VAL:HG23	1.93	0.50
20:LD:214:LEU:HD21	20:LD:221:ARG:HH21	1.77	0.50
1:C1:2838:OMC:H5	1:C1:2906:G:H1	1.60	0.50
1:C1:3026:C:OP2	33:LR:62:ARG:NH2	2.44	0.50
42:Lc:43:LYS:HB3	42:Lc:104:LEU:HD21	1.94	0.50
54:CC:361:LEU:O	56:CJ:666:LYS:NZ	2.38	0.50
55:CD:349:THR:OG1	55:CD:401:GLU:OE2	2.28	0.50
10:CQ:18:GLY:HA3	10:CQ:31:PHE:O	2.11	0.50
42:Lc:98:ALA:HB2	42:Lc:104:LEU:HD13	1.94	0.50
1:C1:967:U:H2'	1:C1:968:U:C6	2.47	0.50
1:C1:3289:G:O6	1:C1:3298:U:O4	2.28	0.50
1:C1:2376:A:H2'	1:C1:2377:G:H8	1.77	0.50
53:Lq:10:TRP:O	53:Lq:14:ARG:HB3	2.12	0.50
55:CD:422:ARG:NH1	55:CD:436:GLU:OE2	2.45	0.50
56:CJ:266:ALA:HB1	56:CJ:269:ALA:HB3	1.94	0.50
11:Cb:15:ARG:NH2	11:Cb:18:ASP:OD2	2.45	0.50
31:LP:52:ILE:HA	31:LP:85:VAL:HG12	1.94	0.50
55:CD:317:SER:OG	55:CD:318:GLN:N	2.43	0.50
1:C1:2632:A:OP1	25:LJ:96:ASN:ND2	2.42	0.49
1:C1:2659:G:O2'	1:C1:2664:A:N1	2.42	0.49
23:LG:84:THR:HG22	23:LG:182:ILE:HG22	1.93	0.49
42:Lc:26:VAL:HG12	42:Lc:95:ILE:HA	1.94	0.49
5:CH:186:VAL:HG23	5:CH:187:THR:HG23	1.93	0.49
24:LH:75:LEU:HD13	24:LH:108:VAL:HG13	1.95	0.49
54:CC:500:ASN:ND2	54:CC:591:ILE:O	2.36	0.49
1:C1:1202:C:O2'	1:C1:1269:A:N1	2.40	0.49
1:C1:2615:A:N6	1:C1:2672:U:O2'	2.44	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:Ch:40:ASN:OD1	15:Ch:48:GLN:NE2	2.37	0.49
40:LZ:120:ARG:HE	40:LZ:125:LYS:HB2	1.78	0.49
1:C1:505:G:O2'	19:LC:343:GLU:OE1	2.29	0.49
1:C1:2197:G:HO2'	12:Cd:2:GLY:N	2.10	0.49
2:C2:103:G:OP2	2:C2:105:A:O2'	2.26	0.49
12:Cd:411:ILE:HG13	12:Cd:439:LEU:HD11	1.94	0.49
33:LR:105:LEU:HD23	33:LR:138:LEU:HD23	1.93	0.49
37:LV:106:ASN:OD1	37:LV:110:GLU:N	2.45	0.49
1:C1:1582:A:N6	38:LX:83:GLU:OE2	2.42	0.49
1:C1:1624:C:OP1	1:C1:1800:C:O2'	2.28	0.49
1:C1:2734:U:H1'	41:La:58:MET:HE1	1.95	0.49
8:CN:107:VAL:HG23	8:CN:108:ILE:HG13	1.95	0.49
55:CD:338:LEU:HD13	55:CD:342:LEU:HD21	1.94	0.49
1:C1:1929:G:OP2	33:LR:135:LYS:NZ	2.33	0.49
6:CK:53:GLN:O	6:CK:57:GLN:HG3	2.13	0.49
6:CK:154:PRO:HG2	6:CK:249:PRO:HB2	1.94	0.49
46:Lg:42:ALA:HB3	46:Lg:51:LYS:HG2	1.95	0.49
54:CC:721:ARG:HH12	54:CC:774:LEU:HD22	1.78	0.49
1:C1:92:G:N2	1:C1:95:G:O2'	2.46	0.49
3:C4:10:C:OP2	13:Cf:59:ARG:NH1	2.46	0.49
10:CQ:83:ARG:O	10:CQ:87:GLN:HG2	2.13	0.49
1:C1:1607:U:O2'	1:C1:1792:G:O6	2.31	0.49
1:C1:3284:G:H21	1:C1:3303:A:H2	1.61	0.49
40:LZ:45:ILE:HG23	40:LZ:67:ILE:HG23	1.94	0.49
56:CJ:197:TYR:O	56:CJ:207:LEU:HA	2.12	0.49
1:C1:2588:U:H3	1:C1:2608:G:H1	1.61	0.48
1:C1:2796:A:O2'	1:C1:2810:A:N6	2.46	0.48
1:C1:3110:A:H4'	1:C1:3234:C:H1'	1.95	0.48
20:LD:214:LEU:HD12	20:LD:226:PHE:HE2	1.78	0.48
30:LO:62:MET:HA	30:LO:72:PRO:HD2	1.94	0.48
1:C1:3002:A:H4'	18:LB:13:SER:HB2	1.95	0.48
18:LB:313:VAL:HG23	18:LB:365:GLU:HG3	1.95	0.48
27:LL:189:ARG:HB2	48:Li:18:ARG:HD3	1.95	0.48
1:C1:338:G:O2'	2:C2:25:G:N3	2.46	0.48
1:C1:448:C:H41	21:LE:15:ARG:HH21	1.59	0.48
1:C1:1766:G:H2'	1:C1:1767:A:C8	2.48	0.48
1:C1:2320:A:H2'	1:C1:2321:A:H8	1.78	0.48
54:CC:327:TRP:HB3	54:CC:330:GLU:HG3	1.95	0.48
54:CC:462:ASP:OD2	54:CC:464:THR:OG1	2.27	0.48
22:CM:102:PRO:HB2	22:CM:105:PRO:HD2	1.95	0.48
20:LD:208:ALA:HB2	20:LD:239:LEU:HD12	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:LE:199:LYS:O	28:LM:117:ARG:NH2	2.45	0.48
54:CC:358:PRO:HA	54:CC:361:LEU:HD23	1.95	0.48
1:C1:1548:A:N7	56:CJ:19:ARG:NH1	2.61	0.48
1:C1:1816:C:O2'	1:C1:1822:A:N1	2.42	0.48
1:C1:2320:A:H2'	1:C1:2321:A:C8	2.49	0.48
13:Cf:113:MET:HB2	13:Cf:261:ARG:HB3	1.95	0.48
15:Ch:465:SER:OG	15:Ch:466:LYS:N	2.44	0.48
18:LB:219:ILE:HG12	18:LB:277:THR:HG23	1.94	0.48
19:LC:30:PRO:HD2	19:LC:278:PRO:HG2	1.96	0.48
20:LD:214:LEU:HB3	20:LD:222:TYR:HB2	1.95	0.48
21:LE:131:GLU:HA	21:LE:134:LYS:HE2	1.95	0.48
28:LM:23:GLU:OE2	34:LS:158:LYS:NZ	2.44	0.48
34:LS:12:ARG:HB3	34:LS:24:LEU:HD23	1.94	0.48
1:C1:230:G:H2'	1:C1:231:A:C8	2.49	0.48
1:C1:2729:G:H2'	1:C1:2732:C:H5	1.79	0.48
21:LE:61:LEU:HD11	21:LE:103:ILE:HG13	1.94	0.48
40:LZ:69:PRO:HG3	40:LZ:114:LYS:HB2	1.95	0.48
1:C1:736:G:H2'	1:C1:737:A:H8	1.77	0.48
2:C2:133:C:H2'	2:C2:134:G:H8	1.79	0.48
5:CH:250:LEU:HD11	5:CH:334:VAL:HG11	1.95	0.48
5:CH:440:ILE:HG13	10:CQ:1:MET:HE2	1.95	0.48
54:CC:529:PRO:HB2	55:CD:227:SER:HB3	1.95	0.48
29:LN:75:VAL:HG11	29:LN:80:THR:HG22	1.95	0.48
40:LZ:95:ILE:HG22	40:LZ:99:THR:HG21	1.95	0.48
44:Le:80:VAL:HA	44:Le:83:VAL:HG12	1.96	0.48
56:CJ:75:GLU:HG3	56:CJ:77:LEU:H	1.79	0.48
56:CJ:459:GLN:NE2	56:CJ:483:PRO:O	2.46	0.48
1:C1:3179:G:H2'	1:C1:3180:G:H8	1.79	0.48
34:LS:109:ASP:OD1	34:LS:113:ARG:NH1	2.47	0.48
1:C1:382:A:H5''	31:LP:16:ARG:HG3	1.96	0.47
1:C1:979:A:N6	1:C1:1033:U:O4	2.47	0.47
27:LL:17:HIS:HB3	27:LL:20:ARG:HD3	1.95	0.47
31:LP:122:ALA:HB3	31:LP:143:PRO:HG2	1.96	0.47
15:Ch:421:SER:O	15:Ch:428:THR:HA	2.14	0.47
23:LG:159:ASP:OD1	23:LG:159:ASP:N	2.44	0.47
1:C1:3179:G:H2'	1:C1:3180:G:C8	2.50	0.47
15:Ch:136:SER:OG	15:Ch:517:ASN:OXT	2.31	0.47
25:LJ:22:ILE:HG12	25:LJ:126:MET:HG2	1.95	0.47
43:Ld:39:ARG:O	43:Ld:43:GLU:HG2	2.14	0.47
55:CD:106:ALA:HB3	55:CD:484:VAL:HB	1.96	0.47
1:C1:278:A:H8	1:C1:297:G:H1'	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:300:A:H2'	1:C1:301:A:H8	1.78	0.47
10:CQ:16:SER:HB3	18:LB:73:VAL:HG11	1.96	0.47
18:LB:90:VAL:HG22	18:LB:104:THR:HG23	1.96	0.47
32:LQ:94:ARG:O	32:LQ:98:ASN:ND2	2.45	0.47
56:CJ:128:ARG:HD2	56:CJ:128:ARG:HA	1.68	0.47
6:CK:241:ARG:NH1	12:Cd:79:ASN:OD1	2.46	0.47
40:LZ:108:GLU:HG3	54:CC:773:LYS:HE3	1.97	0.47
55:CD:30:GLU:HA	55:CD:33:ARG:HE	1.79	0.47
1:C1:684:C:H2'	1:C1:685:G:C8	2.49	0.47
1:C1:2576:U:H1'	1:C1:2577:G:H5'	1.96	0.47
15:Ch:378:ALA:HA	15:Ch:384:MET:HG2	1.97	0.47
1:C1:20:U:H2'	1:C1:21:A:C8	2.50	0.47
1:C1:36:A:H2'	1:C1:37:C:H6	1.80	0.47
1:C1:1077:U:H5	35:LT:120:LYS:HA	1.80	0.47
1:C1:1879:G:O2'	1:C1:2297:U:O4	2.28	0.47
8:CN:233:ILE:HA	8:CN:237:MET:HB2	1.95	0.47
54:CC:711:LYS:HG3	54:CC:759:ILE:HD13	1.96	0.47
1:C1:21:A:H2'	1:C1:22:G:C8	2.50	0.47
1:C1:2479:U:O2'	1:C1:2554:A:N1	2.47	0.47
1:C1:2523:G:H2'	1:C1:2524:G:H8	1.78	0.47
4:CF:64:ARG:NH1	4:CF:65:ILE:O	2.47	0.47
19:LC:290:LEU:HD21	32:LQ:152:ASP:HB2	1.97	0.47
21:LE:87:PHE:HB3	21:LE:162:GLN:NE2	2.30	0.47
26:LK:16:ARG:HB3	26:LK:57:ARG:HD2	1.96	0.47
55:CD:309:ASP:HB3	55:CD:312:VAL:HG12	1.97	0.47
1:C1:1045:A:N3	35:LT:130:ARG:NH2	2.62	0.47
1:C1:1159:C:H4'	30:LO:91:PRO:HD3	1.96	0.47
2:C2:9:A:H2'	2:C2:10:A:C8	2.50	0.47
25:LJ:94:ARG:O	25:LJ:157:ARG:NH2	2.47	0.47
1:C1:958:G:OP2	32:LQ:78:ARG:NH2	2.47	0.47
1:C1:2518:G:C6	17:LA:64:ARG:HD2	2.50	0.47
32:LQ:126:MET:O	32:LQ:146:GLY:HA3	2.15	0.47
54:CC:459:VAL:HG13	54:CC:791:ALA:HB2	1.97	0.47
1:C1:604:G:H2'	1:C1:605:G:C8	2.50	0.46
8:CN:4:ARG:HB3	8:CN:208:LEU:HA	1.97	0.46
56:CJ:460:TRP:HB2	56:CJ:476:TYR:CG	2.50	0.46
1:C1:2164:G:H21	1:C1:2205:A:H62	1.63	0.46
5:CH:595:ARG:HB2	38:LX:83:GLU:OE1	2.15	0.46
21:LE:98:ASN:HB3	21:LE:101:TYR:HD1	1.80	0.46
23:LG:119:ILE:HG13	54:CC:291:ILE:HG21	1.98	0.46
40:LZ:108:GLU:HG3	54:CC:773:LYS:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C2:38:U:H5'	47:Lh:83:LEU:HD13	1.97	0.46
21:LE:55:GLY:O	21:LE:109:VAL:N	2.44	0.46
55:CD:109:GLU:OE1	55:CD:481:LYS:NZ	2.38	0.46
1:C1:333:C:OP2	19:LC:199:ARG:NH1	2.36	0.46
1:C1:357:G:OP2	49:Lj:52:LYS:NZ	2.38	0.46
1:C1:586:G:H1	1:C1:597:G:H5''	1.80	0.46
33:LR:98:ARG:NH1	33:LR:130:ASN:OD1	2.46	0.46
40:LZ:71:ILE:HD11	40:LZ:106:ARG:HB2	1.97	0.46
1:C1:619:A:H2'	1:C1:620:G:C8	2.51	0.46
1:C1:2368:C:H4'	6:CK:142:THR:HG21	1.98	0.46
1:C1:2925:G:H2'	1:C1:2926:A:C8	2.50	0.46
2:C2:75:G:OP2	39:LY:73:TYR:OH	2.24	0.46
22:LF:182:TYR:CZ	22:LF:203:GLN:HG2	2.51	0.46
28:LM:112:LEU:HD22	28:LM:116:ASP:HB3	1.97	0.46
1:C1:203:A:N3	19:LC:228:ASN:ND2	2.57	0.46
1:C1:277:A:N1	1:C1:2744:A:O2'	2.49	0.46
1:C1:716:G:H5''	32:LQ:71:PRO:HB2	1.97	0.46
6:CK:87:PRO:HD2	6:CK:90:LEU:HD12	1.96	0.46
13:Cf:34:ARG:HB3	13:Cf:46:MET:HE1	1.97	0.46
13:Cf:105:MET:HA	13:Cf:111:LEU:H	1.81	0.46
28:LM:38:ARG:NH2	34:LS:96:GLU:OE1	2.38	0.46
31:LP:40:LYS:HD3	31:LP:113:ILE:HG22	1.96	0.46
56:CJ:238:LEU:HA	56:CJ:241:VAL:HG12	1.98	0.46
10:CQ:43:LYS:NZ	11:Cb:18:ASP:OD1	2.37	0.46
30:LO:11:ASP:HB2	30:LO:119:LYS:HB3	1.98	0.46
35:LT:155:ALA:O	35:LT:158:THR:OG1	2.30	0.46
48:Li:43:SER:HB3	48:Li:46:THR:HG22	1.97	0.46
56:CJ:188:SER:O	56:CJ:466:ASN:ND2	2.34	0.46
1:C1:464:C:H2'	1:C1:465:G:H8	1.80	0.46
1:C1:2683:OMU:HM23	1:C1:2683:OMU:H1'	1.72	0.46
6:CK:174:PRO:HG2	6:CK:177:LEU:HD12	1.98	0.46
20:LD:116:ASP:OD1	20:LD:116:ASP:N	2.40	0.46
1:C1:630:U:H2'	1:C1:631:U:C2	2.51	0.46
1:C1:652:A:H2'	1:C1:653:A:C8	2.51	0.46
1:C1:2092:U:H2'	1:C1:2093:G:C8	2.51	0.46
1:C1:2478:A:N1	1:C1:2553:C:N4	2.60	0.46
1:C1:3288:A:H2'	1:C1:3289:G:H8	1.81	0.46
5:CH:544:ILE:O	5:CH:549:ARG:NH1	2.44	0.46
15:Ch:84:ARG:HB2	15:Ch:127:GLN:OE1	2.16	0.46
54:CC:484:THR:O	55:CD:462:LYS:NZ	2.48	0.46
56:CJ:381:GLN:HG2	56:CJ:382:PRO:HD3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2147:U:OP1	17:LA:209:HIS:NE2	2.37	0.46
1:C1:2327:G:H22	1:C1:2359:G:H1'	1.81	0.46
50:Lk:26:LYS:NZ	50:Lk:28:ASN:OD1	2.41	0.46
1:C1:696:G:N2	1:C1:699:A:OP2	2.45	0.45
1:C1:1177:G:H2'	1:C1:1178:A:C8	2.51	0.45
1:C1:1915:G:OP1	12:Cd:452:GLY:N	2.36	0.45
4:CF:14:GLN:O	6:CK:71:ARG:NH2	2.49	0.45
14:Cg:36:VAL:HG13	14:Cg:54:VAL:HG21	1.98	0.45
22:LF:184:ILE:HG23	22:LF:189:ASP:HB3	1.98	0.45
1:C1:1041:U:OP2	22:LF:104:LYS:NZ	2.50	0.45
1:C1:1214:A:H5''	1:C1:1215:C:H5'	1.98	0.45
1:C1:1785:C:H2'	1:C1:1786:G:H8	1.81	0.45
54:CC:411:TYR:HE2	56:CJ:34:ARG:HD2	1.80	0.45
1:C1:2383:C:H2'	1:C1:2384:OMU:H6	1.98	0.45
4:CF:148:GLU:HG3	4:CF:214:ILE:HG12	1.98	0.45
4:CF:183:ASP:OD1	4:CF:184:GLU:N	2.49	0.45
4:CF:227:TRP:HB2	4:CF:234:VAL:HG22	1.98	0.45
12:Cd:358:PRO:HD2	12:Cd:400:ARG:HG2	1.98	0.45
19:LC:303:PRO:O	22:LF:32:ARG:NH1	2.49	0.45
56:CJ:189:PHE:HB3	56:CJ:196:TYR:HB2	1.98	0.45
1:C1:364:G:O2'	1:C1:389:A2M:N6	2.47	0.45
1:C1:2123:G:H2'	1:C1:2124:G:H8	1.82	0.45
1:C1:2169:G:H2'	1:C1:2170:A:C8	2.51	0.45
1:C1:2330:A:H2'	1:C1:2331:A:C8	2.51	0.45
1:C1:3204:C:H2'	1:C1:3205:G:C8	2.51	0.45
14:Cg:168:SER:O	14:Cg:175:ARG:NH2	2.49	0.45
19:LC:353:LYS:O	22:LF:77:GLN:NE2	2.38	0.45
20:LD:207:VAL:O	20:LD:211:MET:HG3	2.17	0.45
41:La:101:VAL:HG22	41:La:124:VAL:HB	1.99	0.45
1:C1:842:G:H8	17:LA:183:SER:HB3	1.82	0.45
9:CO:106:ILE:HG23	9:CO:107:VAL:HG13	1.98	0.45
1:C1:2633:A:H5''	25:LJ:106:GLY:HA3	1.99	0.45
1:C1:2974:A:H2'	1:C1:2975:G:H8	1.82	0.45
1:C1:3120:C:H2'	1:C1:3121:G:H8	1.82	0.45
1:C1:3184:C:O2	9:CO:93:ARG:NH2	2.38	0.45
5:CH:587:LEU:HD22	38:LX:146:LEU:HD13	1.98	0.45
15:Ch:379:SER:OG	15:Ch:380:ASP:N	2.49	0.45
18:LB:10:ARG:NH2	18:LB:264:THR:O	2.50	0.45
29:LN:5:LYS:HG3	48:Li:49:VAL:HG11	1.97	0.45
29:LN:14:LYS:HA	29:LN:19:VAL:HG11	1.99	0.45
33:LR:105:LEU:HD22	33:LR:135:LYS:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
56:CJ:50:ARG:NH1	56:CJ:58:THR:O	2.50	0.45
1:C1:980:A:H2'	1:C1:981:G:C8	2.51	0.45
1:C1:1811:U:O2'	2:C2:114:G:OP1	2.29	0.45
1:C1:2181:G:H2'	1:C1:2182:A:H8	1.82	0.45
1:C1:2225:A:H2'	1:C1:2226:C:C6	2.51	0.45
1:C1:2706:A:H2'	1:C1:2707:A:C8	2.52	0.45
15:Ch:242:PRO:HB3	15:Ch:335:LEU:HD22	1.98	0.45
18:LB:190:ALA:O	18:LB:194:GLU:HG2	2.17	0.45
43:Ld:14:ASP:HB3	43:Ld:97:LEU:HD21	1.98	0.45
54:CC:486:ARG:NH2	55:CD:112:ASP:OD2	2.50	0.45
