



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:04 PM UTC

PDB ID : 5LJ5 / pdb_00005lj5
EMDB ID : EMD-4057
Title : Overall structure 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 : 10.00 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
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

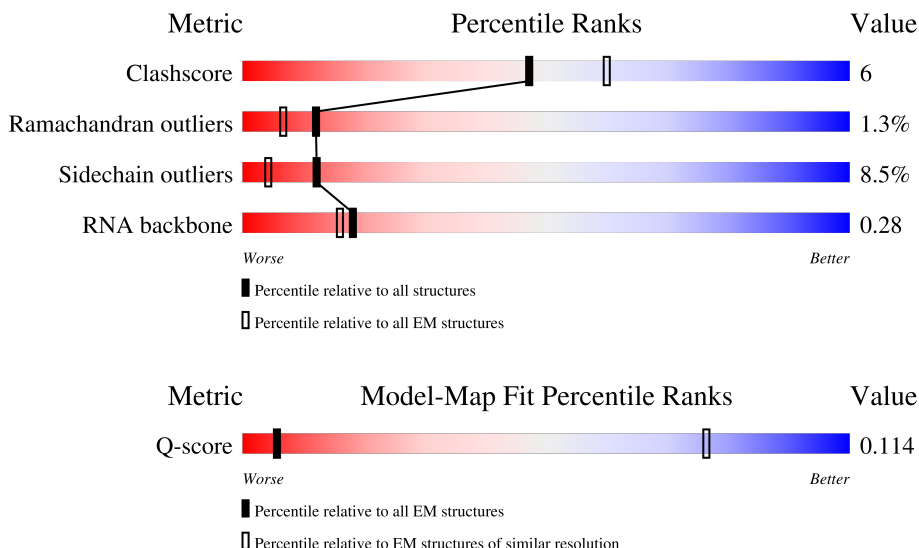
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 10.00 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.



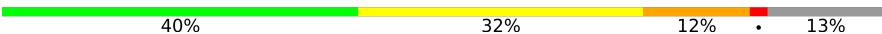
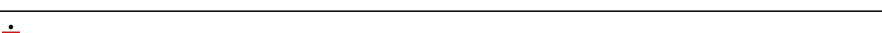
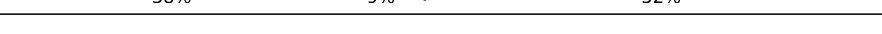
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	147 (9.50 - 10.50)

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	U	179	
2	E	16	
3	I	76	

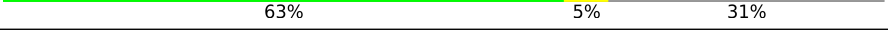
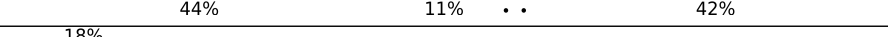
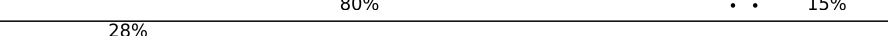
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Mol	Chain	Length	Quality of chain
4	Z	1175	
5	V	112	
6	A	2413	
7	B	2163	
8	D	278	
9	F	179	
10	C	1008	
11	G	235	
12	H	591	
13	J	451	
14	K	379	
15	L	157	
16	M	339	
17	N	364	
18	O	590	
19	P	175	
20	R	135	
21	S	687	
22	T	859	
23	b	196	
23	k	196	
24	d	101	
24	n	101	
25	e	94	
25	p	94	

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Mol	Chain	Length	Quality of chain
26	f	86	
26	q	86	
27	g	77	
27	r	77	
28	h	146	
28	l	146	
29	j	110	
29	m	110	
30	W	238	
31	Y	111	
32	Q	1071	
33	t	503	
33	u	503	
33	v	503	
33	w	503	
34	s	175	
35	x	188	

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
37	ZN	N	401	-	-	X	-
37	ZN	N	402	-	-	X	-

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 85476 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	2168	Total	C	N	O	S	0	0
			16919	10835	2966	3060	58		

- Molecule 7 is a protein called Pre-mRNA-splicing helicase BRR2.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	B	1707	Total	C	N	O	1	0
			8462	5048	1707	1707		

- Molecule 8 is a protein called Protein CWC16.

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

- Molecule 9 is a protein called Pre-mRNA-splicing factor CWC25.

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

- Molecule 10 is a protein called Pre-mRNA-splicing factor SNU114.

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

- Molecule 11 is a protein called Pre-mRNA-splicing factor ISY1.

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

- Molecule 12 is a protein called CWC22.

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

- Molecule 13 is a protein called Pre-mRNA-splicing factor PRP46.

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

- Molecule 14 is a protein called Pre-mRNA-processing protein 45.

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

- Molecule 15 is a protein called Pre-mRNA-splicing factor BUD31.

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

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	252	Total	C	N	O	S	0	0
			2012	1277	354	370	11		

- Molecule 17 is a protein called Pre-mRNA-splicing factor SLT11.

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

- Molecule 18 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	283	Total	C	N	O	S	0	0
			2068	1285	385	392	6		

- Molecule 19 is a protein called CWC15.

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

- Molecule 20 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
20	R	97	Total	C	N	O	0	0
			544	325	106	113		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	464	Total	C	N	O	S	0	0
			3121	1949	581	584	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor SYF1.

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

- Molecule 23 is a protein called Small nuclear ribonucleoprotein-associated protein B.

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

- Molecule 24 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

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

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

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

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

- Molecule 27 is a protein called Small nuclear ribonucleoprotein G.

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

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D2.

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

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

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

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein B''.

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

- Molecule 32 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	Q	619	Total	C	N	O	0	0
			3066	1828	619	619		

- Molecule 33 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	t	438	Total	C	N	O	0	0
			2171	1295	438	438		
33	u	437	Total	C	N	O	0	0
			2166	1292	437	437		
33	v	426	Total	C	N	O	0	0
			2111	1259	426	426		
33	w	435	Total	C	N	O	0	0
			2156	1286	435	435		

- Molecule 34 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	110	Total	C	N	O	0	0
			548	328	110	110		

- Molecule 35 is a protein called unknown.

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

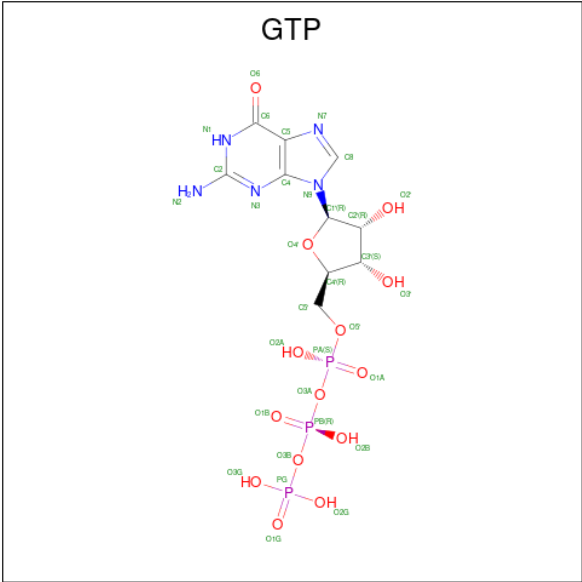
- Molecule 36 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 37 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

- Molecule 38 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

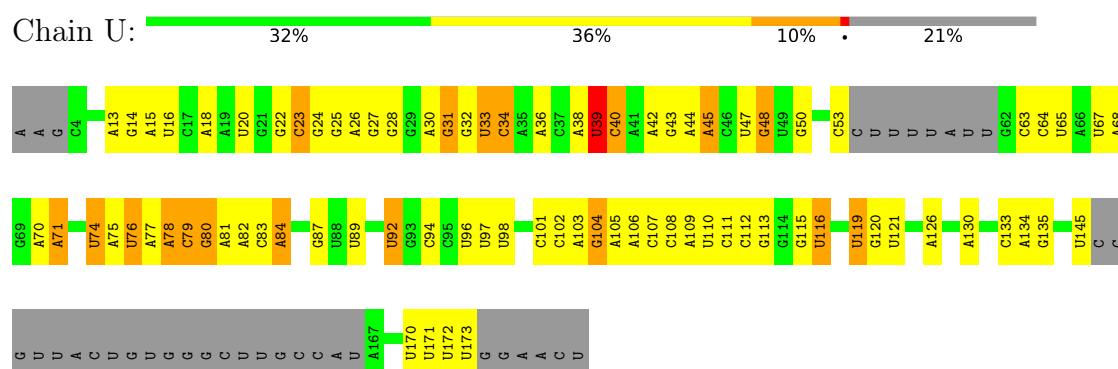


Mol	Chain	Residues	Atoms					AltConf
38	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

3 Residue-property plots [i](#)

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

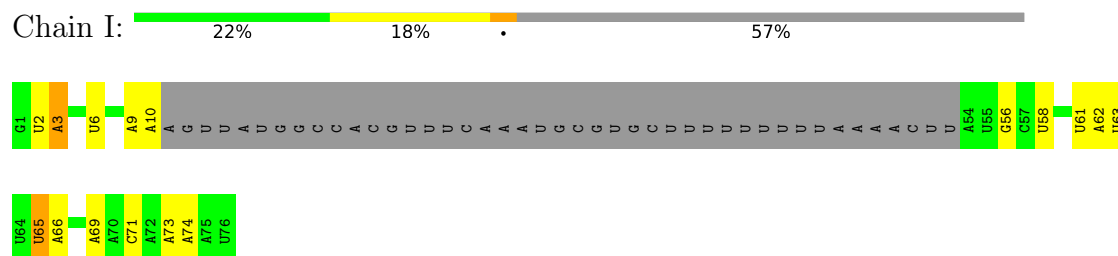
- Molecule 1: U5 snRNA (small nuclear RNA)



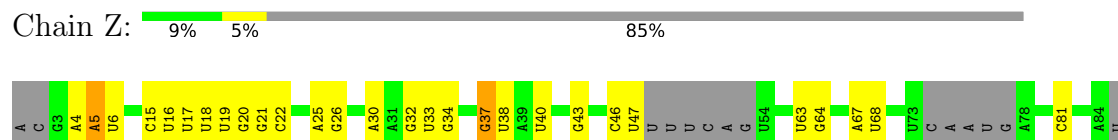
- Molecule 2: Exon 1 (5' exon) of UBC4 pre-mRNA

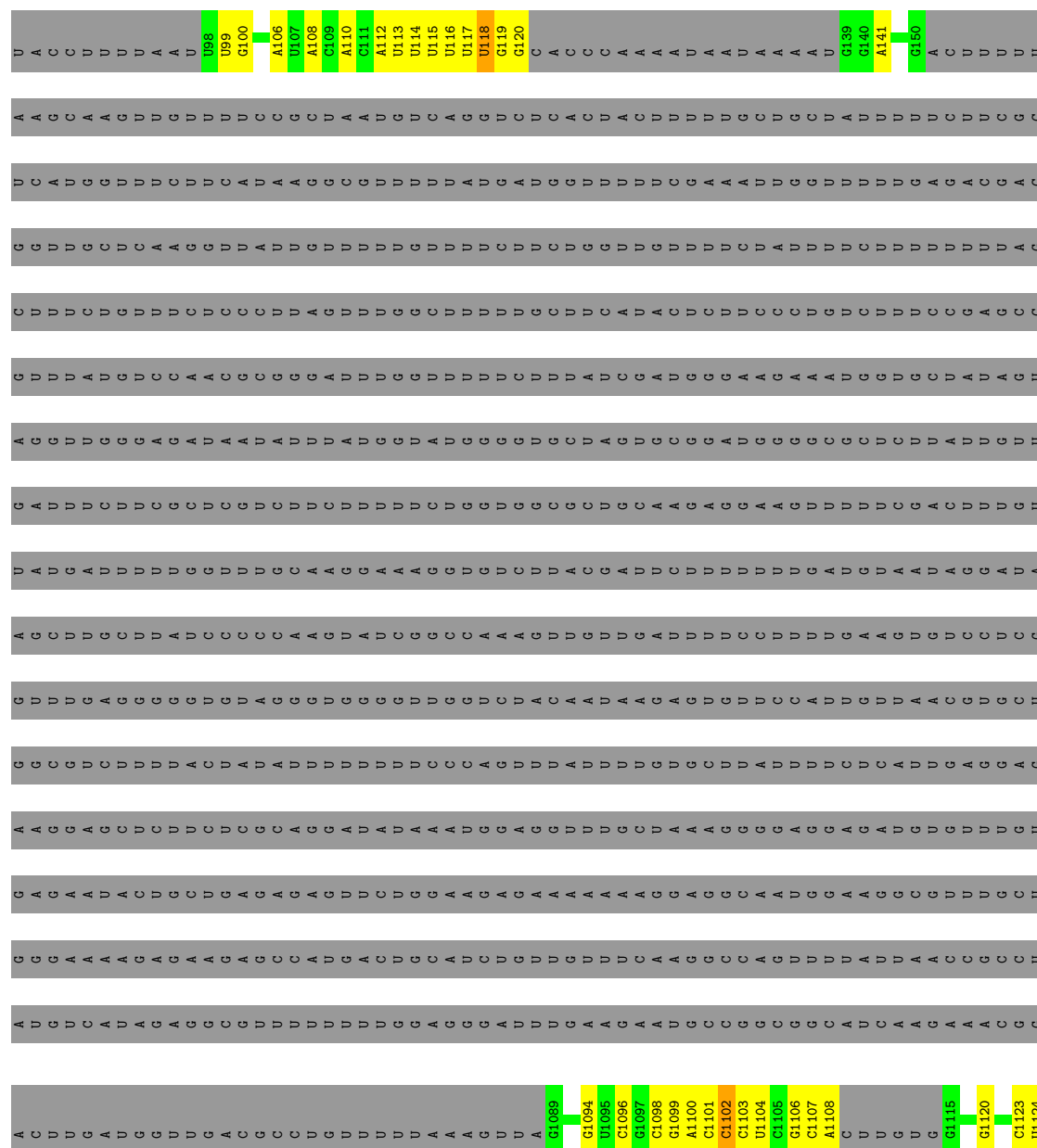


- Molecule 3: Intron of UBC4 pre-mRNA



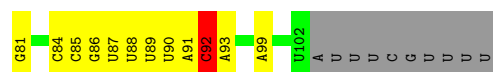
- Molecule 4: U2 snRNA (small nuclear RNA)





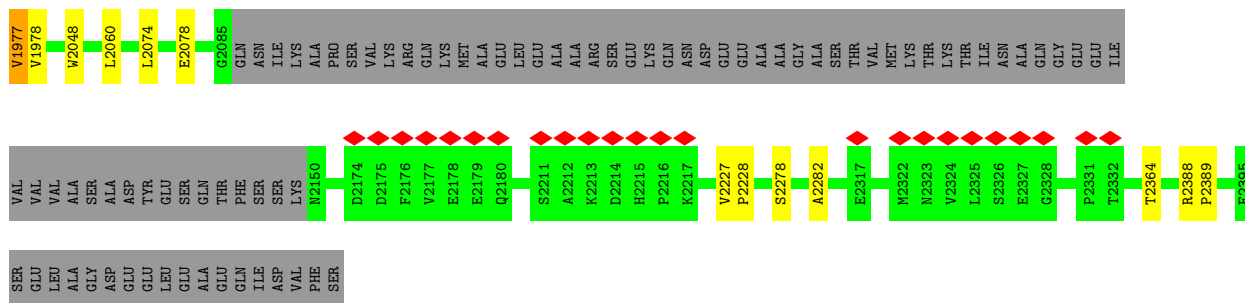
- Molecule 5: U6 snRNA (small nuclear RNA)

Chain V: 40% 32% 12% 13%

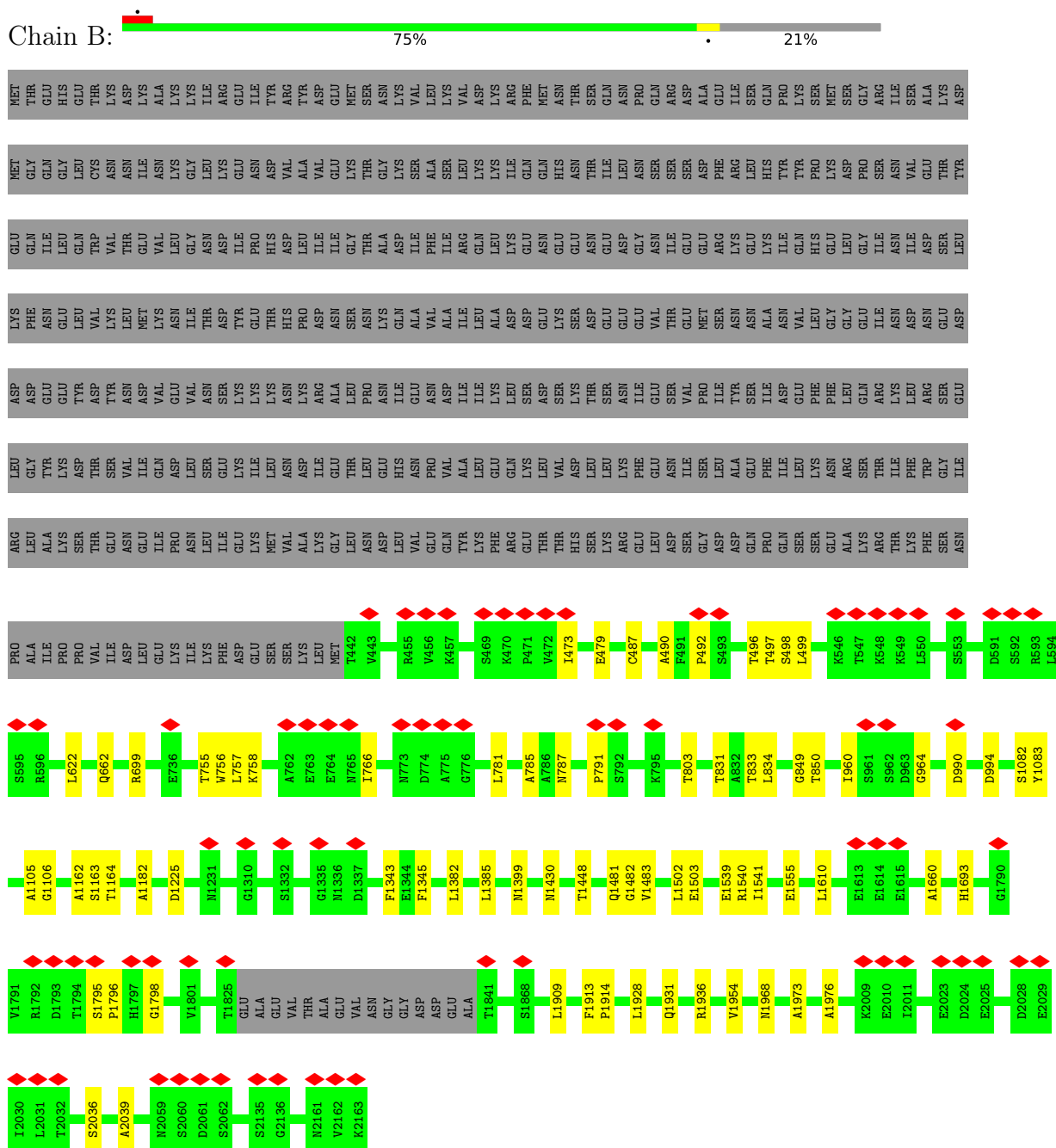


- Molecule 6: Pre-mRNA-splicing factor 8





- Molecule 7: Pre-mRNA-splicing helicase BRR2



- Molecule 8: Protein CWC16

Chain D: 

THR	LYS	GLY	LYS	ILE	GLN	LYS	SER	SER	THR	VAL	VAL	THR	THR	ASN	GLY	GLY	ARG	THR	LYS	ASP	ASP	LEU	LYS	THR	THR	ASN	GLN	PRO	GLY	ASN	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR
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- Molecule 9: Pre-mRNA-splicing factor CWC25

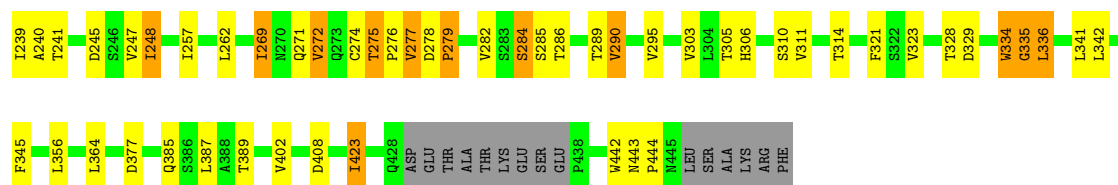
Chain F: 

ARG	THR	PRO	ASP	SER	THR	LYS	THR	LYS	ARG	ALA	MET	SER	SER	GLN	ARG	GLY	LYS	PRO	PRO	LEU	SER	LYS	THR	ASP	LEU	ASP	TYR														
TYR	LEU	GLY	LYS	LYS	LEU	SER	ILE	ASN	GLN	PRO	ALA	THR	THR	ILE	SER	ALA	SER	GLY	ALA	ALA	THR	SER	ILE	SER	SER	GLN	LYS	LYS	LEU	LYS	ASP	PRO	MET	SER	LYS	PHE	LYS	VAL	THR	LYS	GLN
MET	S3	L6	R20	V23	E27	I31	Q34	R48	GLU	LEU	ASN	GLU	LEU	LEU	ASN	GLU	THR	LYS	ASN	ASP	LEU	ALA	LYS	LYS	SER	GLY	LEU	GLU	TRP	MET	TYR	GLN	ASP	ALA	LYS	LEU	SER	ASP	GLU	LYS	GLU

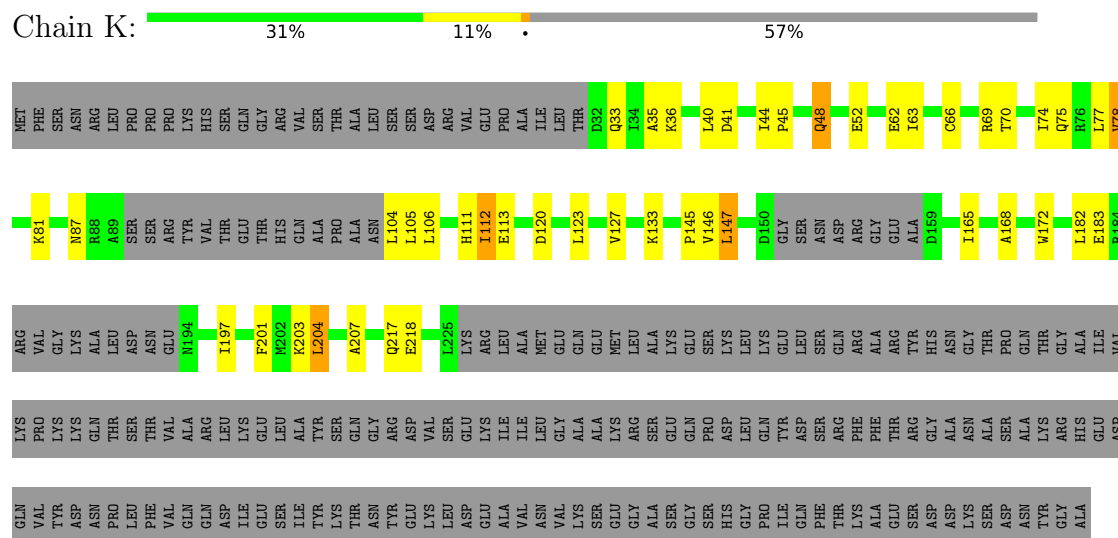
- Molecule 10: Pre-mRNA-splicing factor SNU114

Chain C: 

