



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 21, 2017 – 03:36 PM EST

PDB ID : 5MQ0
EMDB ID: : EMD-3541
Title : Structure of a spliceosome remodeled for exon ligation
Authors : Fica, S.M.; Oubridge, C.; Galej, W.P.; Wilkinson, M.E.; Newman, A.J.; Bai, X.-C.; Nagai, K.
Deposited on : 2016-12-19
Resolution : 4.17 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

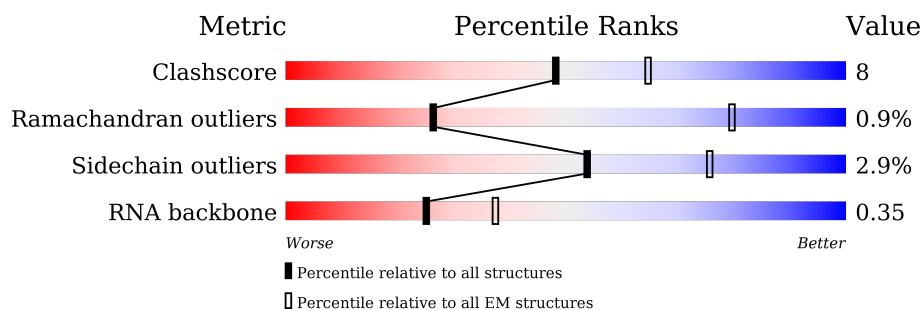
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.17 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.
















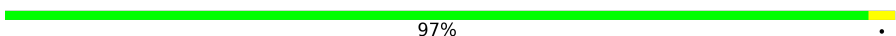











Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686
RNA backbone	3027	244

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	I	95	
2	E	20	
3	2	1175	
4	6	112	
5	5	179	
6	A	2413	
7	C	1008	
8	H	577	


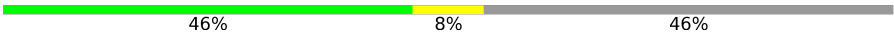


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Mol	Chain	Length	Quality of chain
9	J	451	
10	K	379	
11	L	157	
12	M	339	
13	N	364	
14	O	590	
15	P	175	
16	R	135	
17	S	687	
18	T	877	
19	a	251	
20	c	382	
21	o	455	
22	X	68	
23	y	215	
24	b	196	
24	k	196	
25	d	101	
25	n	101	
26	e	94	
26	p	94	
27	f	86	
27	q	86	
28	g	77	
28	r	77	

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Mol	Chain	Length	Quality of chain
29	h	146	
29	l	146	
30	j	110	
30	m	110	
31	V	1145	
32	W	238	
33	Y	111	
34	3	3	
35	s	175	
36	t	503	
36	u	503	
36	v	503	
36	w	503	

2 Entry composition

There are 41 unique types of molecules in this entry. The entry contains 77441 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 Yeast UBC4 gene for ubiquitin-conjugating enzyme.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	I	34	Total	C	N	O	P	0	0
			714	321	118	241	34		

- Molecule 2 is a RNA chain called 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 S.cerevisiae chromosome II reading frame ORF YBR230c.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	2	155	Total	C	N	O	P	0	0
			3271	1462	547	1107	155		

- Molecule 4 is a RNA chain called Saccharomyces cerevisiae strain T.52_2H chromosome XII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	6	99	Total	C	N	O	P	0	0
			2108	944	375	690	99		

- Molecule 5 is a RNA chain called Saccharomyces cerevisiae strain WI_C_MBSP_4 chromosome VII sequence.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	5	141	Total	C	N	O	P	0	0
			2999	1342	530	986	141		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1914	Total	C	N	O	S	0	0
			15199	9832	2669	2645	53		

- Molecule 7 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	874	Total	C	N	O	S	0	0
			6562	4265	1104	1168	25		

- Molecule 8 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	401	Total	C	N	O	S	0	0
			3261	2104	544	595	18		

- Molecule 9 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	J	342	Total	C	N	O	S	0	0
			2690	1699	475	506	10		

- Molecule 10 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	K	187	Total	C	N	O	S	0	0
			1458	908	269	276	5		

- Molecule 11 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	L	155	Total	C	N	O	S	0	0
			1162	737	217	198	10		

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	M	252	Total	C	N	O	S	0	0
			2016	1281	356	368	11		

- Molecule 13 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	N	227	Total	C	N	O	S	0	0
			1798	1139	309	335	15		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	211	Total	C	N	O	S	0	0
			1755	1102	320	327	6		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	69	Total	C	N	O	S	0	0
			565	358	112	94	1		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	R	108	Total	C	N	O		0	0
			614	369	121	124			

- Molecule 17 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	S	468	Total	C	N	O	S	0	0
			3229	2025	599	598	7		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SYF1,PRE-MRNASPLICING FACTOR SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	T	633	Total	C	N	O		0	0
			3154	1888	633	633			

- Molecule 19 is a protein called Pre-mRNA-splicing factor 18.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	137	Total	C	N	O	S	0	0
			1119	726	194	196	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	c	103	Total	C	N	O	S	0	0
			786	498	142	144	2		

- Molecule 21 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	o	313	Total	C	N	O	S	0	0
			2425	1537	429	451	8		

- Molecule 22 is a protein called UNKNOWN PROTEIN.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	68	Total	C	N	O	0	0
			338	202	68	68		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	y	83	Total	C	N	O	S	0	0
			679	420	125	133	1		

- Molecule 24 is a protein called Small nuclear ribonucleoprotein-associated protein B.

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

- Molecule 25 is a protein called Small nuclear ribonucleoprotein Sm D3.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	e	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
26	p	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

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

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

- Molecule 28 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
28	r	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
29	l	79	Total	C	N	O	S	0	0
			618	393	107	116	2		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
30	m	93	Total	C	N	O	S	0	0
			726	468	136	118	4		

- Molecule 31 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	V	645	Total	C	N	O	0	0
			3189	1899	645	645		

- Molecule 32 is a protein called U2 small nuclear ribonucleoprotein A'.

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

- Molecule 33 is a protein called U2 small nuclear ribonucleoprotein B''.

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

- Molecule 34 is a RNA chain called 3'-EXON OF UBC4 PRE-MRNA, BOUND BY PRP22 HELICASE.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	3	3	Total	C	N	O	P	0	0
			60	27	6	24	3		

- Molecule 35 is a protein called Pre-mRNA-splicing factor SNT309.

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

- Molecule 36 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	t	438	Total	C	N	O	0	0
			2171	1295	438	438		
36	u	116	Total	C	N	O	0	0
			578	346	116	116		
36	v	118	Total	C	N	O	0	0
			588	352	118	118		
36	w	435	Total	C	N	O	0	0
			2156	1286	435	435		

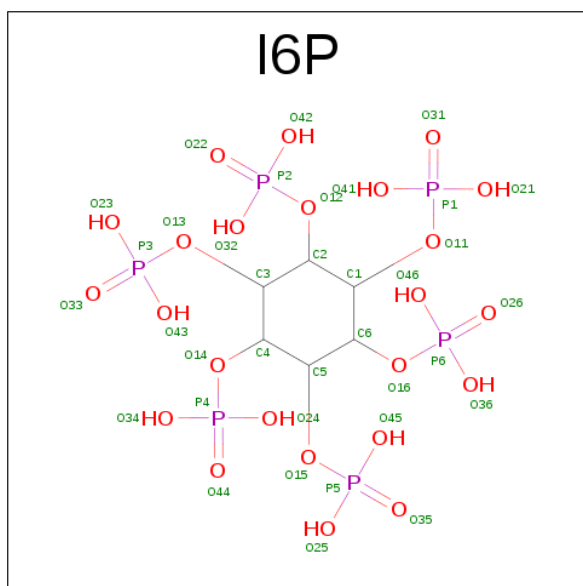
- Molecule 37 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
37	6	3	Total	Mg	0
			3	3	

- Molecule 38 is POTASSIUM ION (three-letter code: K) (formula: K).

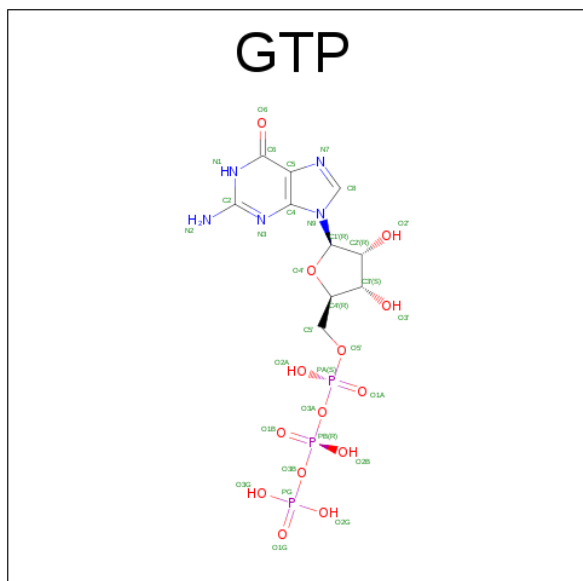
Mol	Chain	Residues	Atoms			AltConf
38	6	2	Total	K		0
			2	2		

- Molecule 39 is INOSITOL 1,2,3,4,5,6-HEXAKISPHOSPHATE (three-letter code: I6P) (formula: $C_6H_{18}O_{24}P_6$).



Mol	Chain	Residues	Atoms				AltConf
39	A	1	Total	C	O	P	0
			36	6	24	6	

- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

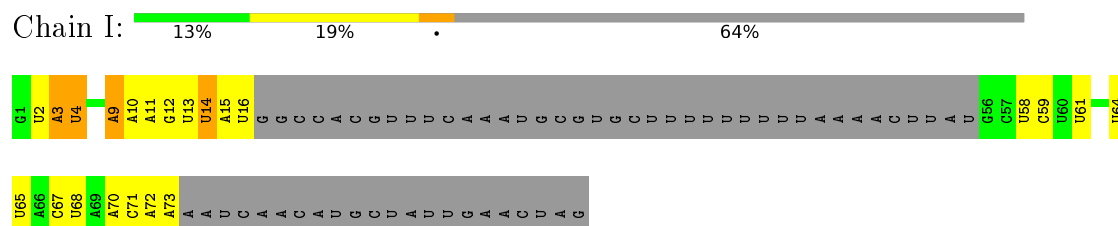
- Molecule 41 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

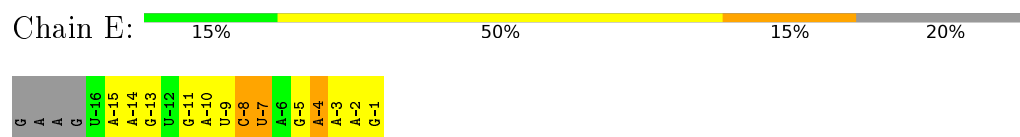
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

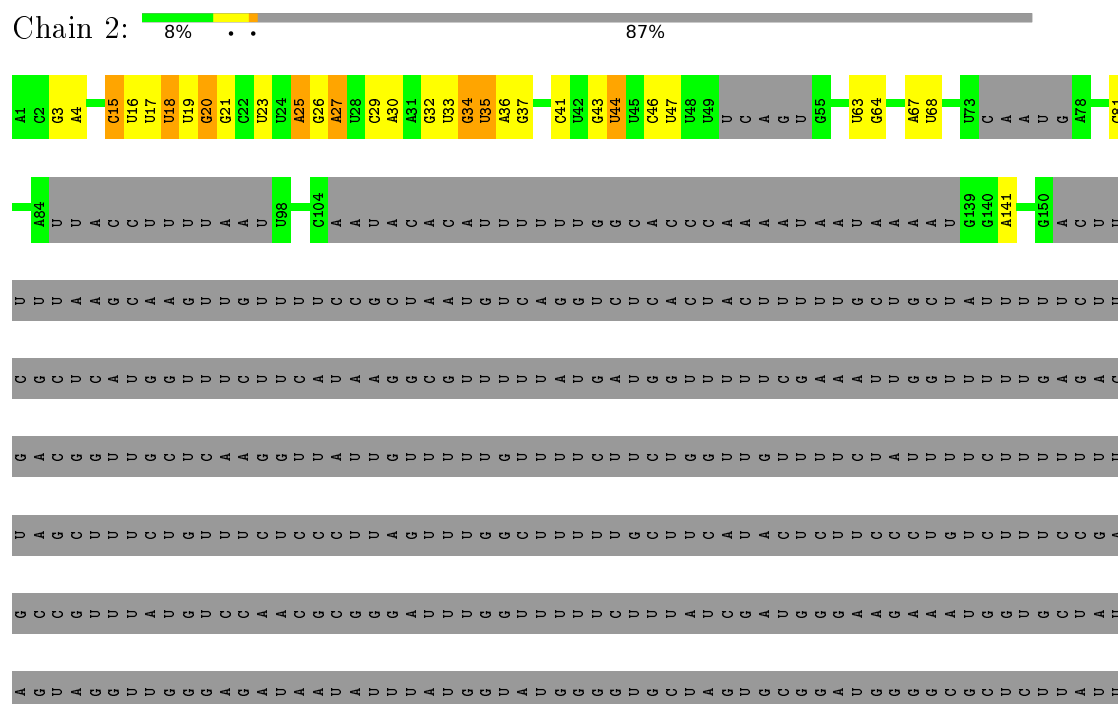
- Molecule 1: Yeast UBC4 gene for ubiquitin-conjugating enzyme



- Molecule 2: 5'-EXON OF UBC4 PRE-MRNA



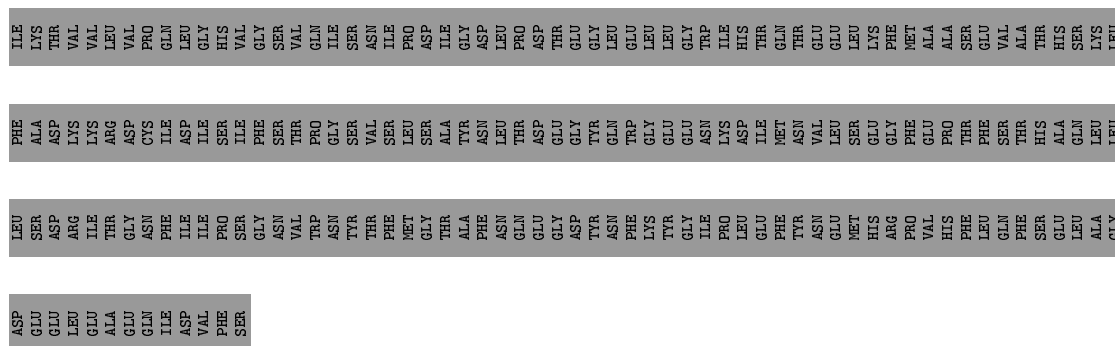
- Molecule 3: S.cerevisiae chromosome II reading frame ORF YBR230c



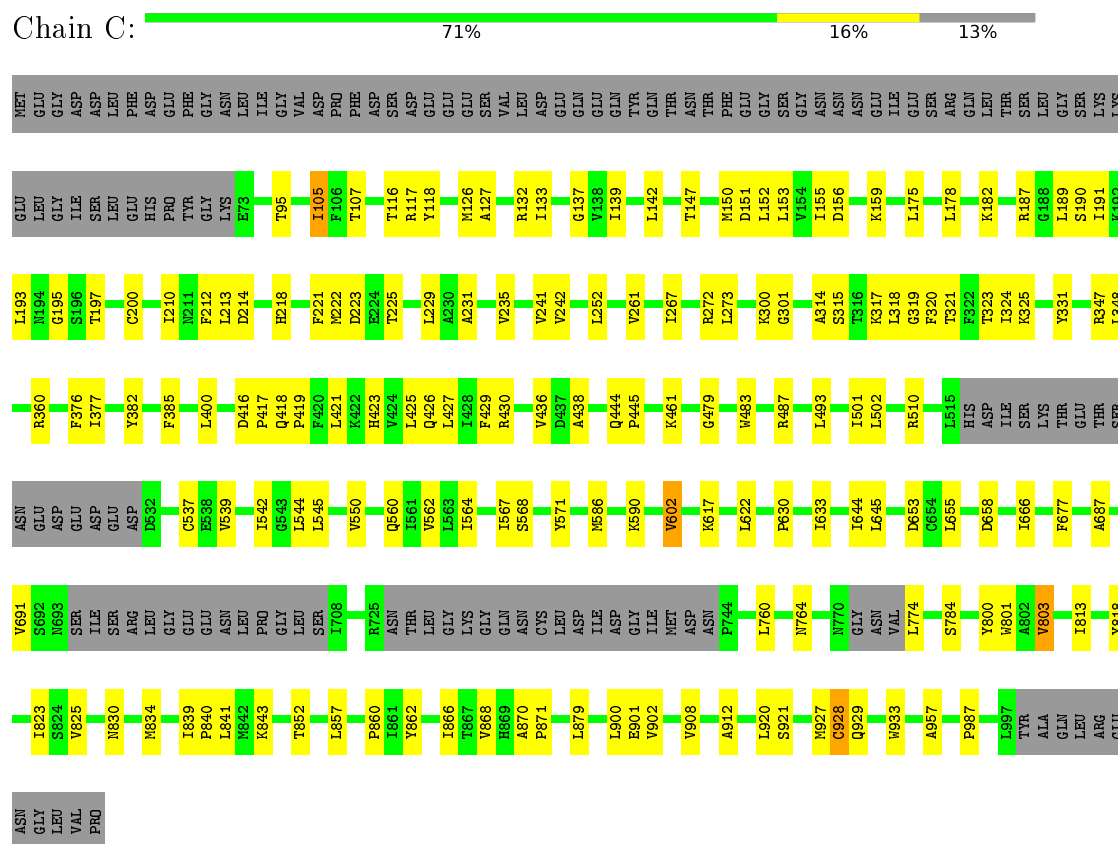
Device Type	Percentage
Smartphones	64%
Tablets	15%
Other mobile devices	21%