54:CC:487:GLN:OE1	54:CC:490:SER:OG	2.31	0.45
54:CC:496:ASP:OD1	54:CC:496:ASP:N	2.45	0.45
54:CC:721:ARG:HA	54:CC:721:ARG:HD2	1.71	0.45
1:C1:70:C:O2'	1:C1:102:G:O2'	2.27	0.45
2:C2:97:A:OP1	47:Lh:72:ARG:NH2	2.46	0.45
38:LX:109:LYS:HE3	38:LX:109:LYS:HB2	1.79	0.45
54:CC:531:VAL:HA	54:CC:535:LEU:HD23	1.98	0.45
1:C1:2400:G:O6	1:C1:2473:U:O4	2.35	0.45
21:LE:16:THR:HG23	22:LF:4:THR:HA	1.98	0.45
50:Lk:25:ILE:HG13	50:Lk:68:ILE:HD11	1.99	0.45
52:Lp:32:THR:O	52:Lp:37:TYR:OH	2.29	0.45
54:CC:521:ILE:O	54:CC:584:ARG:HA	2.17	0.45
1:C1:224:U:H2'	1:C1:225:A:C8	2.52	0.44
1:C1:404:U:H2'	1:C1:405:G:H8	1.81	0.44
1:C1:1809:G:O2'	56:CJ:2:GLY:N	2.45	0.44
4:CF:43:PHE:HB3	4:CF:223:LEU:HD23	1.99	0.44
40:LZ:82:THR:HG22	46:Lg:94:PHE:CE1	2.52	0.44
47:Lh:29:THR:O	47:Lh:33:GLN:HG2	2.18	0.44
54:CC:338:MET:O	56:CJ:45:ARG:NH1	2.38	0.44
56:CJ:177:HIS:NE2	56:CJ:268:LEU:O	2.50	0.44
56:CJ:266:ALA:HB3	56:CJ:270:ALA:HB2	1.99	0.44
1:C1:1264:U:H2'	1:C1:1265:G:C8	2.51	0.44
5:CH:429:ASN:ND2	5:CH:431:GLU:OE2	2.50	0.44
22:LF:92:VAL:O	22:LF:120:GLY:HA2	2.17	0.44
32:LQ:149:LEU:HD23	32:LQ:153:GLN:HB3	1.98	0.44
45:Lf:20:ARG:NH2	45:Lf:22:ARG:O	2.48	0.44
56:CJ:379:PRO:HB2	56:CJ:382:PRO:HD2	1.98	0.44
1:C1:2221:U:H2'	1:C1:2222:A:H8	1.83	0.44
1:C1:2615:A:H2'	1:C1:2616:A:C8	2.52	0.44
5:CH:19:ILE:HG21	5:CH:59:LYS:HE2	1.99	0.44
27:LL:52:ASP:OD2	27:LL:52:ASP:N	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1476:G:OP2	1:C1:1476:G:N2	2.46	0.44
1:C1:1596:U:H2'	1:C1:1597:G:C8	2.53	0.44
1:C1:2218:A:N6	1:C1:2226:C:O2	2.51	0.44
34:LS:138:PRO:HA	34:LS:141:LYS:HB2	2.00	0.44
54:CC:516:ALA:HB2	54:CC:594:ILE:HD11	1.99	0.44
56:CJ:177:HIS:HA	56:CJ:180:ILE:HG12	2.00	0.44
1:C1:669:U:O4	19:LC:119:LYS:NZ	2.42	0.44
24:LH:7:GLU:HA	24:LH:92:LEU:O	2.17	0.44
1:C1:768:A:H4'	1:C1:769:G:H5'	1.99	0.44
1:C1:2958:G:H2'	1:C1:2959:U:C6	2.53	0.44
4:CF:100:VAL:HG12	4:CF:243:ARG:HH12	1.83	0.44
13:Cf:23:ILE:HD13	14:Cg:97:PRO:HD2	2.00	0.44
15:Ch:148:PRO:HB3	15:Ch:508:LYS:HA	1.99	0.44
54:CC:375:PRO:O	54:CC:376:GLU:HG3	2.18	0.44
1:C1:390:A:H4'	1:C1:391:U:H3'	2.00	0.44
1:C1:788:A:N3	1:C1:2771:C:O2'	2.47	0.44
1:C1:813:G:O2'	1:C1:1844:A:N3	2.44	0.44
1:C1:1576:C:H2'	1:C1:1577:C:C6	2.53	0.44
1:C1:2113:G:O2'	1:C1:2152:U:OP1	2.32	0.44
1:C1:2384:OMU:HM23	1:C1:2384:OMU:H1'	1.69	0.44
1:C1:2919:C:H2'	1:C1:2920:G:H8	1.83	0.44
1:C1:3249:C:O2'	31:LP:69:ARG:O	2.26	0.44
24:LH:154:ARG:HG2	24:LH:162:VAL:HG22	2.00	0.44
1:C1:282:U:H2'	1:C1:283:G:H8	1.83	0.44
1:C1:1054:U:O4	1:C1:1070:G:O6	2.36	0.44
1:C1:1211:A:H5''	4:CF:203:SER:HB3	1.98	0.44
6:CK:2:PRO:HB2	6:CK:6:TYR:CG	2.53	0.44
48:Li:64:ARG:HA	48:Li:67:ILE:HG22	1.99	0.44
53:Lq:31:ASP:HB3	53:Lq:34:ASN:HB2	1.99	0.44
55:CD:443:ARG:HA	55:CD:443:ARG:HD2	1.83	0.44
1:C1:405:G:OP1	31:LP:62:ARG:NH1	2.51	0.44
13:Cf:249:HIS:ND1	13:Cf:250:GLY:O	2.51	0.44
19:LC:352:PRO:HB2	22:LF:77:GLN:NE2	2.33	0.44
42:Lc:47:ILE:HA	42:Lc:92:THR:HG22	2.00	0.44
1:C1:2069:A:H2'	1:C1:2070:A:C8	2.53	0.43
1:C1:2376:A:H2'	1:C1:2377:G:C8	2.53	0.43
5:CH:341:GLU:OE2	5:CH:345:GLN:NE2	2.46	0.43
15:Ch:502:LEU:HD22	15:Ch:514:THR:HG22	2.00	0.43
18:LB:242:LYS:HD2	18:LB:242:LYS:HA	1.83	0.43
33:LR:44:LEU:HD22	33:LR:49:LEU:HD22	2.00	0.43
1:C1:2103:U:OP2	5:CH:657:LYS:NZ	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C4:23:A:N3	3:C4:119:U:O2'	2.43	0.43
45:Lf:16:LEU:HD11	45:Lf:33:LYS:HB2	2.00	0.43
52:Lp:85:ARG:HG3	52:Lp:86:LEU:HD12	2.00	0.43
56:CJ:46:GLU:OE1	56:CJ:50:ARG:NH2	2.45	0.43
1:C1:230:G:H2'	1:C1:231:A:H8	1.84	0.43
1:C1:970:U:H2'	1:C1:971:A:C8	2.53	0.43
1:C1:1100:G:H2'	1:C1:1101:C:C6	2.53	0.43
1:C1:3079:U:H1'	1:C1:3080:A:H5''	2.00	0.43
5:CH:361:LEU:HA	5:CH:364:VAL:HG12	2.00	0.43
18:LB:92:TYR:HB2	18:LB:158:VAL:HB	2.00	0.43
19:LC:236:PRO:HG2	19:LC:239:ALA:HB3	2.00	0.43
54:CC:492:LYS:HE2	54:CC:495:GLY:HA2	2.00	0.43
1:C1:213:A:HO2'	1:C1:214:G:H21	1.61	0.43
1:C1:1395:G:H5''	44:Le:125:ALA:HB2	2.01	0.43
1:C1:2956:U:H2'	1:C1:2957:C:C6	2.53	0.43
1:C1:2971:U:H2'	1:C1:2972:U:C6	2.53	0.43
3:C4:6:C:O3'	20:LD:50:ARG:NH2	2.48	0.43
7:CL:52:ASP:OD2	34:LS:80:ARG:NH1	2.51	0.43
14:Cg:150:ASP:O	14:Cg:170:ARG:NH1	2.40	0.43
16:Cz:72:LYS:HE2	16:Cz:72:LYS:HB3	1.87	0.43
18:LB:123:TYR:CZ	18:LB:124:LYS:HG3	2.53	0.43
38:LX:90:GLU:OE2	38:LX:90:GLU:N	2.51	0.43
56:CJ:198:GLN:HA	56:CJ:206:ILE:O	2.18	0.43
1:C1:767:G:OP2	32:LQ:91:SER:OG	2.22	0.43
1:C1:1046:G:C6	35:LT:109:VAL:HG22	2.54	0.43
1:C1:1584:U:H2'	1:C1:1585:A:O4'	2.18	0.43
1:C1:3152:C:O2'	1:C1:3154:U:OP1	2.34	0.43
13:Cf:98:HIS:CD2	13:Cf:120:PRO:HG3	2.53	0.43
47:Lh:34:LEU:HD23	47:Lh:34:LEU:HA	1.89	0.43
1:C1:464:C:H2'	1:C1:465:G:C8	2.54	0.43
1:C1:644:A:H2'	1:C1:645:A:C8	2.54	0.43
15:Ch:88:HIS:HB2	15:Ch:121:THR:HB	1.99	0.43
15:Ch:362:GLU:O	15:Ch:366:LYS:HG3	2.18	0.43
1:C1:231:A:H2'	1:C1:232:A:C8	2.54	0.43
1:C1:1931:U:H2'	1:C1:1932:G:C8	2.54	0.43
1:C1:2224:G:H3'	1:C1:2225:A:H8	1.84	0.43
1:C1:2986:G:H2'	1:C1:2987:A:C8	2.53	0.43
21:LE:163:LYS:O	21:LE:167:LYS:HG2	2.19	0.43
23:LG:186:LYS:HB2	23:LG:197:THR:HG23	2.00	0.43
1:C1:804:G:H2'	1:C1:805:C:C6	2.54	0.43
1:C1:1595:C:H2'	1:C1:1596:U:C6	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:2157:G:C6	12:Cd:311:ILE:HG21	2.54	0.43
7:CL:69:ILE:HG21	35:LT:160:ILE:HG21	2.00	0.43
15:Ch:41:PHE:CD2	15:Ch:69:LEU:HD13	2.50	0.43
23:LG:195:LYS:O	56:CJ:97:ARG:NH2	2.50	0.43
1:C1:1511:G:O2'	1:C1:1568:A:N3	2.44	0.43
1:C1:1894:G:O2'	33:LR:82:LYS:O	2.30	0.43
1:C1:2112:A:N6	1:C1:2150:G:O2'	2.44	0.43
1:C1:2974:A:H2'	1:C1:2975:G:C8	2.53	0.43
16:Cz:77:GLN:HA	16:Cz:80:ILE:HG22	2.01	0.43
1:C1:1186:A:H62	1:C1:1283:G:H21	1.66	0.43
1:C1:1676:A:H2'	1:C1:1677:A:C8	2.54	0.43
3:C4:93:G:H2'	3:C4:94:A:C8	2.53	0.43
25:LJ:162:ARG:HG2	25:LJ:166:GLN:NE2	2.34	0.43
1:C1:948:U:H2'	1:C1:949:A:C8	2.52	0.42
1:C1:1698:A:H2'	1:C1:1699:G:C8	2.54	0.42
1:C1:2751:A:H2'	1:C1:2752:G:H8	1.84	0.42
1:C1:2790:G:H2'	1:C1:2791:C:C6	2.54	0.42
1:C1:2839:U:H1'	18:LB:251:ALA:HB3	2.01	0.42
6:CK:132:MET:HE1	6:CK:214:VAL:HG11	2.01	0.42
12:Cd:235:VAL:O	12:Cd:329:VAL:HA	2.19	0.42
18:LB:161:VAL:HG13	18:LB:184:ILE:HD11	2.01	0.42
26:LK:159:GLU:N	26:LK:159:GLU:OE2	2.51	0.42
48:Li:102:ILE:HA	48:Li:105:GLU:HG3	2.00	0.42
54:CC:658:CYS:HB3	54:CC:668:LYS:HB3	2.00	0.42
1:C1:410:A:H2'	1:C1:411:A:C8	2.54	0.42
5:CH:140:LYS:HE3	5:CH:140:LYS:HB2	1.87	0.42
20:LD:93:THR:O	20:LD:161:ARG:NH1	2.47	0.42
35:LT:145:ASP:OD1	35:LT:145:ASP:N	2.52	0.42
55:CD:50:LEU:HA	55:CD:50:LEU:HD23	1.74	0.42
55:CD:155:LEU:HB2	55:CD:168:SER:HB3	2.01	0.42
1:C1:1728:G:OP2	50:Lk:35:LYS:NZ	2.49	0.42
1:C1:1733:G:OP1	50:Lk:77:ARG:NH1	2.46	0.42
3:C4:11:A:N1	3:C4:67:G:O2'	2.44	0.42
8:CN:15:VAL:HA	8:CN:61:ARG:HG2	2.00	0.42
11:Cb:41:ALA:HA	11:Cb:44:LEU:HD12	2.01	0.42
13:Cf:48:ASP:OD2	13:Cf:123:TYR:OH	2.30	0.42
18:LB:244:HIS:ND1	18:LB:245:LYS:HG3	2.35	0.42
24:LH:122:GLY:HA3	24:LH:226:ILE:HD12	2.00	0.42
54:CC:336:ASN:OD1	54:CC:336:ASN:N	2.52	0.42
1:C1:866:A:OP1	49:Lj:5:THR:OG1	2.31	0.42
1:C1:966:G:O4'	35:LT:79:ARG:NH2	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1345:G:H2'	1:C1:1346:A:C8	2.54	0.42
1:C1:1731:G:H5'	50:Lk:26:LYS:HE2	2.02	0.42
1:C1:1877:G:OP2	11:Cb:11:LYS:NZ	2.39	0.42
1:C1:1905:U:O2'	1:C1:1907:G:N7	2.47	0.42
1:C1:3109:U:H3	1:C1:3338:C:N4	2.15	0.42
5:CH:168:THR:HA	5:CH:216:GLN:O	2.20	0.42
6:CK:25:ARG:HD2	16:Cz:27:LYS:HE2	2.02	0.42
27:LL:141:ASP:OD1	27:LL:142:GLN:NE2	2.53	0.42
40:LZ:81:PRO:HB2	42:Lc:65:MET:HE2	2.01	0.42
52:Lp:48:ARG:HB2	52:Lp:58:LYS:NZ	2.34	0.42
1:C1:1395:G:OP1	44:Le:106:ARG:NH2	2.52	0.42
1:C1:1517:A:H2'	1:C1:1518:A:C8	2.55	0.42
1:C1:1658:G:O6	36:LU:81:ARG:NH2	2.52	0.42
1:C1:2642:U:H2'	1:C1:2643:C:C6	2.54	0.42
1:C1:3111:C:C4	1:C1:3113:A:H1'	2.54	0.42
23:LG:158:ASN:C	23:LG:158:ASN:HD22	2.28	0.42
54:CC:794:ASP:OD1	54:CC:794:ASP:N	2.51	0.42
1:C1:1779:A:H2'	1:C1:1780:A:H8	1.81	0.42
1:C1:1812:OMC:H2'	1:C1:1813:G:C8	2.53	0.42
1:C1:2176:A:N3	1:C1:2560:A:O2'	2.45	0.42
5:CH:131:ALA:O	5:CH:135:MET:HG3	2.20	0.42
12:Cd:125:ASP:HA	12:Cd:128:LYS:HG2	2.01	0.42
13:Cf:117:TYR:O	13:Cf:255:PHE:HA	2.20	0.42
28:LM:20:LEU:HD21	28:LM:30:ILE:HD11	2.02	0.42
40:LZ:4:LEU:HD21	40:LZ:81:PRO:HG3	2.02	0.42
44:Le:19:MET:HE2	44:Le:51:LEU:HD21	2.01	0.42
56:CJ:183:HIS:O	56:CJ:186:ARG:NH1	2.53	0.42
1:C1:575:G:H2'	1:C1:576:A:C8	2.55	0.42
1:C1:1095:A:O2'	1:C1:1353:G:H4'	2.19	0.42
1:C1:3137:A:H2'	1:C1:3138:A:H8	1.85	0.42
5:CH:288:LYS:HG2	57:CH:701:GTP:C6	2.55	0.42
13:Cf:103:VAL:HG22	13:Cf:113:MET:HG2	2.02	0.42
19:LC:35:ILE:HD12	19:LC:121:PHE:CE2	2.54	0.42
23:LG:56:PRO:HD2	23:LG:59:ILE:HD12	2.02	0.42
30:LO:170:TYR:CE2	30:LO:174:LYS:HD2	2.55	0.42
32:LQ:90:VAL:HG13	32:LQ:94:ARG:HD2	2.01	0.42
40:LZ:22:VAL:HG12	40:LZ:44:GLY:HA3	2.01	0.42
53:Lq:133:LEU:HD23	53:Lq:133:LEU:HA	1.91	0.42
55:CD:30:GLU:HG3	55:CD:33:ARG:HE	1.84	0.42
55:CD:175:GLY:HA2	55:CD:203:TRP:HH2	1.84	0.42
56:CJ:38:ILE:O	56:CJ:130:ARG:NH1	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:122:A:O2'	54:CC:287:GLU:OE2	2.32	0.42
13:Cf:104:ARG:HB3	13:Cf:112:ASP:OD1	2.19	0.42
22:LF:114:LEU:HD21	22:LF:121:VAL:HG22	2.00	0.42
24:LH:64:VAL:HG12	24:LH:119:VAL:HG21	2.01	0.42
36:LU:120:ASP:OD1	36:LU:120:ASP:N	2.50	0.42
1:C1:159:U:H2'	1:C1:160:G:C8	2.54	0.42
1:C1:243:U:O2'	1:C1:244:G:O5'	2.31	0.42
1:C1:524:A:H2'	1:C1:525:A:C8	2.55	0.42
2:C2:119:C:OP1	56:CJ:25:LYS:NZ	2.40	0.42
15:Ch:464:GLY:HA3	15:Ch:494:VAL:HG21	2.02	0.42
27:LL:195:VAL:HG21	48:Li:20:LEU:HD21	2.01	0.42
1:C1:37:C:H4'	1:C1:790:A:H2	1.85	0.42
1:C1:42:G:H21	1:C1:2571:U:H4'	1.85	0.42
1:C1:575:G:H2'	1:C1:576:A:H8	1.85	0.42
1:C1:2149:U:H2'	1:C1:2150:G:O4'	2.19	0.42
1:C1:2159:C:H2'	1:C1:2160:C:C6	2.55	0.42
1:C1:2802:U:O2'	1:C1:2805:U:O4	2.29	0.42
1:C1:3266:A:H2'	1:C1:3267:G:C8	2.55	0.42
4:CF:91:ARG:O	4:CF:94:ARG:NH1	2.53	0.42
5:CH:191:THR:HA	5:CH:192:PRO:HD3	1.90	0.42
5:CH:301:MET:O	5:CH:305:ILE:HG13	2.20	0.42
19:LC:301:ARG:NE	32:LQ:69:GLU:OE2	2.47	0.42
23:LG:60:ARG:O	23:LG:64:GLN:HG3	2.19	0.42
25:LJ:162:ARG:HG2	25:LJ:166:GLN:HE22	1.85	0.42
30:LO:35:VAL:HG22	30:LO:105:LYS:HB2	2.02	0.42
30:LO:114:TYR:O	30:LO:119:LYS:NZ	2.53	0.42
34:LS:141:LYS:HD2	34:LS:141:LYS:HA	1.90	0.42
55:CD:145:ARG:NH2	55:CD:207:GLU:OE2	2.43	0.42
1:C1:269:A:H2'	1:C1:270:G:C8	2.55	0.41
1:C1:491:C:H5''	21:LE:100:ARG:HG3	2.01	0.41
1:C1:2728:A:H2'	1:C1:2729:G:C8	2.55	0.41
14:Cg:56:ARG:NH2	14:Cg:57:ASP:OD1	2.53	0.41
15:Ch:166:SER:OG	15:Ch:167:GLY:N	2.53	0.41
15:Ch:194:GLY:O	15:Ch:206:THR:HA	2.20	0.41
17:LA:129:THR:HG1	17:LA:132:ASN:HD22	1.66	0.41
50:Lk:37:LYS:HB3	50:Lk:44:LEU:HD11	2.02	0.41
54:CC:334:PRO:HA	54:CC:335:PRO:HD3	1.94	0.41
1:C1:2069:A:H2'	1:C1:2070:A:H8	1.84	0.41
1:C1:3118:C:O2'	1:C1:3119:A:H8	2.03	0.41
3:C4:17:A:OP1	25:LJ:154:ARG:NH2	2.49	0.41
8:CN:98:GLU:OE2	10:CQ:74:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:LO:129:LEU:HD22	34:LS:156:VAL:HG13	2.02	0.41
43:Ld:52:MET:HB3	43:Ld:85:ARG:HD3	2.02	0.41
55:CD:399:GLU:HG2	55:CD:470:LYS:HD3	2.01	0.41
1:C1:1223:A2M:OP2	26:LK:92:ARG:NH2	2.53	0.41
1:C1:1889:A:H2'	1:C1:1890:A:C8	2.55	0.41
3:C4:88:G:O2'	3:C4:91:A:N6	2.53	0.41
13:Cf:112:ASP:OD1	13:Cf:112:ASP:N	2.53	0.41
