Full wwPDB EM Validation Report ⓘ

Nov 9, 2022 – 03:58 AM JST

PDB ID	:	6ICZ
EMDB ID	:	EMD-9645
Title	:	Cryo-EM structure of a human post-catalytic spliceosome (P complex) at 3.0 angstrom
Authors	:	Zhang, X.; Zhan, X.; Yan, C.; Shi, Y.
Deposited on	:	2018-09-07
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

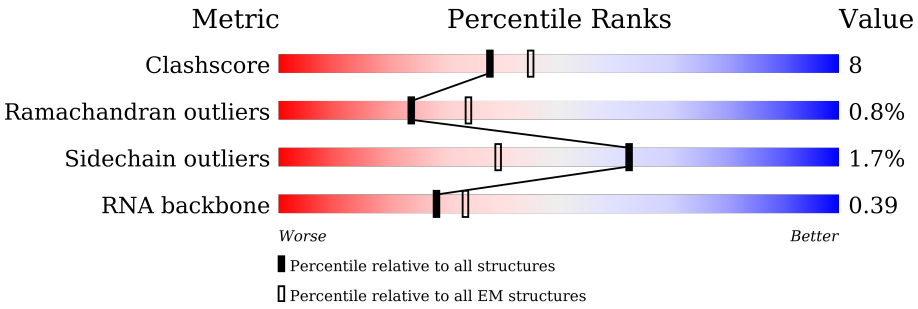
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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 <=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	v	148	97% 97% ·
2	w	174	52% 51% ·· 48%
3	u	411	94% 93% · 6%
4	x	703	· · 96%
5	A	2335	12% 81% 15% ·
6	B	117	14% 26% 38% 17% · 17%
7	C	972	· 74% 17% · 8%

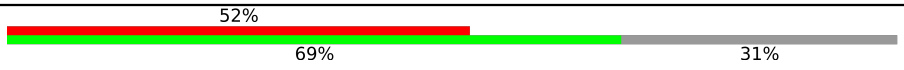
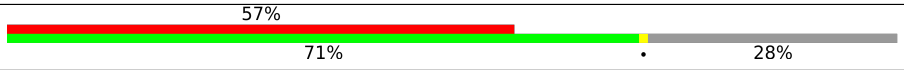
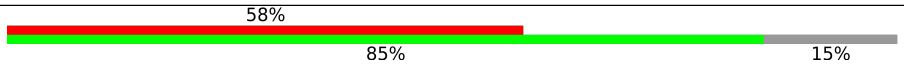
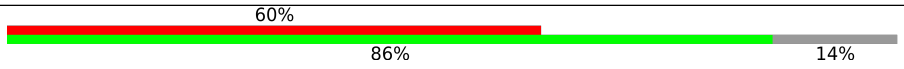
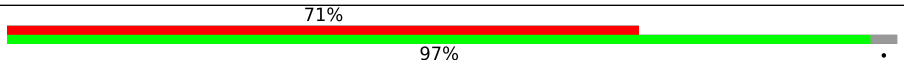
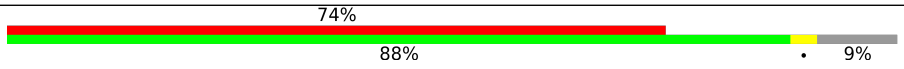
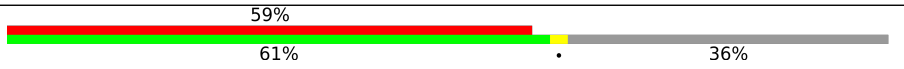
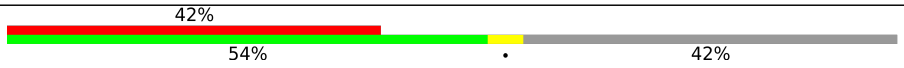
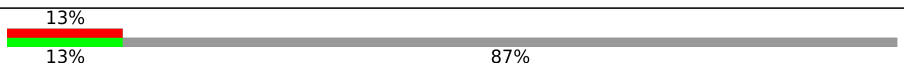
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	E	357	62% 22% 15%
9	F	107	44% 34% 12% 9%
10	G	273	6% 12% 8% 9% 69%
11	H	188	37% 16% 16% 39% 26%
12	J	848	33% 62% 5% 33%
13	L	802	27% 50% 6% 43%
14	M	243	42% 9% 47%
15	N	144	76% 17% 6%
16	O	420	53% 15% 32%
17	P	229	43% 5% 52%
18	R	536	38% 10% 51%
19	S	166	78% 18%
20	T	514	43% 16% 39%
21	U	2752	99%
22	V	908	28% 47% 50%
23	W	579	69% 17% 12%
24	X	184	14% 43% 7% 50%
25	Z	586	34% 7% 59%
26	I	855	57% 60% 6% 34%
27	y	301	24% 26% 74%
28	Q	1485	89% 89% 11%
29	a	126	44% 64% 36%
29	h	126	56% 64% 36%
30	b	231	28% 37% 63%
30	i	231	33% 37% 63%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
31	c	119	
31	j	119	
32	d	118	
32	k	118	
33	f	86	
33	m	86	
34	e	92	
34	l	92	
35	g	76	
35	n	76	
36	o	255	
37	p	225	
38	Y	1220	
39	K	225	
40	q	504	
40	r	504	
40	s	504	
40	t	504	
41	D	2136	

2 Entry composition

There are 46 unique types of molecules in this entry. The entry contains 97900 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 protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
1	v	144	711	423	144	144	0	0

- Molecule 2 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	w	91	445	263	91	91	0	0

- Molecule 3 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	u	386	1907	1135	386	386	0	0

- Molecule 4 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	x	25	124	74	25	25	0	0

- Molecule 5 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	2253	17837	11432	3157	3177	71	0	0

- Molecule 6 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
6	B	97	2040	914	339	690	97	0	0

- Molecule 7 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	C	894	Total	C	N	O	S	0	0
			7066	4520	1178	1334	34		

- Molecule 8 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	E	303	Total	C	N	O	S	0	0
			2366	1487	415	451	13		

- Molecule 9 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	97	Total	C	N	O	P	0	0
			2075	928	381	669	97		

- Molecule 10 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	G	84	Total	C	N	O	P	0	0
			1549	684	218	563	84		

- Molecule 11 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	H	140	Total	C	N	O	P	0	0
			2966	1326	510	990	140		

- Molecule 12 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	J	571	Total	C	N	O	S	0	0
			3829	2385	720	718	6		

- Molecule 13 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	L	454	Total	C	N	O	S	0	0
			3064	1884	596	578	6		

- Molecule 14 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	130	Total	C	N	O	S	0	0
			1098	684	204	208	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	N	143	Total	C	N	O	S	0	0
			1184	746	217	209	12		

- Molecule 16 is a protein called Pre-mRNA-splicing factor RBM22.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	285	Total	C	N	O	S	0	0
			2296	1442	408	426	20		

- Molecule 17 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	110	Total	C	N	O	S	0	0
			929	569	182	176	2		

- Molecule 18 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
18	R	261	Total	C	N	O	P	S	0	0
			2073	1300	373	386	2	12		

- Molecule 19 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	159	Total	C	N	O	S	0	0
			1236	787	215	227	7		

- Molecule 20 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	313	Total	C	N	O	S	0	0
			2461	1554	447	452	8		

- Molecule 21 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	26	Total	C	N	O	S	0	0
			193	120	36	36	1		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	452	Total	C	N	O	S	0	0
			2765	1723	508	523	11		

- Molecule 23 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	508	Total	C	N	O	S	0	0
			4122	2623	714	761	24		

- Molecule 24 is a protein called PRKR-interacting protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	92	Total	C	N	O	S	0	0
			701	432	133	132	4		

- Molecule 25 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Z	242	Total	C	N	O	S	0	0
			1999	1260	357	374	8		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
26	I	564	Total	C	N	O	0	0
			2782	1654	564	564		

- Molecule 27 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	y	79	Total	C	N	O	0	0
			390	232	79	79		

- Molecule 28 is a protein called RNA helicase aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
28	Q	1322	Total	C	N	O	4	0
			6562	3918	1322	1322		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms				AltConf	Trace
29	h	81	Total	C	N	O	0	0
			398	236	81	81		
29	a	81	Total	C	N	O	0	0
			399	237	81	81		

- Molecule 30 is a protein called Small nuclear ribonucleoprotein-associated protein.