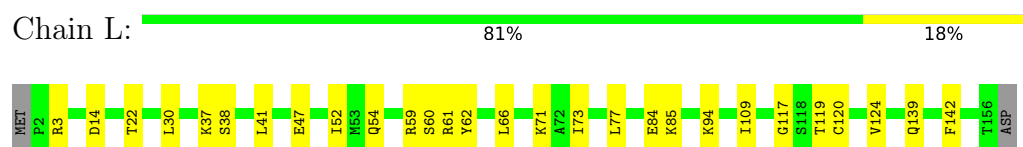
MET	GLU	GLY	ASP	LEU	PHE	ASP	GLY	ASN	ILE	GLY	VAL	ASP	PRO	PHE	ASP	SER	ASP	GLU	GLY	GLY	THR	THR	PHE	GLY	SER	SER	GLY	ASN	ASN	ASN	ASN	GLU	GLU	ILE	GLY	THR	LEU	THR	VAL	GLY	SER	LYS							
GLU	LEU	GLY	ILE	SER	LEU	PHE	GLU	HIS	ASP	PRO	TYR	GLY	ASN	LEU	ILE	GLY	VAL	H103	T104	I105	F106	SER	VAL	LEU	ASP	GLU	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN							
L193	C200	T201	S207	R208	M209	L210	N211	F212	L213	V219	R220	D222	D223	E224	T225	A226	V227	A228	L229	E230	A231	L234	V235	L236	V241	V242	Q251	L252	Q255	N259	V261	C264	F265	V266	I267	V138	I139	L152	L153	D156	W172	I185	I191	K192					
Q301	I311	I312	F313	A314	S315	L318	G319	F320	T321	F322	T323	V328	S335	I336	T345	N358	I379	F380	L381	I384	F385	L389	S390	N391	L399	L400	R401	V406	N407	L408	Q418	P419	F420	L421	V424	L427	Q431	Q432	L435	V436	Q560	D437	A438						
L439	Q444	P445	E446	T447	L448	W449	A470	H471	V472	L473	K474	T475	V486	R487	L488	L492	L493	V499	R500	I501	T504	I518	SER	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR						
V562	L563	I564	I567	I572	R573	S574	A575	T576	L577	K590	T598	T599	V602	I605	V606	L607	Q608	P609	L610	L615	P616	K617	L618	L619	D620	ASP	A621	I625	S626	V632	I633	I634	E641	I644	M652	D653	C654	L655	L656	F657	D658	Y663	G664	L665	I666	S764			
F677	N693	SER	ILE	ARG	LEU	GLY	GLY	GLU	GLU	ASN	LEU	PRO	GLY	LEU	SER	LEU	ASN	R725	ASN	THR	LEU	GLY	LYS	GLY	GLN	ASN	CYS	LEU	ASP	ILE	GLY	ILE	MET	ASP	ASN	F744	K749	T753	L760	V766	S767	F768	Y769	N770	GLY	ASN	VAL	L774	S784



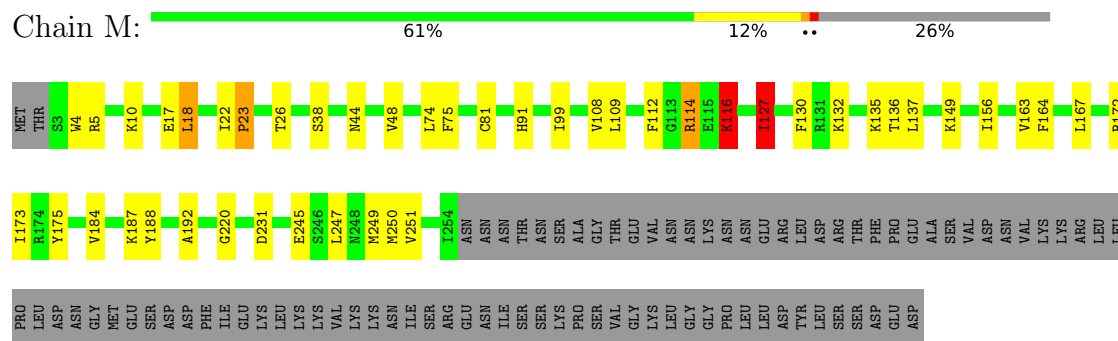
• Molecule 14: Pre-mRNA-processing protein 45



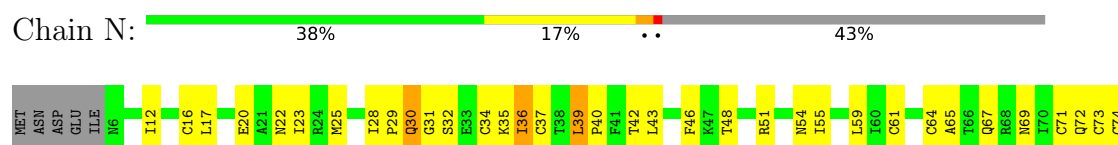
• Molecule 15: Pre-mRNA-splicing factor BUD31

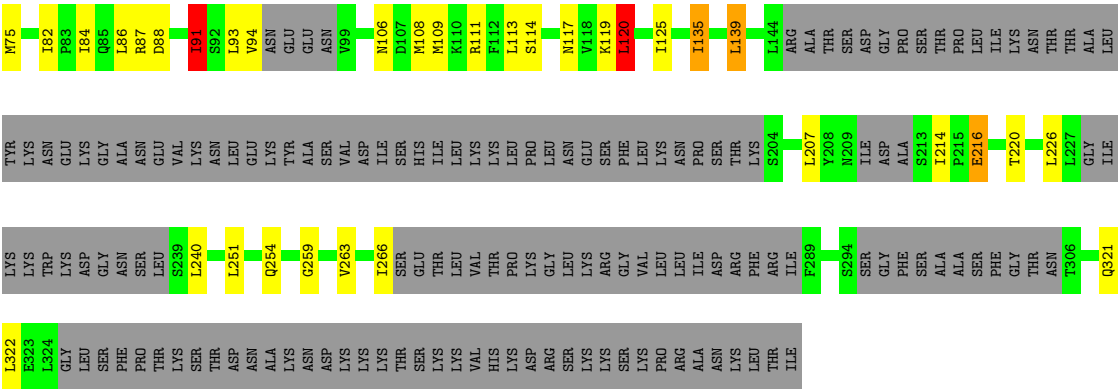


• Molecule 16: Pre-mRNA-splicing factor CWC2

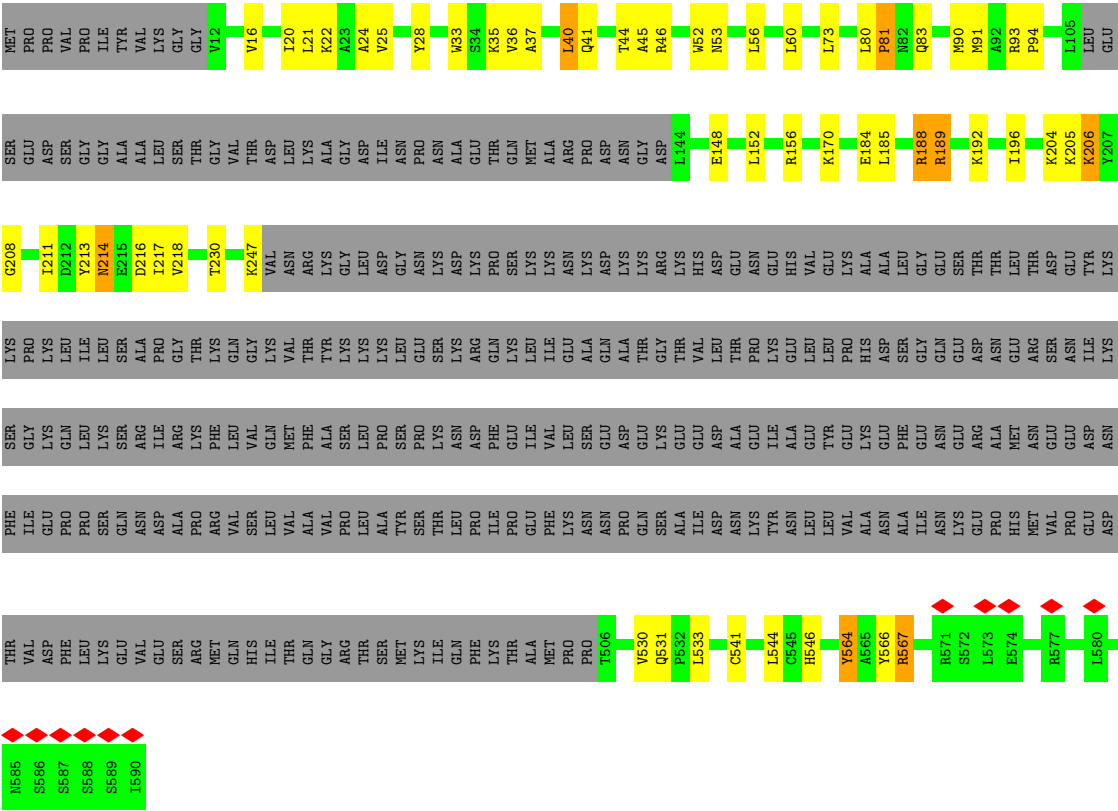
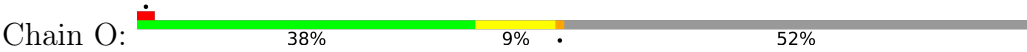


• Molecule 17: Pre-mRNA-splicing factor SLT11

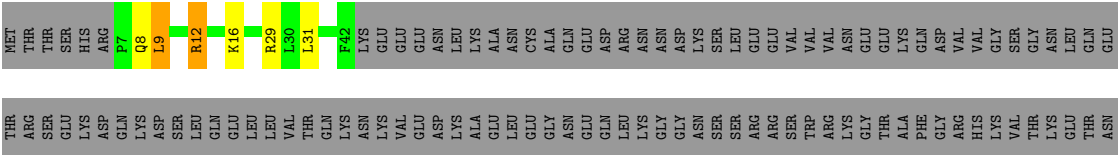




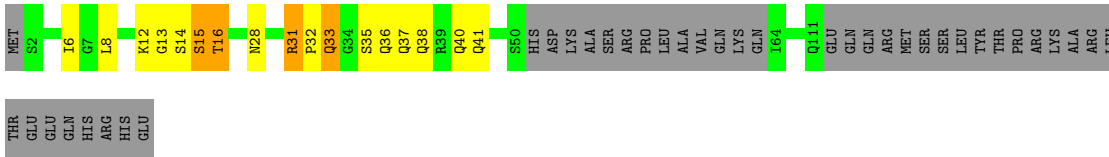
● Molecule 18: Pre-mRNA-splicing factor CEF1



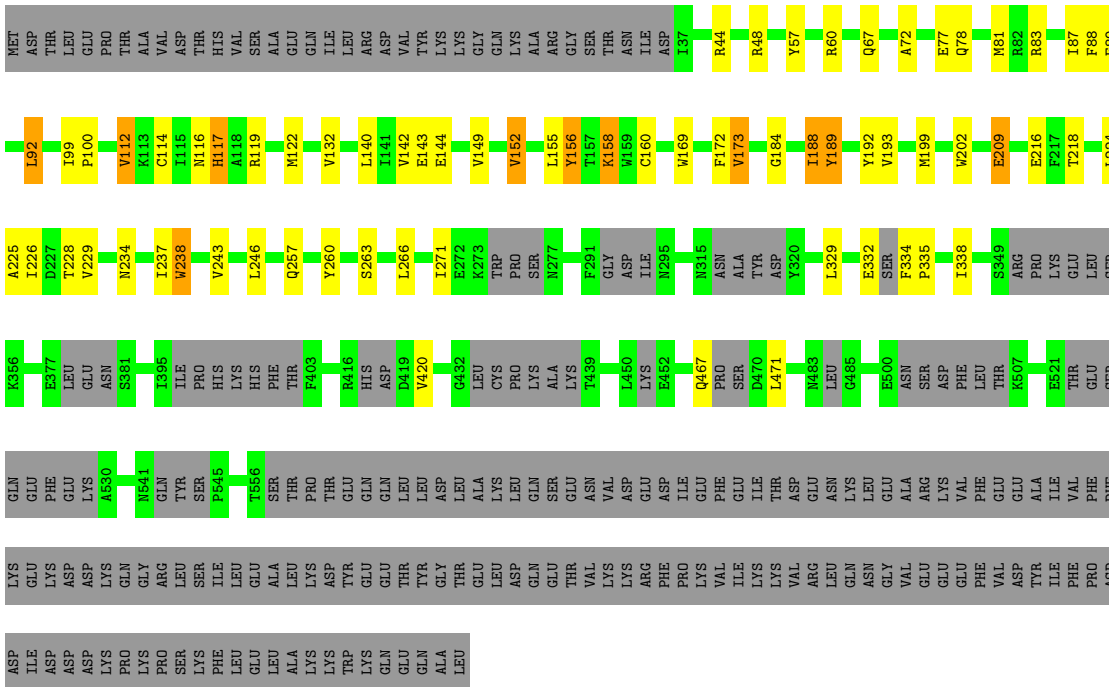
● Molecule 19: CWC15



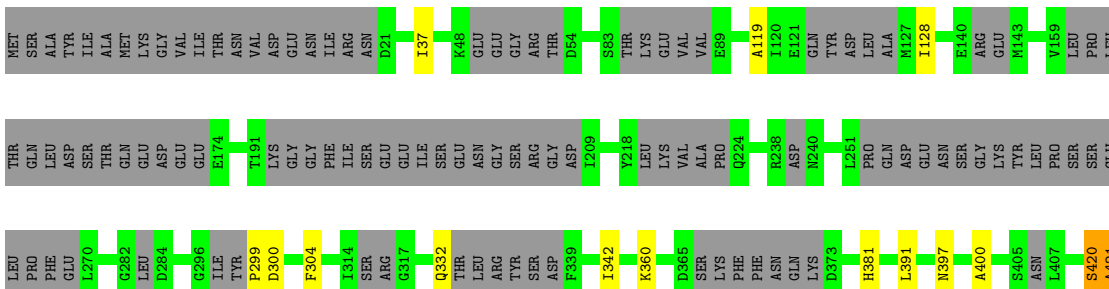
- Molecule 20: Pre-mRNA-splicing factor CWC21

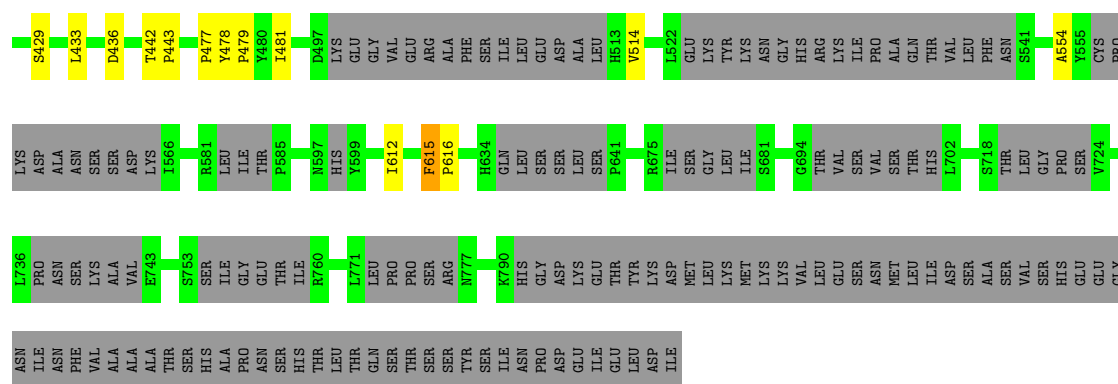


- Molecule 21: Pre-mRNA-splicing factor CLF1



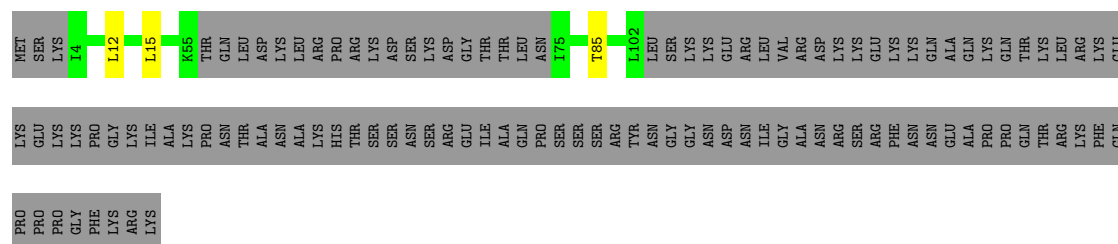
- Molecule 22: Pre-mRNA-splicing factor SYF1





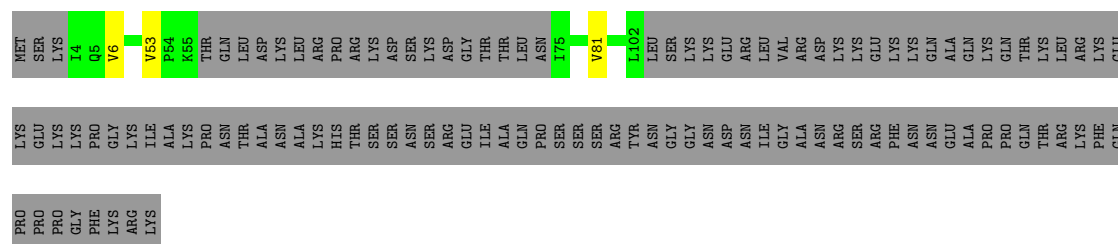
• Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain b: 39% 59%



• Molecule 23: Small nuclear ribonucleoprotein-associated protein B

Chain k: 39% 59%



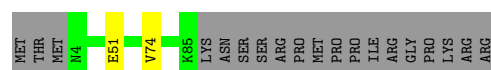
• Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain d: 69% 10% 19%



• Molecule 24: Small nuclear ribonucleoprotein Sm D3

Chain n: 79% 19%



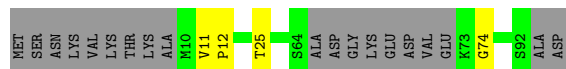
- Molecule 25: Small nuclear ribonucleoprotein E

Chain e: 



- Molecule 25: Small nuclear ribonucleoprotein E

Chain p: 



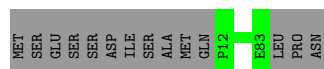
- Molecule 26: Small nuclear ribonucleoprotein F

Chain f: 



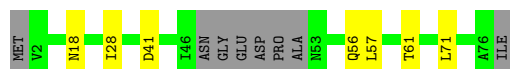
- Molecule 26: Small nuclear ribonucleoprotein F

Chain q: 



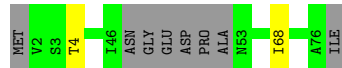
- Molecule 27: Small nuclear ribonucleoprotein G

Chain g: 



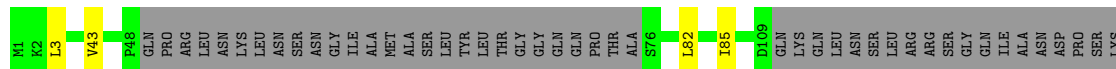
- Molecule 27: Small nuclear ribonucleoprotein G

Chain r: 



- Molecule 28: Small nuclear ribonucleoprotein Sm D1

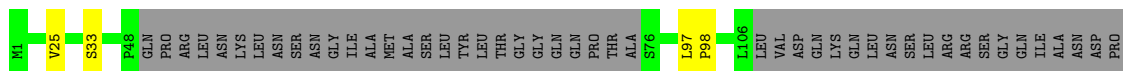
Chain h: 



LYS
ARG
ARG
ARG
ASP
PHE
GLY
ALA
PRO
ALA
ALA
ASN
LYS
LYS
PRO
ARG
ARG
GLY
LEU

- Molecule 28: Small nuclear ribonucleoprotein Sm D1

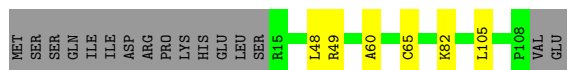
Chain l:  51% 46%



SER
LYS
LYS
ARG
ARG
ARG
ASP
PHE
GLY
GLY
ALA
ALA
PRO
PRO
ALA
ALA
ASN
LYS
LYS
ASN
PRO
SER
ARG
ARG
GLY
LEU

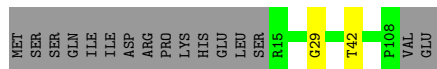
- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain j:  80% 5% 15%



- Molecule 29: Small nuclear ribonucleoprotein Sm D2

Chain m:  84% 15%



- Molecule 30: U2 small nuclear ribonucleoprotein A'

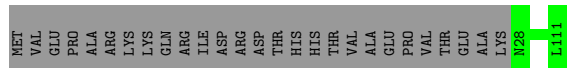
Chain W:  63% 5% 31%



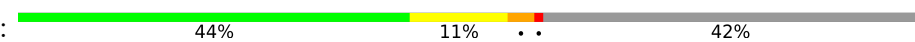
LYS
THR
MET
GLU
ILE
MET
ASN
LEU
VAL
VAL
SER
LYS
LYS
MET
THR
VAL
THR
VAL
GLU
ARG
ASN
GLU
LEU
LYS
LYS
LYS
GLN
LEU
ALA
GLU
THR
THR
SER
LEU
GLU
GLU
ILE
ALA
ALA
ARG
LEU
GLU
GLU
LEU
LEU
LEU
LEU
GLY
GLY
VAL

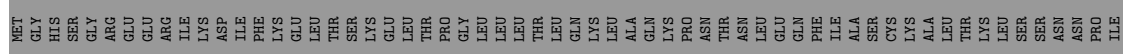
- Molecule 31: U2 small nuclear ribonucleoprotein B''

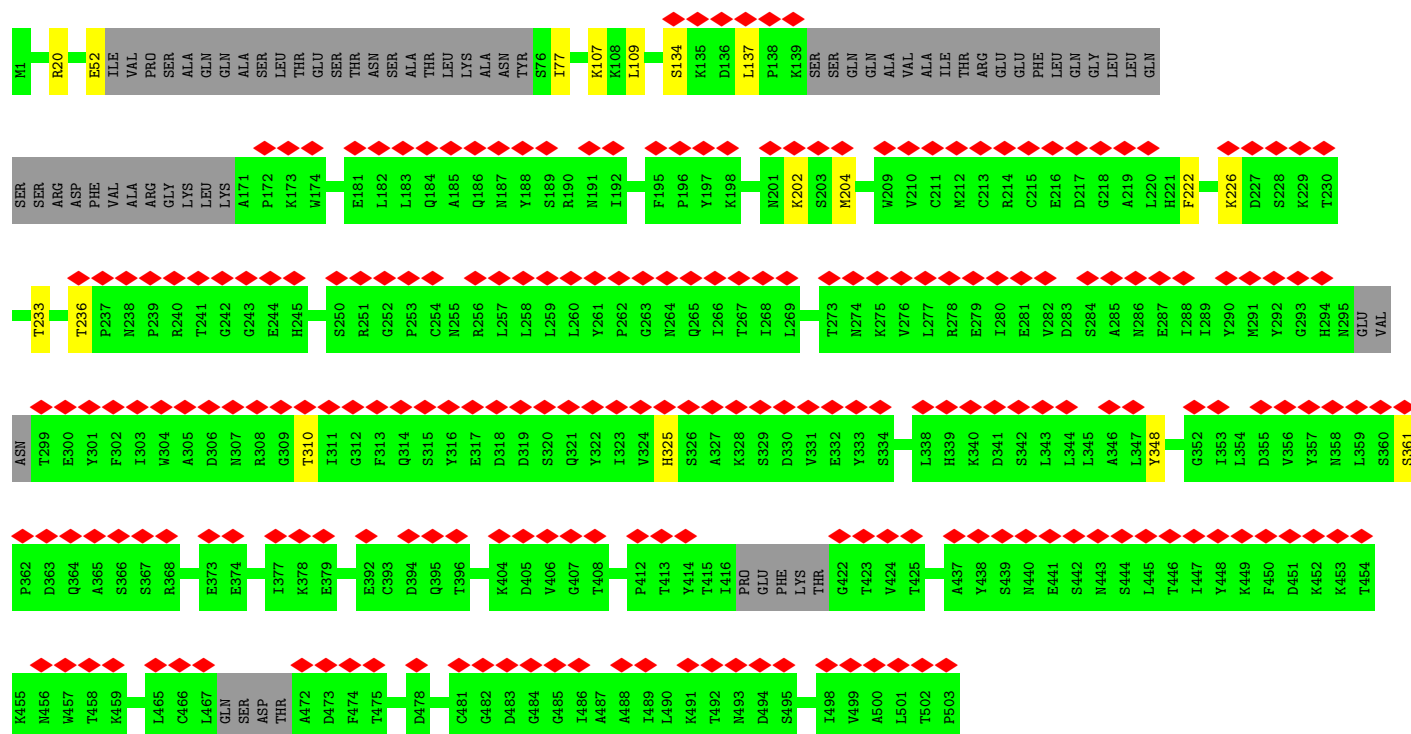
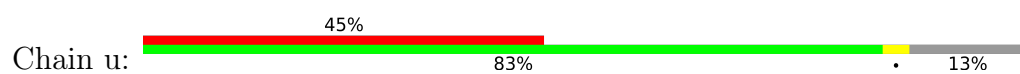
Chain Y:  76% 24%