WORLDWIDE
PDB
PROTEIN DATA BANK

 **EMDataBank**
Unified Data Resource for 3DEM



- Molecule 7: Pre-mRNA-splicing factor SNU114

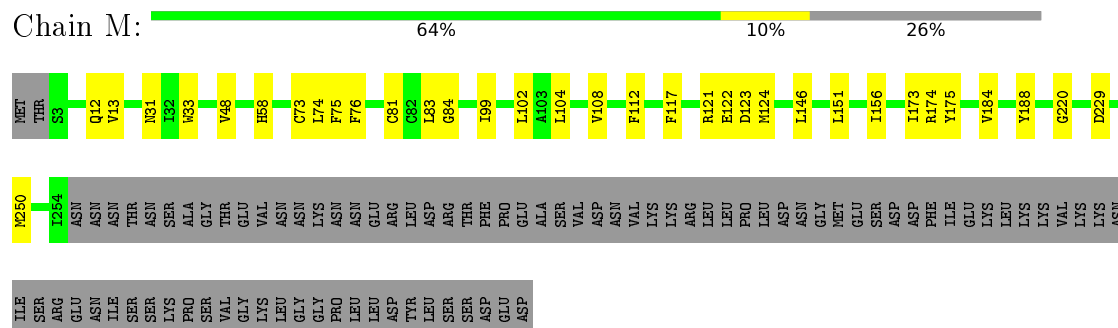


- Molecule 8: Pre-mRNA-splicing factor CWC22

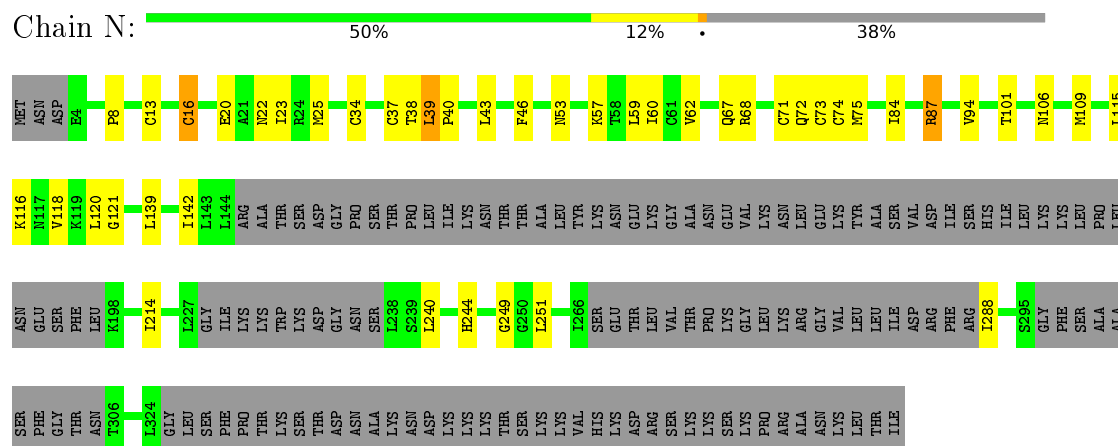




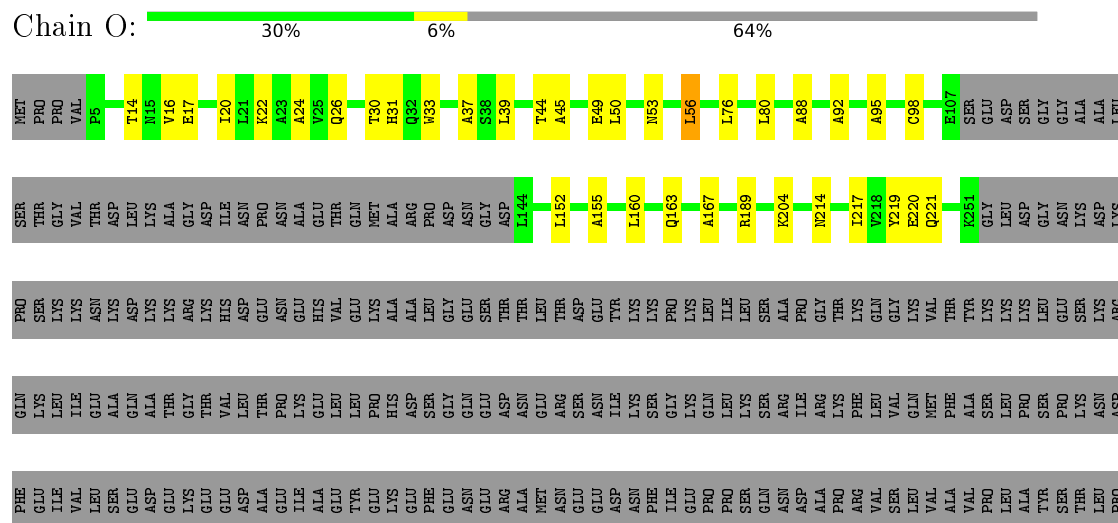
• Molecule 12: Pre-mRNA-splicing factor CWC2



• Molecule 13: Pre-mRNA-splicing factor SLT11



• Molecule 14: Pre-mRNA-splicing factor CEF1



ILE	PRO	GLU	PHE	LYS	ASN	ASN	PRO	GLN	SER	ALA	ILE	ASP	ASN	TYR	ASN	LEU	LEU	VAL	ALA	ASN	ALA	ILE	ASN	LYS	GLU	PRO	HIS	MET	VAL	PRO	GLU	ASP	THR	GLN	ASP	PHE	LEU	LYS	GLU	VAL	GLU	SER	ARG	MET	GLN	HIS	ILE	THR	GLN	GLY	ARG	THR	GLY	SER	LEU	GLN	ILE	THR	GLY	ARG	LYS	ILE	GLN	LYS	PHE
LYS	THR	ALA	MET	PRO	PRO	THR	GLU	VAL	LEU	LEU	GLU	SER	ILE	GLN	LYS	VAL	GLU	SER	ILE	GLN	ALA	GLN	LEU	GLN	LYS	LEU	GLN	HIS	VAL	GLN	ASN	ASN	GLU	MET	CYS	SER	THR	LEU	CYS	HIS	SER	LEU	PRO	ALA	LEU	ILE	GLU	THR	GLY	GLN	ARG	LYS	TYR												
TYR	ALA	ASP	TYR	TYR	ALA	TYR	ARG	GLN	GLU	ILE	ARG	SER	LEU	GLY	GLU	ARG	LYS	ARG	LEU	GLN	ALA	ALA	MET	LEU	ASN	SER	SER	SER	ILE																																				

• Molecule 15: Pre-mRNA-splicing factor CWC15

Chain P:  35% 61%

GLY	Y156	V174	R175																																																								
ASP	GLN	LYS	ASP	LEU	GLN	LEU	VAL	THR	GLN	LYS	ASN	LYS	VAL	GLU	ASP	LYS	ALA	GLU	LEU	GLU	GLY	ASN	GLN	GLU	LEU	LYS	GLY	GLY	ASN	SER	SER	ARG	ARG	S126	W127	R135	HIS	LYS	VAL	THR	LYS	GLU	THR	VAL	GLN	GLY	SER	ILE	LYS	GLU	HIS	ALA	THR	LYS	LYS	ALA	GLU	SER	LYS
MET	THR	S4	R6	L9	H34	R40	K41	F42	LYS	GLU	GLU	ASN	GLU	GLU	ASN	LEU	ALA	ALA	CYS	ALA	GLN	GLU	ASP	SER	ASN	LYS	ASP	SER	LEU	GLU	GLU	VAL	MET	ASN	GLU	GLU	LYS	GLN	ASP	VAL	VAL	GLY	GLY	GLY	ASN	LEU	GLN	GLU	THR	ARG	SER	LYS	GLU	LYS					

• Molecule 16: Pre-mRNA-splicing factor CWC21

Chain R:  72% 7% 20%

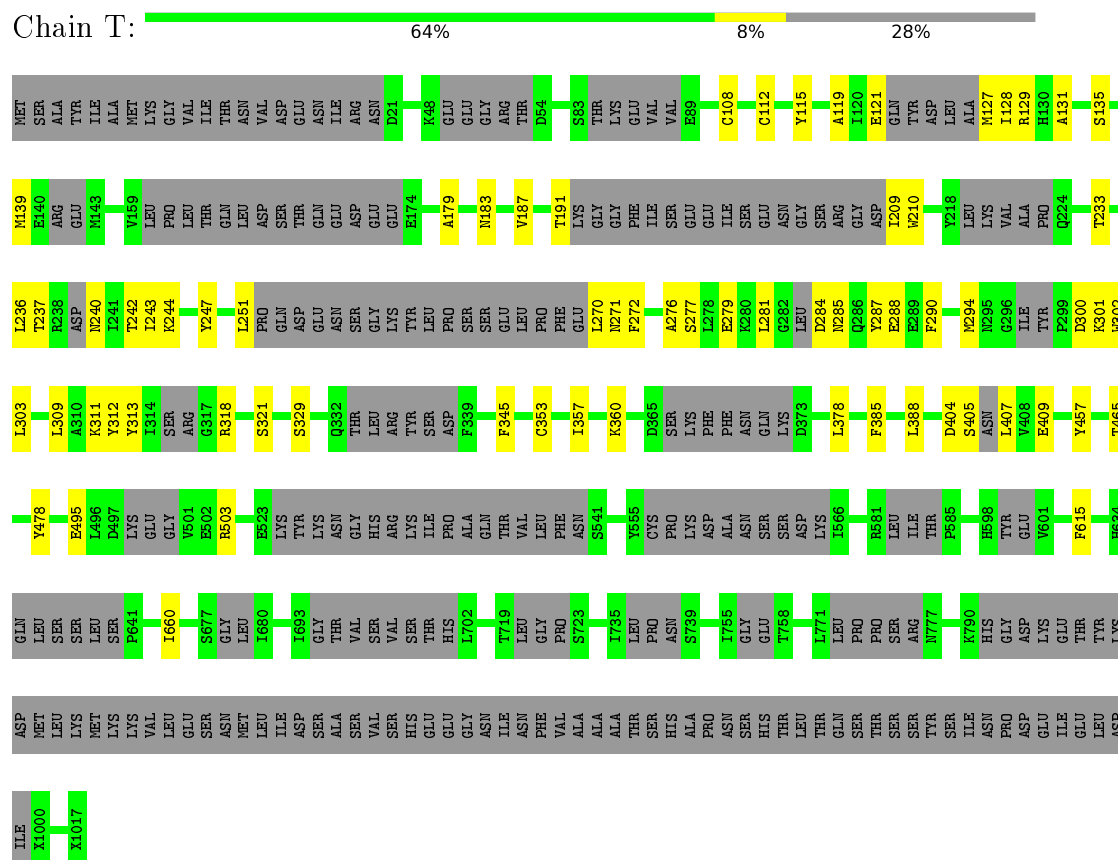
MET	S2	L8	K9	G13	S14	S15	S16	S17	G18	H19	S50	HIS	ASP	GLN	ALA	SER	ARG	PRO	L58	H67	R71	L102	L106	M116	SER	SER	LEU	TYR	THR	PRO	ARG	LYS	ALA	ARG	LEU	THR	GLU	GLN	HIS	ARG	HIS	GLU
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• Molecule 17: Pre-mRNA-splicing factor CLF1

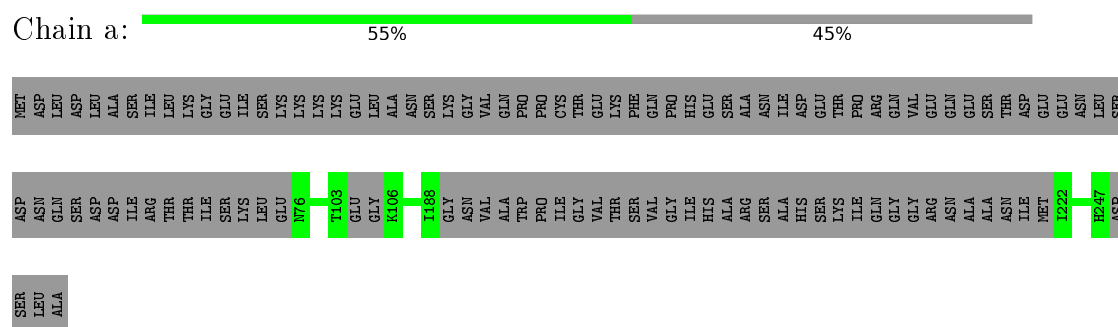
Chain S:  60% 7% 32%

TRP	LYS	GLN	GLU	GLN	ALA	LEU	TYR	GLU	GLN	GLU	GLN	GLU	GLN	ASP	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GLU	GLN	GL
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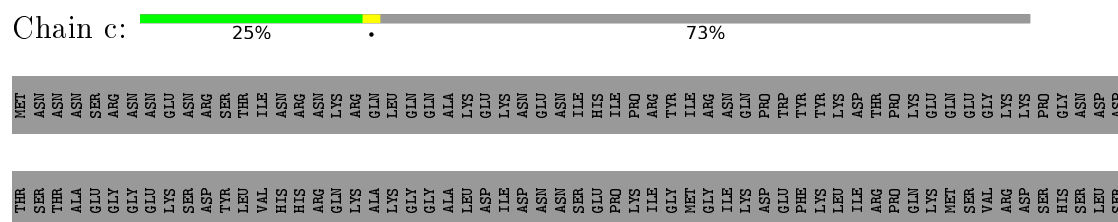
• Molecule 18: Pre-mRNA-splicing factor SYF1,PRE-MRNASPLICING FACTOR SYF1

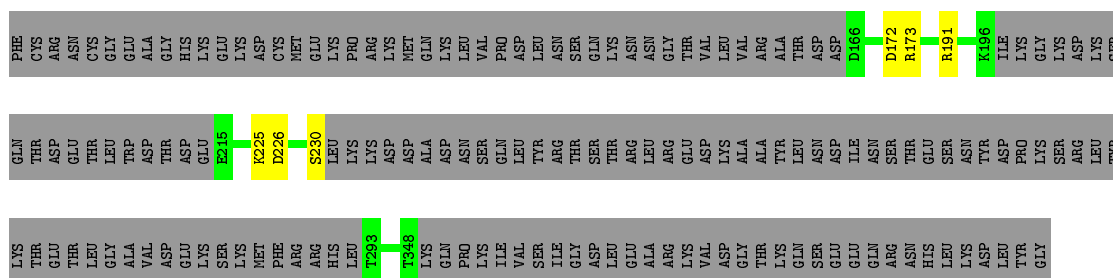


• Molecule 19: Pre-mRNA-splicing factor 18

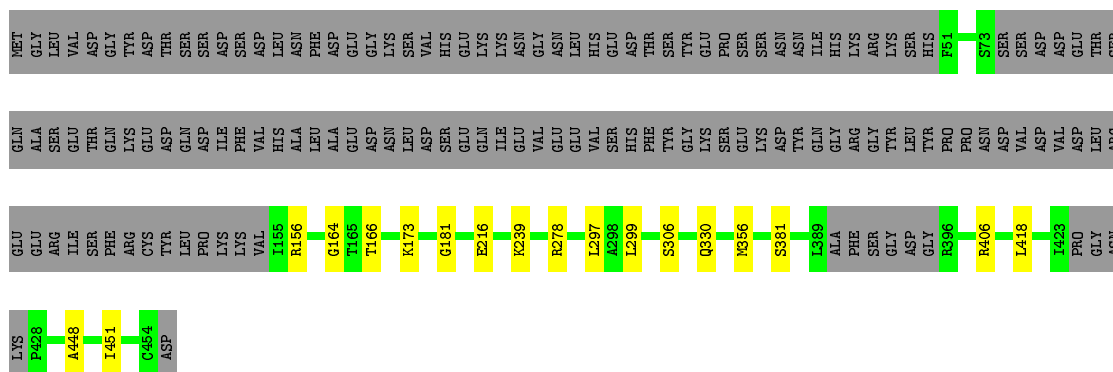


• Molecule 20: Pre-mRNA-splicing factor SLU7





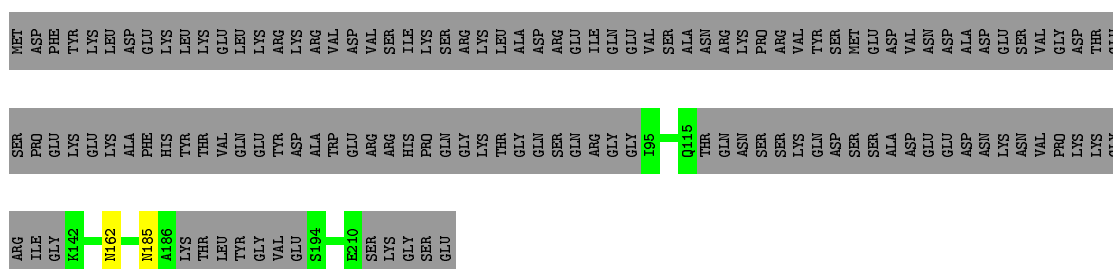
- Molecule 21: Pre-mRNA-processing factor 17



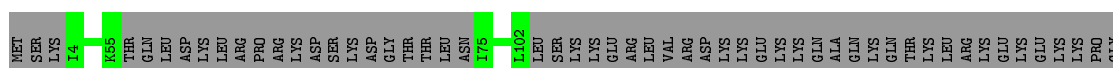
- Molecule 22: UNKNOWN PROTEIN



- Molecule 23: Pre-mRNA-splicing factor SYF2



- Molecule 24: Small nuclear ribonucleoprotein-associated protein B



LYS ILE ALA LYS PRO ASN THR ALA ASN ALA LYS HIS THR SER SER ASN SER ARG GLU ILE ALA GLN PRO SER SER SER ARG TYR ASN GLY GLY ASN ASP ASN ILE GLY ALA ASN ARG SER ARG PHE VAL ASN ASP ASN ALA PRO PRO GLN THR ARG LYS PHE GLN PRO PRO GLY PHE LYS

ARG
LYS

- Molecule 24: Small nuclear ribonucleoprotein-associated protein B


Chain k:  39% . 59%

MET SER I4 K19 K85 THR LYS LEU ASP LYS LEU PRO ARG LYS ASP SER SER ASP GLY THR LEU ASN I75 V81 L84 L102 SER LYS LYS GLU ARG LEU VAL ARG ASP LYS LYS ARG PHE THR ALA GLN LYS THR LYS LEU ARG LYS GLU

