



Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 07:26 PM UTC

PDB ID : 8I9P / pdb_00008i9p
EMDB ID : EMD-35279
Title : Cryo-EM structure of a Chaetomium thermophilum pre-60S ribosomal subunit
- State Mak16
Authors : Lau, B.; Huang, Z.; Beckmann, R.; Hurt, E.; Cheng, J.
Deposited on : 2023-02-07
Resolution : 3.00 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
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

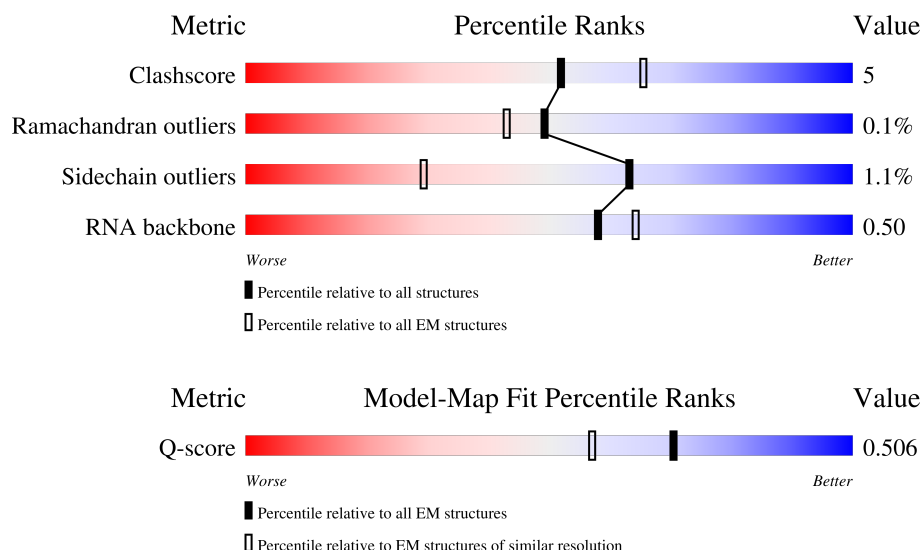
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.00 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.



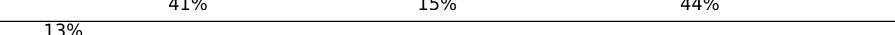
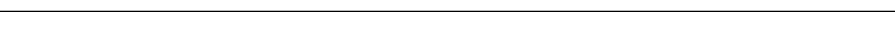
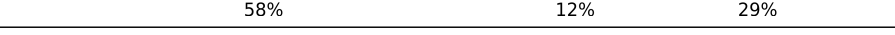
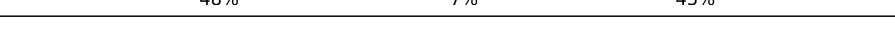
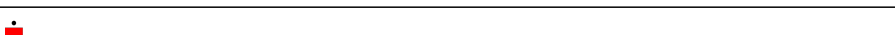
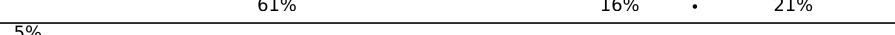
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	3341	
2	C2	306	
3	CA	316	

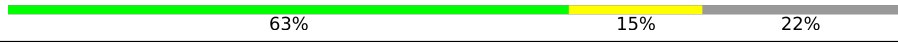
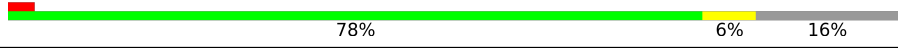
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Mol	Chain	Length	Quality of chain
4	CB	391	
5	CC	801	
6	CE	598	
7	CI	414	
8	CJ	679	
9	CM	249	
9	LF	249	
10	CR	237	
11	CU	451	
12	LC	365	
13	LE	200	
14	LG	262	
15	LL	213	
16	LM	142	
17	LN	203	
18	LO	204	
19	LP	187	
20	LQ	213	
21	LS	174	
22	LT	160	
23	LX	156	
24	LY	138	
25	Le	131	
26	Lf	109	
27	Lh	935	

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Mol	Chain	Length	Quality of chain
28	Li	110	
29	Lj	95	
30	Cc	282	
31	Cd	436	
32	Ce	336	

2 Entry composition

There are 33 unique types of molecules in this entry. The entry contains 80799 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 RNA (3341-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	C1	1307	Total	C	N	O	P	0	0
			27990	12490	5103	9090	1307		

- Molecule 2 is a RNA chain called RNA (306-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C2	256	Total	C	N	O	P	0	0
			5456	2435	974	1791	256		

- Molecule 3 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	CA	260	Total	C	N	O	S	0	0
			2144	1371	393	373	7		

- Molecule 4 is a protein called Ribosome biogenesis protein C8F11.04.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	CB	269	Total	C	N	O	S	0	0
			2140	1370	377	390	3		

- Molecule 5 is a protein called Ribosome biogenesis protein ERB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	CC	258	Total	C	N	O	S	0	0
			2159	1378	362	412	7		

- Molecule 6 is a protein called RNA helicase.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	CE	463	Total	C	N	O	S	0	0
			3673	2352	643	667	11		

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
CE	543	LYS	-	insertion	UNP G0RYU9
CE	544	SER	-	insertion	UNP G0RYU9
CE	545	PHE	-	insertion	UNP G0RYU9
CE	546	GLY	-	insertion	UNP G0RYU9
CE	547	PHE	-	insertion	UNP G0RYU9
CE	548	SER	-	insertion	UNP G0RYU9
CE	549	THR	-	insertion	UNP G0RYU9
CE	550	PRO	-	insertion	UNP G0RYU9
CE	551	PRO	-	insertion	UNP G0RYU9
CE	552	ARG	-	insertion	UNP G0RYU9
CE	553	VAL	-	insertion	UNP G0RYU9
CE	554	ASP	-	insertion	UNP G0RYU9
CE	555	ILE	-	insertion	UNP G0RYU9
CE	556	THR	-	insertion	UNP G0RYU9
CE	557	LEU	-	insertion	UNP G0RYU9
CE	558	SER	-	insertion	UNP G0RYU9
CE	559	ALA	-	insertion	UNP G0RYU9
CE	560	SER	-	insertion	UNP G0RYU9
CE	561	LEU	-	insertion	UNP G0RYU9
CE	562	SER	-	insertion	UNP G0RYU9
CE	563	ARG	-	insertion	UNP G0RYU9
CE	564	ASP	-	insertion	UNP G0RYU9
CE	565	LYS	-	insertion	UNP G0RYU9
CE	566	LYS	-	insertion	UNP G0RYU9
CE	567	PRO	-	insertion	UNP G0RYU9
CE	568	GLN	-	insertion	UNP G0RYU9
CE	569	GLY	-	insertion	UNP G0RYU9
CE	570	ARG	-	insertion	UNP G0RYU9
CE	571	ARG	-	insertion	UNP G0RYU9
CE	572	ALA	-	insertion	UNP G0RYU9
CE	573	TYR	-	insertion	UNP G0RYU9
CE	574	GLY	-	insertion	UNP G0RYU9
CE	575	SER	-	insertion	UNP G0RYU9
CE	576	GLN	-	insertion	UNP G0RYU9
CE	577	PRO	-	insertion	UNP G0RYU9
CE	578	ARG	-	insertion	UNP G0RYU9
CE	579	GLN	-	insertion	UNP G0RYU9
CE	580	GLY	-	insertion	UNP G0RYU9
CE	581	GLY	-	insertion	UNP G0RYU9
CE	582	ARG	-	insertion	UNP G0RYU9
CE	583	TYR	-	insertion	UNP G0RYU9
CE	584	LYS	-	insertion	UNP G0RYU9

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	CI	146	Total	C	N	O	S	0	0
			1196	763	224	204	5		

- Molecule 8 is a protein called Pescadillo homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	CJ	380	Total	C	N	O	S	0	0
			3109	2003	547	549	10		

- Molecule 9 is a protein called 60S ribosomal protein l7-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	CM	187	Total	C	N	O	S	0	0
			1525	987	278	257	3		
9	LF	240	Total	C	N	O	S	0	0
			1967	1264	368	332	3		

- Molecule 10 is a protein called Nucleolar protein 16.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	CR	167	Total	C	N	O	S	0	0
			1354	827	278	247	2		

- Molecule 11 is a protein called rRNA-processing protein EBP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	CU	116	Total	C	N	O	S	0	0
			924	576	169	176	3		

- Molecule 12 is a protein called 60S ribosomal protein L4-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	LC	362	Total	C	N	O	S	0	0
			2752	1738	526	479	9		

- Molecule 13 is a protein called 60S ribosomal protein L6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	LE	170	Total	C	N	O	S	0	0
			1338	861	241	233	3		

- Molecule 14 is a protein called 60S ribosomal protein L8.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	LG	185	Total	C	N	O	S	0	0
			1482	958	265	254	5		

- Molecule 15 is a protein called 60S ribosomal protein L13.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	LL	117	Total	C	N	O	S	0	0
			964	608	206	148	2		

- Molecule 16 is a protein called 60S ribosomal protein L14-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	LM	128	Total	C	N	O	S	0	0
			1037	661	201	174	1		

- Molecule 17 is a protein called Ribosomal protein L15.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	LN	183	Total	C	N	O	S	0	0
			1563	974	332	253	4		

- Molecule 18 is a protein called 60S ribosomal protein L16-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	LO	204	Total	C	N	O	S	0	0
			1618	1039	306	267	6		

- Molecule 19 is a protein called 60S ribosomal protein l17-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	LP	154	Total	C	N	O	S	0	0
			1212	758	233	218	3		

- Molecule 20 is a protein called Ribosomal protein L18-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	LQ	129	Total	C	N	O	S	0	0
			1021	646	200	173	2		

- Molecule 21 is a protein called 60S ribosomal protein L20.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	LS	174	Total	C	N	O	S	0	0
			1433	922	267	239	5		

- Molecule 22 is a protein called 60S ribosomal protein l21-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	LT	126	Total	C	N	O	S	0	0
			1014	643	196	173	2		

- Molecule 23 is a protein called 60S ribosomal protein L25-like protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
23	LX	22	Total	C	N	O	0	0
			148	91	31	26		

- Molecule 24 is a protein called 60S ribosomal protein L26-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	LY	134	Total	C	N	O	S	0	0
			1065	664	215	184	2		

- Molecule 25 is a protein called 60S ribosomal protein L32-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Le	131	Total	C	N	O	S	0	0
			1055	663	213	172	7		

- Molecule 26 is a protein called 60S ribosomal protein l33-like protein.

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

- Molecule 27 is a protein called dolichyl-diphosphooligosaccharide--protein glycotransferase.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Lh	121	Total	C	N	O	0	0
			995	633	196	166		

- Molecule 28 is a protein called 60S ribosomal protein L36.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	Li	88	Total	C	N	O	S	0	0
			731	449	162	119	1		

- Molecule 29 is a protein called Ribosomal protein L37.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Lj	74	Total	C	N	O	S	0	0
			595	365	132	93	5		

- Molecule 30 is a protein called Ribosomal RNA-processing protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	Cc	236	Total	C	N	O	S	0	0
			1898	1208	337	343	10		

- Molecule 31 is a protein called Brix domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	Cd	343	Total	C	N	O	S	0	0
			2768	1746	534	484	4		

- Molecule 32 is a protein called Protein MAK16.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	Ce	194	Total	C	N	O	S	0	0
			1609	1020	304	276	9		

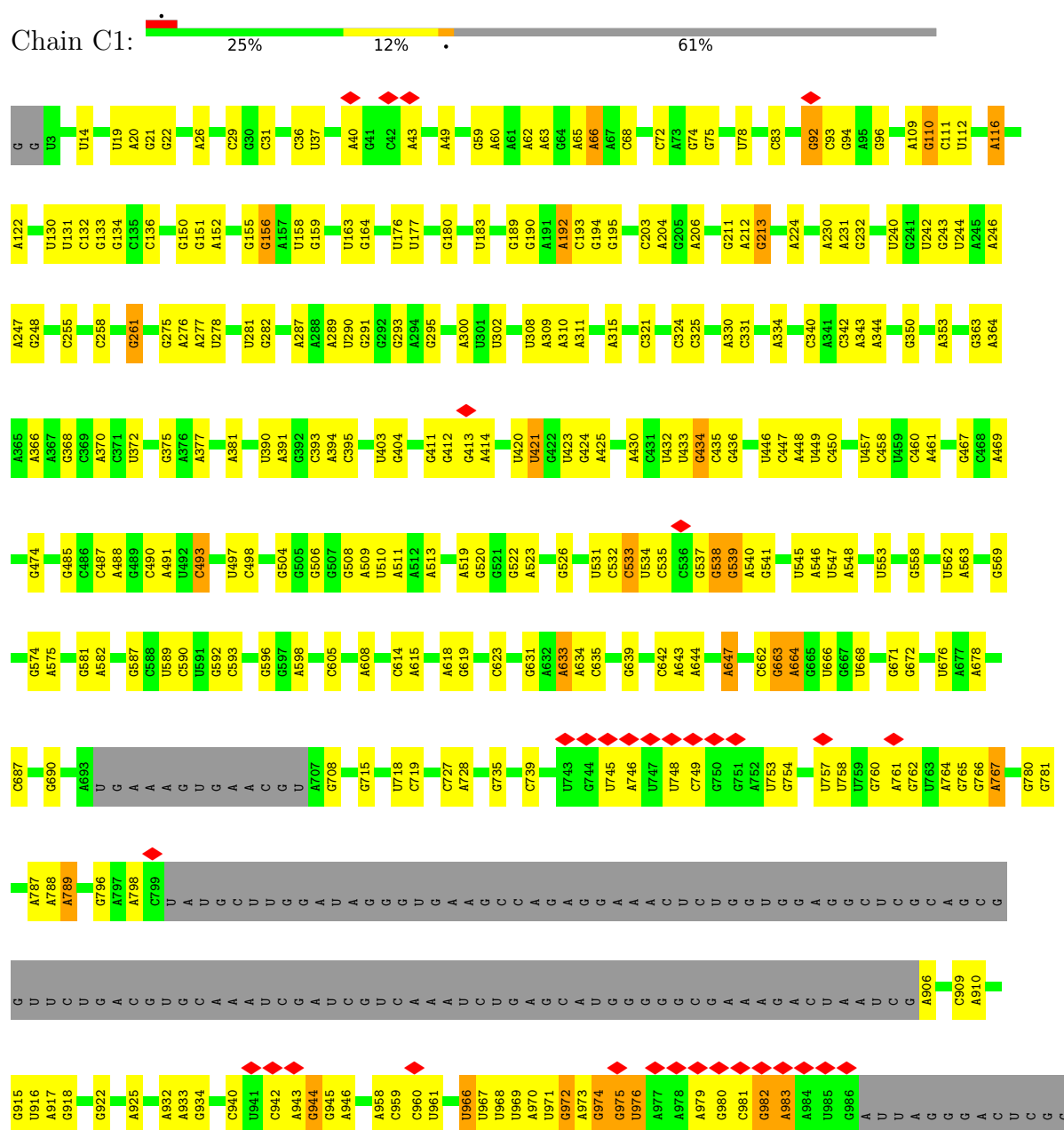
- Molecule 33 is ZINC ION (CCD ID: ZN) (formula: Zn).

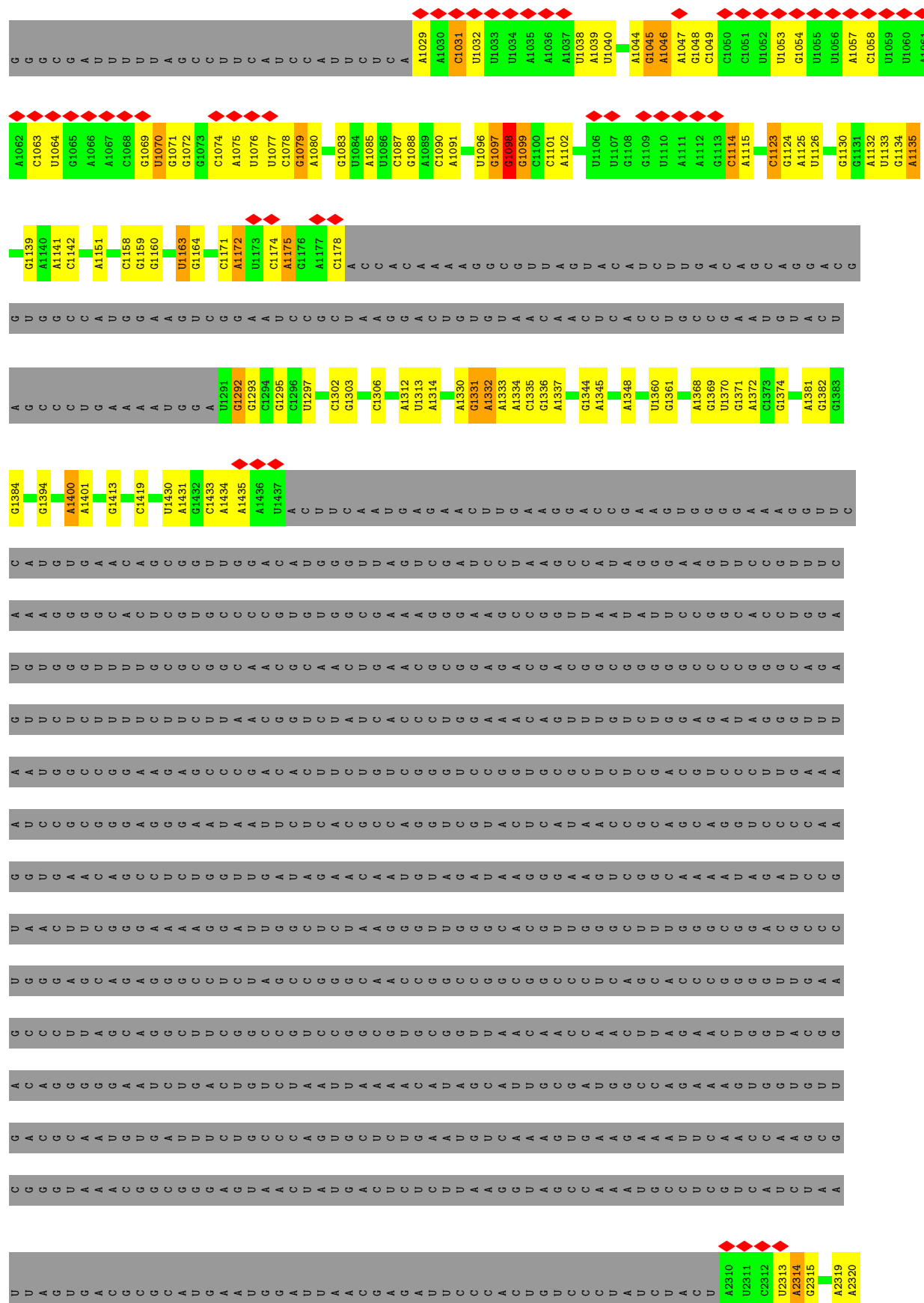
Mol	Chain	Residues	Atoms		AltConf
33	Lj	1	Total	Zn	0
			1	1	
33	Ce	1	Total	Zn	0
			1	1	

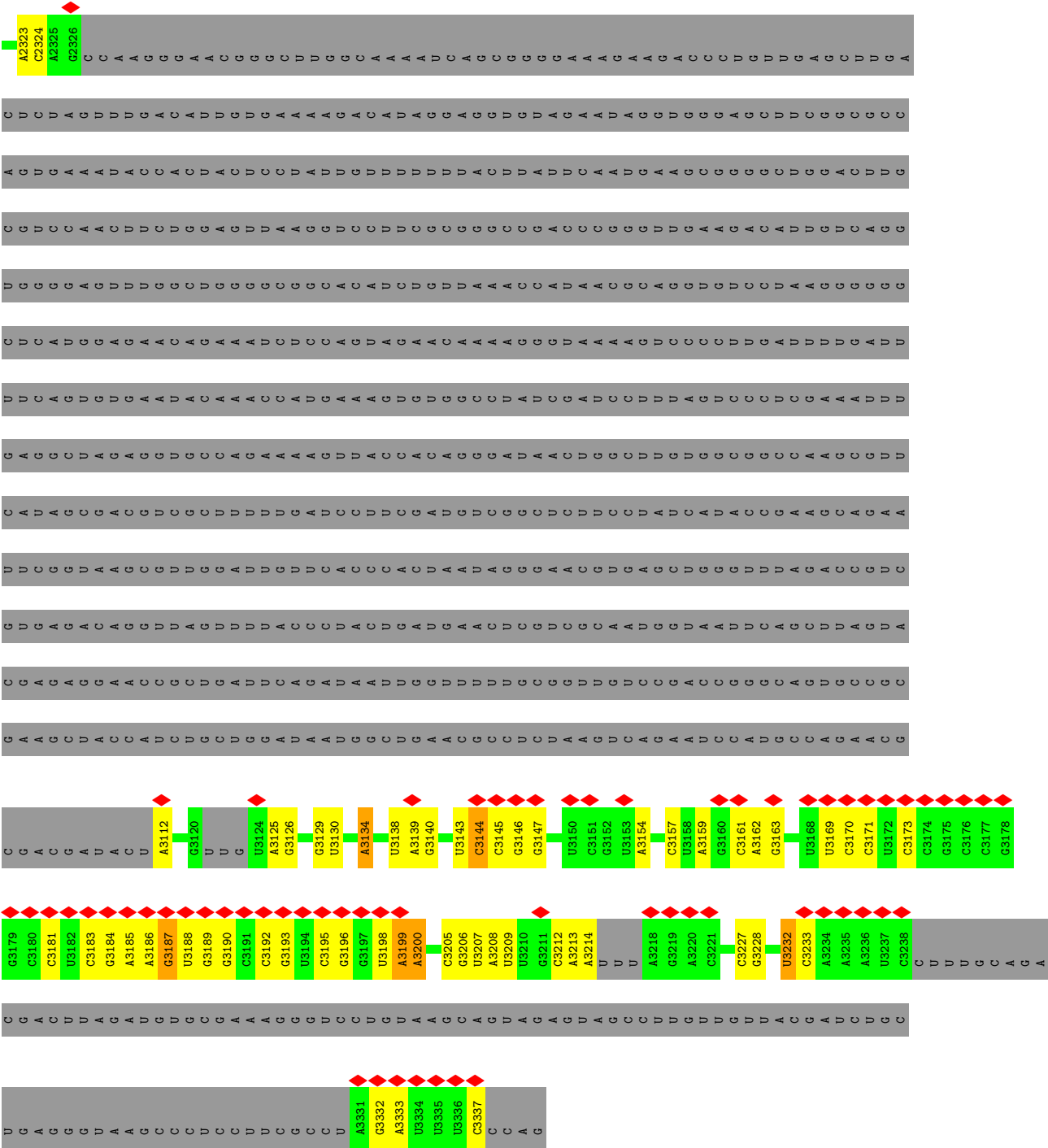
3 Residue-property plots

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

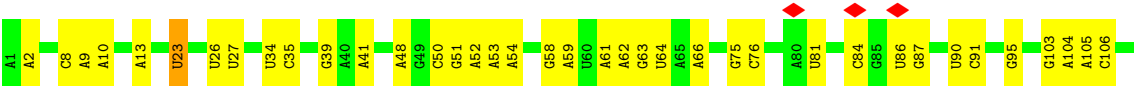
• Molecule 1: RNA (3341-MER)