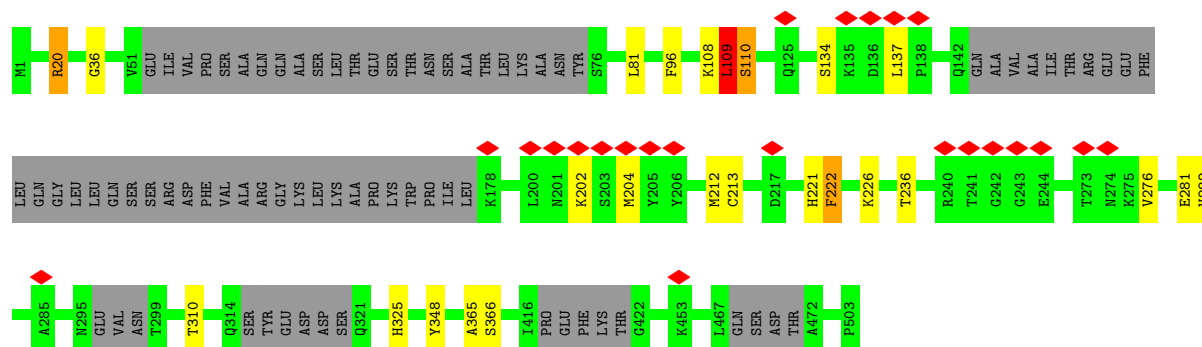
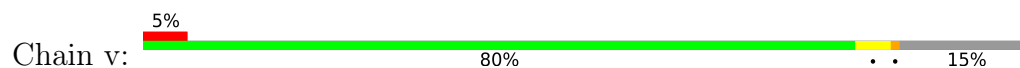
- Molecule 32: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

Chain Q:  44% 11% 42%

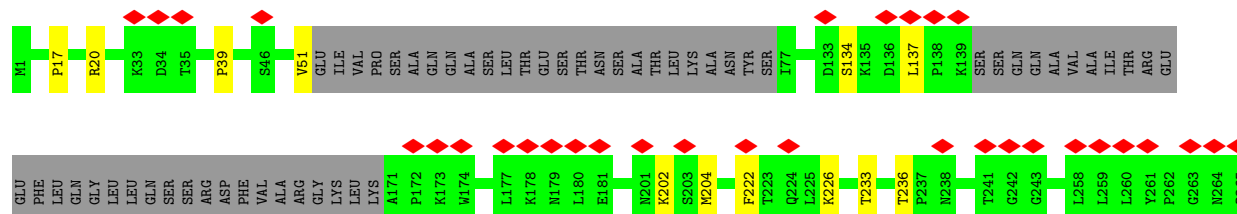
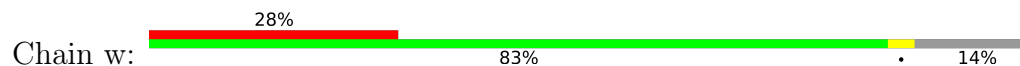


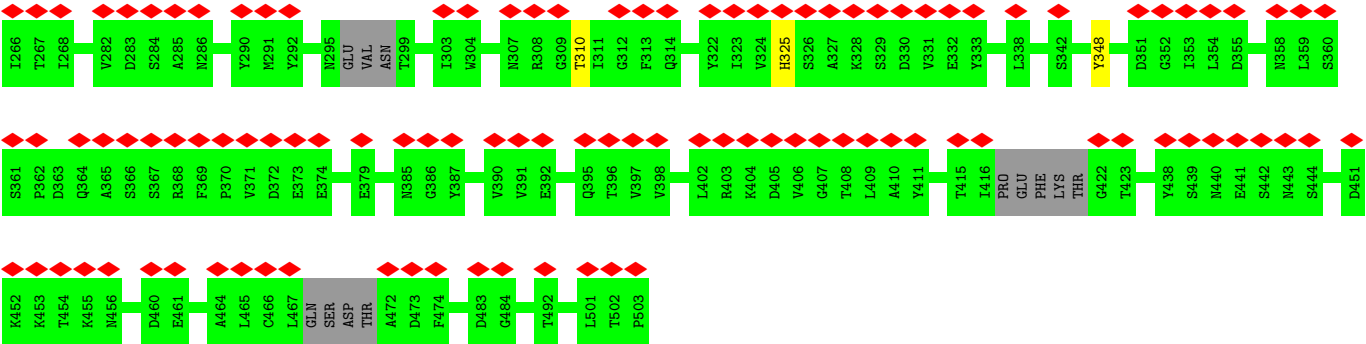


• Molecule 33: Pre-mRNA-processing factor 19

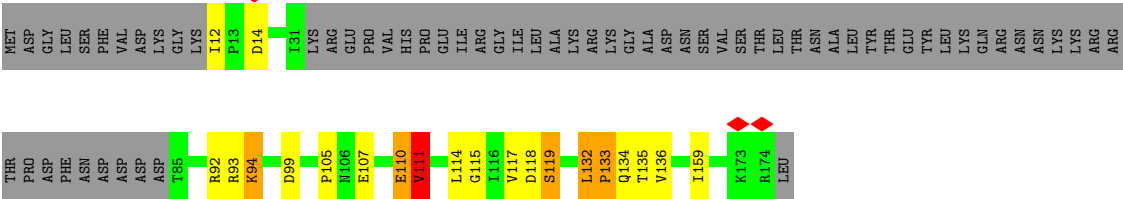


• Molecule 33: Pre-mRNA-processing factor 19





• Molecule 34: Pre-mRNA-splicing factor SNT309



• Molecule 35: unknown



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	15872	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	0.073	Depositor
Minimum map value	-0.018	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.006	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: MG, ZN, GTP

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	0.41	0/2310	0.87	9/3594 (0.3%)
6	A	0.58	1/17321 (0.0%)	1.06	26/23534 (0.1%)
7	B	0.88	0/8463	1.19	17/11800 (0.1%)
8	D	0.49	0/929	0.81	0/1243
9	F	0.53	0/325	1.20	0/442
10	C	0.55	0/6902	1.02	7/9386 (0.1%)
11	G	0.52	0/839	1.10	0/1126
12	H	0.55	0/2667	1.35	4/3630 (0.1%)
13	J	0.59	0/2613	0.88	2/3551 (0.1%)
14	K	0.53	0/1308	1.05	4/1765 (0.2%)
15	L	0.52	0/1294	1.05	2/1732 (0.1%)
16	M	0.51	0/2058	0.97	2/2769 (0.1%)
17	N	0.55	0/1680	1.03	2/2258 (0.1%)
18	O	0.70	0/2091	1.28	6/2824 (0.2%)
19	P	0.61	0/282	0.88	1/380 (0.3%)
20	R	0.52	0/545	1.35	3/748 (0.4%)
21	S	0.53	0/3155	1.32	2/4298 (0.0%)
22	T	0.48	0/2918	1.49	12/4032 (0.3%)
23	b	0.53	0/636	0.71	0/856
23	k	0.49	0/394	0.99	2/546 (0.4%)
24	d	0.53	0/634	0.88	2/859 (0.2%)
24	n	0.48	0/403	1.14	4/559 (0.7%)
25	e	0.61	0/585	0.84	0/795
25	p	0.49	0/367	1.28	6/507 (1.2%)
26	f	0.57	0/585	0.85	0/791
26	q	0.50	0/353	1.01	0/489
27	g	0.55	0/532	0.76	0/715
27	r	0.48	0/338	0.90	2/467 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
28	h	0.50	0/649	0.77	0/880
28	l	0.52	0/390	1.23	4/541 (0.7%)
29	j	0.55	0/753	0.89	0/1013
29	m	0.50	0/466	1.18	4/649 (0.6%)
30	W	0.50	0/814	1.18	10/1134 (0.9%)
31	Y	0.49	0/415	1.08	0/577
32	Q	0.88	1/3061 (0.0%)	1.89	81/4260 (1.9%)
33	t	0.76	0/2165	1.14	10/3010 (0.3%)
33	u	0.81	1/2160 (0.0%)	1.15	11/3003 (0.4%)
33	v	0.84	2/2104 (0.1%)	1.23	14/2923 (0.5%)
33	w	0.76	0/2150	1.12	9/2989 (0.3%)
34	s	0.98	1/546 (0.2%)	1.45	11/760 (1.4%)
All	All	0.62	6/86729 (0.0%)	1.12	277/120679 (0.2%)

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
11	G	0	1
16	M	0	1
18	O	0	2
21	S	0	1
32	Q	0	45
33	t	0	1
33	v	0	1
33	w	0	1
34	s	0	2
All	All	0	57

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	v	109	LEU	C-N	8.00	1.44	1.33
33	v	134	SER	C-O	-5.76	1.17	1.24
34	s	133	PRO	CA-C	5.59	1.60	1.52
32	Q	708	LYS	N-CA	5.22	1.52	1.46
33	u	77	ILE	C-N	5.14	1.40	1.33
6	A	632	ILE	N-CA	5.10	1.52	1.46

All (277) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Q	403	THR	N-CA-C	15.89	128.68	111.36
32	Q	404	GLN	N-CA-C	15.28	121.67	108.07
32	Q	402	VAL	N-CA-C	14.99	125.99	107.70
12	H	87	ILE	CA-C-N	14.31	134.45	118.85
12	H	87	ILE	C-N-CA	14.31	134.45	118.85
33	v	134	SER	CA-C-O	-11.53	108.20	120.42
32	Q	429	VAL	N-CA-C	11.38	122.23	110.62
32	Q	745	PHE	CA-C-N	10.90	141.32	121.70
32	Q	745	PHE	C-N-CA	10.90	141.32	121.70
22	T	615	PHE	CA-C-N	10.69	131.39	120.38
22	T	615	PHE	C-N-CA	10.69	131.39	120.38
33	v	137	LEU	CA-C-N	10.18	130.35	119.05
33	v	137	LEU	C-N-CA	10.18	130.35	119.05
34	s	132	LEU	CA-C-N	10.08	132.44	119.84
34	s	132	LEU	C-N-CA	10.08	132.44	119.84
28	l	33	SER	CA-C-N	9.88	130.02	119.05
28	l	33	SER	C-N-CA	9.88	130.02	119.05
10	C	106	PHE	N-CA-C	9.81	124.05	109.24
29	m	29	GLY	CA-C-N	9.69	129.80	119.05
29	m	29	GLY	C-N-CA	9.69	129.80	119.05
32	Q	745	PHE	O-C-N	-9.46	111.52	122.68
32	Q	902	ILE	CA-C-N	9.40	132.18	120.72
32	Q	902	ILE	C-N-CA	9.40	132.18	120.72
1	U	39	U	C2'-C3'-O3'	9.12	127.38	113.70
18	O	564	TYR	CB-CA-C	9.09	122.71	111.43
33	u	137	LEU	CA-C-N	8.98	128.71	119.19
33	u	137	LEU	C-N-CA	8.98	128.71	119.19
28	l	97	LEU	CA-C-N	8.96	131.04	119.84
28	l	97	LEU	C-N-CA	8.96	131.04	119.84
18	O	564	TYR	O-C-N	-8.84	114.61	123.62
13	J	141	TRP	N-CA-C	8.59	123.50	112.34
30	W	43	MET	CA-C-N	8.58	128.72	119.28
30	W	43	MET	C-N-CA	8.58	128.72	119.28
33	v	110	SER	N-CA-C	8.49	120.54	111.28
32	Q	747	ASP	N-CA-C	8.49	119.47	108.34
1	U	83	C	C4'-C3'-O3'	-8.47	100.29	113.00
32	Q	654	ILE	CB-CA-C	8.40	125.07	111.29
33	t	137	LEU	CA-C-N	8.29	127.88	118.85
33	t	137	LEU	C-N-CA	8.29	127.88	118.85
5	V	92	C	C2'-C3'-O3'	8.27	121.91	109.50
17	N	91	ILE	N-CA-CB	8.20	120.14	110.55
30	W	4	THR	CA-C-N	7.87	127.43	118.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	W	4	THR	C-N-CA	7.87	127.43	118.85
34	s	135	THR	CA-C-O	-7.80	112.20	120.55
5	V	34	A	C2'-C3'-O3'	-7.75	102.07	113.70
33	v	134	SER	O-C-N	7.75	130.98	122.15
32	Q	430	GLY	N-CA-C	7.74	122.13	112.14
20	R	38	GLN	N-CA-C	-7.69	102.89	111.28
22	T	436	ASP	CA-C-N	7.59	127.30	119.56
22	T	436	ASP	C-N-CA	7.59	127.30	119.56
32	Q	748	LYS	CA-C-N	7.55	128.16	120.38
32	Q	748	LYS	C-N-CA	7.55	128.16	120.38
24	n	51	GLU	CA-C-N	7.46	127.49	119.28
24	n	51	GLU	C-N-CA	7.46	127.49	119.28
32	Q	574	GLU	N-CA-CB	-7.35	98.98	109.94
23	k	53	VAL	CA-C-N	7.27	127.25	119.76
23	k	53	VAL	C-N-CA	7.27	127.25	119.76
7	B	1541	ILE	N-CA-C	7.15	117.94	110.72
25	p	12	PRO	CA-C-N	7.10	127.09	119.28
25	p	12	PRO	C-N-CA	7.10	127.09	119.28
32	Q	400	ILE	CA-C-N	7.04	134.64	121.97
32	Q	400	ILE	C-N-CA	7.04	134.64	121.97
32	Q	477	GLU	CA-C-N	7.01	134.93	121.54
32	Q	477	GLU	C-N-CA	7.01	134.93	121.54
10	C	379	ILE	O-C-N	7.00	125.04	120.07
32	Q	573	GLN	CA-C-N	6.99	129.97	120.54
32	Q	573	GLN	C-N-CA	6.99	129.97	120.54
32	Q	470	VAL	CA-C-N	6.92	134.43	121.97
32	Q	470	VAL	C-N-CA	6.92	134.43	121.97
32	Q	401	VAL	CA-C-N	-6.86	115.11	121.97
32	Q	401	VAL	C-N-CA	-6.86	115.11	121.97
33	u	134	SER	CA-C-O	-6.84	112.10	119.97
32	Q	447	LYS	N-CA-C	6.82	125.33	110.80
32	Q	446	LEU	N-CA-C	6.82	121.76	113.38
29	m	42	THR	CA-C-N	6.81	126.80	119.78
29	m	42	THR	C-N-CA	6.81	126.80	119.78
21	S	420	VAL	O-C-N	6.80	124.77	120.42
32	Q	405	PRO	N-CA-C	6.79	122.47	113.57
6	A	882	ILE	N-CA-CB	6.78	118.49	110.55
10	C	379	ILE	N-CA-CB	6.73	114.74	110.50
32	Q	642	GLU	N-CA-C	6.71	118.59	111.28
7	B	787	ASN	N-CA-C	6.70	118.24	111.07
22	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
18	O	531	GLN	CA-C-N	6.68	128.19	119.84
18	O	531	GLN	C-N-CA	6.68	128.19	119.84
7	B	699	ARG	CA-C-N	-6.68	112.88	119.76
7	B	699	ARG	C-N-CA	-6.68	112.88	119.76
32	Q	388	TYR	CA-C-N	6.66	130.05	120.79
32	Q	388	TYR	C-N-CA	6.66	130.05	120.79
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
32	Q	916	ALA	N-CA-C	6.60	121.74	113.43
33	w	39	PRO	N-CA-CB	6.59	110.51	103.39
6	A	1339	LEU	N-CA-C	-6.56	104.21	111.36
22	T	612	ILE	O-C-N	6.56	124.62	120.42
30	W	11	ALA	CA-C-N	6.53	128.00	119.84
30	W	11	ALA	C-N-CA	6.53	128.00	119.84
14	K	145	PRO	N-CA-C	6.52	122.02	114.20
7	B	473	ILE	CB-CA-C	-6.50	105.27	112.68
7	B	831	THR	N-CA-C	-6.50	101.17	110.59
24	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
24	n	74	VAL	CA-C-N	6.42	126.37	120.21
24	n	74	VAL	C-N-CA	6.42	126.37	120.21
33	v	222	PHE	N-CA-C	-6.38	97.68	108.26
32	Q	394	ASN	CB-CA-C	6.37	121.22	111.85
6	A	969	ILE	N-CA-C	6.30	116.95	107.75
22	T	304	PHE	N-CA-C	-6.24	104.48	111.28
22	T	478	TYR	CA-C-N	6.22	127.62	119.84
22	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
10	C	766	TRP	N-CA-C	6.21	118.31	110.24
32	Q	369	VAL	CA-C-N	6.17	133.08	121.97
32	Q	369	VAL	C-N-CA	6.17	133.08	121.97
30	W	67	ILE	CA-C-N	6.16	127.55	119.84
30	W	67	ILE	C-N-CA	6.16	127.55	119.84
22	T	442	THR	CA-C-N	6.16	127.54	119.84
22	T	442	THR	C-N-CA	6.16	127.54	119.84
7	B	1909	LEU	CA-C-N	6.15	126.05	119.28
7	B	1909	LEU	C-N-CA	6.15	126.05	119.28
6	A	1795	LYS	O-C-N	6.12	125.22	120.38
33	w	137	LEU	CA-C-N	6.07	125.63	119.19
33	w	137	LEU	C-N-CA	6.07	125.63	119.19
32	Q	651	ARG	CB-CA-C	6.07	118.86	109.03
30	W	148	VAL	CA-C-N	6.07	125.62	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	W	148	VAL	C-N-CA	6.07	125.62	119.19
7	B	803	THR	N-CA-C	-6.05	100.14	109.52
25	p	25	THR	CA-C-N	5.97	125.89	119.85
25	p	25	THR	C-N-CA	5.97	125.89	119.85
33	v	226	LYS	N-CA-C	-5.96	106.62	114.31
33	u	226	LYS	N-CA-C	-5.96	106.62	114.31
33	w	226	LYS	N-CA-C	-5.96	106.63	114.31
5	V	72	C	C4'-C3'-O3'	-5.95	104.07	113.00
32	Q	384	ALA	CB-CA-C	5.95	122.43	109.99
27	r	4	THR	CA-C-N	5.94	125.70	119.76
27	r	4	THR	C-N-CA	5.94	125.70	119.76
33	t	226	LYS	N-CA-C	-5.93	106.66	114.31
32	Q	690	ALA	N-CA-C	5.93	120.80	113.50
5	V	92	C	C4'-C3'-O3'	5.89	118.24	109.40
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
32	Q	892	PRO	N-CA-CB	5.82	106.18	102.92
7	B	1430	ASN	CA-C-N	-5.81	115.38	122.64
7	B	1430	ASN	C-N-CA	-5.81	115.38	122.64
6	A	770	MET	N-CA-C	5.79	114.97	108.25
10	C	129	ILE	N-CA-C	5.76	113.58	107.76
34	s	132	LEU	N-CA-C	5.76	122.54	109.81
6	A	214	THR	N-CA-CB	5.76	118.36	110.01
34	s	117	VAL	CA-C-O	5.75	124.12	119.29
34	s	159	ILE	CA-C-O	5.73	127.41	121.05
18	O	567	ARG	CA-C-O	-5.71	114.37	120.42
32	Q	483	ASP	CB-CA-C	5.71	121.14	110.70
6	A	1401	SER	N-CA-C	5.68	117.62	110.24
32	Q	916	ALA	N-CA-CB	-5.67	100.87	110.51
20	R	33	GLN	N-CA-C	-5.64	105.21	111.36
7	B	849	GLY	N-CA-C	5.63	120.38	113.79
10	C	966	PHE	CB-CA-C	-5.63	102.04	110.88
32	Q	474	GLU	CB-CA-C	5.61	119.70	111.73
16	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
34	s	132	LEU	CA-C-O	5.57	127.79	120.16
34	s	135	THR	O-C-N	5.55	128.88	122.17
32	Q	472	ILE	N-CA-C	-5.55	101.03	108.35
33	v	202	LYS	N-CA-C	-5.53	106.48	113.18
32	Q	402	VAL	CB-CA-C	-5.52	106.56	111.74
33	w	202	LYS	N-CA-C	-5.51	106.51	113.18
32	Q	471	ILE	N-CA-CB	5.50	120.30	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	u	202	LYS	N-CA-C	-5.50	106.53	113.18
22	T	420	SER	N-CA-C	5.49	117.44	108.76
14	K	69	ARG	N-CA-C	-5.49	104.98	110.97
14	K	78	VAL	N-CA-CB	5.48	117.99	110.54
32	Q	371	ILE	CA-C-N	5.47	130.75	122.98
32	Q	371	ILE	C-N-CA	5.47	130.75	122.98
7	B	850	THR	CB-CA-C	-5.47	102.78	111.48
6	A	851	ARG	CB-CA-C	-5.47	102.29	110.88
17	N	322	LEU	N-CA-C	5.47	119.67	112.89
21	S	271	ILE	N-CA-CB	5.47	117.98	110.54
33	t	202	LYS	N-CA-C	-5.47	106.57	113.18
7	B	1225	ASP	N-CA-C	5.46	116.25	108.54
7	B	662	GLN	N-CA-C	5.46	122.43	110.80
7	B	1954	VAL	N-CA-C	5.45	118.75	111.44
33	v	204	MET	N-CA-C	5.42	118.69	112.57
33	u	204	MET	N-CA-C	5.41	118.69	112.57
32	Q	960	SER	N-CA-C	-5.40	107.94	114.75
6	A	737	ARG	N-CA-C	5.39	122.29	110.80
33	w	204	MET	N-CA-C	5.38	118.65	112.57
33	t	204	MET	N-CA-C	5.37	118.64	112.57
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
25	p	11	VAL	CA-C-N	5.32	125.86	120.38
25	p	11	VAL	C-N-CA	5.32	125.86	120.38
19	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
32	Q	700	ARG	CB-CA-C	5.31	118.74	110.67
32	Q	750	PRO	N-CA-C	5.30	123.39	112.47
32	Q	401	VAL	O-C-N	-5.28	115.97	122.57
32	Q	898	LYS	CA-C-N	5.26	127.33	120.28
32	Q	898	LYS	C-N-CA	5.26	127.33	120.28
10	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
32	Q	829	ASP	CB-CA-C	5.24	120.38	109.95
6	A	1942	ASP	O-C-N	5.24	125.14	120.48
32	Q	749	PRO	CA-C-N	5.23	126.38	119.84
32	Q	749	PRO	C-N-CA	5.23	126.38	119.84
33	t	236	THR	CA-C-N	-5.22	114.86	120.03
33	t	236	THR	C-N-CA	-5.22	114.86	120.03
12	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