13:Cf:232:ILE:HG23	13:Cf:244:VAL:HG13	2.01	0.41
19:LC:34:ASP:OD1	19:LC:34:ASP:N	2.52	0.41
27:LL:195:VAL:HG22	48:Li:20:LEU:HD11	2.02	0.41
45:Lf:55:TYR:CZ	45:Lf:67:ARG:HB2	2.55	0.41
55:CD:116:ALA:HB3	55:CD:149:ALA:HB3	2.02	0.41
55:CD:151:TYR:OH	55:CD:181:LYS:NZ	2.49	0.41
1:C1:514:A:O2'	34:LS:69:PRO:HD2	2.21	0.41
1:C1:714:G:N1	1:C1:725:C:OP2	2.45	0.41
1:C1:1100:G:H2'	1:C1:1101:C:H6	1.86	0.41
1:C1:1623:A:H5''	1:C1:1624:C:C5	2.56	0.41
2:C2:74:U:C4	39:LY:73:TYR:HD1	2.38	0.41
5:CH:365:MET:HA	5:CH:368:ILE:HG12	2.02	0.41
5:CH:587:LEU:HD21	38:LX:90:GLU:OE2	2.20	0.41
6:CK:133:PHE:HB3	6:CK:149:ARG:HB3	2.01	0.41
17:LA:61:VAL:HG11	17:LA:88:ILE:HD11	2.03	0.41
1:C1:656:U:H2'	1:C1:657:U:C6	2.56	0.41
1:C1:2130:A:H2'	1:C1:2131:A:C8	2.55	0.41
1:C1:2160:C:O2'	1:C1:2161:A:O4'	2.39	0.41
1:C1:2532:C:H4'	40:LZ:55:ARG:HB2	2.03	0.41
1:C1:3287:U:H2'	1:C1:3288:A:C8	2.55	0.41
5:CH:641:HIS:HB2	31:LP:136:ILE:HD12	2.03	0.41
54:CC:521:ILE:HB	54:CC:585:ILE:HB	2.03	0.41
1:C1:462:A:H2'	1:C1:463:C:C6	2.55	0.41
24:LH:207:ARG:HE	24:LH:207:ARG:HB3	1.72	0.41
53:Lq:120:ARG:HE	53:Lq:123:ARG:NH2	2.19	0.41
54:CC:502:VAL:O	54:CC:503:ARG:NH1	2.49	0.41
56:CJ:99:ASP:OD2	56:CJ:102:ASN:ND2	2.53	0.41
1:C1:2884:C:H2'	1:C1:2885:A:C4	2.55	0.41
1:C1:3137:A:OP1	30:LO:38:ARG:NH2	2.53	0.41
4:CF:183:ASP:HB3	4:CF:187:GLU:H	1.85	0.41
5:CH:357:ILE:HG23	5:CH:361:LEU:HB3	2.03	0.41
6:CK:244:GLN:HB2	6:CK:260:LEU:HD21	2.02	0.41
37:LV:34:ARG:HE	37:LV:66:LYS:HE2	1.85	0.41
54:CC:543:LEU:HD12	54:CC:582:LEU:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:404:U:H2'	1:C1:405:G:C8	2.56	0.41
1:C1:1067:A:H4'	35:LT:35:ARG:NH1	2.36	0.41
1:C1:1191:C:H4'	4:CF:4:SER:HA	2.03	0.41
1:C1:1638:G:H2'	1:C1:1639:A:C8	2.55	0.41
1:C1:2713:G:OP2	14:Cg:119:ARG:NH2	2.48	0.41
15:Ch:85:PHE:HA	15:Ch:123:SER:O	2.21	0.41
18:LB:180:MET:HE2	18:LB:182:ILE:HG12	2.02	0.41
21:LE:58:LEU:HD11	21:LE:72:LEU:HB2	2.03	0.41
25:LJ:47:VAL:O	25:LJ:68:VAL:HA	2.19	0.41
1:C1:88:U:H2'	1:C1:89:A:C8	2.56	0.41
1:C1:1252:U:H1'	1:C1:1255:C:H5	1.86	0.41
1:C1:1589:C:H5'	38:LX:92:GLN:OE1	2.21	0.41
1:C1:2882:U:H2'	12:Cd:221:ARG:HD3	2.03	0.41
1:C1:3225:G:H2'	1:C1:3226:C:C6	2.56	0.41
4:CF:10:TYR:OH	6:CK:69:GLU:OE2	2.29	0.41
5:CH:284:ILE:HB	5:CH:316:ILE:HD13	2.03	0.41
10:CQ:66:ASP:HB3	10:CQ:69:LEU:HG	2.02	0.41
18:LB:164:HIS:HA	18:LB:178:HIS:O	2.21	0.41
22:LF:242:ASN:O	22:LF:246:ARG:HG2	2.21	0.41
26:LK:15:LEU:HD22	26:LK:28:LEU:HD21	2.03	0.41
27:LL:192:ALA:HB2	48:Li:19:GLY:HA2	2.01	0.41
29:LN:38:ARG:HB2	29:LN:62:TYR:CZ	2.56	0.41
30:LO:129:LEU:HD11	34:LS:170:PRO:HG2	2.03	0.41
36:LU:22:ILE:HB	36:LU:109:VAL:HG22	2.03	0.41
38:LX:71:ASP:H	38:LX:74:LYS:HB2	1.85	0.41
43:Ld:14:ASP:OD2	43:Ld:87:ARG:NH2	2.53	0.41
54:CC:399:PHE:CE1	56:CJ:209:LEU:HD22	2.56	0.41
55:CD:367:ILE:HD11	55:CD:391:VAL:HG11	2.03	0.41
1:C1:151:G:H5''	1:C1:152:G:H2'	2.02	0.41
1:C1:371:A:H4'	39:LY:90:THR:HG22	2.03	0.41
1:C1:430:G:O6	53:Lq:134:ARG:NH1	2.47	0.41
1:C1:804:G:H2'	1:C1:805:C:H6	1.86	0.41
1:C1:2080:A:O2'	1:C1:3038:G:O2'	2.37	0.41
17:LA:40:TYR:HA	17:LA:91:GLY:HA3	2.02	0.41
19:LC:273:LYS:HE2	19:LC:273:LYS:HB2	1.87	0.41
20:LD:113:LEU:HB3	20:LD:115:LEU:HD13	2.03	0.41
21:LE:194:LYS:HB3	21:LE:196:HIS:CE1	2.56	0.41
24:LH:10:ILE:HG12	24:LH:109:ARG:HG3	2.03	0.41
24:LH:138:VAL:HG11	24:LH:183:LEU:HD11	2.03	0.41
26:LK:114:ARG:HA	26:LK:117:ARG:HG2	2.02	0.41
43:Ld:33:PHE:HB3	43:Ld:73:LYS:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
54:CC:654:ARG:NH1	54:CC:675:LYS:O	2.54	0.41
55:CD:320:HIS:HB3	55:CD:338:LEU:O	2.21	0.41
1:C1:568:U:OP1	22:LF:246:ARG:NH2	2.48	0.40
1:C1:743:A:C2	1:C1:753:A:H1'	2.56	0.40
1:C1:957:C:H2'	1:C1:958:G:C8	2.56	0.40
1:C1:1901:A:H2'	1:C1:1902:A:C8	2.56	0.40
1:C1:2889:A:H2'	1:C1:2890:C:C6	2.56	0.40
3:C4:3:G:O3'	3:C4:25:G:N2	2.47	0.40
5:CH:163:ASN:O	5:CH:216:GLN:NE2	2.54	0.40
6:CK:165:PRO:HG2	12:Cd:326:GLN:HE21	1.86	0.40
10:CQ:1:MET:N	18:LB:71:GLU:OE2	2.47	0.40
18:LB:237:LYS:HE2	18:LB:237:LYS:HB2	1.80	0.40
54:CC:642:HIS:HB2	54:CC:647:LEU:HB2	2.02	0.40
1:C1:1584:U:H4'	1:C1:1815:A:H4'	2.03	0.40
1:C1:1917:OMU:H1'	1:C1:1917:OMU:HM23	1.87	0.40
1:C1:2923:G:O2'	12:Cd:30:ARG:NH2	2.47	0.40
1:C1:3157:C:H2'	1:C1:3158:C:O4'	2.20	0.40
2:C2:57:C:H4'	2:C2:63:G:N7	2.37	0.40
3:C4:4:U:H2'	3:C4:5:A:C8	2.56	0.40
8:CN:104:LEU:HA	8:CN:107:VAL:HG22	2.04	0.40
12:Cd:47:ILE:HB	12:Cd:56:LYS:HB3	2.04	0.40
38:LX:62:LYS:HB2	38:LX:62:LYS:HE3	1.90	0.40
55:CD:10:ALA:HA	55:CD:11:PRO:HD3	1.93	0.40
55:CD:151:TYR:O	55:CD:179:SER:OG	2.28	0.40
1:C1:268:U:H2'	1:C1:269:A:C8	2.55	0.40
1:C1:927:C:H2'	1:C1:928:C:C6	2.56	0.40
1:C1:1777:A:H2'	1:C1:1778:A:C8	2.56	0.40
1:C1:2101:A:C4	49:Lj:3:LYS:HB3	2.56	0.40
1:C1:2219:A:N6	1:C1:2221:U:OP1	2.54	0.40
1:C1:2800:G:O2'	7:CL:44:GLU:OE2	2.27	0.40
1:C1:2833:G:OP2	1:C1:2833:G:N2	2.41	0.40
1:C1:3238:U:H2'	1:C1:3239:C:H6	1.85	0.40
2:C2:26:U:H2'	2:C2:27:U:C6	2.56	0.40
11:Cb:65:LEU:HD12	11:Cb:68:HIS:CD2	2.56	0.40
30:LO:26:LYS:HA	30:LO:26:LYS:HD2	1.86	0.40
55:CD:186:LEU:HD11	55:CD:240:ILE:HD11	2.02	0.40
1:C1:134:G:O2'	54:CC:302:ARG:O	2.39	0.40
1:C1:1049:G:H2'	1:C1:1050:C:C6	2.57	0.40
1:C1:2226:C:H2'	1:C1:2227:U:H6	1.87	0.40
1:C1:2476:U:OP1	23:LG:248:ARG:NH2	2.43	0.40
1:C1:2751:A:H2'	1:C1:2752:G:C8	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:Cd:298:ARG:NH1	12:Cd:299:ALA:O	2.55	0.40
14:Cg:173:LYS:HA	14:Cg:176:GLU:HG2	2.03	0.40
15:Ch:86:ARG:HB2	15:Ch:123:SER:HB2	2.03	0.40
21:LE:196:HIS:CD2	21:LE:197:LEU:HG	2.57	0.40
25:LJ:113:LEU:HD11	25:LJ:126:MET:HE1	2.03	0.40
31:LP:180:ILE:HD13	31:LP:180:ILE:HA	1.99	0.40
33:LR:61:SER:O	33:LR:65:GLU:HG2	2.22	0.40
54:CC:664:LEU:HD23	54:CC:664:LEU:HA	1.97	0.40
56:CJ:130:ARG:HD3	56:CJ:233:PHE:CZ	2.56	0.40
1:C1:2172:U:O2'	1:C1:2175:C:N4	2.54	0.40
7:CL:59:PHE:HA	7:CL:60:PRO:HD3	1.96	0.40
7:CL:61:TYR:HB3	7:CL:64:ARG:HD2	2.03	0.40
29:LN:200:TRP:O	29:LN:203:ARG:HD3	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	CF	243/270 (90%)	241 (99%)	2 (1%)	0	100	100
5	CH	621/661 (94%)	612 (99%)	9 (1%)	0	100	100
6	CK	231/261 (88%)	225 (97%)	6 (3%)	0	100	100
7	CL	77/558 (14%)	77 (100%)	0	0	100	100
8	CN	244/246 (99%)	238 (98%)	6 (2%)	0	100	100
9	CO	56/120 (47%)	56 (100%)	0	0	100	100
10	CQ	181/225 (80%)	180 (99%)	1 (1%)	0	100	100
11	Cb	99/117 (85%)	98 (99%)	1 (1%)	0	100	100
12	Cd	458/627 (73%)	449 (98%)	9 (2%)	0	100	100
13	Cf	281/350 (80%)	279 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	Cg	186/202 (92%)	184 (99%)	2 (1%)	0	100	100
15	Ch	484/517 (94%)	469 (97%)	15 (3%)	0	100	100
16	Cz	99/123 (80%)	98 (99%)	1 (1%)	0	100	100
17	LA	189/254 (74%)	186 (98%)	3 (2%)	0	100	100
18	LB	387/392 (99%)	380 (98%)	7 (2%)	0	100	100
19	LC	361/365 (99%)	355 (98%)	6 (2%)	0	100	100
20	LD	282/304 (93%)	280 (99%)	2 (1%)	0	100	100
21	LE	187/200 (94%)	183 (98%)	4 (2%)	0	100	100
22	CM	130/249 (52%)	126 (97%)	4 (3%)	0	100	100
22	LF	246/249 (99%)	241 (98%)	5 (2%)	0	100	100
23	LG	233/262 (89%)	230 (99%)	3 (1%)	0	100	100
24	LH	188/229 (82%)	185 (98%)	3 (2%)	0	100	100
25	LJ	167/173 (96%)	166 (99%)	1 (1%)	0	100	100
26	LK	156/165 (94%)	153 (98%)	3 (2%)	0	100	100
27	LL	201/213 (94%)	200 (100%)	1 (0%)	0	100	100
28	LM	139/142 (98%)	135 (97%)	4 (3%)	0	100	100
29	LN	200/203 (98%)	194 (97%)	6 (3%)	0	100	100
30	LO	201/204 (98%)	199 (99%)	2 (1%)	0	100	100
31	LP	167/187 (89%)	164 (98%)	3 (2%)	0	100	100
32	LQ	148/213 (70%)	145 (98%)	3 (2%)	0	100	100
33	LR	153/2898 (5%)	152 (99%)	1 (1%)	0	100	100
34	LS	172/174 (99%)	169 (98%)	3 (2%)	0	100	100
35	LT	127/160 (79%)	124 (98%)	3 (2%)	0	100	100
36	LU	103/127 (81%)	100 (97%)	3 (3%)	0	100	100
37	LV	133/139 (96%)	132 (99%)	1 (1%)	0	100	100
38	LX	120/156 (77%)	119 (99%)	1 (1%)	0	100	100
39	LY	131/138 (95%)	125 (95%)	6 (5%)	0	100	100
40	LZ	133/135 (98%)	131 (98%)	2 (2%)	0	100	100
41	La	104/149 (70%)	104 (100%)	0	0	100	100
42	Lc	93/108 (86%)	93 (100%)	0	0	100	100
43	Ld	108/120 (90%)	107 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
44	Le	124/131 (95%)	123 (99%)	1 (1%)	0	100	100
45	Lf	106/109 (97%)	106 (100%)	0	0	100	100
46	Lg	116/119 (98%)	114 (98%)	2 (2%)	0	100	100
47	Lh	111/935 (12%)	110 (99%)	1 (1%)	0	100	100
48	Li	99/110 (90%)	99 (100%)	0	0	100	100
49	Lj	86/95 (90%)	84 (98%)	2 (2%)	0	100	100
50	Lk	74/94 (79%)	71 (96%)	3 (4%)	0	100	100
51	Ll	48/51 (94%)	46 (96%)	2 (4%)	0	100	100
52	Lp	89/92 (97%)	87 (98%)	2 (2%)	0	100	100
53	Lq	137/147 (93%)	133 (97%)	4 (3%)	0	100	100
54	CC	493/801 (62%)	481 (98%)	12 (2%)	0	100	100
55	CD	441/495 (89%)	430 (98%)	11 (2%)	0	100	100
56	CJ	483/679 (71%)	471 (98%)	12 (2%)	0	100	100
All	All	10626/16443 (65%)	10439 (98%)	187 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
4	CF	212/236 (90%)	211 (100%)	1 (0%)	81	89
5	CH	543/575 (94%)	543 (100%)	0	100	100
6	CK	206/225 (92%)	206 (100%)	0	100	100
7	CL	61/458 (13%)	61 (100%)	0	100	100
8	CN	205/206 (100%)	205 (100%)	0	100	100
9	CO	48/99 (48%)	48 (100%)	0	100	100
10	CQ	144/192 (75%)	144 (100%)	0	100	100
11	Cb	85/101 (84%)	85 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	Cd	403/541 (74%)	403 (100%)	0	100	100
13	Cf	250/310 (81%)	250 (100%)	0	100	100
14	Cg	158/176 (90%)	158 (100%)	0	100	100
15	Ch	408/436 (94%)	408 (100%)	0	100	100
16	Cz	89/107 (83%)	89 (100%)	0	100	100
17	LA	150/198 (76%)	150 (100%)	0	100	100
18	LB	329/331 (99%)	329 (100%)	0	100	100
19	LC	282/285 (99%)	282 (100%)	0	100	100
20	LD	221/253 (87%)	221 (100%)	0	100	100
21	LE	157/166 (95%)	157 (100%)	0	100	100
22	CM	10/215 (5%)	10 (100%)	0	100	100
22	LF	213/215 (99%)	213 (100%)	0	100	100
23	LG	200/222 (90%)	200 (100%)	0	100	100
24	LH	167/200 (84%)	167 (100%)	0	100	100
25	LJ	140/150 (93%)	140 (100%)	0	100	100
26	LK	127/136 (93%)	127 (100%)	0	100	100
27	LL	158/176 (90%)	158 (100%)	0	100	100
28	LM	116/117 (99%)	116 (100%)	0	100	100
29	LN	179/180 (99%)	179 (100%)	0	100	100
30	LO	162/163 (99%)	162 (100%)	0	100	100
31	LP	133/152 (88%)	133 (100%)	0	100	100
32	LQ	128/178 (72%)	128 (100%)	0	100	100
33	LR	125/2396 (5%)	125 (100%)	0	100	100
34	LS	152/154 (99%)	152 (100%)	0	100	100
35	LT	110/135 (82%)	110 (100%)	0	100	100
36	LU	92/108 (85%)	92 (100%)	0	100	100
37	LV	98/102 (96%)	98 (100%)	0	100	100
38	LX	107/129 (83%)	107 (100%)	0	100	100
39	LY	116/119 (98%)	116 (100%)	0	100	100
40	LZ	121/121 (100%)	121 (100%)	0	100	100
41	La	93/122 (76%)	93 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
42	Lc	76/88 (86%)	76 (100%)	0	100	100
43	Ld	90/105 (86%)	90 (100%)	0	100	100
44	Le	109/114 (96%)	109 (100%)	0	100	100
45	Lf	89/90 (99%)	89 (100%)	0	100	100
46	Lg	95/102 (93%)	95 (100%)	0	100	100
47	Lh	102/781 (13%)	102 (100%)	0	100	100
48	Li	85/93 (91%)	85 (100%)	0	100	100
49	Lj	72/78 (92%)	72 (100%)	0	100	100
50	Lk	73/88 (83%)	73 (100%)	0	100	100
51	Ll	45/46 (98%)	45 (100%)	0	100	100
52	Lp	73/74 (99%)	73 (100%)	0	100	100
53	Lq	109/112 (97%)	109 (100%)	0	100	100
54	CC	408/710 (58%)	408 (100%)	0	100	100
55	CD	365/410 (89%)	365 (100%)	0	100	100
56	CJ	301/579 (52%)	301 (100%)	0	100	100
All	All	8790/13855 (63%)	8789 (100%)	1 (0%)	100	100