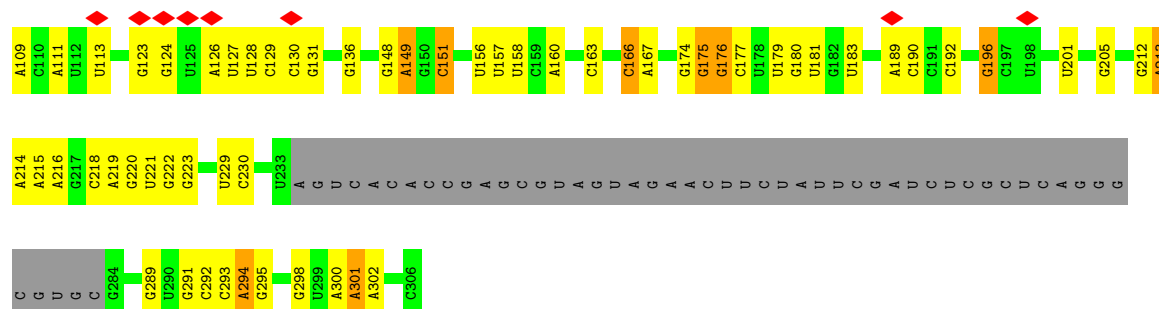




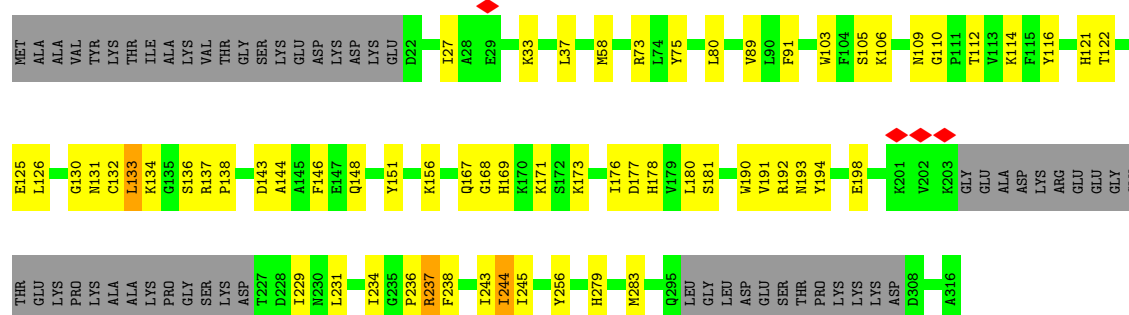


• Molecule 2: RNA (306-MER)

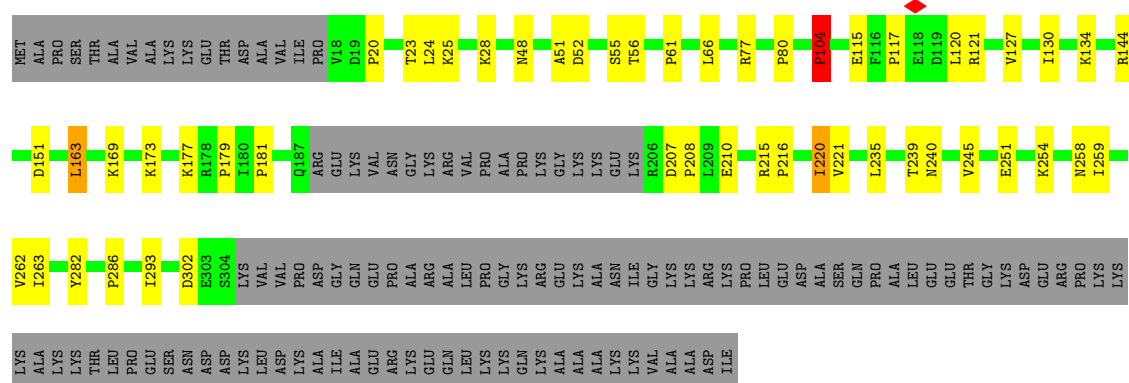




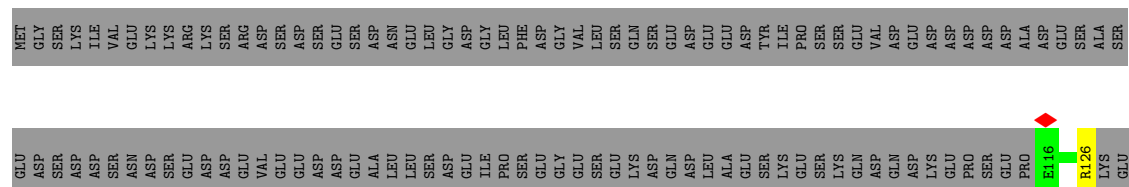
• Molecule 3: Brix domain-containing protein

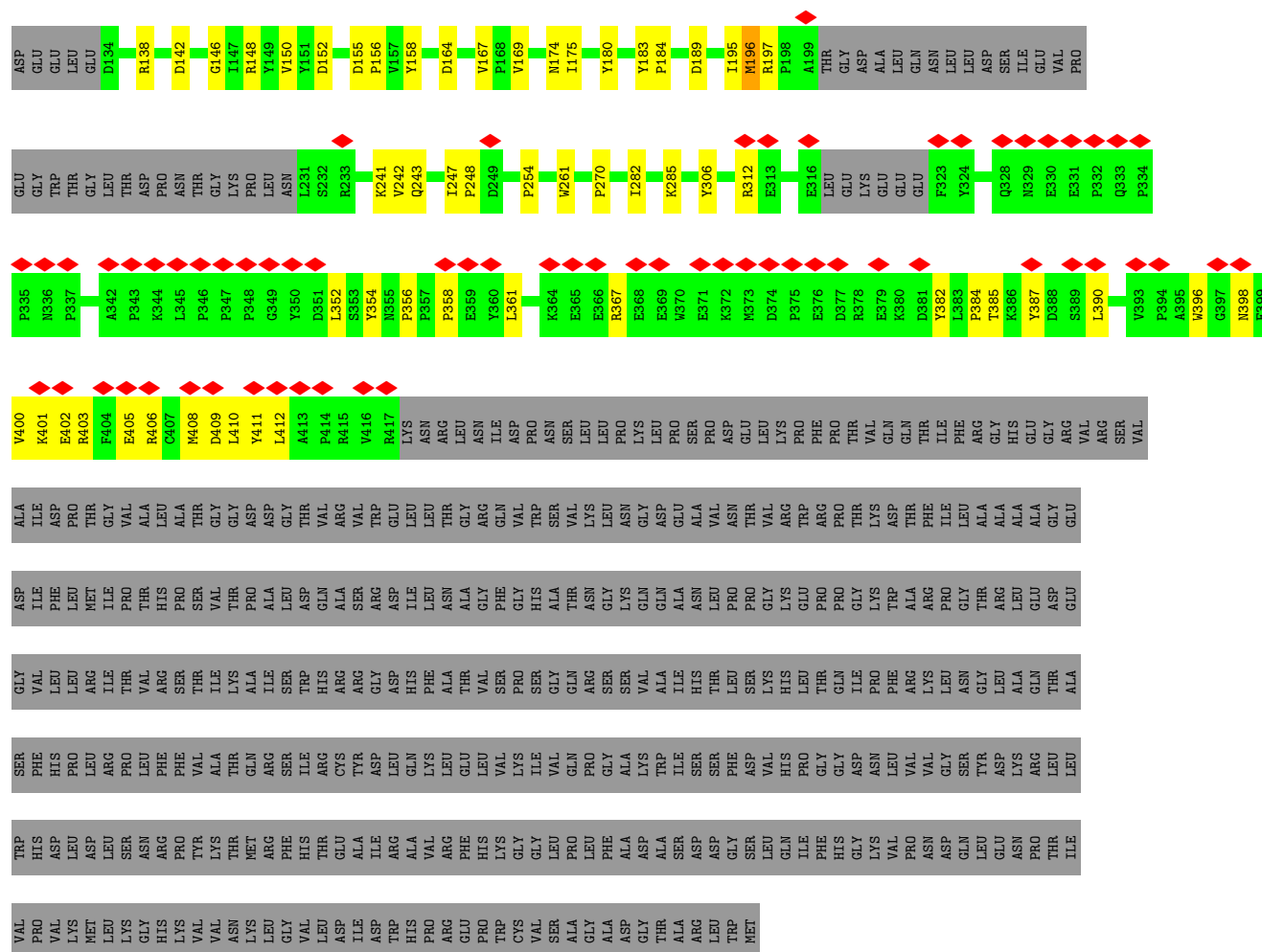


• Molecule 4: Ribosome biogenesis protein C8F11.04

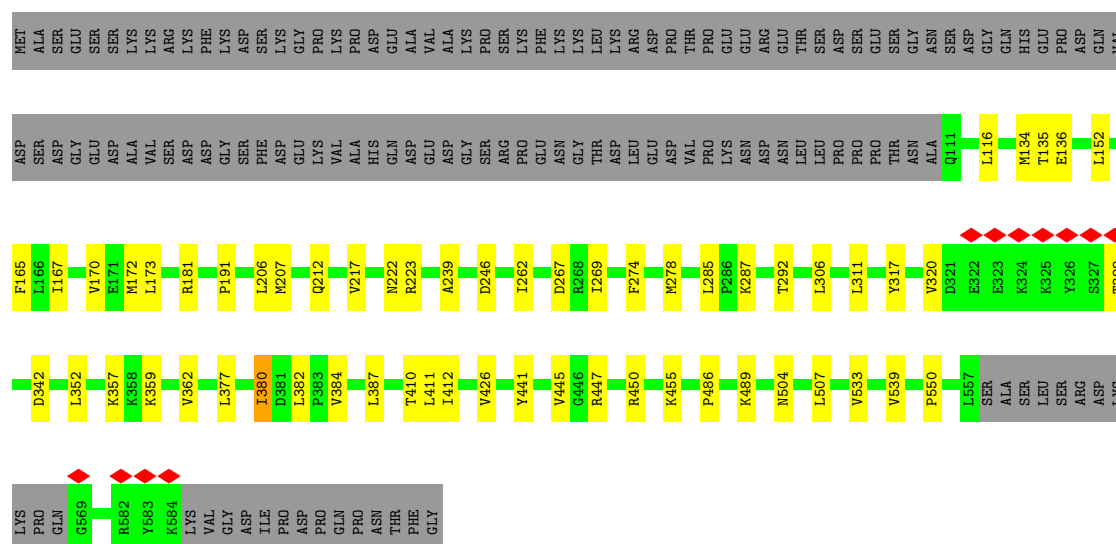


• Molecule 5: Ribosome biogenesis protein ERB1



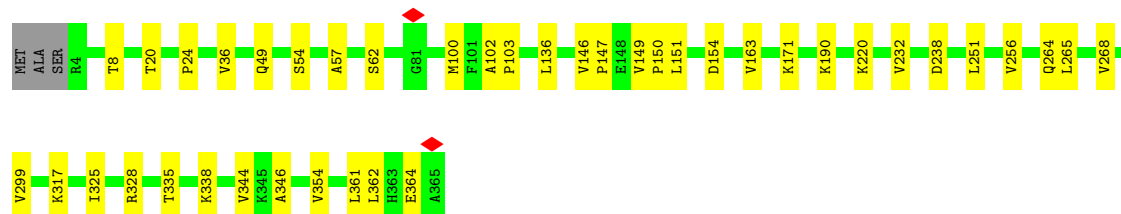
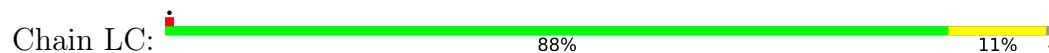


• Molecule 6: RNA helicase

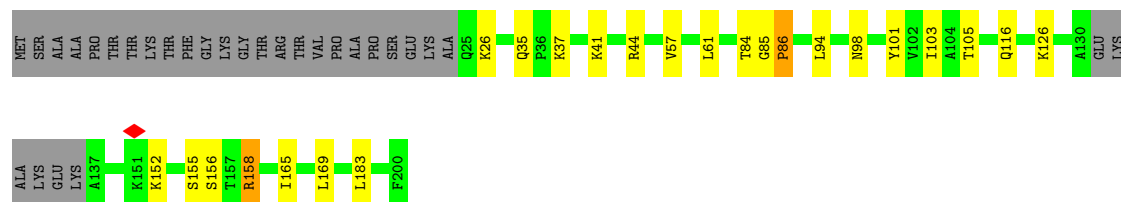


• Molecule 7: Putative RNA-binding protein

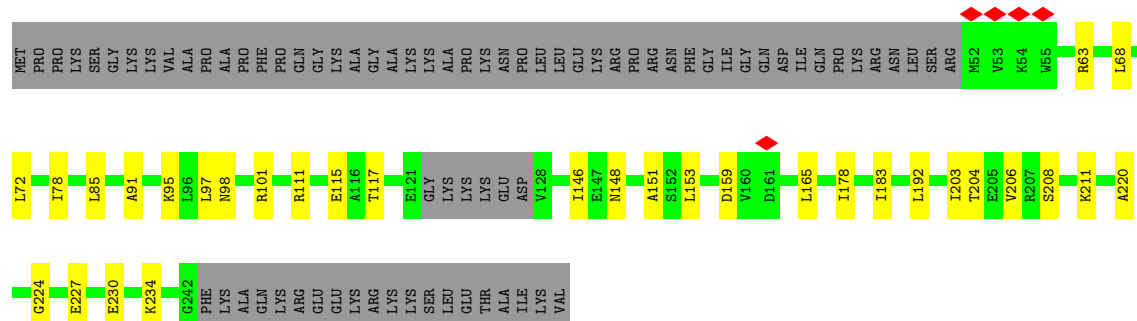
- Molecule 12: 60S ribosomal protein L4-like protein



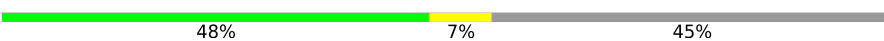
- Molecule 13: 60S ribosomal protein L6

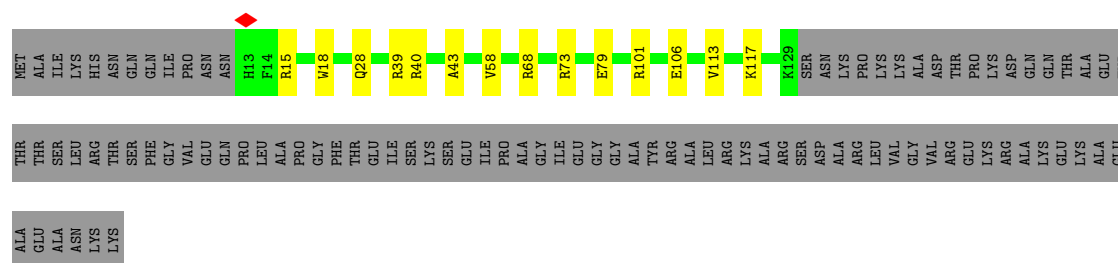


- Molecule 14: 60S ribosomal protein L8



- Molecule 15: 60S ribosomal protein L13

Chain LL: 



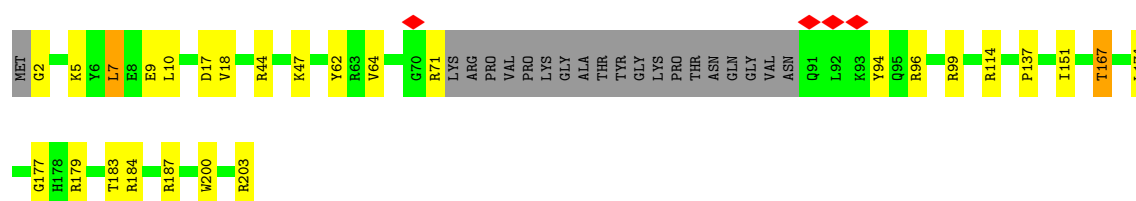
- Molecule 16: 60S ribosomal protein L14-like protein

Chain LM: 



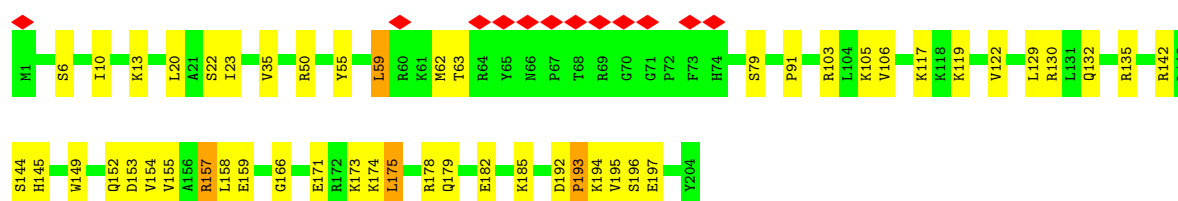
- Molecule 17: Ribosomal protein L15

Chain LN: 



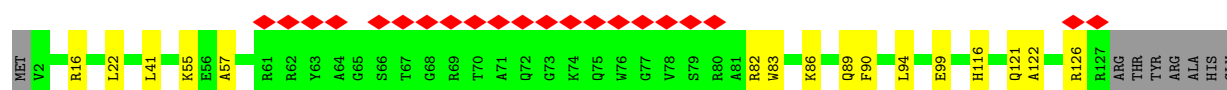
- Molecule 18: 60S ribosomal protein L16-like protein

Chain LO: 



- Molecule 19: 60S ribosomal protein l17-like protein

Chain LP: 

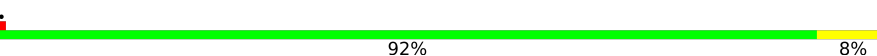


- Molecule 24: 60S ribosomal protein L26-like protein

Chain LY:  86% 11% ..

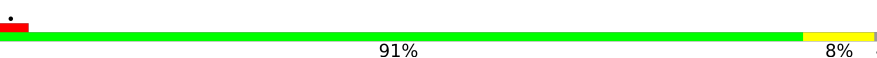


- Molecule 25: 60S ribosomal protein L32-like protein

Chain Le:  92% 8%



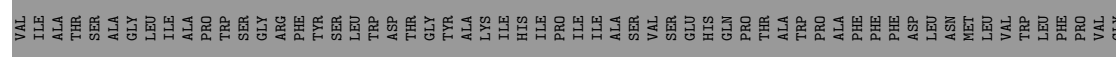
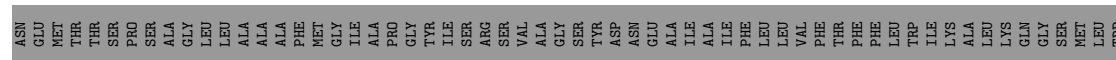
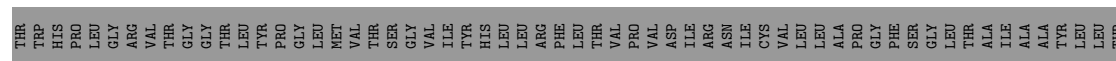
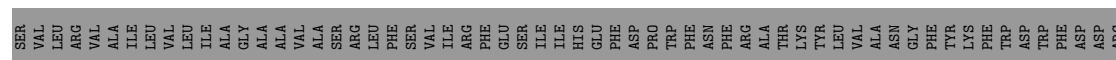
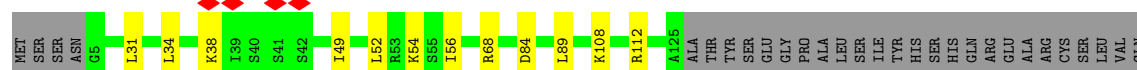
- Molecule 26: 60S ribosomal protein l33-like protein

Chain Lf:  91% 8%



- Molecule 27: dolichyl-diphosphooligosaccharide--protein glycotransferase

Chain Lh:  12% 87%



[illegible]

- Molecule 28: 60S ribosomal protein L36



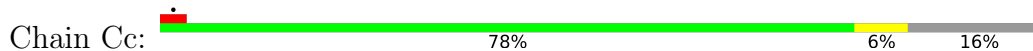
MET	GLU	ASP	ALA	THR	PRO	ALA	PRO	VAL	GLU	ARG	THR	GLY	LEU	ILE	ARG	GLY	LEU	ASN	LYS	G23	K32	R38 K39	R45	L52 I53	R64 R65	E68	K74	R77	T98	R91	K95	R101	E105	H110
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------------	-----	------------	------------	-----	-----	-----	-----	-----	-----	------	------	------

- Molecule 29: Ribosomal protein L37



MET	THR	LYS	GLY	THR	SER	SER	PHE	GLY	GLY	ARG	HIS	ASN	K14	R20	L27	K32	V33	C34	W49	T59	R63	M64	L67	S68	P71	R72	R73	F74	K75	R87	PRO	ALA	VAL	SER	THR	SER	SER
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- Molecule 30: Ribosomal RNA-processing protein 1

[illegible]

