



Full wwPDB EM Validation Report ⓘ

Mar 19, 2026 – 08:35 PM UTC

PDB ID : 5LJ3 / pdb_00005lj3
EMDB ID : EMD-4055
Title : Structure of the core of the yeast spliceosome immediately after branching
Authors : Galej, W.P.; Wilkinson, M.F.; Fica, S.M.; Oubridge, C.; Newman, A.J.; Nagai, K.
Deposited on : 2016-07-17
Resolution : 3.80 Å(reported)

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

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

A user guide is available at

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

The types of validation reports are described at

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

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

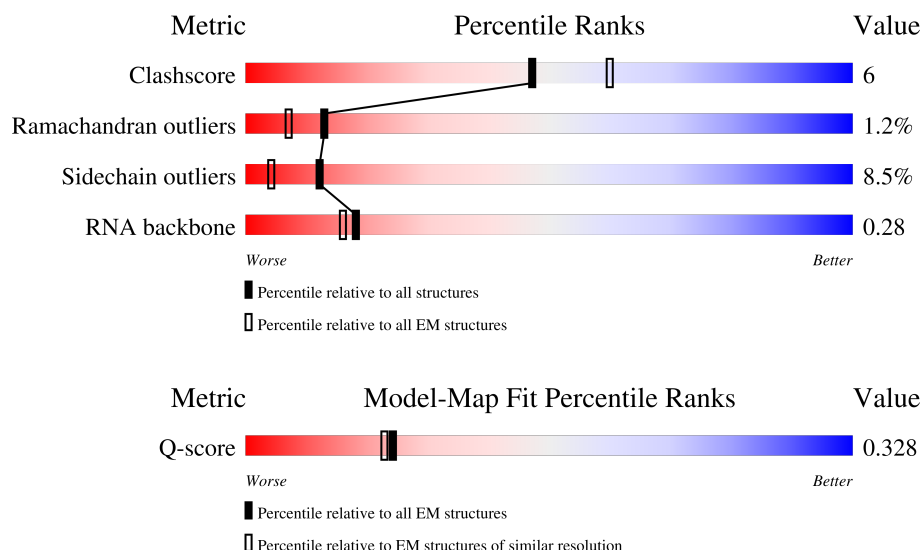
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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.



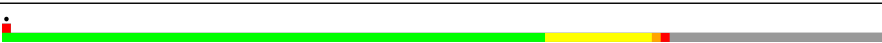
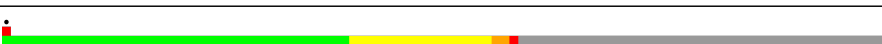
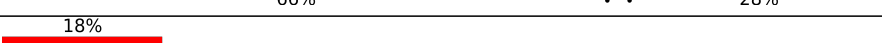
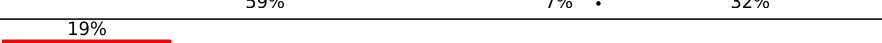
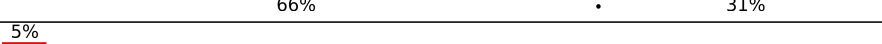
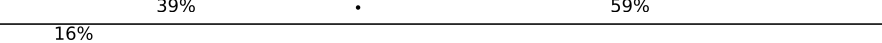
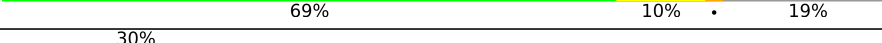
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	U	179	
2	E	16	
3	I	76	

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Mol	Chain	Length	Quality of chain
4	Z	1175	
5	V	112	
6	A	2413	
7	D	278	
8	F	179	
9	C	1008	
10	G	235	
11	H	591	
12	J	451	
13	K	379	
14	L	157	
15	M	339	
16	N	364	
17	O	590	
18	P	175	
19	R	135	
20	S	687	
21	T	859	
22	b	196	
22	k	196	
23	d	101	
23	n	101	
24	e	94	
24	p	94	
25	f	86	

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Mol	Chain	Length	Quality of chain
25	q	86	
26	g	77	
26	r	77	
27	h	146	
27	l	146	
28	j	110	
28	m	110	
29	W	238	
30	Y	111	
31	x	132	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
33	ZN	N	401	-	-	X	-
33	ZN	N	402	-	-	X	-

2 Entry composition

There are 34 unique types of molecules in this entry. The entry contains 63161 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 U5 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	U	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

- Molecule 2 is a RNA chain called Exon 1 (5' exon) of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	16	Total	C	N	O	P	0	0
			346	155	66	109	16		

- Molecule 3 is a RNA chain called Intron of UBC4 pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	33	Total	C	N	O	P	0	0
			693	312	116	232	33		

- Molecule 4 is a RNA chain called U2 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Z	171	Total	C	N	O	P	0	0
			3610	1614	604	1221	171		

- Molecule 5 is a RNA chain called U6 snRNA (small nuclear RNA).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	V	97	Total	C	N	O	P	0	0
			2066	925	368	676	97		

- Molecule 6 is a protein called Pre-mRNA-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1922	Total	C	N	O	S	0	0
			15704	10112	2720	2814	58		

- Molecule 7 is a protein called Protein CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	114	Total	C	N	O	S	0	0
			912	577	165	162	8		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC25.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	F	46	Total	C	N	O	0	0
			321	203	61	57		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	C	882	Total	C	N	O	S	0	0
			6756	4393	1133	1203	27		

- Molecule 10 is a protein called ISY1.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	97	Total	C	N	O	S	0	0
			823	513	154	155	1		

- Molecule 11 is a protein called CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	399	Total	C	N	O	S	0	0
			2639	1657	468	506	8		

- Molecule 12 is a protein called PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	326	Total	C	N	O	S	0	0
			2556	1616	454	476	10		

- Molecule 13 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	K	163	Total	C	N	O	S	0	0
			1289	808	236	240	5		

- Molecule 14 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	L	155	Total	C	N	O	S	0	0
			1270	797	238	225	10		

- Molecule 15 is a protein called CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	252	Total	C	N	O	S	0	0
			2010	1275	354	370	11		

- Molecule 16 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	N	209	Total	C	N	O	S	0	0
			1658	1055	287	301	15		

- Molecule 17 is a protein called CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	O	198	Total	C	N	O	S	0	0
			1645	1032	300	307	6		

- Molecule 18 is a protein called CWC15.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	P	36	Total	C	N	O	0	0
			275	176	53	46		

- Molecule 19 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	R	97	Total	C	N	O	0	0
			550	328	109	113		

- Molecule 20 is a protein called CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	S	464	Total	C	N	O	S	0	0
			3120	1948	581	584	7		

- Molecule 21 is a protein called SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	T	592	Total	C	N	O	0	0
			2946	1762	592	592		

- Molecule 22 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
22	k	80	Total	C	N	O		0	0
			396	236	80	80			

- Molecule 23 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
23	n	82	Total	C	N	O		0	0
			404	240	82	82			

- Molecule 24 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
24	p	75	Total	C	N	O		0	0
			369	219	75	75			

- Molecule 25 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
25	q	72	Total	C	N	O		0	0
			354	210	72	72			

- Molecule 26 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
26	r	69	Total	C	N	O		0	0
			340	202	69	69			

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
27	l	79	Total	C	N	O		0	0
			392	234	79	79			

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
28	m	94	Total	C	N	O		0	0
			467	279	94	94			

- Molecule 29 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	W	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 30 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	Y	84	Total	C	N	O	0	0
			416	248	84	84		

- Molecule 31 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	x	132	Total	C	N	O	0	0
			660	396	132	132		

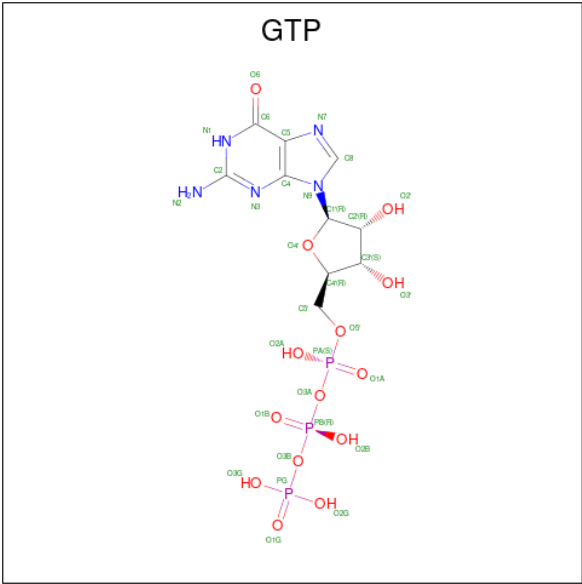
- Molecule 32 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
32	E	1	Total	Mg	0
			1	1	
32	V	1	Total	Mg	0
			1	1	

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

Mol	Chain	Residues	Atoms		AltConf
33	D	1	Total	Zn	0
			1	1	
33	L	3	Total	Zn	0
			3	3	
33	M	1	Total	Zn	0
			1	1	
33	N	2	Total	Zn	0
			2	2	

- Molecule 34 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

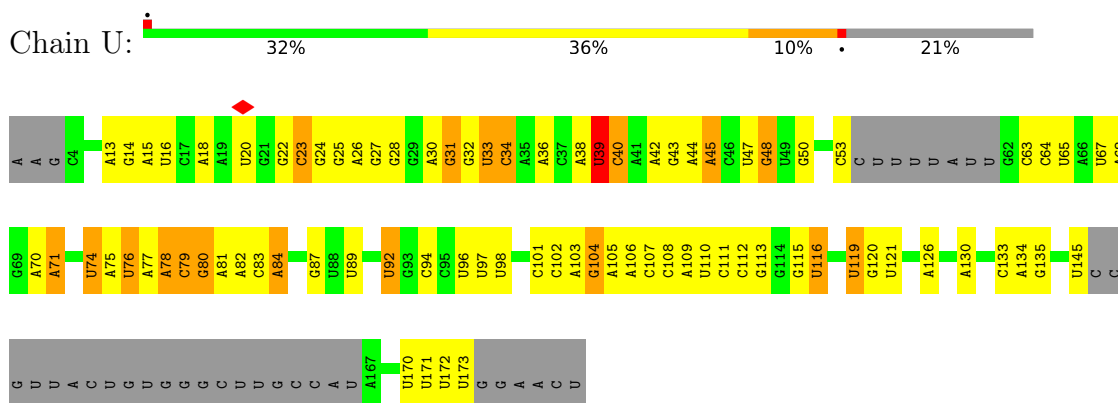


Mol	Chain	Residues	Atoms					AltConf
34	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

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.

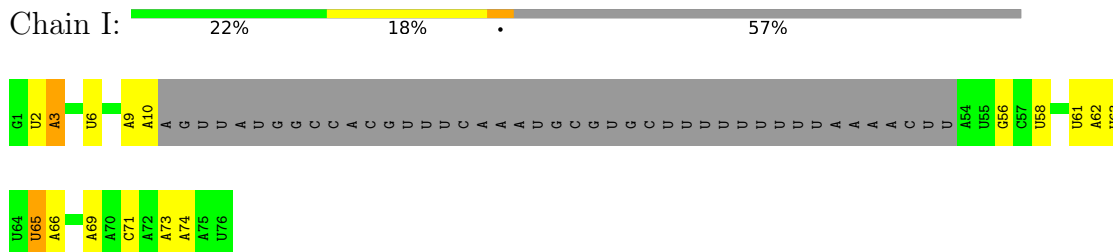
- Molecule 1: U5 snRNA (small nuclear RNA)



- Molecule 2: Exon 1 (5' exon) of UBC4 pre-mRNA

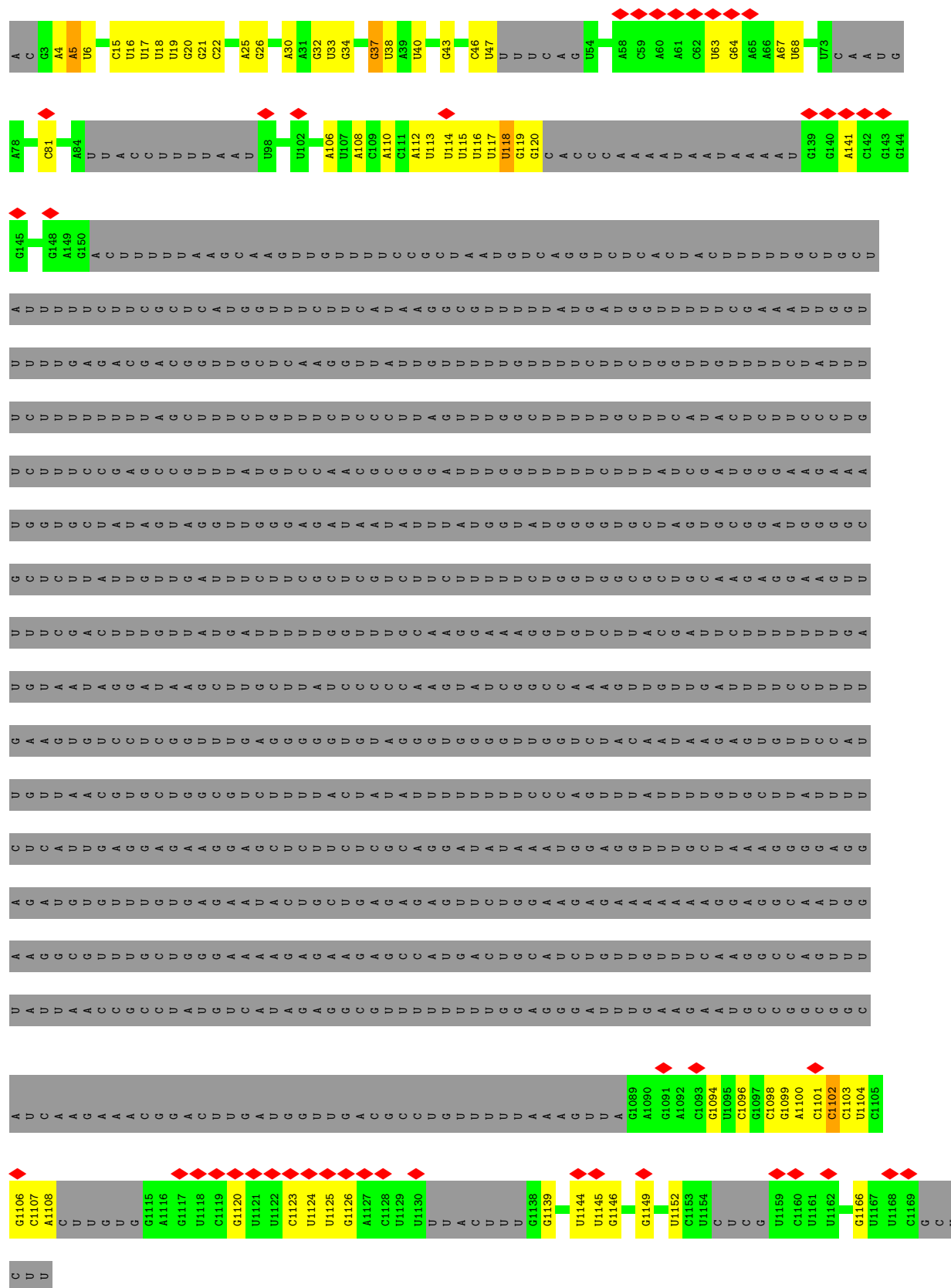


- Molecule 3: Intron of UBC4 pre-mRNA

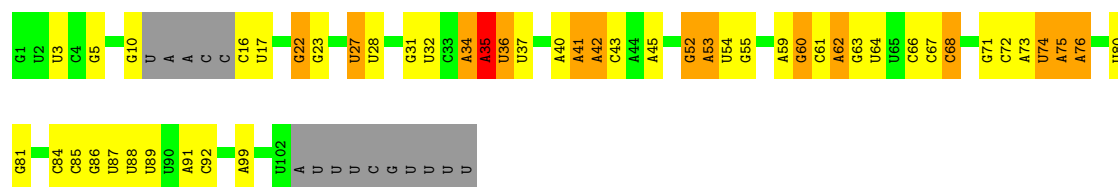


- Molecule 4: U2 snRNA (small nuclear RNA)

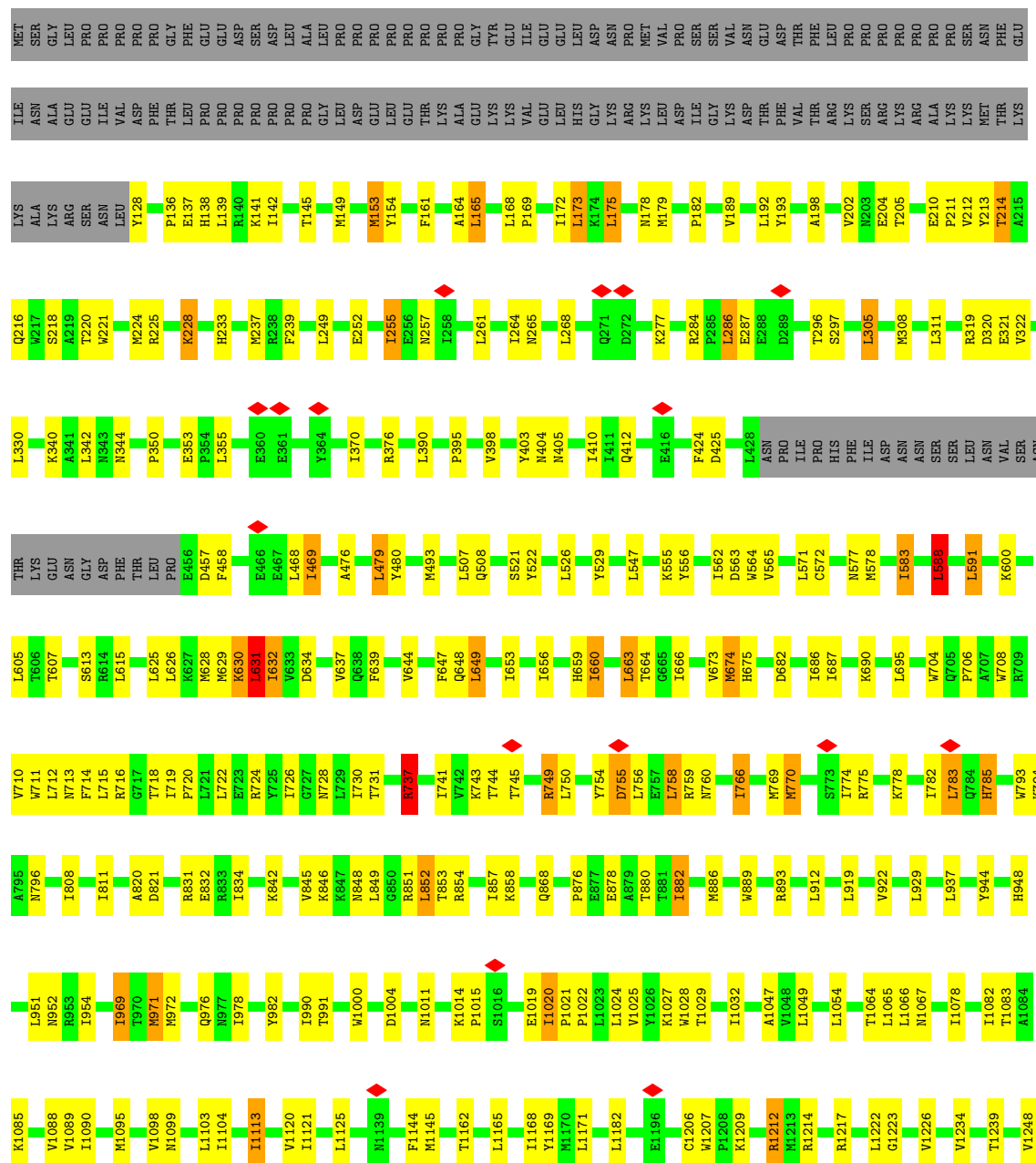


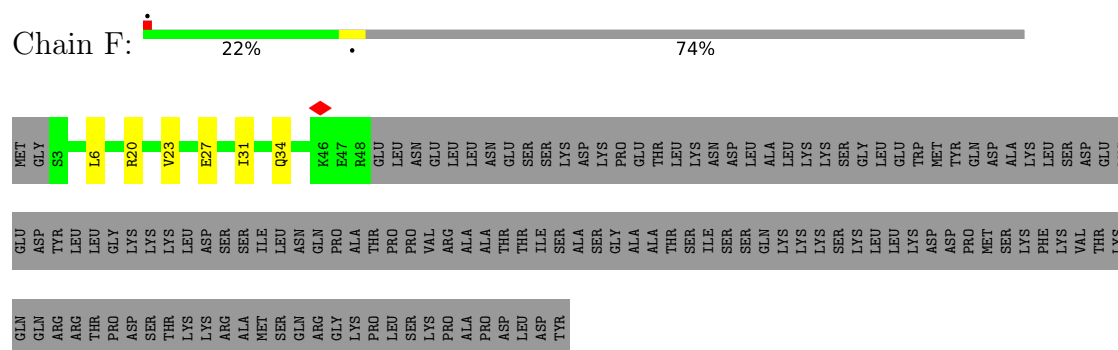


- Molecule 5: U6 snRNA (small nuclear RNA)