LYS GLU LYS LYS PRO GLY LYS ILE ALA LYS PRO ASN THR ALA ASN ALA HIS THR SER SER ASN SER ARG GLU ILE ALA GLN PRO SER SER SER ARG TYR ASN GLY GLY ASN ASP ASN ILE GLY VAL ALA ASN ARG ARG SER PHE LYS ASN GLU ALA PRO GLN THR ARG LYS PHE GLN


PRO
PRO
PRO
GLY
PHE
LYS
ARG
LYS

- Molecule 25: Small nuclear ribonucleoprotein Sm D3

Chain d:  81% 19%


MET THR MET I4 K85 LYS ASN SER SER ARG PRO MET PRO PRO ILE ARG GLY PRO LYS ARG ARG

- Molecule 25: Small nuclear ribonucleoprotein Sm D3

Chain n:  78% . 19%

MET THR MET I4 S20 Q43 D76 K85 LYS ASN SER SER ARG PRO MET PRO PRO ILE ARG GLY PRO LYS ARG ARG

- Molecule 26: Small nuclear ribonucleoprotein E

Chain e:  78% . 20%


MET SER ASN LYS VAL LYS THR LYS ALA M10 T25 S64 ALA ASP GLY LYS GLU ASP VAL VAL GLU K73 S92 ALA ASP

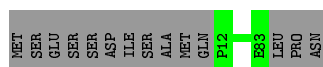
- Molecule 26: Small nuclear ribonucleoprotein E

Chain p:  73% 6% 20%

MET SER ASN LYS VAL LYS THR LYS ALA M10 I54 S64 ALA ASP GLY LYS GLU ASP VAL VAL GLU K73 G74 L77 G78 K79 I80 L81 L82 S92 ALA ASP

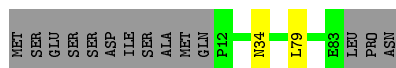
- Molecule 27: Small nuclear ribonucleoprotein F

Chain f:  84% 16%



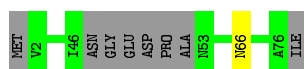
- Molecule 27: Small nuclear ribonucleoprotein F

Chain q: 81% 16%



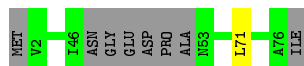
- Molecule 28: Small nuclear ribonucleoprotein G

Chain g: 88% 10%



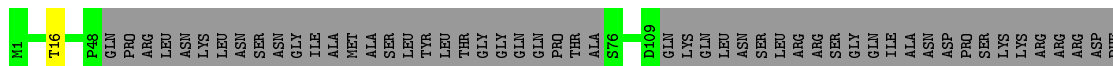
- Molecule 28: Small nuclear ribonucleoprotein G

Chain r: 88% 10%



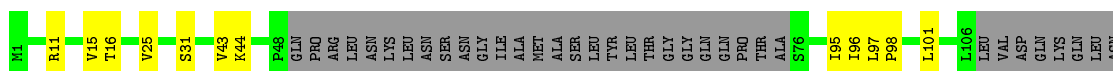
- Molecule 29: Small nuclear ribonucleoprotein Sm D1

Chain h: 55% 44%



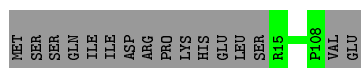
- Molecule 29: Small nuclear ribonucleoprotein Sm D1

Chain l: 46% 8% 46%

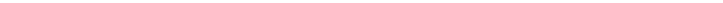


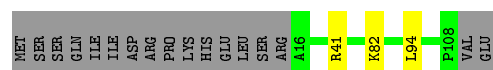
- Molecule 30: Small nuclear ribonucleoprotein Sm D2

Chain j: 85% 15%



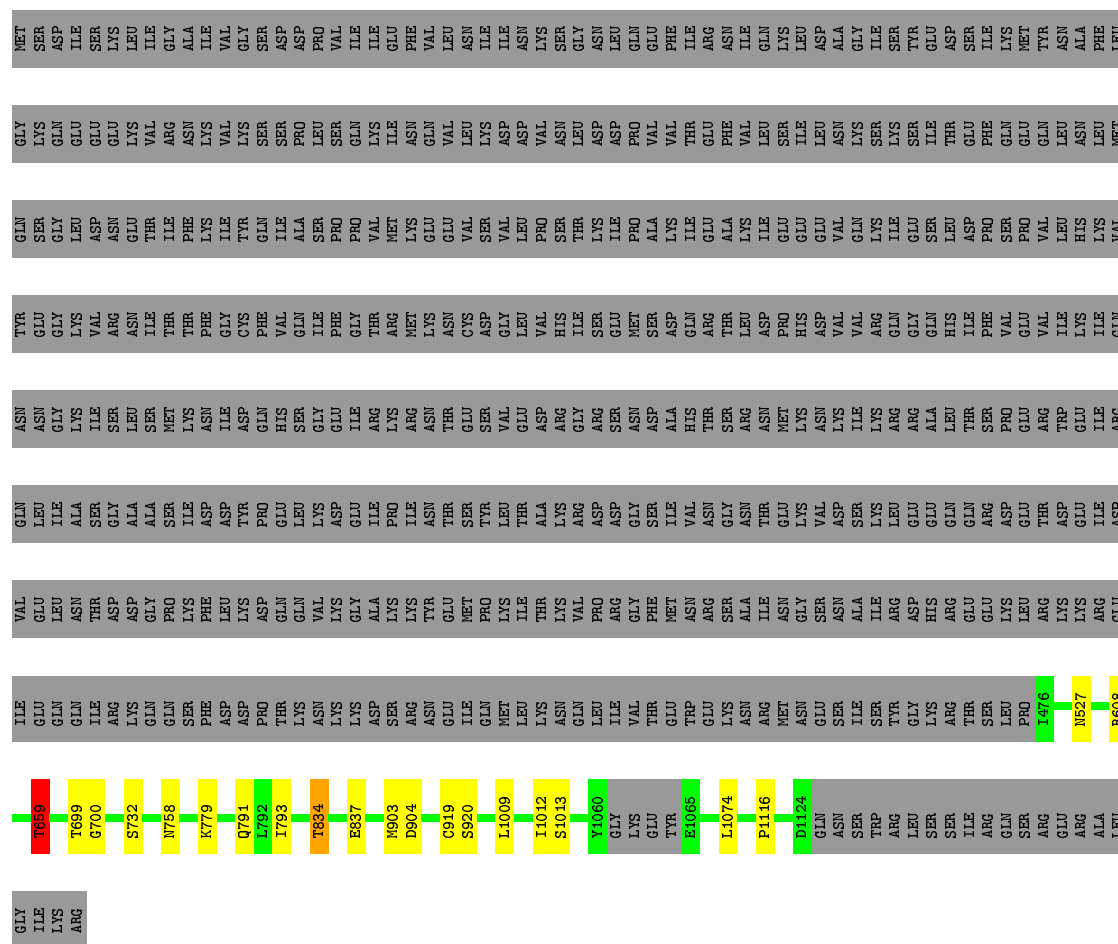
- Molecule 30: Small nuclear ribonucleoprotein Sm D2

Chain m:  82% • 15%



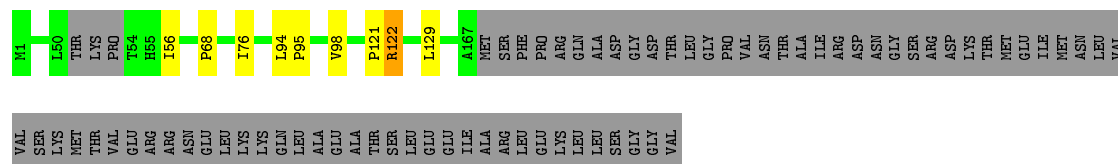
- Molecule 31: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22

Chain V: 54% . 44%



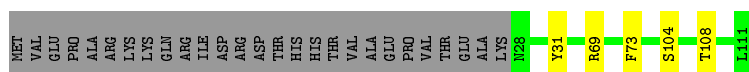
- Molecule 32: U2 small nuclear ribonucleoprotein A'

Chain W:  65% . 31%



- Molecule 33: U2 small nuclear ribonucleoprotein B''

Chain Y:  71% 5% 24%



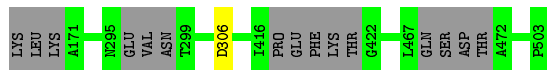
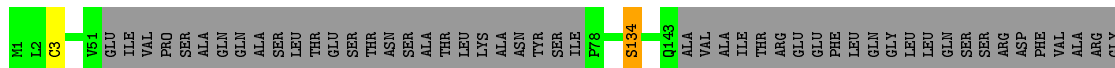
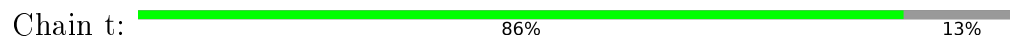
- Molecule 34: 3'-EXON OF UBC4 PRE-MRNA, BOUND BY PRP22 HELICASE



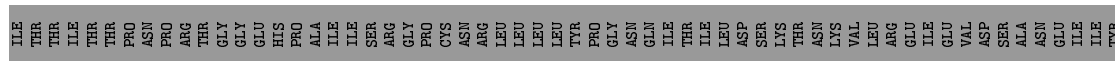
- Molecule 35: Pre-mRNA-splicing factor SNT309

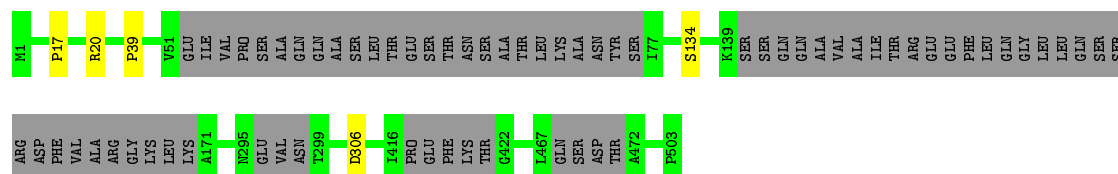
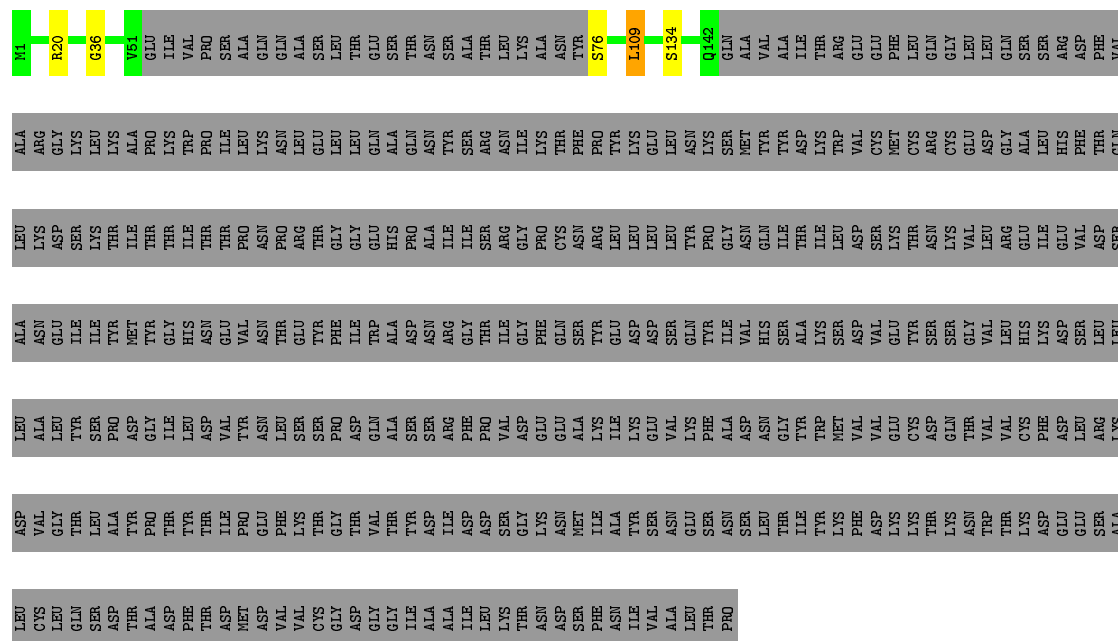


- Molecule 36: Pre-mRNA-processing factor 19



- Molecule 36: Pre-mRNA-processing factor 19





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	29527	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	81000	Depositor
Image detector	Not provided	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, MG, K, I6P, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	I	0.33	0/795	0.83	1/1231 (0.1%)
10	K	0.44	0/1480	0.75	0/2000
11	L	0.46	0/1186	0.72	0/1606
12	M	0.41	0/2062	0.66	0/2772
13	N	0.41	0/1823	0.71	0/2456
14	O	0.46	0/1781	0.78	0/2385
15	P	0.39	0/580	0.66	0/776
16	R	0.41	0/617	0.68	0/848
17	S	0.47	0/3269	0.76	0/4446
18	T	0.42	0/3036	0.71	0/4197
19	a	0.38	0/1141	0.61	0/1546
2	E	0.34	0/388	0.78	0/603
20	c	0.45	1/798 (0.1%)	0.60	0/1074
21	o	0.41	0/2491	0.64	0/3384
23	y	0.34	0/681	0.54	0/902
24	b	0.36	0/636	0.63	0/856
24	k	0.35	0/636	0.58	0/856
25	d	0.35	0/634	0.56	0/859
25	n	0.37	0/634	0.53	0/859
26	e	0.41	0/585	0.61	0/795
26	p	0.40	0/585	0.56	0/795
27	f	0.40	0/585	0.57	0/791
27	q	0.40	0/585	0.61	0/791
28	g	0.50	0/532	0.61	0/715
28	r	0.35	0/529	0.50	0/711
29	h	0.38	0/649	0.54	0/880
29	l	0.40	0/623	0.64	0/844
3	2	0.27	0/3639	0.72	0/5643
30	j	0.36	0/753	0.57	0/1013
30	m	0.37	0/738	0.61	0/995
31	V	0.57	2/3186 (0.1%)	1.53	9/4434 (0.2%)
32	W	0.31	0/814	0.53	0/1134

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
33	Y	0.32	0/415	0.55	0/577
34	3	0.19	0/65	0.65	0/98
35	s	0.57	0/546	0.80	0/760
36	t	0.46	0/2165	0.71	3/3010 (0.1%)
36	u	0.57	0/576	0.78	0/802
36	v	0.59	0/586	0.89	3/816 (0.4%)
36	w	0.47	0/2150	0.68	2/2989 (0.1%)
4	6	0.33	0/2357	0.72	1/3667 (0.0%)
5	5	0.32	0/3351	0.73	0/5213
6	A	0.46	0/15598	0.73	0/21212
7	C	0.42	0/6703	0.69	0/9138
8	H	0.48	0/3314	0.77	0/4463
9	J	0.47	0/2749	0.74	0/3735
All	All	0.43	3/79046 (0.0%)	0.76	19/109677 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
15	P	0	1
21	o	0	1
24	k	0	1
31	V	0	3
35	s	0	2
36	t	0	2
36	v	0	1
36	w	0	1
7	C	0	1
9	J	0	1
All	All	0	14

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	V	1009	LEU	C-N	7.26	1.50	1.34
20	c	230	SER	C-O	6.14	1.35	1.23
31	V	834	THR	C-N	-5.27	1.22	1.34

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	V	834	THR	C-N-CA	-46.64	5.11	121.70
31	V	834	THR	CA-C-N	-38.77	31.91	117.20
31	V	1009	LEU	O-C-N	27.39	166.52	122.70
31	V	1009	LEU	CA-C-N	-22.51	67.67	117.20
31	V	1009	LEU	C-N-CA	-18.95	74.32	121.70
31	V	659	THR	O-C-N	-18.65	92.86	122.70
31	V	659	THR	C-N-CA	-15.15	83.82	121.70
31	V	834	THR	O-C-N	-13.32	101.39	122.70
31	V	659	THR	CA-C-N	-12.68	89.30	117.20
36	t	134	SER	CA-C-O	-7.90	103.51	120.10
4	6	45	A	C2'-C3'-O3'	7.15	125.23	109.50
36	t	134	SER	O-C-N	6.00	132.31	122.70
36	w	39	PRO	N-CA-CB	6.00	110.50	103.30
36	v	134	SER	CA-C-O	-5.68	108.18	120.10
36	v	76	SER	N-CA-CB	5.29	118.44	110.50
1	I	9	A	C4'-C3'-O3'	5.26	123.53	113.00
36	v	134	SER	O-C-N	5.19	131.01	122.70
36	t	306	ASP	CB-CA-C	-5.11	100.17	110.40
36	w	306	ASP	CB-CA-C	-5.10	100.19	110.40

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
7	C	105	ILE	Peptide
9	J	194	HIS	Peptide
15	P	5	HIS	Peptide
31	V	659	THR	Mainchain
31	V	834	THR	Mainchain,Peptide
24	k	84	LEU	Peptide
21	o	239	LYS	Peptide
35	s	111	VAL	Peptide
35	s	132	LEU	Peptide
36	t	134	SER	Mainchain
36	t	3	CYS	Mainchain
36	v	109	LEU	Mainchain
36	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	I	714	0	361	6	0
2	E	346	0	173	11	0
3	2	3271	0	1660	26	0
4	6	2108	0	1063	29	0
5	5	2999	0	1515	34	0
6	A	15199	0	14954	262	0
7	C	6562	0	6486	105	0
8	H	3261	0	3323	91	0
9	J	2690	0	2690	85	0
10	K	1458	0	1468	20	0
11	L	1162	0	1111	19	0
12	M	2016	0	1985	32	0
13	N	1798	0	1842	38	0
14	O	1755	0	1794	24	0
15	P	565	0	555	7	0
16	R	614	0	390	8	0
17	S	3229	0	2573	37	0
18	T	3154	0	1331	94	0
19	a	1119	0	1164	0	0
20	c	786	0	719	0	0
21	o	2425	0	2253	0	0
22	X	338	0	70	1	0
23	y	679	0	706	0	0
24	b	631	0	670	0	0
24	k	631	0	665	0	0
25	d	625	0	647	0	0
25	n	625	0	647	0	0
26	e	575	0	597	0	0
26	p	575	0	597	0	0
27	f	573	0	572	0	0
27	q	573	0	572	0	0
28	g	529	0	557	0	0
28	r	526	0	555	0	0
29	h	644	0	686	0	0
29	l	618	0	660	0	0
30	j	741	0	778	0	0
30	m	726	0	754	0	0
31	V	3189	0	1412	12	0
32	W	816	0	340	1	0
33	Y	416	0	182	14	0
34	3	60	0	31	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	s	548	0	219	0	0
36	t	2171	0	945	0	0
36	u	578	0	246	0	0
36	v	588	0	250	0	0
36	w	2156	0	938	0	0
37	6	3	0	0	0	0
38	6	2	0	0	0	0
39	A	36	0	6	0	0
40	C	32	0	12	0	0
41	L	3	0	0	0	0
41	M	1	0	0	0	0
41	N	2	0	0	0	0
All	All	77441	0	63724	846	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 8.