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	Q	844	THR	N-CA-CB	5.19	117.75	110.12
32	Q	959	THR	CA-C-N	5.19	130.55	121.52
32	Q	959	THR	C-N-CA	5.19	130.55	121.52
33	v	348	TYR	N-CA-C	5.18	116.17	108.60
14	K	74	ILE	N-CA-CB	5.18	117.59	110.54
15	L	14	ASP	N-CA-C	5.18	117.34	111.02
33	w	236	THR	CA-C-N	-5.18	114.90	120.03
33	w	236	THR	C-N-CA	-5.18	114.90	120.03
32	Q	814	VAL	N-CA-C	5.18	114.86	109.01
34	s	134	GLN	N-CA-C	-5.17	104.90	111.11
33	t	348	TYR	N-CA-C	5.17	116.14	108.60
32	Q	705	ASP	CA-C-N	-5.17	111.67	121.54
32	Q	705	ASP	C-N-CA	-5.17	111.67	121.54
32	Q	483	ASP	N-CA-CB	-5.15	102.53	110.20
6	A	1752	VAL	N-CA-CB	5.15	117.54	110.54
32	Q	391	GLY	CA-C-N	5.15	128.92	120.63
32	Q	391	GLY	C-N-CA	5.15	128.92	120.63
33	u	236	THR	CA-C-N	-5.14	114.94	120.03
33	u	236	THR	C-N-CA	-5.14	114.94	120.03
7	B	1481	GLN	N-CA-C	5.14	119.19	113.02
33	w	348	TYR	N-CA-C	5.13	116.09	108.60
32	Q	784	PRO	CA-C-N	5.13	132.13	123.01
32	Q	784	PRO	C-N-CA	5.13	132.13	123.01
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
33	u	348	TYR	N-CA-C	5.12	116.07	108.60
32	Q	486	LEU	N-CA-CB	5.12	117.59	109.82
32	Q	442	GLU	CA-C-N	5.11	131.30	121.54
32	Q	442	GLU	C-N-CA	5.11	131.30	121.54
32	Q	384	ALA	N-CA-CB	5.10	118.72	110.40
32	Q	917	LYS	CA-C-N	5.10	131.15	121.97
32	Q	917	LYS	C-N-CA	5.10	131.15	121.97
33	v	236	THR	CA-C-N	-5.10	114.98	120.03
33	v	236	THR	C-N-CA	-5.10	114.98	120.03
32	Q	495	ARG	CA-C-N	5.09	131.08	123.24
32	Q	495	ARG	C-N-CA	5.09	131.08	123.24
6	A	1657	ILE	O-C-N	5.08	126.89	121.91
16	M	167	LEU	N-CA-C	5.08	118.74	112.54
34	s	110	GLU	N-CA-C	5.08	117.80	110.28
18	O	41	GLN	N-CA-C	5.08	118.25	111.75
32	Q	896	SER	N-CA-C	5.07	121.61	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	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
34	s	111	VAL	N-CA-C	5.06	119.87	109.34
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
15	L	47	GLU	CA-C-O	-5.06	115.49	120.90
33	v	109	LEU	CA-C-N	5.06	127.06	120.28
33	v	109	LEU	C-N-CA	5.06	127.06	120.28
12	H	440	LEU	N-CA-CB	5.05	117.33	110.01
20	R	31	ARG	N-CA-C	5.05	120.97	109.81
32	Q	897	GLY	N-CA-C	5.04	125.14	113.18
6	A	766	ILE	CB-CA-C	5.04	118.95	112.14
13	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
32	Q	371	ILE	O-C-N	5.04	128.10	122.61
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
33	t	361	SER	CA-C-N	5.02	125.04	119.32
33	t	361	SER	C-N-CA	5.02	125.04	119.32
32	Q	402	VAL	CA-C-N	5.01	127.41	120.29
32	Q	402	VAL	C-N-CA	5.01	127.41	120.29
32	Q	445	LYS	CB-CA-C	-5.01	100.20	109.37
33	u	361	SER	CA-C-N	5.01	125.03	119.32
33	u	361	SER	C-N-CA	5.01	125.03	119.32
2	E	-10	A	C2'-C3'-O3'	5.00	117.01	109.50

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	403	TYR	Peptide
11	G	3	ARG	Peptide
16	M	231	ASP	Peptide
18	O	567	ARG	Mainchain
18	O	83	GLN	Peptide
32	Q	367	GLN	Peptide
32	Q	390	GLU	Peptide
32	Q	399	SER	Peptide
32	Q	429	VAL	Peptide
32	Q	439	THR	Peptide
32	Q	441	SER	Peptide

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Mol	Chain	Res	Type	Group
32	Q	442	GLU	Peptide
32	Q	444	THR	Peptide
32	Q	445	LYS	Peptide
32	Q	446	LEU	Peptide
32	Q	465	ASP	Peptide
32	Q	468	SER	Peptide
32	Q	501	LEU	Peptide
32	Q	541	VAL	Peptide
32	Q	543	ASP	Peptide
32	Q	628	HIS	Peptide
32	Q	662	LYS	Peptide
32	Q	705	ASP	Peptide
32	Q	706	THR	Peptide
32	Q	707	PHE	Peptide
32	Q	733	SER	Peptide
32	Q	736	VAL	Peptide
32	Q	737	THR	Peptide
32	Q	744	PRO	Peptide
32	Q	745	PHE	Peptide
32	Q	747	ASP	Peptide
32	Q	748	LYS	Peptide
32	Q	749	PRO	Peptide
32	Q	797	VAL	Peptide
32	Q	798	ARG	Peptide
32	Q	833	ASN	Peptide
32	Q	856	ASN	Peptide
32	Q	857	PHE	Peptide
32	Q	889	GLN	Peptide
32	Q	893	VAL	Peptide
32	Q	895	SER	Peptide
32	Q	896	SER	Peptide
32	Q	911	PHE	Peptide
32	Q	915	ALA	Peptide
32	Q	916	ALA	Peptide
32	Q	923	ASN	Peptide
32	Q	924	TYR	Peptide
32	Q	944	LEU	Peptide
32	Q	960	SER	Peptide
32	Q	977	GLU	Peptide
21	S	237	ILE	Peptide
34	s	111	VAL	Peptide
34	s	132	LEU	Peptide