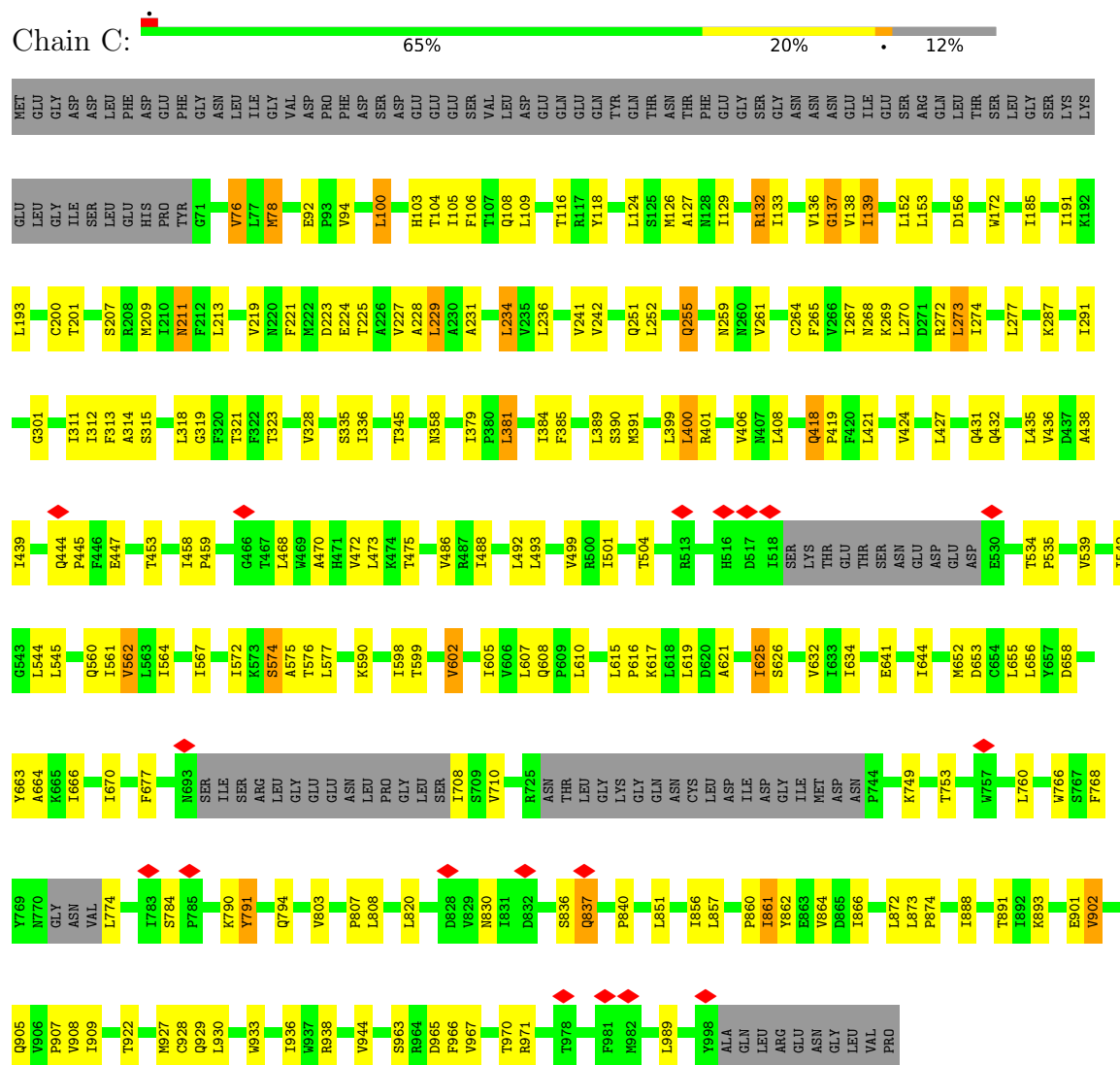


Chain A: 61% 16% 2% 21%



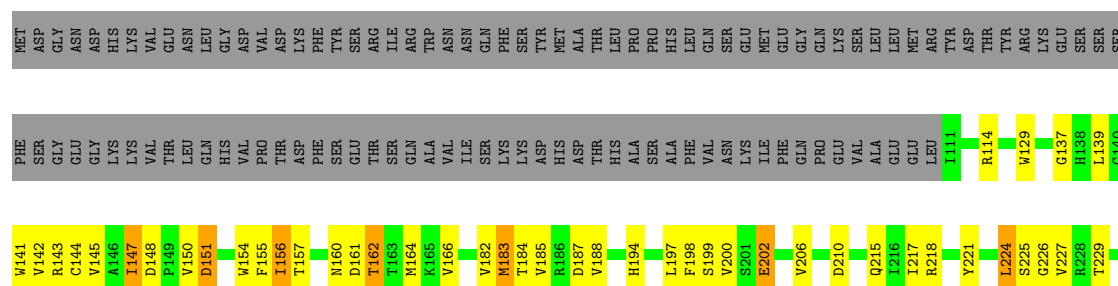
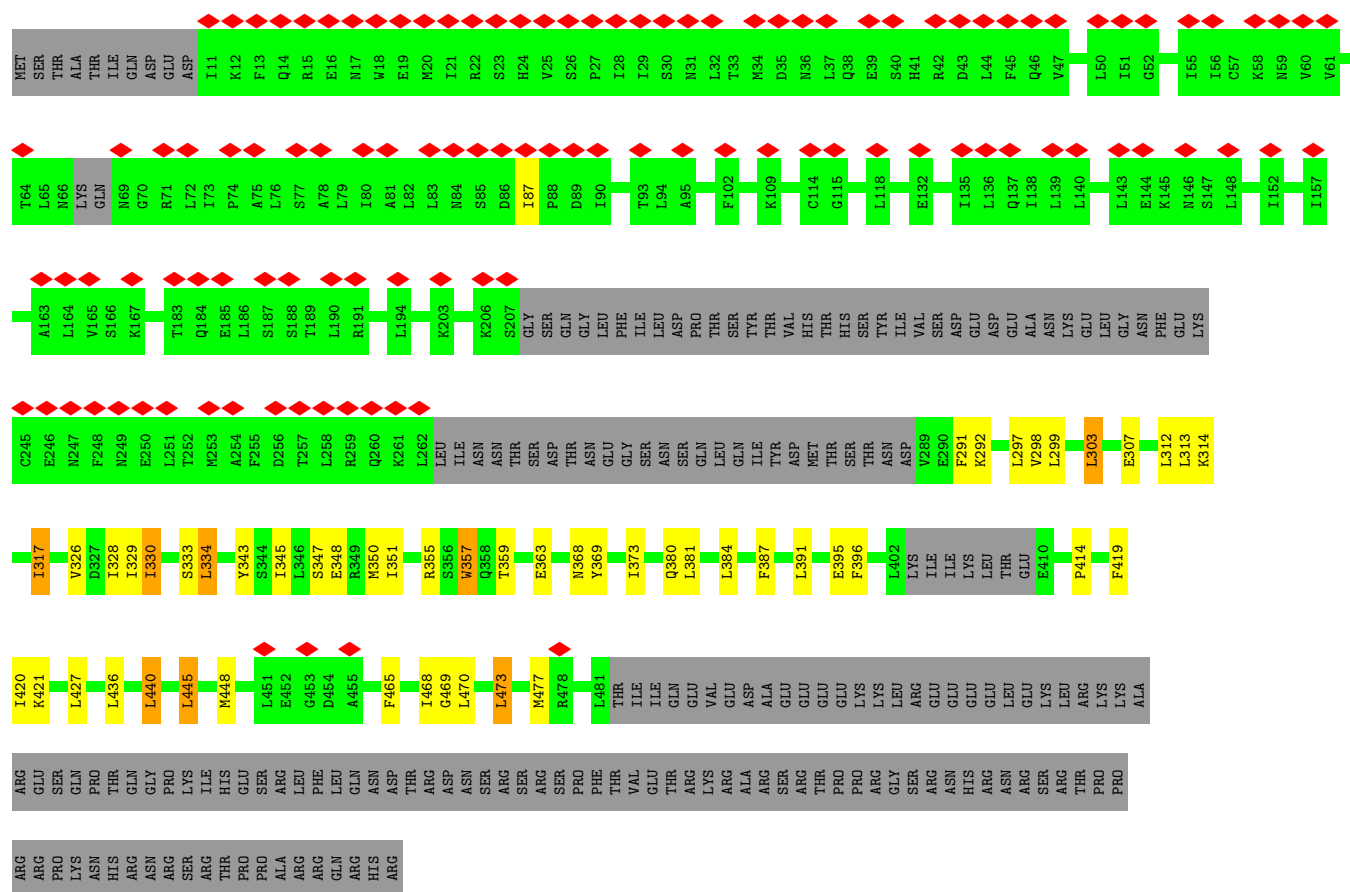


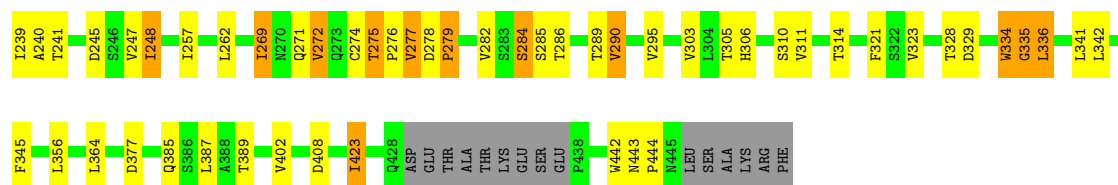
- Molecule 9: Pre-mRNA-splicing factor SNU114



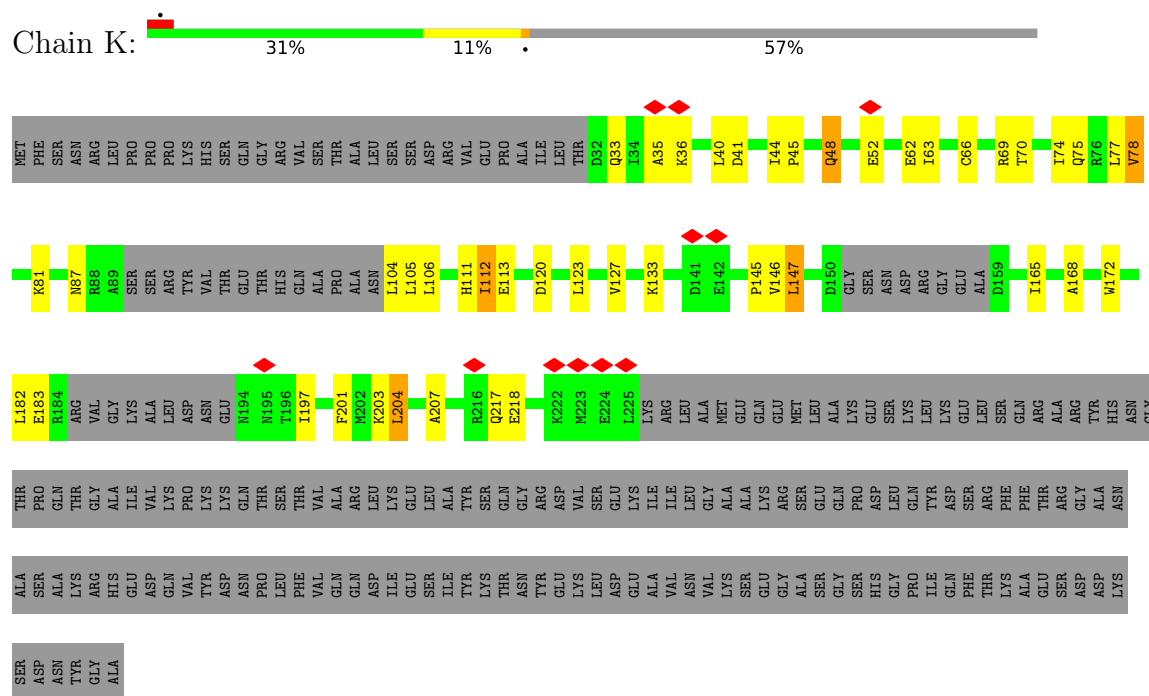
- Molecule 10: ISY1



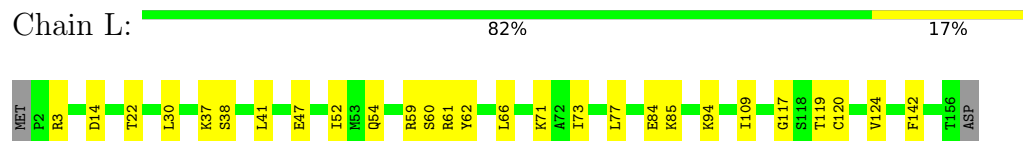




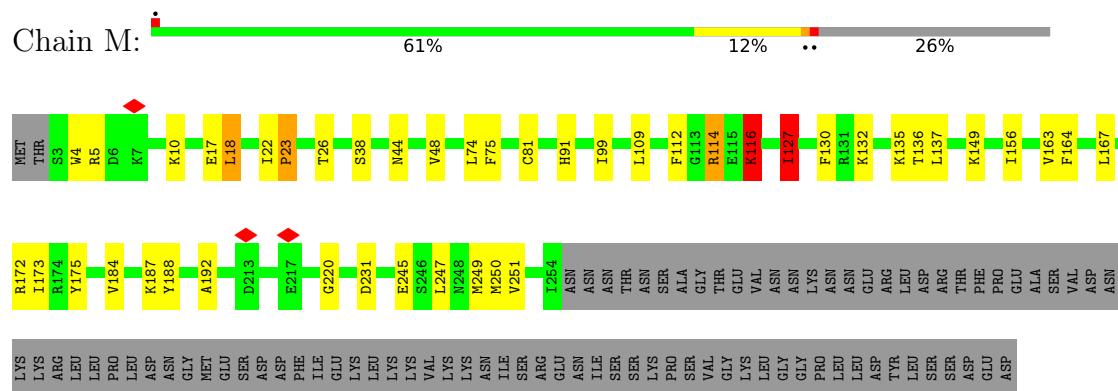
- Molecule 13: Pre-mRNA-processing protein 45



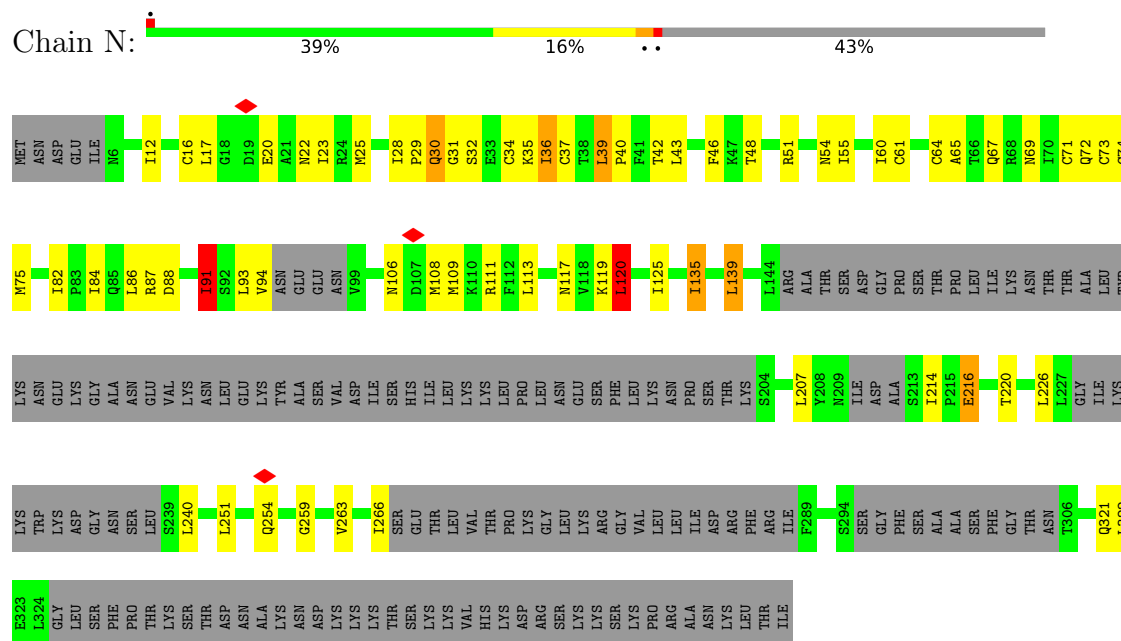
- Molecule 14: Pre-mRNA-splicing factor BUD31



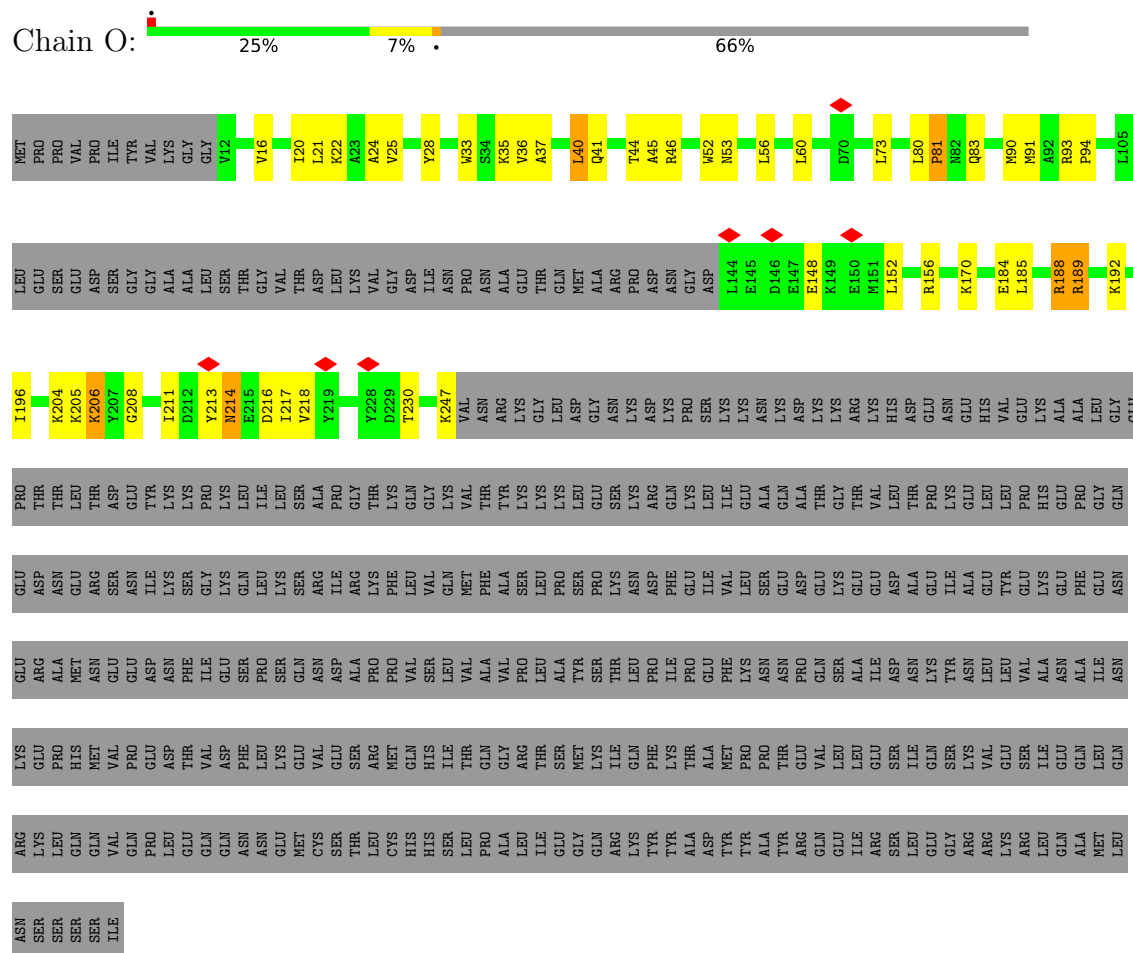
- Molecule 15: CWC2



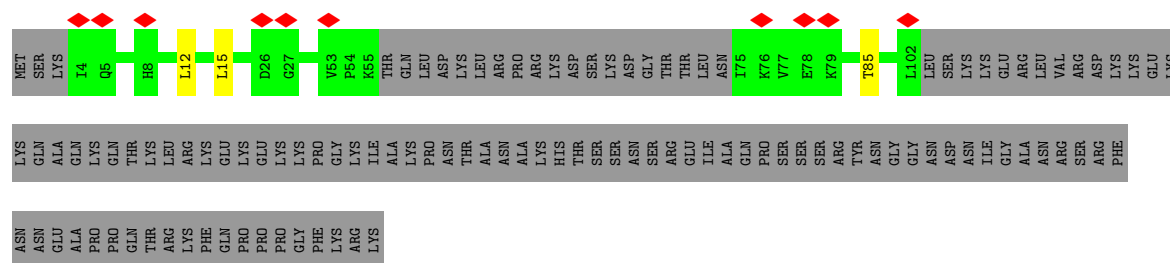
- Molecule 16: Pre-mRNA-splicing factor SLT11



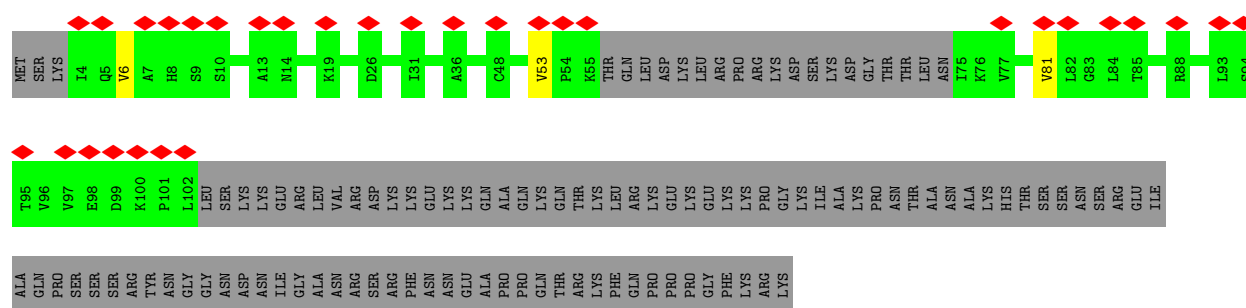
• Molecule 17: CEF1



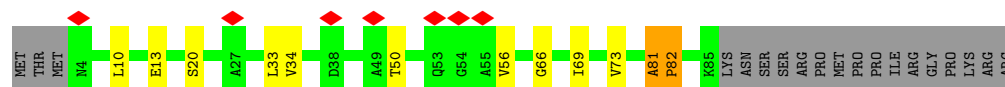
• Molecule 18: CWC15



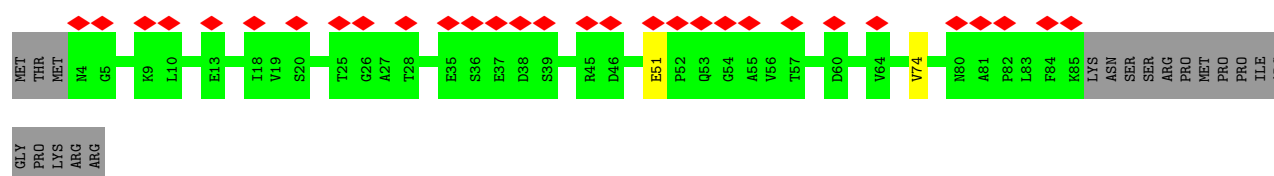
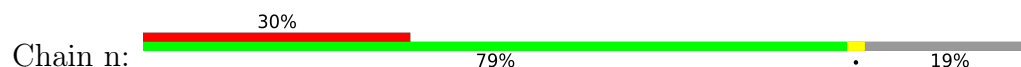
• Molecule 22: Small nuclear ribonucleoprotein-associated protein B



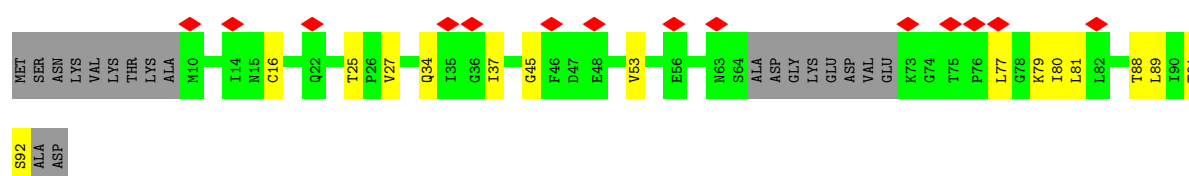
• Molecule 23: Small nuclear ribonucleoprotein Sm D3