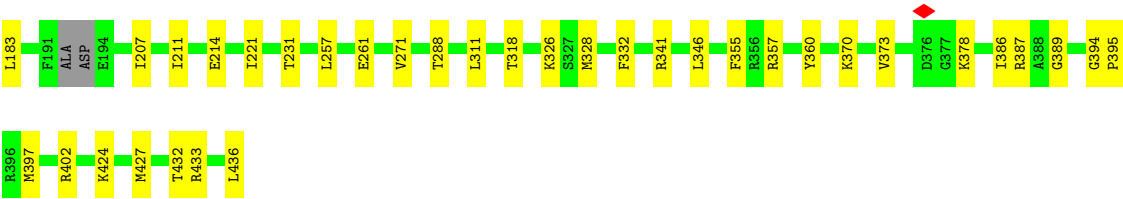
I225 M228 R244 R258 ARG PRO ASN SER SER GLN ASP HTS ASP THR LYS ASP MET GLY ASP SER ASP SER TRP GLU GLY PHE ASP ASP

- Molecule 31: Brix domain-containing protein

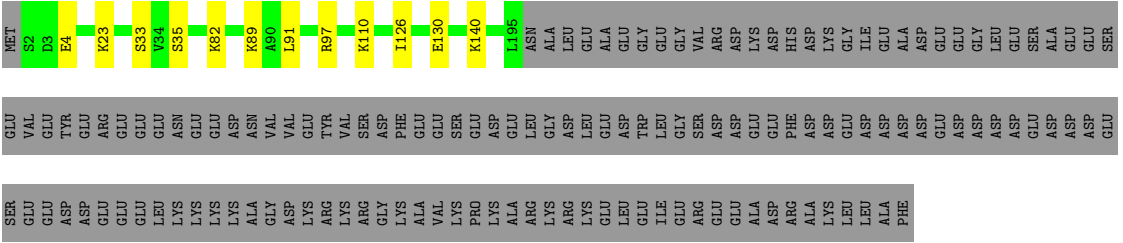


MET	ALA	ALA	SER	LYS	SER	LYS	ASP	L9	K23	K32	R43	R46	E50	R60	I69	R73	D76	D77	LEU	ASP	ASP	D81	R94	R95	E96	VAL	ALA	GLU	ALA	ALA	ALA	ALA	ARG	ASP	ASP	GLN	VAL	VAL	ASP	LYS
-----	-----	-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

ASN	ASP	GLU	ASN	GLU	LYS	ARG	ASP	ASP	ASP	ILE	ASP	SER	MET	LEU	GLY	SER	ASP	ASP	GLU	GLY	ALA	LYS	LYS	GLU	GLU	GLY	GLN	ARG	GLN	GLN	PRO	THR	ILE	SER	SER	THR	THR	ASN	L776	ASP	LEU	THR	P180
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------	-----	-----	-----	------



• Molecule 32: Protein MAK16



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	83243	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 ($e^-/\text{\AA}^2$)	44	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.449	Depositor
Minimum map value	-0.224	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	438.9, 438.9, 438.9	wwPDB
Map dimensions	420, 420, 420	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: ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	C1	0.19	0/31321	0.34	2/48825 (0.0%)
2	C2	0.18	0/6097	0.36	0/9499
3	CA	0.44	0/2190	0.75	2/2940 (0.1%)
4	CB	0.50	1/2188 (0.0%)	0.83	6/2975 (0.2%)
5	CC	0.32	0/2224	0.63	1/3024 (0.0%)
6	CE	0.32	0/3743	0.56	2/5045 (0.0%)
7	CI	0.38	0/1225	0.79	3/1645 (0.2%)
8	CJ	0.23	0/3189	0.59	4/4309 (0.1%)
9	CM	0.30	0/1555	0.72	1/2091 (0.0%)
9	LF	0.33	0/2004	0.57	1/2686 (0.0%)
10	CR	0.43	0/1369	0.63	0/1828
11	CU	0.32	0/935	0.75	1/1256 (0.1%)
12	LC	0.41	0/2809	0.64	2/3787 (0.1%)
13	LE	0.67	0/1363	0.88	1/1833 (0.1%)
14	LG	0.34	0/1504	0.60	0/2018
15	LL	0.34	0/983	0.53	0/1318
16	LM	0.48	0/1056	0.72	0/1419
17	LN	0.57	0/1595	0.75	0/2132
18	LO	0.26	0/1652	0.72	6/2215 (0.3%)
19	LP	0.32	0/1231	0.55	1/1658 (0.1%)
20	LQ	0.49	0/1033	0.70	0/1391
21	LS	0.72	0/1468	0.91	0/1975
22	LT	0.34	0/1033	0.67	1/1389 (0.1%)
23	LX	0.14	0/148	0.36	0/194
24	LY	0.36	0/1079	0.58	0/1443
25	Le	0.50	0/1073	0.66	0/1431
26	Lf	0.76	0/883	0.90	0/1187
27	Lh	0.27	0/1006	0.49	0/1338
28	Li	0.44	0/738	0.69	0/971
29	Lj	0.18	0/606	0.41	0/803
30	Cc	0.18	0/1934	0.49	0/2614
31	Cd	0.25	0/2822	0.53	0/3790

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
32	Ce	0.19	0/1638	0.43	0/2196
All	All	0.32	1/85694 (0.0%)	0.53	34/123225 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
18	LO	0	1
22	LT	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	CB	115	GLU	N-CA	5.11	1.49	1.46

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	LO	193	PRO	CA-N-CD	-8.57	100.01	112.00
8	CJ	147	MET	CB-CG-SD	7.71	135.84	112.70
9	CM	210	PRO	CA-N-CD	-7.34	101.73	112.00
18	LO	171	GLU	CA-CB-CG	6.92	127.95	114.10
8	CJ	147	MET	CA-CB-CG	6.89	127.88	114.10
12	LC	163	VAL	N-CA-C	-6.74	106.73	113.20
4	CB	302	ASP	N-CA-C	-6.42	106.66	114.75
6	CE	380	ILE	CA-C-N	6.17	131.16	122.46
6	CE	380	ILE	C-N-CA	6.17	131.16	122.46
1	C1	1123	C	N3-C4-N4	-6.05	99.86	118.00
18	LO	175	LEU	CA-CB-CG	6.05	137.46	116.30
4	CB	216	PRO	CA-C-N	5.96	125.10	120.33
4	CB	216	PRO	C-N-CA	5.96	125.10	120.33
4	CB	239	THR	N-CA-C	5.89	117.70	111.28
12	LC	163	VAL	CB-CA-C	5.84	116.48	110.70
7	CI	311	GLN	CA-CB-CG	5.75	125.59	114.10
22	LT	115	LEU	CA-CB-CG	5.69	136.21	116.30
18	LO	59	LEU	CA-CB-CG	5.66	136.10	116.30
4	CB	115	GLU	CB-CA-C	-5.63	108.95	117.07
1	C1	1098	G	N1-C6-O6	-5.49	103.42	119.90
5	CC	196	MET	CB-CG-SD	5.47	129.10	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	CB	104	PRO	CA-N-CD	-5.46	104.36	112.00
19	LP	55	LYS	CB-CG-CD	5.43	123.79	111.30
7	CI	310	GLU	CA-C-N	-5.41	112.15	121.66
7	CI	310	GLU	C-N-CA	-5.41	112.15	121.66
8	CJ	193	LYS	CB-CG-CD	5.31	123.51	111.30
18	LO	157	ARG	CA-CB-CG	5.28	124.67	114.10
3	CA	237	ARG	CA-C-N	-5.18	113.73	122.29
3	CA	237	ARG	C-N-CA	-5.18	113.73	122.29
13	LE	156	SER	N-CA-C	-5.18	107.34	113.97
8	CJ	267	GLU	CA-CB-CG	5.14	124.39	114.10
11	CU	286	LYS	CA-CB-CG	5.14	124.39	114.10
9	LF	60	GLU	CA-CB-CG	5.10	124.31	114.10
18	LO	157	ARG	N-CA-CB	5.01	117.33	110.07

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
18	LO	192	ASP	Peptide
22	LT	92	ARG	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C1	27990	0	14115	219	0
2	C2	5456	0	2762	41	0
3	CA	2144	0	2178	45	0
4	CB	2140	0	2195	29	0
5	CC	2159	0	2081	50	0
6	CE	3673	0	3778	36	0
7	CI	1196	0	1202	24	0
8	CJ	3109	0	3122	74	0
9	CM	1525	0	1604	36	0
9	LF	1967	0	2080	23	0
10	CR	1354	0	1400	16	0
11	CU	924	0	951	28	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	LC	2752	0	2878	27	0
13	LE	1338	0	1423	12	0
14	LG	1482	0	1610	21	0
15	LL	964	0	1041	13	0
16	LM	1037	0	1110	13	0
17	LN	1563	0	1618	19	0
18	LO	1618	0	1714	37	0
19	LP	1212	0	1250	11	0
20	LQ	1021	0	1118	7	0
21	LS	1433	0	1496	21	0
22	LT	1014	0	1073	21	0
23	LX	148	0	163	2	0
24	LY	1065	0	1156	10	0
25	Le	1055	0	1133	9	0
26	Lf	862	0	891	5	0
27	Lh	995	0	1110	11	0
28	Li	731	0	797	12	0
29	Lj	595	0	625	12	0
30	Cc	1898	0	1931	10	0
31	Cd	2768	0	2860	31	0
32	Ce	1609	0	1682	9	0
33	Ce	1	0	0	0	0
33	Lj	1	0	0	0	0
All	All	80799	0	66147	777	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 5.