All (846) 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)
18:T:119:ALA:HB2	18:T:131:ALA:CB	1.25	1.63
18:T:119:ALA:CB	18:T:131:ALA:HB3	1.40	1.48
18:T:237:THR:N	18:T:240:ASN:N	1.73	1.34
18:T:300:ASP:CB	18:T:303:LEU:CB	2.06	1.33
18:T:119:ALA:HB1	18:T:128:ILE:CA	1.58	1.33
18:T:128:ILE:H	18:T:183:ASN:CB	1.45	1.29
18:T:119:ALA:CB	18:T:128:ILE:HA	1.61	1.29
18:T:271:ASN:HA	18:T:294:MET:O	1.27	1.28
34:3:2:U:C2'	34:3:3:U:H5'	1.63	1.28
8:H:312:LEU:HA	8:H:315:LEU:CD2	1.64	1.27
34:3:2:U:H2'	34:3:3:U:C5'	1.64	1.26
8:H:311:LYS:O	8:H:315:LEU:CD2	1.85	1.24
3:2:1107:C:C4	33:Y:31:TYR:CB	2.23	1.21
8:H:312:LEU:CA	8:H:315:LEU:HD23	1.72	1.19
18:T:285:ASN:HA	18:T:311:LYS:CB	1.73	1.19
12:M:108:VAL:CG1	13:N:59:LEU:HD22	1.72	1.19
18:T:128:ILE:N	18:T:183:ASN:CB	2.06	1.18
8:H:312:LEU:CA	8:H:315:LEU:CD2	2.21	1.18
3:2:1107:C:N3	33:Y:31:TYR:CB	2.06	1.18
8:H:312:LEU:O	8:H:315:LEU:HD23	1.44	1.18
12:M:108:VAL:CG1	13:N:59:LEU:CD2	2.21	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:312:LEU:C	8:H:315:LEU:HD23	1.61	1.17
18:T:191:THR:CB	18:T:209:ILE:CB	2.24	1.14
8:H:311:LYS:O	8:H:315:LEU:HD22	1.38	1.13
18:T:357:ILE:CB	18:T:385:PHE:CB	2.29	1.11
18:T:119:ALA:HB1	18:T:128:ILE:C	1.72	1.09
18:T:119:ALA:HB1	18:T:128:ILE:HA	1.11	1.08
18:T:115:TYR:O	18:T:131:ALA:HB1	1.53	1.06
8:H:312:LEU:HA	8:H:315:LEU:HD21	1.39	1.04
8:H:315:LEU:H	8:H:315:LEU:HD22	1.22	1.03
12:M:108:VAL:HG13	13:N:59:LEU:HD22	1.40	1.03
18:T:271:ASN:CA	18:T:294:MET:O	2.06	1.03
3:2:1106:G:C6	33:Y:69:ARG:O	2.11	1.02
8:H:317:ILE:HD11	8:H:322:LYS:HG2	1.42	1.01
18:T:313:TYR:HA	18:T:318:ARG:CB	1.91	1.00
18:T:300:ASP:C	18:T:303:LEU:H	1.64	1.00
18:T:288:GLU:CB	18:T:311:LYS:CB	2.42	0.98
18:T:300:ASP:C	18:T:301:LYS:N	2.16	0.98
18:T:128:ILE:CB	18:T:183:ASN:CB	2.42	0.97
12:M:108:VAL:HG13	13:N:59:LEU:CD2	1.91	0.96
3:2:1106:G:O6	33:Y:69:ARG:O	1.83	0.95
8:H:312:LEU:HA	8:H:315:LEU:HD23	1.31	0.95
18:T:404:ASP:CB	18:T:409:GLU:CB	2.45	0.94
8:H:312:LEU:C	8:H:315:LEU:CD2	2.35	0.94
18:T:237:THR:H	18:T:240:ASN:N	1.54	0.94
18:T:119:ALA:CA	18:T:128:ILE:HA	1.97	0.93
12:M:108:VAL:HG11	13:N:59:LEU:HD22	1.47	0.93
6:A:904:THR:O	31:V:1116:PRO:CB	2.17	0.93
8:H:311:LYS:O	8:H:315:LEU:HD21	1.66	0.92
18:T:119:ALA:HB1	18:T:128:ILE:O	1.70	0.91
12:M:108:VAL:CG1	13:N:59:LEU:HD21	1.97	0.91
18:T:119:ALA:C	18:T:128:ILE:HA	1.90	0.91
8:H:317:ILE:HD11	8:H:322:LYS:CG	1.99	0.90
18:T:119:ALA:CB	18:T:131:ALA:CB	2.19	0.90
18:T:119:ALA:HB2	18:T:131:ALA:HB2	1.50	0.89
31:V:732:SER:CB	34:3:2:U:OP2	2.22	0.87
8:H:312:LEU:CA	8:H:315:LEU:HD21	1.99	0.86
18:T:284:ASP:C	18:T:311:LYS:HA	1.95	0.85
18:T:128:ILE:CA	18:T:183:ASN:CB	2.54	0.85
3:2:1108:A:N6	33:Y:108:THR:CB	2.40	0.84
31:V:700:GLY:HA3	34:3:1:U:OP2	1.76	0.84
18:T:312:TYR:CB	18:T:321:SER:CB	2.55	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:119:ALA:CB	18:T:128:ILE:O	2.26	0.83
9:J:355:THR:HG21	9:J:404:CYS:HA	1.59	0.83
7:C:142:LEU:HD11	7:C:189:LEU:HD22	1.61	0.82
9:J:156:ILE:HD13	9:J:197:LEU:HD21	1.59	0.82
8:H:311:LYS:C	8:H:315:LEU:HD21	2.00	0.82
12:M:108:VAL:HG21	13:N:73:CYS:O	1.78	0.81
8:H:312:LEU:O	8:H:315:LEU:CD2	2.25	0.81
18:T:187:VAL:CB	18:T:210:TRP:CB	2.60	0.80
7:C:139:ILE:HD12	7:C:225:THR:HG23	1.62	0.79
31:V:903:MET:C	31:V:904:ASP:N	2.35	0.79
9:J:240:ALA:HB1	9:J:248:ILE:HD11	1.65	0.78
12:M:108:VAL:HG12	13:N:59:LEU:HD21	1.65	0.78
6:A:139:LEU:HD12	6:A:193:TYR:CG	2.18	0.78
18:T:285:ASN:CA	18:T:311:LYS:CB	2.59	0.78
18:T:237:THR:CA	18:T:240:ASN:N	2.47	0.78
14:O:16:VAL:HG22	14:O:152:LEU:HD21	1.66	0.77
11:L:41:LEU:HD23	11:L:44:LYS:HB2	1.65	0.77
8:H:136:LEU:HD22	8:H:169:THR:HG21	1.66	0.77
18:T:271:ASN:HA	18:T:294:MET:C	2.04	0.77
3:2:25:A:OP1	6:A:854:ARG:HD2	1.83	0.77
9:J:342:LEU:HD21	10:K:55:VAL:HG21	1.66	0.77
6:A:856:TRP:CD1	15:P:174:VAL:HG21	2.19	0.77
6:A:1350:ILE:HG23	6:A:1356:LEU:HD23	1.68	0.76
8:H:317:ILE:O	8:H:317:ILE:HD12	1.85	0.76
18:T:300:ASP:O	18:T:303:LEU:N	2.18	0.76
3:2:1108:A:C2	33:Y:73:PHE:CB	2.69	0.76
9:J:248:ILE:HG23	9:J:262:LEU:HB2	1.67	0.76
8:H:315:LEU:H	8:H:315:LEU:CD2	1.98	0.76
8:H:317:ILE:CD1	8:H:322:LYS:HG3	2.15	0.76
3:2:1106:G:N1	33:Y:69:ARG:O	2.19	0.75
18:T:233:THR:O	18:T:240:ASN:N	2.19	0.75
7:C:493:LEU:HD22	7:C:542:ILE:HD11	1.68	0.75
6:A:1020:ILE:HG22	6:A:1022:PRO:HD2	1.71	0.73
8:H:311:LYS:C	8:H:315:LEU:CD2	2.56	0.73
7:C:539:VAL:HG13	7:C:564:ILE:HG23	1.71	0.73
8:H:317:ILE:CD1	8:H:322:LYS:CG	2.66	0.73
8:H:315:LEU:N	8:H:315:LEU:HD22	2.02	0.72
18:T:244:LYS:CB	18:T:276:ALA:HA	2.20	0.72
8:H:316:LYS:HG3	8:H:316:LYS:O	1.90	0.71
6:A:1391:PRO:HG2	6:A:1547:ILE:HD11	1.70	0.71
18:T:300:ASP:C	18:T:303:LEU:N	2.41	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:140:LEU:HD21	17:S:155:LEU:HD22	1.71	0.71
6:A:1082:ILE:HD13	6:A:1113:ILE:HD11	1.72	0.71
18:T:251:LEU:CB	18:T:272:PHE:CB	2.69	0.71
31:V:699:THR:O	34:3:1:U:H4'	1.89	0.71
18:T:244:LYS:CB	18:T:279:GLU:CB	2.68	0.71
18:T:300:ASP:C	18:T:302:TRP:N	2.44	0.71
18:T:236:LEU:C	18:T:240:ASN:N	2.43	0.71
6:A:1634:LEU:HD21	6:A:1641:LEU:HD12	1.73	0.70
12:M:104:LEU:HD21	13:N:16:CYS:HA	1.73	0.70
17:S:209:GLU:HB3	17:S:218:THR:HG22	1.71	0.70
6:A:518:VAL:HG21	6:A:689:TYR:CD2	2.26	0.70
18:T:270:LEU:O	18:T:294:MET:HA	1.92	0.70
18:T:119:ALA:HA	18:T:127:MET:O	1.92	0.69
6:A:377:VAL:HG11	7:C:912:ALA:HB3	1.73	0.69
9:J:403:LEU:HD11	9:J:419:ALA:HB2	1.74	0.69
6:A:621:LEU:HD23	6:A:722:LEU:HD21	1.73	0.69
18:T:108:CYS:CB	18:T:139:MET:CB	2.72	0.68
18:T:236:LEU:CB	18:T:242:THR:CB	2.72	0.68
18:T:277:SER:CB	18:T:290:PHE:CB	2.71	0.68
12:M:108:VAL:HG11	13:N:59:LEU:CD2	2.09	0.68
7:C:633:ILE:HB	7:C:645:LEU:HD12	1.76	0.68
18:T:353:CYS:CB	18:T:388:LEU:CB	2.72	0.68
9:J:230:VAL:HG22	9:J:241:THR:HG22	1.75	0.68
4:6:79:A:OP1	4:6:81:G:O2'	2.12	0.68
5:5:101:C:OP1	6:A:672:LYS:N	2.26	0.67
6:A:1067:ASN:HB2	6:A:1083:THR:HG21	1.76	0.67
9:J:144:CYS:SG	9:J:188:VAL:N	2.68	0.67
34:3:2:U:C2'	34:3:3:U:C5'	2.45	0.66
6:A:857:ILE:HD11	6:A:969:ILE:HD11	1.76	0.66
8:H:317:ILE:C	8:H:317:ILE:HD12	2.15	0.66
3:2:1107:C:N4	33:Y:31:TYR:CB	2.57	0.66
18:T:233:THR:O	18:T:240:ASN:HA	1.95	0.66
14:O:37:ALA:HB2	14:O:45:ALA:HA	1.76	0.66
6:A:1092:PHE:CZ	6:A:1093:LYS:HG3	2.31	0.66
7:C:193:LEU:HD12	7:C:213:LEU:HB3	1.78	0.66
5:5:38:A:H2'	5:5:39:U:O4'	1.96	0.65
7:C:142:LEU:HD13	7:C:218:HIS:HB2	1.78	0.65
9:J:333:SER:HB2	9:J:343:THR:HG23	1.79	0.65
34:3:2:U:C5	34:3:3:U:C5	2.85	0.65
7:C:155:ILE:HD11	7:C:175:LEU:HD23	1.78	0.65
8:H:132:GLU:HB2	8:H:135:ILE:HD11	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:330:ILE:O	8:H:334:LEU:HD23	1.97	0.64
12:M:250:MET:SD	13:N:139:LEU:HD21	2.37	0.64
18:T:244:LYS:O	18:T:276:ALA:HB2	1.96	0.64
5:5:45:A:H61	5:5:74:U:H3	1.46	0.64
6:A:569:LEU:HD21	6:A:637:VAL:HG21	1.80	0.64
6:A:228:LYS:HG3	6:A:695:LEU:HD11	1.80	0.64
7:C:197:THR:HG21	7:C:544:LEU:HD22	1.79	0.64
18:T:281:LEU:CB	18:T:287:TYR:CB	2.76	0.64
18:T:119:ALA:C	18:T:128:ILE:CA	2.65	0.64
6:A:1961:LEU:HD13	6:A:2083:ILE:HG21	1.78	0.63
3:2:1107:C:C2	33:Y:31:TYR:CB	2.82	0.63
31:V:608:ARG:O	31:V:837:GLU:CB	2.46	0.63
31:V:920:SER:N	31:V:1012:ILE:O	2.31	0.63
8:H:49:ILE:HB	8:H:56:ILE:HD13	1.80	0.63
31:V:779:LYS:O	34:3:1:U:H1'	1.98	0.63
8:H:334:LEU:HD21	8:H:384:LEU:HD12	1.81	0.63
12:M:250:MET:HB2	13:N:139:LEU:HD11	1.81	0.62
2:E:-3:A:H2'	2:E:-2:A:O4'	2.00	0.62
18:T:233:THR:O	18:T:240:ASN:CA	2.48	0.62
3:2:1108:A:H62	33:Y:108:THR:CB	2.13	0.61
6:A:1375:LEU:HD12	6:A:1383:PHE:CZ	2.35	0.61
6:A:1422:ILE:HD12	6:A:1422:ILE:O	2.00	0.61
14:O:16:VAL:CG2	14:O:152:LEU:HD21	2.31	0.61
6:A:388:PRO:HB2	6:A:398:VAL:HG11	1.82	0.61
9:J:145:VAL:HG22	9:J:157:THR:HG22	1.81	0.61
7:C:839:ILE:HB	7:C:840:PRO:HD3	1.81	0.61
14:O:24:ALA:HB2	14:O:39:LEU:HD23	1.83	0.61
7:C:483:TRP:CH2	7:C:550:VAL:HG11	2.36	0.60
18:T:129:ARG:H	18:T:183:ASN:CB	2.14	0.60
6:A:664:THR:O	6:A:666:ILE:N	2.34	0.60
5:5:45:A:N6	5:5:74:U:H3	1.99	0.59
6:A:585:ARG:HD3	12:M:33:TRP:CE2	2.38	0.59
7:C:691:VAL:HG12	7:C:841:LEU:HD22	1.83	0.59
9:J:277:VAL:HG22	9:J:278:ASP:H	1.67	0.59
6:A:1092:PHE:O	6:A:1093:LYS:C	2.39	0.59
6:A:677:ILE:HG21	6:A:1621:VAL:HG12	1.85	0.59
6:A:1126:LEU:HD11	6:A:1161:TYR:CD2	2.36	0.59
7:C:241:VAL:HG11	7:C:273:LEU:CD2	2.33	0.59
8:H:312:LEU:N	8:H:315:LEU:HD21	2.17	0.59
8:H:421:LYS:HB2	8:H:468:ILE:HD11	1.84	0.59
4:6:2:U:H2'	4:6:3:U:O4'	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:966:PRO:HB3	6:A:1089:VAL:HB	1.84	0.59
14:O:214:ASN:ND2	17:S:44:ARG:O	2.35	0.58
6:A:374:ILE:HG22	6:A:376:ARG:HG2	1.84	0.58
6:A:1023:LEU:HD13	6:A:1451:PHE:CE1	2.38	0.58
18:T:271:ASN:N	18:T:294:MET:O	2.35	0.58
18:T:329:SER:CB	18:T:345:PHE:CB	2.81	0.58
9:J:373:LEU:HD13	9:J:389:THR:CG2	2.33	0.58
6:A:1632:ILE:HD11	6:A:1649:PHE:CE2	2.39	0.58
6:A:779:ALA:HA	6:A:782:ILE:HD12	1.85	0.58
6:A:1422:ILE:HD13	6:A:1425:PHE:CZ	2.38	0.58
8:H:61:VAL:HG23	8:H:101:MET:SD	2.44	0.58
6:A:660:ILE:HG21	6:A:711:TRP:CH2	2.39	0.57
18:T:247:TYR:O	18:T:272:PHE:CB	2.51	0.57
18:T:236:LEU:CB	18:T:242:THR:H	2.17	0.57
18:T:284:ASP:O	18:T:311:LYS:HA	2.04	0.57
6:A:671:TYR:CZ	6:A:674:MET:HG3	2.39	0.57
6:A:585:ARG:HD3	12:M:33:TRP:CD2	2.40	0.57
9:J:200:VAL:HG11	9:J:230:VAL:HG23	1.87	0.57
9:J:265:HIS:CE1	9:J:291:ARG:HG2	2.40	0.57
6:A:1350:ILE:HD12	6:A:1356:LEU:CD2	2.34	0.57
17:S:270:ALA:HB1	17:S:280:LEU:HD11	1.85	0.57
18:T:309:LEU:HA	18:T:321:SER:CB	2.35	0.57
4:6:63:G:H2'	4:6:64:U:C6	2.39	0.57
6:A:1814:VAL:O	6:A:1818:ARG:HG2	2.04	0.57
7:C:562:VAL:HG23	7:C:564:ILE:HD11	1.87	0.57
8:H:334:LEU:HD12	8:H:380:GLN:HB3	1.87	0.57
6:A:1286:TRP:CE2	6:A:1302:LEU:HD11	2.40	0.57
6:A:1968:ALA:HA	6:A:2012:LEU:HD22	1.87	0.57
7:C:191:ILE:HG23	7:C:221:PHE:CE1	2.40	0.57
6:A:1426:ARG:HD2	16:R:8:LEU:HD12	1.87	0.56
8:H:200:ILE:O	8:H:204:ASP:N	2.35	0.56
2:E:-4:A:OP1	6:A:668:ARG:NE	2.38	0.56
18:T:112:CYS:HA	18:T:135:SER:CB	2.35	0.56
3:2:1106:G:H1	33:Y:69:ARG:CB	2.18	0.56
8:H:351:ILE:HG21	8:H:395:GLU:HB3	1.85	0.56
7:C:323:THR:CG2	7:C:438:ALA:HB2	2.36	0.56
6:A:1023:LEU:HA	6:A:1451:PHE:CZ	2.40	0.56
6:A:176:LEU:HD22	6:A:632:ILE:HD11	1.86	0.56
12:M:108:VAL:HG22	13:N:75:MET:HG2	1.86	0.56
14:O:20:ILE:HD11	14:O:152:LEU:HD22	1.86	0.56
18:T:119:ALA:CB	18:T:127:MET:O	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1309:ILE:HG12	6:A:1356:LEU:HD13	1.88	0.56
1:I:3:A:C2	1:I:4:U:C2	2.94	0.56
5:5:110:U:H2'	5:5:111:C:O4'	2.06	0.56
7:C:687:ALA:HB3	7:C:852:THR:HG21	1.88	0.56
1:I:67:C:H2'	1:I:68:U:O4'	2.06	0.56
6:A:1882:LEU:HD11	6:A:1991:ILE:HG21	1.88	0.55
9:J:164:MET:HE1	9:J:185:VAL:HG11	1.88	0.55
9:J:324:ALA:HB3	9:J:356:LEU:HD21	1.89	0.55
14:O:17:GLU:HA	14:O:20:ILE:HD12	1.88	0.55
17:S:149:VAL:HA	17:S:152:VAL:HG12	1.89	0.55
17:S:250:PHE:CE2	17:S:266:LEU:HD13	2.42	0.55
5:5:23:C:O4'	5:5:23:C:O2	2.25	0.55
6:A:1543:ARG:O	6:A:1547:ILE:HD12	2.06	0.55
8:H:25:VAL:HG23	8:H:44:LEU:HD13	1.89	0.55
3:2:34:G:O2'	3:2:35:U:H6	1.90	0.55
6:A:255:ILE:HD11	6:A:637:VAL:HG13	1.89	0.55
17:S:193:VAL:HG11	17:S:202:TRP:CZ2	2.42	0.55
18:T:129:ARG:CB	18:T:187:VAL:CB	2.85	0.55
6:A:1973:LYS:HB3	6:A:2039:LEU:HD12	1.89	0.55
6:A:343:ASN:HD21	6:A:354:PRO:HA	1.72	0.55
6:A:742:VAL:HG21	9:J:224:LEU:HA	1.89	0.55
7:C:900:LEU:O	7:C:902:VAL:N	2.39	0.55
4:6:70:U:OP2	6:A:737:ARG:NH2	2.40	0.55
4:6:61:C:H2'	4:6:62:A:O4'	2.07	0.54
11:L:29:GLN:HB3	11:L:55:LEU:HD11	1.88	0.54
6:A:615:LEU:HD13	6:A:619:PHE:CD2	2.41	0.54
4:6:35:A:H2'	12:M:75:PHE:CE1	2.42	0.54
6:A:624:GLU:HB3	6:A:666:ILE:HG12	1.89	0.54
17:S:251:ALA:HB1	17:S:267:TYR:OH	2.07	0.54
13:N:240:LEU:HD13	13:N:251:LEU:HD13	1.89	0.54
6:A:1158:ILE:HG12	6:A:1172:PHE:CE1	2.43	0.54
7:C:823:ILE:CG2	7:C:825:VAL:HG23	2.37	0.54
8:H:309:ALA:O	8:H:313:LEU:HD13	2.07	0.54
6:A:898:ILE:HB	6:A:1074:VAL:HG12	1.89	0.54
8:H:21:ILE:HG22	8:H:47:VAL:HG23	1.88	0.54
5:5:65:U:H2'	5:5:66:A:C8	2.43	0.54
18:T:281:LEU:CB	18:T:287:TYR:HA	2.37	0.54
18:T:405:SER:O	18:T:407:LEU:N	2.41	0.54
13:N:16:CYS:HB2	13:N:74:CYS:SG	2.47	0.54
8:H:60:VAL:HG13	8:H:76:LEU:HD21	1.89	0.54
9:J:321:PHE:HB2	10:K:57:LEU:HD12	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:L:30:LEU:HD13	11:L:55:LEU:HD22	1.89	0.54
6:A:1624:LEU:HD21	6:A:1635:HIS:CE1	2.43	0.54
17:S:99:ILE:N	17:S:100:PRO:CD	2.71	0.54
32:W:121:PRO:O	32:W:122:ARG:CB	2.56	0.54
4:6:62:A:H61	15:P:5:HIS:HB2	1.73	0.53
6:A:857:ILE:HD11	6:A:969:ILE:CD1	2.38	0.53
7:C:116:THR:HG21	7:C:118:TYR:CZ	2.42	0.53
3:2:34:G:HO2'	3:2:35:U:H6	1.55	0.53
6:A:1632:ILE:HG21	6:A:1645:LEU:HD13	1.90	0.53
6:A:673:VAL:HG22	6:A:714:PHE:CE1	2.44	0.53
5:5:39:U:H2'	5:5:40:C:C6	2.43	0.53
5:5:43:G:N2	5:5:46:C:OP1	2.41	0.53
13:N:13:CYS:SG	13:N:16:CYS:HB2	2.48	0.53
3:2:1107:C:N3	33:Y:104:SER:HA	2.23	0.53
6:A:1699:ALA:HB2	6:A:1767:TYR:CD1	2.43	0.53
9:J:277:VAL:HG11	9:J:321:PHE:HZ	1.74	0.53
18:T:119:ALA:HB2	18:T:131:ALA:HB3	0.56	0.53
5:5:123:U:H2'	5:5:124:C:C6	2.43	0.53
6:A:1283:GLU:N	8:H:345:ILE:HD11	2.24	0.53
7:C:324:ILE:HD12	7:C:325:LYS:N	2.24	0.53
8:H:351:ILE:HD11	8:H:361:TYR:CB	2.39	0.53
9:J:257:ILE:CD1	10:K:78:VAL:HG23	2.39	0.53
9:J:359:ASN:OD1	9:J:360:GLN:N	2.41	0.53
6:A:615:LEU:HD13	6:A:619:PHE:CE2	2.44	0.53
17:S:65:MET:SD	17:S:65:MET:N	2.81	0.53
4:6:52:G:O2'	4:6:53:A:O5'	2.23	0.53
8:H:73:ILE:HG13	8:H:74:PRO:HD3	1.91	0.53
14:O:30:THR:O	14:O:33:TRP:NE1	2.42	0.53
4:6:41:A:H2'	4:6:42:A:O4'	2.09	0.52
6:A:165:LEU:HD21	6:A:578:MET:HB3	1.91	0.52
8:H:51:ILE:HG22	8:H:245:CYS:SG	2.49	0.52