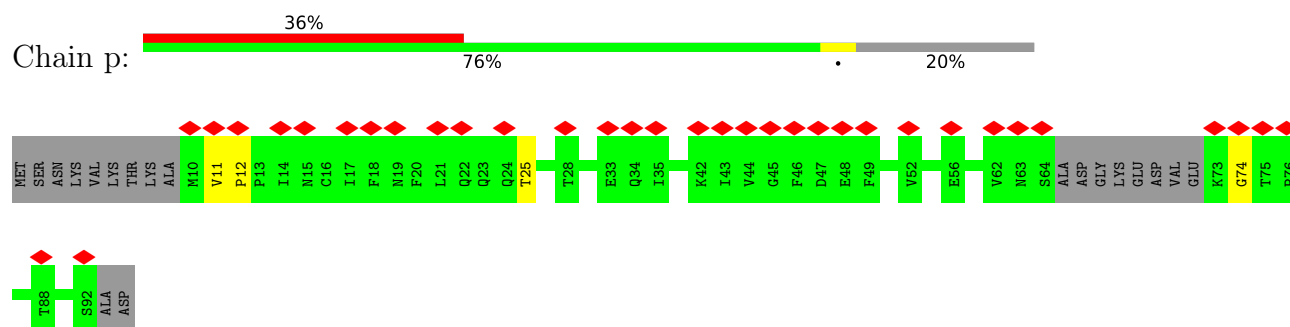
• Molecule 23: Small nuclear ribonucleoprotein Sm D3



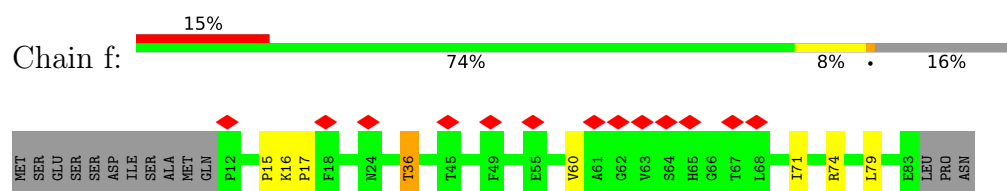
• Molecule 24: Small nuclear ribonucleoprotein E



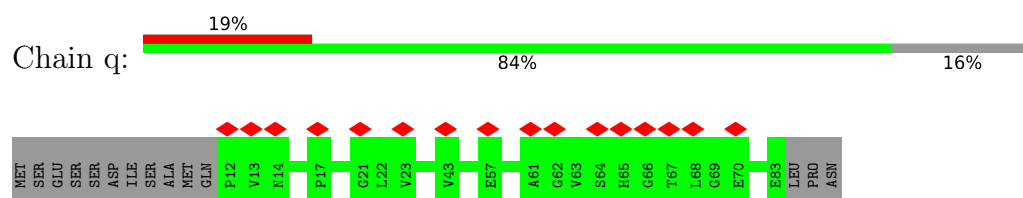
- Molecule 24: Small nuclear ribonucleoprotein E



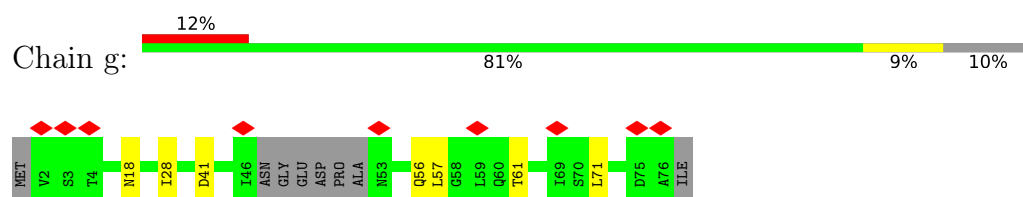
- Molecule 25: Small nuclear ribonucleoprotein F



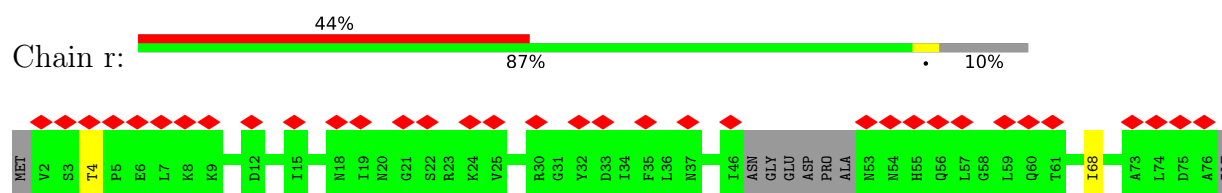
- Molecule 25: Small nuclear ribonucleoprotein F



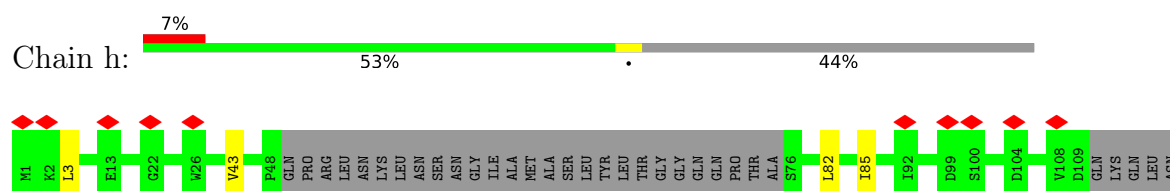
- Molecule 26: Small nuclear ribonucleoprotein G

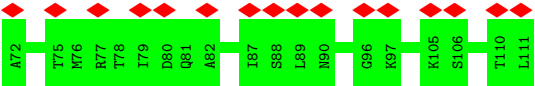
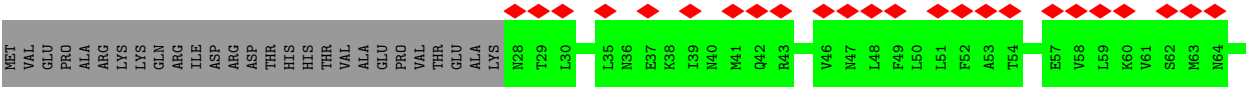


- Molecule 26: Small nuclear ribonucleoprotein G



- Molecule 27: Small nuclear ribonucleoprotein Sm D1





• Molecule 31: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	93106	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 ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	35714	Depositor
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.197	Depositor
Minimum map value	-0.091	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.027	Depositor
Map size (Å)	589.16, 589.16, 589.16	wwPDB
Map dimensions	412, 412, 412	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.43, 1.43, 1.43	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, GTP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	U	0.41	0/3351	0.88	5/5213 (0.1%)
2	E	0.42	0/388	0.80	1/603 (0.2%)
3	I	0.40	0/772	0.81	1/1195 (0.1%)
4	Z	0.40	0/4018	0.76	1/6233 (0.0%)
5	V	0.40	0/2309	0.85	7/3590 (0.2%)
6	A	0.55	1/16107 (0.0%)	1.05	26/21845 (0.1%)
7	D	0.49	0/929	0.81	0/1243
8	F	0.53	0/325	1.20	0/442
9	C	0.55	0/6902	1.02	7/9386 (0.1%)
10	G	0.52	0/839	1.10	0/1126
11	H	0.55	0/2667	1.35	4/3630 (0.1%)
12	J	0.59	0/2613	0.88	2/3551 (0.1%)
13	K	0.53	0/1308	1.05	4/1765 (0.2%)
14	L	0.52	0/1294	1.05	2/1732 (0.1%)
15	M	0.52	0/2056	0.97	2/2766 (0.1%)
16	N	0.55	0/1680	1.03	2/2258 (0.1%)
17	O	0.55	0/1669	1.14	1/2236 (0.0%)
18	P	0.61	0/282	0.88	1/380 (0.3%)
19	R	0.52	0/550	1.29	1/752 (0.1%)
20	S	0.53	0/3154	1.32	2/4297 (0.0%)
21	T	0.48	0/2916	1.48	10/4026 (0.2%)
22	b	0.53	0/636	0.71	0/856
22	k	0.49	0/394	0.99	2/546 (0.4%)
23	d	0.53	0/634	0.88	2/859 (0.2%)
23	n	0.48	0/403	1.14	4/559 (0.7%)
24	e	0.61	0/585	0.84	0/795
24	p	0.49	0/367	1.28	6/507 (1.2%)
25	f	0.57	0/585	0.85	0/791
25	q	0.50	0/353	1.01	0/489
26	g	0.55	0/532	0.76	0/715
26	r	0.48	0/338	0.90	2/467 (0.4%)
27	h	0.50	0/649	0.77	0/880

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
27	l	0.52	0/390	1.23	4/541 (0.7%)
28	j	0.55	0/753	0.89	0/1013
28	m	0.50	0/466	1.18	4/649 (0.6%)
29	W	0.50	0/814	1.18	10/1134 (0.9%)
30	Y	0.49	0/415	1.08	0/577
All	All	0.52	1/64443 (0.0%)	1.05	113/89647 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
6	A	0	2
10	G	0	1
15	M	0	1
17	O	0	1
20	S	0	1
All	All	0	6

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	632	ILE	N-CA	5.10	1.52	1.46

All (113) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	H	87	ILE	CA-C-N	14.31	134.45	118.85
11	H	87	ILE	C-N-CA	14.31	134.45	118.85
21	T	615	PHE	CA-C-N	10.69	131.39	120.38
21	T	615	PHE	C-N-CA	10.69	131.39	120.38
27	l	33	SER	CA-C-N	9.88	130.02	119.05
27	l	33	SER	C-N-CA	9.88	130.02	119.05
9	C	106	PHE	N-CA-C	9.81	124.05	109.24
28	m	29	GLY	CA-C-N	9.69	129.80	119.05
28	m	29	GLY	C-N-CA	9.69	129.80	119.05
1	U	39	U	C2'-C3'-O3'	9.12	127.38	113.70
27	l	97	LEU	CA-C-N	8.96	131.04	119.84
27	l	97	LEU	C-N-CA	8.96	131.04	119.84
12	J	141	TRP	N-CA-C	8.59	123.50	112.34
29	W	43	MET	CA-C-N	8.58	128.72	119.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	W	43	MET	C-N-CA	8.58	128.72	119.28
1	U	83	C	C4'-C3'-O3'	-8.47	100.29	113.00
16	N	91	ILE	N-CA-CB	8.20	120.14	110.55
29	W	4	THR	CA-C-N	7.87	127.43	118.85
29	W	4	THR	C-N-CA	7.87	127.43	118.85
5	V	34	A	C2'-C3'-O3'	-7.75	102.07	113.70
21	T	436	ASP	CA-C-N	7.59	127.30	119.56
21	T	436	ASP	C-N-CA	7.59	127.30	119.56
23	n	51	GLU	CA-C-N	7.46	127.49	119.28
23	n	51	GLU	C-N-CA	7.46	127.49	119.28
22	k	53	VAL	CA-C-N	7.27	127.25	119.76
22	k	53	VAL	C-N-CA	7.27	127.25	119.76
24	p	12	PRO	CA-C-N	7.10	127.09	119.28
24	p	12	PRO	C-N-CA	7.10	127.09	119.28
9	C	379	ILE	O-C-N	7.00	125.04	120.07
28	m	42	THR	CA-C-N	6.81	126.80	119.78
28	m	42	THR	C-N-CA	6.81	126.80	119.78
20	S	420	VAL	O-C-N	6.80	124.77	120.42
6	A	882	ILE	N-CA-CB	6.78	118.49	110.55
9	C	379	ILE	N-CA-CB	6.73	114.74	110.50
21	T	514	VAL	O-C-N	6.70	124.71	120.42
1	U	84	A	C4'-C3'-O3'	-6.68	102.98	113.00
6	A	990	ILE	CB-CA-C	-6.62	103.50	111.97
6	A	769	MET	N-CA-C	6.60	119.07	111.02
6	A	1339	LEU	N-CA-C	-6.56	104.21	111.36
21	T	612	ILE	O-C-N	6.56	124.62	120.42
29	W	11	ALA	CA-C-N	6.53	128.00	119.84
29	W	11	ALA	C-N-CA	6.53	128.00	119.84
13	K	145	PRO	N-CA-C	6.52	122.02	114.20
23	d	81	ALA	C-N-CD	-6.46	106.39	120.60
5	V	35	A	O4'-C4'-C3'	6.44	110.44	104.00
23	n	74	VAL	CA-C-N	6.42	126.37	120.21
23	n	74	VAL	C-N-CA	6.42	126.37	120.21
6	A	969	ILE	N-CA-C	6.30	116.95	107.75
21	T	478	TYR	CA-C-N	6.22	127.62	119.84
21	T	478	TYR	C-N-CA	6.22	127.62	119.84
6	A	1977	VAL	N-CA-CB	6.21	117.82	110.55
9	C	766	TRP	N-CA-C	6.21	118.31	110.24
29	W	67	ILE	CA-C-N	6.16	127.55	119.84
29	W	67	ILE	C-N-CA	6.16	127.55	119.84
21	T	442	THR	CA-C-N	6.16	127.54	119.84
21	T	442	THR	C-N-CA	6.16	127.54	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1795	LYS	O-C-N	6.12	125.22	120.38
29	W	148	VAL	CA-C-N	6.07	125.62	119.19
29	W	148	VAL	C-N-CA	6.07	125.62	119.19
24	p	25	THR	CA-C-N	5.97	125.89	119.85
24	p	25	THR	C-N-CA	5.97	125.89	119.85
5	V	72	C	C4'-C3'-O3'	-5.95	104.07	113.00
26	r	4	THR	CA-C-N	5.94	125.70	119.76
26	r	4	THR	C-N-CA	5.94	125.70	119.76
6	A	1113	ILE	CB-CA-C	-5.89	104.43	111.97
6	A	305	LEU	O-C-N	5.86	125.01	120.38
6	A	770	MET	N-CA-C	5.79	114.97	108.25
9	C	129	ILE	N-CA-C	5.76	113.58	107.76
6	A	214	THR	N-CA-CB	5.76	118.36	110.01
6	A	1401	SER	N-CA-C	5.68	117.62	110.24
9	C	966	PHE	CB-CA-C	-5.63	102.04	110.88
15	M	116	LYS	N-CA-C	-5.59	102.62	110.50
4	Z	118	U	C4'-C3'-O3'	5.57	117.75	109.40
13	K	69	ARG	N-CA-C	-5.49	104.98	110.97
13	K	78	VAL	N-CA-CB	5.48	117.99	110.54
6	A	851	ARG	CB-CA-C	-5.47	102.29	110.88
16	N	322	LEU	N-CA-C	5.47	119.67	112.89
20	S	271	ILE	N-CA-CB	5.47	117.98	110.54
6	A	737	ARG	N-CA-C	5.39	122.29	110.80
6	A	1809	ASN	N-CA-C	-5.34	102.76	110.40
5	V	45	A	C4'-C3'-O3'	-5.34	104.99	113.00
24	p	11	VAL	CA-C-N	5.32	125.86	120.38
24	p	11	VAL	C-N-CA	5.32	125.86	120.38
18	P	12	ARG	N-CA-C	5.32	116.89	108.96
1	U	76	U	C4'-C3'-O3'	5.31	117.36	109.40
9	C	418	GLN	O-C-N	5.26	125.16	120.48
5	V	34	A	C4'-C3'-O3'	5.25	120.87	113.00
6	A	1942	ASP	O-C-N	5.24	125.14	120.48
11	H	330	ILE	N-CA-CB	5.21	116.64	110.55
5	V	35	A	C5'-C4'-C3'	5.20	123.81	116.00
1	U	98	U	C4'-C3'-O3'	-5.20	105.21	113.00
13	K	74	ILE	N-CA-CB	5.18	117.59	110.54
14	L	14	ASP	N-CA-C	5.18	117.34	111.02
6	A	1752	VAL	N-CA-CB	5.15	117.54	110.54
6	A	1611	SER	CA-C-N	-5.12	114.55	119.87
6	A	1611	SER	C-N-CA	-5.12	114.55	119.87
6	A	1029	THR	N-CA-CB	5.12	117.43	110.01
6	A	1657	ILE	O-C-N	5.08	126.89	121.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	M	167	LEU	N-CA-C	5.08	118.74	112.54
17	O	41	GLN	N-CA-C	5.08	118.25	111.75
23	d	81	ALA	N-CA-C	5.07	112.58	108.07
5	V	35	A	C5'-C4'-O4'	5.07	117.40	109.80
6	A	631	LEU	CA-C-N	-5.06	113.24	120.42
6	A	631	LEU	C-N-CA	-5.06	113.24	120.42
14	L	47	GLU	CA-C-O	-5.06	115.49	120.90
11	H	440	LEU	N-CA-CB	5.05	117.33	110.01
19	R	31	ARG	N-CA-C	5.05	120.97	109.81
6	A	766	ILE	CB-CA-C	5.04	118.95	112.14
12	J	335	GLY	N-CA-C	-5.04	102.28	111.15
3	I	65	U	C2'-C3'-O3'	-5.04	106.14	113.70
6	A	404	ASN	N-CA-C	5.03	117.53	110.14
6	A	255	ILE	N-CA-C	-5.02	105.81	110.53
2	E	-10	A	C2'-C3'-O3'	5.00	117.01	109.50

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
10	G	3	ARG	Peptide
15	M	231	ASP	Peptide
17	O	83	GLN	Peptide
20	S	237	ILE	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	U	2999	0	1515	23	0
2	E	346	0	173	5	0
3	I	693	0	351	3	0
4	Z	3610	0	1831	10	0
5	V	2066	0	1043	20	0
6	A	15704	0	15649	254	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	912	0	936	12	0
8	F	321	0	282	6	0
9	C	6756	0	6801	122	0
10	G	823	0	808	11	0
11	H	2639	0	2073	26	0
12	J	2556	0	2551	60	0
13	K	1289	0	1309	20	0
14	L	1270	0	1294	12	0
15	M	2010	0	1964	21	0
16	N	1658	0	1713	55	0
17	O	1645	0	1672	35	0
18	P	275	0	283	4	0
19	R	550	0	356	3	0
20	S	3120	0	2397	44	0
21	T	2946	0	1250	10	0
22	b	631	0	670	2	0
22	k	396	0	169	0	0
23	d	625	0	647	6	0
23	n	404	0	180	0	0
24	e	575	0	597	7	0
24	p	369	0	152	0	0
25	f	573	0	572	4	0
25	q	354	0	153	0	0
26	g	529	0	557	3	0
26	r	340	0	152	0	0
27	h	644	0	686	3	0
27	l	392	0	165	0	0
28	j	741	0	778	3	0
28	m	467	0	199	0	0
29	W	816	0	341	1	0
30	Y	416	0	182	0	0
31	x	660	0	142	7	0
32	E	1	0	0	0	0
32	V	1	0	0	0	0
33	D	1	0	0	1	0
33	L	3	0	0	0	0
33	M	1	0	0	0	0
33	N	2	0	0	4	0
34	C	32	0	12	0	0
All	All	63161	0	52605	692	0