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

Mol	Chain	Res	Type
4	CF	153	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
4	CF	121	GLN
5	CH	14	GLN
5	CH	77	HIS
5	CH	459	GLN
5	CH	533	HIS
6	CK	14	HIS
6	CK	95	ASN
9	CO	14	HIS
10	CQ	70	GLN
10	CQ	87	GLN
10	CQ	130	ASN

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Mol	Chain	Res	Type
11	Cb	68	HIS
13	Cf	26	ASN
14	Cg	121	GLN
15	Ch	133	HIS
17	LA	205	ASN
19	LC	292	ASN
19	LC	297	GLN
20	LD	89	ASN
20	LD	249	GLN
21	LE	162	GLN
21	LE	196	HIS
22	LF	192	HIS
22	LF	200	ASN
23	LG	62	GLN
23	LG	158	ASN
25	LJ	44	GLN
25	LJ	96	ASN
25	LJ	166	GLN
29	LN	95	GLN
29	LN	123	GLN
29	LN	138	ASN
29	LN	153	ASN
31	LP	42	GLN
39	LY	18	HIS
40	LZ	77	ASN
40	LZ	126	ASN
41	La	11	HIS
44	Le	21	HIS
44	Le	79	ASN
48	Li	72	ASN
49	Lj	76	ASN
50	Lk	41	GLN
52	Lp	45	ASN
53	Lq	43	HIS
53	Lq	101	HIS
54	CC	286	ASN
54	CC	328	GLN
54	CC	355	ASN
55	CD	68	ASN
55	CD	271	HIS
55	CD	340	HIS
56	CJ	457	GLN

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Mol	Chain	Res	Type
56	CJ	626	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	3046/3338 (91%)	554 (18%)	24 (0%)
2	C2	151/156 (96%)	20 (13%)	0
3	C4	118/119 (99%)	22 (18%)	0
All	All	3315/3613 (91%)	596 (17%)	24 (0%)

All (596) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	6	G
1	C1	27	A
1	C1	50	A
1	C1	60	G
1	C1	61	A
1	C1	66	A
1	C1	67	A
1	C1	95	G
1	C1	96	A
1	C1	110	A
1	C1	111	G
1	C1	112	C
1	C1	116	A
1	C1	117	A
1	C1	123	A
1	C1	132	U
1	C1	134	G
1	C1	135	G
1	C1	139	G
1	C1	142	U
1	C1	152	G
1	C1	153	A
1	C1	156	G
1	C1	157	G
1	C1	181	G
1	C1	184	U
1	C1	185	U
1	C1	194	C

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Mol	Chain	Res	Type
1	C1	200	G
1	C1	204	C
1	C1	213	A
1	C1	214	G
1	C1	241	U
1	C1	244	G
1	C1	247	A
1	C1	258	A
1	C1	262	G
1	C1	276	G
1	C1	277	A
1	C1	288	A
1	C1	291	U
1	C1	298	U
1	C1	304	U
1	C1	308	C
1	C1	316	A
1	C1	322	C
1	C1	323	G
1	C1	332	C
1	C1	342	A
1	C1	343	C
1	C1	369	G
1	C1	389	A2M
1	C1	392	A
1	C1	394	C
1	C1	395	A
1	C1	396	C
1	C1	414	G
1	C1	415	A
1	C1	434	U
1	C1	435	G
1	C1	443	C
1	C1	445	G
1	C1	446	A
1	C1	447	U
1	C1	448	C
1	C1	458	U
1	C1	459	C
1	C1	460	U
1	C1	469	C
1	C1	470	A

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Mol	Chain	Res	Type
1	C1	471	C
1	C1	472	U
1	C1	479	G
1	C1	512	A
1	C1	514	A
1	C1	527	G
1	C1	535	U
1	C1	536	C
1	C1	537	C
1	C1	545	U
1	C1	547	A
1	C1	548	U
1	C1	549	A
1	C1	570	G
1	C1	583	A
1	C1	588	G
1	C1	592	U
1	C1	593	G
1	C1	595	A
1	C1	597	G
1	C1	599	A
1	C1	608	U
1	C1	609	A
1	C1	610	A
1	C1	624	C
1	C1	632	G
1	C1	634	A
1	C1	648	A
1	C1	650	U
1	C1	665	A
1	C1	669	U
1	C1	678	A
1	C1	693	A
1	C1	700	G
1	C1	703	A
1	C1	704	A
1	C1	719	U
1	C1	720	C
1	C1	721	G
1	C1	747	A
1	C1	748	U
1	C1	756	G

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Mol	Chain	Res	Type
1	C1	757	A
1	C1	759	U
1	C1	761	G
1	C1	762	A
1	C1	763	G
1	C1	767	G
1	C1	782	G
1	C1	790	A
1	C1	799	A
1	C1	812	A
1	C1	826	G
1	C1	830	A
1	C1	843	C
1	C1	857	G
1	C1	862	G
1	C1	877	A
1	C1	889	G
1	C1	891	G
1	C1	896	A
1	C1	898	G
1	C1	899	A
1	C1	903	A
1	C1	905	C
1	C1	906	G
1	C1	919	G
1	C1	926	A
1	C1	931	C
1	C1	933	A
1	C1	934	A
1	C1	935	G
1	C1	937	U
1	C1	940	C
1	C1	941	C
1	C1	943	C
1	C1	944	A
1	C1	945	G
1	C1	947	A
1	C1	955	G
1	C1	956	U
1	C1	963	U
1	C1	964	C
1	C1	976	G

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Mol	Chain	Res	Type
1	C1	977	U
1	C1	983	G
1	C1	984	A
1	C1	1032	C
1	C1	1034	U
1	C1	1040	A
1	C1	1047	A
1	C1	1048	A
1	C1	1049	G
1	C1	1051	C
1	C1	1055	G
1	C1	1058	A
1	C1	1059	C
1	C1	1064	C
1	C1	1065	U
1	C1	1066	G
1	C1	1070	G
1	C1	1075	C
1	C1	1076	A
1	C1	1077	U
1	C1	1078	U
1	C1	1079	C
1	C1	1080	G
1	C1	1081	A
1	C1	1086	A
1	C1	1099	G
1	C1	1109	G
1	C1	1110	G
1	C1	1115	C
1	C1	1118	A
1	C1	1127	U
1	C1	1132	G
1	C1	1136	A
1	C1	1161	G
1	C1	1163	G
1	C1	1164	U
1	C1	1165	G
1	C1	1175	C
1	C1	1176	A
1	C1	1179	C
1	C1	1185	A
1	C1	1188	A

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Mol	Chain	Res	Type
1	C1	1194	U
1	C1	1205	G
1	C1	1209	G
1	C1	1218	U
1	C1	1228	A
1	C1	1241	U
1	C1	1242	A
1	C1	1246	A
1	C1	1248	U
1	C1	1268	G
1	C1	1270	A
1	C1	1278	G
1	C1	1287	A
1	C1	1288	U
1	C1	1290	G
1	C1	1292	U
1	C1	1296	G
1	C1	1313	A
1	C1	1331	A
1	C1	1332	G
1	C1	1333	A
1	C1	1334	A
1	C1	1335	A
1	C1	1336	C
1	C1	1337	G
1	C1	1363	G
1	C1	1369	A
1	C1	1370	G
1	C1	1375	G
1	C1	1382	A
1	C1	1383	G
1	C1	1400	G
1	C1	1401	A
1	C1	1414	G
1	C1	1417	G
1	C1	1420	OMC
1	C1	1429	A
1	C1	1433	OMG
1	C1	1458	G
1	C1	1464	A
1	C1	1466	G
1	C1	1477	U

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Mol	Chain	Res	Type
1	C1	1479	C
1	C1	1485	G
1	C1	1491	OMC
1	C1	1505	U
1	C1	1536	U
1	C1	1538	U
1	C1	1539	C
1	C1	1540	A
1	C1	1542	A
1	C1	1543	G
1	C1	1554	G
1	C1	1560	U
1	C1	1561	G
1	C1	1563	G
1	C1	1567	A
1	C1	1568	A
1	C1	1569	A
1	C1	1570	G
1	C1	1573	A
1	C1	1585	A
1	C1	1586	U
1	C1	1593	A
1	C1	1608	U
1	C1	1609	U
1	C1	1611	C
1	C1	1619	C
1	C1	1622	A
1	C1	1623	A
1	C1	1624	C
1	C1	1638	G
1	C1	1684	A
1	C1	1685	U
1	C1	1697	C
1	C1	1704	U
1	C1	1721	A
1	C1	1722	U
1	C1	1730	A
1	C1	1731	G
1	C1	1745	U
1	C1	1746	G
1	C1	1751	G
1	C1	1758	G

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Mol	Chain	Res	Type
1	C1	1760	G
1	C1	1776	G
1	C1	1777	A
1	C1	1790	G
1	C1	1792	G
1	C1	1793	A
1	C1	1796	A
1	C1	1797	A
1	C1	1800	C
1	C1	1801	U
1	C1	1822	A
1	C1	1826	C
1	C1	1829	C
1	C1	1830	A
1	C1	1846	C
1	C1	1847	A2M
1	C1	1858	G
1	C1	1860	U
1	C1	1866	A
1	C1	1873	A
1	C1	1886	G
1	C1	1887	C
1	C1	1917	OMU
1	C1	1923	C
1	C1	1933	G
1	C1	2055	A
1	C1	2075	U
1	C1	2076	A
1	C1	2084	G
1	C1	2085	G
1	C1	2094	A
1	C1	2121	A
1	C1	2126	C
1	C1	2132	G
1	C1	2151	A
1	C1	2156	U
1	C1	2157	G
1	C1	2158	C
1	C1	2161	A
1	C1	2167	C
1	C1	2168	U
1	C1	2169	G

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Mol	Chain	Res	Type
1	C1	2171	A
1	C1	2172	U
1	C1	2173	G
1	C1	2186	A
1	C1	2188	U
1	C1	2192	A
1	C1	2203	G
1	C1	2205	A
1	C1	2206	A
1	C1	2212	G
1	C1	2216	G
1	C1	2217	U
1	C1	2218	A
1	C1	2219	A
1	C1	2220	C
1	C1	2221	U
1	C1	2222	A
1	C1	2223	U
1	C1	2224	G
1	C1	2225	A
1	C1	2226	C
1	C1	2229	U
1	C1	2230	C
1	C1	2231	U
1	C1	2237	U
1	C1	2279	G
1	C1	2281	U
1	C1	2282	U
1	C1	2284	A
1	C1	2297	U
1	C1	2298	G
1	C1	2299	U
1	C1	2326	A
1	C1	2340	G
1	C1	2348	A
1	C1	2351	U
1	C1	2355	C
1	C1	2356	G
1	C1	2362	A
1	C1	2364	A
1	C1	2373	U
1	C1	2374	U

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Mol	Chain	Res	Type
1	C1	2381	G
1	C1	2382	A
1	C1	2398	G
1	C1	2403	A
1	C1	2406	A
1	C1	2473	U
1	C1	2474	A
1	C1	2477	U
1	C1	2489	C
1	C1	2499	C
1	C1	2500	U
1	C1	2501	U
1	C1	2502	G
1	C1	2503	C
1	C1	2506	C
1	C1	2507	C
1	C1	2508	A
1	C1	2513	C
1	C1	2521	A
1	C1	2526	C
1	C1	2527	C
1	C1	2530	C
1	C1	2531	G
1	C1	2533	G
1	C1	2534	G
1	C1	2544	G
1	C1	2552	A
1	C1	2565	G
1	C1	2566	G
1	C1	2573	G
1	C1	2575	C
1	C1	2576	U
1	C1	2577	G
1	C1	2578	OMG
1	C1	2582	G
1	C1	2584	C
1	C1	2585	A
1	C1	2589	C
1	C1	2606	A
1	C1	2613	C
1	C1	2615	A
1	C1	2633	A

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Mol	Chain	Res	Type
1	C1	2635	A
1	C1	2636	G
1	C1	2647	U
1	C1	2650	A
1	C1	2651	A
1	C1	2656	A
1	C1	2657	G
1	C1	2663	A
1	C1	2664	A
1	C1	2672	U
1	C1	2673	G
1	C1	2674	A
1	C1	2675	U
1	C1	2680	A
1	C1	2682	U
1	C1	2689	G
1	C1	2690	OMU
1	C1	2691	G
1	C1	2708	G
1	C1	2713	G
1	C1	2715	C
1	C1	2717	A
1	C1	2730	U
1	C1	2731	C
1	C1	2732	C
1	C1	2736	G
1	C1	2737	A
1	C1	2750	G
1	C1	2754	U
1	C1	2755	G
1	C1	2756	C
1	C1	2757	C
1	C1	2758	A
1	C1	2761	A
1	C1	2762	A
1	C1	2763	A
1	C1	2769	C
1	C1	2783	G
1	C1	2784	C
1	C1	2785	U
1	C1	2802	U
1	C1	2803	C