All (777) 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:C1:788:A:N6	1:C1:915:G:H1	1.49	1.10
2:C2:223:G:H21	2:C2:301:A:H61	1.11	0.93
2:C2:196:G:H1	2:C2:201:U:H3	0.94	0.91
1:C1:788:A:H62	1:C1:915:G:H1	0.87	0.86
2:C2:223:G:N2	2:C2:301:A:H61	1.73	0.86
27:Lh:34:LEU:O	27:Lh:38:LYS:HB2	1.76	0.85
6:CE:136:GLU:HG2	6:CE:320:VAL:HG22	1.58	0.84
9:CM:87:ALA:HA	9:CM:125:VAL:O	1.83	0.77
1:C1:1053:U:H3	1:C1:1069:G:H1	1.32	0.77
1:C1:3112:A:N7	1:C1:3232:U:O2	2.19	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CE:136:GLU:HG2	6:CE:320:VAL:CG2	2.15	0.76
5:CC:169:VAL:O	5:CC:169:VAL:HG12	1.84	0.75
5:CC:406:ARG:O	5:CC:409:ASP:HB2	1.86	0.73
7:CI:204:ARG:O	7:CI:208:SER:HB2	1.89	0.71
5:CC:396:TRP:HE1	5:CC:398:ASN:HB3	1.57	0.69
3:CA:105:SER:HB2	3:CA:112:THR:HG23	1.75	0.69
1:C1:788:A:N6	1:C1:915:G:N1	2.32	0.69
3:CA:137:ARG:O	11:CU:218:GLN:NE2	2.26	0.69
3:CA:143:ASP:H	3:CA:146:PHE:HD2	1.40	0.68
1:C1:66:A:N6	1:C1:75:G:N2	2.40	0.68
21:LS:8:GLN:HG3	21:LS:26:ARG:HE	1.59	0.68
1:C1:1394:G:OP1	25:Le:106:ARG:NH2	2.26	0.67
1:C1:553:U:OP1	21:LS:67:LYS:NZ	2.28	0.67
3:CA:171:LYS:HG2	5:CC:167:VAL:HG11	1.77	0.67
6:CE:384:VAL:HG12	6:CE:410:THR:CG2	2.25	0.66
18:LO:175:LEU:HD23	18:LO:179:GLN:HE22	1.60	0.66
10:CR:38:SER:O	10:CR:51:ARG:NH2	2.28	0.65
1:C1:1083:G:H5''	9:LF:113:ARG:HD3	1.78	0.65
6:CE:352:LEU:HB3	6:CE:382:LEU:HD21	1.78	0.65
6:CE:377:LEU:HA	6:CE:380:ILE:HG22	1.79	0.65
2:C2:223:G:H21	2:C2:301:A:N6	1.90	0.65
5:CC:306:TYR:H	14:LG:117:THR:HG21	1.60	0.64
9:CM:113:ARG:NH2	9:CM:208:LEU:O	2.30	0.64
11:CU:282:MET:HA	11:CU:285:VAL:HG22	1.80	0.64
19:LP:94:LEU:HB3	19:LP:148:LEU:HD21	1.78	0.64
9:CM:167:ILE:HG23	9:CM:168:PRO:HD2	1.80	0.64
7:CI:321:LYS:NZ	7:CI:325:TYR:O	2.27	0.63
1:C1:281:U:H2'	1:C1:282:G:H8	1.63	0.63
4:CB:25:LYS:HA	4:CB:28:LYS:HG2	1.79	0.63
1:C1:974:G:H1	1:C1:1038:U:H3	1.47	0.62
22:LT:42:ILE:HG22	22:LT:96:VAL:HG12	1.80	0.62
13:LE:61:LEU:HD11	13:LE:103:ILE:HG13	1.80	0.62
1:C1:493:C:O2	13:LE:41:LYS:NZ	2.32	0.62
1:C1:255:C:OP2	6:CE:222:ASN:ND2	2.33	0.62
31:Cd:318:THR:H	31:Cd:436:LEU:HD12	1.65	0.61
8:CJ:169:GLU:OE1	8:CJ:170:ARG:NH1	2.33	0.61
1:C1:14:U:H3	2:C2:136:G:H21	1.48	0.61
1:C1:375:G:O6	31:Cd:43:ARG:NH1	2.33	0.61
2:C2:66:A:OP1	29:Lj:87:ARG:NH2	2.34	0.61
3:CA:109:ASN:O	5:CC:148:ARG:NH2	2.32	0.61
18:LO:132:GLN:HB3	18:LO:135:ARG:HG2	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:Cd:355:PHE:HB3	31:Cd:397:MET:HG2	1.81	0.61
10:CR:39:TRP:HE1	15:LL:40:ARG:HH12	1.49	0.61
3:CA:136:SER:HB3	3:CA:176:ILE:HA	1.83	0.60
9:CM:167:ILE:HG22	9:CM:168:PRO:O	2.01	0.60
10:CR:43:GLU:O	15:LL:40:ARG:NH2	2.34	0.60
17:LN:177:GLY:O	17:LN:184:ARG:NH2	2.33	0.60
2:C2:103:G:OP1	29:Lj:20:ARG:NH2	2.35	0.60
1:C1:796:G:H1	1:C1:906:A:H61	1.50	0.60
17:LN:99:ARG:HB3	17:LN:167:THR:HG21	1.84	0.60
1:C1:672:G:OP1	15:LL:39:ARG:NH2	2.34	0.60
31:Cd:207:ILE:O	31:Cd:231:THR:OG1	2.19	0.60
4:CB:24:LEU:HD13	4:CB:28:LYS:HD3	1.83	0.60
1:C1:281:U:H2'	1:C1:282:G:C8	2.38	0.59
14:LG:165:LEU:HA	17:LN:7:LEU:HD11	1.84	0.59
8:CJ:378:THR:HG21	8:CJ:419:ILE:HG22	1.83	0.59
8:CJ:419:ILE:HD13	8:CJ:456:VAL:HG23	1.85	0.59
1:C1:3173:C:N3	1:C1:3198:U:O2	2.36	0.59
8:CJ:77:LEU:HD22	8:CJ:126:ILE:HD11	1.84	0.59
1:C1:83:C:HO2'	1:C1:687:C:HO2'	1.48	0.59
11:CU:276:VAL:HG12	11:CU:277:ARG:HG2	1.84	0.59
31:Cd:211:ILE:HD13	31:Cd:261:GLU:HB3	1.84	0.59
16:LM:93:LYS:HA	16:LM:96:GLU:HG3	1.85	0.58
3:CA:91:PHE:HB3	3:CA:103:TRP:HB2	1.84	0.58
3:CA:73:ARG:NH1	3:CA:75:TYR:OH	2.36	0.58
3:CA:245:ILE:HB	3:CA:256:TYR:HB3	1.84	0.58
5:CC:408:MET:O	5:CC:412:LEU:N	2.37	0.58
7:CI:298:SER:N	7:CI:301:GLN:OE1	2.37	0.58
17:LN:17:ASP:OD2	28:Li:64:ARG:NH2	2.37	0.58
1:C1:116:A:OP2	17:LN:2:GLY:N	2.36	0.58
4:CB:120:LEU:HD22	4:CB:221:VAL:HG13	1.85	0.58
5:CC:242:VAL:HG23	14:LG:72:LEU:HD21	1.84	0.58
1:C1:116:A:OP1	28:Li:45:ARG:NH1	2.37	0.58
1:C1:189:G:N1	1:C1:192:A:OP2	2.35	0.58
1:C1:403:U:H2'	1:C1:404:G:H8	1.69	0.57
1:C1:3138:U:HO2'	21:LS:172:THR:HG1	1.38	0.57
9:CM:245:ILE:HA	9:CM:248:MET:HB2	1.85	0.57
1:C1:1098:G:H1	1:C1:1123:C:H42	1.50	0.57
31:Cd:180:PRO:HG2	31:Cd:183:LEU:HD12	1.86	0.57
12:LC:36:VAL:HG21	12:LC:251:LEU:HD21	1.85	0.57
1:C1:1046:A:N1	1:C1:1074:C:N3	2.52	0.57
1:C1:1071:G:H2'	1:C1:1072:G:C8	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:780:G:O2'	15:LL:18:TRP:NE1	2.37	0.57
22:LT:92:ARG:HD3	22:LT:92:ARG:H	1.70	0.57
8:CJ:421:ASP:OD1	8:CJ:421:ASP:N	2.37	0.57
28:Li:74:LYS:HD3	28:Li:77:ARG:HD2	1.87	0.57
9:CM:165:GLN:OE1	9:CM:167:ILE:HG13	2.05	0.57
9:LF:124:LYS:HG3	9:LF:197:VAL:HG11	1.86	0.57
31:Cd:77:ASP:OD1	31:Cd:77:ASP:N	2.36	0.57
1:C1:3189:G:H2'	1:C1:3190:G:H8	1.69	0.57
8:CJ:84:GLN:OE1	8:CJ:120:ARG:NH2	2.38	0.57
8:CJ:189:PHE:HA	8:CJ:462:TRP:HE1	1.70	0.57
1:C1:1124:G:N2	1:C1:1125:A:O2'	2.38	0.57
9:LF:156:LYS:HG2	9:LF:157:ARG:HG3	1.86	0.57
18:LO:35:VAL:HG12	18:LO:105:LYS:HB2	1.86	0.57
2:C2:39:G:C2	2:C2:105:A:C2	2.92	0.56
27:Lh:31:LEU:HD12	27:Lh:49:ILE:HD13	1.87	0.56
1:C1:671:G:OP2	15:LL:28:GLN:NE2	2.36	0.56
1:C1:972:G:N2	1:C1:1040:U:O2	2.38	0.56
1:C1:1163:U:O4	18:LO:22:SER:OG	2.23	0.56
8:CJ:141:LEU:HA	8:CJ:144:CYS:HB3	1.86	0.56
8:CJ:163:LYS:HA	9:CM:246:ARG:HH22	1.69	0.56
11:CU:274:GLU:N	11:CU:274:GLU:OE1	2.38	0.56
12:LC:299:VAL:HG21	20:LQ:159:PRO:HB2	1.86	0.56
18:LO:62:MET:HE3	18:LO:63:THR:H	1.69	0.56
3:CA:106:LYS:HB2	3:CA:110:GLY:HA3	1.87	0.56
2:C2:151:C:O2	14:LG:63:ARG:NH2	2.39	0.56
19:LP:41:LEU:HD21	19:LP:99:GLU:HG3	1.86	0.56
1:C1:533:C:C2	1:C1:539:G:C2	2.93	0.56
2:C2:128:U:O4'	8:CJ:14:ARG:NH2	2.39	0.56
5:CC:358:PRO:HA	5:CC:361:LEU:HG	1.86	0.56
25:Le:66:HIS:HB3	32:Ce:23:LYS:HD3	1.87	0.56
1:C1:972:G:C2	1:C1:1040:U:O2	2.58	0.56
1:C1:975:G:N2	1:C1:976:U:O4	2.39	0.56
9:LF:216:PRO:HD3	9:LF:248:MET:HE3	1.87	0.56
18:LO:62:MET:HE3	18:LO:63:THR:HG22	1.86	0.56
1:C1:112:U:OP1	27:Lh:112:ARG:NH2	2.37	0.56
1:C1:261:G:OP1	17:LN:47:LYS:NZ	2.37	0.56
1:C1:533:C:O2	1:C1:539:G:C2	2.59	0.56
13:LE:84:THR:HB	13:LE:94:LEU:HD23	1.87	0.56
6:CE:441:TYR:O	6:CE:445:VAL:HB	2.06	0.55
30:Cc:171:GLU:HG2	30:Cc:172:GLU:HG3	1.88	0.55
9:CM:91:PHE:HB2	9:CM:145:PRO:HG3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C2:103:G:OP2	2:C2:105:A:O2'	2.22	0.55
4:CB:245:VAL:O	4:CB:258:ASN:ND2	2.39	0.55
16:LM:43:GLY:HA3	16:LM:52:THR:HB	1.87	0.55
6:CE:181:ARG:NH2	10:CR:137:GLN:OE1	2.35	0.55
1:C1:420:U:OP2	25:Le:16:LYS:NZ	2.38	0.55
1:C1:538:G:H2'	1:C1:539:G:H8	1.72	0.55
5:CC:411:TYR:HE1	8:CJ:41:GLY:HA2	1.70	0.55
8:CJ:164:MET:HE3	8:CJ:231:VAL:HG11	1.89	0.55
1:C1:642:C:H2'	1:C1:643:A:H8	1.71	0.55
1:C1:1029:A:OP2	1:C1:1031:C:N4	2.39	0.55
5:CC:142:ASP:OD1	5:CC:146:GLY:N	2.36	0.55
2:C2:163:C:O2	9:CM:73:ARG:NH2	2.40	0.55
6:CE:342:ASP:OD1	6:CE:342:ASP:N	2.40	0.55
6:CE:450:ARG:HG2	6:CE:455:LYS:HD2	1.88	0.55
3:CA:27:ILE:H	3:CA:168:GLY:HA3	1.72	0.55
3:CA:151:TYR:HA	11:CU:196:LEU:HD22	1.89	0.55
12:LC:54:SER:HB2	12:LC:57:ALA:HB2	1.89	0.55
1:C1:3134:A:H1'	18:LO:166:GLY:HA3	1.88	0.55
3:CA:133:LEU:HA	3:CA:134:LYS:HZ3	1.72	0.55
5:CC:248:PRO:HG2	5:CC:254:PRO:HB3	1.88	0.55
12:LC:364:GLU:O	21:LS:28:ARG:NH1	2.40	0.55
9:LF:91:PHE:HB2	9:LF:145:PRO:HG3	1.88	0.54
17:LN:200:TRP:O	17:LN:203:ARG:NH1	2.40	0.54
30:Cc:225:ILE:HA	30:Cc:228:MET:HE2	1.88	0.54
1:C1:295:G:OP1	17:LN:179:ARG:NH2	2.40	0.54
1:C1:381:A:OP1	19:LP:16:ARG:NH1	2.40	0.54
4:CB:77:ARG:HB3	4:CB:235:LEU:HB2	1.89	0.54
2:C2:196:G:O6	2:C2:201:U:O4	2.26	0.54
7:CI:249:ASP:HA	7:CI:260:CYS:HB2	1.89	0.54
1:C1:1175:A:N6	1:C1:1297:U:N3	2.56	0.54
3:CA:229:ILE:O	11:CU:252:ARG:NH2	2.38	0.54
4:CB:104:PRO:HD3	4:CB:208:PRO:HB3	1.89	0.54
6:CE:387:LEU:HD13	6:CE:411:LEU:HD11	1.90	0.54
8:CJ:371:THR:HG22	8:CJ:394:ARG:HH21	1.73	0.54
21:LS:74:ASN:HD22	21:LS:135:VAL:HG11	1.73	0.54
14:LG:151:ALA:HA	14:LG:204:THR:HG22	1.90	0.54
1:C1:981:C:H5''	1:C1:982:G:H5'	1.89	0.54
14:LG:97:LEU:HB3	14:LG:192:LEU:HD21	1.90	0.54
20:LQ:56:LEU:HD12	32:Ce:4:GLU:HG2	1.88	0.54
1:C1:92:G:H5'	1:C1:93:C:H5''	1.89	0.53
1:C1:3134:A:OP2	18:LO:173:LYS:NZ	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:246:A:OP2	5:CC:285:LYS:NZ	2.41	0.53
3:CA:33:LYS:HE2	5:CC:156:PRO:HD2	1.90	0.53
18:LO:175:LEU:HD23	18:LO:179:GLN:NE2	2.24	0.53
31:Cd:357:ARG:HB3	31:Cd:394:GLY:HA3	1.90	0.53
1:C1:796:G:H1	1:C1:906:A:N6	2.06	0.53
16:LM:128:ARG:HA	16:LM:131:GLU:HG2	1.91	0.53
8:CJ:191:SER:O	8:CJ:212:TYR:OH	2.25	0.53
12:LC:149:VAL:HG13	12:LC:150:PRO:HD3	1.89	0.53
13:LE:85:GLY:O	13:LE:86:PRO:C	2.50	0.53
9:CM:184:ILE:HG23	9:CM:189:ASP:HB3	1.90	0.53
1:C1:533:C:N3	1:C1:539:G:N1	2.58	0.52
3:CA:144:ALA:HB3	11:CU:225:ARG:HA	1.90	0.52
12:LC:24:PRO:HG2	12:LC:265:LEU:HD23	1.92	0.52
16:LM:13:ARG:HA	21:LS:151:PRO:HA	1.91	0.52
1:C1:735:G:C6	1:C1:760:G:C2	2.98	0.52
1:C1:764:A:H5''	1:C1:765:G:H5'	1.91	0.52
7:CI:192:ALA:HB3	7:CI:259:THR:HB	1.90	0.52
4:CB:151:ASP:HA	4:CB:177:LYS:HE3	1.91	0.52
5:CC:400:VAL:HG22	8:CJ:150:LEU:HD11	1.91	0.52
6:CE:173:LEU:HB3	6:CE:212:GLN:HG2	1.91	0.52
12:LC:136:LEU:HD22	12:LC:149:VAL:HG23	1.92	0.52
27:Lh:68:ARG:NH2	27:Lh:84:ASP:O	2.41	0.52
1:C1:36:C:H4'	1:C1:789:A:H2	1.73	0.52
1:C1:1045:G:C6	22:LT:109:VAL:HG12	2.45	0.52
5:CC:174:ASN:OD1	5:CC:174:ASN:N	2.41	0.52
8:CJ:39:TRP:NE1	8:CJ:232:GLU:OE2	2.38	0.52
11:CU:294:THR:HA	11:CU:297:LYS:HG3	1.92	0.52
1:C1:781:G:H22	12:LC:102:ALA:HA	1.74	0.52
14:LG:208:SER:HA	14:LG:211:LYS:HG3	1.91	0.52
24:LY:36:LYS:HZ1	24:LY:39:ARG:HH11	1.58	0.52
24:LY:54:GLU:HB2	24:LY:107:LYS:HB3	1.91	0.52
1:C1:975:G:H4'	1:C1:976:U:H5'	1.91	0.52
18:LO:117:LYS:O	18:LO:119:LYS:NZ	2.43	0.52
18:LO:182:GLU:HA	18:LO:185:LYS:HE2	1.92	0.52
3:CA:121:HIS:HB2	3:CA:237:ARG:HB2	1.92	0.52
19:LP:122:ALA:HB3	19:LP:143:PRO:HB2	1.91	0.52
1:C1:230:A:H2'	1:C1:231:A:C8	2.44	0.52
2:C2:220:G:OP2	7:CI:274:LYS:NZ	2.43	0.52
1:C1:562:U:H2'	1:C1:563:A:H8	1.75	0.52
1:C1:1171:C:N4	1:C1:1297:U:O2'	2.40	0.52
5:CC:189:ASP:HB3	5:CC:195:ILE:HD11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:1114:C:H2'	1:C1:1115:A:H8	1.74	0.51
30:Cc:168:SER:O	30:Cc:194:ARG:NH2	2.43	0.51
1:C1:631:G:H5'	1:C1:1099:G:H1'	1.92	0.51
6:CE:359:LYS:HG2	6:CE:426:VAL:HG12	1.91	0.51
6:CE:377:LEU:HD22	6:CE:382:LEU:HD23	1.91	0.51
27:Lh:38:LYS:HD3	27:Lh:49:ILE:HG13	1.92	0.51
1:C1:63:A:H5''	17:LN:174:LEU:HD13	1.93	0.51
1:C1:522:G:H2'	1:C1:523:A:C8	2.45	0.51
1:C1:3144:C:O5'	18:LO:178:ARG:NH1	2.44	0.51
5:CC:169:VAL:O	5:CC:169:VAL:CG1	2.54	0.51
6:CE:116:LEU:HD11	6:CE:134:MET:HE1	1.93	0.51
6:CE:362:VAL:HB	6:CE:412:ILE:HG22	1.93	0.51
9:CM:102:PRO:HB2	9:CM:105:PRO:HD2	1.91	0.51
18:LO:153:ASP:O	18:LO:157:ARG:HD2	2.09	0.51
3:CA:234:ILE:O	11:CU:277:ARG:NH2	2.44	0.51
9:CM:237:ARG:HG3	9:CM:240:HIS:HB2	1.93	0.51
11:CU:234:GLU:OE1	11:CU:234:GLU:N	2.43	0.51
22:LT:79:ARG:NH2	22:LT:81:LYS:O	2.43	0.51
1:C1:642:C:H2'	1:C1:643:A:C8	2.45	0.51
1:C1:735:G:C5	1:C1:760:G:N2	2.79	0.51
1:C1:2313:U:H2'	1:C1:2314:A:H8	1.75	0.51
18:LO:154:VAL:O	18:LO:158:LEU:HD23	2.11	0.51
1:C1:2315:G:OP2	19:LP:82:ARG:NH2	2.44	0.50
3:CA:137:ARG:NH2	11:CU:215:SER:O	2.43	0.50
18:LO:129:LEU:HD11	21:LS:170:PRO:HG2	1.93	0.50
5:CC:270:PRO:HB3	14:LG:148:ASN:HA	1.93	0.50
8:CJ:54:ASN:ND2	8:CJ:56:SER:O	2.43	0.50
9:CM:116:GLN:HG2	9:CM:119:ASN:HD21	1.76	0.50
14:LG:91:ALA:O	14:LG:95:LYS:HG3	2.11	0.50
5:CC:138:ARG:HB2	5:CC:150:VAL:HB	1.94	0.50
8:CJ:131:TYR:OH	8:CJ:140:ASP:OD2	2.26	0.50
8:CJ:141:LEU:HD21	8:CJ:238:LEU:HD23	1.94	0.50
8:CJ:410:GLU:O	8:CJ:453:ARG:NH1	2.44	0.50
8:CJ:19:ARG:HE	8:CJ:64:TYR:HE2	1.58	0.50
21:LS:21:ASN:OD1	22:LT:146:ASN:ND2	2.44	0.50
5:CC:242:VAL:HG11	14:LG:68:LEU:HD21	1.92	0.50
8:CJ:41:GLY:HA3	8:CJ:130:ARG:HH12	1.75	0.50
8:CJ:169:GLU:HG2	8:CJ:173:HIS:CE1	2.47	0.50
29:Lj:27:LEU:HA	29:Lj:34:CYS:HA	1.93	0.50
32:Ce:91:LEU:HD22	32:Ce:110:LYS:HD2	1.92	0.50
1:C1:370:A:H4'	24:LY:90:THR:HG22	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:3112:A:N6	1:C1:3232:U:H3	2.10	0.50
3:CA:131:ASN:OD1	3:CA:132:CYS:N	2.44	0.50
1:C1:308:U:H2'	28:Li:39:LYS:HZ3	1.77	0.50
1:C1:1348:A:O2'	25:Le:46:ARG:NH2	2.44	0.50
4:CB:251:GLU:H	4:CB:254:LYS:HE2	1.77	0.50
12:LC:328:ARG:O	9:LF:47:ARG:NH1	2.43	0.50
1:C1:3129:G:N1	1:C1:3157:C:O2	2.45	0.50
4:CB:163:LEU:HD23	4:CB:179:PRO:HG2	1.93	0.50
22:LT:79:ARG:HH21	22:LT:82:HIS:HA	1.76	0.50
31:Cd:46:ARG:O	31:Cd:50:GLU:HG2	2.12	0.50
1:C1:19:U:H2'	1:C1:20:A:C8	2.47	0.50
1:C1:676:U:OP1	12:LC:220:LYS:NZ	2.45	0.50
27:Lh:89:LEU:O	29:Lj:73:ARG:NH2	2.45	0.50
1:C1:1049:C:H4'	22:LT:109:VAL:HG21	1.94	0.49
19:LP:126:ARG:HA	19:LP:140:MET:HE1	1.92	0.49
19:LP:158:GLN:O	31:Cd:341:ARG:NH2	2.45	0.49
12:LC:238:ASP:OD1	12:LC:238:ASP:N	2.43	0.49
17:LN:114:ARG:NH1	17:LN:151:ILE:O	2.45	0.49
1:C1:3188:U:H2'	1:C1:3189:G:C8	2.47	0.49
8:CJ:184:SER:HA	8:CJ:186:ARG:HH21	1.75	0.49
1:C1:531:U:N3	1:C1:541:G:N1	2.60	0.49
1:C1:969:U:O4	1:C1:970:A:N6	2.45	0.49
2:C2:176:G:H2'	2:C2:177:C:H6	1.78	0.49
5:CC:354:TYR:HD2	5:CC:387:TYR:HB2	1.76	0.49
2:C2:175:G:H2'	2:C2:176:G:O4'	2.11	0.49
5:CC:401:LYS:O	5:CC:405:GLU:N	2.43	0.49
9:CM:162:VAL:O	9:CM:165:GLN:NE2	2.45	0.49
12:LC:100:MET:HE3	12:LC:103:PRO:HA	1.94	0.49
31:Cd:357:ARG:HE	31:Cd:394:GLY:HA3	1.78	0.49
4:CB:48:ASN:HB3	4:CB:51:ALA:HB3	1.95	0.49
1:C1:1046:A:N6	1:C1:1074:C:C2	2.80	0.49
6:CE:486:PRO:HB2	6:CE:489:LYS:HG3	1.94	0.49
8:CJ:180:ILE:HA	8:CJ:389:ALA:HA	1.95	0.49
32:Ce:33:SER:OG	32:Ce:35:SER:O	2.30	0.49
1:C1:3195:C:H2'	1:C1:3196:G:H8	1.78	0.49
5:CC:282:ILE:HG22	10:CR:219:GLN:HE21	1.77	0.49
1:C1:1331:G:O6	30:Cc:244:ARG:NH2	2.46	0.49
4:CB:215:ARG:HG3	4:CB:220:ILE:HG13	1.94	0.49
1:C1:538:G:H2'	1:C1:539:G:C8	2.47	0.49
2:C2:179:U:OP1	4:CB:77:ARG:NH2	2.46	0.49
13:LE:155:SER:HB3	13:LE:158:ARG:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:971:U:H4'	22:LT:100:ARG:HG3	1.94	0.48
1:C1:1302:C:H2'	1:C1:1303:G:H8	1.78	0.48
8:CJ:187:LYS:HB2	8:CJ:198:GLN:HB3	1.95	0.48
18:LO:145:HIS:NE2	18:LO:152:GLN:HG3	2.28	0.48
21:LS:12:ARG:HH22	21:LS:15:PRO:HG3	1.78	0.48
1:C1:581:G:O2'	13:LE:35:GLN:O	2.30	0.48
1:C1:972:G:H2'	1:C1:973:A:C8	2.48	0.48
5:CC:396:TRP:NE1	5:CC:398:ASN:HB3	2.27	0.48
7:CI:247:THR:HG21	23:LX:24:ALA:HB1	1.95	0.48
8:CJ:177:HIS:HA	8:CJ:180:ILE:HG12	1.95	0.48
12:LC:361:LEU:HD11	22:LT:148:PRO:HG2	1.94	0.48
13:LE:57:VAL:O	13:LE:105:THR:OG1	2.31	0.48
31:Cd:73:ARG:HH12	31:Cd:436:LEU:HD21	1.78	0.48
1:C1:190:G:N2	1:C1:364:A:C8	2.81	0.48
7:CI:250:LYS:NZ	14:LG:227:GLU:OE2	2.47	0.48
8:CJ:218:ILE:HG22	8:CJ:222:VAL:HG21	1.95	0.48
11:CU:224:LYS:HZ2	11:CU:226:THR:HG23	1.79	0.48
3:CA:126:LEU:HD23	11:CU:285:VAL:HG12	1.95	0.48
3:CA:130:GLY:O	11:CU:277:ARG:NH2	2.46	0.48
3:CA:194:TYR:HB3	3:CA:231:LEU:HB3	1.94	0.48
11:CU:236:ASP:OD1	11:CU:236:ASP:N	2.40	0.48
16:LM:124:LYS:O	16:LM:128:ARG:HB2	2.14	0.48
1:C1:403:U:H2'	1:C1:404:G:C8	2.47	0.48
3:CA:114:LYS:HB3	3:CA:244:ILE:HG13	1.95	0.48
9:CM:162:VAL:HG23	9:CM:165:GLN:HE22	1.78	0.48
1:C1:66:A:N6	1:C1:75:G:C2	2.81	0.48
1:C1:231:A:H2'	1:C1:232:G:C8	2.49	0.48
1:C1:247:A:H2'	1:C1:248:G:C8	2.49	0.48
1:C1:372:U:OP1	31:Cd:60:ARG:NH1	2.45	0.48
1:C1:788:A:H61	1:C1:915:G:H22	1.61	0.48
1:C1:3173:C:H42	1:C1:3198:U:H3	1.61	0.48
7:CI:219:VAL:HG23	7:CI:228:ARG:HB2	1.95	0.48
8:CJ:400:VAL:HG21	9:CM:192:HIS:HB3	1.96	0.48
1:C1:966:U:H5''	9:LF:104:LYS:HG3	1.95	0.48
1:C1:1371:G:O6	12:LC:190:LYS:NZ	2.46	0.48
2:C2:26:U:H2'	2:C2:27:U:C6	2.48	0.48
6:CE:172:MET:HB3	6:CE:172:MET:HE3	1.73	0.48
8:CJ:198:GLN:HA	8:CJ:206:ILE:O	2.13	0.48
8:CJ:372:PHE:O	8:CJ:394:ARG:NH2	2.45	0.48
22:LT:65:TYR:HB3	22:LT:75:ILE:HD11	1.95	0.48
2:C2:13:A:O2'	19:LP:121:GLN:O	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CE:384:VAL:HG12	6:CE:410:THR:HG23	1.95	0.48
14:LG:230:GLU:O	14:LG:234:LYS:NZ	2.47	0.48
1:C1:247:A:H2'	1:C1:248:G:H8	1.78	0.48
8:CJ:173:HIS:O	8:CJ:177:HIS:ND1	2.42	0.48
20:LQ:82:MET:HE3	20:LQ:86:ASN:HB3	1.95	0.48
14:LG:159:ASP:OD1	14:LG:159:ASP:N	2.46	0.47
24:LY:43:ASN:HB3	24:LY:122:LYS:HG3	1.95	0.47
1:C1:37:U:O2	15:LL:15:ARG:NH2	2.47	0.47
1:C1:3125:A:O2'	18:LO:103:ARG:NH1	2.47	0.47
13:LE:98:ASN:HB3	13:LE:101:TYR:HD1	1.79	0.47
27:Lh:31:LEU:HD12	27:Lh:49:ILE:CD1	2.44	0.47
29:Lj:64:MET:O	29:Lj:68:SER:OG	2.29	0.47
1:C1:63:A:N3	1:C1:78:U:O2'	2.43	0.47
1:C1:423:U:H2'	1:C1:424:G:C8	2.49	0.47
1:C1:3184:G:H5'	1:C1:3187:G:H21	1.79	0.47
7:CI:239:GLU:OE1	7:CI:239:GLU:N	2.47	0.47
8:CJ:179:LEU:HD22	8:CJ:184:SER:HB2	1.95	0.47
1:C1:75:G:H5''	15:LL:58:VAL:HB	1.95	0.47
8:CJ:190:LEU:HB2	8:CJ:195:ILE:HG12	1.97	0.47
25:Le:70:SER:OG	25:Le:72:HIS:ND1	2.47	0.47
27:Lh:54:LYS:HA	27:Lh:54:LYS:HD3	1.66	0.47
31:Cd:73:ARG:HH22	31:Cd:436:LEU:HG	1.80	0.47
2:C2:166:C:H2'	2:C2:167:A:H8	1.79	0.47
8:CJ:51:ARG:HH22	8:CJ:55:LYS:HA	1.80	0.47
8:CJ:113:PRO:HG3	8:CJ:120:ARG:HB2	1.96	0.47
12:LC:8:THR:HA	12:LC:20:THR:HG22	1.96	0.47
5:CC:180:TYR:OH	11:CU:272:PHE:N	2.45	0.47
8:CJ:197:TYR:HE2	8:CJ:386:ILE:HD11	1.80	0.47
1:C1:421:U:O2'	26:Lf:90:PRO:O	2.28	0.47
1:C1:1372:A:N6	1:C1:1400:A:O2'	2.47	0.47
2:C2:48:A:O2'	2:C2:51:G:N2	2.48	0.47
17:LN:71:ARG:HB2	17:LN:94:TYR:HB2	1.97	0.47
2:C2:9:A:H2'	2:C2:10:A:C8	2.49	0.47
6:CE:170:VAL:HG22	6:CE:207:MET:HE2	1.97	0.47
5:CC:142:ASP:HB3	5:CC:148:ARG:HB2	1.97	0.47
9:CM:185:ILE:O	9:CM:185:ILE:HG22	2.15	0.47
9:LF:93:ILE:HA	9:LF:119:ASN:O	2.15	0.47
5:CC:152:ASP:OD1	5:CC:152:ASP:N	2.48	0.47
1:C1:423:U:H5''	26:Lf:57:ALA:HB1	1.96	0.46
1:C1:1158:C:H4'	18:LO:91:PRO:HD3	1.97	0.46
2:C2:58:G:O6	29:Lj:63:ARG:NH1	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CB:245:VAL:HG12	4:CB:262:VAL:HG21	1.96	0.46
9:CM:153:LEU:HD13	9:CM:245:ILE:HD11	1.97	0.46
10:CR:206:VAL:HG12	10:CR:209:MET:HE2	1.96	0.46
18:LO:174:LYS:O	18:LO:178:ARG:HG2	2.14	0.46
1:C1:639:G:H2'	1:C1:2323:A:H5'	1.96	0.46
4:CB:282:TYR:OH	7:CI:316:ARG:NH1	2.47	0.46
6:CE:269:ILE:HG22	6:CE:274:PHE:HB2	1.97	0.46
21:LS:124:LEU:HD22	22:LT:154:VAL:HG22	1.98	0.46
1:C1:20:A:H2'	1:C1:21:G:C8	2.50	0.46
1:C1:3157:C:OP1	16:LM:132:ARG:NH2	2.48	0.46
31:Cd:257:LEU:HD22	31:Cd:271:VAL:HG22	1.96	0.46
31:Cd:69:ILE:HG23	31:Cd:432:THR:HG22	1.97	0.46
1:C1:424:G:H2'	1:C1:425:A:C8	2.51	0.46
1:C1:539:G:H2'	1:C1:540:A:H8	1.80	0.46
1:C1:966:U:H2'	1:C1:967:U:C6	2.51	0.46
1:C1:1087:C:H2'	1:C1:1088:G:H8	1.80	0.46
8:CJ:88:GLU:HA	8:CJ:91:ILE:HG22	1.97	0.46
1:C1:3189:G:H2'	1:C1:3190:G:C8	2.50	0.46
2:C2:167:A:O2'	9:CM:82:HIS:NE2	2.48	0.46
3:CA:148:GLN:OE1	11:CU:225:ARG:NE	2.47	0.46
3:CA:180:LEU:HD12	3:CA:193:ASN:HB3	1.98	0.46
10:CR:28:ASN:OD1	15:LL:40:ARG:NH1	2.49	0.46
19:LP:22:LEU:HD13	19:LP:90:PHE:HD2	1.80	0.46
20:LQ:99:LEU:HG	20:LQ:104:GLU:HA	1.96	0.46
25:Le:97:ILE:HG21	25:Le:106:ARG:HG2	1.98	0.46
1:C1:910:A:O2'	29:Lj:49:TRP:O	2.31	0.46