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

All (692) 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)
16:N:34:CYS:SG	16:N:37:CYS:SG	1.40	1.39
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30
16:N:16:CYS:SG	16:N:73:CYS:HB2	1.85	1.16
21:T:360:LYS:CB	21:T:381:HIS:CB	2.36	1.03
16:N:61:CYS:SG	33:N:401:ZN:ZN	1.54	0.94
7:D:88:CYS:SG	33:D:1001:ZN:ZN	1.65	0.85
16:N:16:CYS:SG	16:N:73:CYS:CB	2.65	0.84
15:M:250:MET:HB2	16:N:139:LEU:HD11	1.58	0.83
12:J:210:ASP:HB2	12:J:217:ILE:HD11	1.61	0.83
16:N:61:CYS:O	16:N:64:CYS:SG	2.37	0.82
16:N:220:THR:HG22	16:N:240:LEU:HD12	1.62	0.81
6:A:759:ARG:HD2	6:A:783:LEU:HD13	1.61	0.81
9:C:389:LEU:HD21	9:C:421:LEU:HD12	1.64	0.80
6:A:628:MET:HE3	6:A:660:ILE:HG23	1.64	0.78
5:V:67:C:H2'	5:V:68:C:O4'	1.85	0.76
12:J:323:VAL:HG12	12:J:336:LEU:HD12	1.67	0.75
1:U:45:A:N1	1:U:74:U:C4	2.54	0.75
16:N:113:LEU:HD11	16:N:120:LEU:HD11	1.69	0.75
15:M:22:ILE:HG23	15:M:23:PRO:HD3	1.67	0.74
16:N:37:CYS:SG	33:N:401:ZN:ZN	1.77	0.74
17:O:230:THR:HG23	20:S:116:ASN:HD21	1.53	0.73
5:V:76:A:OP2	6:A:749:ARG:NH1	2.21	0.73
16:N:71:CYS:SG	33:N:402:ZN:ZN	1.77	0.72
6:A:1361:VAL:HG21	6:A:1407:ILE:HD11	1.72	0.72
6:A:1335:TRP:CD1	6:A:1367:ILE:HG13	2.24	0.72
6:A:853:THR:HG23	6:A:971:MET:HG3	1.70	0.71
23:d:50:THR:HG22	23:d:56:VAL:HG12	1.71	0.71
6:A:1335:TRP:CZ2	6:A:1339:LEU:HD13	2.25	0.71
24:e:77:LEU:HD21	24:e:80:ILE:HD12	1.73	0.71
6:A:745:THR:HA	12:J:182:VAL:HG21	1.73	0.70
6:A:631:LEU:HD21	6:A:663:LEU:HD12	1.73	0.70
9:C:406:VAL:HG11	9:C:427:LEU:HB3	1.71	0.70
15:M:250:MET:CB	16:N:139:LEU:HD11	2.21	0.70
9:C:493:LEU:HD21	9:C:539:VAL:HG21	1.74	0.70
20:S:209:GLU:HB3	20:S:218:THR:HG22	1.75	0.69
4:Z:34:G:N2	6:A:1325:SER:OG	2.22	0.68
6:A:1067:ASN:HB2	6:A:1083:THR:HG21	1.76	0.68
27:h:3:LEU:HD11	28:j:60:ALA:HB1	1.75	0.68
27:h:43:VAL:HG11	27:h:85:ILE:HD12	1.76	0.68
6:A:1342:LEU:CD2	6:A:1360:LEU:HD21	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:206:VAL:HG11	12:J:241:THR:HG21	1.76	0.67
9:C:621:ALA:HB2	9:C:664:ALA:HB2	1.76	0.67
9:C:241:VAL:HG11	9:C:273:LEU:HD23	1.76	0.66
17:O:21:LEU:HD12	17:O:40:LEU:HD11	1.76	0.66
6:A:1144:PHE:CD2	6:A:1145:MET:HE2	2.31	0.66
9:C:200:CYS:HB3	9:C:436:VAL:HG21	1.78	0.66
12:J:290:VAL:HG12	12:J:311:VAL:HG11	1.77	0.66
1:U:110:U:H2'	1:U:111:C:O4'	1.95	0.66
6:A:741:ILE:HD11	12:J:224:LEU:HD22	1.78	0.65
6:A:1286:TRP:CE2	6:A:1302:LEU:HD11	2.31	0.65
17:O:60:LEU:HD21	17:O:94:PRO:HB3	1.79	0.65
11:H:299:LEU:HD11	11:H:329:ILE:HG12	1.79	0.65
6:A:716:ARG:O	6:A:720:PRO:HD2	1.97	0.64
9:C:193:LEU:HD11	9:C:228:ALA:HB2	1.78	0.64
16:N:125:ILE:HG21	16:N:135:ILE:HD12	1.80	0.64
12:J:282:VAL:HG11	12:J:323:VAL:HG21	1.80	0.64
16:N:71:CYS:HG	33:N:402:ZN:ZN	1.11	0.64
6:A:1344:THR:O	6:A:1347:ARG:NH1	2.30	0.64
12:J:142:VAL:HG11	12:J:423:ILE:CG2	2.28	0.64
9:C:323:THR:HG21	9:C:438:ALA:HB2	1.81	0.63
6:A:630:LYS:O	6:A:634:ASP:N	2.26	0.63
9:C:501:ILE:HD13	9:C:567:ILE:HG23	1.79	0.63
9:C:872:LEU:HD13	9:C:922:THR:HG22	1.79	0.63
16:N:60:ILE:HB	16:N:64:CYS:SG	2.39	0.63
6:A:886:MET:HE2	6:A:1120:VAL:HG22	1.80	0.63
11:H:445:LEU:HD11	11:H:448:MET:HG3	1.80	0.62
20:S:225:ALA:O	20:S:229:VAL:HG23	1.98	0.62
7:D:63:LYS:HE3	8:F:6:LEU:HD22	1.80	0.62
6:A:213:TYR:HA	6:A:216:GLN:HE21	1.63	0.62
6:A:673:VAL:HG22	6:A:714:PHE:CE1	2.34	0.62
9:C:251:GLN:HG2	9:C:933:TRP:CD2	2.35	0.61
12:J:277:VAL:HG11	12:J:321:PHE:CZ	2.36	0.61
6:A:857:ILE:HD11	6:A:969:ILE:HD11	1.82	0.61
16:N:91:ILE:HD12	16:N:125:ILE:HD12	1.82	0.61
6:A:268:LEU:HD13	6:A:277:LYS:HB2	1.82	0.61
9:C:602:VAL:HG11	9:C:860:PRO:HG3	1.81	0.61
6:A:673:VAL:HG22	6:A:714:PHE:CZ	2.36	0.61
20:S:149:VAL:O	20:S:152:VAL:HG12	2.01	0.61
6:A:628:MET:HE1	6:A:664:THR:HB	1.82	0.61
6:A:1557:LEU:HD13	6:A:1562:PHE:CE2	2.36	0.61
9:C:133:ILE:HD13	9:C:560:GLN:HB3	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:270:LEU:HD11	9:C:313:PHE:HB3	1.82	0.60
16:N:39:LEU:HD13	16:N:40:PRO:HD2	1.84	0.60
6:A:137:GLU:CD	14:L:30:LEU:HG	2.26	0.60
6:A:1738:LEU:HD13	6:A:1779:LEU:HD11	1.84	0.60
4:Z:38:U:O2	10:G:1:MET:N	2.34	0.60
12:J:323:VAL:CG1	12:J:336:LEU:HD12	2.32	0.60
21:T:554:ALA:CB	31:x:120:UNK:CB	2.79	0.60
21:T:554:ALA:HB1	31:x:120:UNK:CB	2.30	0.60
14:L:66:LEU:HD13	14:L:73:ILE:HG13	1.83	0.59
1:U:71:A:N3	1:U:116:U:O2'	2.33	0.59
9:C:656:LEU:HD22	9:C:670:ILE:HD11	1.85	0.59
9:C:866:ILE:HB	9:C:902:VAL:HG13	1.83	0.59
6:A:1032:ILE:HG12	6:A:1171:LEU:HD22	1.83	0.59
16:N:16:CYS:HG	16:N:73:CYS:HB2	1.63	0.59
9:C:499:VAL:HG11	9:C:577:LEU:HD13	1.83	0.59
12:J:164:MET:HE1	12:J:199:SER:HB2	1.84	0.59
20:S:173:VAL:HG23	20:S:188:ILE:HD11	1.85	0.59
6:A:390:LEU:HD21	9:C:605:ILE:HD11	1.85	0.58
12:J:240:ALA:HB1	12:J:248:ILE:HD11	1.82	0.58
12:J:160:ASN:HA	12:J:184:THR:HB	1.85	0.58
16:N:39:LEU:HD23	16:N:111:ARG:HG2	1.85	0.58
11:H:298:VAL:HG11	11:H:312:LEU:HD23	1.84	0.58
6:A:842:LYS:O	6:A:845:VAL:HG12	2.02	0.58
16:N:207:LEU:HD11	16:N:251:LEU:HD11	1.86	0.58
16:N:16:CYS:SG	16:N:71:CYS:SG	3.02	0.58
12:J:248:ILE:HG23	12:J:262:LEU:HB2	1.84	0.58
6:A:1668:ILE:HD13	6:A:1801:SER:HB3	1.86	0.58
17:O:185:LEU:O	17:O:188:ARG:HG3	2.03	0.58
12:J:147:ILE:HD13	12:J:408:ASP:HA	1.84	0.57
16:N:16:CYS:SG	16:N:73:CYS:SG	3.02	0.57
6:A:1632:ILE:HG21	6:A:1645:LEU:HD13	1.85	0.57
17:O:185:LEU:O	17:O:189:ARG:HG2	2.03	0.57
6:A:395:PRO:HB2	6:A:398:VAL:HG21	1.87	0.57
6:A:868:GLN:HE21	17:O:90:MET:HE3	1.70	0.57
6:A:305:LEU:HD21	6:A:476:ALA:HB2	1.85	0.57
14:L:66:LEU:HD13	14:L:73:ILE:CG1	2.34	0.57
6:A:322:VAL:HG23	6:A:508:GLN:HE21	1.70	0.56
6:A:342:LEU:HB3	6:A:344:ASN:HD22	1.70	0.56
6:A:1557:LEU:HD11	6:A:1570:TRP:HB2	1.86	0.56
9:C:328:VAL:HG21	9:C:345:THR:HG22	1.87	0.56
20:S:229:VAL:HG22	20:S:238:TRP:HZ2	1.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:370:ILE:HB	6:A:1418:THR:HG21	1.87	0.56
6:A:969:ILE:HG22	6:A:982:TYR:HA	1.86	0.56
6:A:1049:LEU:HB2	6:A:1258:LEU:HD11	1.86	0.56
6:A:718:THR:O	6:A:719:ILE:C	2.48	0.56
11:H:465:PHE:HB2	11:H:473:LEU:HD23	1.88	0.56
5:V:59:A:H2'	5:V:60:G:O4'	2.05	0.56
6:A:754:TYR:HA	12:J:183:MET:HE3	1.86	0.56
6:A:948:HIS:CE1	6:A:952:ASN:HD21	2.23	0.56
17:O:33:TRP:CE3	17:O:36:VAL:HG11	2.41	0.56
20:S:184:GLY:O	20:S:188:ILE:HG23	2.05	0.56
12:J:289:THR:HG22	12:J:305:THR:HG22	1.88	0.56
16:N:226:LEU:HD13	16:N:266:ILE:HD11	1.87	0.56
6:A:878:GLU:O	6:A:882:ILE:HG23	2.06	0.56
7:D:11:TYR:CD1	10:G:12:LEU:HD21	2.41	0.56
17:O:230:THR:HG21	20:S:117:HIS:ND1	2.21	0.56
6:A:172:ILE:HD13	6:A:625:LEU:HB3	1.88	0.55
6:A:521:SER:HB2	6:A:682:ASP:HA	1.88	0.55
6:A:1417:GLN:HG2	6:A:1418:THR:HG23	1.88	0.55
12:J:277:VAL:HG13	12:J:278:ASP:N	2.20	0.55
16:N:106:ASN:HD21	17:O:208:GLY:HA2	1.71	0.55
14:L:94:LYS:HD2	14:L:109:ILE:HD11	1.87	0.55
6:A:1000:TRP:CZ2	6:A:1510:ILE:HG21	2.41	0.55
6:A:659:HIS:O	6:A:660:ILE:C	2.49	0.55
17:O:37:ALA:HB2	17:O:45:ALA:HA	1.88	0.55
6:A:724:ARG:O	6:A:728:ASN:HB2	2.07	0.55
9:C:472:VAL:HB	9:C:575:ALA:HB3	1.88	0.55
15:M:163:VAL:HG23	15:M:164:PHE:HD1	1.71	0.55
20:S:122:MET:HE1	20:S:142:VAL:HG11	1.87	0.55
1:U:92:U:O2	19:R:12:LYS:NZ	2.39	0.55
6:A:168:LEU:N	6:A:169:PRO:CD	2.69	0.55
6:A:588:LEU:HD13	6:A:591:LEU:CD2	2.37	0.55
6:A:168:LEU:HD21	6:A:626:LEU:HD21	1.89	0.55
6:A:1209:LYS:HA	6:A:1212:ARG:HG2	1.89	0.55
6:A:1933:ILE:HD12	6:A:1948:MET:HE2	1.89	0.55
6:A:424:PHE:CE1	9:C:893:LYS:HB3	2.42	0.54
6:A:1542:TYR:O	6:A:1546:VAL:HG23	2.07	0.54
16:N:106:ASN:HB2	17:O:213:TYR:CG	2.42	0.54
6:A:1169:TYR:CD2	6:A:1262:MET:HE2	2.43	0.54
1:U:45:A:C2	1:U:74:U:O4	2.54	0.54
2:E:-5:G:HO2'	2:E:-4:A:H8	1.55	0.54
6:A:228:LYS:HD2	6:A:695:LEU:HD11	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:17:LEU:CD2	16:N:23:ILE:HD12	2.37	0.54
6:A:175:LEU:HD22	6:A:629:MET:HE2	1.88	0.54
6:A:854:ARG:HG3	6:A:1095:MET:HE1	1.89	0.54
6:A:1562:PHE:O	6:A:1565:THR:OG1	2.24	0.54
16:N:29:PRO:HA	16:N:42:THR:HG22	1.90	0.54
17:O:211:ILE:HD13	20:S:44:ARG:HG3	1.89	0.54
20:S:99:ILE:N	20:S:100:PRO:CD	2.70	0.54
29:W:121:PRO:O	29:W:122:ARG:CB	2.56	0.54
17:O:16:VAL:HG22	17:O:152:LEU:HD21	1.88	0.54
20:S:119:ARG:HA	20:S:122:MET:HE3	1.90	0.54
6:A:141:LYS:HG3	14:L:52:ILE:HD11	1.90	0.54
12:J:164:MET:HE2	12:J:185:VAL:HG21	1.90	0.54
6:A:880:THR:OG1	13:K:207:ALA:HB1	2.08	0.54
6:A:1335:TRP:CH2	6:A:1364:GLU:HG2	2.42	0.54
6:A:1756:PHE:CE1	6:A:1760:THR:HG21	2.43	0.54
7:D:51:CYS:SG	7:D:88:CYS:SG	3.06	0.54
9:C:861:ILE:HD11	9:C:938:ARG:HB2	1.89	0.54
6:A:137:GLU:CD	14:L:52:ILE:HG23	2.33	0.53
9:C:138:VAL:HG23	9:C:236:LEU:HB2	1.90	0.53
9:C:265:PHE:HB2	9:C:311:ILE:HD13	1.89	0.53
1:U:102:C:OP1	6:A:675:HIS:NE2	2.42	0.53
9:C:191:ILE:HG23	9:C:221:PHE:CE2	2.44	0.53
24:e:77:LEU:HD21	24:e:80:ILE:CD1	2.37	0.53
5:V:35:A:C8	14:L:41:LEU:HD13	2.43	0.53
9:C:241:VAL:HG22	9:C:267:ILE:CG2	2.38	0.53
1:U:45:A:N6	1:U:74:U:N3	2.55	0.53
6:A:674:MET:CE	6:A:1621:VAL:HG11	2.38	0.53
6:A:929:LEU:HD11	6:A:1590:LEU:HD23	1.91	0.53
6:A:2060:LEU:HD21	6:A:2078:GLU:HG3	1.89	0.53
12:J:277:VAL:HG11	12:J:321:PHE:HZ	1.71	0.53
6:A:1669:LEU:HD22	6:A:1703:MET:HE3	1.91	0.53
9:C:864:VAL:HG22	9:C:930:LEU:HD23	1.90	0.53
6:A:882:ILE:HD11	6:A:1065:LEU:HD21	1.90	0.53
12:J:306:HIS:CE1	13:K:147:LEU:HD11	2.44	0.53
6:A:210:GLU:O	6:A:214:THR:HG23	2.09	0.53
6:A:588:LEU:HD13	6:A:591:LEU:HD22	1.91	0.53
7:D:101:PRO:HB2	8:F:23:VAL:HG21	1.90	0.53
12:J:142:VAL:HG11	12:J:423:ILE:HG23	1.91	0.53
6:A:161:PHE:HA	6:A:198:ALA:HB1	1.91	0.53
6:A:308:MET:HG3	6:A:479:LEU:HD11	1.89	0.53
9:C:201:THR:HG22	9:C:207:SER:HB3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:126:MET:SD	9:C:132:ARG:NH2	2.82	0.53
6:A:937:LEU:HD22	6:A:1590:LEU:CD2	2.39	0.52
10:G:55:SER:O	10:G:58:ILE:HG22	2.10	0.52
1:U:32:G:H3'	1:U:33:U:C5'	2.38	0.52
9:C:836:SER:O	9:C:840:PRO:HD2	2.09	0.52
12:J:341:LEU:HD23	12:J:342:LEU:N	2.24	0.52
15:M:130:PHE:CE1	16:N:75:MET:HE2	2.44	0.52
21:T:119:ALA:HB1	21:T:128:ILE:CA	2.39	0.52
6:A:937:LEU:HD22	6:A:1590:LEU:HD22	1.91	0.52
13:K:133:LYS:O	16:N:108:MET:HE1	2.09	0.52
6:A:1375:LEU:HD12	6:A:1383:PHE:CE1	2.44	0.52
1:U:45:A:N3	1:U:45:A:H2'	2.24	0.52
13:K:201:PHE:CD2	17:O:80:LEU:HD21	2.45	0.52
21:T:554:ALA:HA	31:x:120:UNK:CB	2.40	0.52
6:A:1339:LEU:HD11	6:A:1360:LEU:HD22	1.92	0.52
12:J:335:GLY:H	12:J:342:LEU:HD13	1.74	0.52
6:A:1207:TRP:O	6:A:1212:ARG:NH1	2.42	0.52
6:A:730:ILE:HD12	6:A:731:THR:N	2.25	0.52
6:A:785:HIS:NE2	13:K:168:ALA:HB2	2.24	0.52
6:A:1090:ILE:HD11	6:A:1104:ILE:CD1	2.40	0.52
6:A:1393:GLU:O	6:A:1394:LEU:HD23	2.10	0.52
6:A:1974:LEU:O	6:A:1977:VAL:HG22	2.10	0.52
9:C:127:ALA:HB2	9:C:209:MET:HE3	1.91	0.52
9:C:539:VAL:HG13	9:C:564:ILE:HG23	1.92	0.52
6:A:1654:TRP:CZ3	6:A:1779:LEU:HD12	2.45	0.51
7:D:51:CYS:SG	7:D:88:CYS:HB3	2.50	0.51
20:S:199:MET:SD	20:S:246:LEU:HD22	2.50	0.51
6:A:212:VAL:HG22	6:A:311:LEU:HD11	1.92	0.51
6:A:808:ILE:HG21	13:K:165:ILE:HD12	1.91	0.51
9:C:626:SER:HB3	9:C:634:ILE:HD12	1.91	0.51
11:H:333:SER:HA	11:H:343:TYR:CE2	2.46	0.51
3:I:2:U:O4	4:Z:37:G:H1'	2.10	0.51
9:C:664:ALA:HB1	9:C:666:ILE:CD1	2.39	0.51
9:C:664:ALA:HB1	9:C:666:ILE:HD12	1.92	0.51
11:H:347:SER:O	11:H:351:ILE:HG12	2.09	0.51
16:N:61:CYS:N	16:N:64:CYS:SG	2.84	0.51
17:O:16:VAL:CG2	17:O:152:LEU:HD21	2.40	0.51
6:A:249:LEU:HD12	6:A:249:LEU:O	2.11	0.51
8:F:34:GLN:HE22	31:x:43:UNK:HA	1.76	0.51
27:h:82:LEU:HD12	27:h:85:ILE:HD11	1.92	0.51
6:A:153:MET:HE3	6:A:154:TYR:CD2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:179:MET:HE1	6:A:653:ILE:HG21	1.93	0.51
6:A:660:ILE:HG21	6:A:711:TRP:CH2	2.45	0.51
6:A:172:ILE:HG23	6:A:629:MET:HG2	1.93	0.51
6:A:1047:ALA:HB3	6:A:1251:TYR:HB3	1.92	0.51
6:A:1375:LEU:HD12	6:A:1383:PHE:HE1	1.76	0.51
9:C:255:GLN:HG2	9:C:598:ILE:HD12	1.92	0.51
12:J:206:VAL:CG1	12:J:241:THR:HG21	2.40	0.51
3:I:2:U:H3'	6:A:607:THR:OG1	2.11	0.51
9:C:963:SER:O	9:C:967:VAL:HG23	2.10	0.51
6:A:458:PHE:CZ	9:C:336:ILE:HD11	2.45	0.51
6:A:1329:THR:HG21	6:A:1601:ILE:HB	1.93	0.51
9:C:872:LEU:HD13	9:C:922:THR:CG2	2.41	0.51
11:H:326:VAL:O	11:H:330:ILE:HG12	2.10	0.51
12:J:275:THR:OG1	12:J:279:PRO:O	2.29	0.51
5:V:27:U:O2'	14:L:124:VAL:HA	2.11	0.50
6:A:350:PRO:HD3	6:A:526:LEU:HD13	1.92	0.50
6:A:741:ILE:CD1	12:J:224:LEU:HD22	2.41	0.50
20:S:172:PHE:CD2	20:S:188:ILE:HD13	2.46	0.50
23:d:81:ALA:HB1	23:d:82:PRO:HB3	1.93	0.50
6:A:713:ASN:O	6:A:716:ARG:HB3	2.11	0.50
6:A:1893:ILE:HD12	6:A:1978:VAL:HG22	1.92	0.50
9:C:139:ILE:HG12	9:C:225:THR:HG23	1.93	0.50
3:I:3:A:OP2	10:G:3:ARG:HA	2.11	0.50
4:Z:4:A:H2'	4:Z:5:A:H5'	1.91	0.50
6:A:249:LEU:HD11	6:A:637:VAL:HG11	1.93	0.50
8:F:31:ILE:HD12	31:x:46:UNK:HA	1.94	0.50
9:C:493:LEU:HD22	9:C:542:ILE:HD11	1.93	0.50
6:A:912:LEU:HD22	6:A:951:LEU:HG	1.94	0.50
9:C:615:LEU:N	9:C:616:PRO:HD2	2.26	0.50
9:C:617:LYS:HB3	9:C:666:ILE:HD11	1.94	0.50
6:A:175:LEU:HD23	6:A:564:TRP:CZ2	2.46	0.50
6:A:182:PRO:HG2	6:A:220:THR:HG21	1.94	0.50
6:A:410:ILE:N	6:A:410:ILE:HD12	2.27	0.50
6:A:674:MET:CE	6:A:674:MET:HA	2.42	0.50
6:A:1282:ASP:C	11:H:345:ILE:HD11	2.36	0.50
8:F:31:ILE:HD11	31:x:45:UNK:CB	2.41	0.50
9:C:133:ILE:HG23	9:C:209:MET:SD	2.52	0.50
9:C:864:VAL:HG22	9:C:930:LEU:CD2	2.42	0.50
17:O:90:MET:HE2	17:O:90:MET:HA	1.93	0.50
17:O:230:THR:HG21	20:S:117:HIS:CE1	2.47	0.50
6:A:1344:THR:HG21	6:A:1537:TRP:CD2	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:J:156:ILE:HG22	12:J:166:VAL:HG22	1.93	0.50
12:J:200:VAL:CG2	12:J:227:VAL:HB	2.41	0.50
9:C:231:ALA:HB2	9:C:473:LEU:HD13	1.93	0.49
5:V:35:A:C8	15:M:75:PHE:CZ	3.00	0.49
6:A:138:HIS:NE2	6:A:142:ILE:HD11	2.27	0.49
6:A:1206:CYS:HG	6:A:1207:TRP:CD1	2.29	0.49
1:U:32:G:C6	1:U:34:C:C4	3.01	0.49
4:Z:4:A:C2'	4:Z:5:A:H5'	2.42	0.49
6:A:793:TRP:CZ2	6:A:820:ALA:HB1	2.48	0.49
6:A:1309:ILE:CG2	6:A:1359:ILE:HD12	2.42	0.49
17:O:230:THR:HG22	20:S:114:CYS:SG	2.53	0.49
10:G:28:ASP:OD1	10:G:28:ASP:N	2.44	0.49
11:H:291:PHE:CE1	11:H:317:ILE:HG21	2.47	0.49
20:S:81:MET:HE3	20:S:112:VAL:HG11	1.94	0.49
24:e:91:THR:HB	26:g:61:THR:HG22	1.94	0.49
9:C:391:MET:HE1	9:C:399:LEU:HD11	1.94	0.49
16:N:37:CYS:SG	16:N:61:CYS:SG	3.11	0.49
6:A:937:LEU:HD13	6:A:1590:LEU:HD11	1.93	0.49
8:F:27:GLU:O	8:F:31:ILE:HG12	2.13	0.49
9:C:116:THR:HG21	9:C:118:TYR:CZ	2.47	0.49
9:C:544:LEU:HD23	9:C:562:VAL:HG12	1.94	0.49
12:J:145:VAL:HG22	12:J:157:THR:HG22	1.94	0.49
6:A:1400:ILE:HG22	6:A:1400:ILE:O	2.12	0.49
9:C:137:GLY:O	9:C:139:ILE:HD12	2.13	0.49
17:O:20:ILE:HD11	17:O:152:LEU:HD22	1.95	0.49
20:S:99:ILE:HD11	20:S:132:VAL:HG11	1.95	0.49
5:V:52:G:H2'	5:V:53:A:C8	2.47	0.49
6:A:1795:LYS:N	6:A:1796:PRO:CD	2.75	0.49
12:J:150:VAL:HG13	12:J:151:ASP:HB3	1.95	0.49
21:T:332:GLN:CB	21:T:342:ILE:CB	2.91	0.49
9:C:607:LEU:HD11	9:C:644:ILE:HD11	1.96	0.48
17:O:24:ALA:O	17:O:28:TYR:N	2.37	0.48
6:A:1557:LEU:HD13	6:A:1562:PHE:CD2	2.48	0.48
9:C:213:LEU:HD11	9:C:561:ILE:HD13	1.95	0.48
11:H:427:LEU:HD23	11:H:436:LEU:HD11	1.95	0.48
6:A:724:ARG:CD	18:P:31:LEU:HD11	2.43	0.48
23:d:66:GLY:HA2	23:d:69:ILE:HD12	1.95	0.48
5:V:41:A:H2'	5:V:42:A:O4'	2.14	0.48
11:H:368:ASN:ND2	11:H:384:LEU:HD11	2.29	0.48
6:A:1669:LEU:HB3	6:A:1681:VAL:HG21	1.95	0.48
12:J:277:VAL:HG22	12:J:278:ASP:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:708:TRP:CE2	6:A:712:LEU:HD11	2.49	0.48
6:A:1223:GLY:CA	6:A:1248:VAL:HG11	2.43	0.48
12:J:147:ILE:HG22	12:J:155:PHE:HB3	1.94	0.48
16:N:65:ALA:O	16:N:69:ASN:N	2.47	0.48
12:J:272:VAL:HG13	12:J:272:VAL:O	2.14	0.48
9:C:241:VAL:HG23	9:C:268:ASN:O	2.14	0.48
16:N:17:LEU:HD21	16:N:23:ILE:HD12	1.96	0.48
6:A:522:TYR:CZ	6:A:686:ILE:HD12	2.48	0.48
6:A:1028:TRP:CZ3	6:A:1162:THR:HG22	2.49	0.48
14:L:22:THR:HG21	14:L:62:TYR:CE1	2.49	0.48
5:V:32:U:C4	16:N:28:ILE:HG21	2.49	0.48
15:M:137:LEU:HD21	15:M:192:ALA:HB1	1.96	0.48
17:O:218:VAL:HB	20:S:89:GLU:HB3	1.96	0.48
6:A:783:LEU:C	6:A:783:LEU:HD12	2.39	0.47
6:A:857:ILE:CD1	6:A:969:ILE:HD11	2.44	0.47
9:C:273:LEU:HD12	9:C:274:ILE:N	2.29	0.47
9:C:625:ILE:HG22	9:C:634:ILE:HD11	1.95	0.47
20:S:140:LEU:HD22	20:S:156:TYR:CE2	2.49	0.47
6:A:165:LEU:HD13	6:A:578:MET:HE2	1.96	0.47
6:A:849:LEU:HD13	6:A:849:LEU:C	2.40	0.47
6:A:1222:LEU:O	6:A:1226:VAL:HG23	2.15	0.47
9:C:229:LEU:HB3	9:C:259:ASN:HD21	1.79	0.47
13:K:41:ASP:HA	13:K:44:ILE:HD12	1.96	0.47
9:C:211:ASN:N	9:C:211:ASN:HD22	2.12	0.47
9:C:873:LEU:HD21	9:C:891:THR:HG21	1.94	0.47
11:H:355:ARG:O	11:H:359:THR:HG23	2.14	0.47
17:O:33:TRP:HA	17:O:36:VAL:HG12	1.96	0.47
20:S:112:VAL:HG13	20:S:114:CYS:HB2	1.96	0.47
21:T:119:ALA:HB1	21:T:128:ILE:HA	1.94	0.47
6:A:522:TYR:CE2	6:A:686:ILE:HD12	2.50	0.47
6:A:1066:LEU:HD11	6:A:1113:ILE:HG23	1.95	0.47
9:C:136:VAL:O	9:C:234:LEU:O	2.33	0.47
12:J:341:LEU:HD22	13:K:45:PRO:HB3	1.96	0.47
6:A:1404:HIS:NE2	6:A:1429:MET:HE2	2.30	0.47
2:E:-5:G:O2'	2:E:-4:A:H8	1.98	0.47
6:A:1234:VAL:HG11	6:A:1239:THR:HG22	1.95	0.47
6:A:1347:ARG:HD2	6:A:1447:TRP:CE2	2.49	0.47
6:A:1388:PHE:CD1	6:A:1397:LEU:HD12	2.50	0.47
9:C:193:LEU:HD12	9:C:213:LEU:HB3	1.97	0.47