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Mol	Chain	Res	Type
1	C1	2804	A
1	C1	2805	U
1	C1	2806	A
1	C1	2812	G
1	C1	2816	C
1	C1	2817	U
1	C1	2826	C
1	C1	2828	U
1	C1	2836	G
1	C1	2846	A
1	C1	2857	G
1	C1	2858	C
1	C1	2863	U
1	C1	2882	U
1	C1	2883	U
1	C1	2884	C
1	C1	2885	A
1	C1	2894	U
1	C1	2895	A
1	C1	2900	A
1	C1	2903	U
1	C1	2905	A
1	C1	2929	C
1	C1	2930	A
1	C1	2931	G
1	C1	2938	U
1	C1	2939	U
1	C1	2940	U
1	C1	2942	C
1	C1	2951	U
1	C1	2955	C
1	C1	2956	U
1	C1	2970	A
1	C1	2980	G
1	C1	3014	U
1	C1	3017	G
1	C1	3036	G
1	C1	3044	A
1	C1	3050	C
1	C1	3051	C
1	C1	3067	G
1	C1	3071	A

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Mol	Chain	Res	Type
1	C1	3080	A
1	C1	3087	A
1	C1	3088	A
1	C1	3089	U
1	C1	3100	A
1	C1	3101	C
1	C1	3102	G
1	C1	3112	U
1	C1	3113	A
1	C1	3118	C
1	C1	3119	A
1	C1	3124	G
1	C1	3125	U
1	C1	3126	A
1	C1	3127	G
1	C1	3131	U
1	C1	3133	U
1	C1	3135	A
1	C1	3141	G
1	C1	3146	C
1	C1	3155	A
1	C1	3162	C
1	C1	3163	A
1	C1	3164	G
1	C1	3168	A
1	C1	3185	G
1	C1	3186	A
1	C1	3188	G
1	C1	3190	G
1	C1	3200	A
1	C1	3201	A
1	C1	3206	C
1	C1	3210	U
1	C1	3211	U
1	C1	3217	U
1	C1	3218	U
1	C1	3228	C
1	C1	3229	G
1	C1	3231	G
1	C1	3245	C
1	C1	3248	A
1	C1	3254	U

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Mol	Chain	Res	Type
1	C1	3257	A
1	C1	3258	U
1	C1	3259	G
1	C1	3260	U
1	C1	3276	A
1	C1	3282	U
1	C1	3291	C
1	C1	3292	U
1	C1	3293	U
1	C1	3295	U
1	C1	3297	G
1	C1	3299	U
1	C1	3302	G
1	C1	3310	G
1	C1	3312	G
1	C1	3319	C
1	C1	3323	C
1	C1	3324	C
1	C1	3325	U
1	C1	3331	U
1	C1	3332	A
1	C1	3338	C
2	C2	34	U
2	C2	35	C
2	C2	38	U
2	C2	49	G
2	C2	59	A
2	C2	62	A
2	C2	63	G
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	95	G
2	C2	104	A
2	C2	106	C
2	C2	113	U
2	C2	116	G
2	C2	125	U
2	C2	127	U
2	C2	129	C
2	C2	131	G
2	C2	152	G

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Mol	Chain	Res	Type
3	C4	7	G
3	C4	22	A
3	C4	29	G
3	C4	41	G
3	C4	52	G
3	C4	54	U
3	C4	55	A
3	C4	64	A
3	C4	66	G
3	C4	75	A
3	C4	76	G
3	C4	81	U
3	C4	83	G
3	C4	84	G
3	C4	85	U
3	C4	86	C
3	C4	89	U
3	C4	90	G
3	C4	93	G
3	C4	97	A
3	C4	101	A
3	C4	111	G

All (24) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	151	G
1	C1	243	U
1	C1	898	G
1	C1	1047	A
1	C1	1064	C
1	C1	1077	U
1	C1	1267	C
1	C1	1537	U
1	C1	1608	U
1	C1	2157	G
1	C1	2160	C
1	C1	2225	A
1	C1	2280	A
1	C1	2575	C
1	C1	2883	U
1	C1	3079	U

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Mol	Chain	Res	Type
1	C1	3132	A
1	C1	3205	G
1	C1	3210	U
1	C1	3230	G
1	C1	3258	U
1	C1	3298	U
1	C1	3301	C
1	C1	3324	C

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

34 non-standard protein/DNA/RNA residues are modelled in this entry.

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
1	OMC	C1	778	1	19,22,23	0.58	0	25,31,34	0.92	1 (4%)
1	OMU	C1	2683	1	19,22,23	3.04	6 (31%)	25,31,34	1.79	4 (16%)
1	A2M	C1	2289	1	22,25,26	4.04	12 (54%)	30,36,39	3.30	15 (50%)
1	A2M	C1	637	1	22,25,26	3.97	11 (50%)	30,36,39	3.31	12 (40%)
1	OMG	C1	2774	1	23,26,27	0.53	0	32,38,41	0.54	0
1	A2M	C1	389	1	22,25,26	4.00	11 (50%)	30,36,39	3.40	15 (50%)
1	OMG	C1	646	1	23,26,27	0.57	0	32,38,41	0.55	0
1	OMG	C1	1433	1	23,26,27	0.56	0	32,38,41	0.47	0
1	OMC	C1	1491	1	19,22,23	0.65	0	25,31,34	0.71	0
1	OMC	C1	2838	1	19,22,23	0.75	1 (5%)	25,31,34	1.55	4 (16%)
1	OMU	C1	1868	1	19,22,23	3.05	6 (31%)	25,31,34	1.92	5 (20%)
1	OMC	C1	1812	1	19,22,23	0.62	0	25,31,34	1.50	2 (8%)
1	OMG	C1	2578	1	23,26,27	0.51	0	32,38,41	0.62	0
1	OMU	C1	2690	1	19,22,23	2.98	7 (36%)	25,31,34	1.84	5 (20%)
1	OMC	C1	2918	1	19,22,23	0.61	0	25,31,34	0.86	1 (4%)
1	OMG	C1	2358	1	23,26,27	0.55	0	32,38,41	0.59	0
1	OMU	C1	2277	1	19,22,23	3.07	6 (31%)	25,31,34	1.76	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	OMU	C1	2380	1	19,22,23	3.05	6 (31%)	25,31,34	1.76	5 (20%)
1	OMG	C1	2876	1	23,26,27	0.52	0	32,38,41	0.51	0
1	OMU	C1	2384	1	19,22,23	3.10	6 (31%)	25,31,34	1.82	5 (20%)
1	OMU	C1	2688	1	19,22,23	3.06	6 (31%)	25,31,34	1.78	5 (20%)
1	OMC	C1	1420	1	19,22,23	0.69	0	25,31,34	1.36	3 (12%)
1	OMG	C1	385	1	23,26,27	0.50	0	32,38,41	0.62	0
1	A2M	C1	848	1	22,25,26	3.99	12 (54%)	30,36,39	3.42	14 (46%)
1	OMG	C1	2881	1	23,26,27	0.51	0	32,38,41	0.46	0
1	OMC	C1	1836	1	19,22,23	0.64	0	25,31,34	0.78	1 (4%)
1	A2M	C1	1223	1	22,25,26	3.99	11 (50%)	30,36,39	3.34	13 (43%)
1	A2M	C1	1847	1	22,25,26	3.97	12 (54%)	30,36,39	3.44	13 (43%)
1	OMC	C1	2300	1	19,22,23	0.62	0	25,31,34	0.81	0
1	OMG	C1	627	1	23,26,27	0.54	0	32,38,41	0.55	0
1	OMU	C1	1917	1	19,22,23	3.05	6 (31%)	25,31,34	1.83	5 (20%)
1	A2M	C1	858	1	22,25,26	4.04	11 (50%)	30,36,39	3.42	12 (40%)
1	A2M	C1	1432	1	22,25,26	3.97	12 (54%)	30,36,39	3.37	11 (36%)
1	OMG	C1	787	1	23,26,27	0.55	0	32,38,41	0.64	1 (3%)

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
1	OMC	C1	778	1	-	0/9/27/28	0/2/2/2
1	OMU	C1	2683	1	-	1/9/27/28	0/2/2/2
1	A2M	C1	2289	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	637	1	-	1/9/27/28	0/3/3/3
1	OMG	C1	2774	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	389	1	-	3/9/27/28	0/3/3/3
1	OMG	C1	646	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	1433	1	-	2/9/27/28	0/3/3/3
1	OMC	C1	1491	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	2838	1	-	2/9/27/28	0/2/2/2
1	OMU	C1	1868	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1812	1	-	1/9/27/28	0/2/2/2
1	OMG	C1	2578	1	-	3/9/27/28	0/3/3/3
1	OMU	C1	2690	1	-	2/9/27/28	0/2/2/2
1	OMC	C1	2918	1	-	0/9/27/28	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMG	C1	2358	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2277	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	2380	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	2876	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	2384	1	-	1/9/27/28	0/2/2/2
1	OMU	C1	2688	1	-	0/9/27/28	0/2/2/2
1	OMC	C1	1420	1	-	3/9/27/28	0/2/2/2
1	OMG	C1	385	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	848	1	-	1/9/27/28	0/3/3/3
1	OMG	C1	2881	1	-	0/9/27/28	0/3/3/3
1	OMC	C1	1836	1	-	0/9/27/28	0/2/2/2
1	A2M	C1	1223	1	-	1/9/27/28	0/3/3/3
1	A2M	C1	1847	1	-	3/9/27/28	0/3/3/3
1	OMC	C1	2300	1	-	0/9/27/28	0/2/2/2
1	OMG	C1	627	1	-	0/9/27/28	0/3/3/3
1	OMU	C1	1917	1	-	2/9/27/28	0/2/2/2
1	A2M	C1	858	1	-	0/9/27/28	0/3/3/3
1	A2M	C1	1432	1	-	0/9/27/28	0/3/3/3
1	OMG	C1	787	1	-	2/9/27/28	0/3/3/3

All (142) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	2289	A2M	C3'-C2'	-13.25	1.24	1.53
1	C1	858	A2M	C3'-C2'	-13.23	1.24	1.53
1	C1	848	A2M	C3'-C2'	-12.97	1.24	1.53
1	C1	637	A2M	C3'-C2'	-12.96	1.24	1.53
1	C1	1223	A2M	C3'-C2'	-12.96	1.24	1.53
1	C1	1847	A2M	C3'-C2'	-12.91	1.24	1.53
1	C1	1432	A2M	C3'-C2'	-12.87	1.24	1.53
1	C1	389	A2M	C3'-C2'	-12.82	1.24	1.53
1	C1	1917	OMU	C2-N1	7.58	1.50	1.38
1	C1	2384	OMU	C2-N1	7.48	1.50	1.38
1	C1	2277	OMU	C2-N1	7.38	1.50	1.38
1	C1	2683	OMU	C2-N1	7.33	1.49	1.38
1	C1	1868	OMU	C2-N1	7.32	1.49	1.38
1	C1	2384	OMU	C2-N3	7.28	1.50	1.38
1	C1	2688	OMU	C2-N1	7.27	1.49	1.38
1	C1	2380	OMU	C2-N1	7.20	1.49	1.38
1	C1	2380	OMU	C2-N3	7.19	1.50	1.38
1	C1	2277	OMU	C2-N3	7.18	1.50	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1868	OMU	C2-N3	7.16	1.50	1.38
1	C1	2683	OMU	C2-N3	7.16	1.50	1.38
1	C1	2688	OMU	C2-N3	7.08	1.50	1.38
1	C1	2690	OMU	C2-N3	6.97	1.50	1.38
1	C1	2690	OMU	C2-N1	6.93	1.49	1.38
1	C1	1917	OMU	C2-N3	6.81	1.49	1.38
1	C1	389	A2M	O4'-C4'	-6.76	1.30	1.45
1	C1	637	A2M	O4'-C4'	-6.72	1.30	1.45
1	C1	1223	A2M	O4'-C4'	-6.67	1.30	1.45
1	C1	2289	A2M	O4'-C4'	-6.62	1.30	1.45
1	C1	1847	A2M	O4'-C4'	-6.54	1.30	1.45
1	C1	1432	A2M	O4'-C4'	-6.52	1.30	1.45
1	C1	858	A2M	O4'-C4'	-6.51	1.30	1.45
1	C1	848	A2M	O4'-C4'	-6.49	1.30	1.45
1	C1	2688	OMU	C6-C5	6.16	1.49	1.35
1	C1	2277	OMU	C6-C5	6.13	1.49	1.35
1	C1	2384	OMU	C6-C5	6.12	1.49	1.35
1	C1	1917	OMU	C6-C5	6.12	1.49	1.35
1	C1	1868	OMU	C6-C5	6.10	1.49	1.35
1	C1	2380	OMU	C6-C5	6.00	1.49	1.35
1	C1	2683	OMU	C6-C5	5.97	1.48	1.35
1	C1	2690	OMU	C6-C5	5.94	1.48	1.35
1	C1	858	A2M	C3'-C4'	5.28	1.66	1.53
1	C1	1432	A2M	C3'-C4'	5.20	1.66	1.53
1	C1	1223	A2M	C3'-C4'	5.17	1.66	1.53
1	C1	2289	A2M	C3'-C4'	5.16	1.66	1.53
1	C1	848	A2M	C3'-C4'	5.15	1.66	1.53
1	C1	1847	A2M	C3'-C4'	4.98	1.65	1.53
1	C1	389	A2M	C3'-C4'	4.96	1.65	1.53
1	C1	637	A2M	C3'-C4'	4.87	1.65	1.53
1	C1	848	A2M	C1'-N9	-4.62	1.33	1.46
1	C1	2289	A2M	C1'-N9	-4.53	1.33	1.46
1	C1	1847	A2M	O4'-C1'	4.49	1.52	1.42
1	C1	2289	A2M	O4'-C1'	4.46	1.52	1.42
1	C1	858	A2M	O4'-C1'	4.44	1.52	1.42
1	C1	2380	OMU	C4-N3	4.39	1.46	1.38
1	C1	1223	A2M	C1'-N9	-4.38	1.34	1.46
1	C1	637	A2M	C1'-N9	-4.37	1.34	1.46
1	C1	1432	A2M	O4'-C1'	4.36	1.52	1.42
1	C1	389	A2M	C6-N6	4.34	1.45	1.34
1	C1	848	A2M	O4'-C1'	4.32	1.52	1.42
1	C1	858	A2M	C6-N6	4.32	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	637	A2M	C6-N6	4.32	1.45	1.34
1	C1	2384	OMU	C4-N3	4.29	1.46	1.38
1	C1	858	A2M	C1'-N9	-4.29	1.34	1.46
1	C1	389	A2M	O4'-C1'	4.28	1.51	1.42
1	C1	389	A2M	C1'-N9	-4.25	1.34	1.46
1	C1	1432	A2M	C6-N6	4.24	1.45	1.34
1	C1	1223	A2M	C6-N6	4.24	1.45	1.34
1	C1	2688	OMU	C4-N3	4.24	1.45	1.38
1	C1	2277	OMU	C4-N3	4.24	1.45	1.38
1	C1	1847	A2M	C1'-N9	-4.23	1.34	1.46
1	C1	2289	A2M	C6-N6	4.23	1.45	1.34
1	C1	1847	A2M	C6-N6	4.23	1.45	1.34
1	C1	1432	A2M	C1'-N9	-4.20	1.34	1.46
1	C1	848	A2M	C6-N6	4.20	1.44	1.34
1	C1	2690	OMU	C4-N3	4.19	1.45	1.38
1	C1	637	A2M	O4'-C1'	4.18	1.51	1.42
1	C1	2683	OMU	C4-N3	4.17	1.45	1.38
1	C1	1223	A2M	O4'-C1'	4.13	1.51	1.42
1	C1	1917	OMU	C4-N3	4.05	1.45	1.38
1	C1	1868	OMU	C4-N3	4.00	1.45	1.38
1	C1	389	A2M	O2'-C2'	3.95	1.52	1.42
1	C1	1432	A2M	O2'-C2'	3.61	1.51	1.42
1	C1	637	A2M	O2'-C2'	3.55	1.51	1.42
1	C1	1223	A2M	O2'-C2'	3.52	1.51	1.42
1	C1	1847	A2M	O2'-C2'	3.50	1.51	1.42
1	C1	858	A2M	O2'-C2'	3.49	1.51	1.42
1	C1	2289	A2M	O2'-C2'	3.42	1.51	1.42
1	C1	848	A2M	O2'-C2'	3.41	1.51	1.42
1	C1	848	A2M	C5-C4	-3.30	1.33	1.39
1	C1	2289	A2M	C5-C4	-3.24	1.33	1.39
1	C1	858	A2M	C5-C4	-3.23	1.33	1.39
1	C1	389	A2M	C2'-C1'	3.18	1.61	1.53
1	C1	1223	A2M	C5-C4	-3.18	1.33	1.39
1	C1	1432	A2M	C5-C4	-3.17	1.33	1.39
1	C1	389	A2M	C5-C4	-3.14	1.33	1.39
1	C1	1847	A2M	C5-C4	-3.05	1.33	1.39
1	C1	389	A2M	C5-N7	-3.03	1.33	1.39
1	C1	637	A2M	C5-C4	-3.02	1.33	1.39
1	C1	1847	A2M	C2'-C1'	2.99	1.60	1.53
1	C1	858	A2M	C2'-C1'	2.91	1.60	1.53
1	C1	1432	A2M	C5-N7	-2.90	1.33	1.39
1	C1	848	A2M	C2'-C1'	2.90	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C1	1223	A2M	C5-N7	-2.88	1.33	1.39
1	C1	1432	A2M	C2'-C1'	2.86	1.60	1.53
1	C1	637	A2M	C2'-C1'	2.86	1.60	1.53
1	C1	1847	A2M	C5-N7	-2.84	1.33	1.39
1	C1	858	A2M	C5-N7	-2.82	1.33	1.39
1	C1	2289	A2M	C2'-C1'	2.82	1.60	1.53
1	C1	1223	A2M	C2'-C1'	2.78	1.60	1.53
1	C1	637	A2M	C5-N7	-2.77	1.34	1.39
1	C1	1917	OMU	C6-N1	2.65	1.44	1.38
1	C1	2688	OMU	C6-N1	2.63	1.44	1.38
1	C1	2380	OMU	C6-N1	2.61	1.44	1.38
1	C1	2384	OMU	C6-N1	2.60	1.44	1.38
1	C1	2277	OMU	C6-N1	2.58	1.44	1.38
1	C1	848	A2M	C5-N7	-2.56	1.34	1.39
1	C1	1868	OMU	C6-N1	2.54	1.44	1.38
1	C1	2289	A2M	C5-N7	-2.54	1.34	1.39
1	C1	2683	OMU	C6-N1	2.50	1.44	1.38
1	C1	2690	OMU	C6-N1	2.49	1.44	1.38
1	C1	1847	A2M	C8-N9	-2.27	1.33	1.37
1	C1	1223	A2M	C8-N9	-2.25	1.33	1.37
1	C1	1432	A2M	C8-N9	-2.24	1.33	1.37
1	C1	848	A2M	C8-N9	-2.22	1.33	1.37
1	C1	2688	OMU	C5-C4	2.21	1.48	1.43
1	C1	2380	OMU	C5-C4	2.18	1.48	1.43
1	C1	1868	OMU	C5-C4	2.18	1.48	1.43
1	C1	858	A2M	C8-N9	-2.17	1.33	1.37
1	C1	2384	OMU	C5-C4	2.16	1.48	1.43
1	C1	389	A2M	C8-N9	-2.14	1.33	1.37
1	C1	2277	OMU	C5-C4	2.13	1.48	1.43
1	C1	1917	OMU	C5-C4	2.13	1.48	1.43
1	C1	2683	OMU	C5-C4	2.13	1.48	1.43
1	C1	637	A2M	C8-N9	-2.11	1.34	1.37
1	C1	2289	A2M	C8-N9	-2.09	1.34	1.37
1	C1	1847	A2M	O3'-C3'	2.09	1.48	1.43
1	C1	848	A2M	O3'-C3'	2.07	1.48	1.43
1	C1	2289	A2M	C4-N9	-2.06	1.33	1.37
1	C1	1432	A2M	O3'-C3'	2.06	1.48	1.43
1	C1	2838	OMC	C4-N3	-2.05	1.30	1.34
1	C1	2690	OMU	C5-C4	2.05	1.48	1.43
1	C1	2690	OMU	O4-C4	-2.01	1.20	1.24