1:C1:1134:G:H3'	1:C1:1135:A:H8	1.80	0.46
2:C2:41:A:H4'	29:Lj:59:THR:HG23	1.98	0.46
4:CB:207:ASP:HB3	4:CB:210:GLU:HG3	1.98	0.46
16:LM:105:GLN:NE2	16:LM:109:ARG:HH21	2.13	0.46
16:LM:123:LEU:HG	18:LO:195:VAL:HG23	1.97	0.46
27:Lh:52:LEU:O	27:Lh:56:ILE:HG13	2.16	0.46
1:C1:1151:A:H4'	9:LF:224:LYS:HD3	1.98	0.46
17:LN:10:LEU:HG	28:Li:53:ILE:HD12	1.97	0.46
3:CA:137:ARG:NH1	3:CA:167:GLN:OE1	2.49	0.46
9:LF:66:ARG:HA	9:LF:66:ARG:HD2	1.67	0.46
22:LT:147:LYS:HD3	22:LT:148:PRO:HD2	1.97	0.46
11:CU:235:ASP:OD1	11:CU:235:ASP:N	2.47	0.46
9:LF:184:ILE:HG23	9:LF:189:ASP:HB2	1.97	0.46
1:C1:715:G:H5''	20:LQ:71:PRO:HB2	1.97	0.45
1:C1:916:U:H2'	1:C1:917:A:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:68:C:OP2	1:C1:293:G:N2	2.42	0.45
1:C1:909:C:H2'	1:C1:910:A:C8	2.50	0.45
25:Le:27:LYS:HB3	25:Le:27:LYS:HE3	1.64	0.45
28:Li:32:LYS:HE3	28:Li:32:LYS:HB3	1.75	0.45
1:C1:506:G:H5''	12:LC:346:ALA:HB2	1.98	0.45
7:CI:301:GLN:CD	7:CI:301:GLN:H	2.23	0.45
25:Le:126:LYS:HA	32:Ce:140:LYS:HE2	1.98	0.45
1:C1:663:G:H2'	1:C1:767:A:H61	1.80	0.45
1:C1:972:G:OP1	22:LT:100:ARG:NH2	2.40	0.45
6:CE:135:THR:OG1	6:CE:136:GLU:N	2.48	0.45
6:CE:217:VAL:O	6:CE:239:ALA:HA	2.16	0.45
6:CE:357:LYS:HE2	6:CE:357:LYS:HB2	1.81	0.45
8:CJ:58:THR:HB	8:CJ:61:THR:HG23	1.98	0.45
8:CJ:400:VAL:O	9:CM:151:ARG:NH1	2.50	0.45
12:LC:264:GLN:O	12:LC:268:VAL:HG13	2.17	0.45
1:C1:959:C:H4'	1:C1:961:U:C2	2.52	0.45
1:C1:1430:U:H2'	1:C1:1431:A:H8	1.82	0.45
5:CC:390:LEU:HD23	5:CC:390:LEU:HA	1.81	0.45
8:CJ:392:CYS:HB3	8:CJ:395:ILE:HD11	1.98	0.45
31:Cd:211:ILE:HB	31:Cd:214:GLU:HB2	1.98	0.45
1:C1:1332:A:H2'	1:C1:1333:A:C8	2.51	0.45
1:C1:3143:U:OP1	18:LO:174:LYS:NZ	2.39	0.45
5:CC:196:MET:HE3	5:CC:196:MET:HA	1.99	0.45
5:CC:352:LEU:HD23	5:CC:382:TYR:CG	2.52	0.45
6:CE:191:PRO:HB3	6:CE:269:ILE:HG12	1.98	0.45
8:CJ:119:PRO:HB3	8:CJ:232:GLU:HB2	1.99	0.45
30:Cc:33:LEU:HD12	30:Cc:77:LEU:HD22	1.98	0.45
1:C1:532:C:N4	1:C1:540:A:H61	2.14	0.45
1:C1:664:A:N1	1:C1:690:G:O2'	2.41	0.45
2:C2:293:C:H4'	2:C2:294:A:H2	1.82	0.45
5:CC:164:ASP:O	5:CC:167:VAL:HG23	2.17	0.45
24:LY:28:VAL:O	24:LY:31:SER:OG	2.34	0.45
30:Cc:60:MET:HE3	30:Cc:60:MET:HB3	1.81	0.45
1:C1:66:A:H61	1:C1:75:G:N2	2.11	0.45
1:C1:618:A:H2'	1:C1:619:G:C8	2.51	0.45
1:C1:1172:A:N3	18:LO:50:ARG:NH2	2.65	0.45
2:C2:130:C:H2'	2:C2:131:G:C8	2.52	0.45
3:CA:169:HIS:NE2	5:CC:158:TYR:OH	2.40	0.45
3:CA:181:SER:O	3:CA:191:VAL:HA	2.17	0.45
3:CA:198:GLU:HG2	3:CA:229:ILE:HG22	1.99	0.45
11:CU:290:ILE:O	11:CU:294:THR:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:LF:102:PRO:HB2	9:LF:105:PRO:HD2	1.99	0.45
18:LO:55:TYR:O	18:LO:59:LEU:HD22	2.17	0.45
29:Lj:64:MET:HE2	29:Lj:67:LEU:HB3	1.99	0.45
31:Cd:94:ARG:NH2	31:Cd:95:ARG:HE	2.14	0.45
1:C1:488:A:O2'	1:C1:3213:A:N1	2.49	0.45
8:CJ:453:ARG:NH2	8:CJ:455:TYR:OH	2.50	0.45
9:CM:185:ILE:O	9:CM:185:ILE:CG2	2.65	0.45
1:C1:155:G:H2'	1:C1:156:G:C8	2.52	0.45
1:C1:662:C:O2'	1:C1:666:U:OP1	2.33	0.45
18:LO:155:VAL:O	18:LO:159:GLU:HB2	2.17	0.45
21:LS:168:LYS:HB2	21:LS:168:LYS:HE3	1.67	0.45
31:Cd:370:LYS:O	31:Cd:387:ARG:NH1	2.50	0.45
1:C1:1172:A:H2'	18:LO:50:ARG:HH21	1.82	0.44
1:C1:3195:C:H2'	1:C1:3196:G:C8	2.52	0.44
10:CR:50:THR:OG1	10:CR:69:ASN:O	2.22	0.44
1:C1:31:C:H4'	17:LN:96:ARG:HG2	2.00	0.44
1:C1:1046:A:N6	1:C1:1074:C:O2	2.50	0.44
2:C2:148:G:H2'	2:C2:149:A:H8	1.82	0.44
11:CU:207:ILE:HD12	11:CU:217:HIS:HB3	2.00	0.44
13:LE:152:LYS:HB2	13:LE:152:LYS:HE3	1.76	0.44
16:LM:96:GLU:O	16:LM:101:LYS:NZ	2.50	0.44
1:C1:3159:A:OP2	16:LM:125:LYS:NZ	2.51	0.44
10:CR:19:MET:HE1	29:Lj:75:LYS:HB2	1.99	0.44
19:LP:86:LYS:HA	19:LP:89:GLN:HG3	1.99	0.44
27:Lh:38:LYS:HE2	27:Lh:38:LYS:HB3	1.84	0.44
3:CA:131:ASN:OD1	11:CU:276:VAL:HB	2.18	0.44
6:CE:285:LEU:O	6:CE:287:LYS:NZ	2.49	0.44
1:C1:447:C:N4	1:C1:448:A:N6	2.64	0.44
1:C1:1070:U:H2'	1:C1:1071:G:C8	2.52	0.44
1:C1:1370:U:O2'	25:Le:100:ASN:O	2.29	0.44
2:C2:205:G:N3	4:CB:240:ASN:ND2	2.63	0.44
6:CE:267:ASP:OD1	6:CE:267:ASP:N	2.49	0.44
9:CM:241:ILE:HD12	9:CM:241:ILE:H	1.83	0.44
11:CU:200:LEU:O	11:CU:204:GLN:N	2.50	0.44
12:LC:151:LEU:HD23	12:LC:256:VAL:HG22	1.99	0.44
17:LN:114:ARG:HG2	17:LN:137:PRO:HG3	2.00	0.44
18:LO:179:GLN:HA	18:LO:182:GLU:HG3	1.98	0.44
30:Cc:215:GLU:OE1	30:Cc:215:GLU:N	2.46	0.44
2:C2:75:G:H2'	2:C2:76:C:C6	2.53	0.44
6:CE:165:PHE:HB2	6:CE:262:ILE:HG12	2.00	0.44
14:LG:98:ASN:HA	14:LG:101:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:290:U:O2'	28:Li:38:ARG:NH1	2.51	0.44
1:C1:966:U:H2'	1:C1:967:U:H6	1.83	0.44
2:C2:8:C:H2'	2:C2:9:A:H8	1.82	0.44
2:C2:23:U:H5''	24:LY:12:ARG:HG3	2.00	0.44
5:CC:367:ARG:HH22	5:CC:385:THR:HA	1.83	0.44
8:CJ:130:ARG:HD3	8:CJ:131:TYR:CZ	2.53	0.44
8:CJ:376:ARG:HH12	9:CM:189:ASP:CG	2.26	0.44
10:CR:132:PRO:HG2	15:LL:106:GLU:HB3	2.00	0.44
1:C1:522:G:H2'	1:C1:523:A:H8	1.83	0.44
1:C1:979:A:H2'	1:C1:980:G:C8	2.53	0.44
1:C1:1292:G:H2'	1:C1:1293:G:C8	2.52	0.44
1:C1:3192:C:H2'	1:C1:3193:G:H8	1.82	0.44
7:CI:218:VAL:HG22	7:CI:231:ALA:HB2	2.00	0.44
8:CJ:84:GLN:HG3	8:CJ:121:TYR:HE1	1.83	0.44
9:CM:190:LEU:HA	9:CM:193:GLU:HB2	1.99	0.44
18:LO:142:ARG:HA	18:LO:145:HIS:HB2	2.00	0.44
22:LT:104:ASP:HA	22:LT:107:ARG:HG2	2.00	0.44
28:Li:88:THR:HB	28:Li:91:ARG:HG3	2.00	0.44
1:C1:461:A:H5'	32:Ce:82:LYS:HB2	2.00	0.43
12:LC:49:GLN:HE21	12:LC:49:GLN:HB3	1.64	0.43
22:LT:42:ILE:O	22:LT:59:GLY:HA2	2.18	0.43
5:CC:356:PRO:HG3	5:CC:384:PRO:HB2	2.00	0.43
7:CI:234:GLU:HB2	7:CI:273:PHE:CZ	2.53	0.43
7:CI:251:TYR:OH	9:CM:53:ARG:NH1	2.51	0.43
21:LS:110:MET:HE3	21:LS:110:MET:HB3	1.90	0.43
1:C1:29:C:H4'	1:C1:62:A:H4'	1.99	0.43
1:C1:423:U:H2'	1:C1:424:G:H8	1.82	0.43
4:CB:80:PRO:HD2	4:CB:181:PRO:HD3	1.99	0.43
8:CJ:191:SER:N	8:CJ:194:GLY:O	2.50	0.43
16:LM:11:TRP:HE1	21:LS:151:PRO:HB2	1.83	0.43
4:CB:117:PRO:HA	4:CB:121:ARG:HB3	2.00	0.43
6:CE:539:VAL:HG22	6:CE:550:PRO:HG3	2.01	0.43
9:LF:113:ARG:HB3	9:LF:210:PRO:HG3	2.01	0.43
18:LO:194:LYS:H	18:LO:194:LYS:HD3	1.82	0.43
1:C1:340:C:O2	1:C1:344:A:O2'	2.35	0.43
1:C1:350:G:N2	1:C1:353:A:OP2	2.40	0.43
2:C2:148:G:H2'	2:C2:149:A:C8	2.54	0.43
5:CC:148:ARG:HE	11:CU:202:ARG:HH22	1.66	0.43
8:CJ:34:ARG:HH21	8:CJ:35:LYS:HG3	1.84	0.43
12:LC:344:VAL:HG11	9:LF:62:ARG:HH11	1.84	0.43
9:LF:173:ALA:O	9:LF:177:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:231:A:H2'	1:C1:232:G:H8	1.84	0.43
1:C1:581:G:H1'	13:LE:37:LYS:HG3	1.99	0.43
5:CC:184:PRO:HA	5:CC:197:ARG:HH12	1.83	0.43
7:CI:197:GLY:HA3	9:CM:58:VAL:HG13	1.98	0.43
8:CJ:99:ASP:OD1	8:CJ:99:ASP:N	2.51	0.43
9:LF:189:ASP:OD1	9:LF:189:ASP:N	2.51	0.43
18:LO:79:SER:HB2	18:LO:106:VAL:HB	2.01	0.43
1:C1:363:G:N1	1:C1:366:A:OP2	2.41	0.43
1:C1:765:G:H2'	20:LQ:97:ARG:HH11	1.84	0.43
1:C1:1344:G:H2'	1:C1:1345:A:C8	2.53	0.43
3:CA:58:MET:HE1	3:CA:180:LEU:HD13	2.01	0.43
8:CJ:187:LYS:HB3	8:CJ:187:LYS:HE3	1.89	0.43
16:LM:31:VAL:HG11	16:LM:54:ARG:NH2	2.34	0.43
32:Ce:97:ARG:HA	32:Ce:97:ARG:HD2	1.89	0.43
1:C1:278:U:O2'	17:LN:179:ARG:O	2.35	0.43
1:C1:532:C:H42	1:C1:540:A:N6	2.16	0.43
31:Cd:32:LYS:HE2	31:Cd:32:LYS:HB3	1.79	0.43
1:C1:574:G:H2'	1:C1:575:A:H8	1.84	0.43
1:C1:910:A:OP1	12:LC:62:SER:OG	2.26	0.43
3:CA:177:ASP:OD1	3:CA:177:ASP:N	2.51	0.43
4:CB:61:PRO:HD2	4:CB:286:PRO:HG3	2.00	0.43
4:CB:169:LYS:HG2	4:CB:173:LYS:HB2	1.99	0.43
4:CB:259:ILE:O	4:CB:263:ILE:HG13	2.19	0.43
9:CM:162:VAL:HG23	9:CM:165:GLN:NE2	2.34	0.43
9:CM:203:GLN:CD	9:CM:203:GLN:H	2.27	0.43
11:CU:198:THR:O	11:CU:202:ARG:HD3	2.19	0.43
18:LO:193:PRO:HA	18:LO:196:SER:OG	2.18	0.43
26:Lf:50:ARG:HH12	26:Lf:70:TRP:HB3	1.84	0.43
31:Cd:76:ASP:OD1	31:Cd:433:ARG:NH1	2.43	0.43
31:Cd:221:ILE:HD11	31:Cd:395:PRO:HG2	2.00	0.43
1:C1:1096:U:H2'	1:C1:1097:G:C8	2.54	0.43
5:CC:175:ILE:HG12	11:CU:274:GLU:OE2	2.19	0.43
10:CR:216:ASN:ND2	10:CR:218:TYR:O	2.52	0.43
14:LG:111:ARG:O	14:LG:115:GLU:HG2	2.19	0.43
18:LO:130:ARG:HD2	18:LO:130:ARG:HA	1.77	0.43
28:Li:65:ARG:HA	28:Li:68:GLU:HG2	2.01	0.43
32:Ce:89:LYS:HZ2	32:Ce:89:LYS:HG3	1.62	0.43
1:C1:243:G:N2	10:CR:191:GLU:OE1	2.52	0.42
2:C2:50:C:OP2	2:C2:51:G:N2	2.47	0.42
3:CA:279:HIS:O	3:CA:283:MET:HG2	2.19	0.42
5:CC:406:ARG:O	5:CC:410:LEU:HD12	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:CE:152:LEU:HG	6:CE:317:TYR:HD1	1.84	0.42
9:CM:89:LEU:HD21	9:CM:122:PHE:HB3	2.01	0.42
12:LC:317:LYS:HB2	12:LC:325:ILE:HG13	2.00	0.42
14:LG:206:VAL:HG23	14:LG:211:LYS:HG2	2.01	0.42
5:CC:261:TRP:HB2	28:Li:105:GLU:HB2	2.01	0.42
8:CJ:245:LEU:HD23	8:CJ:245:LEU:HA	1.89	0.42
21:LS:25:TYR:HB2	21:LS:45:LEU:HD21	1.99	0.42
7:CI:295:ARG:HA	7:CI:296:PRO:HD3	1.87	0.42
8:CJ:72:LEU:HD12	8:CJ:72:LEU:HA	1.92	0.42
12:LC:335:THR:HA	12:LC:338:LYS:HB3	2.02	0.42
18:LO:13:LYS:O	21:LS:169:ARG:NH2	2.43	0.42
27:Lh:108:LYS:H	27:Lh:108:LYS:HG2	1.67	0.42
28:Li:95:LYS:HB2	28:Li:95:LYS:HE2	1.84	0.42
32:Ce:126:ILE:O	32:Ce:130:GLU:HG3	2.19	0.42
1:C1:574:G:H2'	1:C1:575:A:C8	2.54	0.42
1:C1:942:C:H41	11:CU:303:ARG:HH22	1.67	0.42
1:C1:1306:C:H5'	21:LS:2:GLY:HA2	2.00	0.42
6:CE:167:ILE:HD13	6:CE:206:LEU:HD21	2.01	0.42
11:CU:199:ALA:HA	11:CU:202:ARG:HD3	2.01	0.42
9:LF:174:ILE:H	9:LF:174:ILE:HG13	1.65	0.42
2:C2:48:A:H61	2:C2:54:A:N6	2.17	0.42
3:CA:116:TYR:HB2	3:CA:243:ILE:HD11	2.02	0.42
5:CC:155:ASP:HA	5:CC:156:PRO:HD3	1.89	0.42
5:CC:402:GLU:O	5:CC:405:GLU:HB2	2.19	0.42
8:CJ:134:PHE:HE1	8:CJ:241:VAL:HG22	1.84	0.42
9:LF:52:LYS:O	9:LF:55:GLU:HB2	2.18	0.42
1:C1:497:U:H2'	1:C1:498:C:C6	2.54	0.42
1:C1:647:A:N1	1:C1:922:G:O2'	2.52	0.42
6:CE:278:MET:HG2	6:CE:306:LEU:HD11	2.01	0.42
14:LG:85:LEU:HD12	14:LG:183:ILE:HD12	2.02	0.42
17:LN:44:ARG:NH2	17:LN:47:LYS:HG2	2.35	0.42
1:C1:493:C:O5'	13:LE:44:ARG:NH1	2.52	0.42
1:C1:618:A:H2'	1:C1:619:G:H8	1.84	0.42
9:LF:138:PRO:HA	9:LF:234:LEU:HD13	2.02	0.42
19:LP:57:ALA:HA	19:LP:83:TRP:CD1	2.55	0.42
21:LS:77:ILE:HG12	21:LS:126:VAL:HG13	2.01	0.42
22:LT:114:GLU:O	22:LT:118:LYS:HG2	2.19	0.42
24:LY:30:MET:HE3	24:LY:100:PRO:HG3	2.00	0.42
1:C1:324:C:H4'	29:Lj:71:PRO:HB3	2.00	0.42
7:CI:191:ILE:HG23	7:CI:231:ALA:HB3	2.01	0.42
18:LO:193:PRO:O	18:LO:197:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:614:C:H2'	1:C1:615:A:C8	2.55	0.42
1:C1:2313:U:H2'	1:C1:2314:A:C8	2.55	0.42
3:CA:122:THR:OG1	3:CA:125:GLU:OE1	2.29	0.42
8:CJ:40:LYS:HE3	8:CJ:75:GLU:HG3	2.01	0.42
8:CJ:367:PHE:HA	8:CJ:370:PHE:HD2	1.84	0.42
12:LC:362:LEU:HG	21:LS:64:ILE:HG23	2.02	0.42
14:LG:78:ILE:HD11	17:LN:18:VAL:HG13	2.02	0.42
14:LG:220:ALA:O	14:LG:224:GLY:N	2.53	0.42
1:C1:1079:G:N7	22:LT:116:LYS:NZ	2.56	0.42
4:CB:23:THR:HG22	4:CB:293:ILE:HD12	2.01	0.42
8:CJ:26:LEU:HD23	8:CJ:33:PHE:HD1	1.84	0.42
8:CJ:102:ASN:OD1	8:CJ:105:ARG:NH2	2.52	0.42
16:LM:70:PRO:HD3	16:LM:88:TYR:CD2	2.54	0.42
21:LS:88:HIS:HB2	21:LS:90:MET:HE3	2.02	0.42
28:Li:101:ARG:O	28:Li:105:GLU:HG2	2.20	0.42
31:Cd:311:LEU:HD21	31:Cd:332:PHE:CG	2.54	0.42
1:C1:430:A:N1	1:C1:605:C:O2'	2.48	0.41
1:C1:434:G:H2'	1:C1:435:C:C6	2.55	0.41
1:C1:487:C:H2'	1:C1:488:A:H8	1.85	0.41
1:C1:983:A:N1	1:C1:1032:U:O2'	2.53	0.41
1:C1:1087:C:H2'	1:C1:1088:G:C8	2.55	0.41
1:C1:1302:C:H2'	1:C1:1303:G:C8	2.55	0.41
8:CJ:34:ARG:HH21	8:CJ:35:LYS:HE3	1.85	0.41
15:LL:79:GLU:OE1	15:LL:101:ARG:NH2	2.53	0.41
24:LY:130:LYS:HA	24:LY:130:LYS:HD3	1.83	0.41
30:Cc:51:TRP:CE2	30:Cc:93:PHE:HB2	2.54	0.41
30:Cc:126:TRP:CE2	30:Cc:154:LYS:HD3	2.55	0.41
31:Cd:373:VAL:HG23	31:Cd:378:LYS:HA	2.02	0.41
1:C1:945:G:H2'	1:C1:946:A:H8	1.85	0.41
1:C1:1046:A:N1	1:C1:1074:C:C4	2.89	0.41
2:C2:8:C:H2'	2:C2:9:A:C8	2.55	0.41
2:C2:229:U:H2'	2:C2:230:C:C6	2.55	0.41
7:CI:197:GLY:HA2	9:CM:61:TYR:CD2	2.55	0.41
9:CM:51:PHE:HB3	23:LX:31:VAL:HG21	2.02	0.41
9:CM:184:ILE:HD11	9:CM:193:GLU:HG3	2.01	0.41
20:LQ:90:VAL:O	20:LQ:114:VAL:HA	2.20	0.41
1:C1:194:G:H2'	1:C1:195:G:H8	1.86	0.41
1:C1:490:C:H2'	1:C1:491:A:C8	2.55	0.41
1:C1:944:G:H2'	1:C1:945:G:C8	2.55	0.41
2:C2:213:A:OP2	4:CB:144:ARG:NH2	2.50	0.41
6:CE:223:ARG:NE	6:CE:246:ASP:OD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:CJ:171:LEU:HB3	8:CJ:238:LEU:HD12	2.01	0.41
15:LL:113:VAL:O	15:LL:117:LYS:HG3	2.20	0.41
31:Cd:424:LYS:H	31:Cd:427:MET:HE2	1.83	0.41
3:CA:138:PRO:HB3	3:CA:178:HIS:CE1	2.55	0.41
5:CC:312:ARG:HD2	5:CC:312:ARG:HA	1.89	0.41
5:CC:403:ARG:HG2	8:CJ:150:LEU:HD22	2.02	0.41
8:CJ:34:ARG:HD3	8:CJ:226:ILE:HG22	2.03	0.41
8:CJ:127:ILE:HG22	8:CJ:233:PHE:HE1	1.85	0.41
22:LT:45:ASN:H	22:LT:95:HIS:CE1	2.38	0.41
31:Cd:328:MET:HG3	31:Cd:346:LEU:HD13	2.02	0.41
1:C1:1098:G:O6	1:C1:1123:C:N3	2.53	0.41
1:C1:1139:G:O2'	1:C1:1151:A:N3	2.45	0.41
2:C2:298:G:H5''	7:CI:291:ARG:HH22	1.85	0.41
3:CA:37:LEU:HB3	3:CA:89:VAL:HG12	2.03	0.41
7:CI:305:LYS:HD2	7:CI:305:LYS:HA	1.89	0.41
10:CR:45:LEU:HD13	15:LL:43:ALA:HB2	2.03	0.41
26:Lf:87:PHE:O	26:Lf:88:THR:C	2.64	0.41
30:Cc:176:THR:HG22	30:Cc:177:GLN:H	1.84	0.41
31:Cd:326:LYS:HA	31:Cd:326:LYS:HD3	1.88	0.41
1:C1:968:U:O3'	9:LF:127:LYS:NZ	2.43	0.41
1:C1:1053:U:H2'	1:C1:1054:G:H8	1.85	0.41
1:C1:1360:U:H2'	1:C1:1361:G:H8	1.86	0.41
5:CC:411:TYR:CE1	8:CJ:41:GLY:HA2	2.54	0.41
9:CM:76:LYS:HB3	9:CM:76:LYS:HE2	1.89	0.41
10:CR:40:ASN:HB3	10:CR:43:GLU:HB2	2.02	0.41
12:LC:171:LYS:HE2	12:LC:171:LYS:HB3	1.89	0.41
9:LF:94:ARG:O	9:LF:118:ASN:N	2.54	0.41
17:LN:47:LYS:HA	17:LN:47:LYS:HD2	1.82	0.41
29:Lj:32:LYS:HE3	29:Lj:32:LYS:HB3	1.70	0.41
1:C1:72:C:N3	1:C1:74:G:C5	2.89	0.41
1:C1:159:G:OP2	10:CR:227:ARG:NH2	2.54	0.41
4:CB:104:PRO:HG2	4:CB:208:PRO:O	2.21	0.41
6:CE:292:THR:HB	6:CE:311:LEU:HG	2.02	0.41
7:CI:188:VAL:HG22	7:CI:234:GLU:HG3	2.03	0.41
8:CJ:156:SER:HB2	8:CJ:165:ILE:HD12	2.03	0.41
9:CM:141:ALA:HB1	9:CM:237:ARG:HH22	1.86	0.41
18:LO:23:ILE:HD13	18:LO:122:VAL:HG11	2.01	0.41
18:LO:144:SER:HB3	18:LO:149:TRP:HB2	2.02	0.41
26:Lf:105:TYR:HA	26:Lf:106:PRO:C	2.45	0.41
31:Cd:288:THR:HG23	31:Cd:402:ARG:HG3	2.01	0.41
1:C1:436:G:H5''	13:LE:26:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C1:727:C:H2'	1:C1:728:A:H8	1.85	0.41
1:C1:3159:A:N6	1:C1:3199:A:H2'	2.36	0.41
1:C1:3169:U:O2'	1:C1:3200:A:N1	2.44	0.41
3:CA:236:PRO:HB2	3:CA:238:PHE:CE1	2.55	0.41
5:CC:175:ILE:HG23	11:CU:274:GLU:HG3	2.01	0.41
22:LT:131:GLN:HA	22:LT:132:PRO:HD3	1.81	0.41
1:C1:158:U:H2'	1:C1:159:G:C8	2.55	0.41
1:C1:643:A:H2'	1:C1:644:A:C8	2.56	0.41
1:C1:662:C:H2'	1:C1:663:G:O4'	2.21	0.41
1:C1:2319:A:H2'	1:C1:2320:A:H8	1.85	0.41
2:C2:52:A:H2	31:Cd:23:LYS:HE3	1.86	0.41
3:CA:131:ASN:HA	3:CA:234:ILE:HG23	2.02	0.41
3:CA:137:ARG:HE	3:CA:137:ARG:HB3	1.37	0.41
8:CJ:35:LYS:O	8:CJ:38:ILE:HG22	2.20	0.41
8:CJ:190:LEU:HA	8:CJ:195:ILE:HA	2.03	0.41
9:CM:202:LYS:HB2	9:CM:202:LYS:HE2	1.89	0.41
12:LC:154:ASP:N	12:LC:154:ASP:OD1	2.54	0.41
9:LF:92:VAL:O	9:LF:120:GLY:HA2	2.21	0.41
18:LO:10:ILE:HG21	18:LO:20:LEU:HD11	2.03	0.41
22:LT:48:VAL:HG12	22:LT:50:LYS:H	1.86	0.41
24:LY:71:SER:HB3	24:LY:80:HIS:HB2	2.01	0.41
1:C1:533:C:C2	1:C1:539:G:N1	2.89	0.41
3:CA:133:LEU:C	3:CA:134:LYS:HD3	2.46	0.41
4:CB:52:ASP:H	4:CB:55:SER:HG	1.66	0.41
4:CB:104:PRO:CD	4:CB:208:PRO:HB3	2.50	0.41
4:CB:130:ILE:O	4:CB:134:LYS:HG3	2.21	0.41
8:CJ:267:GLU:HB3	8:CJ:380:ARG:NH2	2.36	0.41
10:CR:209:MET:HE1	10:CR:229:LEU:HD11	2.03	0.41
21:LS:146:LYS:HA	21:LS:146:LYS:HD2	1.89	0.41
24:LY:75:LEU:HD23	24:LY:75:LEU:HA	1.79	0.41
31:Cd:386:ILE:HD13	31:Cd:386:ILE:HA	1.94	0.41
1:C1:753:U:H2'	1:C1:754:G:C8	2.57	0.40
1:C1:1090:C:H2'	1:C1:1091:A:H8	1.86	0.40
2:C2:216:A:H2	7:CI:263:VAL:HG22	1.84	0.40
5:CC:241:LYS:HE2	5:CC:241:LYS:HB3	1.81	0.40
5:CC:243:GLN:HG3	5:CC:247:ILE:HD11	2.03	0.40
9:LF:239:GLU:H	9:LF:239:GLU:HG2	1.66	0.40
22:LT:79:ARG:HA	22:LT:79:ARG:HD2	1.86	0.40
1:C1:745:U:O2	1:C1:749:C:N3	2.54	0.40
3:CA:173:LYS:HA	3:CA:173:LYS:HD3	1.79	0.40
4:CB:20:PRO:O	4:CB:23:THR:OG1	2.32	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:CB:52:ASP:O	4:CB:56:THR:OG1	2.34	0.40
5:CC:126:ARG:HA	5:CC:126:ARG:HD2	1.99	0.40
6:CE:504:ASN:HB3	6:CE:507:LEU:HB2	2.02	0.40
17:LN:183:THR:HG22	17:LN:187:ARG:HB2	2.03	0.40
3:CA:190:TRP:HE3	3:CA:192:ARG:HH22	1.68	0.40
5:CC:180:TYR:HA	5:CC:183:TYR:HD1	1.86	0.40
8:CJ:17:MET:HG2	8:CJ:21:GLN:HB2	2.03	0.40
8:CJ:196:TYR:CD1	8:CJ:209:LEU:HD13	2.56	0.40
14:LG:146:ILE:HG23	14:LG:178:ILE:HD13	2.03	0.40
1:C1:110:G:OP2	15:LL:73:ARG:NH2	2.35	0.40
1:C1:194:G:OP1	1:C1:213:G:O2'	2.32	0.40
1:C1:411:G:H2'	1:C1:412:G:C8	2.57	0.40
1:C1:633:A:H3'	1:C1:634:A:H8	1.86	0.40
1:C1:1101:C:H2'	1:C1:1102:A:H8	1.85	0.40
3:CA:146:PHE:HB3	3:CA:156:LYS:HD2	2.03	0.40
6:CE:328:THR:HB	6:CE:447:ARG:HH22	1.86	0.40
8:CJ:51:ARG:O	8:CJ:51:ARG:NE	2.54	0.40
8:CJ:183:HIS:ND1	8:CJ:389:ALA:O	2.55	0.40
8:CJ:367:PHE:HA	8:CJ:370:PHE:CD2	2.56	0.40
8:CJ:419:ILE:HD13	8:CJ:419:ILE:HA	1.92	0.40
18:LO:185:LYS:HE2	18:LO:185:LYS:HB2	1.96	0.40
21:LS:27:MET:HE2	21:LS:27:MET:HB3	2.00	0.40
1:C1:1045:G:H1'	1:C1:1048:G:H1'	2.04	0.40
7:CI:189:MET:HE3	7:CI:260:CYS:HB3	2.04	0.40
8:CJ:454:ILE:HG22	8:CJ:456:VAL:HG13	2.04	0.40
9:CM:187:ILE:O	9:CM:190:LEU:HD12	2.22	0.40
12:LC:146:VAL:HA	12:LC:147:PRO:HD3	1.95	0.40
14:LG:153:LEU:HB3	14:LG:203:ILE:HG22	2.03	0.40
31:CD:360:TYR:HA	31:CD:389:GLY:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	CA	254/316 (80%)	238 (94%)	16 (6%)	0	100	100
4	CB	265/391 (68%)	252 (95%)	12 (4%)	1 (0%)	30	65
5	CC	250/801 (31%)	241 (96%)	9 (4%)	0	100	100
6	CE	459/598 (77%)	440 (96%)	19 (4%)	0	100	100
7	CI	144/414 (35%)	131 (91%)	13 (9%)	0	100	100
8	CJ	374/679 (55%)	359 (96%)	15 (4%)	0	100	100
9	CM	183/249 (74%)	175 (96%)	8 (4%)	0	100	100
9	LF	238/249 (96%)	229 (96%)	9 (4%)	0	100	100
10	CR	159/237 (67%)	152 (96%)	6 (4%)	1 (1%)	21	56
11	CU	114/451 (25%)	113 (99%)	1 (1%)	0	100	100
12	LC	360/365 (99%)	351 (98%)	9 (2%)	0	100	100
13	LE	166/200 (83%)	152 (92%)	13 (8%)	1 (1%)	21	56
14	LG	181/262 (69%)	178 (98%)	3 (2%)	0	100	100
15	LL	115/213 (54%)	113 (98%)	2 (2%)	0	100	100
16	LM	126/142 (89%)	120 (95%)	5 (4%)	1 (1%)	16	50
17	LN	179/203 (88%)	175 (98%)	4 (2%)	0	100	100
18	LO	202/204 (99%)	191 (95%)	11 (5%)	0	100	100
19	LP	150/187 (80%)	148 (99%)	2 (1%)	0	100	100
20	LQ	127/213 (60%)	122 (96%)	5 (4%)	0	100	100
21	LS	172/174 (99%)	164 (95%)	8 (5%)	0	100	100
22	LT	124/160 (78%)	115 (93%)	7 (6%)	2 (2%)	7	34
23	LX	20/156 (13%)	20 (100%)	0	0	100	100
24	LY	132/138 (96%)	129 (98%)	3 (2%)	0	100	100
25	Le	129/131 (98%)	124 (96%)	5 (4%)	0	100	100
26	Lf	106/109 (97%)	101 (95%)	5 (5%)	0	100	100
27	Lh	119/935 (13%)	116 (98%)	3 (2%)	0	100	100
28	Li	86/110 (78%)	84 (98%)	2 (2%)	0	100	100
29	Lj	72/95 (76%)	70 (97%)	2 (3%)	0	100	100
30	Cc	232/282 (82%)	226 (97%)	6 (3%)	0	100	100
31	Cd	334/436 (77%)	317 (95%)	17 (5%)	0	100	100
32	Ce	192/336 (57%)	188 (98%)	4 (2%)	0	100	100
All	All	5764/9436 (61%)	5534 (96%)	224 (4%)	6 (0%)	49	80