9:C:504:THR:HG23	9:C:574:SER:O	2.15	0.47
20:S:229:VAL:HG11	20:S:243:VAL:CG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:687:ILE:HD11	6:A:706:PRO:HG3	1.97	0.47
7:D:23:LEU:HG	10:G:18:GLN:HE22	1.80	0.47
12:J:144:CYS:SG	12:J:187:ASP:HA	2.55	0.47
20:S:225:ALA:O	20:S:228:THR:HG22	2.15	0.47
6:A:468:LEU:HD22	6:A:469:ILE:HG23	1.97	0.46
6:A:1345:TYR:HD1	6:A:1345:TYR:O	1.98	0.46
13:K:104:LEU:HD12	13:K:113:GLU:HA	1.97	0.46
20:S:193:VAL:HG11	20:S:202:TRP:CZ2	2.50	0.46
6:A:876:PRO:HA	13:K:204:LEU:HD22	1.97	0.46
6:A:1417:GLN:CG	6:A:1418:THR:HG23	2.45	0.46
12:J:269:ILE:HA	12:J:285:SER:HA	1.97	0.46
6:A:319:ARG:O	6:A:321:GLU:N	2.48	0.46
7:D:31:LEU:HD11	10:G:31:ARG:NH2	2.30	0.46
9:C:312:ILE:HD13	9:C:435:LEU:HG	1.98	0.46
17:O:25:VAL:HG11	17:O:52:TRP:CH2	2.50	0.46
17:O:214:ASN:HB2	17:O:217:ILE:HD11	1.97	0.46
5:V:71:G:H21	5:V:75:A:H2	1.62	0.46
6:A:1881:THR:HG21	6:A:1920:LEU:CD2	2.46	0.46
12:J:144:CYS:SG	12:J:145:VAL:N	2.89	0.46
6:A:286:LEU:HD13	6:A:287:GLU:N	2.30	0.46
11:H:369:TYR:CE1	11:H:420:ILE:HD11	2.51	0.46
11:H:465:PHE:CB	11:H:473:LEU:HD23	2.46	0.46
15:M:17:GLU:HB2	15:M:18:LEU:HD13	1.97	0.46
5:V:32:U:O4	16:N:28:ILE:HG21	2.16	0.46
6:A:929:LEU:HD11	6:A:1590:LEU:CD2	2.45	0.46
6:A:1275:MET:HE1	6:A:1299:LYS:HD2	1.97	0.46
6:A:1350:ILE:HD13	6:A:1356:LEU:CD2	2.46	0.46
6:A:1428:GLY:O	19:R:16:THR:OG1	2.23	0.46
9:C:493:LEU:CD2	9:C:539:VAL:HG21	2.45	0.46
14:L:94:LYS:CD	14:L:109:ILE:HD11	2.45	0.46
23:d:33:LEU:HD23	23:d:34:VAL:N	2.31	0.46
9:C:873:LEU:N	9:C:874:PRO:CD	2.79	0.46
9:C:928:CYS:SG	9:C:929:GLN:N	2.89	0.46
12:J:248:ILE:HG13	12:J:262:LEU:HD12	1.98	0.46
17:O:230:THR:HG21	20:S:117:HIS:CG	2.51	0.46
11:H:334:LEU:HD21	11:H:384:LEU:HD12	1.98	0.46
15:M:99:ILE:HD13	15:M:188:TYR:CD2	2.51	0.46
1:U:119:U:C2	1:U:120:G:C8	3.04	0.45
6:A:1020:ILE:HB	6:A:1022:PRO:HD2	1.98	0.45
6:A:1357:LEU:HD11	11:H:303:LEU:HD22	1.98	0.45
9:C:501:ILE:CD1	9:C:567:ILE:HG23	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:47:U:H2'	1:U:48:G:C8	2.52	0.45
6:A:1354:GLU:N	6:A:1355:PRO:CD	2.78	0.45
9:C:837:GLN:HE21	9:C:837:GLN:HA	1.81	0.45
11:H:351:ILE:HG21	11:H:395:GLU:HG3	1.98	0.45
12:J:144:CYS:SG	12:J:188:VAL:N	2.88	0.45
12:J:284:SER:OG	12:J:311:VAL:O	2.35	0.45
4:Z:22:C:H4'	6:A:755:ASP:CG	2.42	0.45
6:A:783:LEU:HD12	6:A:783:LEU:O	2.16	0.45
9:C:492:LEU:HD12	9:C:492:LEU:O	2.16	0.45
11:H:330:ILE:HG22	11:H:334:LEU:CD2	2.46	0.45
20:S:169:TRP:CE3	20:S:192:TYR:HB2	2.51	0.45
2:E:-4:A:H2'	2:E:-3:A:C8	2.51	0.45
6:A:628:MET:CE	6:A:664:THR:HB	2.45	0.45
6:A:1286:TRP:CD1	6:A:1448:GLU:HB2	2.52	0.45
6:A:210:GLU:N	6:A:211:PRO:HD2	2.32	0.45
9:C:274:ILE:HG21	9:C:385:PHE:CD2	2.51	0.45
9:C:470:ALA:HB1	9:C:486:VAL:HG12	1.98	0.45
9:C:936:ILE:HG23	9:C:936:ILE:O	2.16	0.45
16:N:216:GLU:O	16:N:220:THR:HG23	2.17	0.45
6:A:1461:TYR:CE1	6:A:1494:LEU:HD13	2.51	0.45
11:H:312:LEU:CD1	11:H:329:ILE:HD11	2.47	0.45
4:Z:5:A:H2'	4:Z:6:U:O4'	2.16	0.45
6:A:507:LEU:HD21	6:A:529:TYR:CE2	2.52	0.45
6:A:583:ILE:HG23	6:A:588:LEU:HD12	1.98	0.45
6:A:1049:LEU:CB	6:A:1258:LEU:HD11	2.47	0.45
12:J:229:THR:HG21	12:J:271:GLN:HA	1.98	0.45
24:e:45:GLY:HA3	24:e:53:VAL:HG12	1.97	0.45
12:J:161:ASP:O	12:J:162:THR:HB	2.17	0.45
20:S:202:TRP:CZ2	20:S:228:THR:HG21	2.52	0.45
6:A:164:ALA:HB3	6:A:578:MET:HE3	1.98	0.45
5:V:63:G:H2'	5:V:64:U:H6	1.82	0.45
6:A:889:TRP:CH2	6:A:893:ARG:HD3	2.52	0.45
6:A:1214:ARG:N	6:A:1255:ASN:OD1	2.50	0.45
6:A:1657:ILE:CD1	6:A:1815:LEU:HD22	2.47	0.45
9:C:862:TYR:CE2	9:C:908:VAL:HG13	2.51	0.45
15:M:81:CYS:SG	15:M:91:HIS:CE1	3.10	0.45
6:A:220:THR:HB	6:A:224:MET:HE3	1.99	0.44
6:A:1560:THR:HG21	6:A:1609:TRP:NE1	2.32	0.44
20:S:140:LEU:HD23	20:S:152:VAL:HG22	1.99	0.44
6:A:173:LEU:HA	6:A:715:LEU:HD13	1.98	0.44
6:A:639:PHE:CG	6:A:649:LEU:HD22	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:N:16:CYS:HB2	16:N:71:CYS:SG	2.57	0.44
9:C:241:VAL:CG1	9:C:273:LEU:HD23	2.46	0.44
9:C:808:LEU:HD22	9:C:944:VAL:HG21	1.99	0.44
16:N:12:ILE:HG23	16:N:16:CYS:SG	2.57	0.44
17:O:80:LEU:O	17:O:81:PRO:C	2.61	0.44
1:U:39:U:H2'	1:U:40:C:O4'	2.18	0.44
6:A:264:ILE:HD11	6:A:647:PHE:N	2.33	0.44
6:A:1090:ILE:HD11	6:A:1104:ILE:HD11	1.99	0.44
6:A:1336:ASN:HB3	6:A:1400:ILE:HD12	1.99	0.44
6:A:1820:ARG:O	6:A:1824:GLN:N	2.50	0.44
9:C:223:ASP:OD1	9:C:224:GLU:N	2.50	0.44
10:G:18:GLN:HG3	10:G:19:GLN:N	2.32	0.44
11:H:292:LYS:CD	11:H:328:ILE:HD11	2.47	0.44
1:U:103:A:O2'	1:U:104:G:O4'	2.24	0.44
6:A:458:PHE:CE2	9:C:336:ILE:HD11	2.52	0.44
6:A:719:ILE:HB	6:A:720:PRO:CD	2.47	0.44
6:A:724:ARG:HD3	18:P:31:LEU:HD11	1.99	0.44
9:C:444:GLN:N	9:C:445:PRO:CD	2.81	0.44
6:A:687:ILE:HD11	6:A:706:PRO:CG	2.48	0.44
9:C:905:GLN:NE2	9:C:936:ILE:HD13	2.32	0.44
12:J:248:ILE:HD13	12:J:272:VAL:HG21	2.00	0.44
21:T:554:ALA:CA	31:x:120:UNK:CB	2.96	0.44
2:E:-4:A:H2'	2:E:-3:A:H8	1.83	0.44
6:A:178:ASN:O	6:A:179:MET:C	2.61	0.44
6:A:674:MET:HE1	6:A:1621:VAL:HG11	2.00	0.44
6:A:759:ARG:CD	6:A:783:LEU:HD13	2.41	0.44
6:A:1371:VAL:HG11	6:A:1397:LEU:HD11	1.98	0.44
9:C:708:ILE:HD12	9:C:708:ILE:N	2.33	0.44
6:A:189:VAL:CG2	6:A:202:VAL:HG13	2.48	0.44
6:A:588:LEU:HD22	6:A:613:SER:HA	2.00	0.44
15:M:114:ARG:NE	15:M:127:ILE:HG21	2.32	0.44
15:M:173:ILE:HG12	15:M:184:VAL:HG13	1.99	0.44
20:S:140:LEU:CD2	20:S:155:LEU:HD22	2.48	0.44
20:S:160:CYS:HB3	20:S:169:TRP:CH2	2.53	0.44
6:A:1372:LYS:HD2	6:A:1378:LYS:HA	2.00	0.43
6:A:1944:LEU:HD23	6:A:1956:ILE:HG23	2.00	0.43
9:C:658:ASP:HB3	9:C:663:TYR:CE2	2.52	0.43
13:K:112:ILE:HD12	16:N:25:MET:HE3	2.00	0.43
15:M:74:LEU:HA	15:M:112:PHE:CE1	2.53	0.43
16:N:125:ILE:HG21	16:N:135:ILE:CD1	2.45	0.43
22:b:85:THR:HG22	23:d:73:VAL:HG22	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:268:LEU:HD13	6:A:277:LYS:CB	2.47	0.43
12:J:129:TRP:HB2	12:J:385:GLN:HE22	1.83	0.43
12:J:156:ILE:HD11	12:J:188:VAL:HG21	2.00	0.43
12:J:277:VAL:HG13	12:J:279:PRO:HD2	2.00	0.43
20:S:229:VAL:HG22	20:S:238:TRP:CZ2	2.50	0.43
6:A:629:MET:HE1	6:A:632:ILE:HD11	1.99	0.43
6:A:1021:PRO:O	6:A:1025:VAL:HG23	2.17	0.43
6:A:1409:ALA:HB3	6:A:1424:HIS:O	2.18	0.43
7:D:43:LEU:HD21	7:D:86:ILE:CD1	2.47	0.43
9:C:862:TYR:CG	9:C:908:VAL:HG22	2.53	0.43
12:J:142:VAL:HG12	12:J:142:VAL:O	2.18	0.43
16:N:91:ILE:CD1	16:N:125:ILE:HD12	2.48	0.43
20:S:193:VAL:HG11	20:S:202:TRP:CH2	2.54	0.43
6:A:239:PHE:CE1	6:A:656:ILE:HD11	2.53	0.43
6:A:796:ASN:HD22	6:A:858:LYS:HG3	1.82	0.43
6:A:1027:LYS:O	6:A:1145:MET:HE1	2.18	0.43
6:A:1375:LEU:CD1	6:A:1614:ILE:HD13	2.49	0.43
9:C:78:MET:HE3	9:C:78:MET:HA	1.99	0.43
9:C:225:THR:HG21	9:C:252:LEU:CD2	2.48	0.43
13:K:35:ALA:CB	20:S:158:LYS:HE3	2.48	0.43
16:N:67:GLN:HB3	16:N:120:LEU:HD23	2.00	0.43
25:f:36:THR:HG21	25:f:60:VAL:HG22	2.00	0.43
9:C:335:SER:HB2	9:C:336:ILE:HD12	1.99	0.43
11:H:350:MET:HE2	11:H:357:TRP:CE2	2.53	0.43
16:N:71:CYS:HB3	16:N:74:CYS:HB2	2.00	0.43
20:S:92:LEU:C	20:S:92:LEU:HD12	2.43	0.43
1:U:79:C:H3'	1:U:80:G:C5'	2.49	0.43
6:A:1085:LYS:O	6:A:1088:VAL:HG13	2.18	0.43
11:H:381:LEU:HD21	11:H:419:PHE:CA	2.49	0.43
16:N:36:ILE:HD11	16:N:75:MET:HE1	1.99	0.43
6:A:834:ILE:CD1	6:A:845:VAL:HG23	2.49	0.43
7:D:11:TYR:CE1	10:G:12:LEU:HD21	2.54	0.43
9:C:888:ILE:HG23	9:C:902:VAL:HG23	2.00	0.43
14:L:73:ILE:HG23	14:L:77:LEU:HD23	2.00	0.43
15:M:250:MET:SD	16:N:139:LEU:HD21	2.59	0.43
6:A:954:ILE:HG23	6:A:991:THR:HG23	2.00	0.43
15:M:247:LEU:HA	15:M:250:MET:HG2	1.99	0.43
17:O:211:ILE:O	20:S:83:ARG:NH2	2.52	0.43
26:g:28:ILE:HG22	26:g:41:ASP:HB3	2.01	0.43
6:A:136:PRO:HB3	6:A:562:ILE:HD13	2.01	0.43
9:C:94:VAL:HG12	12:J:154:TRP:CZ2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:905:GLN:HE22	9:C:936:ILE:HD13	1.84	0.43
20:S:72:ALA:HB1	20:S:88:PHE:CZ	2.54	0.43
6:A:1347:ARG:HD2	6:A:1447:TRP:CD2	2.54	0.43
6:A:1387:VAL:HG12	6:A:1610:TRP:CD2	2.53	0.43
9:C:78:MET:SD	9:C:78:MET:N	2.92	0.43
9:C:242:VAL:HG22	9:C:277:LEU:HD11	2.01	0.43
9:C:381:LEU:HA	9:C:384:ILE:HD12	1.99	0.43
13:K:127:VAL:HG13	16:N:31:GLY:O	2.18	0.43
26:g:56:GLN:C	26:g:57:LEU:HD22	2.43	0.43
1:U:105:A:H2'	1:U:106:A:C8	2.54	0.42
4:Z:26:G:C2	5:V:59:A:C5	3.07	0.42
6:A:305:LEU:HD22	9:C:390:SER:HA	2.01	0.42
6:A:785:HIS:CE1	13:K:168:ALA:HB2	2.54	0.42
6:A:1737:GLN:HE21	6:A:1737:GLN:HA	1.84	0.42
9:C:861:ILE:HA	9:C:907:PRO:HA	2.01	0.42
17:O:211:ILE:HD12	20:S:48:ARG:CZ	2.49	0.42
25:f:16:LYS:N	25:f:17:PRO:CD	2.81	0.42
6:A:556:TYR:CG	13:K:120:ASP:HB3	2.54	0.42
6:A:1089:VAL:HG22	6:A:1098:VAL:HG22	2.01	0.42
9:C:599:THR:HG23	9:C:599:THR:O	2.18	0.42
1:U:74:U:O2	1:U:78:A:C2	2.72	0.42
6:A:139:LEU:HD13	6:A:193:TYR:CD2	2.55	0.42
6:A:852:LEU:HD23	6:A:978:ILE:HD11	2.01	0.42
7:D:49:MET:HE3	7:D:58:ILE:HD11	2.01	0.42
9:C:104:THR:HG23	9:C:105:ILE:HG23	2.00	0.42
9:C:791:TYR:O	9:C:791:TYR:CG	2.72	0.42
10:G:51:LYS:O	10:G:54:VAL:HG12	2.19	0.42
12:J:164:MET:HE1	12:J:199:SER:CB	2.47	0.42
12:J:200:VAL:HG22	12:J:227:VAL:HB	2.01	0.42
16:N:88:ASP:O	16:N:91:ILE:HG23	2.20	0.42
17:O:211:ILE:CD1	20:S:48:ARG:HB2	2.49	0.42
19:R:13:GLY:O	19:R:15:SER:N	2.52	0.42
20:S:155:LEU:C	20:S:155:LEU:HD23	2.44	0.42
24:e:27:VAL:HG22	24:e:92:SER:HB2	2.00	0.42
6:A:1275:MET:HE1	6:A:1299:LYS:CD	2.48	0.42
9:C:132:ARG:NH1	23:d:13:GLU:O	2.53	0.42
9:C:710:VAL:HG22	9:C:820:LEU:HD23	2.01	0.42
14:L:119:THR:HG22	14:L:120:CYS:N	2.34	0.42
16:N:67:GLN:HA	16:N:119:LYS:HA	2.02	0.42
21:T:119:ALA:HB1	21:T:128:ILE:CB	2.50	0.42
25:f:74:ARG:NH1	28:j:65:CYS:SG	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:30:A:H2'	1:U:31:G:O4'	2.20	0.42
5:V:86:G:C2	5:V:87:U:H1'	2.54	0.42
6:A:172:ILE:HG23	6:A:629:MET:CG	2.49	0.42
6:A:179:MET:HE2	6:A:704:TRP:CH2	2.54	0.42
9:C:605:ILE:HD12	9:C:652:MET:HG3	2.01	0.42
1:U:23:C:O2	1:U:23:C:O4'	2.37	0.42
5:V:55:G:N7	17:O:35:LYS:HB3	2.35	0.42
6:A:376:ARG:HG3	9:C:909:ILE:HG21	2.01	0.42
6:A:719:ILE:HB	6:A:720:PRO:HD2	2.01	0.42
6:A:1342:LEU:HD23	6:A:1360:LEU:HD21	2.02	0.42
6:A:1357:LEU:HD11	11:H:303:LEU:CD2	2.49	0.42
9:C:470:ALA:HB2	9:C:488:ILE:HA	2.02	0.42
9:C:472:VAL:HG21	9:C:567:ILE:HG21	2.01	0.42
2:E:-3:A:H2'	2:E:-2:A:O4'	2.19	0.42
4:Z:38:U:OP2	6:A:1643:ILE:HD11	2.20	0.42
6:A:1064:THR:HG22	17:O:81:PRO:HD2	2.02	0.42
6:A:1369:ASN:O	6:A:1373:LEU:N	2.46	0.42
12:J:114:ARG:HB3	13:K:48:GLN:HE22	1.85	0.42
6:A:218:SER:O	6:A:221:TRP:HB3	2.20	0.42
6:A:644:VAL:HG22	6:A:648:GLN:HB2	2.02	0.42
16:N:259:GLY:O	16:N:263:VAL:HG23	2.20	0.42
12:J:183:MET:HE2	12:J:202:GLU:CB	2.50	0.42
13:K:120:ASP:OD2	13:K:123:LEU:HD13	2.20	0.42
15:M:249:MET:SD	16:N:86:LEU:HD13	2.60	0.42
24:e:34:GLN:NE2	24:e:37:ILE:HD12	2.34	0.42
5:V:36:U:O2	5:V:36:U:C2'	2.68	0.42
6:A:164:ALA:CB	6:A:578:MET:HE3	2.50	0.42
6:A:929:LEU:HD12	6:A:1589:LYS:CG	2.50	0.42
9:C:400:LEU:HD12	9:C:408:LEU:HD21	2.02	0.42
15:M:114:ARG:CD	15:M:127:ILE:HG21	2.50	0.42
17:O:22:LYS:HB2	17:O:56:LEU:HD12	2.02	0.42
6:A:756:LEU:CD1	18:P:12:ARG:HD3	2.50	0.41
9:C:418:GLN:HB3	9:C:419:PRO:HD3	2.02	0.41
12:J:334:TRP:CD1	12:J:334:TRP:N	2.88	0.41
16:N:16:CYS:CB	16:N:71:CYS:SG	3.08	0.41
16:N:25:MET:HB3	16:N:46:PHE:HB3	2.01	0.41
20:S:140:LEU:HD21	20:S:155:LEU:HD22	2.01	0.41
1:U:38:A:H2'	1:U:39:U:O4'	2.20	0.41
5:V:61:C:H2'	5:V:62:A:O4'	2.19	0.41
6:A:756:LEU:HD11	18:P:12:ARG:HD3	2.03	0.41
6:A:1169:TYR:CE2	6:A:1262:MET:HE2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:225:THR:HG21	9:C:252:LEU:HD21	2.02	0.41
9:C:608:GLN:HE21	9:C:641:GLU:HG2	1.85	0.41
12:J:276:PRO:HB2	13:K:63:ILE:HD12	2.02	0.41
15:M:48:VAL:HG22	15:M:220:GLY:N	2.36	0.41
15:M:247:LEU:HA	15:M:250:MET:CG	2.51	0.41
5:V:74:U:C5	12:J:221:TYR:CD2	3.07	0.41
6:A:168:LEU:N	6:A:169:PRO:HD2	2.35	0.41
21:T:397:ASN:O	21:T:400:ALA:HB3	2.20	0.41
9:C:273:LEU:HA	9:C:277:LEU:HD12	2.02	0.41
9:C:621:ALA:CB	9:C:664:ALA:HB2	2.48	0.41
22:b:12:LEU:HD12	22:b:15:LEU:HD11	2.02	0.41
6:A:565:VAL:CG1	6:A:637:VAL:HG22	2.51	0.41
7:D:51:CYS:SG	7:D:88:CYS:CB	3.08	0.41
24:e:88:THR:HG22	24:e:89:LEU:HD12	2.01	0.41
6:A:1316:ILE:HD13	6:A:1316:ILE:HA	1.94	0.41
6:A:1749:SER:O	6:A:1752:VAL:HG22	2.20	0.41
11:H:334:LEU:HD12	11:H:380:GLN:HB3	2.02	0.41
6:A:252:GLU:HA	6:A:255:ILE:HD12	2.02	0.41
11:H:330:ILE:HD12	11:H:387:PHE:HE2	1.86	0.41
6:A:1609:TRP:CE3	6:A:1823:LEU:HD13	2.56	0.41
9:C:314:ALA:CB	9:C:321:THR:HG22	2.50	0.41
11:H:292:LYS:HD3	11:H:328:ILE:HD11	2.01	0.41
15:M:156:ILE:HG21	15:M:175:TYR:CE1	2.55	0.41
6:A:480:TYR:OH	9:C:318:LEU:HD21	2.20	0.41
6:A:562:ILE:HG22	6:A:563:ASP:O	2.21	0.41
6:A:666:ILE:HG22	6:A:673:VAL:HG21	2.03	0.41
6:A:758:LEU:HD23	6:A:759:ARG:N	2.36	0.41
6:A:831:ARG:CD	6:A:848:ASN:HD21	2.34	0.41
6:A:937:LEU:HD13	6:A:1590:LEU:HD21	2.01	0.41
6:A:976:GLN:HG3	6:A:1310:LYS:HB3	2.02	0.41
6:A:1014:LYS:N	6:A:1015:PRO:CD	2.84	0.41
9:C:287:LYS:HE3	9:C:291:ILE:HD11	2.03	0.41
12:J:364:LEU:C	12:J:364:LEU:HD23	2.46	0.41
13:K:112:ILE:CD1	16:N:25:MET:HE3	2.50	0.41
16:N:82:ILE:HG22	16:N:86:LEU:HB2	2.02	0.41
5:V:22:G:H2'	5:V:23:G:O4'	2.21	0.41
6:A:370:ILE:HD12	6:A:1418:THR:OG1	2.21	0.40
6:A:390:LEU:N	9:C:653:ASP:OD1	2.54	0.40
6:A:831:ARG:HD3	6:A:848:ASN:HD21	1.86	0.40
6:A:1011:ASN:HD22	6:A:1144:PHE:HA	1.86	0.40
6:A:1969:MET:HE1	6:A:1978:VAL:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:C:152:LEU:HD11	9:C:319:GLY:HA2	2.02	0.40
9:C:632:VAL:HG12	9:C:634:ILE:HG13	2.03	0.40
9:C:677:PHE:HB3	9:C:857:LEU:HD22	2.03	0.40
10:G:4:ASN:C	10:G:4:ASN:HD22	2.29	0.40
20:S:189:TYR:O	20:S:192:TYR:HB3	2.21	0.40
25:f:71:ILE:HG22	28:j:105:LEU:HB3	2.04	0.40
1:U:45:A:N6	1:U:74:U:H3	2.19	0.40
6:A:1620:TYR:CD2	6:A:1621:VAL:HG13	2.56	0.40
9:C:223:ASP:O	9:C:227:VAL:HG23	2.21	0.40
9:C:749:LYS:O	9:C:753:THR:HG23	2.21	0.40
17:O:211:ILE:CD1	20:S:44:ARG:HG3	2.50	0.40
1:U:45:A:OP1	9:C:108:GLN:O	2.40	0.40
6:A:1756:PHE:CZ	6:A:1760:THR:HG21	2.56	0.40
9:C:234:LEU:HD13	9:C:439:ILE:HG23	2.03	0.40
9:C:264:CYS:SG	9:C:312:ILE:HD11	2.61	0.40
9:C:561:ILE:O	9:C:562:VAL:HG13	2.22	0.40
13:K:75:GLN:HA	13:K:78:VAL:HG12	2.03	0.40
16:N:139:LEU:HD13	16:N:139:LEU:C	2.47	0.40
4:Z:1102:C:O2	4:Z:1102:C:C2'	2.69	0.40
5:V:86:G:C2	20:S:57:TYR:CE2	3.10	0.40
6:A:175:LEU:HD22	6:A:629:MET:CE	2.52	0.40
6:A:766:ILE:HG21	6:A:782:ILE:HD13	2.04	0.40
6:A:1223:GLY:HA2	6:A:1248:VAL:HG11	2.02	0.40
6:A:1392:LYS:HB3	6:A:1601:ILE:HD11	2.03	0.40
6:A:1603:ASN:HD22	6:A:1604:ARG:N	2.19	0.40
6:A:1881:THR:HG21	6:A:1920:LEU:HD23	2.02	0.40
9:C:241:VAL:HG22	9:C:267:ILE:HG23	2.04	0.40
9:C:655:LEU:C	9:C:655:LEU:HD23	2.46	0.40
12:J:345:PHE:CE2	12:J:364:LEU:HD22	2.57	0.40
6:A:1054:LEU:HD13	6:A:1121:ILE:HG21	2.03	0.40
6:A:1491:ILE:HD13	6:A:1491:ILE:HA	1.97	0.40
12:J:198:PHE:CD1	12:J:239:ILE:HD13	2.57	0.40
12:J:321:PHE:CE1	12:J:336:LEU:CD2	3.05	0.40
15:M:109:LEU:HA	15:M:116:LYS:HG2	2.03	0.40
16:N:84:ILE:O	16:N:87:ARG:HG3	2.21	0.40
17:O:148:GLU:O	17:O:152:LEU:HD23	2.21	0.40
17:O:211:ILE:HD12	20:S:48:ARG:NE	2.36	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	
6	A	1916/2413 (79%)	1762 (92%)	143 (8%)	11 (1%)	21	54
7	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	6	33
8	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100
9	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	8	36
10	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	11	41
11	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	12	43
12	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	2	21
13	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	21	54
14	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	9	38
15	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	10	40
16	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	8	36
17	O	194/590 (33%)	173 (89%)	17 (9%)	4 (2%)	5	31
18	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	3	25
19	R	91/135 (67%)	80 (88%)	10 (11%)	1 (1%)	11	41
20	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	24	57
21	T	532/859 (62%)	504 (95%)	20 (4%)	8 (2%)	8	36
22	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
22	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	4	27
23	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	9	38
23	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
24	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
24	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	9	37
25	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	9	37
25	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
26	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
26	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	8	36
27	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
27	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	4	27
28	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
28	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
29	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	1	17
30	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
All	All	7089/10809 (66%)	6428 (91%)	577 (8%)	84 (1%)	13	40