All (156) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	1847	A2M	C1'-N9-C8	-9.19	106.71	127.09
1	C1	1432	A2M	C1'-N9-C8	-9.18	106.73	127.09
1	C1	637	A2M	C1'-N9-C8	-9.03	107.05	127.09
1	C1	858	A2M	C1'-N9-C8	-9.03	107.06	127.09
1	C1	1223	A2M	C1'-N9-C8	-8.90	107.35	127.09
1	C1	389	A2M	C1'-N9-C8	-8.89	107.36	127.09
1	C1	848	A2M	C1'-N9-C8	-8.67	107.85	127.09
1	C1	2289	A2M	C1'-N9-C8	-8.29	108.69	127.09
1	C1	1432	A2M	C4-N9-C1'	8.15	145.70	126.63
1	C1	1847	A2M	C4-N9-C1'	8.06	145.47	126.63
1	C1	858	A2M	C4-N9-C1'	7.87	145.03	126.63
1	C1	637	A2M	C4-N9-C1'	7.87	145.03	126.63
1	C1	389	A2M	C4-N9-C1'	7.83	144.95	126.63
1	C1	1223	A2M	C4-N9-C1'	7.67	144.57	126.63
1	C1	848	A2M	C4-N9-C1'	7.13	143.30	126.63
1	C1	2289	A2M	C4-N9-C1'	6.86	142.67	126.63
1	C1	858	A2M	N3-C2-N1	-6.23	119.16	128.58
1	C1	858	A2M	N6-C6-N1	-6.04	104.92	118.38
1	C1	2289	A2M	N3-C2-N1	-6.04	119.44	128.58
1	C1	1847	A2M	N3-C2-N1	-6.00	119.50	128.58
1	C1	1812	OMC	CM2-O2'-C2'	5.88	129.56	114.47
1	C1	1868	OMU	C4-N3-C2	-5.86	119.33	126.61
1	C1	1223	A2M	N3-C2-N1	-5.84	119.74	128.58
1	C1	1432	A2M	N3-C2-N1	-5.83	119.76	128.58
1	C1	1847	A2M	N6-C6-N1	-5.81	105.43	118.38
1	C1	848	A2M	N3-C2-N1	-5.79	119.81	128.58
1	C1	2289	A2M	N6-C6-N1	-5.76	105.56	118.38
1	C1	848	A2M	N6-C6-N1	-5.75	105.56	118.38
1	C1	389	A2M	N3-C2-N1	-5.75	119.88	128.58
1	C1	389	A2M	N6-C6-N1	-5.65	105.78	118.38
1	C1	2690	OMU	C4-N3-C2	-5.64	119.61	126.61
1	C1	637	A2M	N3-C2-N1	-5.60	120.10	128.58
1	C1	1223	A2M	N6-C6-N1	-5.58	105.95	118.38
1	C1	2688	OMU	C4-N3-C2	-5.55	119.72	126.61
1	C1	637	A2M	N6-C6-N1	-5.54	106.03	118.38
1	C1	1432	A2M	N6-C6-N1	-5.45	106.23	118.38
1	C1	2683	OMU	C4-N3-C2	-5.44	119.86	126.61
1	C1	2384	OMU	C4-N3-C2	-5.42	119.88	126.61
1	C1	1917	OMU	C4-N3-C2	-5.41	119.89	126.61
1	C1	2380	OMU	C4-N3-C2	-5.41	119.90	126.61
1	C1	2277	OMU	C4-N3-C2	-5.35	119.97	126.61
1	C1	1432	A2M	C5-C4-N3	-4.95	119.90	126.72
1	C1	1847	A2M	C5-C4-N3	-4.88	120.00	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	389	A2M	C5-C4-N3	-4.84	120.05	126.72
1	C1	858	A2M	C5-C6-N6	4.79	135.14	123.29
1	C1	2838	OMC	C1'-N1-C2	4.73	128.90	118.44
1	C1	858	A2M	C5-C4-N3	-4.73	120.21	126.72
1	C1	1223	A2M	C5-C4-N3	-4.68	120.27	126.72
1	C1	848	A2M	N9-C8-N7	-4.66	107.32	113.94
1	C1	2289	A2M	C5-C6-N6	4.59	134.66	123.29
1	C1	2289	A2M	N9-C8-N7	-4.59	107.43	113.94
1	C1	637	A2M	C5-C4-N3	-4.58	120.42	126.72
1	C1	389	A2M	C5-C6-N6	4.55	134.56	123.29
1	C1	1847	A2M	C5-C6-N6	4.52	134.48	123.29
1	C1	848	A2M	C2'-C1'-N9	-4.51	106.32	113.75
1	C1	637	A2M	C5-C6-N6	4.48	134.38	123.29
1	C1	848	A2M	C5-C4-N3	-4.45	120.59	126.72
1	C1	848	A2M	C5-C6-N6	4.41	134.22	123.29
1	C1	1223	A2M	C5-C6-N6	4.40	134.17	123.29
1	C1	2289	A2M	O4'-C1'-N9	4.34	116.42	108.09
1	C1	1868	OMU	N3-C2-N1	4.31	120.51	114.89
1	C1	1432	A2M	C5-C6-N6	4.28	133.88	123.29
1	C1	848	A2M	O4'-C1'-N9	4.22	116.19	108.09
1	C1	389	A2M	N9-C8-N7	-4.13	108.07	113.94
1	C1	1917	OMU	N3-C2-N1	4.13	120.27	114.89
1	C1	1223	A2M	N9-C8-N7	-4.12	108.08	113.94
1	C1	858	A2M	O4'-C1'-N9	4.12	116.00	108.09
1	C1	2384	OMU	N3-C2-N1	4.08	120.20	114.89
1	C1	1847	A2M	N9-C8-N7	-4.07	108.16	113.94
1	C1	858	A2M	N9-C8-N7	-4.06	108.17	113.94
1	C1	1420	OMC	C1'-N1-C2	4.05	127.38	118.44
1	C1	637	A2M	N9-C8-N7	-4.02	108.24	113.94
1	C1	2289	A2M	C5-C4-N3	-4.01	121.19	126.72
1	C1	2688	OMU	N3-C2-N1	3.98	120.07	114.89
1	C1	1223	A2M	O4'-C1'-N9	3.95	115.68	108.09
1	C1	1432	A2M	O4'-C1'-N9	3.86	115.50	108.09
1	C1	2690	OMU	N3-C2-N1	3.79	119.82	114.89
1	C1	2683	OMU	N3-C2-N1	3.76	119.79	114.89
1	C1	1432	A2M	N9-C8-N7	-3.76	108.61	113.94
1	C1	1847	A2M	O4'-C1'-N9	3.73	115.26	108.09
1	C1	2277	OMU	N3-C2-N1	3.72	119.74	114.89
1	C1	2380	OMU	N3-C2-N1	3.69	119.69	114.89
1	C1	2690	OMU	C5-C4-N3	3.68	119.96	114.80
1	C1	2683	OMU	C5-C4-N3	3.61	119.85	114.80
1	C1	2380	OMU	C5-C4-N3	3.57	119.80	114.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	2688	OMU	C5-C4-N3	3.57	119.80	114.80
1	C1	2277	OMU	C5-C4-N3	3.57	119.80	114.80
1	C1	1432	A2M	C2-N3-C4	3.57	120.54	111.83
1	C1	637	A2M	O4'-C1'-N9	3.54	114.89	108.09
1	C1	1868	OMU	C5-C4-N3	3.54	119.76	114.80
1	C1	1847	A2M	C2-N3-C4	3.53	120.45	111.83
1	C1	858	A2M	C2-N3-C4	3.53	120.44	111.83
1	C1	1917	OMU	C5-C4-N3	3.52	119.73	114.80
1	C1	2838	OMC	C1'-N1-C6	-3.51	113.28	120.78
1	C1	389	A2M	O4'-C1'-N9	3.50	114.80	108.09
1	C1	2384	OMU	C5-C4-N3	3.39	119.55	114.80
1	C1	389	A2M	C2-N3-C4	3.35	120.02	111.83
1	C1	1223	A2M	C2-N3-C4	3.33	119.96	111.83
1	C1	848	A2M	C2-N3-C4	3.33	119.95	111.83
1	C1	637	A2M	C2-N3-C4	3.18	119.60	111.83
1	C1	2289	A2M	C2-N3-C4	3.18	119.59	111.83
1	C1	2690	OMU	O4-C4-C5	-3.04	119.92	125.16
1	C1	848	A2M	C5-N7-C8	3.03	108.21	103.45
1	C1	2838	OMC	O2-C2-N3	-3.01	117.58	122.33
1	C1	389	A2M	C5-N7-C8	3.01	108.19	103.45
1	C1	2683	OMU	O4-C4-C5	-3.00	120.00	125.16
1	C1	2380	OMU	O4-C4-C5	-2.99	120.01	125.16
1	C1	2384	OMU	O4-C4-C5	-2.95	120.07	125.16
1	C1	1432	A2M	N3-C4-N9	2.95	132.18	127.17
1	C1	1847	A2M	C5-N7-C8	2.93	108.06	103.45
1	C1	848	A2M	C4-N9-C8	2.93	108.82	105.74
1	C1	1847	A2M	N3-C4-N9	2.90	132.10	127.17
1	C1	2277	OMU	O4-C4-C5	-2.88	120.19	125.16
1	C1	2289	A2M	C5-N7-C8	2.86	107.95	103.45
1	C1	1223	A2M	N3-C4-N9	2.86	132.03	127.17
1	C1	1812	OMC	C2'-C1'-N1	-2.81	108.91	114.24
1	C1	858	A2M	N3-C4-N9	2.80	131.94	127.17
1	C1	1868	OMU	O4-C4-C5	-2.79	120.35	125.16
1	C1	389	A2M	N3-C4-N9	2.78	131.89	127.17
1	C1	2688	OMU	O4-C4-C5	-2.77	120.38	125.16
1	C1	2289	A2M	C4-N9-C8	2.76	108.64	105.74
1	C1	848	A2M	N3-C4-N9	2.74	131.83	127.17
1	C1	1420	OMC	C1'-N1-C6	-2.74	114.93	120.78
1	C1	1223	A2M	C5-N7-C8	2.74	107.75	103.45
1	C1	637	A2M	N3-C4-N9	2.71	131.78	127.17
1	C1	637	A2M	C5-N7-C8	2.69	107.67	103.45
1	C1	858	A2M	C5-N7-C8	2.65	107.61	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C1	778	OMC	C1'-N1-C2	2.63	124.25	118.44
1	C1	1432	A2M	C5-N7-C8	2.58	107.51	103.45
1	C1	1917	OMU	C1'-N1-C2	2.50	122.07	117.59
1	C1	2838	OMC	O2-C2-N1	2.43	123.65	118.90
1	C1	1917	OMU	O4-C4-C5	-2.42	120.99	125.16
1	C1	1868	OMU	O2-C2-N1	-2.32	119.78	122.80
1	C1	2918	OMC	C1'-N1-C2	2.30	123.52	118.44
1	C1	2289	A2M	C2'-C1'-N9	-2.29	109.99	113.75
1	C1	389	A2M	C4-C5-N7	-2.25	108.01	110.58
1	C1	1223	A2M	C4-N9-C8	2.23	108.08	105.74
1	C1	2289	A2M	N3-C4-N9	2.22	130.94	127.17
1	C1	1847	A2M	C4-C5-N7	-2.21	108.06	110.58
1	C1	848	A2M	C4-C5-N7	-2.19	108.08	110.58
1	C1	2289	A2M	C4'-O4'-C1'	-2.19	104.64	109.47
1	C1	1836	OMC	C1'-N1-C2	2.18	123.26	118.44
1	C1	2289	A2M	C4-C5-N7	-2.16	108.11	110.58
1	C1	2690	OMU	O2-C2-N1	-2.15	120.00	122.80
1	C1	1223	A2M	O4'-C1'-C2'	-2.13	102.93	106.59
1	C1	2688	OMU	O2-C2-N1	-2.09	120.08	122.80
1	C1	1420	OMC	O2-C2-N1	2.07	122.95	118.90
1	C1	637	A2M	C4-N9-C8	2.07	107.91	105.74
1	C1	858	A2M	C4-N9-C8	2.06	107.91	105.74
1	C1	389	A2M	C5-C4-N9	2.06	108.06	105.81
1	C1	389	A2M	C5'-C4'-C3'	-2.06	107.80	115.21
1	C1	787	OMG	C2'-C1'-N9	-2.05	110.34	114.24
1	C1	1847	A2M	C5'-C4'-C3'	-2.02	107.92	115.21
1	C1	389	A2M	C6-C5-C4	2.02	119.94	117.18
1	C1	2384	OMU	C1'-N1-C2	2.02	121.22	117.59
1	C1	2380	OMU	O2-C2-N1	-2.02	120.17	122.80

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C1	389	A2M	O4'-C4'-C5'-O5'
1	C1	389	A2M	C1'-C2'-O2'-CM'
1	C1	637	A2M	C1'-C2'-O2'-CM'
1	C1	1433	OMG	O4'-C4'-C5'-O5'
1	C1	1812	OMC	C3'-C2'-O2'-CM2
1	C1	1917	OMU	O4'-C4'-C5'-O5'
1	C1	2384	OMU	C1'-C2'-O2'-CM2
1	C1	2578	OMG	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
1	C1	2683	OMU	C1'-C2'-O2'-CM2
1	C1	2690	OMU	O4'-C4'-C5'-O5'
1	C1	2838	OMC	O4'-C1'-N1-C2
1	C1	2838	OMC	O4'-C1'-N1-C6
1	C1	1433	OMG	C3'-C4'-C5'-O5'
1	C1	1847	A2M	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C3'-C4'-C5'-O5'
1	C1	2690	OMU	C3'-C4'-C5'-O5'
1	C1	1917	OMU	C3'-C4'-C5'-O5'
1	C1	2578	OMG	C3'-C4'-C5'-O5'
1	C1	389	A2M	C3'-C4'-C5'-O5'
1	C1	848	A2M	O4'-C4'-C5'-O5'
1	C1	2578	OMG	C4'-C5'-O5'-P
1	C1	787	OMG	C3'-C2'-O2'-CM2
1	C1	1223	A2M	O4'-C4'-C5'-O5'
1	C1	1847	A2M	C4'-C5'-O5'-P
1	C1	787	OMG	C1'-C2'-O2'-CM2
1	C1	2277	OMU	C1'-C2'-O2'-CM2
1	C1	1420	OMC	C3'-C2'-O2'-CM2
1	C1	1420	OMC	C2'-C1'-N1-C6
1	C1	1420	OMC	C2'-C1'-N1-C2

There are no ring outliers.

10 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C1	2683	OMU	1	0
1	C1	389	A2M	1	0
1	C1	2838	OMC	1	0
1	C1	1812	OMC	2	0
1	C1	2380	OMU	1	0
1	C1	2384	OMU	2	0
1	C1	1420	OMC	1	0
1	C1	1223	A2M	1	0
1	C1	1917	OMU	1	0
1	C1	1432	A2M	1	0

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 8 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
57	GTP	CH	701	58	33,34,34	0.87	0	50,54,54	1.55	8 (16%)
57	GTP	Cd	1000	58	33,34,34	0.89	0	50,54,54	1.55	8 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
57	GTP	CH	701	58	-	7/22/38/38	0/3/3/3
57	GTP	Cd	1000	58	-	2/22/38/38	0/3/3/3

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	CH	701	GTP	C5-C4-N3	-4.82	120.72	128.39
57	CH	701	GTP	C2-N3-C4	4.54	120.12	112.30
57	Cd	1000	GTP	C5-C4-N3	-4.51	121.21	128.39
57	Cd	1000	GTP	C2-N3-C4	4.37	119.83	112.30
57	CH	701	GTP	N9-C4-N3	3.06	132.06	125.95
57	CH	701	GTP	C2-N1-C6	-2.87	119.91	125.11
57	Cd	1000	GTP	C2-N1-C6	-2.86	119.92	125.11
57	Cd	1000	GTP	N9-C8-N7	-2.81	108.20	113.40
57	Cd	1000	GTP	N9-C4-N3	2.78	131.51	125.95
57	CH	701	GTP	N9-C8-N7	-2.69	108.41	113.40
57	Cd	1000	GTP	O6-C6-C5	-2.53	119.85	126.53
57	CH	701	GTP	C5-C6-N1	2.52	119.67	113.25
57	Cd	1000	GTP	C5-C6-N1	2.45	119.50	113.25
57	CH	701	GTP	C8-N7-C5	2.43	108.60	104.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
57	Cd	1000	GTP	C8-N7-C5	2.43	108.59	104.26
57	CH	701	GTP	O6-C6-C5	-2.34	120.35	126.53

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
57	CH	701	GTP	O4'-C4'-C5'-O5'
57	CH	701	GTP	C3'-C4'-C5'-O5'
57	CH	701	GTP	C5'-O5'-PA-O3A
57	CH	701	GTP	C5'-O5'-PA-O1A
57	CH	701	GTP	C5'-O5'-PA-O2A
57	Cd	1000	GTP	C5'-O5'-PA-O1A
57	CH	701	GTP	PB-O3A-PA-O2A
57	CH	701	GTP	PB-O3A-PA-O1A
57	Cd	1000	GTP	C3'-C4'-C5'-O5'