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Mol	Chain	Res	Type	Group
33	t	3	CYS	Mainchain
33	v	109	LEU	Mainchain
33	w	134	SER	Mainchain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	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	16	0
5	V	2066	0	1042	23	0
6	A	16919	0	16184	261	0
7	B	8462	0	3706	35	0
8	D	912	0	936	12	0
9	F	321	0	282	6	0
10	C	6756	0	6801	122	0
11	G	823	0	808	29	0
12	H	2639	0	2073	26	0
13	J	2556	0	2551	60	0
14	K	1289	0	1309	20	0
15	L	1270	0	1294	13	0
16	M	2012	0	1968	33	0
17	N	1658	0	1712	65	0
18	O	2068	0	1853	42	0
19	P	275	0	283	4	0
20	R	544	0	345	18	0
21	S	3121	0	2399	59	0
22	T	2946	0	1252	16	0
23	b	631	0	670	2	0
23	k	396	0	169	0	0
24	d	625	0	647	6	0
24	n	404	0	180	0	0
25	e	575	0	597	7	0
25	p	369	0	152	0	0
26	f	573	0	572	4	0
26	q	354	0	153	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	g	529	0	557	3	0
27	r	340	0	152	0	0
28	h	644	0	686	3	0
28	l	392	0	165	0	0
29	j	741	0	778	3	0
29	m	467	0	199	0	0
30	W	816	0	341	1	0
31	Y	416	0	182	0	0
32	Q	3066	0	1345	53	0
33	t	2171	0	945	5	0
33	u	2166	0	942	5	0
33	v	2111	0	917	32	0
33	w	2156	0	938	3	0
34	s	548	0	219	10	0
35	x	660	0	142	7	0
36	E	1	0	0	0	0
36	V	1	0	0	0	0
37	D	1	0	0	1	0
37	L	3	0	0	0	0
37	M	1	0	0	0	0
37	N	2	0	0	5	0
38	C	32	0	12	0	0
All	All	85476	0	62328	882	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 (882) 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)
11:G:22:SER:HB2	33:v:276:VAL:N	1.39	1.36
32:Q:434:ARG:O	32:Q:874:ARG:HA	1.26	1.35
17:N:34:CYS:SG	17:N:37:CYS:SG	1.35	1.34
20:R:36:GLN:O	20:R:40:GLN:N	1.60	1.32
1:U:45:A:N1	1:U:74:U:O4	1.65	1.30
11:G:42:LYS:CD	33:v:281:GLU:O	1.83	1.26
21:S:467:GLN:CA	21:S:471:LEU:HA	1.65	1.24
32:Q:472:ILE:CB	32:Q:503:ILE:H	1.55	1.19
32:Q:434:ARG:C	32:Q:874:ARG:HA	1.69	1.18
17:N:16:CYS:SG	17:N:73:CYS:HB2	1.85	1.16
32:Q:435:PHE:HA	32:Q:877:ASP:N	1.61	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:22:SER:CB	33:v:276:VAL:H	1.61	1.12
32:Q:472:ILE:CB	32:Q:503:ILE:N	2.11	1.11
32:Q:472:ILE:CB	32:Q:503:ILE:CA	2.28	1.11
11:G:22:SER:CB	33:v:276:VAL:N	2.13	1.11
11:G:42:LYS:HD3	33:v:281:GLU:O	0.95	1.11
16:M:108:VAL:HG11	17:N:59:LEU:HD13	1.26	1.10
20:R:37:GLN:O	20:R:41:GLN:CB	2.00	1.10
16:M:108:VAL:HG21	17:N:73:CYS:O	1.52	1.09
32:Q:435:PHE:CA	32:Q:877:ASP:H	1.65	1.07
32:Q:672:SER:HA	32:Q:956:LEU:O	1.55	1.05
6:A:2364:THR:H	32:Q:521:PRO:N	1.56	1.03
22:T:360:LYS:CB	22:T:381:HIS:CB	2.36	1.03
21:S:467:GLN:CB	21:S:471:LEU:O	2.07	1.02
11:G:22:SER:HB2	33:v:276:VAL:CA	1.90	1.02
21:S:467:GLN:HA	21:S:471:LEU:HA	1.03	1.01
17:N:61:CYS:HG	37:N:401:ZN:ZN	0.67	1.00
21:S:467:GLN:HA	21:S:471:LEU:CA	1.90	0.99
6:A:2364:THR:N	32:Q:521:PRO:N	2.13	0.96
32:Q:435:PHE:HA	32:Q:877:ASP:H	1.14	0.95
17:N:61:CYS:SG	37:N:401:ZN:ZN	1.54	0.94
33:t:20:ARG:CB	33:u:52:GLU:O	2.16	0.93
32:Q:472:ILE:CB	32:Q:503:ILE:HA	1.98	0.92
22:T:429:SER:O	22:T:433:LEU:N	2.03	0.92
21:S:467:GLN:CA	21:S:471:LEU:CA	2.37	0.92
16:M:108:VAL:HG22	17:N:75:MET:HG2	1.53	0.91
32:Q:472:ILE:CB	32:Q:503:ILE:C	2.43	0.91
34:s:114:LEU:O	34:s:118:ASP:N	2.04	0.90
21:S:332:GLU:CB	21:S:338:ILE:CB	2.51	0.89
21:S:467:GLN:CB	21:S:471:LEU:HA	2.03	0.89
32:Q:472:ILE:CB	32:Q:503:ILE:O	2.22	0.88
20:R:36:GLN:O	20:R:40:GLN:CB	2.21	0.88
21:S:332:GLU:CB	21:S:334:PHE:O	2.22	0.88
16:M:108:VAL:HG11	17:N:59:LEU:CD1	2.03	0.88
21:S:467:GLN:CB	21:S:471:LEU:CA	2.52	0.87
22:T:420:SER:O	22:T:421:ALA:O	1.93	0.87
32:Q:528:ARG:CB	32:Q:530:PHE:N	2.39	0.86
32:Q:673:LEU:H	32:Q:957:LEU:HA	1.38	0.85
33:v:212:MET:O	33:v:222:PHE:HA	1.75	0.85
8:D:88:CYS:SG	37:D:1001:ZN:ZN	1.65	0.85
7:B:479:GLU:HA	7:B:498:SER:CB	2.07	0.85
11:G:22:SER:CB	33:v:276:VAL:O	2.25	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2364:THR:CB	32:Q:521:PRO:N	2.40	0.84
33:v:81:LEU:HA	34:s:99:ASP:CB	2.07	0.84
11:G:22:SER:HB2	33:v:276:VAL:C	2.01	0.84
32:Q:587:PHE:O	32:Q:591:TYR:CB	2.26	0.84
17:N:16:CYS:SG	17:N:73:CYS:CB	2.65	0.84
32:Q:434:ARG:O	32:Q:874:ARG:CA	2.21	0.84
16:M:250:MET:HB2	17:N:139:LEU:HD11	1.58	0.83
20:R:28:ASN:O	20:R:32:PRO:CD	2.27	0.83
13:J:210:ASP:HB2	13:J:217:ILE:HD11	1.61	0.83
7:B:1182:ALA:O	32:Q:496:ARG:HA	1.80	0.82
16:M:108:VAL:HG22	17:N:75:MET:CG	2.10	0.82
18:O:564:TYR:HA	18:O:566:TYR:H	1.44	0.82
17:N:220:THR:HG22	17:N:240:LEU:HD12	1.62	0.81
6:A:759:ARG:HD2	6:A:783:LEU:HD13	1.61	0.81
18:O:564:TYR:CA	18:O:566:TYR:H	1.93	0.81
21:S:329:LEU:HA	21:S:338:ILE:CB	2.10	0.81
10:C:389:LEU:HD21	10:C:421:LEU:HD12	1.64	0.80
20:R:36:GLN:O	20:R:40:GLN:CA	2.29	0.79
32:Q:459:LEU:CB	32:Q:782:LYS:CB	2.60	0.79
11:G:22:SER:HB2	33:v:276:VAL:O	1.83	0.79
6:A:628:MET:HE3	6:A:660:ILE:HG23	1.64	0.78
21:S:467:GLN:CB	21:S:471:LEU:C	2.56	0.77
18:O:564:TYR:HA	18:O:566:TYR:N	2.00	0.77
5:V:67:C:H2'	5:V:68:C:O4'	1.85	0.76
32:Q:586:LYS:O	32:Q:590:VAL:N	2.19	0.76
20:R:37:GLN:O	20:R:41:GLN:N	2.19	0.76
16:M:108:VAL:CG1	17:N:59:LEU:HD13	2.14	0.76
13:J:323:VAL:HG12	13:J:336:LEU:HD12	1.67	0.75
1:U:45:A:N1	1:U:74:U:C4	2.54	0.75
32:Q:434:ARG:C	32:Q:874:ARG:CA	2.57	0.75
17:N:113:LEU:HD11	17:N:120:LEU:HD11	1.69	0.75
16:M:22:ILE:HG23	16:M:23:PRO:HD3	1.67	0.74
17:N:37:CYS:SG	37:N:401:ZN:ZN	1.77	0.74
21:S:332:GLU:CB	21:S:335:PRO:HA	2.18	0.73
32:Q:459:LEU:HA	32:Q:782:LYS:CB	2.17	0.73
18:O:230:THR:HG23	21:S:116:ASN:HD21	1.53	0.73
5:V:76:A:OP2	6:A:749:ARG:NH1	2.21	0.73
16:M:108:VAL:CG1	17:N:59:LEU:HD22	2.20	0.72
17:N:71:CYS:SG	37:N:402:ZN:ZN	1.77	0.72
6:A:1361:VAL:HG21	6:A:1407:ILE:HD11	1.72	0.72
8:D:51:CYS:SG	8:D:88:CYS:HB3	2.30	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
33:v:20:ARG:CB	33:w:51:VAL:CB	2.68	0.71
7:B:1163:SER:CA	32:Q:497:ARG:O	2.32	0.71
24:d:50:THR:HG22	24:d:56:VAL:HG12	1.71	0.71
6:A:1335:TRP:CZ2	6:A:1339:LEU:HD13	2.25	0.71
25:e:77:LEU:HD21	25:e:80:ILE:HD12	1.73	0.71
6:A:745:THR:HA	13:J:182:VAL:HG21	1.73	0.70
6:A:631:LEU:HD21	6:A:663:LEU:HD12	1.73	0.70
10:C:406:VAL:HG11	10:C:427:LEU:HB3	1.71	0.70
16:M:250:MET:CB	17:N:139:LEU:HD11	2.21	0.70
10:C:493:LEU:HD21	10:C:539:VAL:HG21	1.74	0.70
21:S:209:GLU:HB3	21:S:218:THR:HG22	1.75	0.69
32:Q:672:SER:CA	32:Q:956:LEU:O	2.37	0.69
11:G:42:LYS:NZ	33:v:282:VAL:HA	2.08	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
28:h:3:LEU:HD11	29:j:60:ALA:HB1	1.75	0.68
28:h:43:VAL:HG11	28:h:85:ILE:HD12	1.76	0.68
6:A:1342:LEU:CD2	6:A:1360:LEU:HD21	2.24	0.68
13:J:206:VAL:HG11	13:J:241:THR:HG21	1.76	0.67
16:M:108:VAL:HG13	17:N:59:LEU:HD22	1.76	0.67
20:R:28:ASN:O	20:R:32:PRO:HD3	1.93	0.67
32:Q:459:LEU:CA	32:Q:782:LYS:CB	2.72	0.67
32:Q:435:PHE:CA	32:Q:877:ASP:N	2.34	0.67
4:Z:99:U:OP1	33:v:365:ALA:HB2	1.95	0.67
7:B:1163:SER:O	7:B:1164:THR:CB	2.43	0.67
10:C:621:ALA:HB2	10:C:664:ALA:HB2	1.76	0.67
10:C:241:VAL:HG11	10:C:273:LEU:HD23	1.76	0.66
18:O:21:LEU:HD12	18:O:40:LEU:HD11	1.76	0.66
6:A:1144:PHE:CD2	6:A:1145:MET:HE2	2.31	0.66
10:C:200:CYS:HB3	10:C:436:VAL:HG21	1.78	0.66
13:J:290:VAL:HG12	13: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	13:J:224:LEU:HD22	1.78	0.65
16:M:108:VAL:CG2	17:N:75:MET:HG2	2.24	0.65
6:A:1286:TRP:CE2	6:A:1302:LEU:HD11	2.31	0.65
11:G:42:LYS:CG	33:v:281:GLU:O	2.44	0.65
18:O:60:LEU:HD21	18:O:94:PRO:HB3	1.79	0.65
11:G:22:SER:CB	33:v:276:VAL:CA	2.67	0.65
12:H:299:LEU:HD11	12:H:329:ILE:HG12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:716:ARG:O	6:A:720:PRO:HD2	1.97	0.64
10:C:193:LEU:HD11	10:C:228:ALA:HB2	1.78	0.64
34:s:107:GLU:CB	34:s:110:GLU:CB	2.76	0.64
17:N:125:ILE:HG21	17:N:135:ILE:HD12	1.80	0.64
13:J:282:VAL:HG11	13:J:323:VAL:HG21	1.80	0.64
17:N:71:CYS:HG	37:N:402:ZN:ZN	1.11	0.64
6:A:1344:THR:O	6:A:1347:ARG:NH1	2.30	0.64
13:J:142:VAL:HG11	13:J:423:ILE:CG2	2.28	0.64
10:C:323:THR:HG21	10:C:438:ALA:HB2	1.81	0.63
6:A:630:LYS:O	6:A:634:ASP:N	2.26	0.63
10:C:501:ILE:HD13	10:C:567:ILE:HG23	1.79	0.63
10:C:872:LEU:HD13	10:C:922:THR:HG22	1.79	0.63
5:V:90:U:O2'	5:V:92:C:C6	2.52	0.63
6:A:886:MET:HE2	6:A:1120:VAL:HG22	1.80	0.63
22:T:429:SER:O	22:T:433:LEU:CB	2.47	0.62
12:H:445:LEU:HD11	12:H:448:MET:HG3	1.80	0.62
21:S:225:ALA:O	21:S:229:VAL:HG23	1.98	0.62
20:R:37:GLN:C	20:R:41:GLN:H	2.07	0.62
8:D:63:LYS:HE3	9:F:6:LEU:HD22	1.80	0.62
6:A:213:TYR:HA	6:A:216:GLN:HE21	1.63	0.62
5:V:90:U:O2'	5:V:92:C:C5	2.53	0.62
6:A:673:VAL:HG22	6:A:714:PHE:CE1	2.34	0.62
10:C:251:GLN:HG2	10:C:933:TRP:CD2	2.35	0.61
13:J:277:VAL:HG11	13:J:321:PHE:CZ	2.36	0.61
16:M:108:VAL:CG2	17:N:73:CYS:O	2.40	0.61
6:A:857:ILE:HD11	6:A:969:ILE:HD11	1.82	0.61
17:N:91:ILE:HD12	17:N:125:ILE:HD12	1.82	0.61
6:A:268:LEU:HD13	6:A:277:LYS:HB2	1.82	0.61
10:C:602:VAL:HG11	10:C:860:PRO:HG3	1.81	0.61
6:A:673:VAL:HG22	6:A:714:PHE:CZ	2.36	0.61
7:B:1162:ALA:O	32:Q:367:GLN:N	2.34	0.61
21:S:149:VAL:O	21:S:152:VAL:HG12	2.01	0.61
6:A:628:MET:HE1	6:A:664:THR:HB	1.82	0.61
32:Q:435:PHE:CB	32:Q:877:ASP:H	2.12	0.61
15:L:139:GLN:OE1	33:t:453:LYS:CB	2.49	0.61
6:A:1557:LEU:HD13	6:A:1562:PHE:CE2	2.36	0.61
10:C:133:ILE:HD13	10:C:560:GLN:HB3	1.83	0.61
21:S:332:GLU:CB	21:S:334:PHE:C	2.74	0.60
7:B:487:CYS:O	7:B:490:ALA:N	2.33	0.60
10:C:270:LEU:HD11	10:C:313:PHE:HB3	1.82	0.60
17:N:39:LEU:HD13	17:N:40:PRO:HD2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:137:GLU:CD	15: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	11:G:1:MET:N	2.34	0.60
7:B:1973:ALA:O	7:B:1976:ALA:HB3	2.01	0.60
13:J:323:VAL:CG1	13:J:336:LEU:HD12	2.32	0.60
22:T:554:ALA:CB	35:x:120:UNK:CB	2.79	0.60
22:T:554:ALA:HB1	35:x:120:UNK:CB	2.30	0.60
15:L:66:LEU:HD13	15:L:73:ILE:HG13	1.83	0.59
1:U:71:A:N3	1:U:116:U:O2'	2.33	0.59
8:D:51:CYS:SG	8:D:88:CYS:SG	3.00	0.59
10:C:656:LEU:HD22	10:C:670:ILE:HD11	1.85	0.59
10:C:866:ILE:HB	10:C:902:VAL:HG13	1.83	0.59
6:A:1032:ILE:HG12	6:A:1171:LEU:HD22	1.83	0.59
20:R:37:GLN:O	20:R:41:GLN:CA	2.51	0.59
32:Q:402:VAL:CB	32:Q:449:VAL:H	2.15	0.59
17:N:16:CYS:HG	17:N:73:CYS:HB2	1.63	0.59
10:C:499:VAL:HG11	10:C:577:LEU:HD13	1.83	0.59
13:J:164:MET:HE1	13:J:199:SER:HB2	1.84	0.59
21:S:173:VAL:HG23	21:S:188:ILE:HD11	1.85	0.59
32:Q:452:GLY:O	32:Q:784:PRO:CB	2.50	0.59
6:A:390:LEU:HD21	10:C:605:ILE:HD11	1.85	0.58
13:J:240:ALA:HB1	13:J:248:ILE:HD11	1.82	0.58
13:J:160:ASN:HA	13:J:184:THR:HB	1.85	0.58
17:N:39:LEU:HD23	17:N:111:ARG:HG2	1.85	0.58
12:H:298:VAL:HG11	12:H:312:LEU:HD23	1.84	0.58
6:A:842:LYS:O	6:A:845:VAL:HG12	2.02	0.58
17:N:207:LEU:HD11	17:N:251:LEU:HD11	1.86	0.58
17:N:16:CYS:SG	17:N:71:CYS:SG	3.02	0.58
13:J:248:ILE:HG23	13:J:262:LEU:HB2	1.84	0.58
32:Q:425:LEU:HA	32:Q:429:VAL:CB	2.33	0.58
6:A:1668:ILE:HD13	6:A:1801:SER:HB3	1.86	0.58
18:O:185:LEU:O	18:O:188:ARG:HG3	2.03	0.58
13:J:147:ILE:HD13	13:J:408:ASP:HA	1.84	0.57
17:N:16:CYS:SG	17:N:73:CYS:SG	3.02	0.57
7:B:1502:LEU:O	7:B:1503:GLU:C	2.47	0.57
6:A:1632:ILE:HG21	6:A:1645:LEU:HD13	1.85	0.57
18:O:185:LEU:O	18: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	18:O:90:MET:HE3	1.70	0.57
6:A:305:LEU:HD21	6:A:476:ALA:HB2	1.85	0.57
4:Z:100:G:OP2	33:v:365:ALA:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:66:LEU:HD13	15: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
10:C:328:VAL:HG21	10:C:345:THR:HG22	1.87	0.56
21:S:229:VAL:HG22	21:S:238:TRP:HZ2	1.69	0.56
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
32:Q:456:ARG:CB	32:Q:784:PRO:CB	2.83	0.56
6:A:718:THR:O	6:A:719:ILE:C	2.48	0.56
12:H:465:PHE:HB2	12: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	13:J:183:MET:HE3	1.86	0.56
6:A:948:HIS:CE1	6:A:952:ASN:HD21	2.23	0.56
8:D:51:CYS:SG	8:D:88:CYS:CB	2.94	0.56
18:O:33:TRP:CE3	18:O:36:VAL:HG11	2.41	0.56
21:S:184:GLY:O	21:S:188:ILE:HG23	2.05	0.56
13:J:289:THR:HG22	13:J:305:THR:HG22	1.88	0.56
32:Q:673:LEU:N	32:Q:957:LEU:HA	2.17	0.56
17:N:226:LEU:HD13	17:N:266:ILE:HD11	1.87	0.56
32:Q:434:ARG:CB	32:Q:874:ARG:O	2.54	0.56
6:A:878:GLU:O	6:A:882:ILE:HG23	2.06	0.56
8:D:11:TYR:CD1	11:G:12:LEU:HD21	2.41	0.56
18:O:230:THR:HG21	21:S:117:HIS:ND1	2.21	0.56
20:R:31:ARG:N	20:R:32:PRO:CD	2.68	0.56
22:T:420:SER:O	22:T:421:ALA:C	2.49	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
13:J:277:VAL:HG13	13:J:278:ASP:N	2.20	0.55
17:N:106:ASN:HD21	18:O:208:GLY:HA2	1.71	0.55
15:L:94:LYS:HD2	15:L:109:ILE:HD11	1.87	0.55
22:T:299:PRO:O	22:T:300:ASP:C	2.49	0.55
6:A:1000:TRP:CZ2	6:A:1510:ILE:HG21	2.41	0.55
7:B:1795:SER:O	7:B:1798:GLY:N	2.39	0.55
6:A:659:HIS:O	6:A:660:ILE:C	2.49	0.55
18:O:37:ALA:HB2	18:O:45:ALA:HA	1.88	0.55
34:s:114:LEU:O	34:s:118:ASP:CA	2.54	0.55
6:A:724:ARG:O	6:A:728:ASN:HB2	2.07	0.55
10:C:472:VAL:HB	10:C:575:ALA:HB3	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:M:163:VAL:HG23	16:M:164:PHE:HD1	1.71	0.55
21:S:122:MET:HE1	21:S:142:VAL:HG11	1.87	0.55
1:U:92:U:O2	20: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
20:R:28:ASN:O	20:R:32:PRO:HD2	2.04	0.55
32:Q:587:PHE:O	32:Q:591:TYR:N	2.39	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	10:C:893:LYS:HB3	2.42	0.54
6:A:1542:TYR:O	6:A:1546:VAL:HG23	2.07	0.54
17:N:106:ASN:HB2	18: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
5:V:90:U:HO2'	5:V:92:C:H5	1.50	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
6:A:2364:THR:CA	32:Q:521:PRO:N	2.70	0.54
17:N:17:LEU:CD2	17:N:23:ILE:HD12	2.37	0.54
20:R:31:ARG:N	20:R:32:PRO:HD2	2.23	0.54
4:Z:99:U:OP1	33:v:365:ALA:CB	2.56	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
17:N:29:PRO:HA	17:N:42:THR:HG22	1.90	0.54
18:O:211:ILE:HD13	21:S:44:ARG:HG3	1.89	0.54
21:S:99:ILE:N	21:S:100:PRO:CD	2.70	0.54
30:W:121:PRO:O	30:W:122:ARG:CB	2.56	0.54
18:O:16:VAL:HG22	18:O:152:LEU:HD21	1.88	0.54
21:S:119:ARG:HA	21:S:122:MET:HE3	1.90	0.54
6:A:141:LYS:HG3	15:L:52:ILE:HD11	1.90	0.54
13:J:164:MET:HE2	13:J:185:VAL:HG21	1.90	0.54
6:A:880:THR:OG1	14: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
10:C:861:ILE:HD11	10:C:938:ARG:HB2	1.89	0.54
11:G:42:LYS:HZ2	33:v:282:VAL:HA	1.71	0.54
6:A:137:GLU:CD	15:L:52:ILE:HG23	2.33	0.53
10:C:138:VAL:HG23	10:C:236:LEU:HB2	1.90	0.53
10:C:265:PHE:HB2	10:C:311:ILE:HD13	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:U:102:C:OP1	6:A:675:HIS:NE2	2.42	0.53
10:C:191:ILE:HG23	10:C:221:PHE:CE2	2.44	0.53
25:e:77:LEU:HD21	25:e:80:ILE:CD1	2.37	0.53
5:V:35:A:C8	15:L:41:LEU:HD13	2.43	0.53
10:C:241:VAL:HG22	10:C:267:ILE:CG2	2.38	0.53
17:N:64:CYS:SG	17:N:114:SER:HB2	2.48	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
13:J:277:VAL:HG11	13:J:321:PHE:HZ	1.71	0.53
6:A:1669:LEU:HD22	6:A:1703:MET:HE3	1.91	0.53
10:C:864:VAL:HG22	10:C:930:LEU:HD23	1.90	0.53
6:A:882:ILE:HD11	6:A:1065:LEU:HD21	1.90	0.53
13:J:306:HIS:CE1	14: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
8:D:101:PRO:HB2	9:F:23:VAL:HG21	1.90	0.53
13:J:142:VAL:HG11	13: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
10:C:201:THR:HG22	10:C:207:SER:HB3	1.90	0.53
10:C:126:MET:SD	10:C:132:ARG:NH2	2.82	0.53
20:R:36:GLN:C	20:R:40:GLN:CB	2.82	0.53
6:A:937:LEU:HD22	6:A:1590:LEU:CD2	2.39	0.52
7:B:1928:LEU:O	7:B:1931:GLN:N	2.40	0.52
11:G:55:SER:O	11:G:58:ILE:HG22	2.10	0.52
1:U:32:G:H3'	1:U:33:U:C5'	2.38	0.52
10:C:836:SER:O	10:C:840:PRO:HD2	2.09	0.52
13:J:341:LEU:HD23	13:J:342:LEU:N	2.24	0.52
16:M:130:PHE:CE1	17:N:75:MET:HE2	2.44	0.52
22:T:119:ALA:HB1	22:T:128:ILE:CA	2.39	0.52
6:A:937:LEU:HD22	6:A:1590:LEU:HD22	1.91	0.52
14:K:133:LYS:O	17: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
14:K:201:PHE:CD2	18:O:80:LEU:HD21	2.45	0.52
22:T:554:ALA:HA	35:x:120:UNK:CB	2.40	0.52
18:O:564:TYR:C	18:O:566:TYR:H	2.18	0.52
33:v:96:PHE:CB	34:s:92:ARG:CB	2.87	0.52
6:A:1339:LEU:HD11	6:A:1360:LEU:HD22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:1163:SER:N	32:Q:497:ARG:O	2.42	0.52
13:J:335:GLY:H	13:J:342:LEU:HD13	1.74	0.52
4:Z:99:U:P	33:v:365:ALA:HB2	2.49	0.52
4:Z:100:G:OP1	33:v:366:SER:O	2.28	0.52
6:A:1207:TRP:O	6:A:1212:ARG:NH1	2.42	0.52
32:Q:465:ASP:C	32:Q:467:TYR:H	2.18	0.52
6:A:730:ILE:HD12	6:A:731:THR:N	2.25	0.52
6:A:785:HIS:NE2	14: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
10:C:127:ALA:HB2	10:C:209:MET:HE3	1.91	0.52
10:C:539:VAL:HG13	10:C:564:ILE:HG23	1.92	0.52
6:A:1654:TRP:CZ3	6:A:1779:LEU:HD12	2.45	0.51
21:S:199:MET:SD	21:S:246:LEU:HD22	2.50	0.51
32:Q:673:LEU:O	32:Q:958:MET:CB	2.58	0.51
6:A:212:VAL:HG22	6:A:311:LEU:HD11	1.92	0.51
6:A:808:ILE:HG21	14:K:165:ILE:HD12	1.91	0.51
10:C:626:SER:HB3	10:C:634:ILE:HD12	1.91	0.51
12:H:333:SER:HA	12:H:343:TYR:CE2	2.46	0.51
3:I:2:U:O4	4:Z:37:G:H1'	2.10	0.51
10:C:664:ALA:HB1	10:C:666:ILE:CD1	2.39	0.51
10:C:664:ALA:HB1	10:C:666:ILE:HD12	1.92	0.51
12:H:347:SER:O	12:H:351:ILE:HG12	2.09	0.51
18:O:16:VAL:CG2	18:O:152:LEU:HD21	2.40	0.51
6:A:249:LEU:HD12	6:A:249:LEU:O	2.11	0.51
7:B:1105:ALA:O	7:B:1106:GLY:C	2.54	0.51
9:F:34:GLN:HE22	35:x:43:UNK:HA	1.76	0.51
7:B:2036:SER:O	7:B:2039:ALA:HB3	2.11	0.51
28:h:82:LEU:HD12	28:h:85:ILE:HD11	1.92	0.51
6:A:153:MET:HE3	6:A:154:TYR:CD2	2.46	0.51
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
7:B:1399:ASN:O	7:B:1448:THR:HA	2.10	0.51
10:C:255:GLN:HG2	10:C:598:ILE:HD12	1.92	0.51
13:J:206:VAL:CG1	13:J:241:THR:HG21	2.40	0.51
34:s:93:ARG:O	34:s:94:LYS:CB	2.59	0.51
3:I:2:U:H3'	6:A:607:THR:OG1	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:963:SER:O	10:C:967:VAL:HG23	2.10	0.51
32:Q:425:LEU:O	32:Q:429:VAL:CB	2.59	0.51
32:Q:706:THR:C	32:Q:708:LYS:N	2.69	0.51
6:A:458:PHE:CZ	10:C:336:ILE:HD11	2.45	0.51
6:A:1329:THR:HG21	6:A:1601:ILE:HB	1.93	0.51
10:C:872:LEU:HD13	10:C:922:THR:CG2	2.41	0.51
12:H:326:VAL:O	12:H:330:ILE:HG12	2.10	0.51
13:J:275:THR:OG1	13:J:279:PRO:O	2.29	0.51
5:V:27:U:O2'	15: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	13:J:224:LEU:HD22	2.41	0.50
21:S:172:PHE:CD2	21:S:188:ILE:HD13	2.46	0.50
21:S:332:GLU:CB	21:S:335:PRO:CA	2.87	0.50
24:d:81:ALA:HB1	24: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
10:C:139:ILE:HG12	10:C:225:THR:HG23	1.93	0.50
3:I:3:A:OP2	11:G:3:ARG:HA	2.11	0.50
32:Q:840:SER:HA	32:Q:968:THR:HA	1.94	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
9:F:31:ILE:HD12	35:x:46:UNK:HA	1.94	0.50
10:C:493:LEU:HD22	10:C:542:ILE:HD11	1.93	0.50
34:s:114:LEU:O	34:s:118:ASP:CB	2.60	0.50
6:A:912:LEU:HD22	6:A:951:LEU:HG	1.94	0.50
10:C:615:LEU:N	10:C:616:PRO:HD2	2.26	0.50
10:C:617:LYS:HB3	10: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	12:H:345:ILE:HD11	2.36	0.50
9:F:31:ILE:HD11	35:x:45:UNK:CB	2.41	0.50
10:C:133:ILE:HG23	10:C:209:MET:SD	2.52	0.50
10:C:864:VAL:HG22	10:C:930:LEU:CD2	2.42	0.50
18:O:90:MET:HE2	18:O:90:MET:HA	1.93	0.50
18:O:230:THR:HG21	21:S:117:HIS:CE1	2.47	0.50
32:Q:433:ILE:O	32:Q:877:ASP:CB	2.60	0.50
6:A:1344:THR:HG21	6:A:1537:TRP:CD2	2.46	0.50
16:M:108:VAL:CG1	17:N:59:LEU:CD2	2.90	0.50
13:J:156:ILE:HG22	13:J:166:VAL:HG22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:200:VAL:CG2	13:J:227:VAL:HB	2.41	0.50
10:C:231:ALA:HB2	10:C:473:LEU:HD13	1.93	0.49
5:V:35:A:C8	16: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
16:M:108:VAL:HG22	17:N:75:MET:HG3	1.91	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
18:O:230:THR:HG22	21:S:114:CYS:SG	2.53	0.49
11:G:28:ASP:OD1	11:G:28:ASP:N	2.44	0.49
12:H:291:PHE:CE1	12:H:317:ILE:HG21	2.47	0.49
21:S:81:MET:HE3	21:S:112:VAL:HG11	1.94	0.49
25:e:91:THR:HB	27:g:61:THR:HG22	1.94	0.49
10:C:391:MET:HE1	10:C:399:LEU:HD11	1.94	0.49
6:A:937:LEU:HD13	6:A:1590:LEU:HD11	1.93	0.49
9:F:27:GLU:O	9:F:31:ILE:HG12	2.13	0.49
10:C:116:THR:HG21	10:C:118:TYR:CZ	2.47	0.49
10:C:544:LEU:HD23	10:C:562:VAL:HG12	1.94	0.49
13:J:145:VAL:HG22	13:J:157:THR:HG22	1.94	0.49
6:A:1400:ILE:HG22	6:A:1400:ILE:O	2.12	0.49
10:C:137:GLY:O	10:C:139:ILE:HD12	2.13	0.49
18:O:20:ILE:HD11	18:O:152:LEU:HD22	1.95	0.49
21:S:99:ILE:HD11	21: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
13:J:150:VAL:HG13	13:J:151:ASP:HB3	1.95	0.49
22:T:332:GLN:CB	22:T:342:ILE:CB	2.91	0.49
33:t:51:VAL:CB	33:u:20:ARG:CB	2.91	0.49
4:Z:99:U:H5''	33:v:365:ALA:HB1	1.94	0.48
10:C:607:LEU:HD11	10:C:644:ILE:HD11	1.96	0.48
18:O:24:ALA:O	18:O:28:TYR:N	2.37	0.48
6:A:1557:LEU:HD13	6:A:1562:PHE:CD2	2.48	0.48
7:B:479:GLU:CA	7:B:498:SER:CB	2.86	0.48
10:C:213:LEU:HD11	10:C:561:ILE:HD13	1.95	0.48
12:H:427:LEU:HD23	12:H:436:LEU:HD11	1.95	0.48
6:A:724:ARG:CD	19:P:31:LEU:HD11	2.43	0.48
24:d:66:GLY:HA2	24:d:69:ILE:HD12	1.95	0.48
5:V:41:A:H2'	5:V:42:A:O4'	2.14	0.48
12:H:368:ASN:ND2	12:H:384:LEU:HD11	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
32:Q:430:GLY:HA3	32:Q:438:VAL:O	2.14	0.48
6:A:1669:LEU:HB3	6:A:1681:VAL:HG21	1.95	0.48
13:J:277:VAL:HG22	13:J:278:ASP:H	1.79	0.48
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
13:J:147:ILE:HG22	13:J:155:PHE:HB3	1.94	0.48
17:N:65:ALA:O	17:N:69:ASN:N	2.47	0.48
13:J:272:VAL:HG13	13:J:272:VAL:O	2.14	0.48
10:C:241:VAL:HG23	10:C:268:ASN:O	2.14	0.48
17:N:17:LEU:HD21	17: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
15:L:22:THR:HG21	15:L:62:TYR:CE1	2.49	0.48
5:V:32:U:C4	17:N:28:ILE:HG21	2.49	0.48
16:M:137:LEU:HD21	16:M:192:ALA:HB1	1.96	0.48
18:O:218:VAL:HB	21: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
10:C:273:LEU:HD12	10:C:274:ILE:N	2.29	0.47
10:C:625:ILE:HG22	10:C:634:ILE:HD11	1.95	0.47
21:S:140:LEU:HD22	21: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
10:C:229:LEU:HB3	10:C:259:ASN:HD21	1.79	0.47
14:K:41:ASP:HA	14:K:44:ILE:HD12	1.96	0.47
10:C:211:ASN:N	10:C:211:ASN:HD22	2.12	0.47
10:C:873:LEU:HD21	10:C:891:THR:HG21	1.94	0.47
12:H:355:ARG:O	12:H:359:THR:HG23	2.14	0.47
18:O:33:TRP:HA	18:O:36:VAL:HG12	1.96	0.47
21:S:112:VAL:HG13	21:S:114:CYS:HB2	1.96	0.47
22:T:119:ALA:HB1	22:T:128:ILE:HA	1.94	0.47
32:Q:435:PHE:CB	32:Q:874:ARG:C	2.85	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
10:C:136:VAL:O	10:C:234:LEU:O	2.33	0.47
13:J:341:LEU:HD22	14: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1388:PHE:CD1	6:A:1397:LEU:HD12	2.50	0.47
10:C:193:LEU:HD12	10:C:213:LEU:HB3	1.97	0.47
10:C:504:THR:HG23	10:C:574:SER:O	2.15	0.47
21:S:229:VAL:HG11	21:S:243:VAL:CG2	2.45	0.47
33:v:108:LYS:C	33:v:110:SER:N	2.70	0.47
7:B:990:ASP:O	7:B:994:ASP:N	2.45	0.47
6:A:687:ILE:HD11	6:A:706:PRO:HG3	1.97	0.47
8:D:23:LEU:HG	11:G:18:GLN:HE22	1.80	0.47
13:J:144:CYS:SG	13:J:187:ASP:HA	2.55	0.47
21:S:225:ALA:O	21: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
7:B:496:THR:O	7:B:497:THR:CB	2.63	0.46
14:K:104:LEU:HD12	14:K:113:GLU:HA	1.97	0.46
18:O:541:CYS:O	18:O:544:LEU:O	2.33	0.46
21:S:193:VAL:HG11	21:S:202:TRP:CZ2	2.50	0.46
32:Q:401:VAL:O	32:Q:402:VAL:CB	2.62	0.46
6:A:876:PRO:HA	14:K:204:LEU:HD22	1.97	0.46
6:A:1417:GLN:CG	6:A:1418:THR:HG23	2.45	0.46
11:G:22:SER:CA	33:v:276:VAL:CA	2.85	0.46
13:J:269:ILE:HA	13:J:285:SER:HA	1.97	0.46
6:A:319:ARG:O	6:A:321:GLU:N	2.48	0.46
8:D:31:LEU:HD11	11:G:31:ARG:NH2	2.30	0.46
10:C:312:ILE:HD13	10:C:435:LEU:HG	1.98	0.46
18:O:25:VAL:HG11	18:O:52:TRP:CH2	2.50	0.46
18:O:214:ASN:HB2	18: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
13:J:144:CYS:SG	13:J:145:VAL:N	2.89	0.46
6:A:286:LEU:HD13	6:A:287:GLU:N	2.30	0.46
7:B:781:LEU:O	7:B:785:ALA:N	2.41	0.46
12:H:369:TYR:CE1	12:H:420:ILE:HD11	2.51	0.46
12:H:465:PHE:CB	12:H:473:LEU:HD23	2.46	0.46
16:M:17:GLU:HB2	16:M:18:LEU:HD13	1.97	0.46
33:u:222:PHE:O	33:u:233:THR:HA	2.16	0.46
5:V:32:U:O4	17: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	20:R:16:THR:OG1	2.23	0.46
10:C:493:LEU:CD2	10:C:539:VAL:HG21	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:94:LYS:CD	15:L:109:ILE:HD11	2.45	0.46
24:d:33:LEU:HD23	24:d:34:VAL:N	2.31	0.46
33:w:222:PHE:O	33:w:233:THR:HA	2.16	0.46
10:C:873:LEU:N	10:C:874:PRO:CD	2.79	0.46
10:C:928:CYS:SG	10:C:929:GLN:N	2.89	0.46
13:J:248:ILE:HG13	13:J:262:LEU:HD12	1.98	0.46
18:O:230:THR:HG21	21:S:117:HIS:CG	2.51	0.46
32:Q:603:ILE:C	32:Q:605:ASP:H	2.24	0.46
12:H:334:LEU:HD21	12:H:384:LEU:HD12	1.98	0.46
16:M:99:ILE:HD13	16:M:188:TYR:CD2	2.51	0.46
18:O:530:VAL:O	18:O:533:LEU:N	2.48	0.46
34:s:12:ILE:C	34:s:14:ASP:H	2.24	0.46
34:s:115:GLY:O	34:s:119:SER:CB	2.63	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	12:H:303:LEU:HD22	1.98	0.45
10:C:501:ILE:CD1	10:C:567:ILE:HG23	2.46	0.45
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
10:C:837:GLN:HE21	10:C:837:GLN:HA	1.81	0.45
12:H:351:ILE:HG21	12:H:395:GLU:HG3	1.98	0.45
13:J:144:CYS:SG	13:J:188:VAL:N	2.88	0.45
13:J:284:SER:OG	13: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
10:C:492:LEU:HD12	10:C:492:LEU:O	2.16	0.45
12:H:330:ILE:HG22	12:H:334:LEU:CD2	2.46	0.45
21:S:169:TRP:CE3	21:S:192:TYR:HB2	2.51	0.45
33:t:310:THR:HA	33:t:325:HIS:O	2.17	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
10:C:274:ILE:HG21	10:C:385:PHE:CD2	2.51	0.45
10:C:470:ALA:HB1	10:C:486:VAL:HG12	1.98	0.45
10:C:936:ILE:HG23	10:C:936:ILE:O	2.16	0.45
17:N:216:GLU:O	17:N:220:THR:HG23	2.17	0.45
6:A:1461:TYR:CE1	6:A:1494:LEU:HD13	2.51	0.45
7:B:833:THR:O	7:B:834:LEU:C	2.58	0.45
7:B:1343:PHE:O	7:B:1345:PHE:N	2.49	0.45
12:H:312:LEU:CD1	12:H:329:ILE:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
13:J:229:THR:HG21	13:J:271:GLN:HA	1.98	0.45
25:e:45:GLY:HA3	25:e:53:VAL:HG12	1.97	0.45
6:A:2388:ARG:O	6:A:2389:PRO:C	2.57	0.45
13:J:161:ASP:O	13:J:162:THR:HB	2.17	0.45
21:S:202:TRP:CZ2	21: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
10:C:862:TYR:CE2	10:C:908:VAL:HG13	2.51	0.45
16:M:81:CYS:SG	16: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
11:G:22:SER:CA	33:v:276:VAL:O	2.66	0.44
21:S:140:LEU:HD23	21:S:152:VAL:HG22	1.99	0.44
33:v:310:THR:HA	33:v:325:HIS:O	2.16	0.44
6:A:173:LEU:HA	6:A:715:LEU:HD13	1.98	0.44
11:G:22:SER:HA	33:v:276:VAL:O	2.16	0.44
6:A:639:PHE:CG	6:A:649:LEU:HD22	2.52	0.44
7:B:479:GLU:HA	7:B:498:SER:CA	2.46	0.44
17:N:16:CYS:HB2	17:N:71:CYS:SG	2.57	0.44
33:w:310:THR:HA	33:w:325:HIS:O	2.17	0.44
7:B:1082:SER:O	7:B:1083:TYR:C	2.60	0.44
7:B:1382:LEU:O	7:B:1385:LEU:N	2.50	0.44
10:C:241:VAL:CG1	10:C:273:LEU:HD23	2.46	0.44
10:C:808:LEU:HD22	10:C:944:VAL:HG21	1.99	0.44
17:N:12:ILE:HG23	17:N:16:CYS:SG	2.57	0.44
18:O:80:LEU:O	18:O:81:PRO:C	2.61	0.44
33:u:310:THR:HA	33:u:325:HIS:O	2.17	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
10:C:223:ASP:OD1	10:C:224:GLU:N	2.50	0.44
11:G:18:GLN:HG3	11:G:19:GLN:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:H:292:LYS:CD	12: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	10: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	19:P:31:LEU:HD11	1.99	0.44
10:C:444:GLN:N	10:C:445:PRO:CD	2.81	0.44
6:A:687:ILE:HD11	6:A:706:PRO:CG	2.48	0.44
10:C:905:GLN:NE2	10:C:936:ILE:HD13	2.32	0.44
13:J:248:ILE:HD13	13:J:272:VAL:HG21	2.00	0.44
22:T:554:ALA:CA	35:x:120:UNK:CB	2.96	0.44
33:t:222:PHE:O	33:t:233:THR:HA	2.16	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
7:B:498:SER:O	7:B:499:LEU:C	2.60	0.44
10:C:708:ILE:HD12	10: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
16:M:114:ARG:NE	16:M:127:ILE:HG21	2.32	0.44
16:M:173:ILE:HG12	16:M:184:VAL:HG13	1.99	0.44
21:S:140:LEU:CD2	21:S:155:LEU:HD22	2.48	0.44
21:S:160:CYS:HB3	21: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
10:C:658:ASP:HB3	10:C:663:TYR:CE2	2.52	0.43
14:K:112:ILE:HD12	17:N:25:MET:HE3	2.00	0.43
16:M:74:LEU:HA	16:M:112:PHE:CE1	2.53	0.43
17:N:125:ILE:HG21	17:N:135:ILE:CD1	2.45	0.43
23:b:85:THR:HG22	24:d:73:VAL:HG22	1.99	0.43
6:A:268:LEU:HD13	6:A:277:LYS:CB	2.47	0.43
6:A:2278:SER:O	6:A:2282:ALA:HB2	2.18	0.43
11:G:42:LYS:NZ	33:v:282:VAL:CA	2.70	0.43
13:J:129:TRP:HB2	13:J:385:GLN:HE22	1.83	0.43
13:J:156:ILE:HD11	13:J:188:VAL:HG21	2.00	0.43
13:J:277:VAL:HG13	13:J:279:PRO:HD2	2.00	0.43
21:S:229:VAL:HG22	21: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:43:LEU:HD21	8:D:86:ILE:CD1	2.47	0.43
10:C:862:TYR:CG	10:C:908:VAL:HG22	2.53	0.43
13:J:142:VAL:HG12	13:J:142:VAL:O	2.18	0.43
17:N:91:ILE:CD1	17:N:125:ILE:HD12	2.48	0.43
21:S:193:VAL:HG11	21:S:202:TRP:CH2	2.54	0.43
32:Q:469:CYS:O	32:Q:470:VAL:C	2.61	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
10:C:78:MET:HE3	10:C:78:MET:HA	1.99	0.43
10:C:225:THR:HG21	10:C:252:LEU:CD2	2.48	0.43
14:K:35:ALA:CB	21:S:158:LYS:HE3	2.48	0.43
17:N:67:GLN:HB3	17:N:120:LEU:HD23	2.00	0.43
26:f:36:THR:HG21	26:f:60:VAL:HG22	2.00	0.43
10:C:335:SER:HB2	10:C:336:ILE:HD12	1.99	0.43
12:H:350:MET:HE2	12:H:357:TRP:CE2	2.53	0.43
17:N:71:CYS:HB3	17:N:74:CYS:HB2	2.00	0.43
21:S:92:LEU:C	21: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
12:H:381:LEU:HD21	12:H:419:PHE:CA	2.49	0.43
17:N:36:ILE:HD11	17:N:75:MET:HE1	1.99	0.43
6:A:834:ILE:CD1	6:A:845:VAL:HG23	2.49	0.43
8:D:11:TYR:CE1	11:G:12:LEU:HD21	2.54	0.43
10:C:888:ILE:HG23	10:C:902:VAL:HG23	2.00	0.43
15:L:73:ILE:HG23	15:L:77:LEU:HD23	2.00	0.43
16:M:250:MET:SD	17:N:139:LEU:HD21	2.59	0.43
6:A:954:ILE:HG23	6:A:991:THR:HG23	2.00	0.43
16:M:247:LEU:HA	16:M:250:MET:HG2	1.99	0.43
18:O:211:ILE:O	21:S:83:ARG:NH2	2.52	0.43
27:g:28:ILE:HG22	27:g:41:ASP:HB3	2.01	0.43
6:A:136:PRO:HB3	6:A:562:ILE:HD13	2.01	0.43
7:B:1163:SER:O	32:Q:367:GLN:CB	2.67	0.43
10:C:94:VAL:HG12	13:J:154:TRP:CZ2	2.54	0.43
10:C:905:GLN:HE22	10:C:936:ILE:HD13	1.84	0.43
21:S:72:ALA:HB1	21:S:88:PHE:CZ	2.54	0.43
33:u:107:LYS:C	33:u:109:LEU:H	2.25	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
10:C:78:MET:SD	10:C:78:MET:N	2.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:242:VAL:HG22	10:C:277:LEU:HD11	2.01	0.43
10:C:381:LEU:HA	10:C:384:ILE:HD12	1.99	0.43
14:K:127:VAL:HG13	17:N:31:GLY:O	2.18	0.43
27:g:56:GLN:C	27: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	10:C:390:SER:HA	2.01	0.42
6:A:785:HIS:CE1	14:K:168:ALA:HB2	2.54	0.42
6:A:1737:GLN:HE21	6:A:1737:GLN:HA	1.84	0.42
10:C:861:ILE:HA	10:C:907:PRO:HA	2.01	0.42
18:O:211:ILE:HD12	21:S:48:ARG:CZ	2.49	0.42
26:f:16:LYS:N	26:f:17:PRO:CD	2.81	0.42
6:A:556:TYR:CG	14:K:120:ASP:HB3	2.54	0.42
6:A:1089:VAL:HG22	6:A:1098:VAL:HG22	2.01	0.42
7:B:1182:ALA:O	32:Q:496:ARG:CA	2.59	0.42
10:C:599:THR:HG23	10: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:B:1343:PHE:C	7:B:1345:PHE:H	2.26	0.42
7:B:1539:GLU:O	7:B:1540:ARG:C	2.62	0.42
8:D:49:MET:HE3	8:D:58:ILE:HD11	2.01	0.42
10:C:104:THR:HG23	10:C:105:ILE:HG23	2.00	0.42
10:C:791:TYR:O	10:C:791:TYR:CG	2.72	0.42
11:G:51:LYS:O	11:G:54:VAL:HG12	2.19	0.42
13:J:164:MET:HE1	13:J:199:SER:CB	2.47	0.42
13:J:200:VAL:HG22	13:J:227:VAL:HB	2.01	0.42
17:N:88:ASP:O	17:N:91:ILE:HG23	2.20	0.42
18:O:211:ILE:CD1	21:S:48:ARG:HB2	2.49	0.42
20:R:13:GLY:O	20:R:15:SER:N	2.52	0.42
21:S:155:LEU:C	21:S:155:LEU:HD23	2.44	0.42
25:e:27:VAL:HG22	25:e:92:SER:HB2	2.00	0.42
6:A:1275:MET:HE1	6:A:1299:LYS:CD	2.48	0.42
10:C:132:ARG:NH1	24:d:13:GLU:O	2.53	0.42
10:C:710:VAL:HG22	10:C:820:LEU:HD23	2.01	0.42
15:L:119:THR:HG22	15:L:120:CYS:N	2.34	0.42
17:N:67:GLN:HA	17:N:119:LYS:HA	2.02	0.42
22:T:119:ALA:HB1	22:T:128:ILE:CB	2.50	0.42
26:f:74:ARG:NH1	29:j:65:CYS:SG	2.92	0.42
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
10:C:605:ILE:HD12	10:C:652:MET:HG3	2.01	0.42
22:T:420:SER:C	22:T:421:ALA:O	2.60	0.42
1:U:23:C:O2	1:U:23:C:O4'	2.37	0.42
5:V:55:G:N7	18:O:35:LYS:HB3	2.35	0.42
6:A:376:ARG:HG3	10: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	12:H:303:LEU:CD2	2.49	0.42
10:C:470:ALA:HB2	10:C:488:ILE:HA	2.02	0.42
10:C:472:VAL:HG21	10: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	18:O:81:PRO:HD2	2.02	0.42
6:A:1369:ASN:O	6:A:1373:LEU:N	2.46	0.42
13:J:114:ARG:HB3	14: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
7:B:757:LEU:O	7:B:758:LYS:C	2.63	0.42
7:B:1795:SER:O	7:B:1796:PRO:C	2.60	0.42
17:N:259:GLY:O	17:N:263:VAL:HG23	2.20	0.42
11:G:22:SER:HB3	33:v:276:VAL:O	2.13	0.42
13:J:183:MET:HE2	13:J:202:GLU:CB	2.50	0.42
14:K:120:ASP:OD2	14:K:123:LEU:HD13	2.20	0.42
16:M:249:MET:SD	17:N:86:LEU:HD13	2.60	0.42
18:O:564:TYR:CB	18:O:566:TYR:H	2.33	0.42
25:e:34:GLN:NE2	25: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
7:B:1482:GLY:O	7:B:1483:VAL:C	2.62	0.42
10:C:400:LEU:HD12	10:C:408:LEU:HD21	2.02	0.42
16:M:114:ARG:CD	16:M:127:ILE:HG21	2.50	0.42
18:O:22:LYS:HB2	18:O:56:LEU:HD12	2.02	0.42
20:R:32:PRO:HB3	20:R:35:SER:CB	2.50	0.42
6:A:756:LEU:CD1	19:P:12:ARG:HD3	2.50	0.41
10:C:418:GLN:HB3	10:C:419:PRO:HD3	2.02	0.41
13:J:334:TRP:CD1	13:J:334:TRP:N	2.88	0.41
17:N:16:CYS:CB	17:N:71:CYS:SG	3.08	0.41
17:N:25:MET:HB3	17:N:46:PHE:HB3	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:S:140:LEU:HD21	21: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	19:P:12:ARG:HD3	2.03	0.41
6:A:1169:TYR:CE2	6:A:1262:MET:HE2	2.54	0.41
10:C:225:THR:HG21	10:C:252:LEU:HD21	2.02	0.41
10:C:608:GLN:HE21	10:C:641:GLU:HG2	1.85	0.41
13:J:276:PRO:HB2	14:K:63:ILE:HD12	2.02	0.41
16:M:48:VAL:HG22	16:M:220:GLY:N	2.36	0.41
16:M:247:LEU:HA	16:M:250:MET:CG	2.51	0.41
21:S:332:GLU:HA	21:S:334:PHE:CB	2.50	0.41
5:V:74:U:C5	13:J:221:TYR:CD2	3.07	0.41
6:A:168:LEU:N	6:A:169:PRO:HD2	2.35	0.41
22:T:397:ASN:O	22:T:400:ALA:HB3	2.20	0.41
7:B:1610:LEU:O	7:B:1660:ALA:O	2.38	0.41
10:C:273:LEU:HA	10:C:277:LEU:HD12	2.02	0.41
10:C:621:ALA:CB	10:C:664:ALA:HB2	2.48	0.41
23:b:12:LEU:HD12	23:b:15:LEU:HD11	2.02	0.41
32:Q:916:ALA:HB3	32:Q:951:VAL:H	1.85	0.41
33:v:213:CYS:HA	33:v:221:HIS:O	2.19	0.41
6:A:565:VAL:CG1	6:A:637:VAL:HG22	2.51	0.41
25:e:88:THR:HG22	25:e:89:LEU:HD12	2.01	0.41
33:v:81:LEU:CA	34:s:99:ASP:CB	2.89	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
12:H:334:LEU:HD12	12:H:380:GLN:HB3	2.02	0.41
6:A:252:GLU:HA	6:A:255:ILE:HD12	2.02	0.41
6:A:2227:VAL:O	6:A:2228:PRO:C	2.62	0.41
12:H:330:ILE:HD12	12:H:387:PHE:HE2	1.86	0.41
6:A:1609:TRP:CE3	6:A:1823:LEU:HD13	2.56	0.41
10:C:314:ALA:CB	10:C:321:THR:HG22	2.50	0.41
12:H:292:LYS:HD3	12:H:328:ILE:HD11	2.01	0.41
16:M:156:ILE:HG21	16:M:175:TYR:CE1	2.55	0.41
6:A:480:TYR:OH	10: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:C:287:LYS:HE3	10:C:291:ILE:HD11	2.03	0.41
13:J:364:LEU:C	13:J:364:LEU:HD23	2.46	0.41
14:K:112:ILE:CD1	17:N:25:MET:HE3	2.50	0.41
17:N:82:ILE:HG22	17: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	10: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
10:C:152:LEU:HD11	10:C:319:GLY:HA2	2.02	0.40
10:C:632:VAL:HG12	10:C:634:ILE:HG13	2.03	0.40
10:C:677:PHE:HB3	10:C:857:LEU:HD22	2.03	0.40
11:G:4:ASN:C	11:G:4:ASN:HD22	2.29	0.40
21:S:189:TYR:O	21:S:192:TYR:HB3	2.21	0.40
26:f:71:ILE:HG22	29: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
7:B:755:THR:O	7:B:756:TRP:C	2.62	0.40
10:C:223:ASP:O	10:C:227:VAL:HG23	2.21	0.40
10:C:749:LYS:O	10:C:753:THR:HG23	2.21	0.40
18:O:211:ILE:CD1	21:S:44:ARG:HG3	2.50	0.40
1:U:45:A:OP1	10:C:108:GLN:O	2.40	0.40
6:A:1756:PHE:CZ	6:A:1760:THR:HG21	2.56	0.40
7:B:1913:PHE:O	7:B:1914:PRO:C	2.64	0.40
10:C:234:LEU:HD13	10:C:439:ILE:HG23	2.03	0.40
10:C:264:CYS:SG	10:C:312:ILE:HD11	2.61	0.40
10:C:561:ILE:O	10:C:562:VAL:HG13	2.22	0.40
14:K:75:GLN:HA	14:K:78:VAL:HG12	2.03	0.40
17:N:139:LEU:HD13	17: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	21: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
7:B:960:ILE:O	7:B:964:GLY:N	2.54	0.40
10:C:241:VAL:HG22	10:C:267:ILE:HG23	2.04	0.40
10:C:655:LEU:C	10:C:655:LEU:HD23	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:J:345:PHE:CE2	13:J:364:LEU:HD22	2.57	0.40
20:R:31:ARG:O	20:R:33:GLN:N	2.47	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
13:J:198:PHE:CD1	13:J:239:ILE:HD13	2.57	0.40
13:J:321:PHE:CE1	13:J:336:LEU:CD2	3.05	0.40
16:M:109:LEU:HA	16:M:116:LYS:HG2	2.03	0.40
17:N:84:ILE:O	17:N:87:ARG:HG3	2.21	0.40
18:O:148:GLU:O	18:O:152:LEU:HD23	2.21	0.40
18:O:211:ILE:HD12	21: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	2160/2413 (90%)	1997 (92%)	152 (7%)	11 (0%)	24	63
7	B	1704/2163 (79%)	1585 (93%)	111 (6%)	8 (0%)	24	63
8	D	112/278 (40%)	93 (83%)	17 (15%)	2 (2%)	6	34
9	F	44/179 (25%)	41 (93%)	3 (7%)	0	100	100
10	C	872/1008 (86%)	777 (89%)	82 (9%)	13 (2%)	8	40
11	G	95/235 (40%)	89 (94%)	5 (5%)	1 (1%)	11	46
12	H	389/591 (66%)	362 (93%)	23 (6%)	4 (1%)	12	49
13	J	322/451 (71%)	263 (82%)	47 (15%)	12 (4%)	2	20
14	K	155/379 (41%)	146 (94%)	8 (5%)	1 (1%)	21	59
15	L	153/157 (98%)	136 (89%)	15 (10%)	2 (1%)	9	42
16	M	250/339 (74%)	228 (91%)	19 (8%)	3 (1%)	10	44
17	N	195/364 (54%)	178 (91%)	14 (7%)	3 (2%)	8	40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	O	277/590 (47%)	248 (90%)	24 (9%)	5 (2%)	6	34
19	P	34/175 (19%)	28 (82%)	5 (15%)	1 (3%)	3	23
20	R	93/135 (69%)	81 (87%)	11 (12%)	1 (1%)	11	46
21	S	432/687 (63%)	416 (96%)	14 (3%)	2 (0%)	24	63
22	T	536/859 (62%)	506 (94%)	21 (4%)	9 (2%)	7	36
23	b	76/196 (39%)	70 (92%)	6 (8%)	0	100	100
23	k	76/196 (39%)	65 (86%)	9 (12%)	2 (3%)	4	25
24	d	80/101 (79%)	72 (90%)	7 (9%)	1 (1%)	9	42
24	n	80/101 (79%)	66 (82%)	14 (18%)	0	100	100
25	e	71/94 (76%)	68 (96%)	3 (4%)	0	100	100
25	p	71/94 (76%)	63 (89%)	7 (10%)	1 (1%)	9	40
26	f	70/86 (81%)	66 (94%)	3 (4%)	1 (1%)	9	40
26	q	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	g	65/77 (84%)	64 (98%)	1 (2%)	0	100	100
27	r	65/77 (84%)	55 (85%)	9 (14%)	1 (2%)	8	40
28	h	78/146 (53%)	74 (95%)	4 (5%)	0	100	100
28	l	75/146 (51%)	63 (84%)	10 (13%)	2 (3%)	4	25
29	j	92/110 (84%)	87 (95%)	5 (5%)	0	100	100
29	m	92/110 (84%)	84 (91%)	8 (9%)	0	100	100
30	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	1	16
31	Y	82/111 (74%)	77 (94%)	5 (6%)	0	100	100
32	Q	609/1071 (57%)	486 (80%)	73 (12%)	50 (8%)	0	9
33	t	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
33	u	425/503 (84%)	413 (97%)	12 (3%)	0	100	100
33	v	412/503 (82%)	403 (98%)	6 (2%)	3 (1%)	18	56
33	w	423/503 (84%)	414 (98%)	7 (2%)	2 (0%)	24	63
34	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	14
All	All	11527/16230 (71%)	10551 (92%)	821 (7%)	155 (1%)	12	42