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP
6	A	737	ARG
11	H	414	PRO
15	M	127	ILE
16	N	120	LEU
19	R	14	SER
21	T	477	PRO
21	T	481	ILE
21	T	616	PRO
29	W	76	ILE
27	l	98	PRO
26	r	68	ILE
6	A	588	LEU
6	A	1424	HIS
6	A	1639	PRO
6	A	1763	ASN
9	C	76	VAL
9	C	172	TRP
9	C	269	LYS
9	C	432	GLN
9	C	535	PRO
9	C	901	GLU
11	H	469	GLY
12	J	162	THR
12	J	245	ASP
12	J	277	VAL
12	J	328	THR
15	M	23	PRO

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Mol	Chain	Res	Type
17	O	81	PRO
18	P	9	LEU
29	W	122	ARG
22	k	81	VAL
6	A	1593	ALA
7	D	76	LEU
9	C	574	SER
11	H	445	LEU
12	J	442	TRP
14	L	38	SER
16	N	30	GLN
16	N	54	ASN
17	O	214	ASN
20	S	238	TRP
29	W	95	PRO
27	l	25	VAL
6	A	660	ILE
17	O	206	LYS
20	S	112	VAL
21	T	479	PRO
21	T	615	PHE
29	W	68	PRO
29	W	94	LEU
29	W	129	LEU
22	k	6	VAL
6	A	457	ASP
6	A	1491	ILE
7	D	34	MET
9	C	100	LEU
9	C	459	PRO
10	G	41	VAL
12	J	310	SER
12	J	444	PRO
15	M	4	TRP
17	O	216	ASP
21	T	443	PRO
9	C	137	GLY
9	C	807	PRO
11	H	303	LEU
12	J	226	GLY
21	T	391	LEU
12	J	137	GLY

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Mol	Chain	Res	Type
9	C	185	ILE
9	C	301	GLY
12	J	279	PRO
13	K	146	VAL
14	L	117	GLY
25	f	15	PRO
24	p	74	GLY
12	J	443	ASN
21	T	37	ILE
29	W	56	ILE
29	W	98	VAL
6	A	774	ILE
12	J	272	VAL
23	d	82	PRO

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	
6	A	1701/2182 (78%)	1567 (92%)	134 (8%)	11	36
7	D	100/256 (39%)	90 (90%)	10 (10%)	7	28
8	F	26/163 (16%)	25 (96%)	1 (4%)	29	53
9	C	722/910 (79%)	662 (92%)	60 (8%)	10	34
10	G	89/216 (41%)	83 (93%)	6 (7%)	15	41
11	H	185/552 (34%)	167 (90%)	18 (10%)	8	29
12	J	283/398 (71%)	248 (88%)	35 (12%)	4	21
13	K	143/328 (44%)	119 (83%)	24 (17%)	2	13
14	L	138/141 (98%)	128 (93%)	10 (7%)	13	39
15	M	212/295 (72%)	195 (92%)	17 (8%)	11	36
16	N	194/332 (58%)	170 (88%)	24 (12%)	4	21
17	O	174/526 (33%)	156 (90%)	18 (10%)	7	27
18	P	26/152 (17%)	22 (85%)	4 (15%)	2	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	R	24/121 (20%)	20 (83%)	4 (17%)	2	13
20	S	208/633 (33%)	184 (88%)	24 (12%)	5	23
22	b	70/176 (40%)	70 (100%)	0	100	100
23	d	69/89 (78%)	67 (97%)	2 (3%)	37	58
24	e	65/83 (78%)	61 (94%)	4 (6%)	16	42
25	f	63/77 (82%)	61 (97%)	2 (3%)	34	56
26	g	58/66 (88%)	56 (97%)	2 (3%)	32	55
27	h	77/129 (60%)	77 (100%)	0	100	100
28	j	79/103 (77%)	76 (96%)	3 (4%)	29	53
All	All	4706/7928 (59%)	4304 (92%)	402 (8%)	12	33

All (402) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	128	TYR
6	A	145	THR
6	A	149	MET
6	A	153	MET
6	A	165	LEU
6	A	173	LEU
6	A	175	LEU
6	A	192	LEU
6	A	204	GLU
6	A	205	THR
6	A	225	ARG
6	A	228	LYS
6	A	233	HIS
6	A	237	MET
6	A	257	ASN
6	A	261	LEU
6	A	265	ASN
6	A	284	ARG
6	A	286	LEU
6	A	296	THR
6	A	297	SER
6	A	330	LEU
6	A	340	LYS
6	A	353	GLU
6	A	355	LEU

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Mol	Chain	Res	Type
6	A	405	ASN
6	A	412	GLN
6	A	425	ASP
6	A	469	ILE
6	A	479	LEU
6	A	493	MET
6	A	547	LEU
6	A	555	LYS
6	A	571	LEU
6	A	572	CYS
6	A	577	ASN
6	A	583	ILE
6	A	588	LEU
6	A	591	LEU
6	A	600	LYS
6	A	605	LEU
6	A	615	LEU
6	A	630	LYS
6	A	631	LEU
6	A	649	LEU
6	A	663	LEU
6	A	674	MET
6	A	690	LYS
6	A	710	VAL
6	A	722	LEU
6	A	726	ILE
6	A	737	ARG
6	A	743	LYS
6	A	744	THR
6	A	749	ARG
6	A	750	LEU
6	A	755	ASP
6	A	758	LEU
6	A	760	ASN
6	A	770	MET
6	A	775	ARG
6	A	778	LYS
6	A	783	LEU
6	A	785	HIS
6	A	794	LYS
6	A	811	ILE
6	A	821	ASP

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Mol	Chain	Res	Type
6	A	832	GLU
6	A	846	LYS
6	A	852	LEU
6	A	919	LEU
6	A	922	VAL
6	A	944	TYR
6	A	971	MET
6	A	972	MET
6	A	1004	ASP
6	A	1019	GLU
6	A	1020	ILE
6	A	1024	LEU
6	A	1078	ILE
6	A	1082	ILE
6	A	1099	ASN
6	A	1103	LEU
6	A	1125	LEU
6	A	1165	LEU
6	A	1168	ILE
6	A	1182	LEU
6	A	1212	ARG
6	A	1217	ARG
6	A	1277	GLU
6	A	1288	LEU
6	A	1315	ARG
6	A	1317	ARG
6	A	1323	SER
6	A	1326	THR
6	A	1327	THR
6	A	1337	THR
6	A	1338	SER
6	A	1346	PHE
6	A	1347	ARG
6	A	1354	GLU
6	A	1356	LEU
6	A	1373	LEU
6	A	1378	LYS
6	A	1379	MET
6	A	1382	ARG
6	A	1394	LEU
6	A	1429	MET
6	A	1433	ASP

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Mol	Chain	Res	Type
6	A	1434	GLU
6	A	1436	LEU
6	A	1442	ARG
6	A	1491	ILE
6	A	1513	GLU
6	A	1515	LYS
6	A	1520	GLU
6	A	1571	GLU
6	A	1586	GLN
6	A	1589	LYS
6	A	1590	LEU
6	A	1594	GLN
6	A	1598	LEU
6	A	1600	GLN
6	A	1603	ASN
6	A	1644	SER
6	A	1647	GLN
6	A	1668	ILE
6	A	1707	HIS
6	A	1708	GLU
6	A	1737	GLN
6	A	1742	ASP
6	A	1803	ARG
6	A	2048	TRP
6	A	2074	LEU
7	D	3	GLU
7	D	8	ASN
7	D	25	ARG
7	D	47	PHE
7	D	49	MET
7	D	63	LYS
7	D	71	LEU
7	D	79	ILE
7	D	99	THR
7	D	114	ARG
8	F	20	ARG
9	C	76	VAL
9	C	78	MET
9	C	92	GLU
9	C	100	LEU
9	C	103	HIS
9	C	109	LEU

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Mol	Chain	Res	Type
9	C	124	LEU
9	C	132	ARG
9	C	139	ILE
9	C	153	LEU
9	C	156	ASP
9	C	211	ASN
9	C	219	VAL
9	C	229	LEU
9	C	234	LEU
9	C	255	GLN
9	C	261	VAL
9	C	272	ARG
9	C	273	LEU
9	C	315	SER
9	C	358	ASN
9	C	381	LEU
9	C	400	LEU
9	C	401	ARG
9	C	424	VAL
9	C	431	GLN
9	C	447	GLU
9	C	453	THR
9	C	458	ILE
9	C	468	LEU
9	C	475	THR
9	C	534	THR
9	C	545	LEU
9	C	562	VAL
9	C	572	ILE
9	C	576	THR
9	C	590	LYS
9	C	602	VAL
9	C	610	LEU
9	C	619	LEU
9	C	625	ILE
9	C	760	LEU
9	C	768	PHE
9	C	774	LEU
9	C	784	SER
9	C	790	LYS
9	C	791	TYR
9	C	794	GLN

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Mol	Chain	Res	Type
9	C	803	VAL
9	C	830	ASN
9	C	837	GLN
9	C	851	LEU
9	C	856	ILE
9	C	861	ILE
9	C	902	VAL
9	C	927	MET
9	C	965	ASP
9	C	970	THR
9	C	971	ARG
9	C	989	LEU
10	G	18	GLN
10	G	28	ASP
10	G	31	ARG
10	G	33	GLN
10	G	74	GLN
10	G	78	LEU
11	H	297	LEU
11	H	307	GLU
11	H	313	LEU
11	H	314	LYS
11	H	317	ILE
11	H	334	LEU
11	H	348	GLU
11	H	357	TRP
11	H	363	GLU
11	H	373	ILE
11	H	391	LEU
11	H	396	PHE
11	H	421	LYS
11	H	440	LEU
11	H	468	ILE
11	H	470	LEU
11	H	473	LEU
11	H	477	MET
12	J	139	LEU
12	J	143	ARG
12	J	147	ILE
12	J	148	ASP
12	J	151	ASP
12	J	156	ILE

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Mol	Chain	Res	Type
12	J	183	MET
12	J	194	HIS
12	J	197	LEU
12	J	202	GLU
12	J	215	GLN
12	J	218	ARG
12	J	224	LEU
12	J	225	SER
12	J	247	VAL
12	J	248	ILE
12	J	257	ILE
12	J	269	ILE
12	J	274	CYS
12	J	275	THR
12	J	284	SER
12	J	286	THR
12	J	290	VAL
12	J	295	VAL
12	J	303	VAL
12	J	314	THR
12	J	329	ASP
12	J	334	TRP
12	J	336	LEU
12	J	356	LEU
12	J	377	ASP
12	J	387	LEU
12	J	389	THR
12	J	402	VAL
12	J	423	ILE
13	K	33	GLN
13	K	36	LYS
13	K	40	LEU
13	K	48	GLN
13	K	52	GLU
13	K	62	GLU
13	K	66	CYS
13	K	70	THR
13	K	77	LEU
13	K	81	LYS
13	K	87	ASN
13	K	105	LEU
13	K	106	LEU

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Mol	Chain	Res	Type
13	K	111	HIS
13	K	112	ILE
13	K	147	LEU
13	K	172	TRP
13	K	182	LEU
13	K	183	GLU
13	K	197	ILE
13	K	203	LYS
13	K	204	LEU
13	K	217	GLN
13	K	218	GLU
14	L	3	ARG
14	L	37	LYS
14	L	54	GLN
14	L	59	ARG
14	L	60	SER
14	L	61	ARG
14	L	71	LYS
14	L	84	GLU
14	L	85	LYS
14	L	142	PHE
15	M	5	ARG
15	M	10	LYS
15	M	18	LEU
15	M	26	THR
15	M	38	SER
15	M	44	ASN
15	M	114	ARG
15	M	116	LYS
15	M	127	ILE
15	M	132	LYS
15	M	135	LYS
15	M	136	THR
15	M	149	LYS
15	M	172	ARG
15	M	187	LYS
15	M	245	GLU
15	M	251	VAL
16	N	20	GLU
16	N	22	ASN
16	N	30	GLN
16	N	32	SER