9:J:200:VAL:HG21	9:J:227:VAL:CG1	2.39	0.52
4:6:35:A:N1	12:M:81:CYS:HA	2.24	0.52
3:2:1108:A:N1	33:Y:73:PHE:CB	2.72	0.52
6:A:1375:LEU:HD12	6:A:1383:PHE:HZ	1.72	0.52
6:A:889:TRP:O	6:A:893:ARG:HG2	2.09	0.52
7:C:323:THR:HG21	7:C:438:ALA:HB2	1.91	0.52
17:S:225:ALA:O	17:S:228:THR:HG22	2.09	0.52
6:A:1257:ASN:OD1	6:A:1270:LEU:HD13	2.09	0.52
6:A:1372:LYS:HB3	6:A:1378:LYS:HA	1.91	0.52
7:C:539:VAL:HG13	7:C:564:ILE:CG2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:6:75:A:H8	5:5:98:U:HO2'	1.58	0.52
6:A:915:ALA:HB1	6:A:993:ALA:HB1	1.90	0.52
8:H:58:LYS:HA	8:H:61:VAL:HG12	1.92	0.52
11:L:90:LEU:HB2	11:L:106:LEU:HD11	1.91	0.52
6:A:868:GLN:O	10:K:197:ILE:HA	2.10	0.52
7:C:242:VAL:HG21	7:C:272:ARG:HE	1.74	0.52
1:I:58:U:H2'	1:I:59:C:O4'	2.10	0.52
11:L:104:CYS:SG	11:L:105:CYS:N	2.83	0.52
5:5:30:A:H2'	5:5:31:G:O4'	2.09	0.52
5:5:62:G:H2'	5:5:63:C:O4'	2.10	0.52
6:A:1422:ILE:HD11	8:H:306:ASP:CG	2.30	0.52
9:J:200:VAL:CG2	9:J:227:VAL:HB	2.40	0.51
7:C:318:LEU:HD22	7:C:421:LEU:CD2	2.40	0.51
7:C:823:ILE:HG22	7:C:825:VAL:HG23	1.92	0.51
9:J:144:CYS:SG	9:J:187:ASP:HA	2.51	0.51
9:J:290:VAL:HG11	9:J:334:TRP:CZ3	2.45	0.51
6:A:1067:ASN:CB	6:A:1083:THR:HG21	2.40	0.51
18:T:233:THR:HA	18:T:243:ILE:N	2.22	0.51
7:C:139:ILE:CG2	7:C:252:LEU:HD22	2.40	0.51
8:H:83:LEU:HD21	8:H:90:ILE:HB	1.93	0.51
9:J:145:VAL:N	9:J:404:CYS:SG	2.84	0.51
6:A:1624:LEU:HD22	6:A:1633:PHE:HB3	1.93	0.51
6:A:168:LEU:N	6:A:169:PRO:HD2	2.26	0.51
6:A:1823:LEU:O	6:A:1825:ILE:HG23	2.10	0.51
6:A:627:LYS:HG2	6:A:664:THR:HB	1.92	0.51
9:J:284:SER:OG	9:J:311:VAL:O	2.28	0.51
6:A:849:LEU:HD23	6:A:978:ILE:HG21	1.92	0.51
7:C:241:VAL:HG11	7:C:273:LEU:HD23	1.93	0.51
6:A:355:LEU:HD23	6:A:356:TYR:CE2	2.46	0.51
6:A:687:ILE:HD11	6:A:706:PRO:HG3	1.93	0.51
7:C:116:THR:HG21	7:C:118:TYR:CE1	2.46	0.51
14:O:20:ILE:HD11	14:O:152:LEU:CD2	2.41	0.51
6:A:1407:ILE:HG21	6:A:1426:ARG:NH2	2.26	0.51
7:C:147:THR:HG1	7:C:190:SER:HG	1.58	0.51
6:A:1400:ILE:HG21	6:A:1440:ILE:HD12	1.93	0.51
7:C:324:ILE:HG22	7:C:377:ILE:HD13	1.92	0.51
7:C:385:PHE:CE1	7:C:425:LEU:HD11	2.46	0.51
8:H:312:LEU:N	8:H:315:LEU:CD2	2.74	0.51
18:T:115:TYR:O	18:T:131:ALA:CB	2.43	0.51
6:A:1454:SER:HA	6:A:1487:GLY:HA2	1.93	0.50
2:E:-9:U:O2	2:E:-9:U:H2'	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:74:PRO:HA	8:H:123:ILE:HD12	1.92	0.50
7:C:418:GLN:HB3	7:C:419:PRO:HD3	1.92	0.50
7:C:655:LEU:C	7:C:655:LEU:HD23	2.32	0.50
8:H:181:LEU:HD13	8:H:194:LEU:HD22	1.92	0.50
6:A:806:ALA:N	6:A:807:PRO:HD2	2.26	0.50
11:L:33:ALA:HB1	11:L:52:ILE:HG22	1.93	0.50
18:T:119:ALA:CA	18:T:127:MET:O	2.58	0.50
6:A:138:HIS:HB2	11:L:52:ILE:HD11	1.93	0.50
1:I:14:U:C6	12:M:229:ASP:HB3	2.47	0.50
6:A:1387:VAL:HG12	6:A:1610:TRP:CD2	2.47	0.50
6:A:522:TYR:CZ	6:A:686:ILE:HD12	2.47	0.50
6:A:687:ILE:HD11	6:A:706:PRO:CG	2.41	0.50
9:J:324:ALA:CB	9:J:364:LEU:HD11	2.42	0.50
13:N:34:CYS:SG	13:N:37:CYS:N	2.83	0.50
3:2:1108:A:H62	33:Y:108:THR:CA	2.25	0.50
6:A:338:ASN:O	6:A:342:LEU:HG	2.11	0.50
8:H:94:LEU:HA	8:H:97:GLU:HG2	1.94	0.50
9:J:269:ILE:HA	9:J:285:SER:HA	1.93	0.50
6:A:1212:ARG:HA	6:A:1259:LEU:HD11	1.93	0.50
6:A:1925:PRO:O	6:A:1929:GLN:N	2.45	0.50
7:C:241:VAL:HG22	7:C:267:ILE:CG2	2.42	0.50
6:A:139:LEU:HD13	6:A:562:ILE:HD11	1.94	0.49
7:C:314:ALA:CB	7:C:321:THR:HG22	2.42	0.49
9:J:277:VAL:HG11	9:J:321:PHE:CZ	2.47	0.49
6:A:194:HIS:CD2	10:K:122:LEU:HD23	2.46	0.49
5:5:103:A:OP2	6:A:675:HIS:NE2	2.44	0.49
5:5:76:U:O3'	6:A:334:LYS:NZ	2.42	0.49
9:J:357:SER:O	9:J:365:PHE:HB3	2.11	0.49
17:S:285:LEU:HD21	17:S:302:SER:CB	2.41	0.49
18:T:404:ASP:CB	18:T:409:GLU:CA	2.90	0.49
6:A:1426:ARG:CD	16:R:8:LEU:HD12	2.43	0.49
9:J:242:ALA:HB2	9:J:248:ILE:HA	1.92	0.49
9:J:334:TRP:HD1	9:J:341:LEU:HA	1.78	0.49
6:A:1407:ILE:HG21	6:A:1426:ARG:HH21	1.77	0.49
6:A:1391:PRO:CG	6:A:1547:ILE:HD11	2.42	0.49
6:A:468:LEU:HD21	7:C:382:TYR:HB3	1.95	0.49
9:J:242:ALA:HB1	9:J:269:ILE:CG2	2.43	0.49
11:L:29:GLN:CB	11:L:55:LEU:HD11	2.43	0.49
6:A:660:ILE:HG21	6:A:711:TRP:CZ2	2.48	0.49
6:A:173:LEU:HD13	6:A:715:LEU:HB2	1.94	0.49
6:A:461:LEU:HD11	7:C:331:TYR:HB3	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:165:LEU:HD12	6:A:622:MET:HG2	1.94	0.49
6:A:834:ILE:HD13	6:A:845:VAL:HG23	1.93	0.49
12:M:74:LEU:HA	12:M:112:PHE:CE1	2.47	0.49
3:2:3:G:H2'	3:2:4:A:O4'	2.13	0.49
6:A:1855:THR:HG21	6:A:1966:SER:HB3	1.93	0.49
9:J:327:CYS:SG	9:J:328:THR:N	2.86	0.49
7:C:493:LEU:CD2	7:C:542:ILE:HD11	2.40	0.49
7:C:800:TYR:O	7:C:803:VAL:HG12	2.13	0.49
10:K:174:ASN:HD21	10:K:185:ARG:HH22	1.61	0.49
18:T:233:THR:HA	18:T:243:ILE:H	1.78	0.49
6:A:1754:ALA:O	6:A:1758:ASP:HB2	2.12	0.49
9:J:403:LEU:CD1	9:J:419:ALA:HB2	2.42	0.49
9:J:200:VAL:CG1	9:J:230:VAL:HG23	2.43	0.49
10:K:182:LEU:HD11	14:O:22:LYS:CG	2.43	0.49
34:3:2:U:H2'	34:3:3:U:H5'	0.71	0.48
14:O:14:THR:HG23	14:O:17:GLU:HB2	1.95	0.48
17:S:185:VAL:O	17:S:188:ILE:HG13	2.13	0.48
18:T:119:ALA:O	18:T:128:ILE:N	2.46	0.48
6:A:166:LYS:HE3	6:A:730:ILE:HD11	1.95	0.48
7:C:315:SER:HB3	7:C:320:PHE:CE1	2.48	0.48
8:H:47:VAL:HG13	8:H:49:ILE:HG23	1.94	0.48
8:H:58:LYS:O	8:H:61:VAL:HG12	2.13	0.48
18:T:237:THR:CB	18:T:240:ASN:CB	2.91	0.48
6:A:1862:VAL:HG13	6:A:1870:VAL:HG13	1.95	0.48
6:A:336:PHE:HB3	6:A:530:VAL:HG21	1.93	0.48
9:J:238:LEU:HD21	9:J:250:LEU:HD22	1.94	0.48
14:O:30:THR:HG23	14:O:31:HIS:CE1	2.48	0.48
6:A:1267:VAL:HG22	6:A:1302:LEU:CD2	2.44	0.48
6:A:343:ASN:HD21	6:A:354:PRO:CA	2.25	0.48
6:A:480:TYR:OH	7:C:317:LYS:NZ	2.46	0.48
7:C:318:LEU:HD13	7:C:421:LEU:HD21	1.95	0.48
9:J:289:THR:HG22	9:J:305:THR:HG22	1.94	0.48
12:M:250:MET:CG	13:N:139:LEU:HD11	2.43	0.48
18:T:236:LEU:CB	18:T:240:ASN:N	2.77	0.48
6:A:632:ILE:HG22	6:A:656:ILE:HG21	1.95	0.48
13:N:25:MET:CB	13:N:46:PHE:HB3	2.44	0.48
6:A:1967:ALA:HB1	6:A:2015:LEU:HB3	1.96	0.48
7:C:801:TRP:HB3	7:C:843:LYS:HD3	1.96	0.48
7:C:862:TYR:CE2	7:C:908:VAL:HG13	2.48	0.48
8:H:143:LEU:HD11	8:H:151:VAL:HG11	1.95	0.48
1:I:3:A:N6	4:6:51:A:O4'	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:S:140:LEU:CD2	17:S:155:LEU:HD22	2.41	0.48
22:X:88:UNK:O	22:X:91:UNK:N	2.46	0.48
6:A:238:ARG:NH2	6:A:1694:MET:O	2.46	0.48
6:A:355:LEU:HD23	6:A:356:TYR:CZ	2.49	0.48
6:A:766:ILE:HG21	6:A:782:ILE:HD13	1.95	0.48
9:J:344:ASN:HD22	10:K:45:PRO:HG3	1.78	0.48
8:H:44:LEU:O	8:H:47:VAL:HG12	2.13	0.48
12:M:99:ILE:HD13	12:M:188:TYR:CD2	2.49	0.48
10:K:185:ARG:NH1	14:O:26:GLN:O	2.43	0.48
17:S:107:ASP:O	17:S:111:LYS:HG2	2.14	0.48
6:A:379:ILE:HD11	6:A:391:TYR:CD1	2.49	0.48
9:J:376:TYR:HD1	9:J:383:LYS:HA	1.78	0.48
3:2:46:C:H2'	3:2:47:U:C6	2.49	0.48
4:6:70:U:H2'	4:6:71:G:O4'	2.14	0.48
6:A:1033:ASN:HB2	6:A:1288:LEU:HD23	1.94	0.48
8:H:135:ILE:HD12	8:H:162:LEU:HD21	1.95	0.48
6:A:182:PRO:HB2	6:A:264:ILE:HD11	1.95	0.47
6:A:209:ILE:HG21	6:A:303:PHE:HE2	1.79	0.47
12:M:250:MET:CB	13:N:139:LEU:HD11	2.44	0.47
8:H:80:ILE:HD12	8:H:94:LEU:HD13	1.96	0.47
9:J:276:PRO:HB2	10:K:63:ILE:HD12	1.95	0.47
17:S:140:LEU:HD22	17:S:152:VAL:HG23	1.95	0.47
7:C:222:MET:HE1	7:C:225:THR:HG21	1.95	0.47
8:H:351:ILE:HD11	8:H:361:TYR:HB2	1.95	0.47
18:T:281:LEU:CB	18:T:287:TYR:CA	2.92	0.47
6:A:1565:THR:HG21	6:A:1825:ILE:HD11	1.95	0.47
7:C:150:MET:HG3	7:C:214:ASP:CB	2.44	0.47
16:R:8:LEU:HD23	16:R:9:LYS:N	2.29	0.47
7:C:150:MET:HB3	7:C:178:LEU:HD22	1.95	0.47
3:2:34:G:O2'	3:2:35:U:C6	2.66	0.47
6:A:1344:THR:HG21	6:A:1537:TRP:CD2	2.49	0.47
6:A:1991:ILE:HG23	6:A:1992:TYR:CD2	2.50	0.47
6:A:636:HIS:CE1	6:A:653:ILE:HD11	2.49	0.47
7:C:222:MET:CE	7:C:252:LEU:HD21	2.45	0.47
14:O:88:ALA:HB2	14:O:95:ALA:HA	1.96	0.47
6:A:1347:ARG:HD3	6:A:1444:ILE:HG22	1.96	0.47
5:5:110:U:C2	5:5:111:C:C6	3.03	0.47
6:A:2015:LEU:HD22	6:A:2022:ALA:HB1	1.96	0.47
9:J:147:ILE:HD11	9:J:169:LEU:HD11	1.97	0.47
13:N:116:LYS:HB3	13:N:118:VAL:HG22	1.96	0.47
18:T:404:ASP:CB	18:T:409:GLU:HA	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:625:LEU:HD22	6:A:715:LEU:HD21	1.96	0.47
13:N:8:PRO:HB2	13:N:62:VAL:HG11	1.97	0.47
18:T:119:ALA:HA	18:T:127:MET:C	2.36	0.47
5:5:93:G:C2	5:5:102:C:C2	3.03	0.47
7:C:319:GLY:O	7:C:426:GLN:NE2	2.48	0.47
9:J:290:VAL:HG12	9:J:304:LEU:HB2	1.96	0.47
5:5:106:A:O2'	9:J:213:LYS:NZ	2.30	0.46
5:5:25:G:N3	5:5:25:G:H2'	2.30	0.46
6:A:161:PHE:CE1	6:A:198:ALA:HA	2.50	0.46
6:A:611:LYS:O	6:A:614:ARG:HG2	2.16	0.46
9:J:156:ILE:HG22	9:J:166:VAL:HG13	1.97	0.46
11:L:41:LEU:HD21	12:M:83:LEU:HD21	1.96	0.46
14:O:217:ILE:HD11	17:S:82:ARG:CZ	2.45	0.46
6:A:1107:LEU:HB2	6:A:1110:ALA:HB2	1.98	0.46
6:A:165:LEU:HD13	6:A:578:MET:HE2	1.97	0.46
7:C:222:MET:HE1	7:C:252:LEU:HD21	1.97	0.46
10:K:180:VAL:HG12	10:K:185:ARG:NH1	2.30	0.46
14:O:76:LEU:O	14:O:80:LEU:N	2.43	0.46
5:5:88:U:O2'	9:J:216:ILE:HD11	2.15	0.46
6:A:228:LYS:CG	6:A:695:LEU:HD11	2.42	0.46
16:R:67:HIS:O	16:R:71:ARG:CB	2.64	0.46
31:V:919:CYS:HA	31:V:1013:SER:HA	1.97	0.46
6:A:637:VAL:O	6:A:641:LEU:N	2.46	0.46
6:A:522:TYR:CE1	6:A:686:ILE:HD12	2.50	0.46
7:C:241:VAL:HG11	7:C:273:LEU:HD22	1.97	0.46
8:H:60:VAL:HG13	8:H:76:LEU:HD11	1.98	0.46
11:L:22:THR:HG21	11:L:62:TYR:CE1	2.50	0.46
17:S:128:THR:HB	17:S:129:LEU:HD12	1.96	0.46
6:A:1354:GLU:N	6:A:1355:PRO:CD	2.79	0.46
8:H:45:PHE:CZ	8:H:258:LEU:HB3	2.50	0.46
1:I:64:U:H2'	1:I:65:U:O4'	2.16	0.46
9:J:277:VAL:HG22	9:J:278:ASP:N	2.29	0.46
9:J:365:PHE:CE1	9:J:373:LEU:HG	2.50	0.46
11:L:78:TYR:OH	11:L:92:ILE:HG21	2.16	0.46
14:O:214:ASN:HD22	17:S:44:ARG:HG3	1.80	0.46
6:A:1204:ARG:NH2	6:A:1260:PHE:HA	2.31	0.46
6:A:209:ILE:HB	6:A:212:VAL:HB	1.97	0.46
9:J:407:PHE:CZ	9:J:414:LEU:HD13	2.51	0.46
6:A:1961:LEU:HD12	6:A:1963:LEU:HG	1.98	0.46
8:H:402:LEU:HD22	8:H:420:ILE:HD11	1.98	0.46
11:L:67:TYR:HE1	11:L:75:LYS:HA	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:284:ASP:O	18:T:311:LYS:CB	2.63	0.46
12:M:121:ARG:O	12:M:123:ASP:N	2.48	0.46
6:A:191:VAL:O	6:A:559:GLN:HA	2.16	0.46
6:A:719:ILE:N	6:A:720:PRO:CD	2.79	0.46
6:A:789:ALA:HB2	6:A:799:TRP:CE2	2.51	0.46
6:A:831:ARG:HG3	6:A:852:LEU:CD1	2.46	0.46
17:S:72:ALA:HB1	17:S:88:PHE:CZ	2.50	0.46
18:T:119:ALA:CA	18:T:131:ALA:CB	2.92	0.46
6:A:1082:ILE:HG23	6:A:1109:PHE:HE1	1.81	0.46
7:C:152:LEU:HD21	7:C:319:GLY:HA2	1.97	0.46
8:H:148:LEU:HA	8:H:151:VAL:HG12	1.97	0.46
11:L:61:ARG:O	11:L:61:ARG:HD3	2.16	0.46
14:O:189:ARG:NE	17:S:38:LEU:HD12	2.31	0.46
6:A:1165:LEU:HD21	6:A:1514:PHE:CE1	2.51	0.45
6:A:1701:ILE:HB	6:A:1734:PHE:HB2	1.99	0.45
9:J:227:VAL:HA	9:J:243:GLY:HA3	1.98	0.45
9:J:198:PHE:CD1	9:J:239:ILE:HD13	2.50	0.45
12:M:146:LEU:HD13	12:M:151:LEU:HD12	1.96	0.45
6:A:1165:LEU:HD21	6:A:1514:PHE:HE1	1.81	0.45
6:A:1651:ALA:HB2	6:A:1911:TRP:CH2	2.51	0.45
4:6:39:G:C6	12:M:117:PHE:HD2	2.33	0.45
17:S:285:LEU:HD22	17:S:299:GLU:HA	1.99	0.45
17:S:300:THR:O	17:S:304:LYS:CB	2.64	0.45
6:A:1875:ILE:HG22	6:A:1876:ASN:N	2.31	0.45
6:A:995:LEU:O	6:A:999:LEU:HG	2.16	0.45
18:T:300:ASP:C	18:T:301:LYS:C	2.75	0.45
6:A:1850:LEU:HD11	6:A:1881:THR:HG22	1.97	0.45
6:A:831:ARG:HG3	6:A:852:LEU:HD13	1.99	0.45
10:K:134:VAL:HG11	13:N:115:LEU:HD11	1.97	0.45
17:S:199:MET:HB2	17:S:242:GLU:HB3	1.98	0.45
18:T:285:ASN:HA	18:T:311:LYS:CA	2.42	0.45
5:5:35:A:H2'	5:5:36:A:C8	2.52	0.45
6:A:518:VAL:HG21	6:A:689:TYR:CE2	2.51	0.45
6:A:674:MET:HA	6:A:677:ILE:HD12	1.98	0.45
7:C:235:VAL:HG23	7:C:261:VAL:HG11	1.99	0.45
7:C:879:LEU:HD11	7:C:921:SER:OG	2.16	0.45
9:J:291:ARG:HD3	9:J:303:VAL:HG23	1.99	0.45
9:J:341:LEU:HD23	9:J:342:LEU:N	2.31	0.45
31:V:791:GLN:HA	31:V:1074:LEU:CB	2.47	0.45
6:A:1865:THR:CG2	6:A:1871:ALA:HB2	2.46	0.45
18:T:284:ASP:C	18:T:311:LYS:CA	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:27:A:OP1	6:A:1093:LYS:NZ	2.40	0.45
5:5:80:G:C4	5:5:82:A:C2	3.05	0.45
6:A:721:LEU:HD11	6:A:725:TYR:CZ	2.52	0.45
7:C:200:CYS:HB3	7:C:436:VAL:HG21	1.99	0.45
7:C:152:LEU:HD11	7:C:319:GLY:HA2	1.97	0.45
7:C:493:LEU:HD21	7:C:539:VAL:HG21	1.98	0.45
13:N:67:GLN:HG2	13:N:120:LEU:HD23	1.99	0.45
7:C:126:MET:SD	7:C:132:ARG:NH2	2.90	0.45
6:A:376:ARG:NH1	7:C:957:ALA:O	2.49	0.45
9:J:209:TRP:HA	9:J:216:ILE:HA	1.99	0.45
12:M:121:ARG:O	12:M:124:MET:N	2.49	0.45
12:M:12:GLN:HE22	12:M:58:HIS:HB3	1.81	0.45
13:N:94:VAL:HG23	13:N:142:ILE:HD12	1.99	0.45
9:J:198:PHE:CE1	9:J:239:ILE:HD13	2.51	0.44
9:J:242:ALA:HB1	9:J:269:ILE:HG21	1.99	0.44
6:A:1047:ALA:HB3	6:A:1251:TYR:HB3	1.98	0.44
6:A:330:LEU:HD21	6:A:386:ALA:HB2	1.98	0.44
7:C:691:VAL:CG1	7:C:841:LEU:HD22	2.46	0.44
6:A:138:HIS:CE1	11:L:49:LEU:HD11	2.52	0.44
14:O:22:LYS:HB2	14:O:56:LEU:HD11	1.99	0.44
9:J:296:VAL:HG23	10:K:73:TYR:CG	2.52	0.44
4:6:69:C:C2	4:6:78:G:C2	3.05	0.44
8:H:317:ILE:C	8:H:317:ILE:CD1	2.86	0.44
18:T:457:TYR:CB	18:T:465:THR:HA	2.48	0.44
5:5:15:A:N7	5:5:133:C:N4	2.65	0.44
6:A:1689:ARG:NH1	6:A:1692:TYR:OH	2.51	0.44
6:A:203:ASN:HA	6:A:548:LEU:HD23	1.99	0.44
13:N:43:LEU:HD21	13:N:57:LYS:HB2	1.99	0.44
4:6:62:A:C4	4:6:63:G:C8	3.06	0.44
6:A:461:LEU:HD11	7:C:331:TYR:CB	2.46	0.44
7:C:318:LEU:HD22	7:C:421:LEU:HD22	1.98	0.44
6:A:1182:LEU:HD11	15:P:127:TRP:HZ2	1.81	0.44
6:A:1624:LEU:HD21	6:A:1635:HIS:ND1	2.32	0.44
7:C:155:ILE:CD1	7:C:175:LEU:HD23	2.47	0.44
7:C:416:ASP:HB3	7:C:417:PRO:HD2	1.99	0.44
8:H:73:ILE:CG1	8:H:74:PRO:HD3	2.48	0.44
12:M:48:VAL:HG22	12:M:220:GLY:N	2.33	0.44
16:R:102:LEU:O	16:R:106:LEU:CB	2.66	0.44
18:T:119:ALA:O	18:T:128:ILE:CA	2.65	0.44
5:5:103:A:C4	5:5:104:G:C8	3.06	0.44
6:A:1328:PHE:CD2	6:A:1603:ASN:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:150:MET:SD	7:C:212:PHE:HB3	2.58	0.44