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	CB	104	PRO
10	CR	130	ALA
16	LM	22	LEU
13	LE	86	PRO
22	LT	44	VAL
22	LT	81	LYS

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	
3	CA	231/276 (84%)	228 (99%)	3 (1%)	61	81
4	CB	231/329 (70%)	226 (98%)	5 (2%)	45	74
5	CC	240/710 (34%)	240 (100%)	0	100	100
6	CE	398/517 (77%)	397 (100%)	1 (0%)	86	91
7	CI	121/336 (36%)	119 (98%)	2 (2%)	53	78
8	CJ	332/579 (57%)	330 (99%)	2 (1%)	78	88
9	CM	161/215 (75%)	157 (98%)	4 (2%)	42	72
9	LF	206/215 (96%)	205 (100%)	1 (0%)	81	89
10	CR	144/206 (70%)	139 (96%)	5 (4%)	32	65
11	CU	99/376 (26%)	97 (98%)	2 (2%)	48	76
12	LC	283/285 (99%)	281 (99%)	2 (1%)	76	86
13	LE	143/166 (86%)	137 (96%)	6 (4%)	26	61
14	LG	158/222 (71%)	158 (100%)	0	100	100
15	LL	99/176 (56%)	98 (99%)	1 (1%)	68	84
16	LM	108/117 (92%)	107 (99%)	1 (1%)	70	85
17	LN	164/180 (91%)	158 (96%)	6 (4%)	30	64
18	LO	163/163 (100%)	162 (99%)	1 (1%)	78	88
19	LP	125/152 (82%)	123 (98%)	2 (2%)	55	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
20	LQ	110/178 (62%)	106 (96%)	4 (4%)	31	65
21	LS	154/154 (100%)	149 (97%)	5 (3%)	34	67
22	LT	109/135 (81%)	109 (100%)	0	100	100
23	LX	12/129 (9%)	12 (100%)	0	100	100
24	LY	117/119 (98%)	116 (99%)	1 (1%)	70	85
25	Le	114/114 (100%)	114 (100%)	0	100	100
26	Lf	89/90 (99%)	88 (99%)	1 (1%)	65	83
27	Lh	108/781 (14%)	108 (100%)	0	100	100
28	Li	75/93 (81%)	74 (99%)	1 (1%)	61	81
29	Lj	61/78 (78%)	61 (100%)	0	100	100
30	Cc	204/244 (84%)	203 (100%)	1 (0%)	81	89
31	Cd	291/367 (79%)	291 (100%)	0	100	100
32	Ce	173/297 (58%)	173 (100%)	0	100	100
All	All	5023/7999 (63%)	4966 (99%)	57 (1%)	63	83

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	CA	80	LEU
3	CA	133	LEU
3	CA	244	ILE
4	CB	66	LEU
4	CB	104	PRO
4	CB	127	VAL
4	CB	163	LEU
4	CB	220	ILE
6	CE	533	VAL
7	CI	323	MET
7	CI	327	PHE
8	CJ	30	LEU
8	CJ	144	CYS
9	CM	60	GLU
9	CM	95	ILE
9	CM	96	LYS
9	CM	241	ILE
10	CR	10	ARG
10	CR	127	GLU

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Mol	Chain	Res	Type
10	CR	134	GLN
10	CR	164	SER
10	CR	211	ARG
11	CU	226	THR
11	CU	276	VAL
12	LC	232	VAL
12	LC	354	VAL
13	LE	116	GLN
13	LE	126	LYS
13	LE	158	ARG
13	LE	165	ILE
13	LE	169	LEU
13	LE	183	LEU
9	LF	77	GLN
15	LL	68	ARG
16	LM	20	LEU
17	LN	5	LYS
17	LN	7	LEU
17	LN	9	GLU
17	LN	62	TYR
17	LN	64	VAL
17	LN	167	THR
18	LO	6	SER
19	LP	116	HIS
19	LP	148	LEU
20	LQ	92	LEU
20	LQ	113	THR
20	LQ	114	VAL
20	LQ	156	LEU
21	LS	79	LEU
21	LS	129	LEU
21	LS	133	GLU
21	LS	144	VAL
21	LS	159	ILE
24	LY	75	LEU
26	Lf	68	VAL
28	Li	52	LEU
30	Cc	176	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
3	CA	85	ASN
3	CA	119	ASN
3	CA	121	HIS
3	CA	246	GLN
4	CB	22	GLN
4	CB	47	GLN
4	CB	211	ASN
5	CC	166	ASN
5	CC	290	GLN
6	CE	210	HIS
6	CE	222	ASN
6	CE	405	ASN
6	CE	492	ASN
6	CE	494	GLN
6	CE	504	ASN
9	CM	77	GLN
9	CM	119	ASN
10	CR	216	ASN
10	CR	219	GLN
10	CR	220	GLN
11	CU	191	ASN
11	CU	218	GLN
11	CU	246	GLN
12	LC	60	GLN
12	LC	284	GLN
12	LC	330	ASN
13	LE	116	GLN
9	LF	64	GLN
9	LF	99	ASN
9	LF	178	ASN
9	LF	206	ASN
9	LF	249	ASN
14	LG	92	GLN
16	LM	105	GLN
17	LN	32	GLN
18	LO	43	ASN
21	LS	8	GLN
21	LS	62	ASN
22	LT	139	HIS
22	LT	146	ASN
25	Le	79	ASN
27	Lh	37	GLN
28	Li	24	HIS

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Mol	Chain	Res	Type
28	Li	47	GLN
30	Cc	37	GLN
30	Cc	223	GLN
31	Cd	208	ASN
31	Cd	314	ASN
32	Ce	13	GLN
32	Ce	39	ASN
32	Ce	55	GLN
32	Ce	93	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C1	1297/3341 (38%)	256 (19%)	10 (0%)
2	C2	254/306 (83%)	59 (23%)	3 (1%)
All	All	1551/3647 (42%)	315 (20%)	13 (0%)

All (315) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C1	22	G
1	C1	26	A
1	C1	40	A
1	C1	43	A
1	C1	49	A
1	C1	59	G
1	C1	60	A
1	C1	65	A
1	C1	66	A
1	C1	92	G
1	C1	94	G
1	C1	96	G
1	C1	109	A
1	C1	110	G
1	C1	111	C
1	C1	116	A
1	C1	122	A
1	C1	130	U
1	C1	131	U
1	C1	132	C
1	C1	133	G

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Mol	Chain	Res	Type
1	C1	134	G
1	C1	136	C
1	C1	150	G
1	C1	151	G
1	C1	152	A
1	C1	156	G
1	C1	163	U
1	C1	164	G
1	C1	176	U
1	C1	177	U
1	C1	180	G
1	C1	183	U
1	C1	192	A
1	C1	193	C
1	C1	203	C
1	C1	204	A
1	C1	206	A
1	C1	211	G
1	C1	212	A
1	C1	213	G
1	C1	224	A
1	C1	240	U
1	C1	242	U
1	C1	244	U
1	C1	258	C
1	C1	261	G
1	C1	275	G
1	C1	276	A
1	C1	277	A
1	C1	287	A
1	C1	289	A
1	C1	291	G
1	C1	300	A
1	C1	302	U
1	C1	309	A
1	C1	310	A
1	C1	311	A
1	C1	315	A
1	C1	321	C
1	C1	325	C
1	C1	330	A
1	C1	331	C

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Mol	Chain	Res	Type
1	C1	334	A
1	C1	342	C
1	C1	343	A
1	C1	368	G
1	C1	377	A
1	C1	390	U
1	C1	391	A
1	C1	393	C
1	C1	394	A
1	C1	395	C
1	C1	413	G
1	C1	414	A
1	C1	421	U
1	C1	432	U
1	C1	433	U
1	C1	434	G
1	C1	446	U
1	C1	449	U
1	C1	450	C
1	C1	457	U
1	C1	458	C
1	C1	460	C
1	C1	467	G
1	C1	469	A
1	C1	474	G
1	C1	485	G
1	C1	493	C
1	C1	504	G
1	C1	508	G
1	C1	509	A
1	C1	511	A
1	C1	513	A
1	C1	520	G
1	C1	526	G
1	C1	533	C
1	C1	534	U
1	C1	535	C
1	C1	537	G
1	C1	538	G
1	C1	539	G
1	C1	545	U
1	C1	546	A

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Mol	Chain	Res	Type
1	C1	547	U
1	C1	548	A
1	C1	558	G
1	C1	569	G
1	C1	582	A
1	C1	587	G
1	C1	589	U
1	C1	590	C
1	C1	592	G
1	C1	593	C
1	C1	596	G
1	C1	598	A
1	C1	608	A
1	C1	623	C
1	C1	633	A
1	C1	635	C
1	C1	647	A
1	C1	663	G
1	C1	664	A
1	C1	668	U
1	C1	678	A
1	C1	708	G
1	C1	718	U
1	C1	719	C
1	C1	739	C
1	C1	746	A
1	C1	748	U
1	C1	757	U
1	C1	758	U
1	C1	761	A
1	C1	762	G
1	C1	766	G
1	C1	767	A
1	C1	787	A
1	C1	789	A
1	C1	798	A
1	C1	918	G
1	C1	925	A
1	C1	932	A
1	C1	933	A
1	C1	934	G
1	C1	940	C