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Mol	Chain	Res	Type
16	N	35	LYS
16	N	36	ILE
16	N	39	LEU
16	N	43	LEU
16	N	48	THR
16	N	51	ARG
16	N	55	ILE
16	N	72	GLN
16	N	91	ILE
16	N	93	LEU
16	N	94	VAL
16	N	109	MET
16	N	117	ASN
16	N	120	LEU
16	N	135	ILE
16	N	139	LEU
16	N	214	ILE
16	N	216	GLU
16	N	254	GLN
16	N	321	GLN
17	O	40	LEU
17	O	44	THR
17	O	46	ARG
17	O	53	ASN
17	O	73	LEU
17	O	91	MET
17	O	93	ARG
17	O	156	ARG
17	O	170	LYS
17	O	184	GLU
17	O	188	ARG
17	O	189	ARG
17	O	192	LYS
17	O	196	ILE
17	O	204	LYS
17	O	205	LYS
17	O	206	LYS
17	O	247	LYS
18	P	8	GLN
18	P	9	LEU
18	P	16	LYS
18	P	29	ARG

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Mol	Chain	Res	Type
19	R	6	ILE
19	R	8	LEU
19	R	15	SER
19	R	16	THR
20	S	60	ARG
20	S	67	GLN
20	S	77	GLU
20	S	78	GLN
20	S	87	ILE
20	S	92	LEU
20	S	117	HIS
20	S	143	GLU
20	S	144	GLU
20	S	152	VAL
20	S	156	TYR
20	S	158	LYS
20	S	173	VAL
20	S	188	ILE
20	S	189	TYR
20	S	209	GLU
20	S	216	GLU
20	S	224	LEU
20	S	226	ILE
20	S	234	ASN
20	S	257	GLN
20	S	260	TYR
20	S	263	SER
20	S	266	LEU
23	d	10	LEU
23	d	20	SER
24	e	16	CYS
24	e	25	THR
24	e	79	LYS
24	e	81	LEU
25	f	36	THR
25	f	79	LEU
26	g	18	ASN
26	g	71	LEU
28	j	48	LEU
28	j	49	ARG
28	j	82	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92)

such sidechains are listed below:

Mol	Chain	Res	Type
6	A	194	HIS
6	A	216	GLN
6	A	257	ASN
6	A	310	ASN
6	A	326	ASN
6	A	344	ASN
6	A	392	ASN
6	A	412	GLN
6	A	508	GLN
6	A	617	ASN
6	A	638	GLN
6	A	643	ASN
6	A	658	ASN
6	A	692	ASN
6	A	705	GLN
6	A	733	GLN
6	A	760	ASN
6	A	830	ASN
6	A	848	ASN
6	A	946	ASN
6	A	948	HIS
6	A	961	GLN
6	A	1086	ASN
6	A	1368	GLN
6	A	1449	ASN
6	A	1522	ASN
6	A	1603	ASN
6	A	1615	ASN
6	A	1737	GLN
6	A	2018	ASN
7	D	8	ASN
9	C	108	GLN
9	C	128	ASN
9	C	143	HIS
9	C	158	HIS
9	C	167	ASN
9	C	180	ASN
9	C	260	ASN
9	C	289	ASN
9	C	290	HIS
9	C	358	ASN
9	C	418	GLN

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Mol	Chain	Res	Type
9	C	423	HIS
9	C	426	GLN
9	C	432	GLN
9	C	554	HIS
9	C	608	GLN
9	C	693	ASN
9	C	776	ASN
9	C	837	GLN
9	C	929	GLN
10	G	19	GLN
10	G	33	GLN
11	H	247	ASN
11	H	390	HIS
12	J	194	HIS
12	J	214	ASN
12	J	273	GLN
12	J	280	GLN
12	J	317	HIS
12	J	360	GLN
13	K	33	GLN
13	K	48	GLN
13	K	50	ASN
13	K	210	ASN
14	L	46	ASN
14	L	58	GLN
14	L	115	ASN
15	M	44	ASN
16	N	22	ASN
17	O	26	GLN
17	O	72	GLN
20	S	61	ASN
20	S	78	GLN
20	S	79	HIS
20	S	167	ASN
20	S	179	GLN
20	S	200	GLN
20	S	212	HIS
20	S	214	ASN
22	b	40	HIS
22	b	46	ASN
23	d	17	HIS
24	e	15	ASN

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Mol	Chain	Res	Type
24	e	34	GLN
25	f	25	HIS
26	g	18	ASN
26	g	20	ASN
26	g	66	ASN
27	h	86	ASN
28	j	28	HIS
28	j	64	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	U	138/179 (77%)	68 (49%)	13 (9%)
2	E	15/16 (93%)	10 (66%)	2 (13%)
3	I	31/76 (40%)	15 (48%)	0
4	Z	162/1175 (13%)	58 (35%)	11 (6%)
5	V	96/112 (85%)	35 (36%)	5 (5%)
All	All	442/1558 (28%)	186 (42%)	31 (7%)

All (186) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	13	A
1	U	14	G
1	U	15	A
1	U	16	U
1	U	18	A
1	U	20	U
1	U	22	G
1	U	23	C
1	U	24	G
1	U	25	G
1	U	26	A
1	U	27	G
1	U	28	G
1	U	31	G
1	U	33	U
1	U	34	C
1	U	36	A
1	U	39	U
1	U	40	C

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Mol	Chain	Res	Type
1	U	42	A
1	U	43	G
1	U	44	A
1	U	48	G
1	U	50	G
1	U	53	C
1	U	63	C
1	U	65	U
1	U	67	U
1	U	68	A
1	U	70	A
1	U	71	A
1	U	74	U
1	U	75	A
1	U	76	U
1	U	77	A
1	U	78	A
1	U	79	C
1	U	80	G
1	U	81	A
1	U	82	A
1	U	84	A
1	U	87	G
1	U	89	U
1	U	92	U
1	U	94	C
1	U	96	U
1	U	97	U
1	U	101	C
1	U	104	G
1	U	107	C
1	U	108	C
1	U	109	A
1	U	112	C
1	U	113	G
1	U	115	G
1	U	116	U
1	U	119	U
1	U	121	U
1	U	126	A
1	U	130	A
1	U	133	C

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Mol	Chain	Res	Type
1	U	134	A
1	U	135	G
1	U	145	U
1	U	170	U
1	U	171	U
1	U	172	U
1	U	173	U
2	E	-14	A
2	E	-11	G
2	E	-10	A
2	E	-9	U
2	E	-8	C
2	E	-7	U
2	E	-6	A
2	E	-5	G
2	E	-4	A
2	E	-1	G
3	I	3	A
3	I	6	U
3	I	9	A
3	I	10	A
3	I	56	G
3	I	58	U
3	I	61	U
3	I	62	A
3	I	63	U
3	I	65	U
3	I	66	A
3	I	69	A
3	I	71	C
3	I	73	A
3	I	74	A
4	Z	5	A
4	Z	15	C
4	Z	16	U
4	Z	17	U
4	Z	18	U
4	Z	19	U
4	Z	20	G
4	Z	21	G
4	Z	25	A
4	Z	30	A

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Mol	Chain	Res	Type
4	Z	32	G
4	Z	33	U
4	Z	37	G
4	Z	40	U
4	Z	43	G
4	Z	46	C
4	Z	47	U
4	Z	63	U
4	Z	64	G
4	Z	67	A
4	Z	68	U
4	Z	81	C
4	Z	106	A
4	Z	108	A
4	Z	110	A
4	Z	112	A
4	Z	113	U
4	Z	114	U
4	Z	115	U
4	Z	116	U
4	Z	117	U
4	Z	119	G
4	Z	120	G
4	Z	141	A
4	Z	1094	G
4	Z	1096	C
4	Z	1098	C
4	Z	1099	G
4	Z	1100	A
4	Z	1101	C
4	Z	1102	C
4	Z	1103	C
4	Z	1104	U
4	Z	1106	G
4	Z	1107	C
4	Z	1108	A
4	Z	1120	G
4	Z	1123	C
4	Z	1124	U
4	Z	1125	U
4	Z	1126	G
4	Z	1139	G

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Mol	Chain	Res	Type
4	Z	1144	U
4	Z	1145	U
4	Z	1146	G
4	Z	1149	G
4	Z	1152	U
4	Z	1166	G
5	V	3	U
5	V	5	G
5	V	10	G
5	V	17	U
5	V	22	G
5	V	27	U
5	V	28	U
5	V	31	G
5	V	34	A
5	V	35	A
5	V	36	U
5	V	37	U
5	V	40	A
5	V	41	A
5	V	42	A
5	V	43	C
5	V	52	G
5	V	53	A
5	V	54	U
5	V	62	A
5	V	66	C
5	V	68	C
5	V	73	A
5	V	74	U
5	V	75	A
5	V	76	A
5	V	80	U
5	V	81	G
5	V	84	C
5	V	85	C
5	V	88	U
5	V	89	U
5	V	91	A
5	V	92	C
5	V	99	A

All (31) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	U	23	C
1	U	24	G
1	U	26	A
1	U	27	G
1	U	33	U
1	U	39	U
1	U	43	G
1	U	45	A
1	U	64	C
1	U	76	U
1	U	78	A
1	U	96	U
1	U	172	U
2	E	-10	A
2	E	-9	U
4	Z	16	U
4	Z	19	U
4	Z	20	G
4	Z	32	G
4	Z	112	A
4	Z	114	U
4	Z	115	U
4	Z	118	U
4	Z	1123	C
4	Z	1124	U
4	Z	1145	U
5	V	16	C
5	V	53	A
5	V	60	G
5	V	74	U
5	V	84	C

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 10 ligands modelled in this entry, 9 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	GTP	C	1101	-	33,34,34	1.09	3 (9%)	50,54,54	1.77	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
34	GTP	C	1101	-	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	C	1101	GTP	C5-C4	2.70	1.46	1.38
34	C	1101	GTP	C5-N7	-2.61	1.33	1.39
34	C	1101	GTP	C6-N1	-2.39	1.34	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	1101	GTP	C5-C4-N3	-5.96	118.91	128.39
34	C	1101	GTP	C2-N3-C4	5.05	121.00	112.30
34	C	1101	GTP	N9-C4-N3	4.57	135.08	125.95
34	C	1101	GTP	C6-C5-N7	3.18	136.08	130.29
34	C	1101	GTP	O6-C6-C5	-2.83	119.07	126.53
34	C	1101	GTP	C4-C5-N7	-2.33	106.97	110.67
34	C	1101	GTP	C5-C6-N1	2.28	119.06	113.25
34	C	1101	GTP	O2B-PB-O1B	2.05	121.97	112.44

There are no chirality outliers.

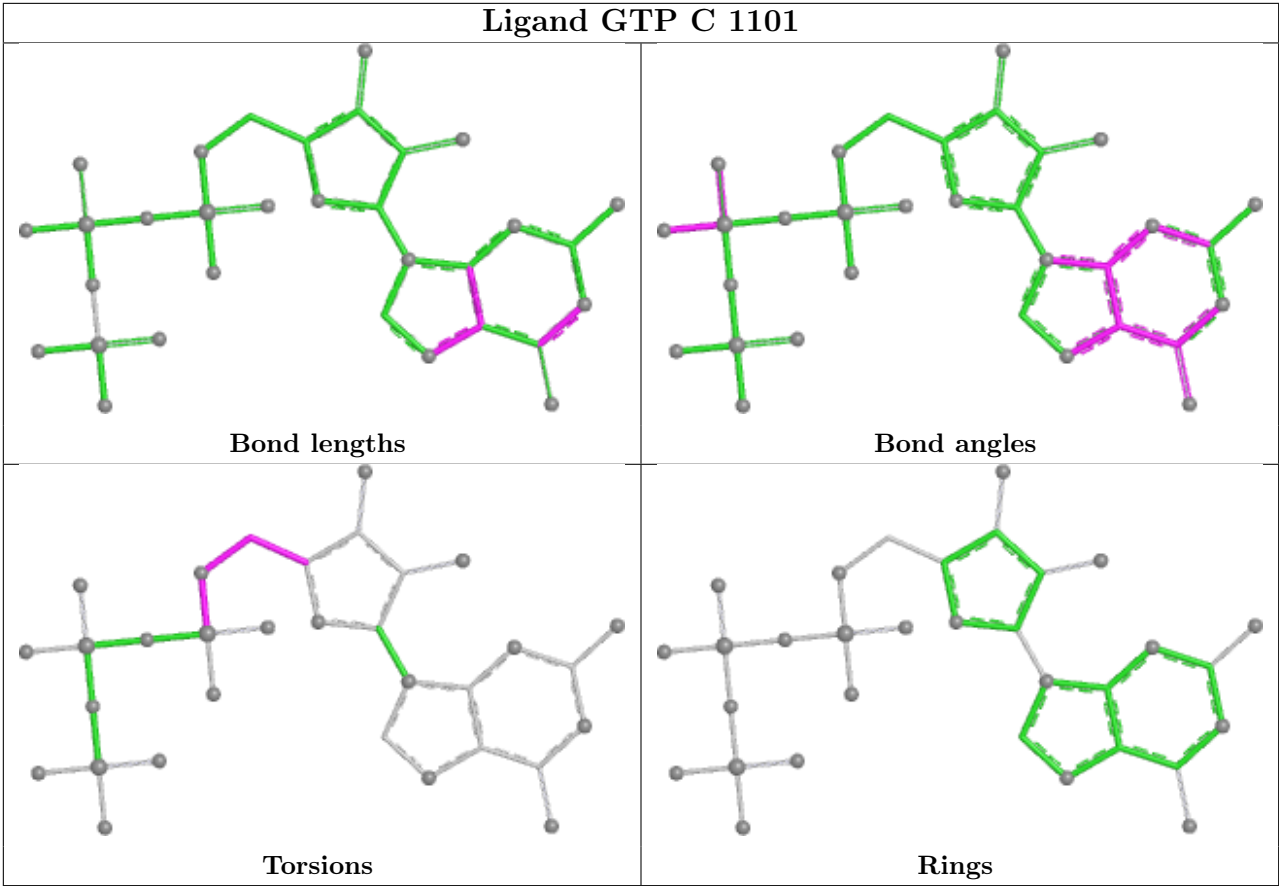
All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	C	1101	GTP	C5'-O5'-PA-O3A
34	C	1101	GTP	C5'-O5'-PA-O1A
34	C	1101	GTP	C3'-C4'-C5'-O5'
34	C	1101	GTP	O4'-C4'-C5'-O5'
34	C	1101	GTP	C4'-C5'-O5'-PA

There are no ring outliers.

No monomer is involved in short contacts.

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
31	x	4
21	T	2
19	R	1
5	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	54:UNK	C	55:UNK	N	111.76
1	x	110:UNK	C	111:UNK	N	53.94
1	x	36:UNK	C	37:UNK	N	49.39

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	87:UNK	C	88:UNK	N	31.03
1	T	419:LYS	C	420:SER	N	5.13
1	R	35:SER	C	36:GLN	N	4.69
1	V	92:C	O3'	93:A	P	3.22
1	T	431:ALA	C	432:ILE	N	3.17

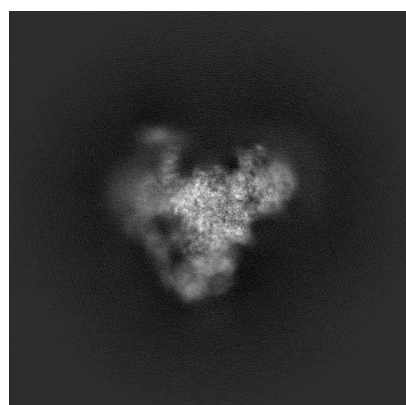
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4055. These allow visual inspection of the internal detail of the map and identification of artifacts.

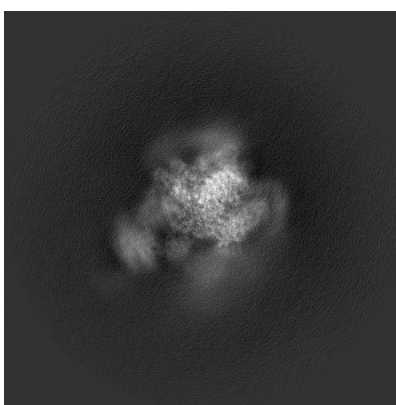
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

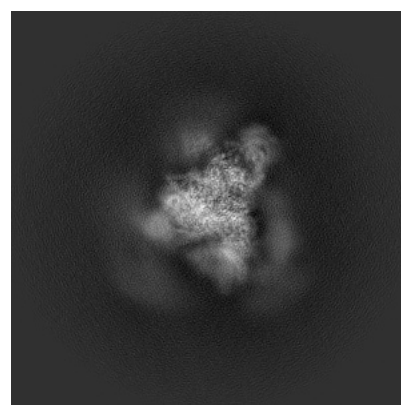
6.1.1 Primary map



X



Y

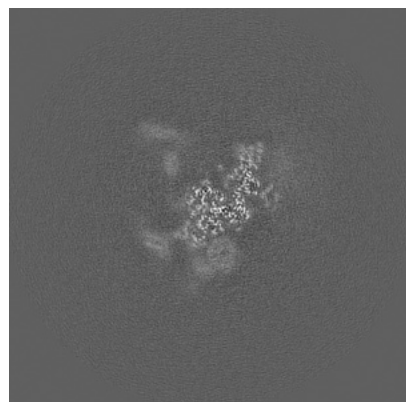


Z

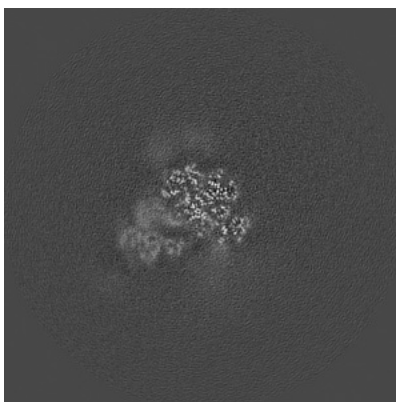
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

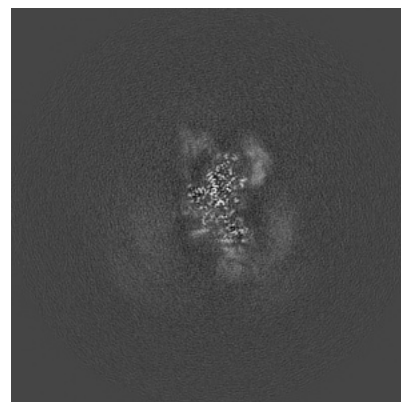
6.2.1 Primary map



X Index: 206



Y Index: 206

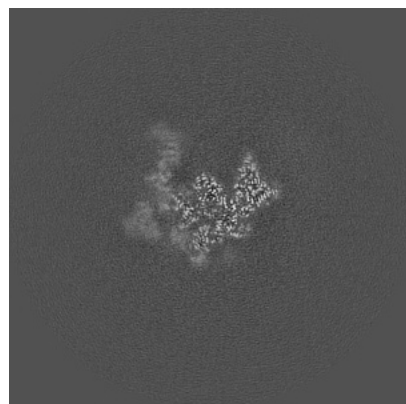


Z Index: 206

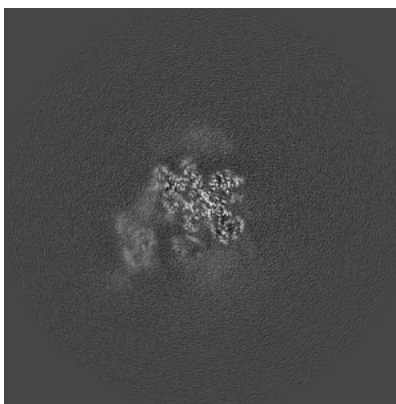
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

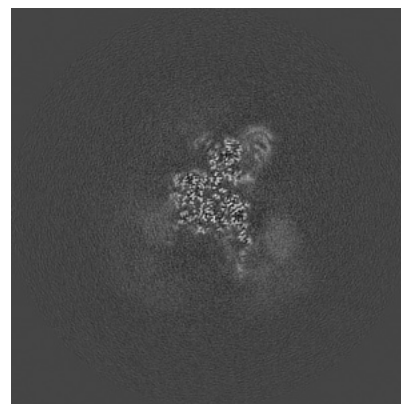
6.3.1 Primary map



X Index: 225



Y Index: 197

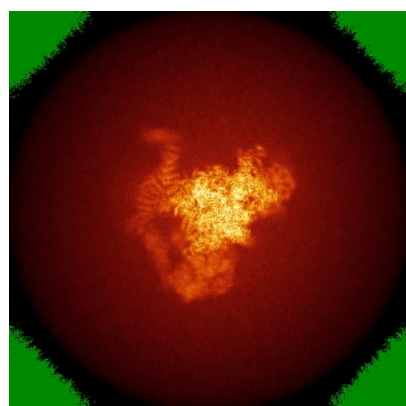


Z Index: 221

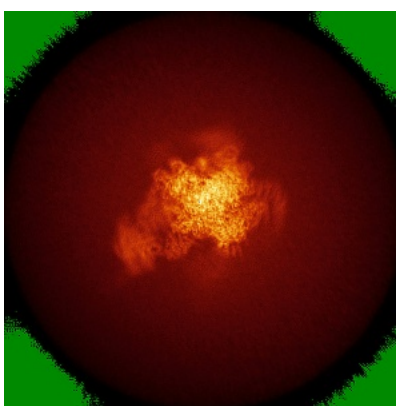
The images above show the largest variance slices of the map in three orthogonal directions.