2:E:-15:A:H2'	2:E:-15:A:N3	2.32	0.44
13:N:60:ILE:HG13	13:N:72:GLN:HG3	1.98	0.44
13:N:68:ARG:HB3	13:N:84:ILE:HD12	2.00	0.44
18:T:119:ALA:HB3	18:T:131:ALA:HB3	1.72	0.44
6:A:137:GLU:HG3	11:L:30:LEU:HD23	2.00	0.44
6:A:1508:HIS:O	6:A:1511:ARG:HG2	2.17	0.44
6:A:181:HIS:HB3	6:A:182:PRO:HD2	2.00	0.44
6:A:660:ILE:HA	6:A:660:ILE:HD12	1.94	0.44
7:C:231:ALA:O	7:C:487:ARG:NH1	2.51	0.44
8:H:355:ARG:O	8:H:359:THR:HG23	2.18	0.44
9:J:324:ALA:CB	9:J:356:LEU:HD21	2.48	0.44
3:2:20:G:C2	15:P:6:ARG:HD3	2.52	0.44
6:A:1082:ILE:HG23	6:A:1109:PHE:CE1	2.53	0.43
7:C:187:ARG:NH2	7:C:653:ASP:OD2	2.51	0.43
7:C:760:LEU:HD23	7:C:764:ASN:HD21	1.82	0.43
8:H:298:VAL:HG13	8:H:311:LYS:HB3	2.00	0.43
9:J:181:HIS:CE1	9:J:201:SER:HG	2.36	0.43
9:J:181:HIS:CG	9:J:201:SER:HG	2.34	0.43
9:J:229:THR:HG21	9:J:271:GLN:HA	1.99	0.43
6:A:1054:LEU:HD13	6:A:1121:ILE:HD13	1.99	0.43
6:A:1974:LEU:O	6:A:1977:VAL:HG12	2.18	0.43
6:A:996:ASP:OD2	6:A:1511:ARG:NH1	2.49	0.43
7:C:105:ILE:HG22	7:C:182:LYS:HB3	2.00	0.43
7:C:423:HIS:CE1	7:C:427:LEU:HD11	2.53	0.43
7:C:501:ILE:HD13	7:C:567:ILE:HG23	2.00	0.43
2:E:-14:A:O2'	2:E:-13:G:O4'	2.25	0.43
8:H:189:THR:O	8:H:192:GLU:HG2	2.18	0.43
8:H:98:LEU:O	8:H:101:MET:HG2	2.18	0.43
13:N:71:CYS:SG	13:N:72:GLN:N	2.92	0.43
4:6:1:G:H2'	4:6:2:U:C6	2.53	0.43
3:2:43:G:H2'	3:2:44:U:H5'	2.01	0.43
18:T:121:GLU:C	18:T:179:ALA:HB1	2.39	0.43
5:5:111:C:H2'	5:5:112:C:C6	2.54	0.43
6:A:1353:THR:HG23	6:A:1356:LEU:HB3	1.99	0.43
7:C:866:ILE:HG22	7:C:868:VAL:HG13	1.99	0.43
9:J:250:LEU:HD11	9:J:262:LEU:HD11	2.00	0.43
9:J:341:LEU:HD22	10:K:45:PRO:HA	2.01	0.43
13:N:214:ILE:O	13:N:244:HIS:NE2	2.43	0.43
6:A:1170:MET:HE3	6:A:1230:ILE:HG13	1.99	0.43
6:A:1999:ILE:HG22	6:A:2000:SER:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:342:LEU:HD22	6:A:392:ASN:ND2	2.34	0.43
5:5:112:C:H1'	6:A:716:ARG:HG3	1.99	0.43
7:C:151:ASP:CB	7:C:175:LEU:O	2.67	0.43
17:S:126:ILE:HD12	17:S:136:TRP:CD2	2.53	0.43
17:S:534:TYR:HA	17:S:551:PHE:CB	2.49	0.43
4:6:78:G:O2'	6:A:611:LYS:HD3	2.19	0.43
6:A:239:PHE:HA	6:A:240:PRO:C	2.39	0.43
6:A:521:SER:HB2	6:A:682:ASP:HA	2.00	0.43
13:N:71:CYS:SG	13:N:73:CYS:N	2.80	0.43
5:5:74:U:O2	5:5:78:A:C4	2.72	0.43
6:A:137:GLU:OE1	11:L:34:GLN:NE2	2.52	0.43
6:A:905:TYR:HB2	6:A:908:ASP:HB2	2.01	0.43
7:C:567:ILE:HG22	7:C:571:TYR:CE1	2.53	0.43
7:C:622:LEU:HD21	7:C:644:ILE:HD11	2.01	0.43
8:H:17:ASN:O	8:H:20:MET:HG2	2.19	0.43
9:J:217:ILE:HG23	15:P:34:HIS:CG	2.54	0.43
31:V:779:LYS:O	34:3:1:U:C1'	2.67	0.43
6:A:1069:LEU:HB3	6:A:1116:TYR:HE2	1.84	0.43
6:A:1069:LEU:HB3	6:A:1116:TYR:CE2	2.54	0.43
6:A:1886:THR:O	6:A:1996:LEU:HD11	2.18	0.43
7:C:444:GLN:N	7:C:445:PRO:CD	2.82	0.43
8:H:423:LEU:HD23	8:H:427:LEU:HD13	2.01	0.43
3:2:36:A:H2'	3:2:37:G:C8	2.54	0.42
5:5:102:C:OP1	6:A:675:HIS:NE2	2.52	0.42
6:A:1087:ASN:HD21	6:A:1098:VAL:CG1	2.32	0.42
7:C:107:THR:HG21	7:C:479:GLY:HA2	2.01	0.42
7:C:137:GLY:HA2	7:C:213:LEU:HB2	2.01	0.42
8:H:351:ILE:HD13	8:H:358:GLN:HA	2.00	0.42
9:J:271:GLN:HB3	9:J:314:THR:HG22	2.01	0.42
4:6:35:A:O2'	11:L:40:LYS:HE2	2.19	0.42
5:5:74:U:O2	5:5:78:A:C2	2.72	0.42
4:6:72:C:OP2	6:A:732:ARG:NH2	2.52	0.42
6:A:1207:TRP:CZ2	6:A:1268:ARG:HB2	2.55	0.42
6:A:226:ARG:O	6:A:229:ARG:HB2	2.19	0.42
8:H:143:LEU:CD1	8:H:151:VAL:HG21	2.49	0.42
8:H:44:LEU:HD23	8:H:79:LEU:HD21	2.01	0.42
10:K:75:GLN:O	10:K:78:VAL:HG12	2.19	0.42
18:T:112:CYS:CA	18:T:135:SER:CB	2.96	0.42
6:A:1278:VAL:O	6:A:1278:VAL:HG23	2.19	0.42
6:A:1033:ASN:HD22	6:A:1288:LEU:HB3	1.85	0.42
6:A:637:VAL:O	6:A:641:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:314:ALA:HB2	7:C:321:THR:HG22	2.01	0.42
7:C:825:VAL:HG22	7:C:834:MET:SD	2.59	0.42
7:C:928:CYS:SG	7:C:929:GLN:N	2.92	0.42
6:A:1351:VAL:HA	8:H:303:LEU:HD21	2.01	0.42
9:J:282:VAL:HG11	9:J:323:VAL:HG21	2.01	0.42
6:A:1082:ILE:HG21	6:A:1113:ILE:CD1	2.50	0.42
6:A:1400:ILE:CG2	6:A:1440:ILE:HB	2.49	0.42
7:C:195:GLY:C	7:C:545:LEU:HD13	2.39	0.42
7:C:602:VAL:HG11	7:C:860:PRO:HG3	2.01	0.42
8:H:28:ILE:HG12	8:H:43:ASP:HB3	2.02	0.42
9:J:142:VAL:CG1	9:J:157:THR:HB	2.50	0.42
9:J:334:TRP:CD1	9:J:341:LEU:HA	2.54	0.42
13:N:39:LEU:HD13	13:N:40:PRO:HD2	2.01	0.42
18:T:271:ASN:O	18:T:294:MET:CB	2.67	0.42
6:A:834:ILE:CD1	6:A:845:VAL:HG23	2.50	0.42
7:C:617:LYS:HB3	7:C:666:ILE:HD11	2.01	0.42
13:N:101:THR:HG22	13:N:120:LEU:HB3	2.02	0.42
4:6:30:G:OP1	11:L:115:ASN:N	2.44	0.42
6:A:1608:LEU:HG	6:A:1823:LEU:HD21	2.01	0.42
6:A:229:ARG:HG2	6:A:695:LEU:HD23	2.01	0.42
6:A:460:PRO:HB3	7:C:376:PHE:HA	2.02	0.42
6:A:688:TYR:O	6:A:692:ASN:N	2.53	0.42
2:E:-8:C:H2'	2:E:-7:U:O4'	2.20	0.42
9:J:216:ILE:C	9:J:216:ILE:HD12	2.39	0.42
6:A:1369:ASN:O	6:A:1373:LEU:CB	2.67	0.42
6:A:139:LEU:HD12	6:A:193:TYR:CD2	2.55	0.42
6:A:1553:ILE:HG21	6:A:1570:TRP:CE3	2.54	0.42
6:A:165:LEU:CD2	6:A:578:MET:HB3	2.49	0.42
6:A:654:HIS:CE1	6:A:658:ASN:OD1	2.72	0.42
2:E:-13:G:C2	8:H:316:LYS:HD2	2.55	0.42
12:M:173:ILE:HG12	12:M:184:VAL:HG13	2.02	0.42
6:A:200:THR:OG1	6:A:574:GLN:NE2	2.53	0.42
6:A:719:ILE:N	6:A:720:PRO:HD2	2.34	0.42
7:C:229:LEU:HD22	7:C:235:VAL:HG21	2.02	0.42
9:J:250:LEU:CD1	9:J:295:VAL:HG23	2.50	0.42
9:J:326:ALA:HB2	9:J:356:LEU:HD13	2.01	0.42
4:6:71:G:N2	4:6:74:U:OP2	2.47	0.42
6:A:1125:LEU:HD22	6:A:1170:MET:HE1	2.02	0.42
6:A:1634:LEU:HD21	6:A:1641:LEU:CD1	2.46	0.42
6:A:2078:GLU:O	6:A:2082:ILE:HD12	2.19	0.42
6:A:754:TYR:HA	9:J:183:MET:CE	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:780:ARG:HA	6:A:780:ARG:NE	2.35	0.42
7:C:178:LEU:N	7:C:178:LEU:HD12	2.35	0.42
9:J:187:ASP:O	9:J:200:VAL:HG12	2.20	0.42
6:A:556:TYR:CG	10:K:120:ASP:HB3	2.54	0.42
17:S:140:LEU:HD13	17:S:156:TYR:CZ	2.54	0.42
4:6:52:G:H2'	4:6:53:A:C8	2.55	0.42
4:6:91:A:C2	17:S:99:ILE:HG21	2.55	0.42
6:A:1887:GLY:O	6:A:1991:ILE:HG22	2.20	0.42
6:A:330:LEU:HD12	7:C:920:LEU:HD21	2.01	0.42
3:2:20:G:O4'	6:A:780:ARG:HD3	2.19	0.42
8:H:334:LEU:CD1	8:H:380:GLN:HB3	2.48	0.42
8:H:462:ILE:HG23	8:H:473:LEU:HD13	2.02	0.42
9:J:111:ILE:HG22	17:S:194:MET:O	2.19	0.42
9:J:223:HIS:CG	9:J:227:VAL:CG2	3.03	0.42
9:J:327:CYS:SG	9:J:330:ASP:N	2.93	0.42
12:M:156:ILE:HG21	12:M:175:TYR:CE1	2.54	0.42
6:A:1282:ASP:C	8:H:345:ILE:HD11	2.40	0.41
6:A:1805:ILE:HG23	6:A:1809:ASN:HB2	2.02	0.41
6:A:207:ARG:HD2	6:A:298:TYR:O	2.19	0.41
6:A:209:ILE:HG23	6:A:301:TRP:CE2	2.55	0.41
6:A:165:LEU:HD11	6:A:579:LEU:HD23	2.02	0.41
6:A:168:LEU:HD21	6:A:626:LEU:HD11	2.00	0.41
8:H:463:ASN:O	8:H:466:THR:OG1	2.29	0.41
31:V:779:LYS:HA	31:V:793:ILE:O	2.20	0.41
6:A:841:GLU:HB2	6:A:844:MET:CB	2.50	0.41
7:C:152:LEU:HD21	7:C:319:GLY:CA	2.50	0.41
7:C:200:CYS:SG	7:C:210:ILE:HD12	2.60	0.41
7:C:870:ALA:N	7:C:871:PRO:HD2	2.35	0.41
6:A:1442:ARG:HG3	8:H:300:LYS:O	2.20	0.41
6:A:1468:ALA:O	6:A:1472:ASN:N	2.53	0.41
6:A:1974:LEU:O	6:A:1978:VAL:HG23	2.20	0.41
6:A:708:TRP:CZ2	6:A:712:LEU:HD11	2.54	0.41
8:H:373:ILE:HD11	8:H:419:PHE:CD2	2.55	0.41
9:J:244:ARG:HA	9:J:268:PRO:HB3	2.01	0.41
18:T:119:ALA:CB	18:T:131:ALA:HB2	2.28	0.41
6:A:2075:THR:O	6:A:2079:ILE:HG12	2.20	0.41
6:A:714:PHE:CE1	6:A:718:THR:HG21	2.56	0.41
8:H:42:ARG:O	8:H:45:PHE:HB3	2.20	0.41
10:K:110:HIS:NE2	13:N:20:GLU:O	2.52	0.41
14:O:39:LEU:HD11	14:O:155:ALA:CB	2.50	0.41
7:C:95:THR:HG21	15:P:40:ARG:NH2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:-9:U:O4'	16:R:19:HIS:HB2	2.20	0.41
4:6:57:U:H2'	4:6:58:C:O4'	2.20	0.41
6:A:1107:LEU:HD23	6:A:1109:PHE:CZ	2.56	0.41
6:A:1609:TRP:HE3	6:A:1823:LEU:HD13	1.85	0.41
6:A:766:ILE:CG2	6:A:782:ILE:HD13	2.50	0.41
7:C:347:ARG:O	7:C:348:LEU:C	2.58	0.41
2:E:-5:G:OP2	6:A:1377:SER:O	2.38	0.41
6:A:818:SER:HB3	9:J:141:TRP:CZ2	2.55	0.41
9:J:311:VAL:HA	9:J:326:ALA:O	2.20	0.41
9:J:358:ILE:HG22	9:J:359:ASN:O	2.20	0.41
14:O:219:TYR:O	14:O:221:GLN:N	2.54	0.41
17:S:185:VAL:HG22	17:S:189:TYR:CE2	2.55	0.41
17:S:47:GLN:HG2	17:S:51:ARG:HE	1.86	0.41
18:T:119:ALA:CB	18:T:128:ILE:CA	2.39	0.41
3:2:15:C:HO2'	3:2:18:U:H3	1.68	0.41
6:A:583:ILE:HD11	6:A:619:PHE:CZ	2.55	0.41
7:C:212:PHE:O	7:C:213:LEU:HD23	2.20	0.41
8:H:50:LEU:HB2	8:H:251:LEU:HD22	2.02	0.41
13:N:139:LEU:HD13	13:N:139:LEU:C	2.40	0.41
10:K:112:ILE:HD11	13:N:23:ILE:HB	2.02	0.41
16:R:16:THR:OG1	16:R:17:SER:N	2.53	0.41
17:S:140:LEU:CD2	17:S:152:VAL:HG23	2.51	0.41
17:S:367:TRP:O	17:S:371:ILE:N	2.44	0.41
6:A:1879:ILE:HD11	6:A:1894:ILE:HD11	2.02	0.41
8:H:49:ILE:CG2	8:H:56:ILE:HG21	2.51	0.41
13:N:84:ILE:O	13:N:87:ARG:HG3	2.20	0.41
14:O:163:GLN:HB3	14:O:167:ALA:HB3	2.02	0.41
4:6:31:G:N1	13:N:53:ASN:O	2.54	0.41
6:A:305:LEU:HD21	6:A:476:ALA:HB2	2.02	0.41
6:A:593:LEU:HD23	6:A:593:LEU:HA	1.94	0.41
5:5:130:A:H2'	5:5:131:A:C8	2.56	0.41
6:A:1857:VAL:HG22	6:A:1878:CYS:O	2.21	0.41
6:A:1935:VAL:O	6:A:1959:THR:HG22	2.21	0.41
8:H:391:LEU:HA	8:H:391:LEU:HD23	1.95	0.41
9:J:146:ALA:HB3	9:J:188:VAL:HG23	2.03	0.41
5:5:45:A:N6	5:5:74:U:N3	2.56	0.41
6:A:506:PHE:CD2	6:A:525:LEU:HD13	2.56	0.41
7:C:502:LEU:HD21	7:C:510:ARG:HH21	1.85	0.41
7:C:133:ILE:HD13	7:C:560:GLN:HB3	2.01	0.41
11:L:52:ILE:HD12	11:L:52:ILE:C	2.42	0.41
17:S:199:MET:SD	17:S:246:LEU:HD22	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:5:93:G:H4'	16:R:13:GLY:HA2	2.03	0.41
4:6:42:A:H2'	4:6:43:C:O4'	2.21	0.41
6:A:1654:TRP:CZ3	6:A:1779:LEU:HD12	2.55	0.41
6:A:218:SER:CB	6:A:315:SER:HA	2.51	0.41
2:E:-5:G:O3'	6:A:667:TYR:HE1	2.04	0.41
6:A:695:LEU:HD13	6:A:696:GLY:N	2.35	0.41
6:A:762:VAL:HG22	6:A:815:TYR:CG	2.56	0.41
7:C:117:ARG:NH1	7:C:156:ASP:O	2.54	0.41
7:C:126:MET:SD	7:C:132:ARG:HG2	2.60	0.41
7:C:677:PHE:CD1	7:C:857:LEU:HD11	2.56	0.41
7:C:813:ILE:HD13	7:C:818:TYR:OH	2.21	0.41
17:S:185:VAL:HG22	17:S:189:TYR:CZ	2.56	0.41
4:6:69:C:C2	4:6:78:G:N2	2.89	0.40
6:A:1066:LEU:HD21	6:A:1113:ILE:HG21	2.03	0.40
6:A:1632:ILE:HD11	6:A:1649:PHE:CD2	2.56	0.40
6:A:1632:ILE:HG21	6:A:1645:LEU:CD1	2.50	0.40
8:H:333:SER:HA	8:H:343:TYR:CE2	2.56	0.40
8:H:474:THR:HA	8:H:477:MET:HG2	2.04	0.40
8:H:65:LEU:HD12	8:H:117:ILE:HD11	2.03	0.40
18:T:495:GLU:CB	18:T:503:ARG:CB	2.98	0.40
6:A:1995:TRP:CD1	6:A:1995:TRP:N	2.89	0.40
7:C:139:ILE:CD1	7:C:225:THR:HG23	2.40	0.40
8:H:151:VAL:O	8:H:154:VAL:HG12	2.21	0.40
9:J:200:VAL:HG21	9:J:227:VAL:HG12	2.03	0.40
12:M:73:CYS:O	12:M:76:PHE:HB3	2.21	0.40
10:K:146:VAL:N	17:S:128:THR:O	2.52	0.40
5:5:103:A:O2'	5:5:104:G:H5''	2.20	0.40
6:A:507:LEU:HD21	6:A:529:TYR:CD2	2.55	0.40
2:E:-5:G:C4	6:A:671:TYR:CE1	3.09	0.40
6:A:919:LEU:HA	6:A:919:LEU:HD23	1.95	0.40
7:C:320:PHE:HB2	7:C:429:PHE:HD2	1.86	0.40
8:H:124:LEU:O	8:H:129:VAL:HG23	2.21	0.40
9:J:213:LYS:HZ2	9:J:215:GLN:HG3	1.86	0.40
10:K:170:SER:O	10:K:185:ARG:NH2	2.48	0.40
5:5:104:G:OP2	6:A:531:LEU:HD11	2.22	0.40
6:A:1553:ILE:HG21	6:A:1570:TRP:CZ3	2.57	0.40
6:A:1879:ILE:HD12	6:A:1892:LYS:HB3	2.02	0.40
6:A:781:THR:O	6:A:785:HIS:HB2	2.22	0.40
7:C:127:ALA:HA	7:C:133:ILE:HD11	2.02	0.40
4:6:85:C:O2	14:O:167:ALA:HA	2.22	0.40
6:A:1967:ALA:HB2	6:A:2016:LYS:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:239:PHE:HE1	6:A:635:THR:HG22	1.87	0.40
9:J:150:VAL:HG11	15:P:40:ARG:NH2	2.37	0.40
14:O:33:TRP:CD1	14:O:49:GLU:HG3	2.57	0.40
17:S:155:LEU:C	17:S:155:LEU:HD23	2.42	0.40
18:T:360:LYS:CB	18:T:378:LEU:O	2.70	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	1906/2413 (79%)	1733 (91%)	161 (8%)	12 (1%)	30	74
7	C	864/1008 (86%)	771 (89%)	87 (10%)	6 (1%)	26	71
8	H	393/577 (68%)	353 (90%)	36 (9%)	4 (1%)	19	65
9	J	340/451 (75%)	295 (87%)	39 (12%)	6 (2%)	11	55
10	K	183/379 (48%)	163 (89%)	17 (9%)	3 (2%)	12	57
11	L	153/157 (98%)	136 (89%)	16 (10%)	1 (1%)	26	71
12	M	250/339 (74%)	236 (94%)	12 (5%)	2 (1%)	24	70
13	N	217/364 (60%)	191 (88%)	22 (10%)	4 (2%)	11	55
14	O	207/590 (35%)	193 (93%)	11 (5%)	3 (1%)	14	59
15	P	63/175 (36%)	56 (89%)	7 (11%)	0	100	100
16	R	104/135 (77%)	91 (88%)	12 (12%)	1 (1%)	19	65
17	S	438/687 (64%)	415 (95%)	20 (5%)	3 (1%)	26	71
18	T	557/877 (64%)	532 (96%)	22 (4%)	3 (0%)	34	77
19	a	131/251 (52%)	123 (94%)	8 (6%)	0	100	100
20	c	97/382 (25%)	87 (90%)	8 (8%)	2 (2%)	9	52
21	o	305/455 (67%)	251 (82%)	46 (15%)	8 (3%)	7	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
23	y	77/215 (36%)	76 (99%)	1 (1%)	0	100	100
24	b	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
24	k	76/196 (39%)	68 (90%)	7 (9%)	1 (1%)	15	61
25	d	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
25	n	80/101 (79%)	74 (92%)	6 (8%)	0	100	100
26	e	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
26	p	71/94 (76%)	66 (93%)	4 (6%)	1 (1%)	14	59
27	f	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	q	70/86 (81%)	65 (93%)	5 (7%)	0	100	100
28	g	65/77 (84%)	63 (97%)	2 (3%)	0	100	100
28	r	65/77 (84%)	57 (88%)	8 (12%)	0	100	100
29	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
29	l	75/146 (51%)	65 (87%)	8 (11%)	2 (3%)	6	47
30	j	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
30	m	91/110 (83%)	84 (92%)	7 (8%)	0	100	100
31	V	639/1145 (56%)	602 (94%)	34 (5%)	3 (0%)	34	77
32	W	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	3	32
33	Y	82/111 (74%)	76 (93%)	6 (7%)	0	100	100
35	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	2	28
36	t	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
36	u	112/503 (22%)	104 (93%)	8 (7%)	0	100	100
36	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	7	48
36	w	423/503 (84%)	414 (98%)	7 (2%)	2 (0%)	34	77
All	All	9407/14756 (64%)	8598 (91%)	725 (8%)	84 (1%)	26	67