All (155) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	320	ASP

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Mol	Chain	Res	Type
6	A	737	ARG
7	B	766	ILE
12	H	414	PRO
16	M	127	ILE
17	N	120	LEU
20	R	14	SER
22	T	421	ALA
22	T	477	PRO
22	T	481	ILE
22	T	616	PRO
30	W	76	ILE
28	l	98	PRO
27	r	68	ILE
32	Q	370	VAL
32	Q	380	THR
32	Q	399	SER
32	Q	400	ILE
32	Q	401	VAL
32	Q	440	ASP
32	Q	443	CYS
32	Q	466	LYS
32	Q	470	VAL
32	Q	471	ILE
32	Q	478	ARG
32	Q	502	ILE
32	Q	503	ILE
32	Q	546	GLU
32	Q	653	VAL
32	Q	654	ILE
32	Q	655	ASP
32	Q	707	PHE
32	Q	737	THR
32	Q	748	LYS
32	Q	749	PRO
32	Q	799	ASN
32	Q	836	PHE
32	Q	917	LYS
32	Q	925	VAL
32	Q	948	PRO
34	s	94	LYS
34	s	111	VAL
34	s	133	PRO

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Mol	Chain	Res	Type
6	A	588	LEU
6	A	1424	HIS
6	A	1639	PRO
6	A	1763	ASN
7	B	1693	HIS
10	C	76	VAL
10	C	172	TRP
10	C	269	LYS
10	C	432	GLN
10	C	535	PRO
10	C	901	GLU
12	H	469	GLY
13	J	162	THR
13	J	245	ASP
13	J	277	VAL
13	J	328	THR
16	M	23	PRO
18	O	81	PRO
19	P	9	LEU
30	W	122	ARG
23	k	81	VAL
32	Q	369	VAL
32	Q	374	GLU
32	Q	395	ASP
32	Q	856	ASN
32	Q	857	PHE
32	Q	894	ILE
32	Q	896	SER
32	Q	942	HIS
33	v	109	LEU
34	s	105	PRO
34	s	136	VAL
6	A	1593	ALA
7	B	492	PRO
7	B	1936	ARG
8	D	76	LEU
10	C	574	SER
12	H	445	LEU
13	J	442	TRP
15	L	38	SER
17	N	30	GLN
17	N	54	ASN

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Mol	Chain	Res	Type
18	O	214	ASN
18	O	546	HIS
21	S	238	TRP
30	W	95	PRO
28	I	25	VAL
32	Q	451	ASP
32	Q	604	ASN
32	Q	644	SER
32	Q	746	ILE
32	Q	824	ARG
32	Q	929	THR
32	Q	944	LEU
33	v	20	ARG
6	A	660	ILE
7	B	1555	GLU
7	B	1968	ASN
18	O	206	LYS
21	S	112	VAL
22	T	479	PRO
22	T	615	PHE
30	W	68	PRO
30	W	94	LEU
30	W	129	LEU
23	k	6	VAL
32	Q	504	THR
32	Q	738	ASP
32	Q	839	LYS
32	Q	927	LEU
33	w	20	ARG
34	s	119	SER
6	A	457	ASP
6	A	1491	ILE
8	D	34	MET
10	C	100	LEU
10	C	459	PRO
11	G	41	VAL
13	J	310	SER
13	J	444	PRO
16	M	4	TRP
18	O	216	ASP
22	T	443	PRO
32	Q	541	VAL

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Mol	Chain	Res	Type
32	Q	704	GLU
32	Q	708	LYS
33	w	17	PRO
7	B	622	LEU
10	C	137	GLY
10	C	807	PRO
12	H	303	LEU
13	J	226	GLY
22	T	391	LEU
32	Q	821	PRO
13	J	137	GLY
32	Q	750	PRO
7	B	791	PRO
10	C	185	ILE
10	C	301	GLY
13	J	279	PRO
14	K	146	VAL
15	L	117	GLY
26	f	15	PRO
25	p	74	GLY
13	J	443	ASN
22	T	37	ILE
30	W	56	ILE
30	W	98	VAL
33	v	36	GLY
6	A	774	ILE
13	J	272	VAL
24	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	32
8	D	100/256 (39%)	90 (90%)	10 (10%)	7	24
9	F	26/163 (16%)	25 (96%)	1 (4%)	29	50