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Mol	Chain	Res	Type
1	C1	943	A
1	C1	944	G
1	C1	958	A
1	C1	960	C
1	C1	966	U
1	C1	972	G
1	C1	974	G
1	C1	975	G
1	C1	976	U
1	C1	982	G
1	C1	983	A
1	C1	1031	C
1	C1	1039	A
1	C1	1045	G
1	C1	1046	A
1	C1	1047	A
1	C1	1057	A
1	C1	1058	C
1	C1	1063	C
1	C1	1064	U
1	C1	1070	U
1	C1	1075	A
1	C1	1076	U
1	C1	1077	U
1	C1	1078	C
1	C1	1079	G
1	C1	1080	A
1	C1	1085	A
1	C1	1097	G
1	C1	1098	G
1	C1	1099	G
1	C1	1114	C
1	C1	1126	U
1	C1	1130	G
1	C1	1132	A
1	C1	1133	U
1	C1	1135	A
1	C1	1141	A
1	C1	1142	C
1	C1	1160	G
1	C1	1163	U
1	C1	1164	G

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Mol	Chain	Res	Type
1	C1	1172	A
1	C1	1174	C
1	C1	1175	A
1	C1	1178	C
1	C1	1292	G
1	C1	1295	G
1	C1	1312	A
1	C1	1313	U
1	C1	1314	A
1	C1	1330	A
1	C1	1331	G
1	C1	1332	A
1	C1	1334	A
1	C1	1335	C
1	C1	1336	G
1	C1	1337	A
1	C1	1368	A
1	C1	1369	G
1	C1	1374	G
1	C1	1381	A
1	C1	1382	G
1	C1	1384	G
1	C1	1400	A
1	C1	1401	A
1	C1	1413	G
1	C1	1419	C
1	C1	1433	C
1	C1	1434	A
1	C1	1435	A
1	C1	2314	A
1	C1	2324	C
1	C1	3126	G
1	C1	3130	U
1	C1	3134	A
1	C1	3139	A
1	C1	3140	G
1	C1	3144	C
1	C1	3145	C
1	C1	3146	G
1	C1	3147	G
1	C1	3154	A
1	C1	3161	C

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Mol	Chain	Res	Type
1	C1	3162	A
1	C1	3163	G
1	C1	3170	C
1	C1	3171	C
1	C1	3181	C
1	C1	3183	C
1	C1	3185	A
1	C1	3186	A
1	C1	3187	G
1	C1	3199	A
1	C1	3200	A
1	C1	3205	C
1	C1	3206	G
1	C1	3207	U
1	C1	3208	A
1	C1	3209	U
1	C1	3212	C
1	C1	3214	A
1	C1	3227	C
1	C1	3228	G
1	C1	3232	U
1	C1	3233	C
1	C1	3332	G
1	C1	3333	A
1	C1	3337	C
2	C2	2	A
2	C2	23	U
2	C2	34	U
2	C2	35	C
2	C2	53	A
2	C2	59	A
2	C2	61	A
2	C2	62	A
2	C2	63	G
2	C2	64	U
2	C2	81	U
2	C2	84	C
2	C2	86	U
2	C2	87	G
2	C2	90	U
2	C2	91	C
2	C2	95	G

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Mol	Chain	Res	Type
2	C2	104	A
2	C2	106	C
2	C2	109	A
2	C2	111	A
2	C2	113	U
2	C2	124	G
2	C2	126	A
2	C2	127	U
2	C2	129	C
2	C2	149	A
2	C2	151	C
2	C2	156	U
2	C2	157	U
2	C2	158	U
2	C2	160	A
2	C2	166	C
2	C2	174	G
2	C2	175	G
2	C2	176	G
2	C2	180	G
2	C2	181	U
2	C2	183	U
2	C2	189	A
2	C2	190	C
2	C2	192	C
2	C2	196	G
2	C2	212	G
2	C2	213	A
2	C2	214	A
2	C2	215	A
2	C2	218	C
2	C2	219	A
2	C2	221	U
2	C2	222	G
2	C2	289	G
2	C2	291	G
2	C2	292	C
2	C2	294	A
2	C2	295	G
2	C2	300	A
2	C2	301	A
2	C2	302	A

All (13) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C1	150	G
1	C1	432	U
1	C1	510	U
1	C1	519	A
1	C1	538	G
1	C1	1044	A
1	C1	1046	A
1	C1	1159	G
1	C1	3162	A
1	C1	3207	U
2	C2	123	G
2	C2	174	G
2	C2	175	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

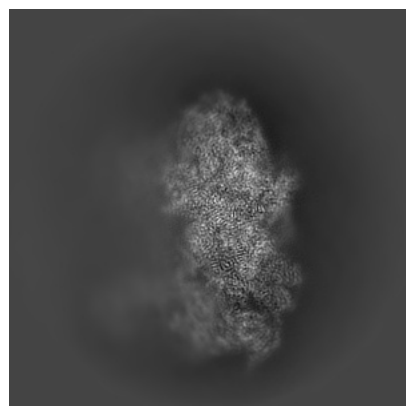
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35279. These allow visual inspection of the internal detail of the map and identification of artifacts.

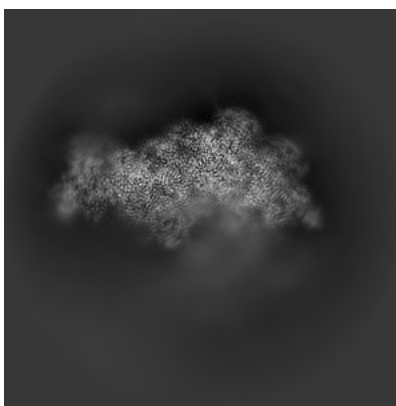
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

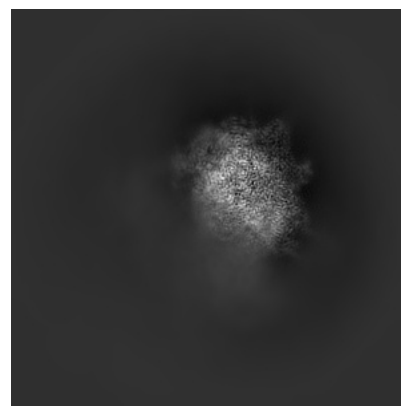
6.1.1 Primary map



X

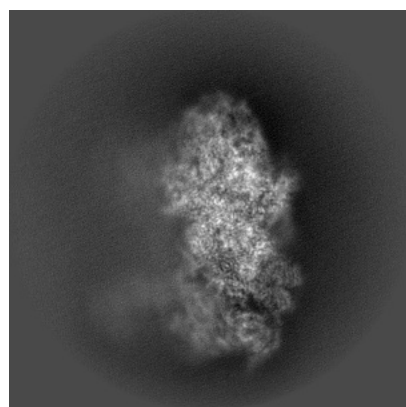


Y

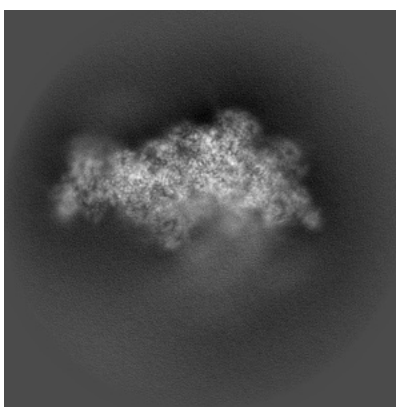


Z

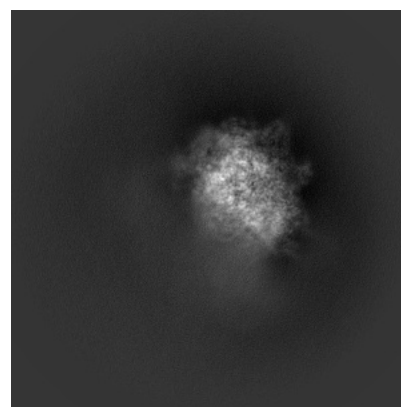
6.1.2 Raw map



X



Y

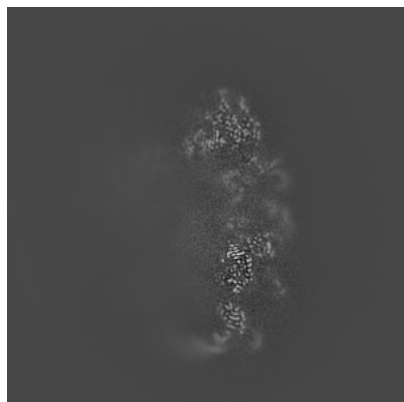


Z

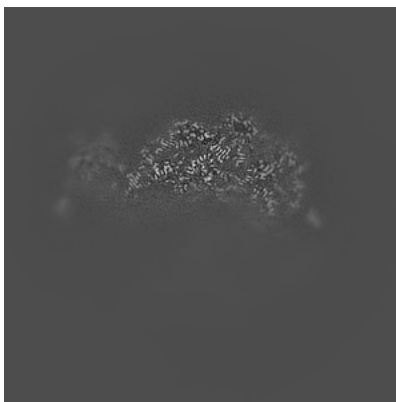
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

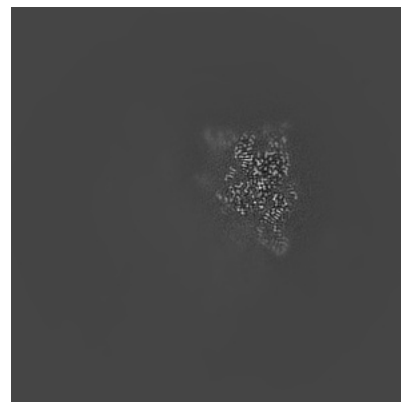
6.2.1 Primary map



X Index: 210

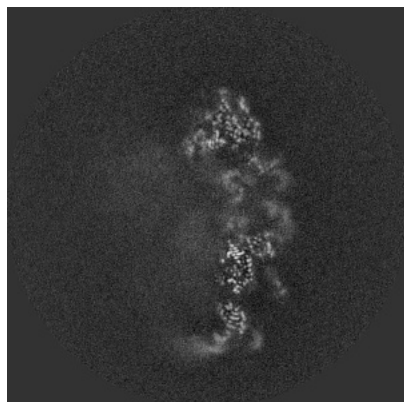


Y Index: 210

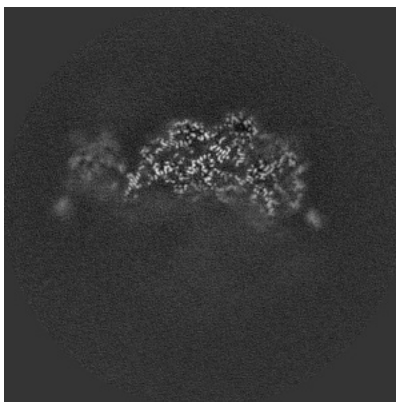


Z Index: 210

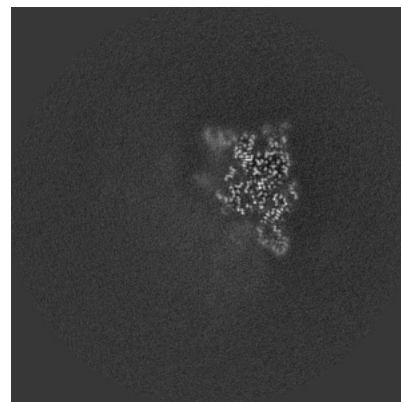
6.2.2 Raw map



X Index: 210



Y Index: 210

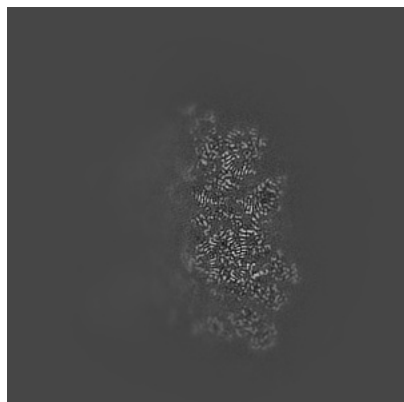


Z Index: 210

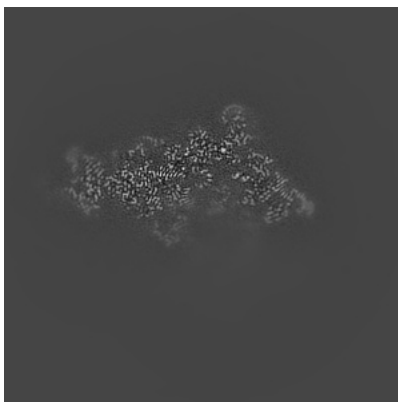
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

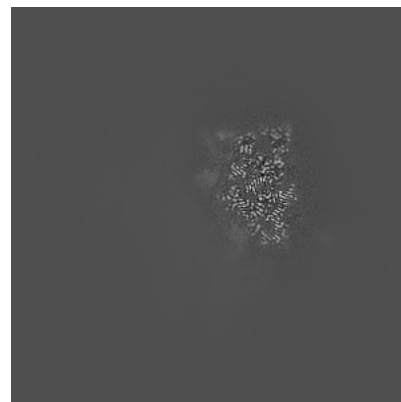
6.3.1 Primary map



X Index: 244

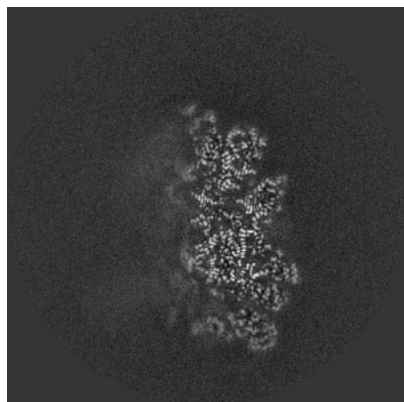


Y Index: 247

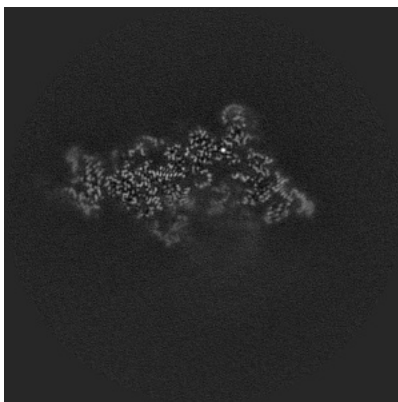


Z Index: 216

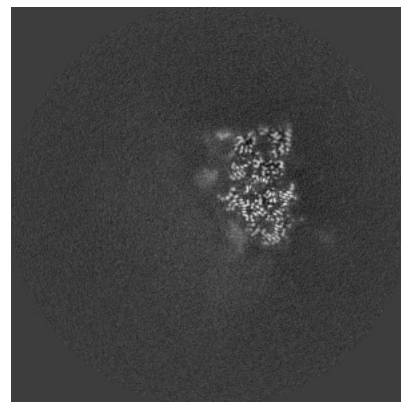
6.3.2 Raw map



X Index: 244



Y Index: 247

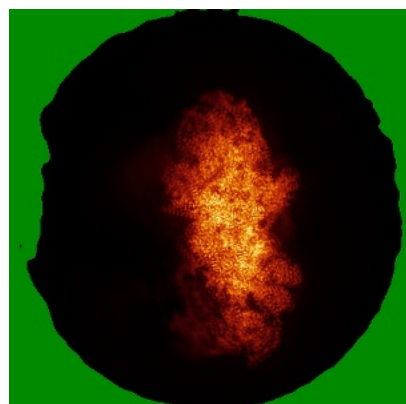


Z Index: 217

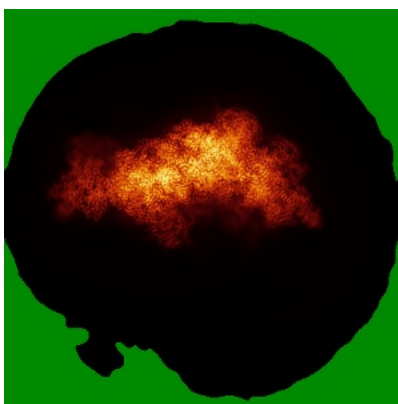
The images above show the largest variance slices of the map in three orthogonal directions.

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

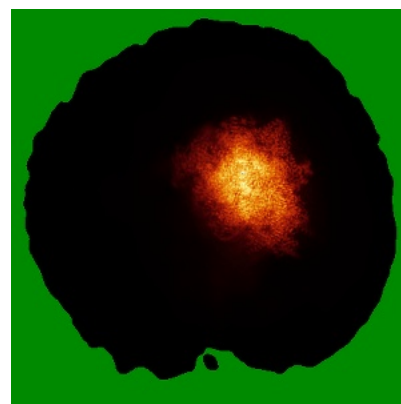
6.4.1 Primary map



X

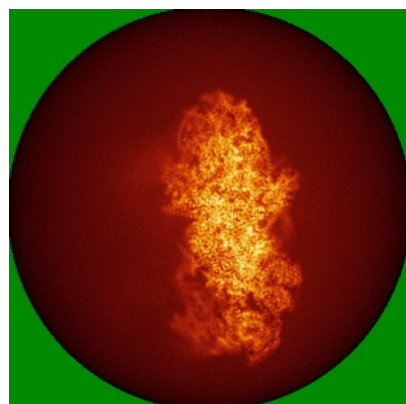


Y

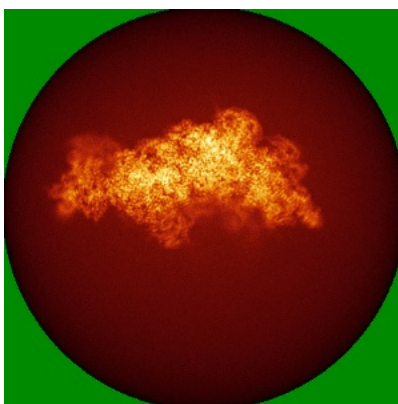


Z

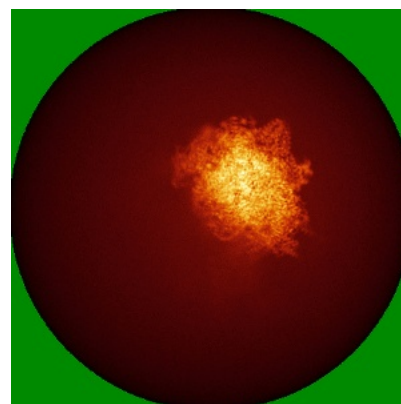
6.4.2 Raw map



X



Y

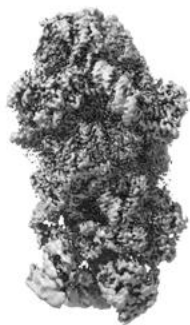


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

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

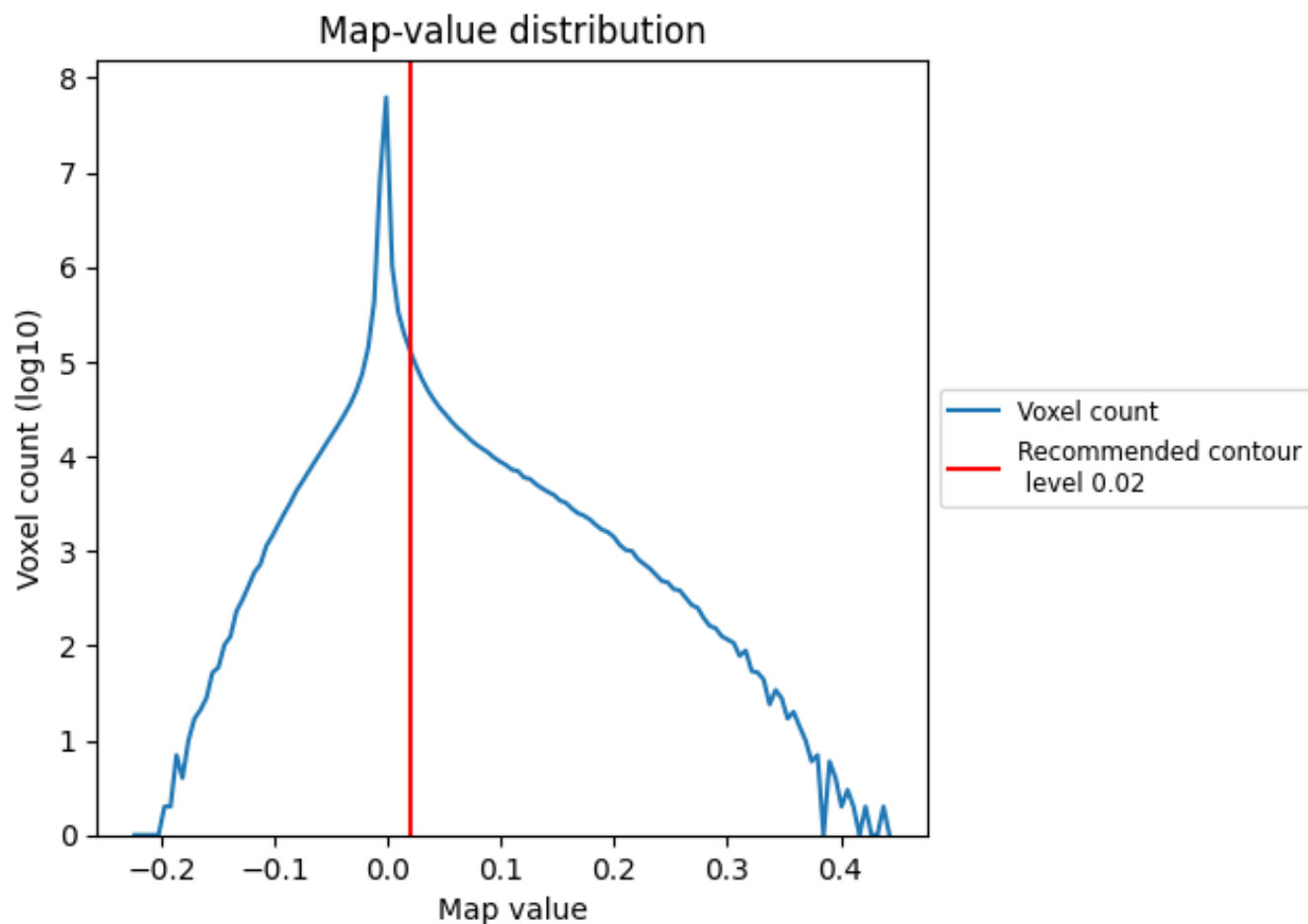
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