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	487	ASN
6	A	742	VAL
6	A	1620	TYR
7	C	568	SER
7	C	901	GLU
8	H	414	PRO

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Mol	Chain	Res	Type
10	K	108	ASN
10	K	188	LYS
17	S	238	TRP
18	T	478	TYR
20	c	226	ASP
21	o	173	LYS
21	o	418	LEU
31	V	527	ASN
31	V	659	THR
32	W	76	ILE
35	s	94	LYS
35	s	111	VAL
35	s	133	PRO
6	A	2069	VAL
7	C	927	MET
9	J	226	GLY
9	J	287	ASP
9	J	400	ARG
10	K	193	GLU
12	M	84	GLY
12	M	122	GLU
14	O	204	LYS
14	O	220	GLU
20	c	172	ASP
21	o	164	GLY
21	o	181	GLY
21	o	381	SER
31	V	758	ASN
32	W	122	ARG
35	s	105	PRO
35	s	136	VAL
36	v	109	LEU
6	A	511	ASP
6	A	1622	GLY
8	H	109	LYS
9	J	162	THR
13	N	16	CYS
13	N	249	GLY
16	R	14	SER
24	k	81	VAL
32	W	95	PRO
36	v	20	ARG

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Mol	Chain	Res	Type
6	A	418	ASP
7	C	159	LYS
8	H	67	LYS
9	J	277	VAL
13	N	38	THR
14	O	92	ALA
18	T	615	PHE
21	o	306	SER
29	l	31	SER
32	W	68	PRO
32	W	94	LEU
32	W	129	LEU
35	s	119	SER
36	w	20	ARG
6	A	322	VAL
6	A	1093	LYS
6	A	1405	ILE
9	J	318	PRO
17	S	235	LEU
29	l	98	PRO
36	w	17	PRO
8	H	353	PHE
18	T	660	ILE
21	o	297	LEU
21	o	448	ALA
6	A	1984	PRO
6	A	665	GLY
11	L	152	GLY
13	N	121	GLY
17	S	237	ILE
26	p	74	GLY
7	C	301	GLY
7	C	987	PRO
32	W	56	ILE
32	W	98	VAL
36	v	36	GLY