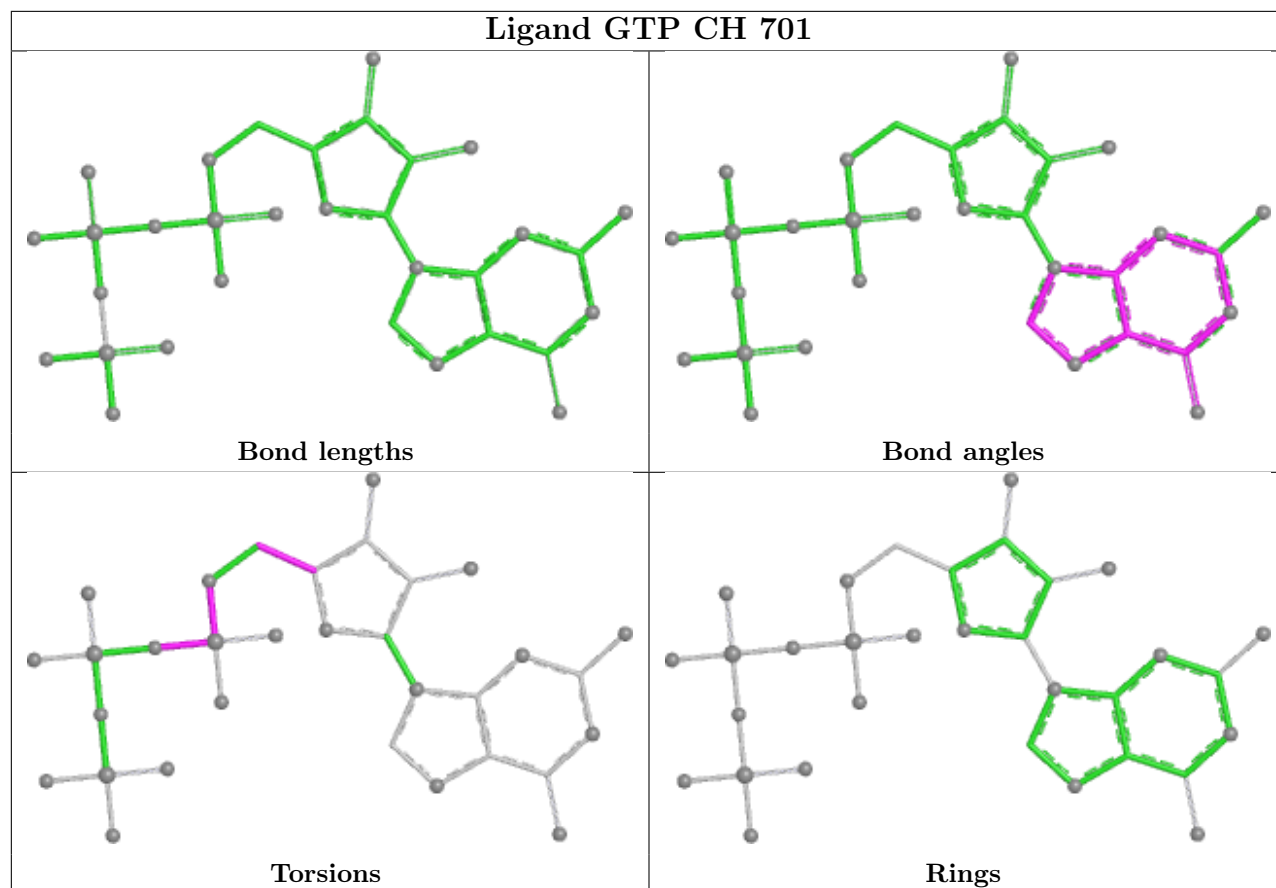
There are no ring outliers.

1 monomer is involved in 1 short contact:

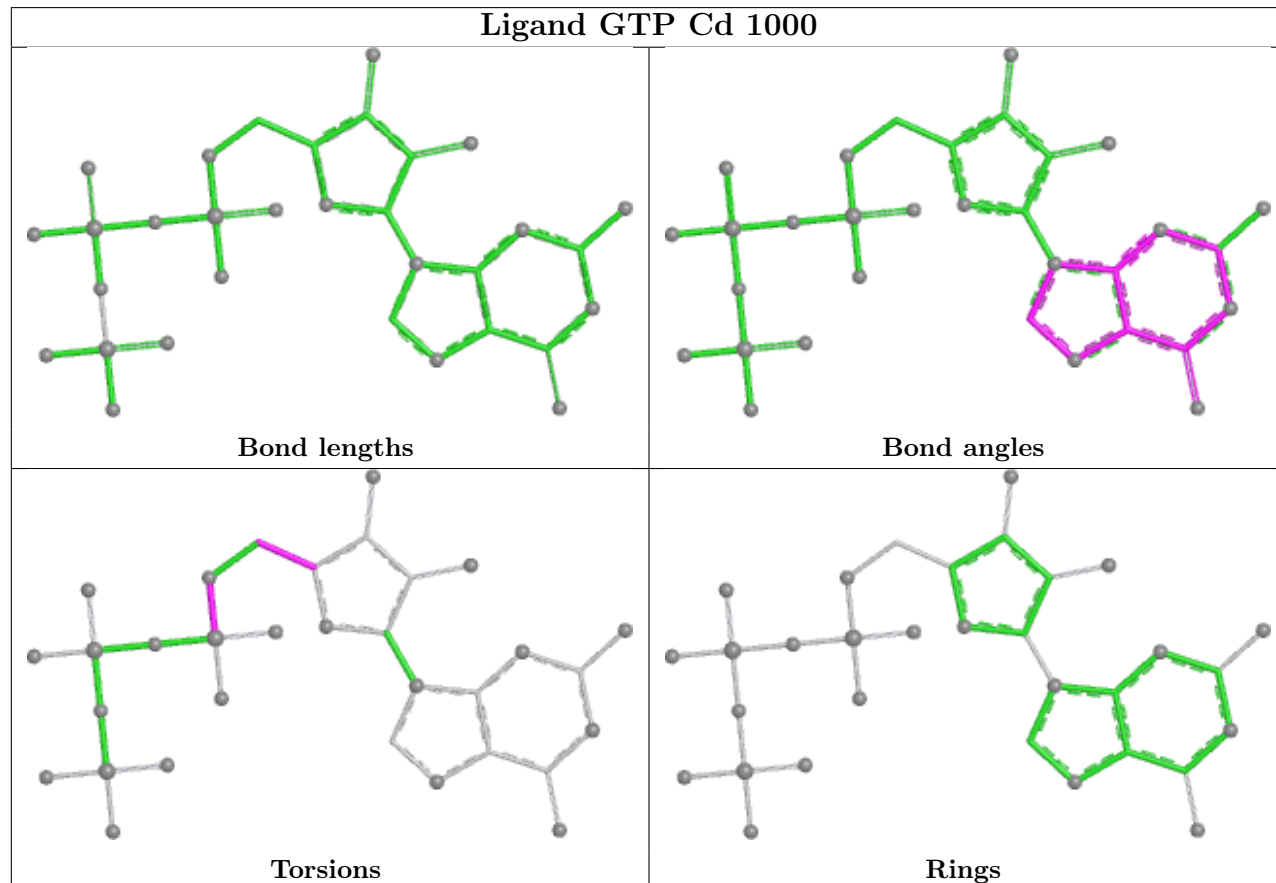
Mol	Chain	Res	Type	Clashes	Symm-Clashes
57	CH	701	GTP	1	0

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

Ligand GTP CH 701



Ligand GTP Cd 1000



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.

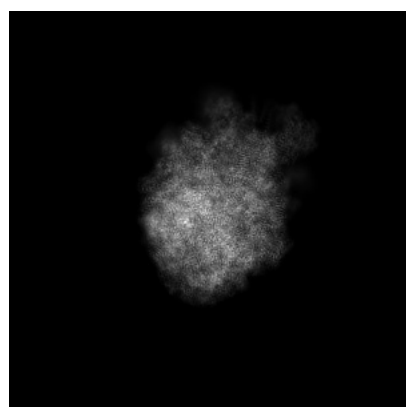
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17951. These allow visual inspection of the internal detail of the map and identification of artifacts.

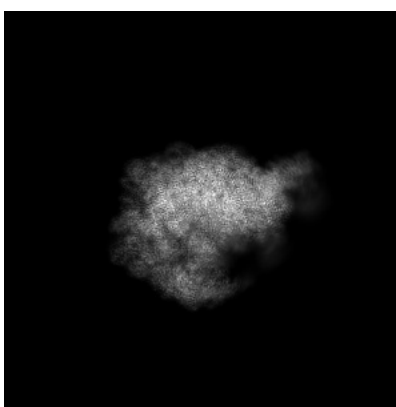
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

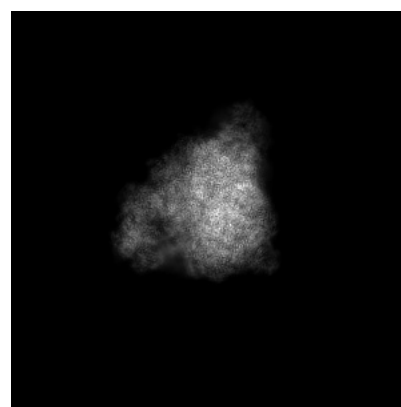
6.1.1 Primary map



X



Y

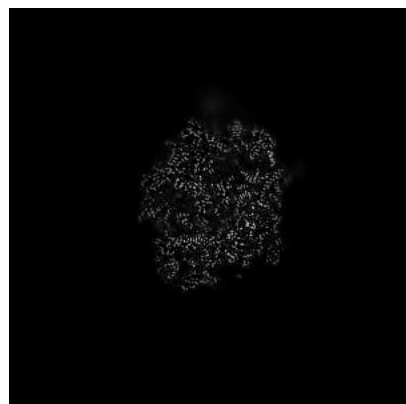


Z

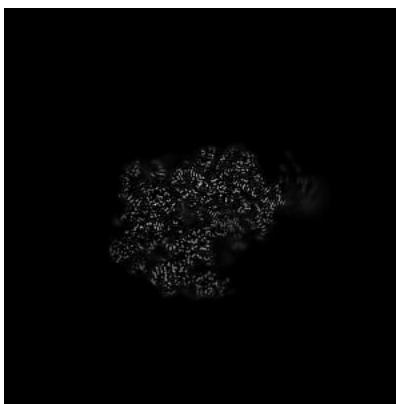
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

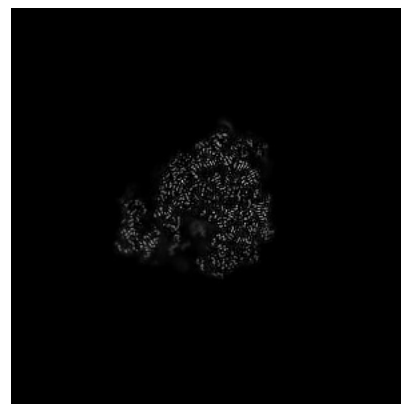
6.2.1 Primary map



X Index: 250



Y Index: 250

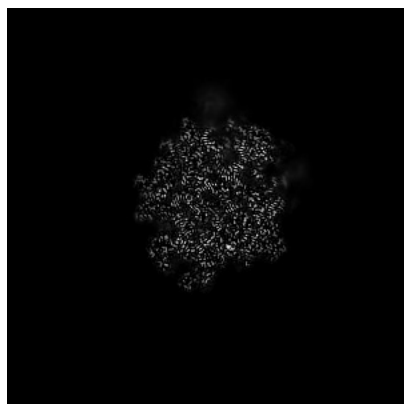


Z Index: 250

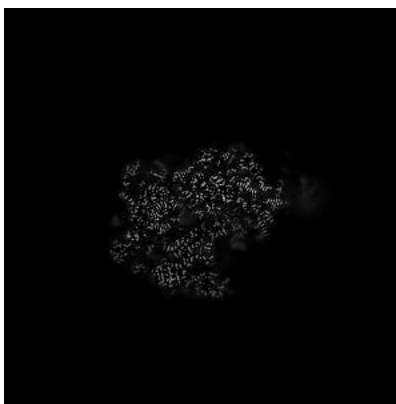
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

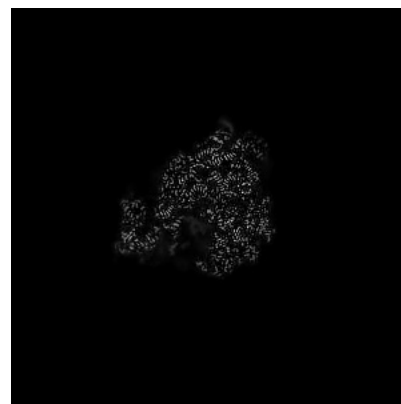
6.3.1 Primary map



X Index: 259



Y Index: 248

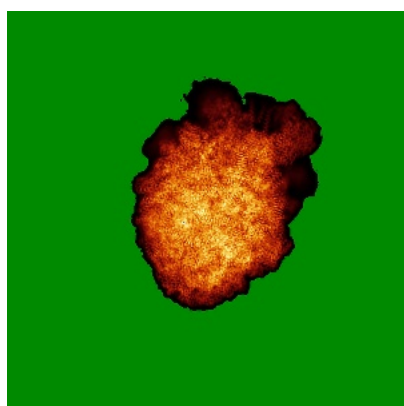


Z Index: 252

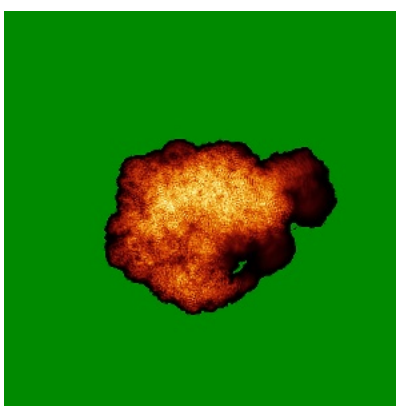
The images above show the largest variance slices of the map in three orthogonal directions.

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

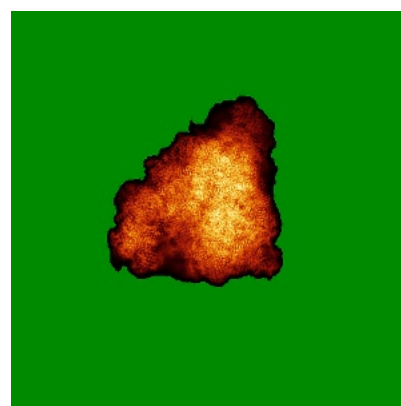
6.4.1 Primary map



X



Y

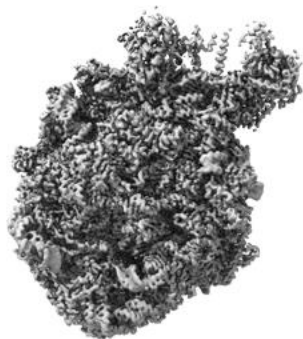


Z

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](#)

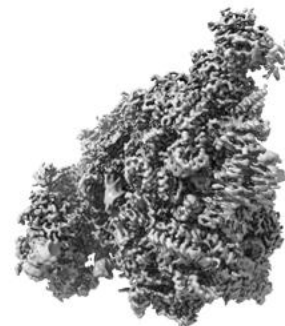
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.7. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

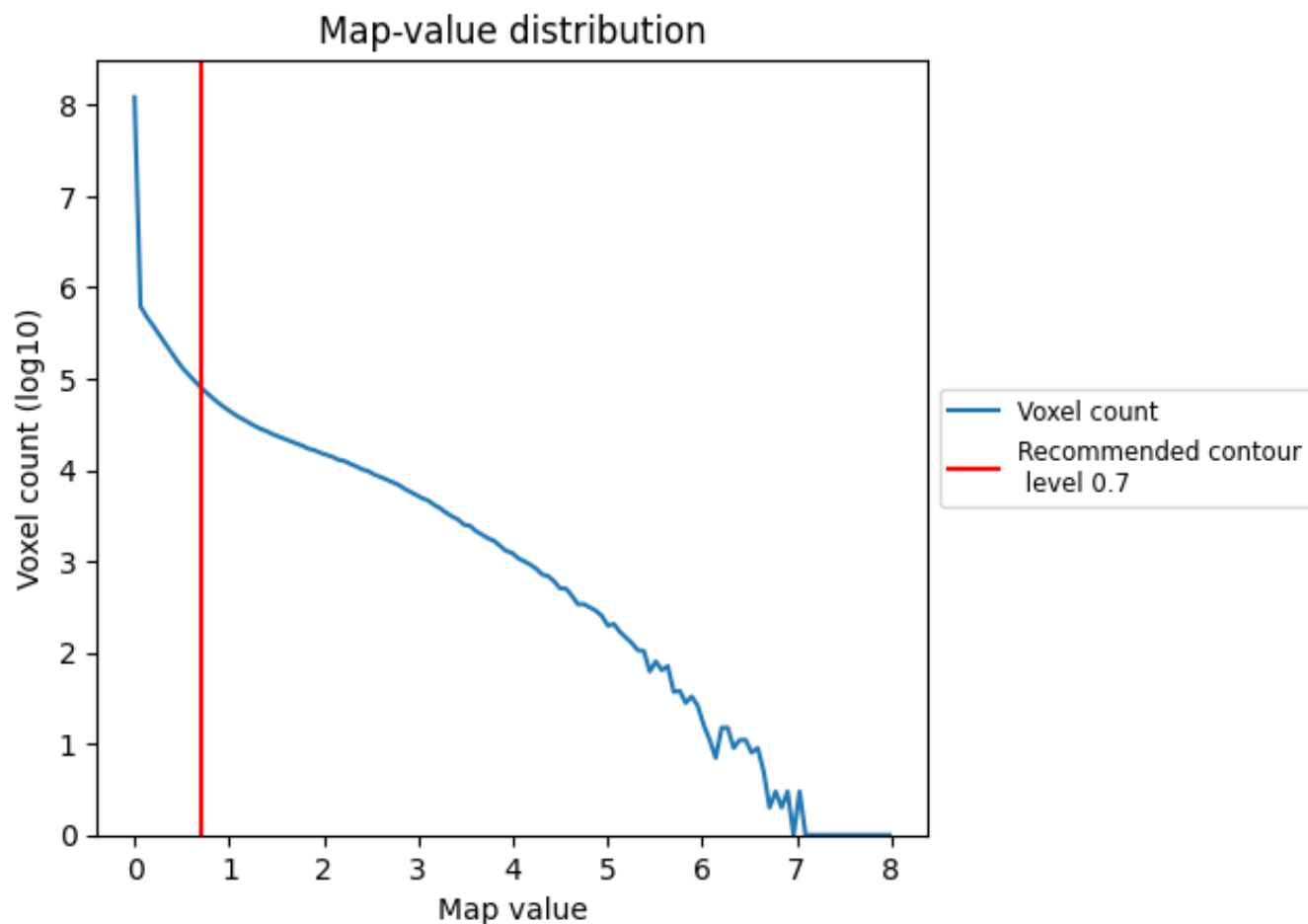
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