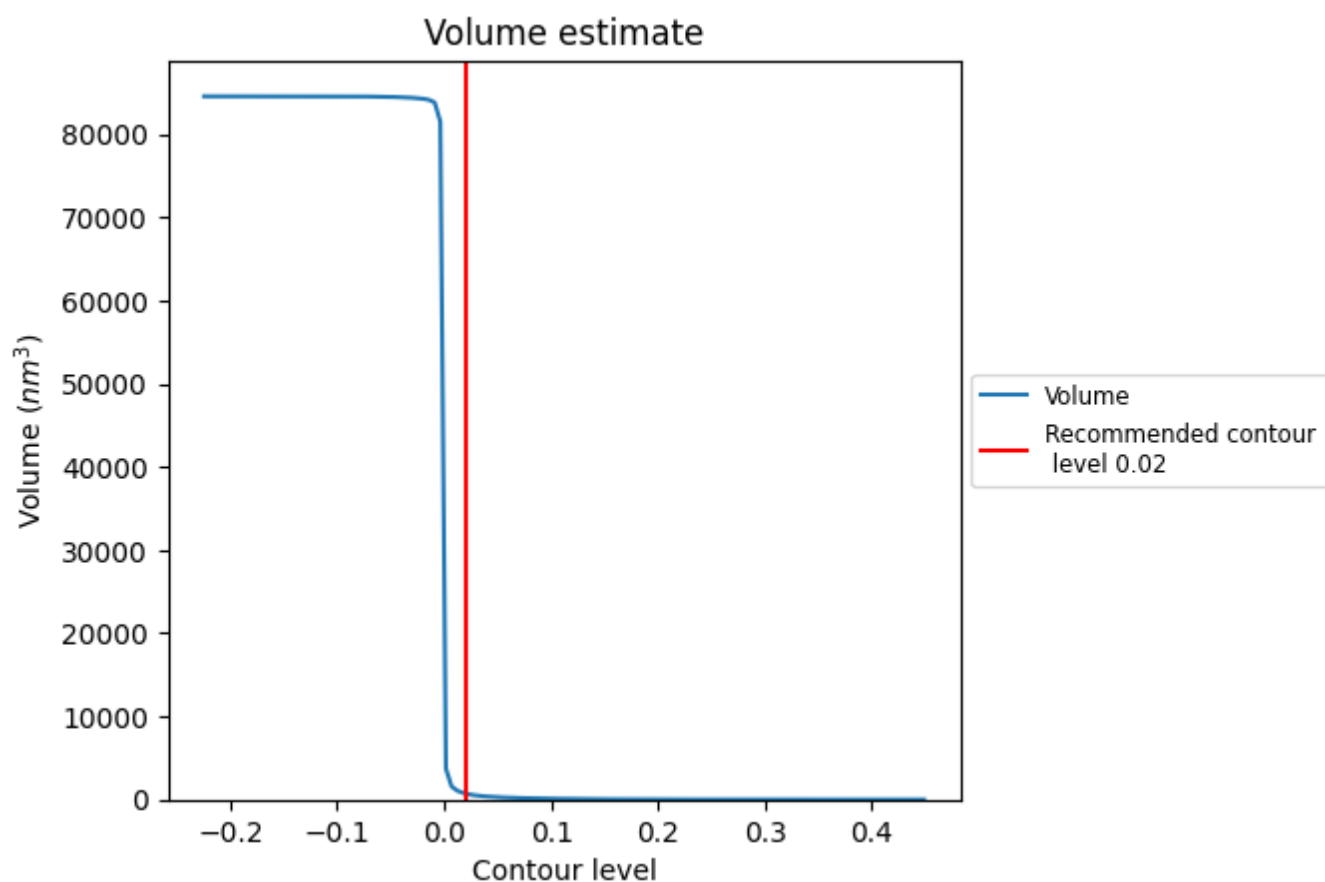
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

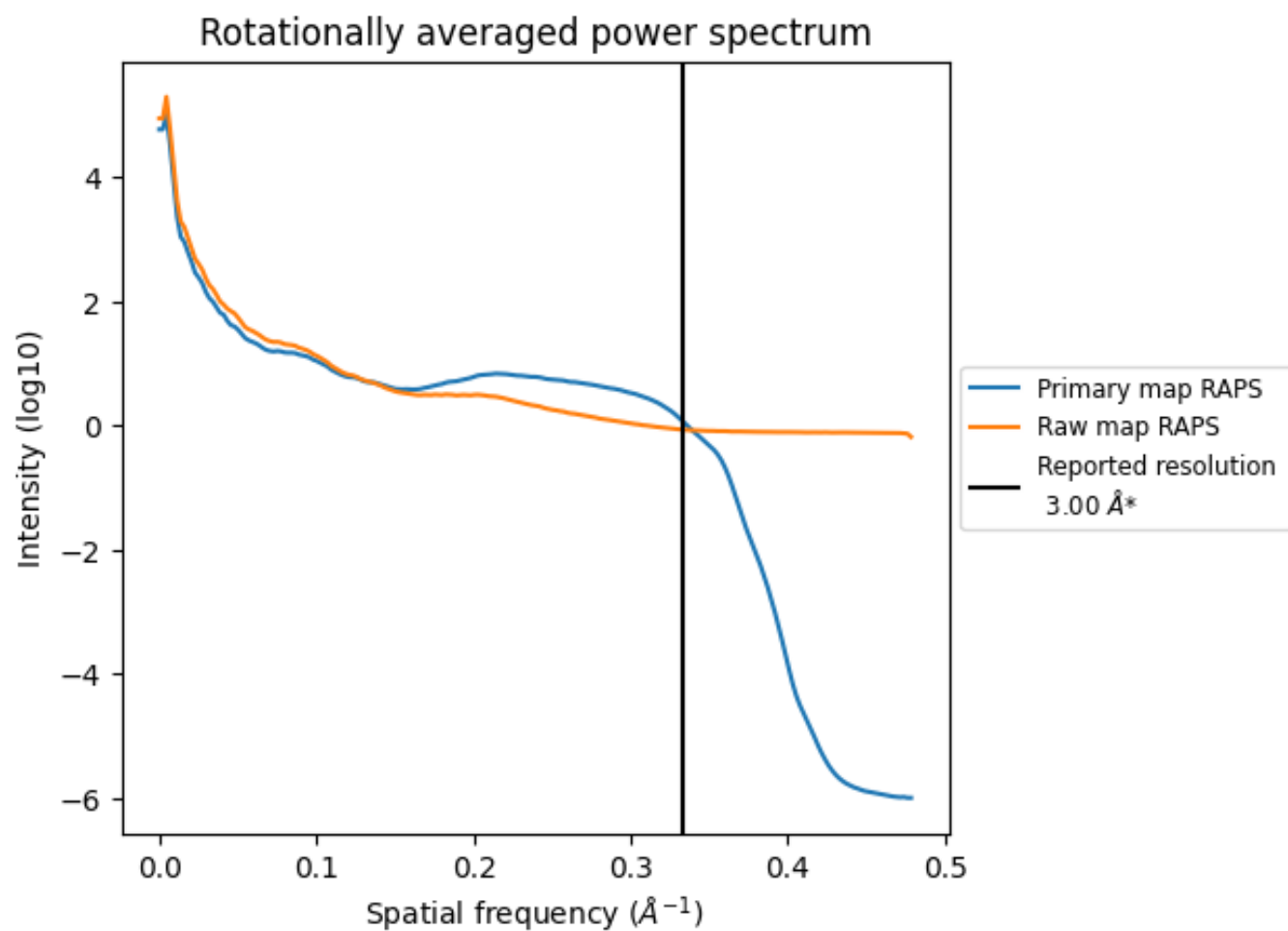
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 730 nm^3 ; this corresponds to an approximate mass of 660 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 ⓘ

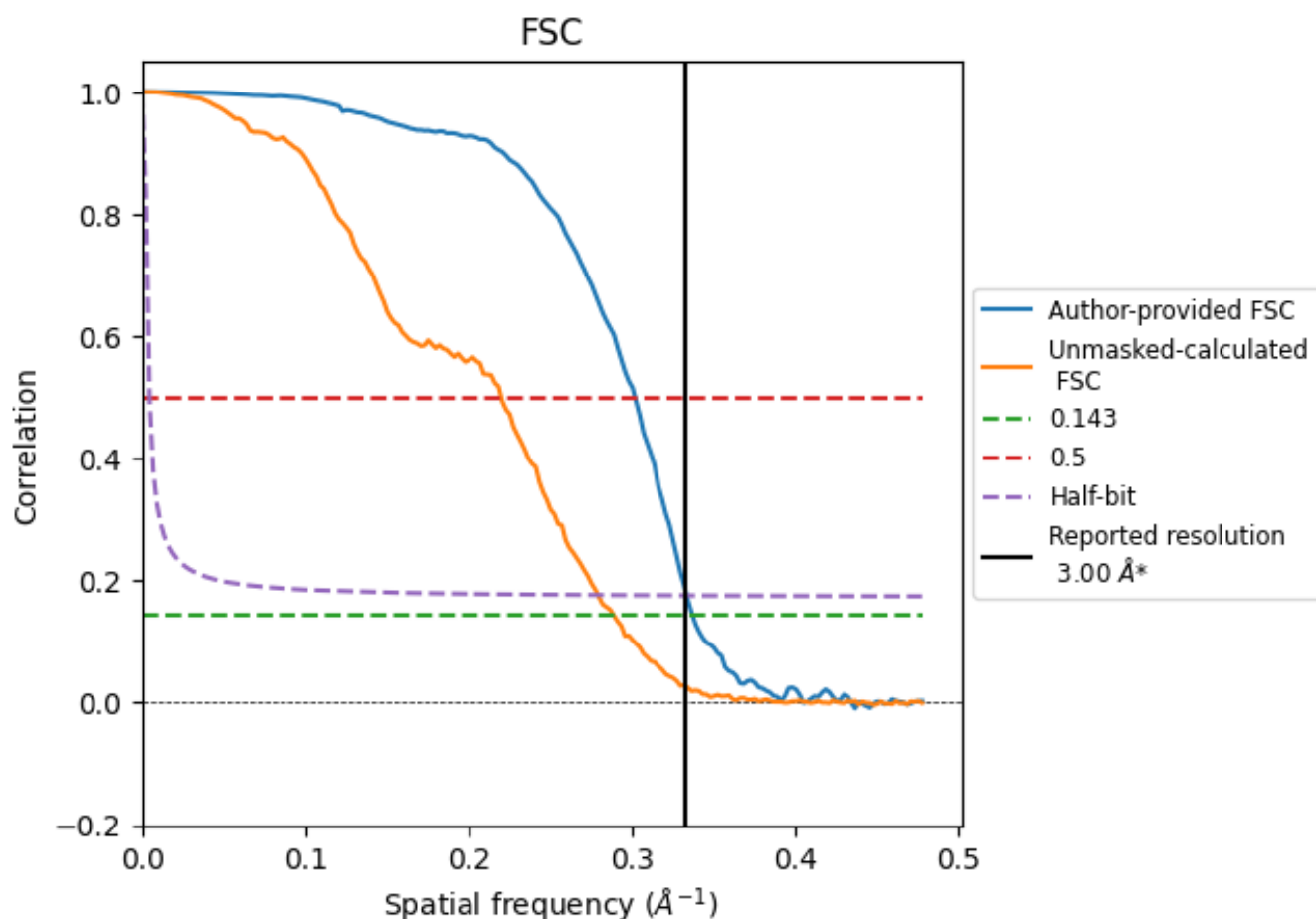


*Reported resolution corresponds to spatial frequency of 0.333 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.333 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

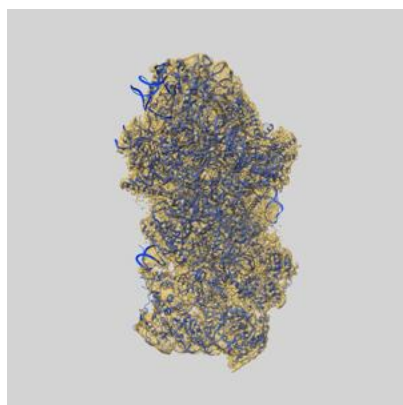
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	2.96	3.31	2.99
Unmasked-calculated*	3.46	4.54	3.58

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.46 differs from the reported value 3.0 by more than 10 %

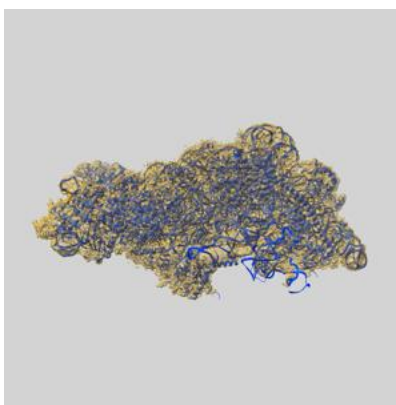
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35279 and PDB model 8I9P. Per-residue inclusion information can be found in section 3 on page 11.

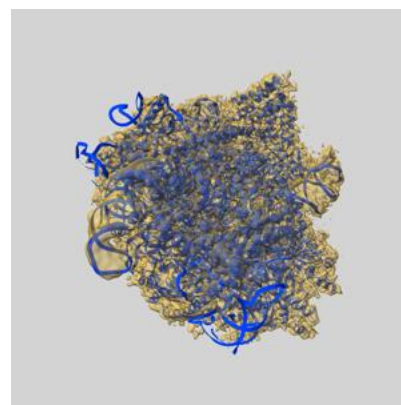
9.1 Map-model overlay [i](#)



X



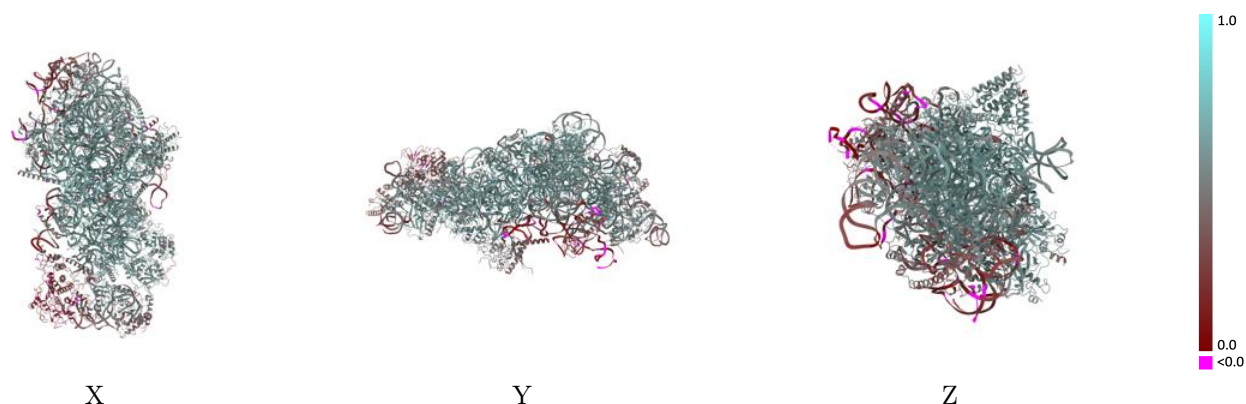
Y



Z

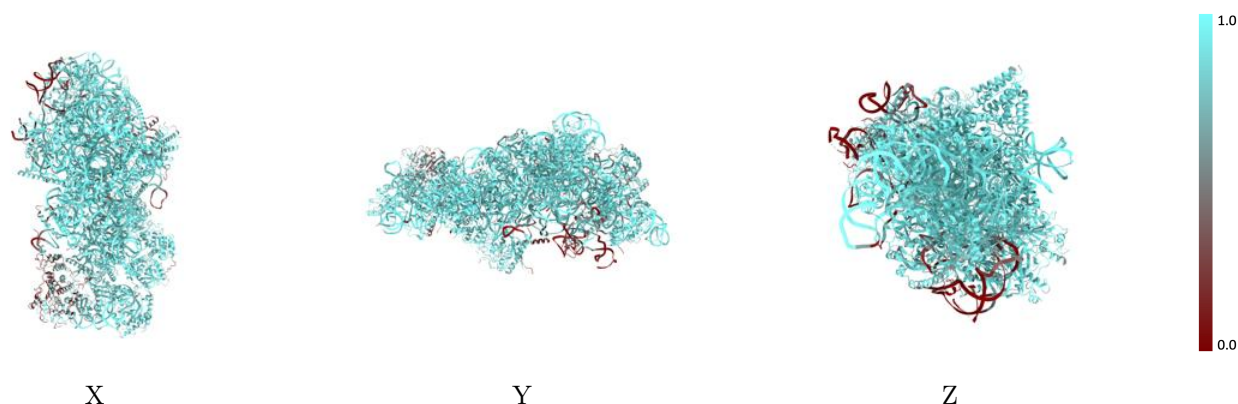
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



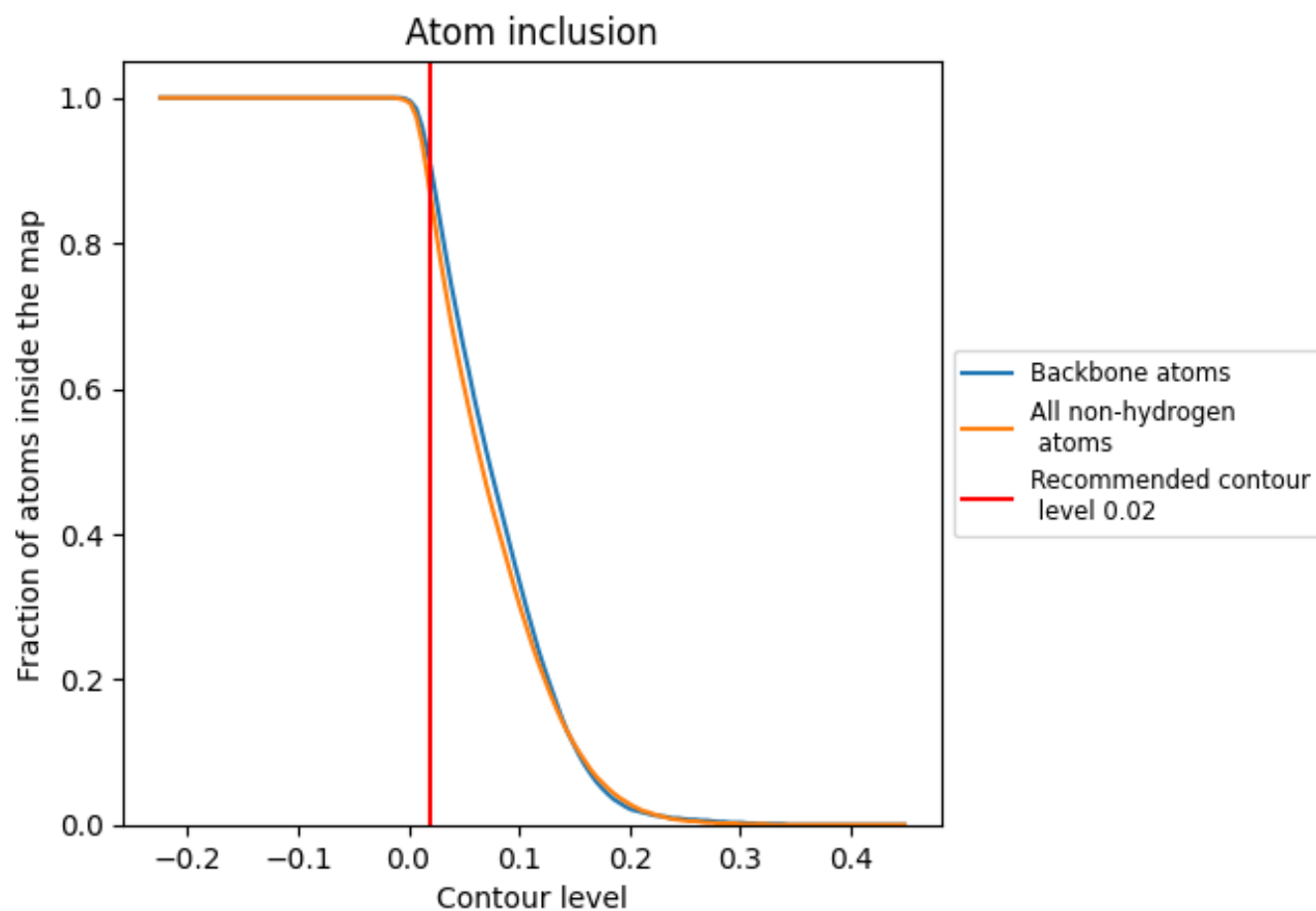
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 87% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8660	 0.5060
C1	 0.8530	 0.4980
C2	 0.9190	 0.4810
CA	 0.9000	 0.5070
CB	 0.8900	 0.4860
CC	 0.6640	 0.3660
CE	 0.9270	 0.5530
CI	 0.9090	 0.4980
CJ	 0.5190	 0.2470
CM	 0.6790	 0.3310
CR	 0.9540	 0.5940
CU	 0.7270	 0.3630
Cc	 0.9220	 0.5550
Cd	 0.9390	 0.5730
Ce	 0.9780	 0.6160
LC	 0.9710	 0.6190
LE	 0.9110	 0.5320
LF	 0.9580	 0.5880
LG	 0.9460	 0.5920
LL	 0.9650	 0.6190
LM	 0.8960	 0.4910
LN	 0.9640	 0.6240
LO	 0.8560	 0.4570
LP	 0.7840	 0.4880
LQ	 0.9800	 0.6070
LS	 0.8940	 0.5010
LT	 0.5030	 0.3290
LX	 0.5270	 0.4450
LY	 0.9520	 0.6040
Le	 0.9700	 0.6300
Lf	 0.9510	 0.5980
Lh	 0.9130	 0.5490
Li	 0.9540	 0.5890
Lj	 0.9750	 0.6310