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	1577/2182 (72%)	1549 (98%)	28 (2%)	66	87
7	C	681/910 (75%)	662 (97%)	19 (3%)	51	80
8	H	366/538 (68%)	357 (98%)	9 (2%)	55	82
9	J	299/397 (75%)	280 (94%)	19 (6%)	22	61
10	K	159/328 (48%)	152 (96%)	7 (4%)	35	72
11	L	112/141 (79%)	105 (94%)	7 (6%)	22	62
12	M	214/296 (72%)	210 (98%)	4 (2%)	65	86
13	N	211/332 (64%)	205 (97%)	6 (3%)	51	80
14	O	187/525 (36%)	181 (97%)	6 (3%)	46	78
15	P	56/151 (37%)	54 (96%)	2 (4%)	42	76
16	R	25/121 (21%)	24 (96%)	1 (4%)	38	73
17	S	230/633 (36%)	221 (96%)	9 (4%)	39	74
18	T	1/786 (0%)	1 (100%)	0	100	100
19	a	125/225 (56%)	125 (100%)	0	100	100
20	c	71/346 (20%)	68 (96%)	3 (4%)	36	72
21	o	256/413 (62%)	247 (96%)	9 (4%)	43	77
23	y	76/193 (39%)	74 (97%)	2 (3%)	54	81
24	b	70/176 (40%)	70 (100%)	0	100	100
24	k	70/176 (40%)	69 (99%)	1 (1%)	74	89
25	d	69/89 (78%)	69 (100%)	0	100	100
25	n	69/89 (78%)	66 (96%)	3 (4%)	35	72
26	e	65/83 (78%)	63 (97%)	2 (3%)	47	79
26	p	65/83 (78%)	60 (92%)	5 (8%)	16	55
27	f	63/77 (82%)	63 (100%)	0	100	100
27	q	63/77 (82%)	61 (97%)	2 (3%)	46	78
28	g	58/66 (88%)	57 (98%)	1 (2%)	68	88
28	r	57/66 (86%)	56 (98%)	1 (2%)	66	87
29	h	77/129 (60%)	76 (99%)	1 (1%)	76	90
29	l	73/129 (57%)	63 (86%)	10 (14%)	4	29
30	j	79/103 (77%)	79 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
30	m	77/103 (75%)	74 (96%)	3 (4%)	39 74
All	All	5601/9963 (56%)	5441 (97%)	160 (3%)	54 79

All (160) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	155	ASN
6	A	175	LEU
6	A	196	SER
6	A	233	HIS
6	A	326	ASN
6	A	527	LYS
6	A	537	THR
6	A	588	LEU
6	A	632	ILE
6	A	716	ARG
6	A	753	TYR
6	A	756	LEU
6	A	760	ASN
6	A	1094	ASP
6	A	1140	ASN
6	A	1165	LEU
6	A	1212	ARG
6	A	1337	THR
6	A	1346	PHE
6	A	1511	ARG
6	A	1650	ARG
6	A	1663	PHE
6	A	1757	LEU
6	A	1803	ARG
6	A	1940	MET
6	A	1951	PHE
6	A	1995	TRP
6	A	1997	ASP
7	C	153	LEU
7	C	223	ASP
7	C	300	LYS
7	C	360	ARG
7	C	400	LEU
7	C	430	ARG
7	C	461	LYS
7	C	537	CYS

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Mol	Chain	Res	Type
7	C	586	MET
7	C	590	LYS
7	C	602	VAL
7	C	630	PRO
7	C	658	ASP
7	C	774	LEU
7	C	784	SER
7	C	803	VAL
7	C	830	ASN
7	C	928	CYS
7	C	933	TRP
8	H	84	ASN
8	H	130	ILE
8	H	193	SER
8	H	315	LEU
8	H	320	ASN
8	H	357	TRP
8	H	399	MET
8	H	419	PHE
8	H	421	LYS
9	J	110	LEU
9	J	152	ASN
9	J	156	ILE
9	J	162	THR
9	J	218	ARG
9	J	238	LEU
9	J	261	THR
9	J	274	CYS
9	J	286	THR
9	J	290	VAL
9	J	303	VAL
9	J	323	VAL
9	J	329	ASP
9	J	343	THR
9	J	356	LEU
9	J	386	SER
9	J	443	ASN
9	J	446	LEU
9	J	450	ARG
10	K	37	ASN
10	K	62	GLU
10	K	132	ARG

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Mol	Chain	Res	Type
10	K	179	THR
10	K	190	LEU
10	K	195	ASN
10	K	202	MET
11	L	30	LEU
11	L	52	ILE
11	L	55	LEU
11	L	75	LYS
11	L	142	PHE
11	L	153	CYS
11	L	155	SER
12	M	13	VAL
12	M	31	ASN
12	M	102	LEU
12	M	174	ARG
13	N	22	ASN
13	N	39	LEU
13	N	87	ARG
13	N	106	ASN
13	N	109	MET
13	N	288	ILE
14	O	44	THR
14	O	50	LEU
14	O	53	ASN
14	O	56	LEU
14	O	98	CYS
14	O	160	LEU
15	P	9	LEU
15	P	175	ARG
16	R	17	SER
17	S	65	MET
17	S	124	ARG
17	S	128	THR
17	S	143	GLU
17	S	147	ASN
17	S	156	TYR
17	S	232	LEU
17	S	237	ILE
17	S	266	LEU
20	c	173	ARG
20	c	191	ARG
20	c	225	LYS

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Mol	Chain	Res	Type
21	o	156	ARG
21	o	166	THR
21	o	216	GLU
21	o	278	ARG
21	o	299	LEU
21	o	330	GLN
21	o	356	MET
21	o	406	ARG
21	o	451	ILE
23	y	162	ASN
23	y	185	ASN
26	e	25	THR
26	e	92	SER
28	g	66	ASN
29	h	16	THR
24	k	19	LYS
29	l	11	ARG
29	l	15	VAL
29	l	16	THR
29	l	25	VAL
29	l	43	VAL
29	l	44	LYS
29	l	95	ILE
29	l	96	ILE
29	l	97	LEU
29	l	101	LEU
30	m	41	ARG
30	m	82	LYS
30	m	94	LEU
25	n	20	SER
25	n	43	GLN
25	n	76	ASP
28	r	71	LEU
26	p	54	ILE
26	p	77	LEU
26	p	79	LYS
26	p	81	LEU
26	p	82	LEU
27	q	34	ASN
27	q	79	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (59) such sidechains are listed below:

Mol	Chain	Res	Type
6	A	155	ASN
6	A	326	ASN
6	A	344	ASN
6	A	542	HIS
6	A	617	ASN
6	A	636	HIS
6	A	713	ASN
6	A	828	HIS
6	A	848	ASN
6	A	1030	GLN
6	A	1115	GLN
6	A	1140	ASN
6	A	1369	ASN
6	A	1856	ASN
6	A	2018	ASN
7	C	143	HIS
7	C	194	ASN
7	C	211	ASN
7	C	218	HIS
7	C	289	ASN
7	C	358	ASN
7	C	423	HIS
7	C	431	GLN
7	C	683	ASN
7	C	764	ASN
7	C	776	ASN
7	C	830	ASN
8	H	320	ASN
9	J	271	GLN
9	J	443	ASN
10	K	86	ASN
10	K	171	ASN
10	K	192	ASN
10	K	195	ASN
11	L	116	ASN
12	M	12	GLN
12	M	31	ASN
12	M	39	GLN
14	O	83	GLN
15	P	34	HIS
17	S	79	HIS
17	S	147	ASN
17	S	236	GLN

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Mol	Chain	Res	Type
17	S	248	ASN
17	S	252	HIS
19	a	246	ASN
20	c	332	ASN
21	o	183	ASN
21	o	259	ASN
21	o	330	GLN
23	y	99	GLN
23	y	144	GLN
23	y	185	ASN
29	h	94	GLN
29	l	14	GLN
29	l	21	ASN
29	l	86	ASN
29	l	94	GLN
28	r	53	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	32/95 (33%)	14 (43%)	4 (12%)
2	E	15/20 (75%)	5 (33%)	1 (6%)
3	2	146/1175 (12%)	49 (33%)	5 (3%)
34	3	2/3 (66%)	2 (100%)	0
4	6	98/112 (87%)	37 (37%)	3 (3%)
5	5	138/179 (77%)	61 (44%)	3 (2%)
All	All	431/1584 (27%)	168 (38%)	16 (3%)

All (168) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	2	U
1	I	3	A
1	I	4	U
1	I	10	A
1	I	11	A
1	I	13	U
1	I	14	U
1	I	15	A
1	I	16	U
1	I	61	U

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Mol	Chain	Res	Type
1	I	70	A
1	I	71	C
1	I	72	A
1	I	73	A
2	E	-11	G
2	E	-10	A
2	E	-8	C
2	E	-4	A
2	E	-1	G
3	2	15	C
3	2	16	U
3	2	17	U
3	2	18	U
3	2	19	U
3	2	20	G
3	2	21	G
3	2	23	U
3	2	25	A
3	2	26	G
3	2	27	A
3	2	29	C
3	2	30	A
3	2	32	G
3	2	33	U
3	2	34	G
3	2	35	U
3	2	41	C
3	2	44	U
3	2	63	U
3	2	64	G
3	2	67	A
3	2	68	U
3	2	81	C
3	2	141	A
3	2	1094	G
3	2	1096	C
3	2	1098	C
3	2	1099	G
3	2	1100	A
3	2	1101	C
3	2	1102	C
3	2	1103	C

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Mol	Chain	Res	Type
3	2	1104	U
3	2	1106	G
3	2	1107	C
3	2	1108	A
3	2	1120	G
3	2	1123	C
3	2	1124	U
3	2	1125	U
3	2	1126	G
3	2	1139	G
3	2	1144	U
3	2	1145	U
3	2	1146	G
3	2	1149	G
3	2	1152	U
3	2	1166	G
4	6	8	A
4	6	10	G
4	6	17	U
4	6	19	C
4	6	20	G
4	6	21	U
4	6	27	U
4	6	28	U
4	6	29	U
4	6	34	A
4	6	35	A
4	6	36	U
4	6	37	U
4	6	40	A
4	6	41	A
4	6	43	C
4	6	46	U
4	6	49	A
4	6	50	G
4	6	51	A
4	6	52	G
4	6	54	U
4	6	55	G
4	6	59	A
4	6	68	C
4	6	72	C

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Mol	Chain	Res	Type
4	6	73	A
4	6	74	U
4	6	75	A
4	6	80	U
4	6	84	C
4	6	85	C
4	6	88	U
4	6	90	U
4	6	91	A
4	6	92	C
4	6	93	A
5	5	10	U
5	5	14	G
5	5	15	A
5	5	16	U
5	5	17	C
5	5	20	U
5	5	24	G
5	5	25	G
5	5	26	A
5	5	27	G
5	5	28	G
5	5	31	G
5	5	33	U
5	5	34	C
5	5	40	C
5	5	41	A
5	5	42	A
5	5	43	G
5	5	44	A
5	5	45	A
5	5	46	C
5	5	52	G
5	5	63	C
5	5	64	C
5	5	67	U
5	5	68	A
5	5	69	G
5	5	70	A
5	5	71	A
5	5	75	A
5	5	76	U

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Mol	Chain	Res	Type
5	5	77	A
5	5	78	A
5	5	80	G
5	5	81	A
5	5	82	A
5	5	89	U
5	5	92	U
5	5	95	C
5	5	97	U
5	5	101	C
5	5	108	C
5	5	109	A
5	5	113	G
5	5	116	U
5	5	121	U
5	5	126	A
5	5	129	G
5	5	130	A
5	5	131	A
5	5	133	C
5	5	134	A
5	5	135	G
5	5	136	G
5	5	140	A
5	5	142	C
5	5	145	U
5	5	169	U
5	5	170	U
5	5	171	U
5	5	172	U
34	3	2	U
34	3	3	U

All (16) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	9	A
1	I	12	G
1	I	13	U
1	I	70	A
2	E	-7	U
3	2	15	C

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Mol	Chain	Res	Type
3	2	17	U
3	2	1123	C
3	2	1124	U
3	2	1145	U
4	6	16	C
4	6	45	A
4	6	92	C
5	5	27	G
5	5	39	U
5	5	45	A

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
39	I6P	A	3001	-	30,36,36	0.66	0	60,60,60	1.17	6 (10%)
40	GTP	C	1101	-	26,34,34	1.06	2 (7%)	29,54,54	1.95	8 (27%)

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
39	I6P	A	3001	-	-	0/30/54/54	0/1/1/1
40	GTP	C	1101	-	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C	1101	GTP	C5-C4	2.68	1.46	1.40
40	C	1101	GTP	C6-C5	3.34	1.48	1.41

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	C	1101	GTP	C1'-N9-C4	-3.90	122.45	126.81
40	C	1101	GTP	C6-C5-C4	-3.78	116.54	120.86
40	C	1101	GTP	N3-C2-N1	-3.71	122.51	127.56
40	C	1101	GTP	C5-C6-N1	-3.49	118.96	123.52
39	A	3001	I6P	O13-P3-O33	-2.46	101.61	107.48
39	A	3001	I6P	O34-P4-O24	2.02	114.86	107.44
40	C	1101	GTP	O3G-PG-O2G	2.05	114.97	107.44
39	A	3001	I6P	C5-C4-C3	2.06	115.02	110.48
40	C	1101	GTP	O2B-PB-O1B	2.08	123.40	112.56
40	C	1101	GTP	O4'-C1'-N9	2.13	112.14	108.11
39	A	3001	I6P	O36-P6-O46	2.15	115.34	107.44
39	A	3001	I6P	O21-P1-O41	2.29	115.85	107.44
39	A	3001	I6P	C2-C3-C4	2.82	116.69	110.48
40	C	1101	GTP	C6-N1-C2	4.83	121.55	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	X	1
18	T	1
31	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	27:UNK	C	86:UNK	N	8.48
1	V	903:MET	C	904:ASP	N	2.35
1	T	300:ASP	C	301:LYS	N	2.16