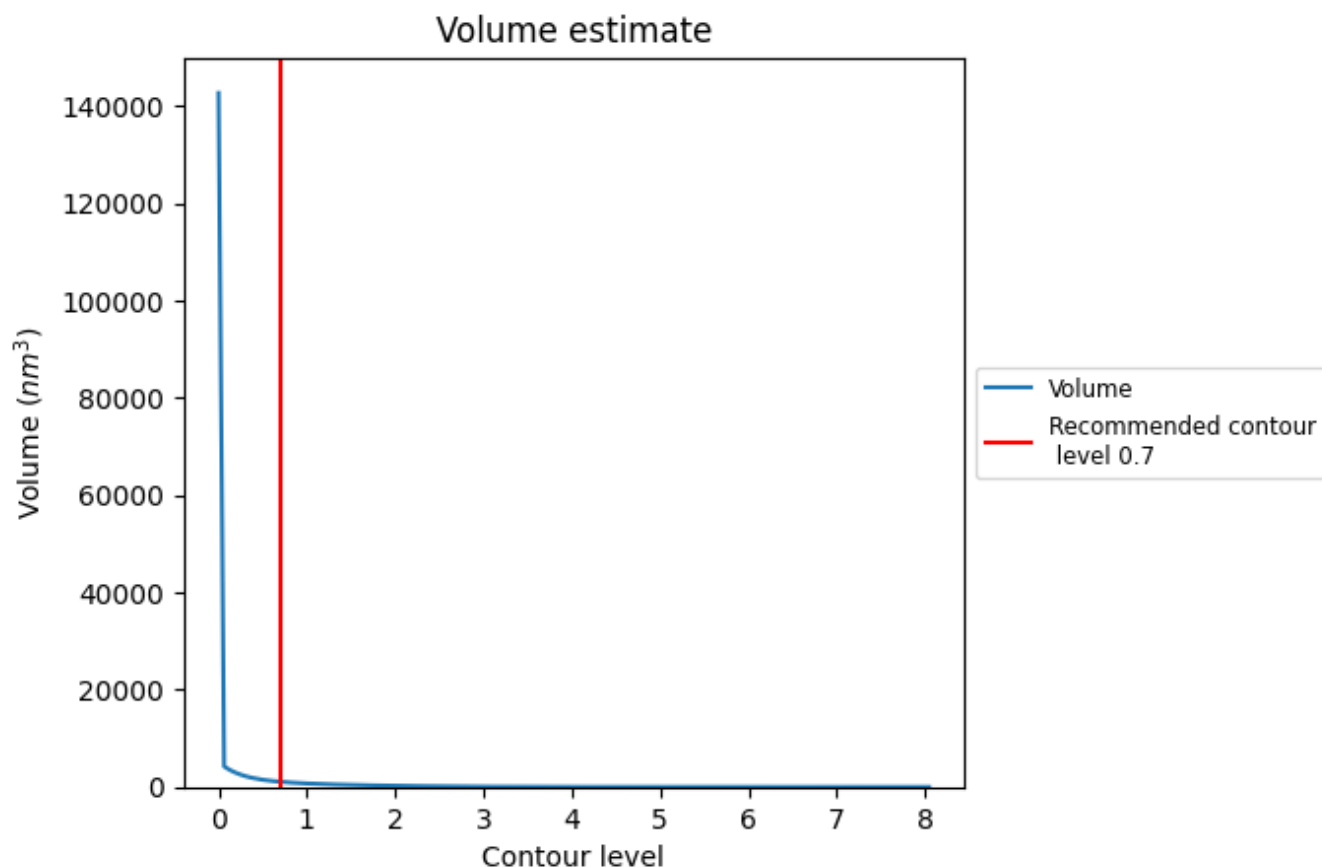
This section contains the results of statistical analysis of the map.

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.

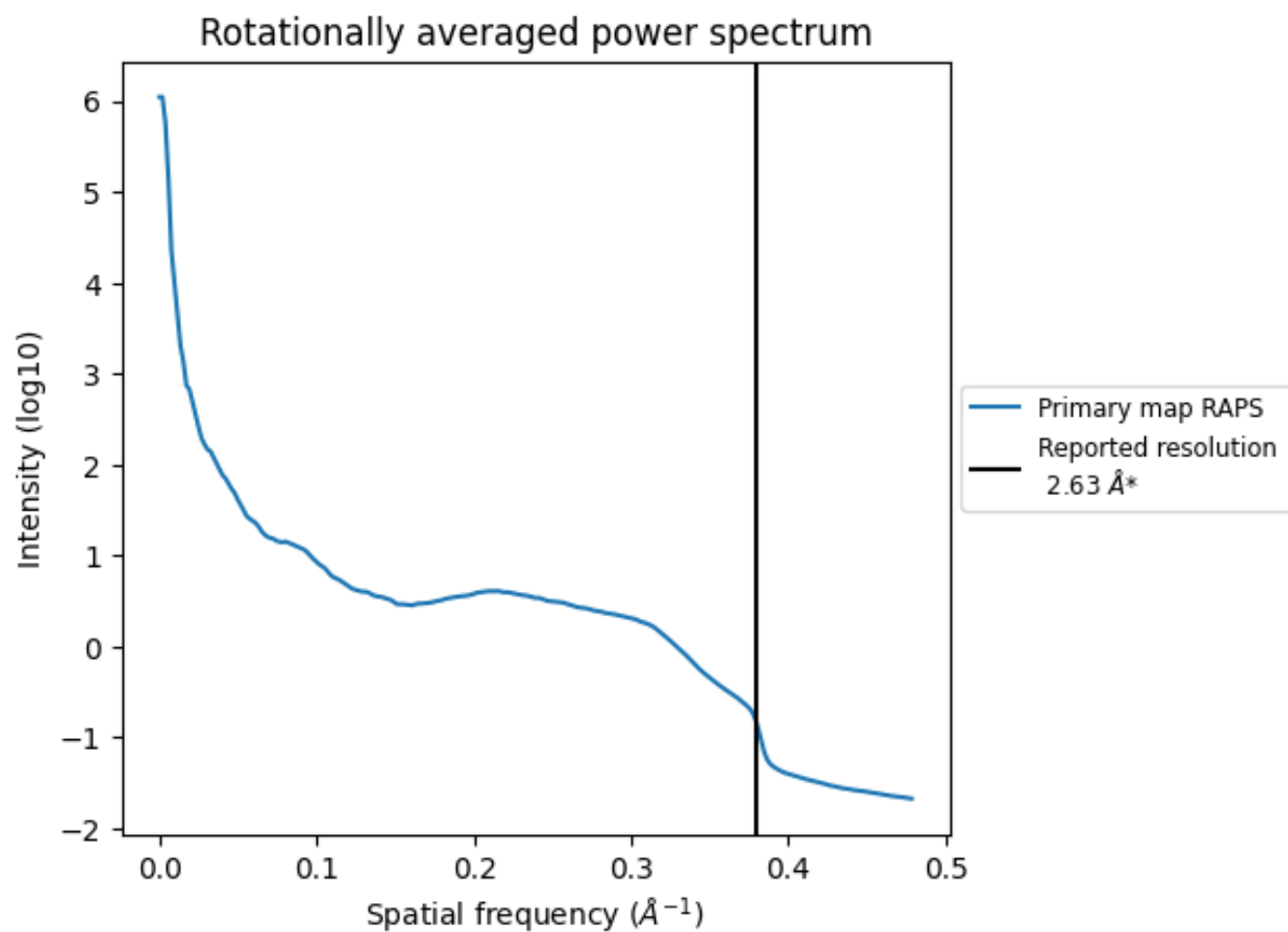
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1068 nm³; this corresponds to an approximate mass of 965 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 0.380 Å⁻¹

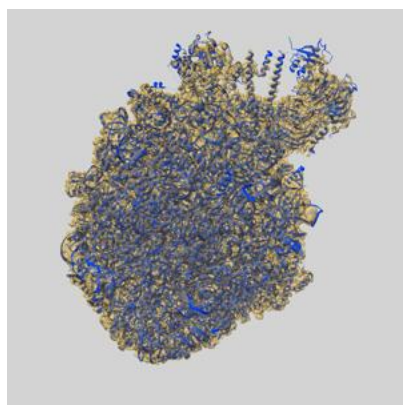
8 Fourier-Shell correlation

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

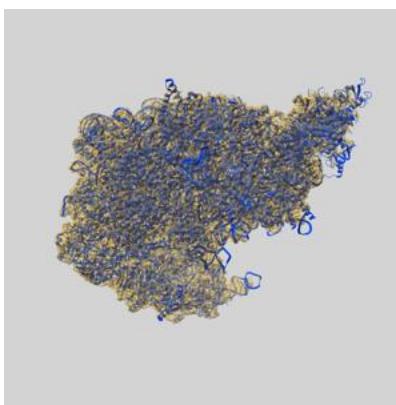
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-17951 and PDB model 8PV2. Per-residue inclusion information can be found in section [3](#) on page [16](#).

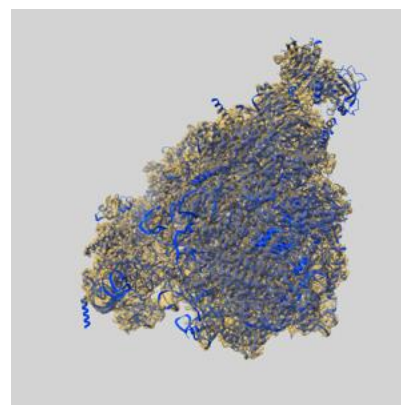
9.1 Map-model overlay [i](#)



X



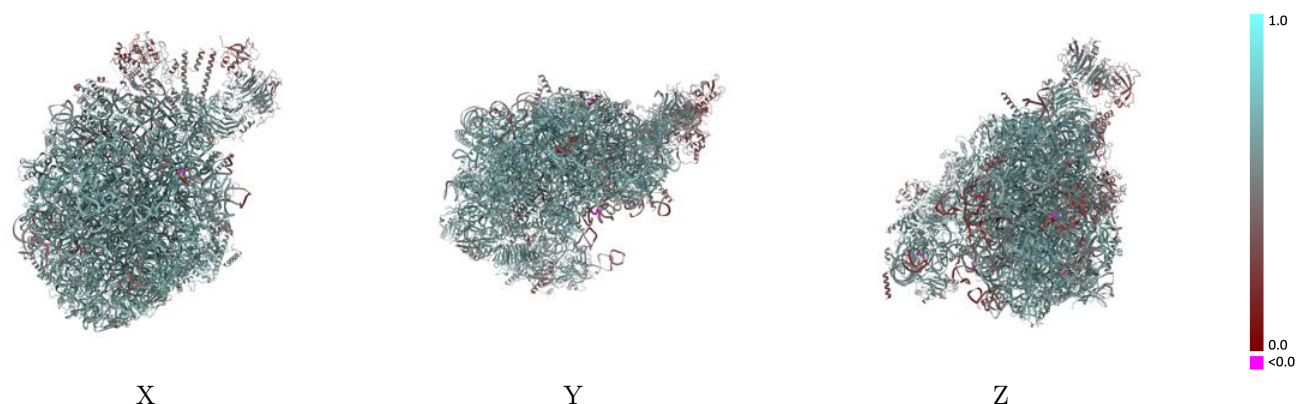
Y



Z

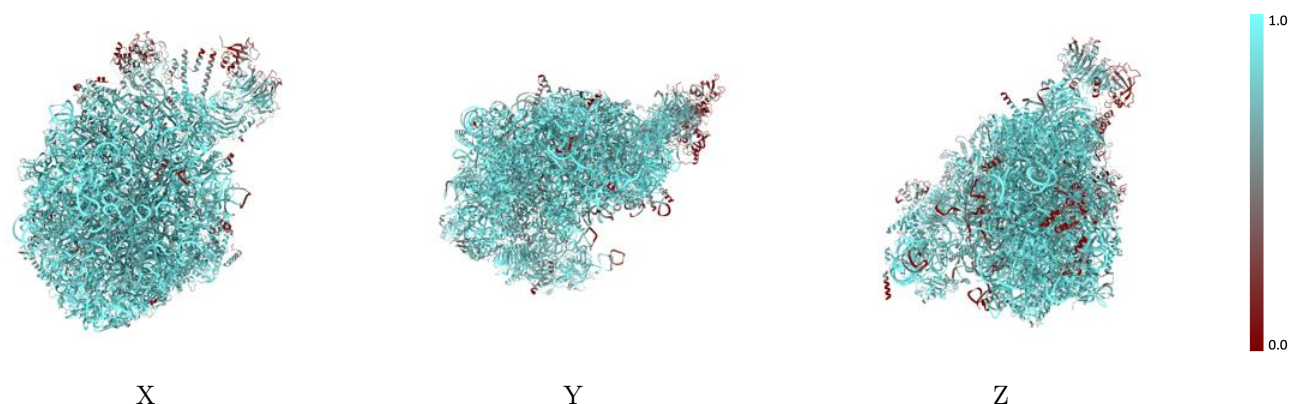
The images above show the 3D surface view of the map at the recommended contour level 0.7 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



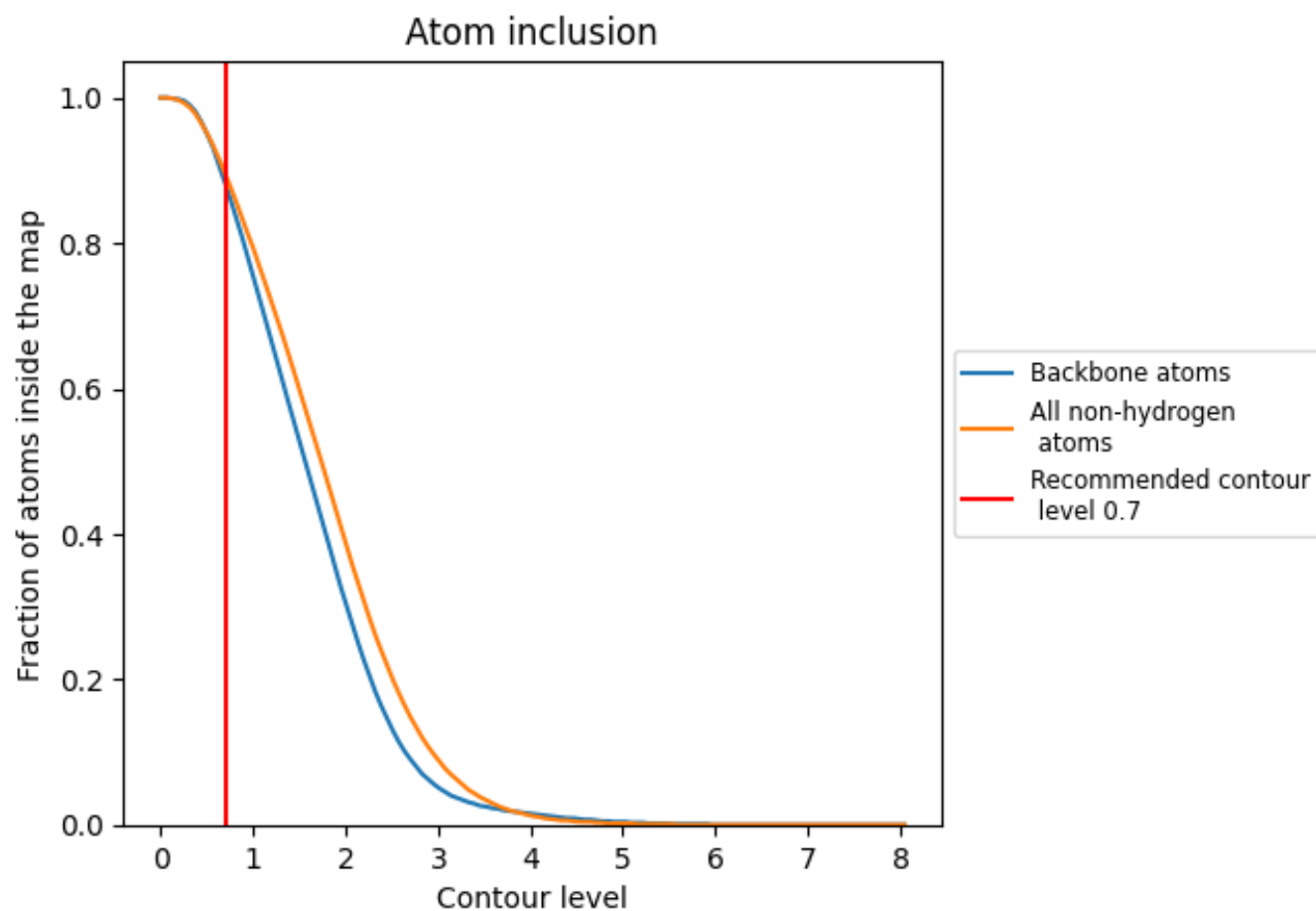
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.7).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 90% 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 (0.7) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8950	 0.6000
C1	 0.9400	 0.6070
C2	 0.9850	 0.6490
C4	 0.8850	 0.5460
CC	 0.8020	 0.5510
CD	 0.5410	 0.4540
CF	 0.8550	 0.5830
CH	 0.8550	 0.6040
CJ	 0.6710	 0.4640
CK	 0.9490	 0.6510
CL	 0.8040	 0.5690
CM	 0.2020	 0.2870
CN	 0.9210	 0.6280
CO	 0.8270	 0.6100
CQ	 0.8340	 0.6030
Cb	 0.9210	 0.6280
Cd	 0.9140	 0.6220
Cf	 0.9090	 0.5990
Cg	 0.8630	 0.5730
Ch	 0.8510	 0.5820
Cz	 0.7610	 0.5310
LA	 0.9100	 0.6250
LB	 0.9560	 0.6650
LC	 0.9470	 0.6460
LD	 0.8810	 0.5830
LE	 0.8510	 0.5890
LF	 0.9110	 0.6310
LG	 0.8580	 0.5820
LH	 0.9150	 0.6360
LJ	 0.8540	 0.5390
LK	 0.7600	 0.5280
LL	 0.8740	 0.6080
LM	 0.9230	 0.6290
LN	 0.9550	 0.6540
LO	 0.9670	 0.6630



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Chain	Atom inclusion	Q-score
LP	 0.9510	 0.6540
LQ	 0.9050	 0.6200
LR	 0.9280	 0.6290
LS	 0.9410	 0.6380
LT	 0.7370	 0.5190
LU	 0.8560	 0.5800
LV	 0.9600	 0.6610
LX	 0.9240	 0.6140
LY	 0.9150	 0.6260
LZ	 0.9320	 0.6090
La	 0.9210	 0.6240
Lc	 0.8820	 0.5940
Ld	 0.9210	 0.6520
Le	 0.9550	 0.6590
Lf	 0.9760	 0.6700
Lg	 0.9000	 0.6120
Lh	 0.8860	 0.6000
Li	 0.8190	 0.5650
Lj	 0.9810	 0.6780
Lk	 0.8190	 0.5470
Ll	 0.9880	 0.6830
Lp	 0.8750	 0.6000
Lq	 0.9180	 0.6140