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	C	722/910 (79%)	662 (92%)	60 (8%)	10	30
11	G	89/216 (41%)	83 (93%)	6 (7%)	15	36
12	H	185/552 (34%)	167 (90%)	18 (10%)	8	24
13	J	283/397 (71%)	248 (88%)	35 (12%)	4	17
14	K	143/328 (44%)	119 (83%)	24 (17%)	2	10
15	L	138/141 (98%)	128 (93%)	10 (7%)	13	35
16	M	213/296 (72%)	196 (92%)	17 (8%)	11	31
17	N	194/332 (58%)	170 (88%)	24 (12%)	4	17
18	O	174/525 (33%)	156 (90%)	18 (10%)	7	23
19	P	26/152 (17%)	22 (85%)	4 (15%)	2	12
20	R	23/121 (19%)	19 (83%)	4 (17%)	2	9
21	S	208/633 (33%)	184 (88%)	24 (12%)	5	18
23	b	70/176 (40%)	70 (100%)	0	100	100
24	d	69/89 (78%)	67 (97%)	2 (3%)	37	58
25	e	65/83 (78%)	61 (94%)	4 (6%)	16	38
26	f	63/77 (82%)	61 (97%)	2 (3%)	34	56
27	g	58/66 (88%)	56 (97%)	2 (3%)	32	54
28	h	77/129 (60%)	77 (100%)	0	100	100
29	j	79/103 (77%)	76 (96%)	3 (4%)	29	50
All	All	4706/7927 (59%)	4304 (92%)	402 (8%)	12	29

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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
8	D	3	GLU
8	D	8	ASN
8	D	25	ARG

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Mol	Chain	Res	Type
8	D	47	PHE
8	D	49	MET
8	D	63	LYS
8	D	71	LEU
8	D	79	ILE
8	D	99	THR
8	D	114	ARG
9	F	20	ARG
10	C	76	VAL
10	C	78	MET
10	C	92	GLU
10	C	100	LEU
10	C	103	HIS
10	C	109	LEU
10	C	124	LEU
10	C	132	ARG
10	C	139	ILE
10	C	153	LEU
10	C	156	ASP
10	C	211	ASN
10	C	219	VAL
10	C	229	LEU
10	C	234	LEU
10	C	255	GLN
10	C	261	VAL
10	C	272	ARG
10	C	273	LEU
10	C	315	SER
10	C	358	ASN
10	C	381	LEU
10	C	400	LEU
10	C	401	ARG
10	C	424	VAL
10	C	431	GLN
10	C	447	GLU
10	C	453	THR
10	C	458	ILE
10	C	468	LEU
10	C	475	THR
10	C	534	THR
10	C	545	LEU
10	C	562	VAL

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Mol	Chain	Res	Type
10	C	572	ILE
10	C	576	THR
10	C	590	LYS
10	C	602	VAL
10	C	610	LEU
10	C	619	LEU
10	C	625	ILE
10	C	760	LEU
10	C	768	PHE
10	C	774	LEU
10	C	784	SER
10	C	790	LYS
10	C	791	TYR
10	C	794	GLN
10	C	803	VAL
10	C	830	ASN
10	C	837	GLN
10	C	851	LEU
10	C	856	ILE
10	C	861	ILE
10	C	902	VAL
10	C	927	MET
10	C	965	ASP
10	C	970	THR
10	C	971	ARG
10	C	989	LEU
11	G	18	GLN
11	G	28	ASP
11	G	31	ARG
11	G	33	GLN
11	G	74	GLN
11	G	78	LEU
12	H	297	LEU
12	H	307	GLU
12	H	313	LEU
12	H	314	LYS
12	H	317	ILE
12	H	334	LEU
12	H	348	GLU
12	H	357	TRP
12	H	363	GLU
12	H	373	ILE

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Mol	Chain	Res	Type
12	H	391	LEU
12	H	396	PHE
12	H	421	LYS
12	H	440	LEU
12	H	468	ILE
12	H	470	LEU
12	H	473	LEU
12	H	477	MET
13	J	139	LEU
13	J	143	ARG
13	J	147	ILE
13	J	148	ASP
13	J	151	ASP
13	J	156	ILE
13	J	183	MET
13	J	194	HIS
13	J	197	LEU
13	J	202	GLU
13	J	215	GLN
13	J	218	ARG
13	J	224	LEU
13	J	225	SER
13	J	247	VAL
13	J	248	ILE
13	J	257	ILE
13	J	269	ILE
13	J	274	CYS
13	J	275	THR
13	J	284	SER
13	J	286	THR
13	J	290	VAL
13	J	295	VAL
13	J	303	VAL
13	J	314	THR
13	J	329	ASP
13	J	334	TRP
13	J	336	LEU
13	J	356	LEU
13	J	377	ASP
13	J	387	LEU
13	J	389	THR
13	J	402	VAL

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Mol	Chain	Res	Type
13	J	423	ILE
14	K	33	GLN
14	K	36	LYS
14	K	40	LEU
14	K	48	GLN
14	K	52	GLU
14	K	62	GLU
14	K	66	CYS
14	K	70	THR
14	K	77	LEU
14	K	81	LYS
14	K	87	ASN
14	K	105	LEU
14	K	106	LEU
14	K	111	HIS
14	K	112	ILE
14	K	147	LEU
14	K	172	TRP
14	K	182	LEU
14	K	183	GLU
14	K	197	ILE
14	K	203	LYS
14	K	204	LEU
14	K	217	GLN
14	K	218	GLU
15	L	3	ARG
15	L	37	LYS
15	L	54	GLN
15	L	59	ARG
15	L	60	SER
15	L	61	ARG
15	L	71	LYS
15	L	84	GLU
15	L	85	LYS
15	L	142	PHE
16	M	5	ARG
16	M	10	LYS
16	M	18	LEU
16	M	26	THR
16	M	38	SER
16	M	44	ASN
16	M	114	ARG

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Mol	Chain	Res	Type
16	M	116	LYS
16	M	127	ILE
16	M	132	LYS
16	M	135	LYS
16	M	136	THR
16	M	149	LYS
16	M	172	ARG
16	M	187	LYS
16	M	245	GLU
16	M	251	VAL
17	N	20	GLU
17	N	22	ASN
17	N	30	GLN
17	N	32	SER
17	N	35	LYS
17	N	36	ILE
17	N	39	LEU
17	N	43	LEU
17	N	48	THR
17	N	51	ARG
17	N	55	ILE
17	N	72	GLN
17	N	91	ILE
17	N	93	LEU
17	N	94	VAL
17	N	109	MET
17	N	117	ASN
17	N	120	LEU
17	N	135	ILE
17	N	139	LEU
17	N	214	ILE
17	N	216	GLU
17	N	254	GLN
17	N	321	GLN
18	O	40	LEU
18	O	44	THR
18	O	46	ARG
18	O	53	ASN
18	O	73	LEU
18	O	91	MET
18	O	93	ARG
18	O	156	ARG

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Mol	Chain	Res	Type
18	O	170	LYS
18	O	184	GLU
18	O	188	ARG
18	O	189	ARG
18	O	192	LYS
18	O	196	ILE
18	O	204	LYS
18	O	205	LYS
18	O	206	LYS
18	O	247	LYS
19	P	8	GLN
19	P	9	LEU
19	P	16	LYS
19	P	29	ARG
20	R	6	ILE
20	R	8	LEU
20	R	15	SER
20	R	16	THR
21	S	60	ARG
21	S	67	GLN
21	S	77	GLU
21	S	78	GLN
21	S	87	ILE
21	S	92	LEU
21	S	117	HIS
21	S	143	GLU
21	S	144	GLU
21	S	152	VAL
21	S	156	TYR
21	S	158	LYS
21	S	173	VAL
21	S	188	ILE
21	S	189	TYR
21	S	209	GLU
21	S	216	GLU
21	S	224	LEU
21	S	226	ILE
21	S	234	ASN
21	S	257	GLN
21	S	260	TYR
21	S	263	SER
21	S	266	LEU

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Mol	Chain	Res	Type
24	d	10	LEU
24	d	20	SER
25	e	16	CYS
25	e	25	THR
25	e	79	LYS
25	e	81	LEU
26	f	36	THR
26	f	79	LEU
27	g	18	ASN
27	g	71	LEU
29	j	48	LEU
29	j	49	ARG
29	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

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Mol	Chain	Res	Type
6	A	1522	ASN
6	A	1603	ASN
6	A	1615	ASN
6	A	1737	GLN
6	A	2018	ASN
8	D	8	ASN
10	C	108	GLN
10	C	128	ASN
10	C	143	HIS
10	C	158	HIS
10	C	167	ASN
10	C	180	ASN
10	C	260	ASN
10	C	289	ASN
10	C	290	HIS
10	C	358	ASN
10	C	418	GLN
10	C	423	HIS
10	C	426	GLN
10	C	432	GLN
10	C	554	HIS
10	C	608	GLN
10	C	693	ASN
10	C	776	ASN
10	C	837	GLN
10	C	929	GLN
11	G	19	GLN
11	G	33	GLN
12	H	247	ASN
12	H	390	HIS
13	J	194	HIS
13	J	214	ASN
13	J	273	GLN
13	J	280	GLN
13	J	317	HIS
13	J	360	GLN
14	K	33	GLN
14	K	48	GLN
14	K	50	ASN
14	K	210	ASN
15	L	46	ASN
15	L	58	GLN

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Mol	Chain	Res	Type
15	L	115	ASN
16	M	44	ASN
17	N	22	ASN
18	O	26	GLN
18	O	72	GLN
21	S	61	ASN
21	S	78	GLN
21	S	79	HIS
21	S	167	ASN
21	S	179	GLN
21	S	200	GLN
21	S	212	HIS
21	S	214	ASN
23	b	40	HIS
23	b	46	ASN
24	d	17	HIS
25	e	15	ASN
25	e	34	GLN
26	f	25	HIS
27	g	18	ASN
27	g	20	ASN
27	g	66	ASN
28	h	86	ASN
29	j	28	HIS
29	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%)	36 (37%)	6 (6%)
All	All	442/1558 (28%)	187 (42%)	32 (7%)

All (187) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	U	13	A
1	U	14	G

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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	93	A
5	V	99	A

All (32) 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

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Mol	Chain	Res	Type
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	V	92	C

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 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	$\# Z > 2$
38	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
38	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)
38	C	1101	GTP	C5-C4	2.70	1.46	1.38
38	C	1101	GTP	C5-N7	-2.61	1.33	1.39
38	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(°)
38	C	1101	GTP	C5-C4-N3	-5.96	118.91	128.39
38	C	1101	GTP	C2-N3-C4	5.05	121.00	112.30
38	C	1101	GTP	N9-C4-N3	4.57	135.08	125.95
38	C	1101	GTP	C6-C5-N7	3.18	136.08	130.29
38	C	1101	GTP	O6-C6-C5	-2.83	119.07	126.53
38	C	1101	GTP	C4-C5-N7	-2.33	106.97	110.67
38	C	1101	GTP	C5-C6-N1	2.28	119.06	113.25
38	C	1101	GTP	O2B-PB-O1B	2.05	121.97	112.44

There are no chirality outliers.

All (5) torsion outliers are listed below:

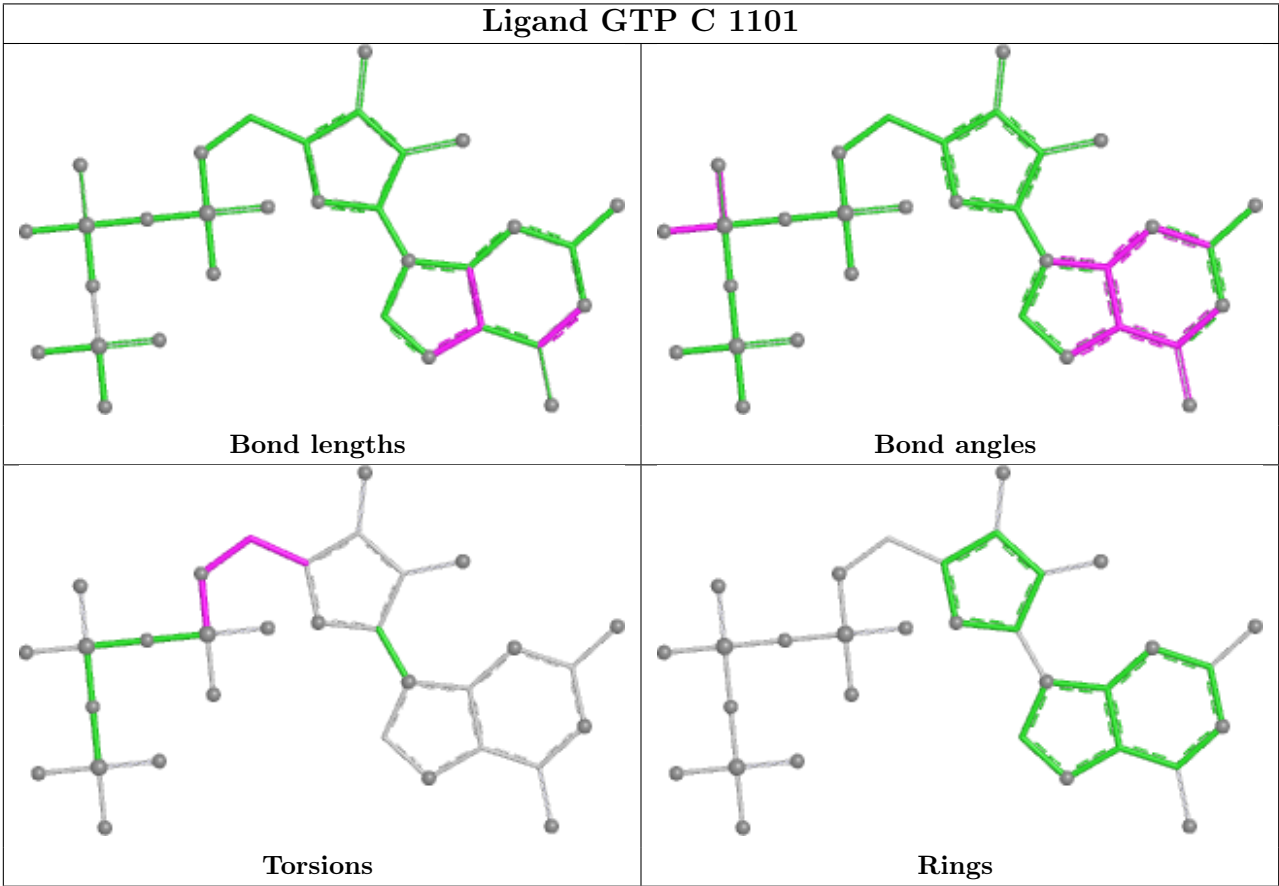
Mol	Chain	Res	Type	Atoms
38	C	1101	GTP	C5'-O5'-PA-O3A
38	C	1101	GTP	C5'-O5'-PA-O1A
38	C	1101	GTP	C3'-C4'-C5'-O5'
38	C	1101	GTP	O4'-C4'-C5'-O5'
38	C	1101	GTP	C4'-C5'-O5'-PA

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
35	x	4

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

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	x	36:UNK	C	37:UNK	N	49.39
1	x	87:UNK	C	88:UNK	N	31.03

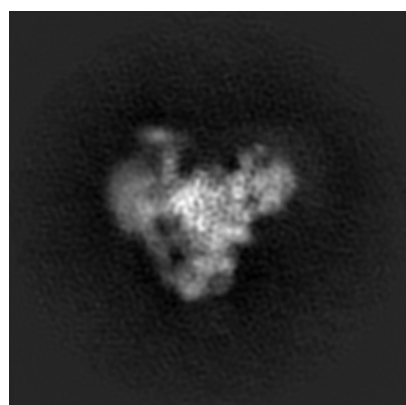
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4057. These allow visual inspection of the internal detail of the map and identification of artifacts.

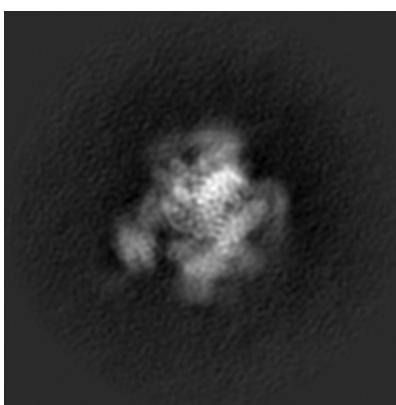
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

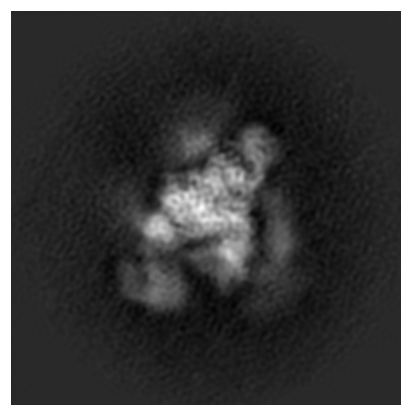
6.1.1 Primary map



X



Y

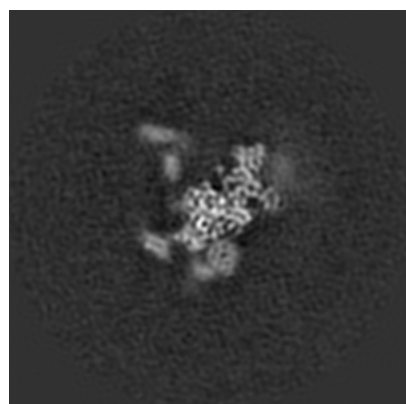


Z

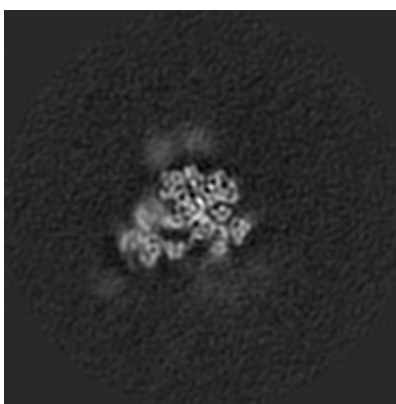
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

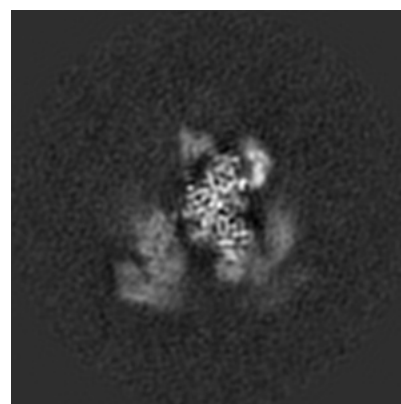
6.2.1 Primary map



X Index: 206



Y Index: 206

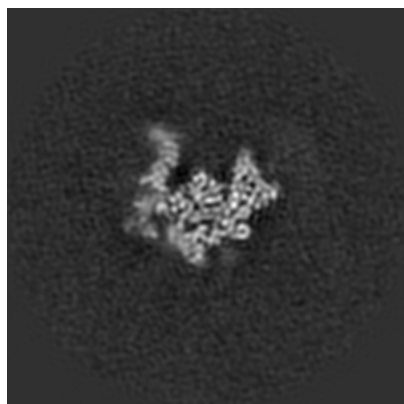


Z Index: 206

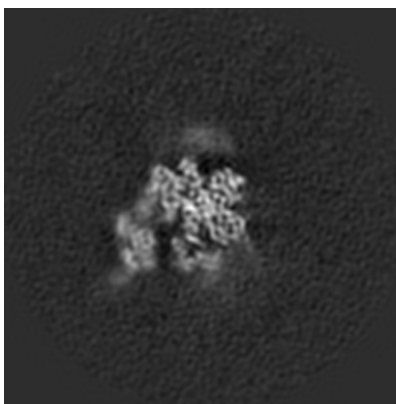
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

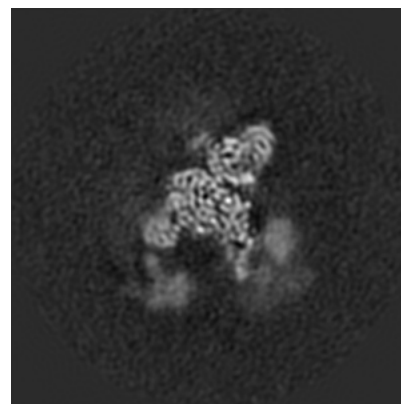
6.3.1 Primary map



X Index: 228



Y Index: 196

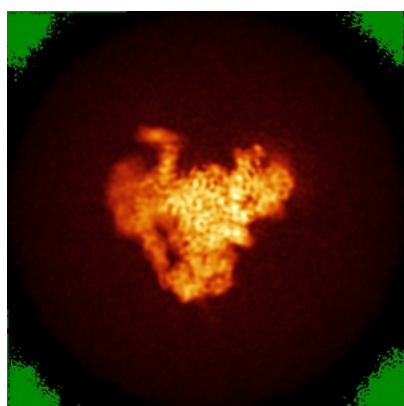


Z Index: 221

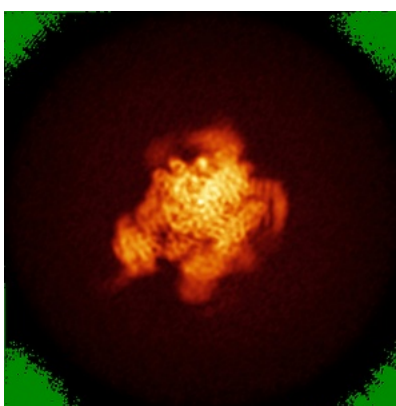
The images above show the largest variance slices of the map in three orthogonal directions.