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

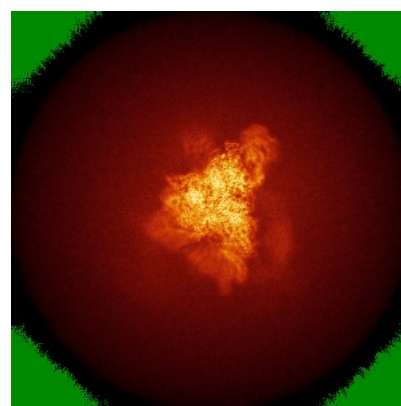
6.4.1 Primary map



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

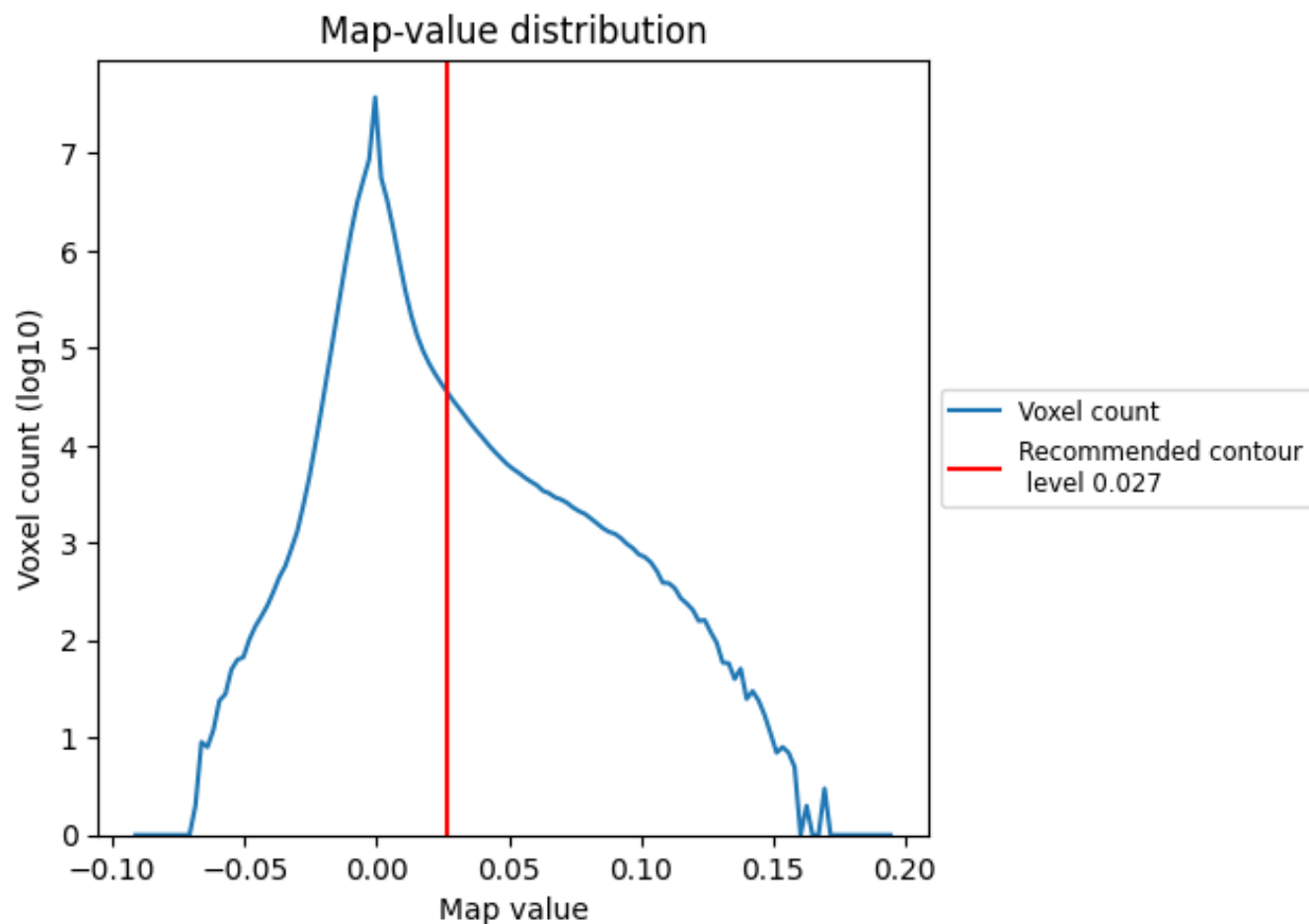
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

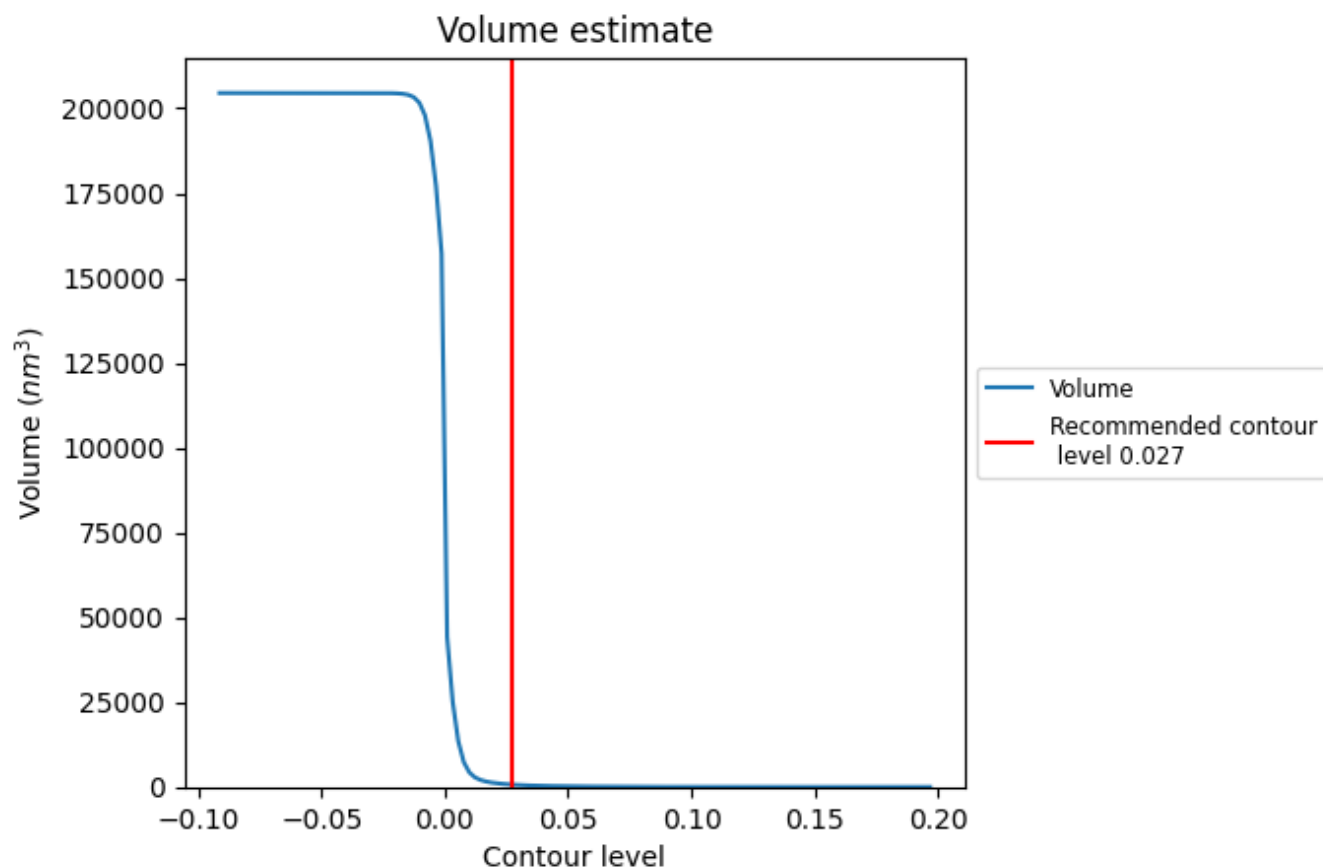
This section contains the results of statistical analysis of the map.

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.

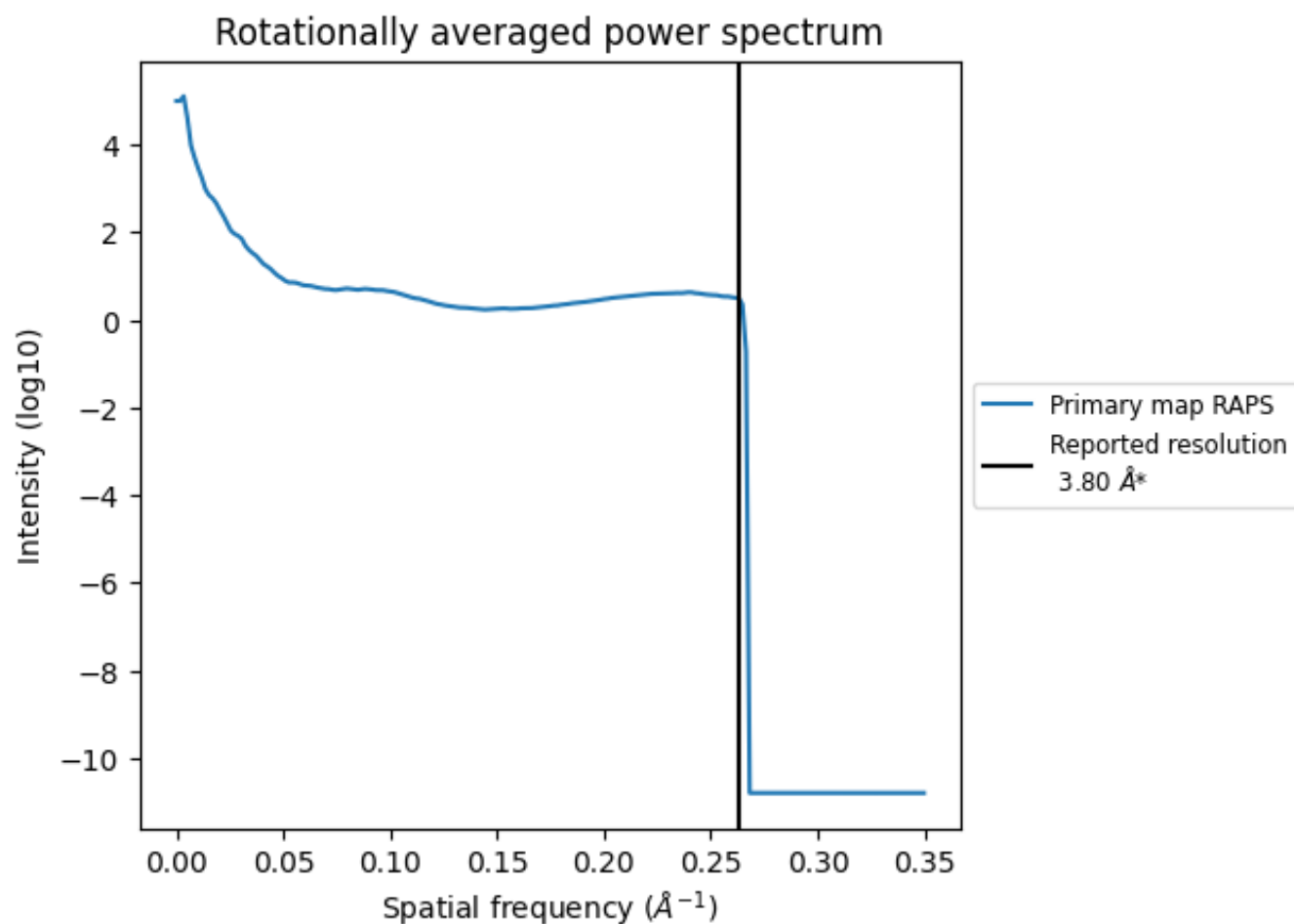
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 699 nm³; this corresponds to an approximate mass of 632 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 ⓘ

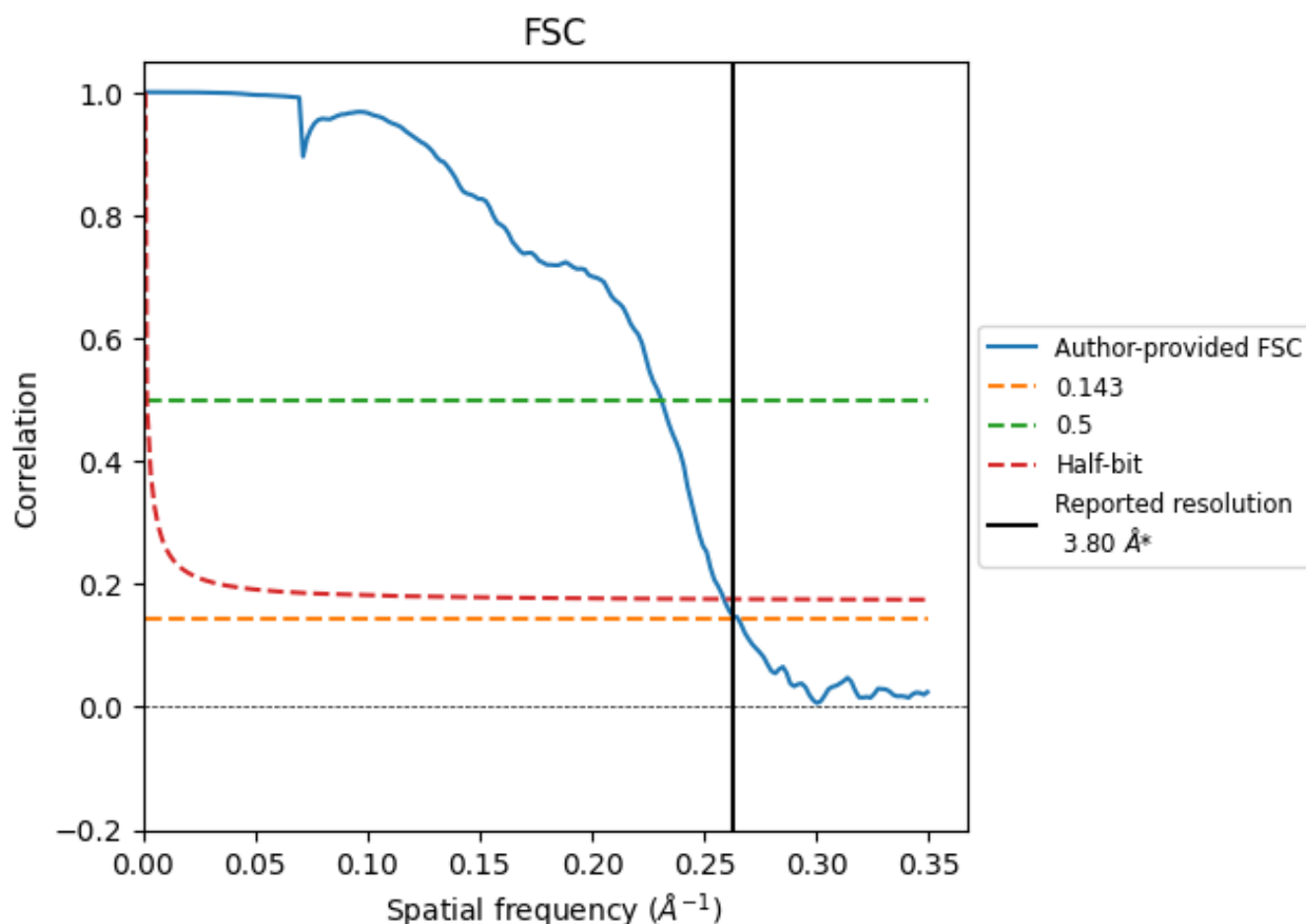


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

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 0.263 Å⁻¹

8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.77	4.33	3.86
Unmasked-calculated*	-	-	-

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

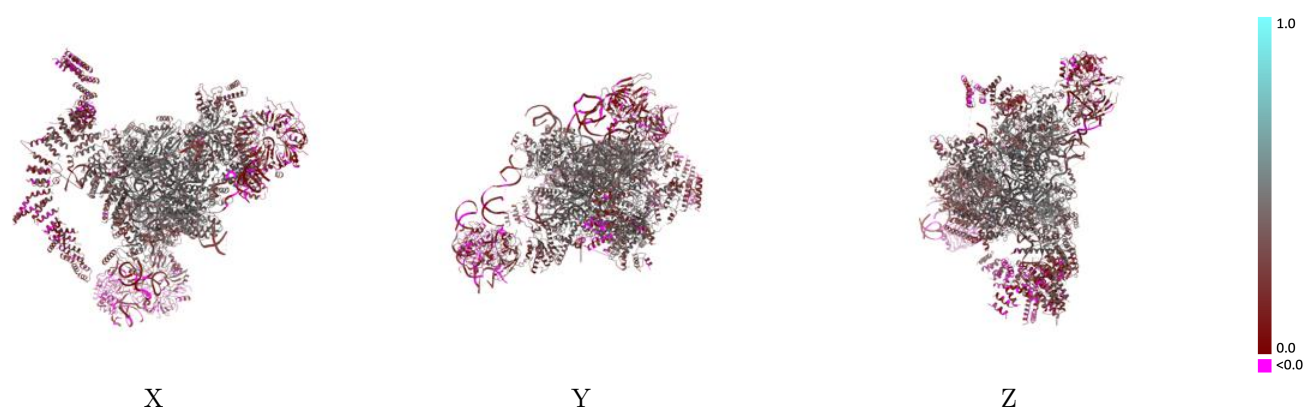
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-4055 and PDB model 5LJ3. Per-residue inclusion information can be found in section 3 on page 11.

9.1 Map-model overlay [i](#)

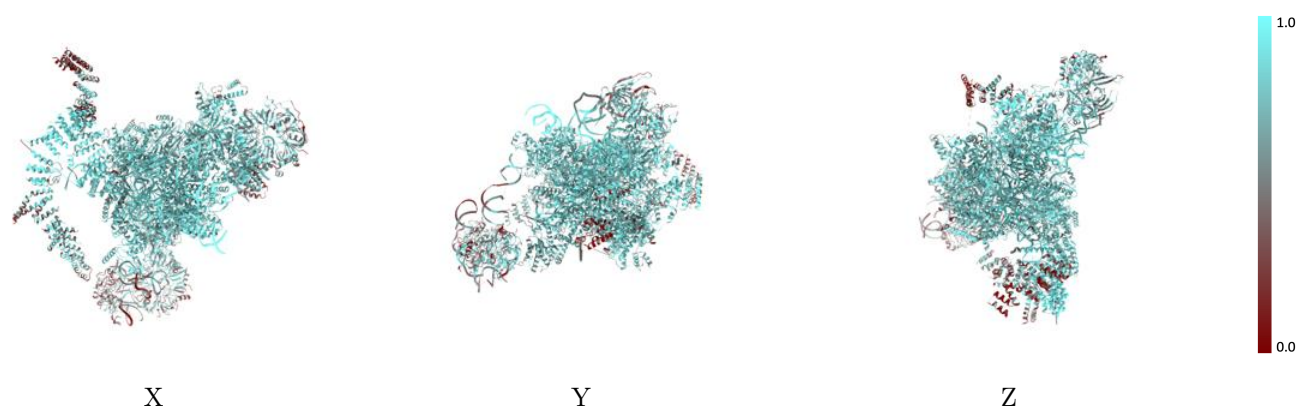
This section was not generated.

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



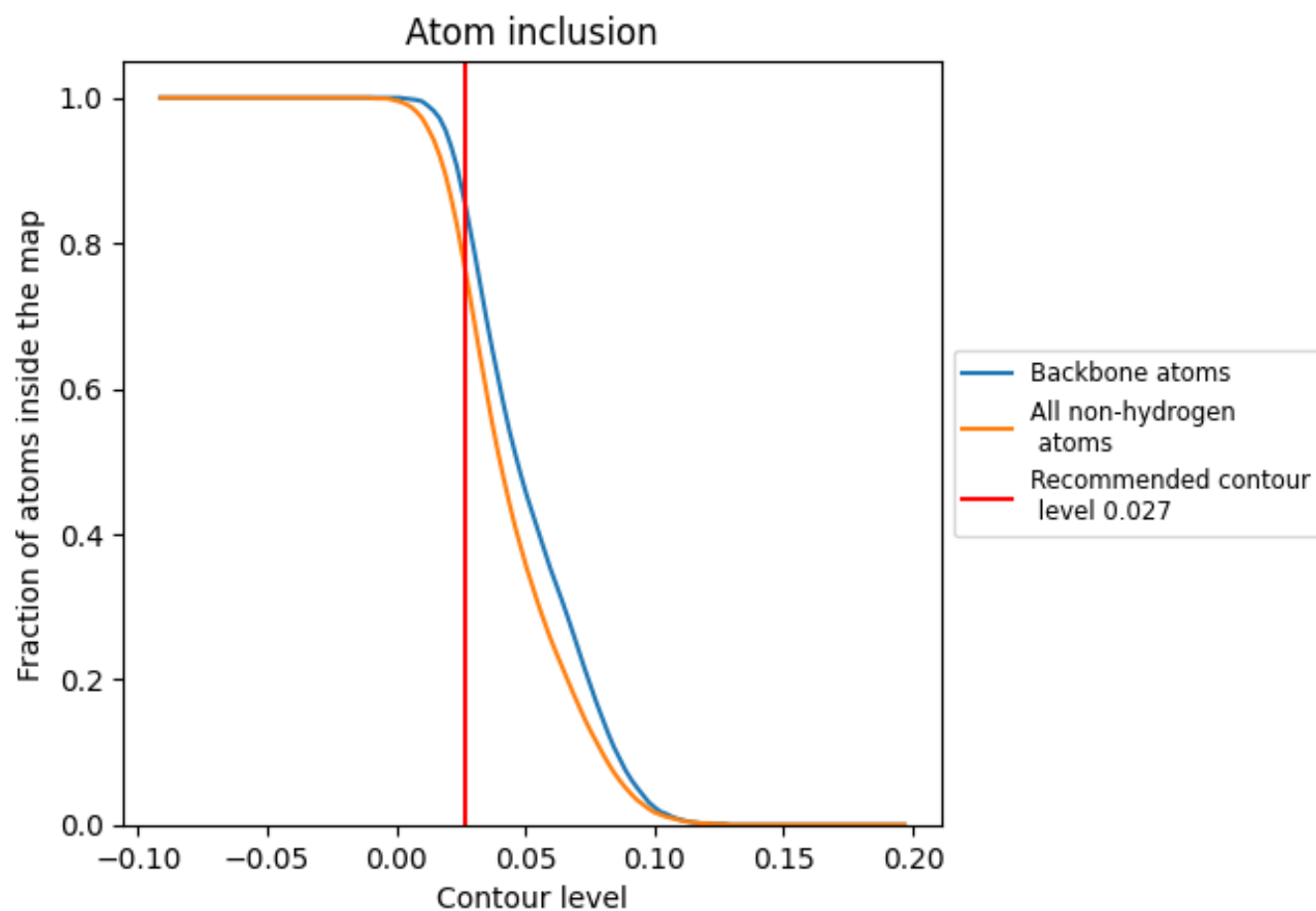
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.027).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 76% 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 (0.027) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7580	 0.3280
A	 0.8060	 0.4030
C	 0.8210	 0.4000
D	 0.8160	 0.4470
E	 0.8730	 0.3790
F	 0.7540	 0.4070
G	 0.7620	 0.3730
H	 0.6400	 0.2920
I	 0.8460	 0.3550
J	 0.8530	 0.4480
K	 0.7530	 0.4000
L	 0.8500	 0.4130
M	 0.8270	 0.4050
N	 0.8050	 0.3720
O	 0.7520	 0.3480
P	 0.8910	 0.4710
R	 0.7720	 0.3030
S	 0.6930	 0.3080
T	 0.6800	 0.1940
U	 0.8720	 0.2820
V	 0.9360	 0.3840
W	 0.3480	 0.0310
Y	 0.4880	 0.0440
Z	 0.5860	 0.1400
b	 0.6580	 0.2180
d	 0.7200	 0.3150
e	 0.6290	 0.1410
f	 0.6170	 0.1160
g	 0.6540	 0.2000
h	 0.6180	 0.1670
j	 0.5950	 0.1050
k	 0.5830	 0.1470
l	 0.7400	 0.2760
m	 0.6940	 0.2170
n	 0.5520	 0.1460



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Chain	Atom inclusion	Q-score
p	 0.5090	 0.1000
q	 0.7230	 0.2400
r	 0.4760	 0.0880
x	 0.8470	 0.3030