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

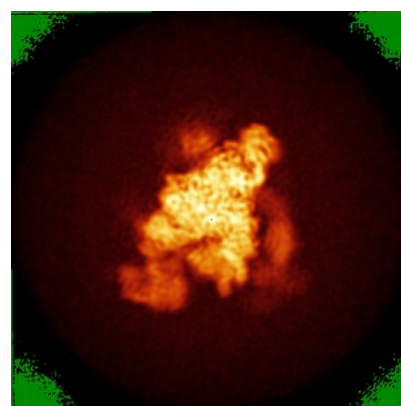
6.4.1 Primary map



X



Y

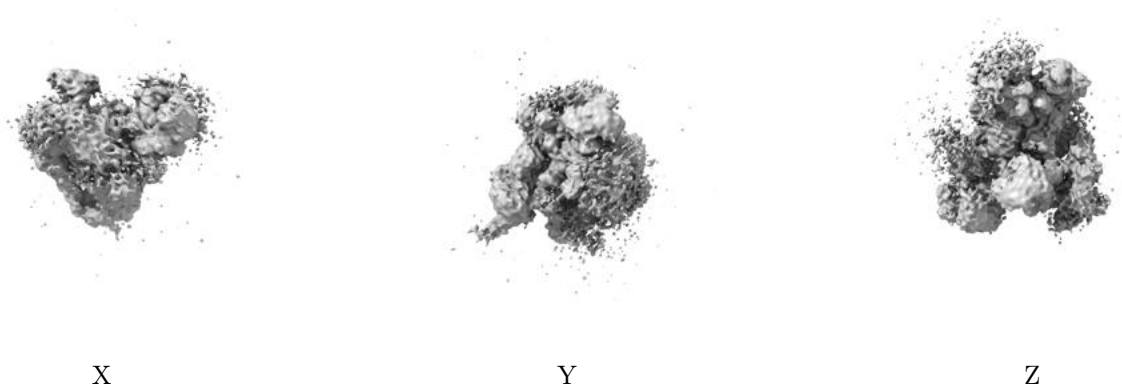


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.006. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

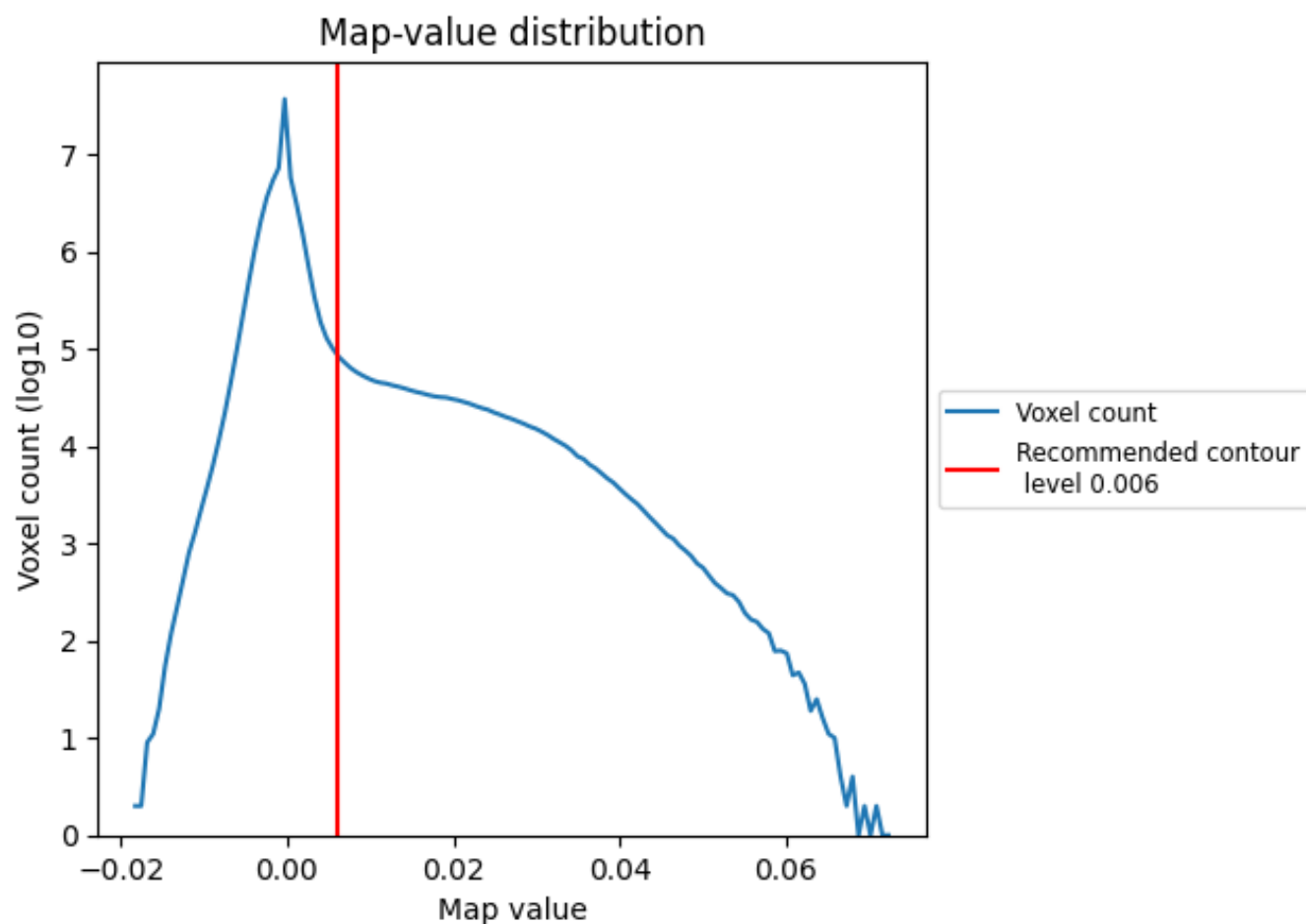
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

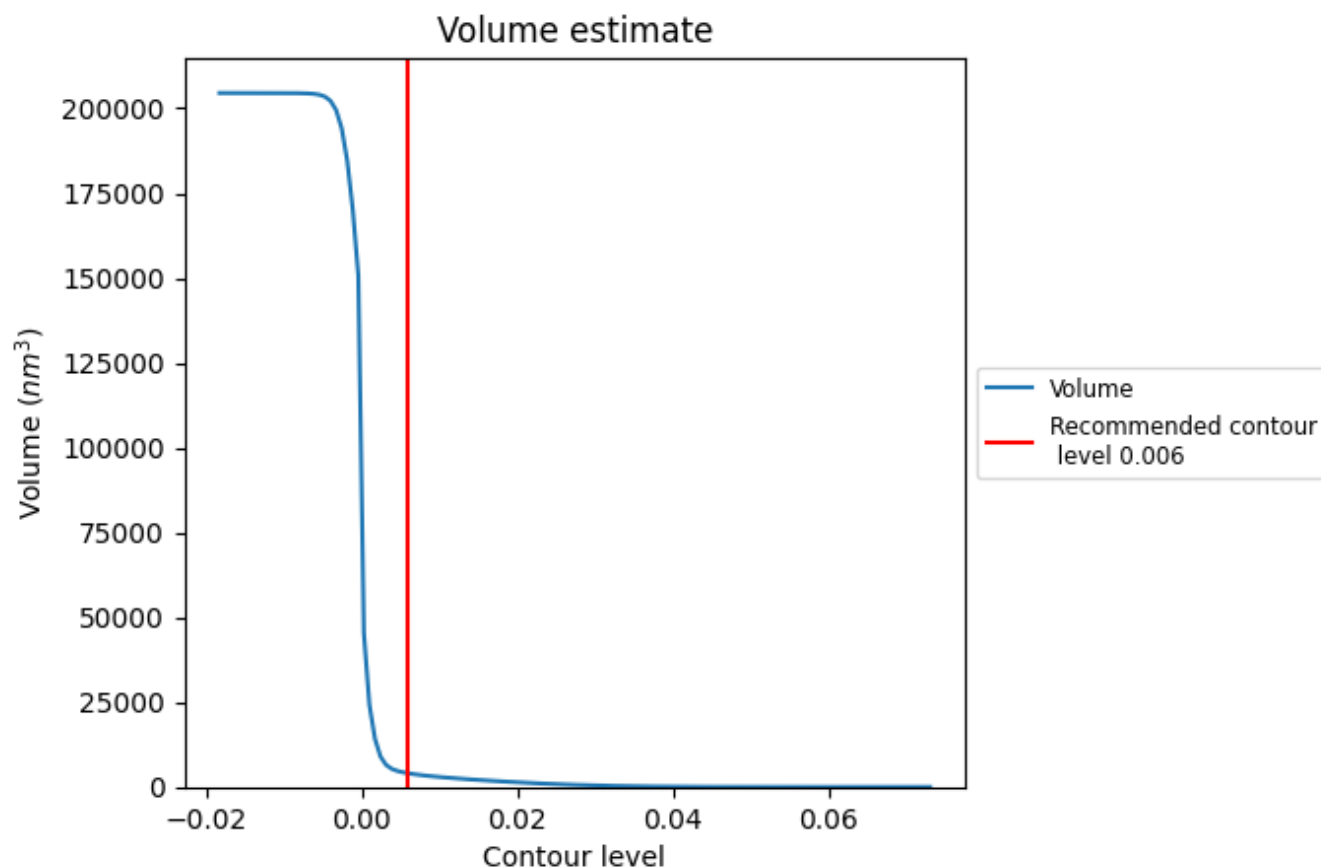
This section contains the results of statistical analysis of the map.

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.

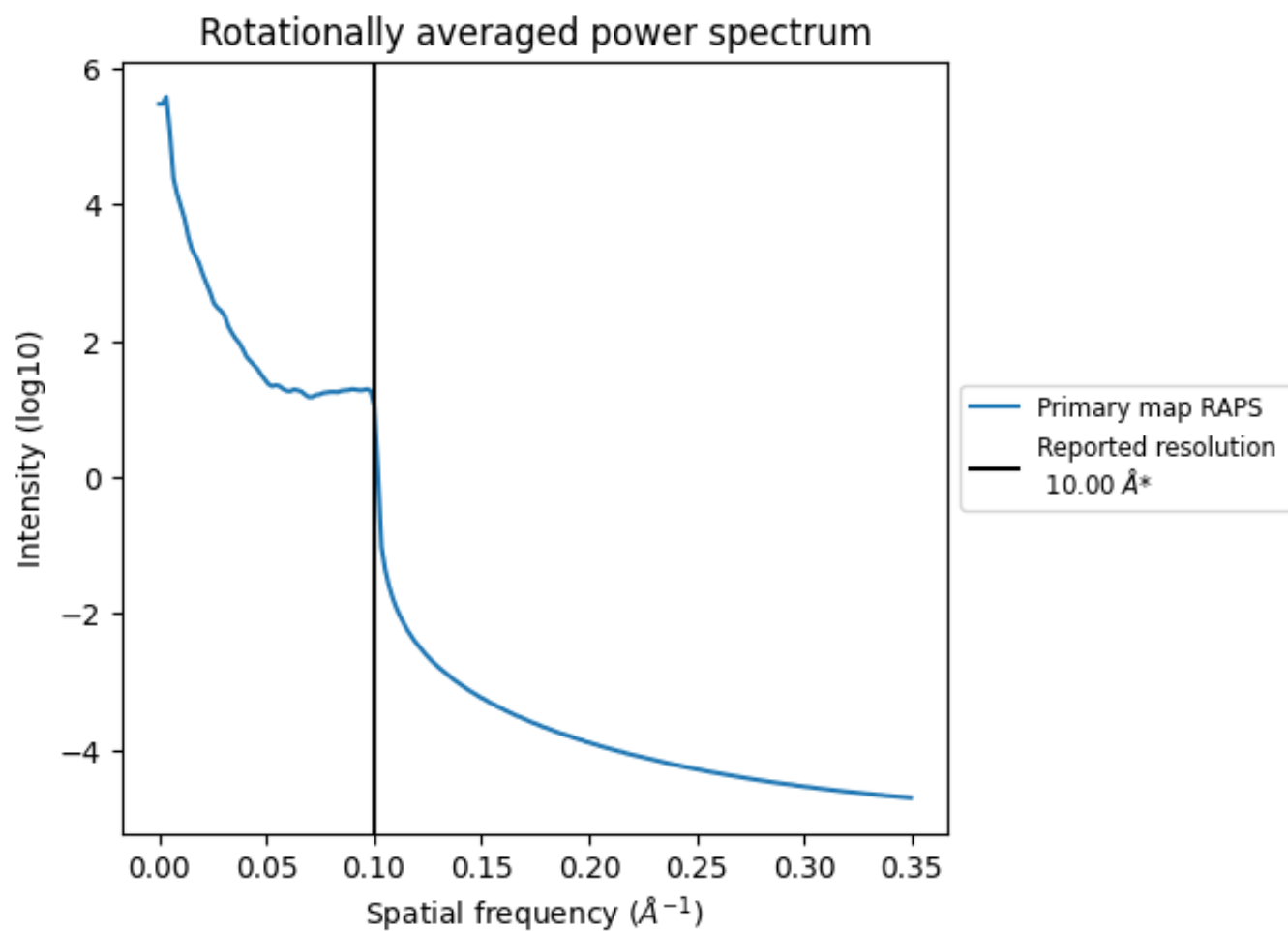
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 4018 nm^3 ; this corresponds to an approximate mass of 3629 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 ⓘ

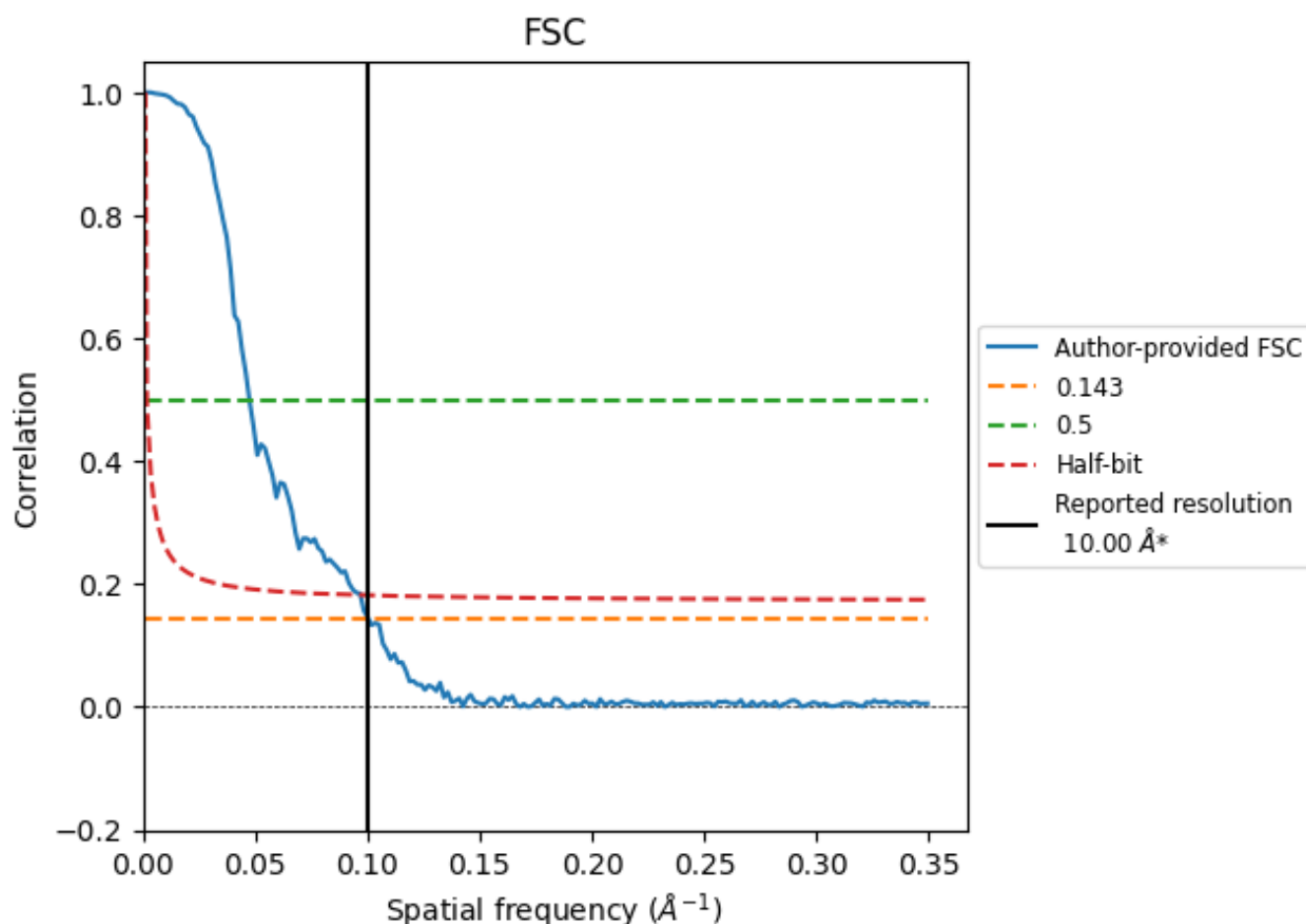


*Reported resolution corresponds to spatial frequency of 0.100 Å⁻¹

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 0.100 Å⁻¹

8.2 Resolution estimates [i](#)

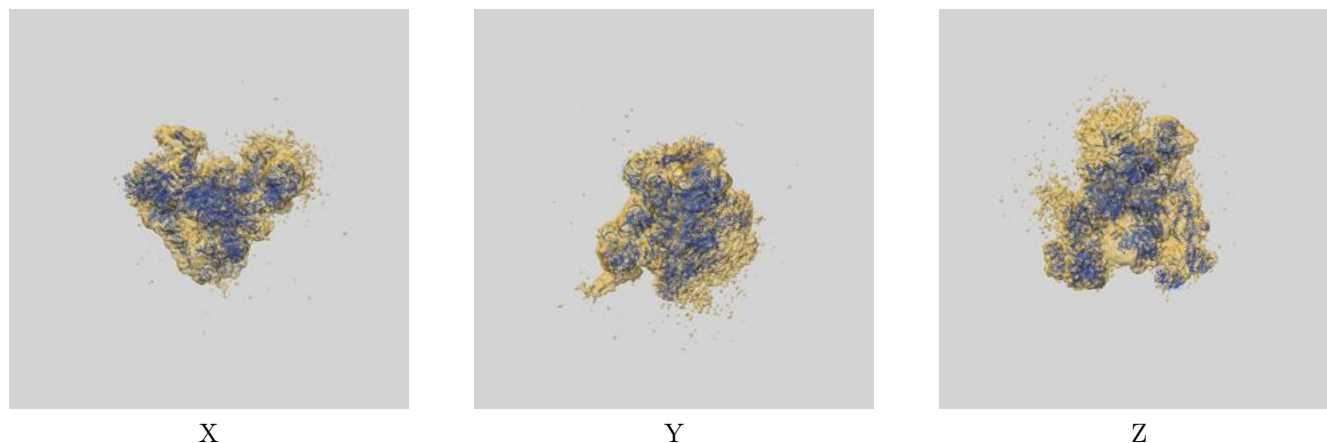
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	10.00	-	-
Author-provided FSC curve	9.95	21.10	10.32
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

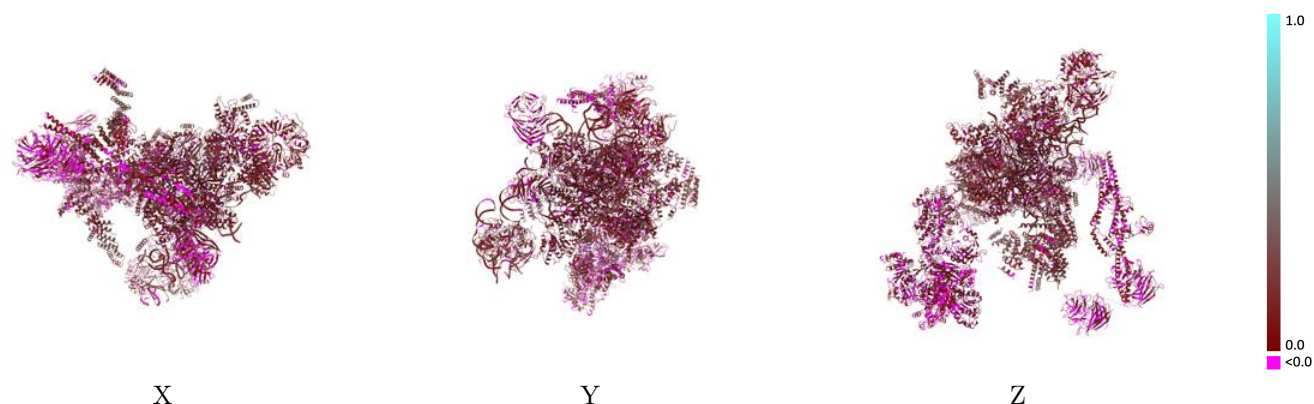
This section contains information regarding the fit between EMDB map EMD-4057 and PDB model 5LJ5. Per-residue inclusion information can be found in section 3 on page 12.

9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.006 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](#)

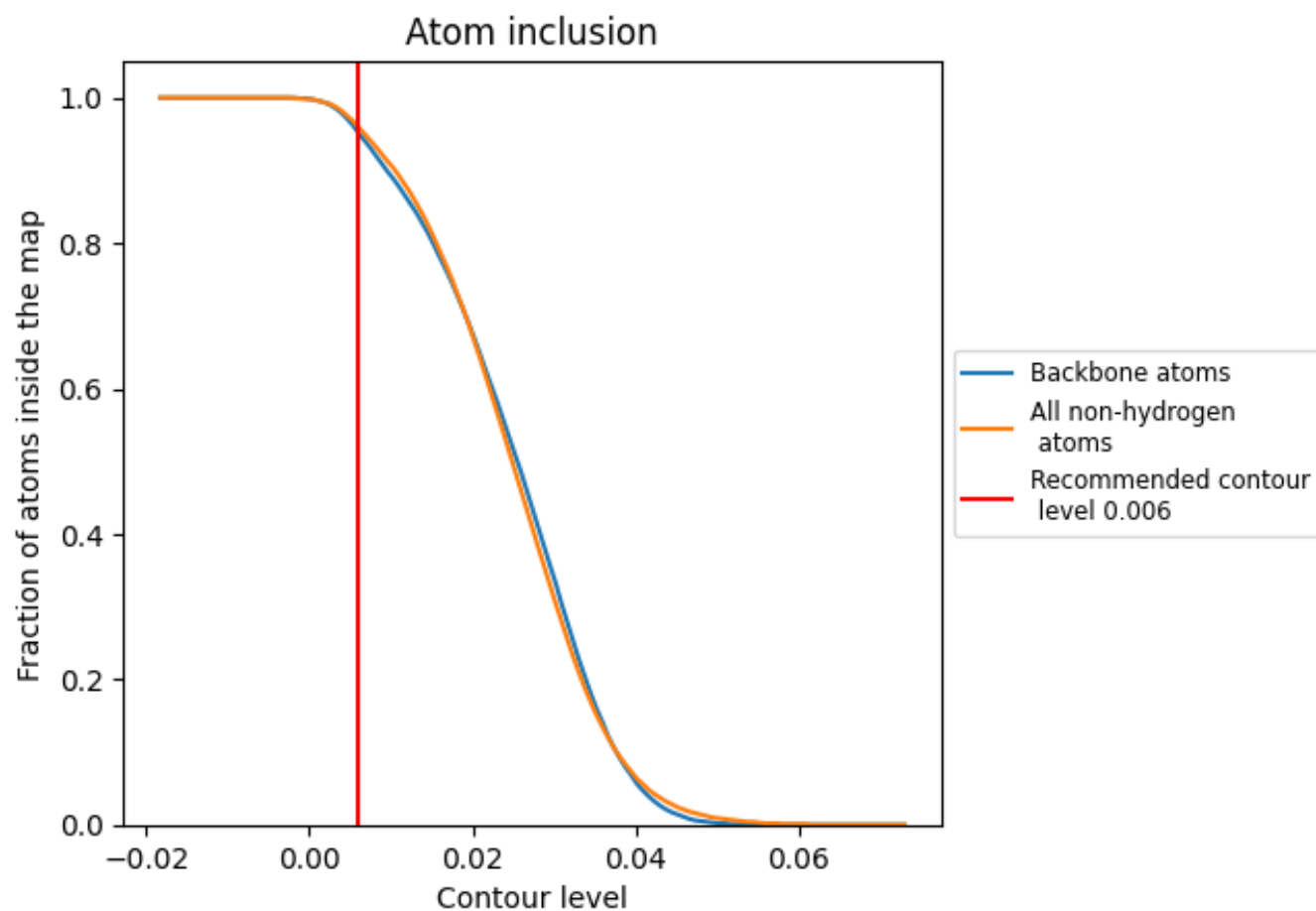


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 96% 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 (0.006) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9600	 0.1140
A	 0.9820	 0.1130
B	 0.9520	 0.0430
C	 0.9890	 0.1230
D	 0.9820	 0.1110
E	 1.0000	 0.1490
F	 0.9910	 0.1550
G	 0.9910	 0.1270
H	 0.9960	 0.1600
I	 1.0000	 0.1410
J	 0.9900	 0.1030
K	 0.9870	 0.1390
L	 0.9990	 0.1210
M	 0.9880	 0.1220
N	 0.9910	 0.1370
O	 0.9600	 0.1170
P	 0.9890	 0.0910
Q	 0.9970	 0.0980
R	 0.9980	 0.2170
S	 0.9940	 0.1570
T	 1.0000	 0.2110
U	 1.0000	 0.1590
V	 1.0000	 0.1670
W	 0.9990	 0.1180
Y	 1.0000	 0.1230
Z	 1.0000	 0.1350
b	 1.0000	 0.1000
d	 1.0000	 0.1240
e	 1.0000	 0.1180
f	 0.9980	 0.1080
g	 0.9940	 0.1040
h	 0.9980	 0.1150
j	 0.9990	 0.1240
k	 1.0000	 0.1330
l	 1.0000	 0.1610



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Chain	Atom inclusion	Q-score
m	 1.0000	 0.1750
n	 1.0000	 0.1600
p	 1.0000	 0.1770
q	 1.0000	 0.1890
r	 0.9970	 0.1630
s	 0.9640	 0.0670
t	 0.7890	 0.0310
u	 0.4930	 0.0330
v	 0.9440	 0.0720
w	 0.6830	 0.0100
x	 1.0000	 0.2770