Mol	Chain	Residues	Atoms				AltConf	Trace
30	i	86	Total	C	N	O	0	0
			424	252	86	86		
30	b	86	Total	C	N	O	0	0
			424	252	86	86		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms				AltConf	Trace
31	j	82	Total	C	N	O	0	0
			406	242	82	82		
31	c	82	Total	C	N	O	0	0
			406	242	82	82		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	k	85	Total	C	N	O	0	0
			422	252	85	85		
32	d	97	Total	C	N	O	0	0
			480	286	97	97		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	m	73	Total	C	N	O	0	0
			356	210	73	73		
33	f	74	Total	C	N	O	0	0
			361	213	74	74		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	l	79	Total 391	C 233	N 79	O 79	0	0
34	e	79	Total 391	C 233	N 79	O 79	0	0

- Molecule 35 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms				AltConf	Trace
35	n	69	Total 339	C 201	N 69	O 69	0	0
35	g	74	Total 363	C 215	N 74	O 74	0	0

- Molecule 36 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	o	162	Total 804	C 480	N 162	O 162	0	0

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein B".

Mol	Chain	Residues	Atoms				AltConf	Trace
37	p	94	Total 464	C 276	N 94	O 94	0	0

- Molecule 38 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	Y	713	Total 2917	C 1486	N 716	O 714	S 1	0	0

- Molecule 39 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	K	152	Total 757	C 453	N 152	O 152	0	0

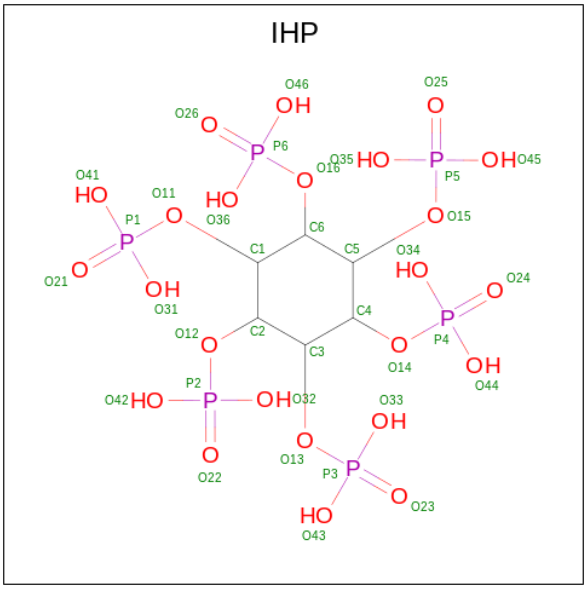
- Molecule 40 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
40	q	132	Total	C	N	O	0	0
			659	395	132	132		
40	r	131	Total	C	N	O	0	0
			654	392	131	131		
40	s	67	Total	C	N	O	0	0
			335	201	67	67		
40	t	67	Total	C	N	O	0	0
			335	201	67	67		

- Molecule 41 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

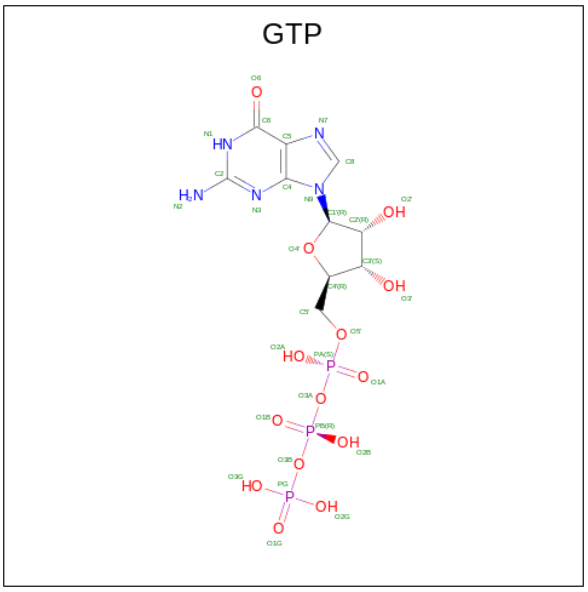
Mol	Chain	Residues	Atoms				AltConf	Trace
41	D	1722	Total	C	N	O	0	0
			8530	5086	1722	1722		

- Molecule 42 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$).



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

- Molecule 43 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

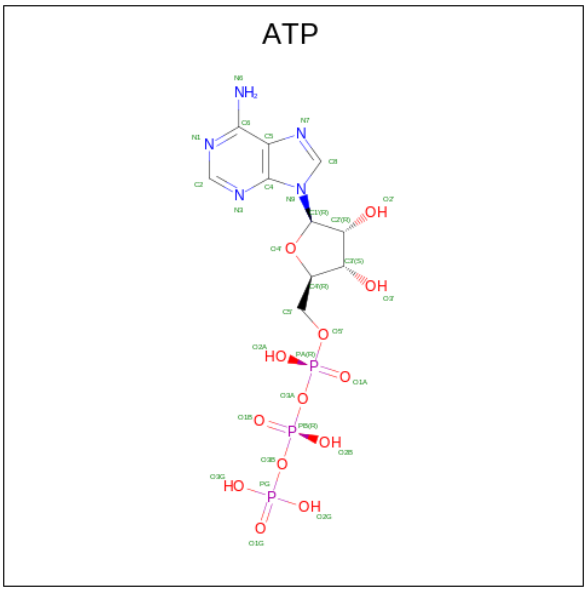
- Molecule 44 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
44	C	1	Total	Mg	0
			1	1	
44	F	6	Total	Mg	0
			6	6	
44	Q	2	Total	Mg	0
			2	2	

- Molecule 45 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
45	N	3	Total	Zn	0
			3	3	
45	O	3	Total	Zn	0
			3	3	
45	Z	1	Total	Zn	0
			1	1	

- Molecule 46 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



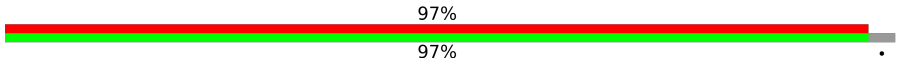
Mol	Chain	Residues	Atoms					AltConf
46	Q	1	Total	C	N	O	P	0
			31	10	5	13	3	

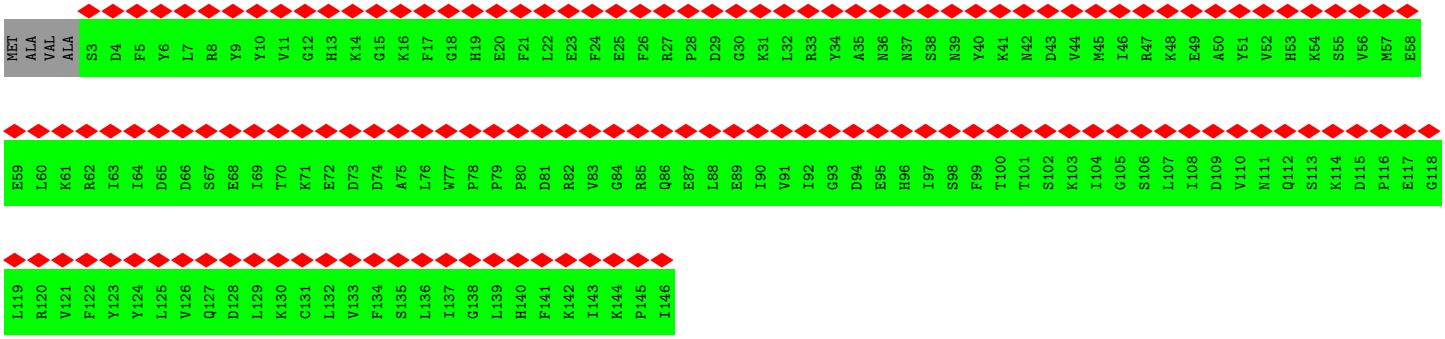
3 Residue-property plots (i)

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: Protein mago nashi homolog 2

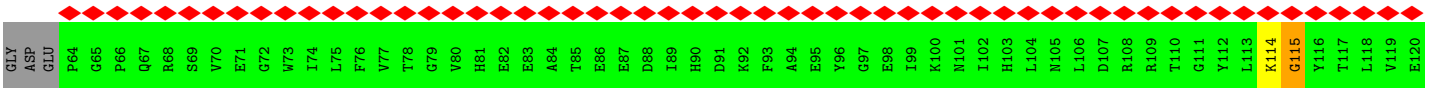
Chain v:





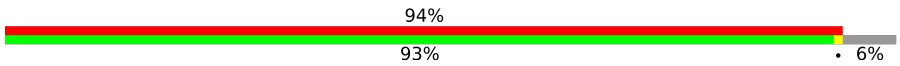
• Molecule 2: RNA-binding protein 8A

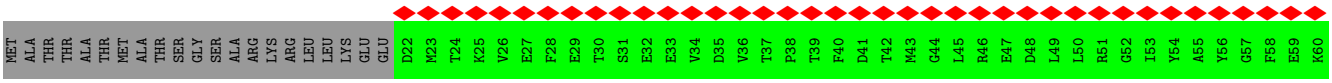
Chain w:

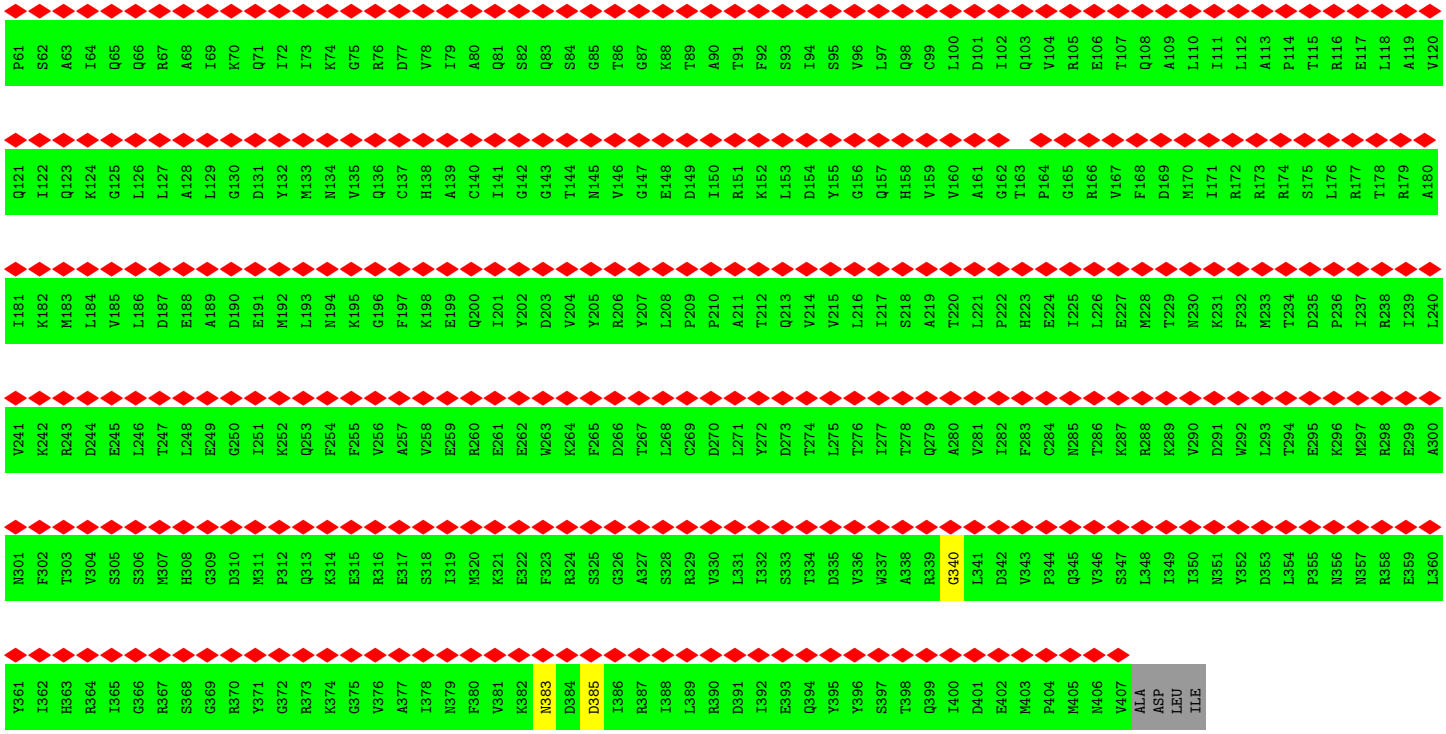


• Molecule 3: Eukaryotic initiation factor 4A-III

Chain u:

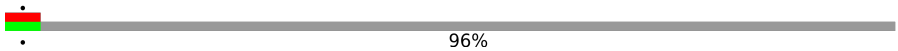


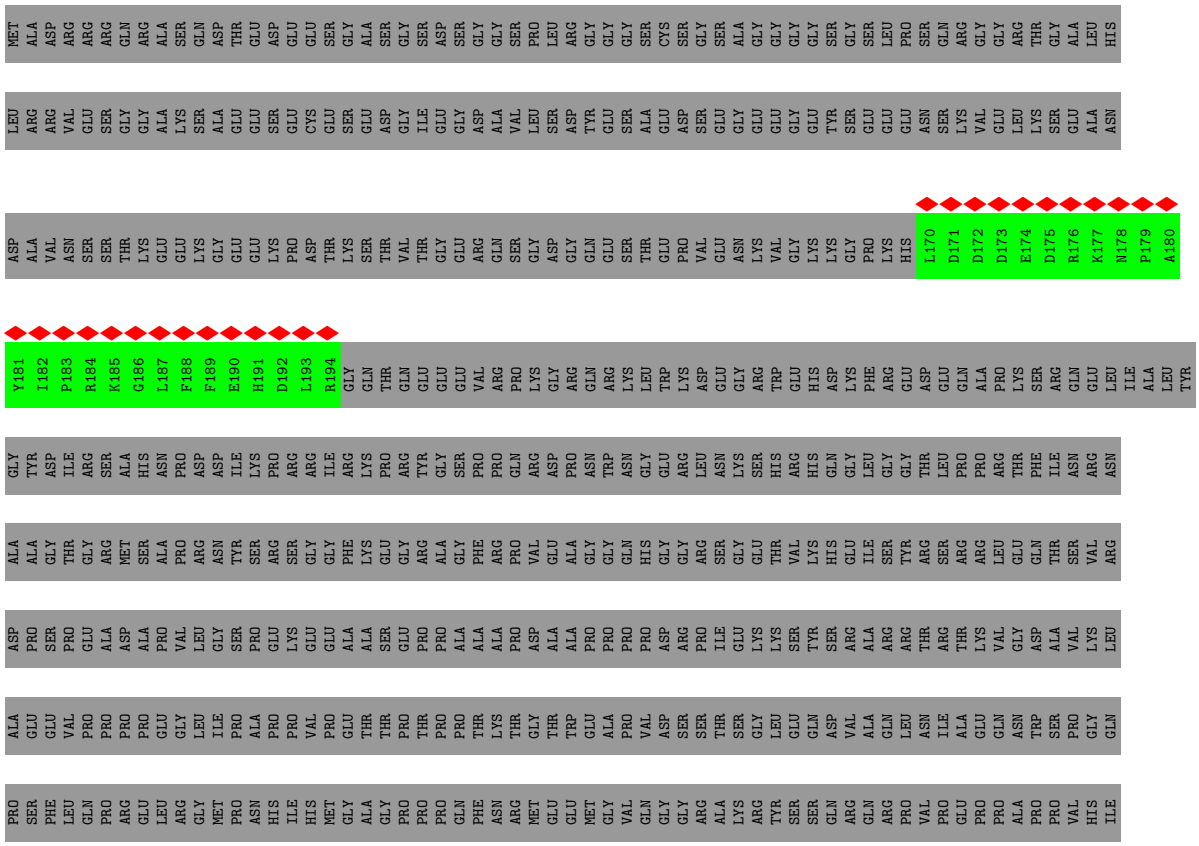


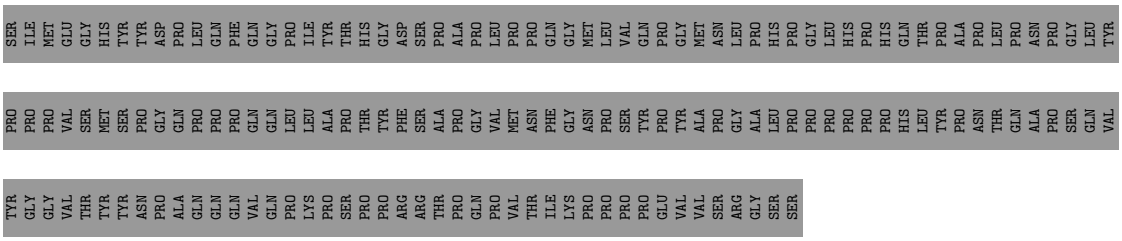


- Molecule 4: Protein CASC3

Chain x:

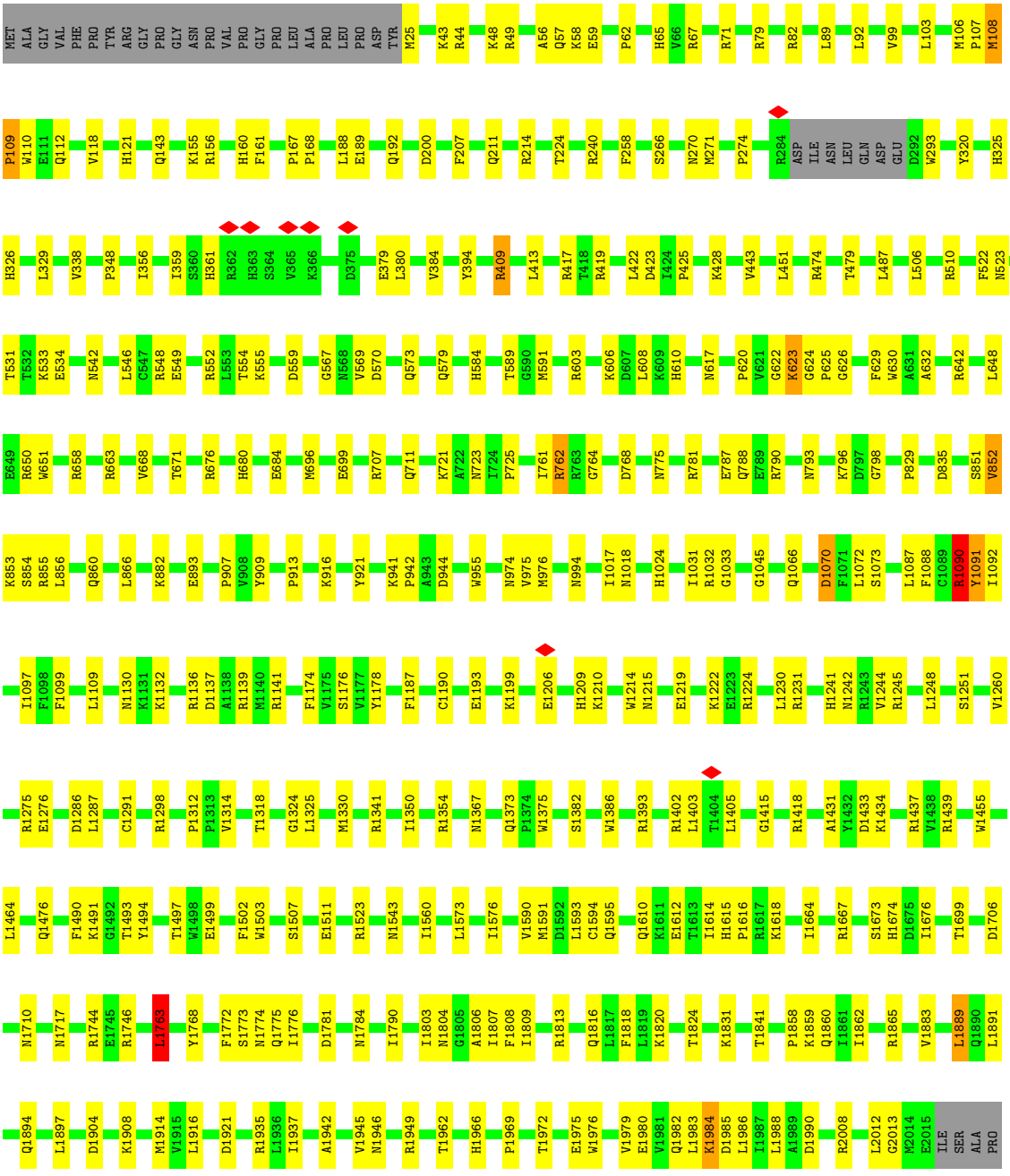


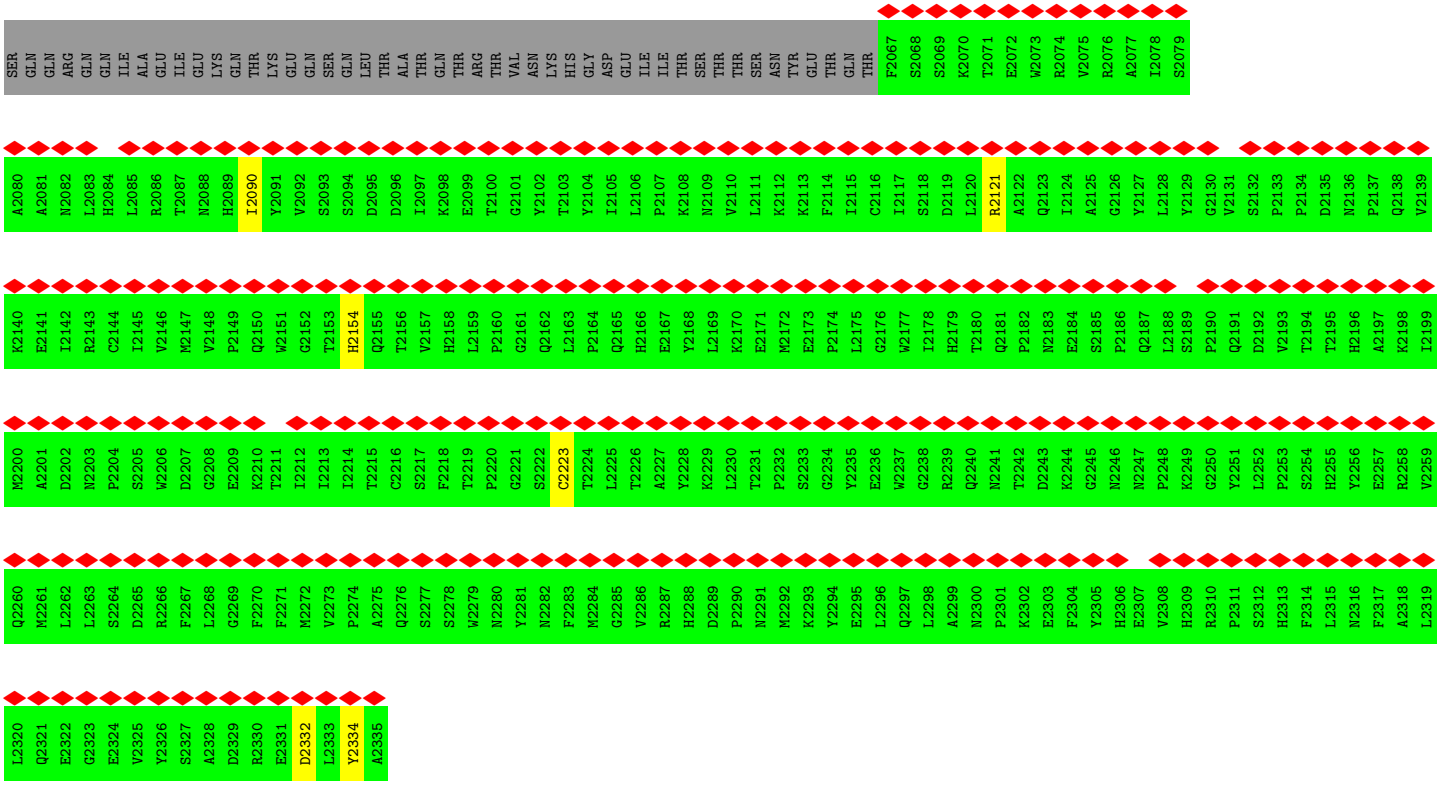




• Molecule 5: Pre-mRNA-processing-splicing factor 8

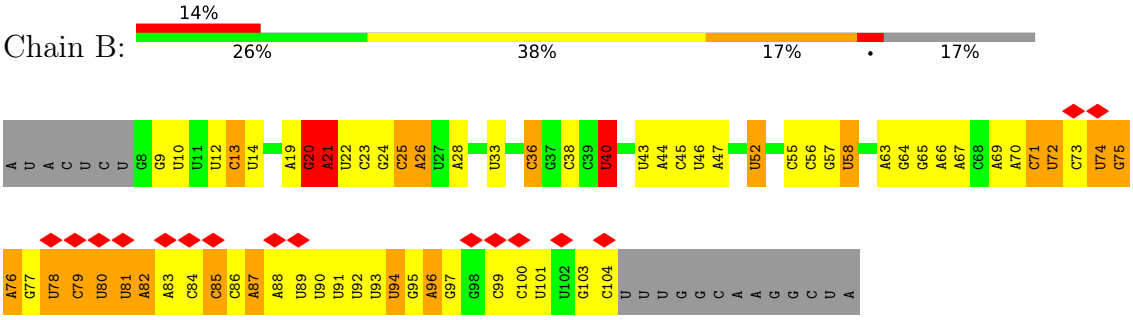
Chain A:





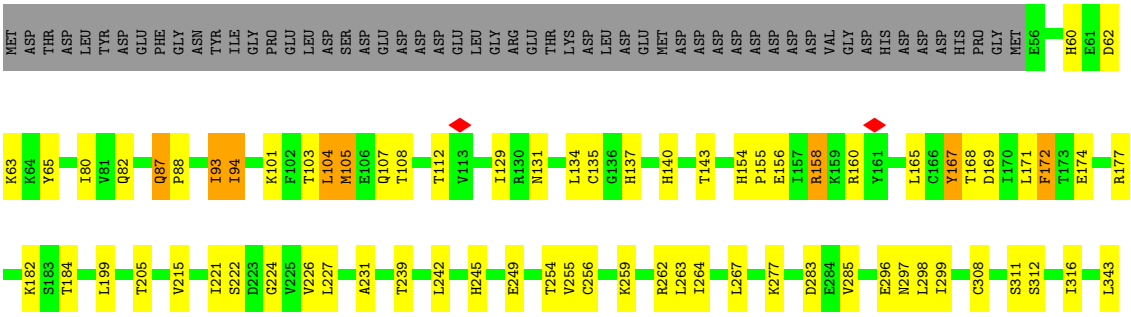
• Molecule 6: U5snRNA

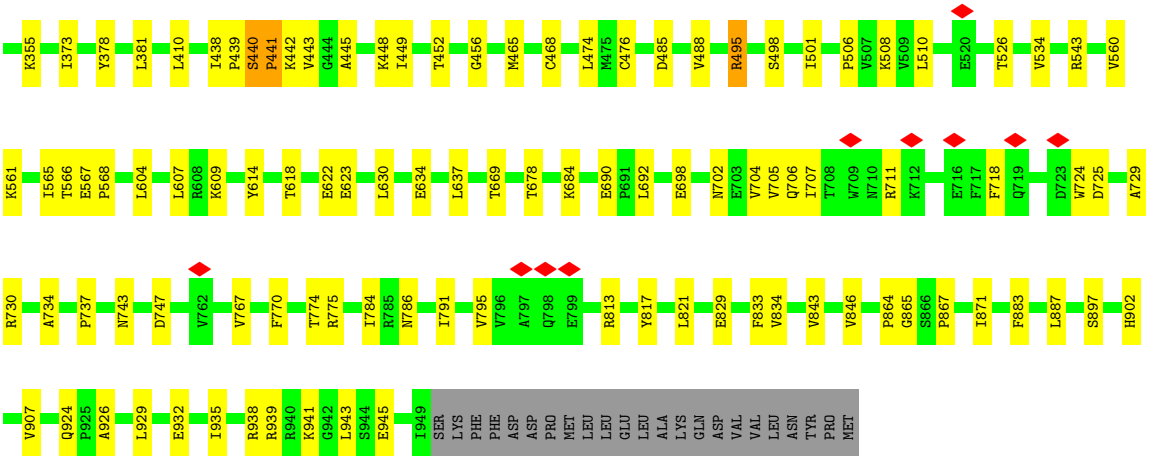
Chain B:



• Molecule 7: 116 kDa U5 small nuclear ribonucleoprotein component

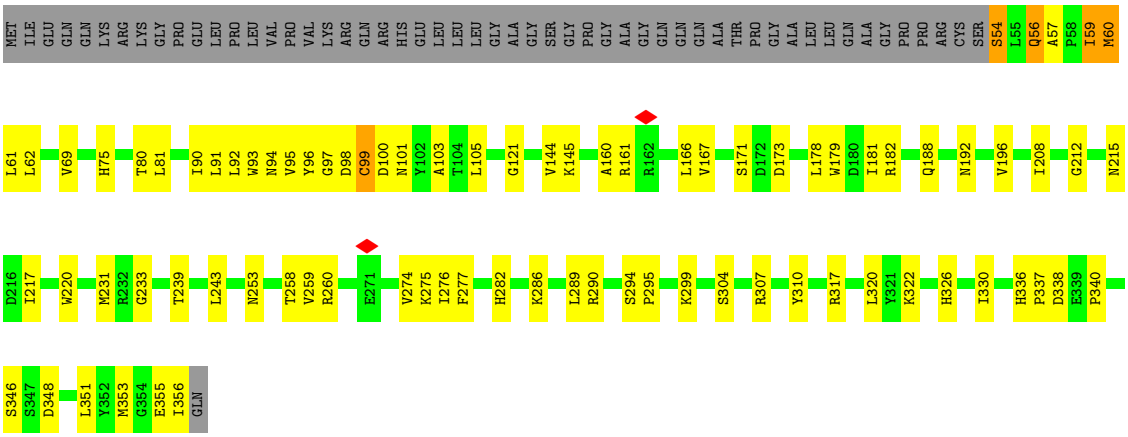
Chain C:





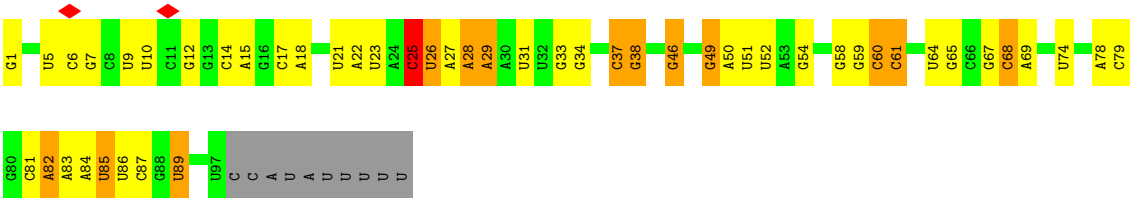
• Molecule 8: U5 small nuclear ribonucleoprotein 40 kDa protein

Chain E:



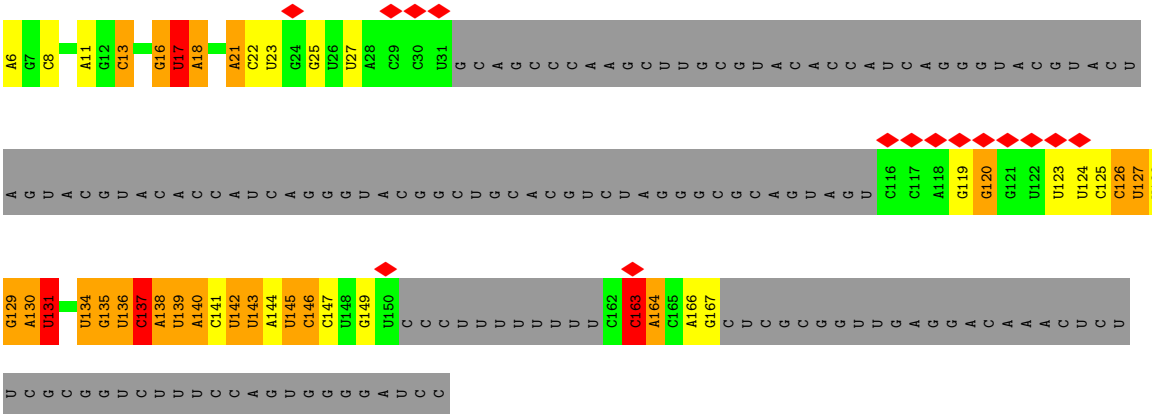
• Molecule 9: U6snRNA

Chain F:



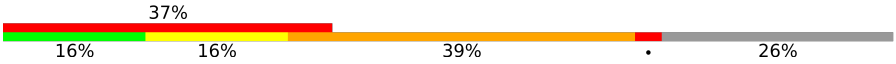
• Molecule 10: pre-mRNA

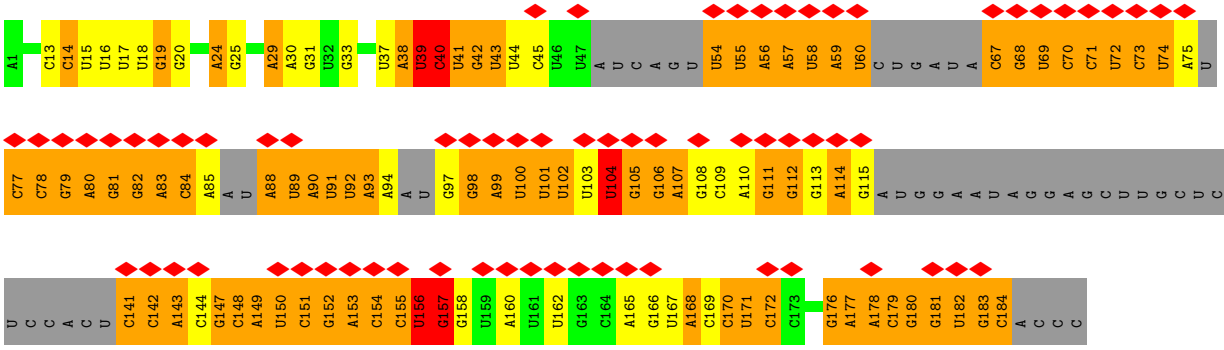
Chain G:



• Molecule 11: U2snRNA

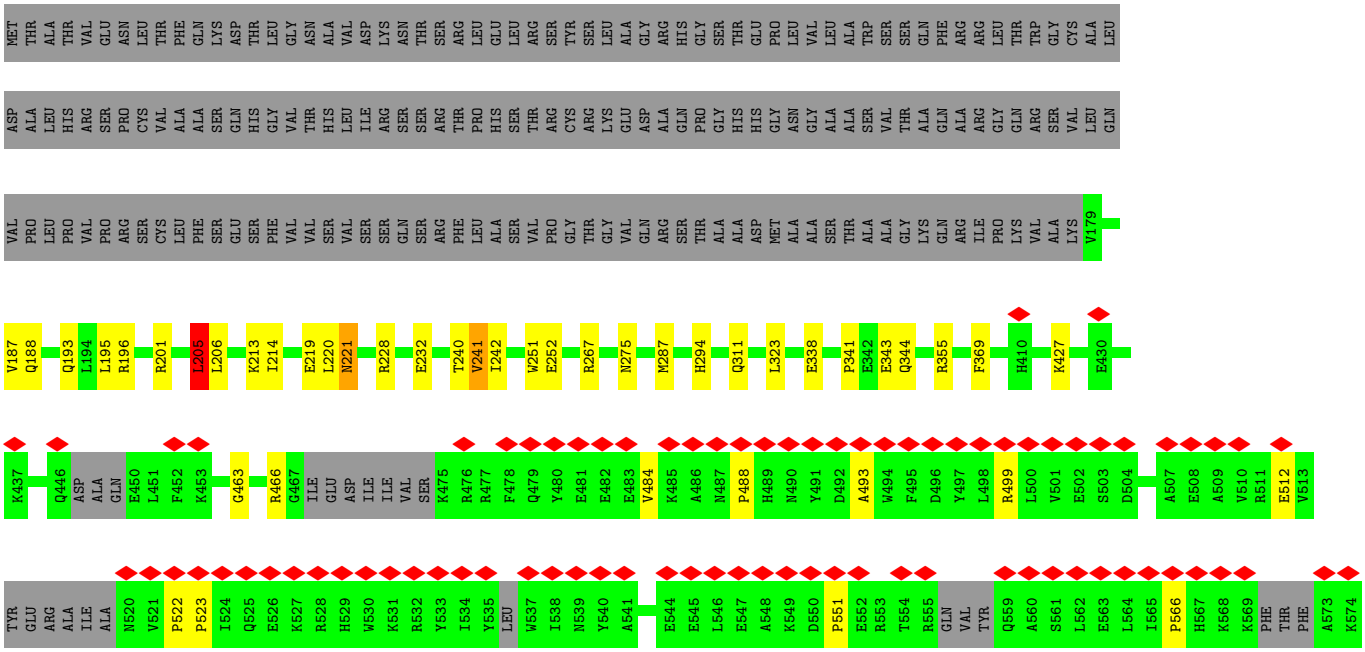
Chain H:

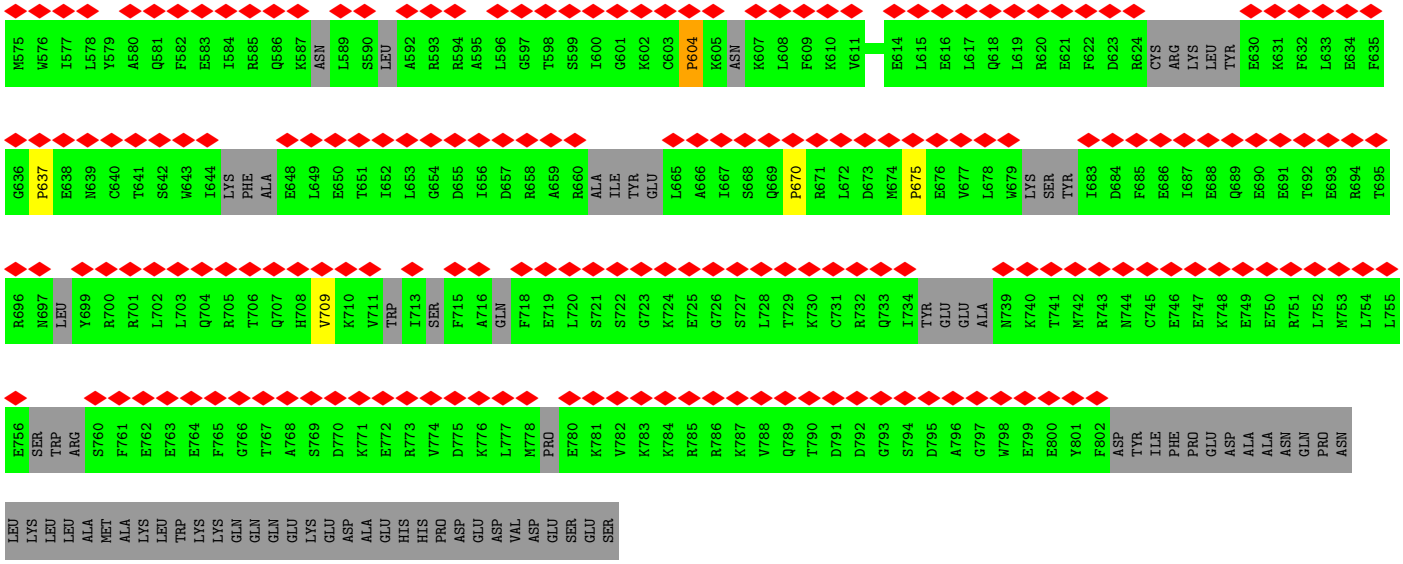




• Molecule 12: Crooked neck-like protein 1

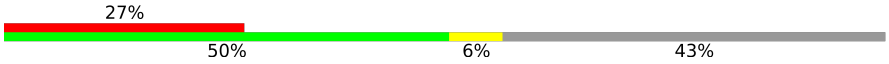
Chain J:

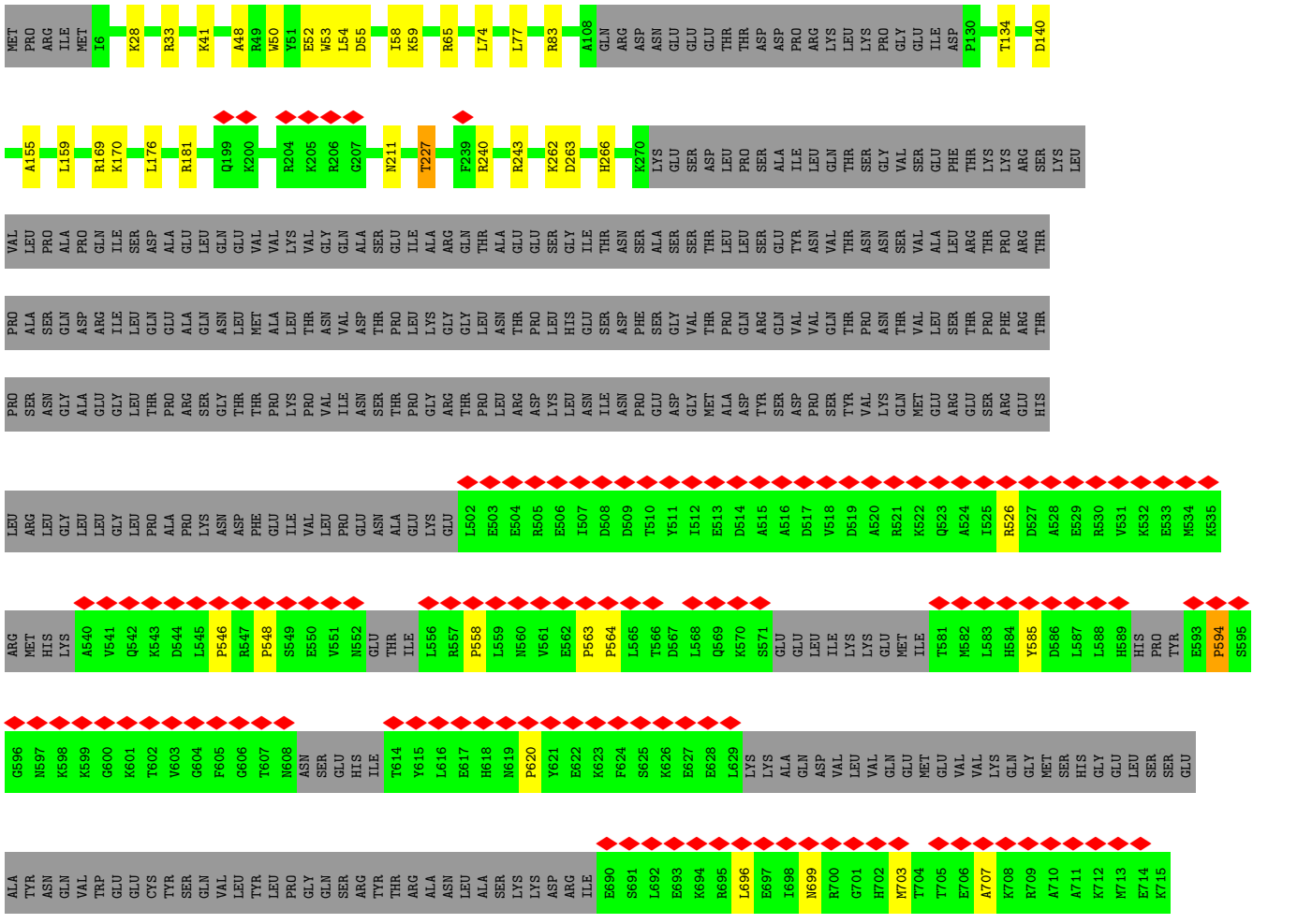


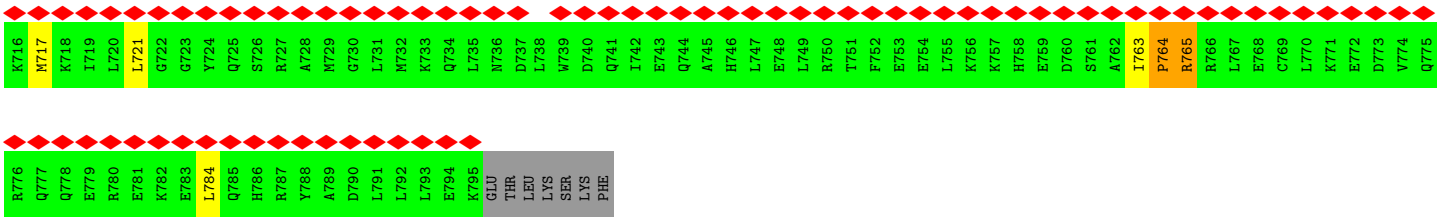


• Molecule 13: Cell division cycle 5-like protein

Chain L:

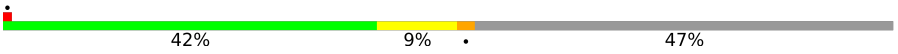


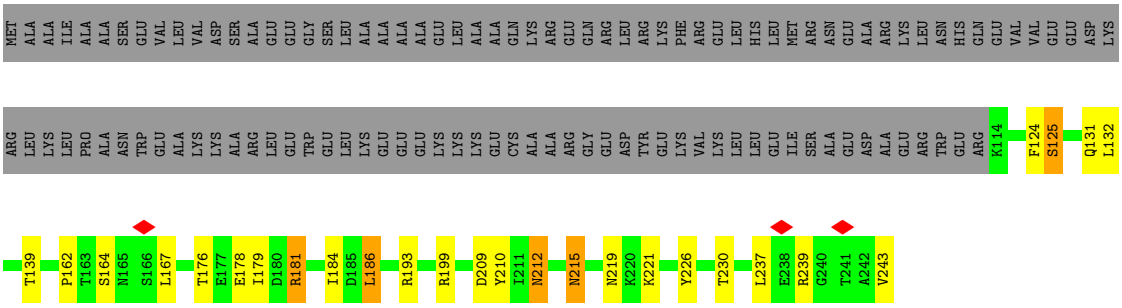




• Molecule 14: Pre-mRNA-splicing factor SYF2

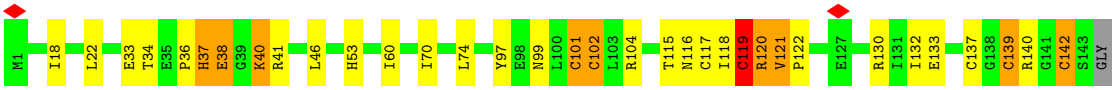
Chain M:





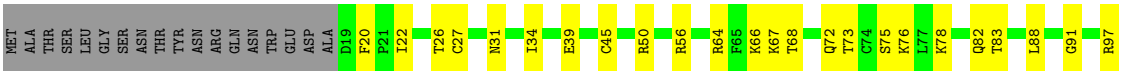
• Molecule 15: Protein BUD31 homolog

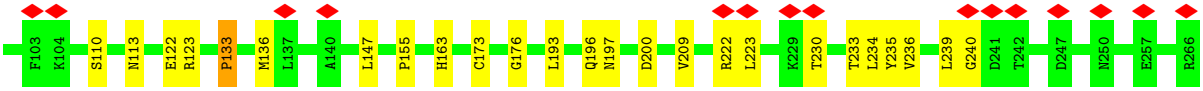
Chain N:

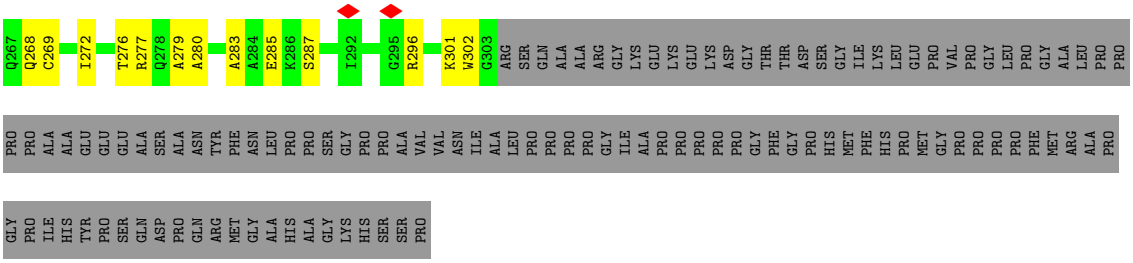


• Molecule 16: Pre-mRNA-splicing factor RBM22

Chain O:

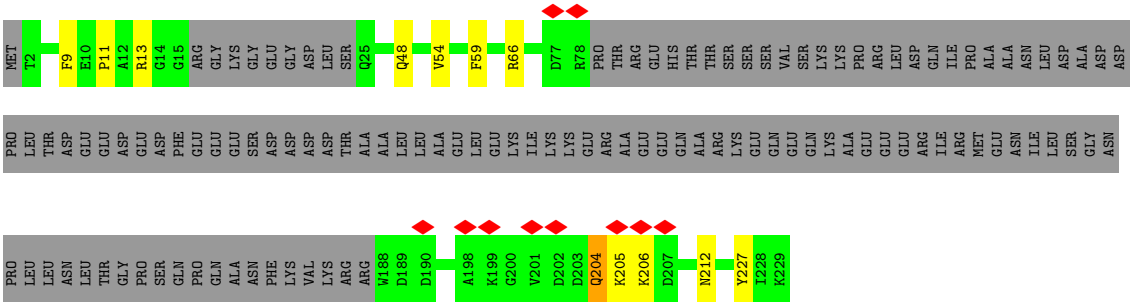






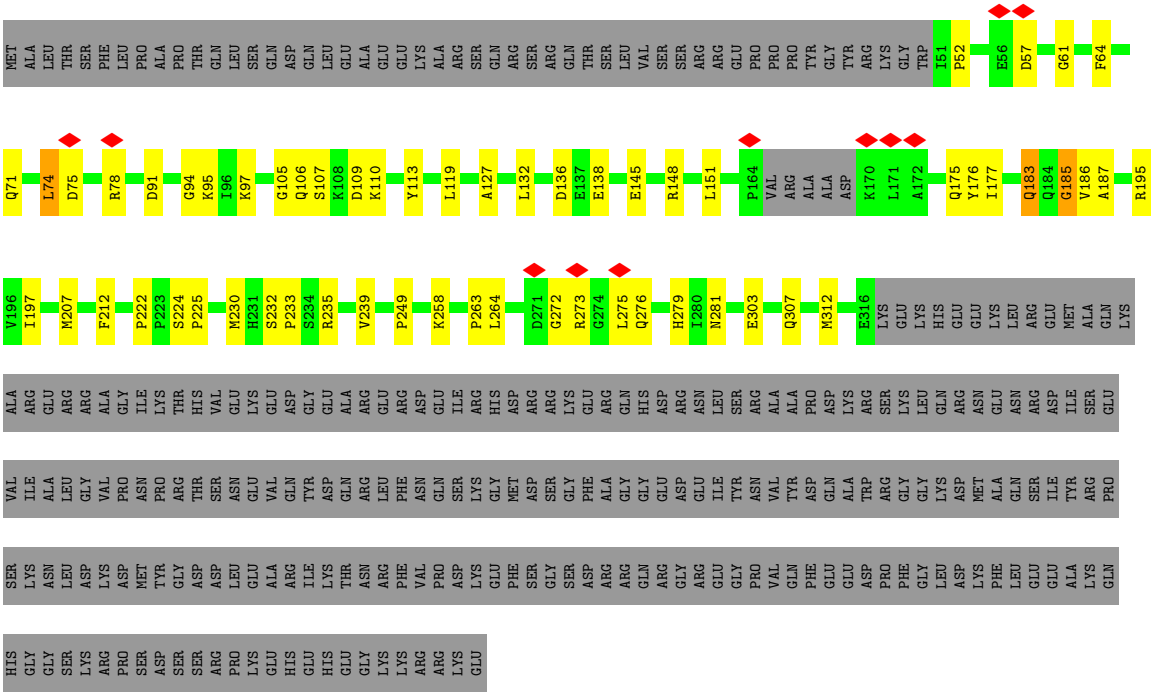
• Molecule 17: Spliceosome-associated protein CWC15 homolog

Chain P:



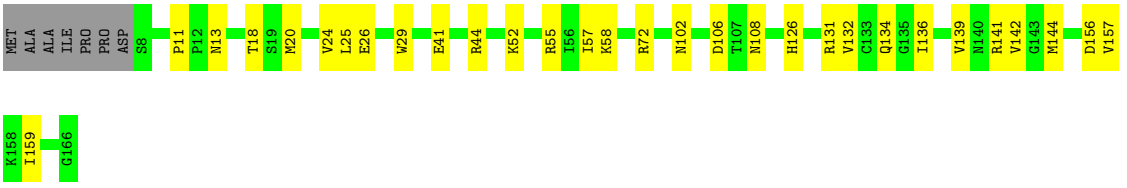
• Molecule 18: SNW domain-containing protein 1

Chain R:



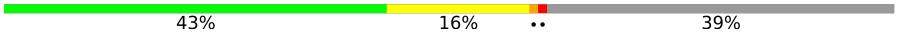
• Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1

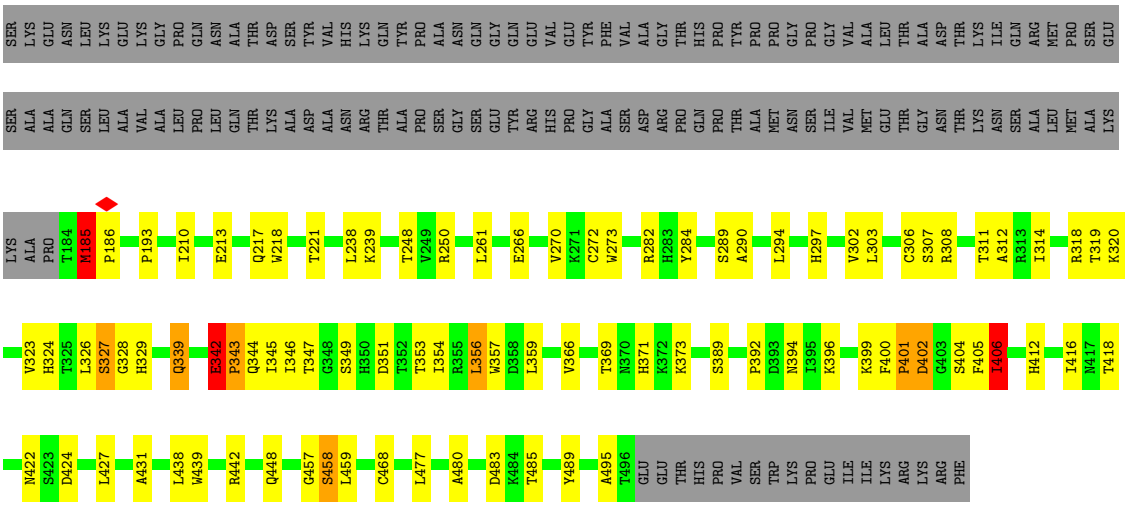
Chain S:



• Molecule 20: Pleiotropic regulator 1

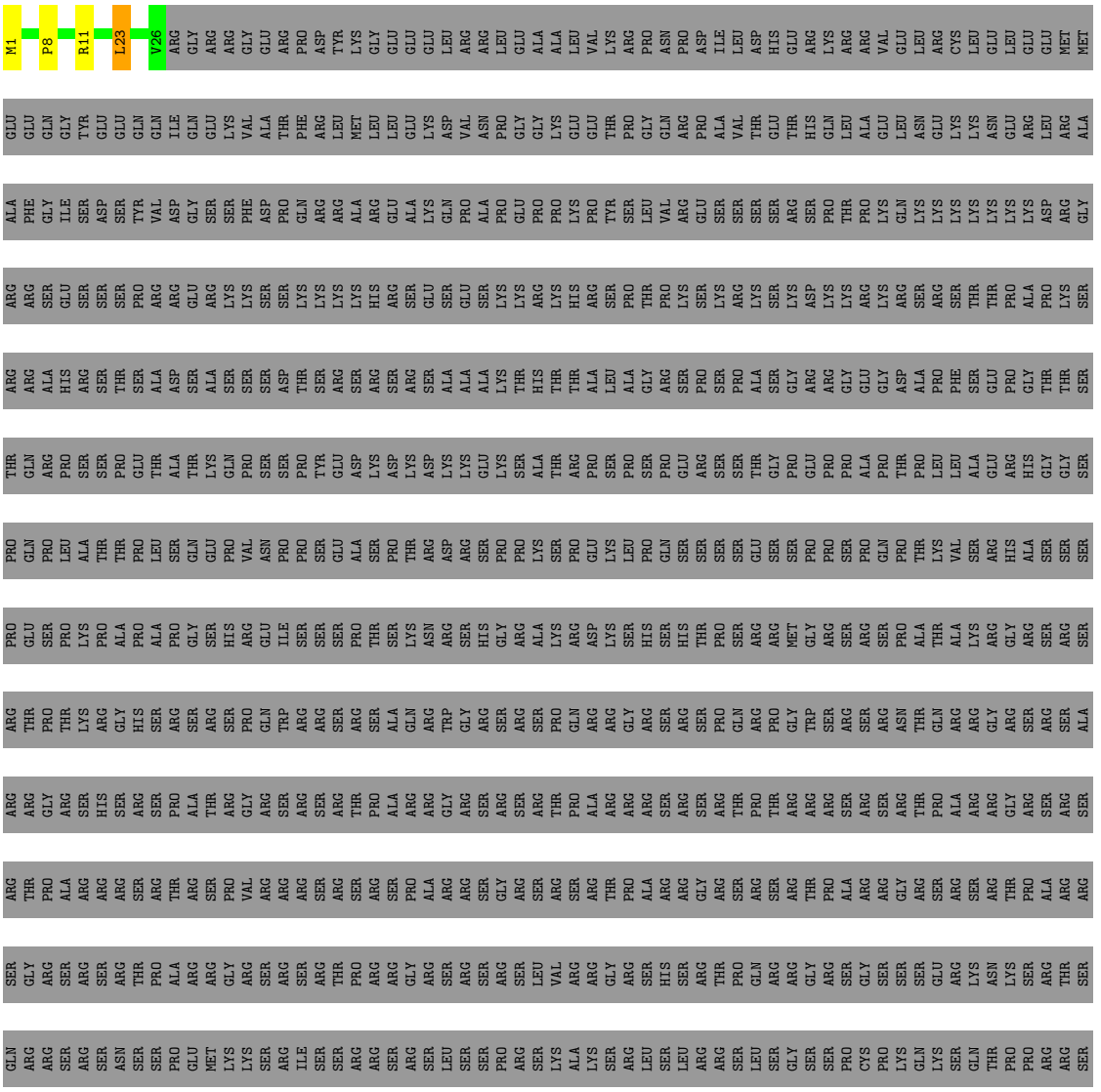
Chain T:

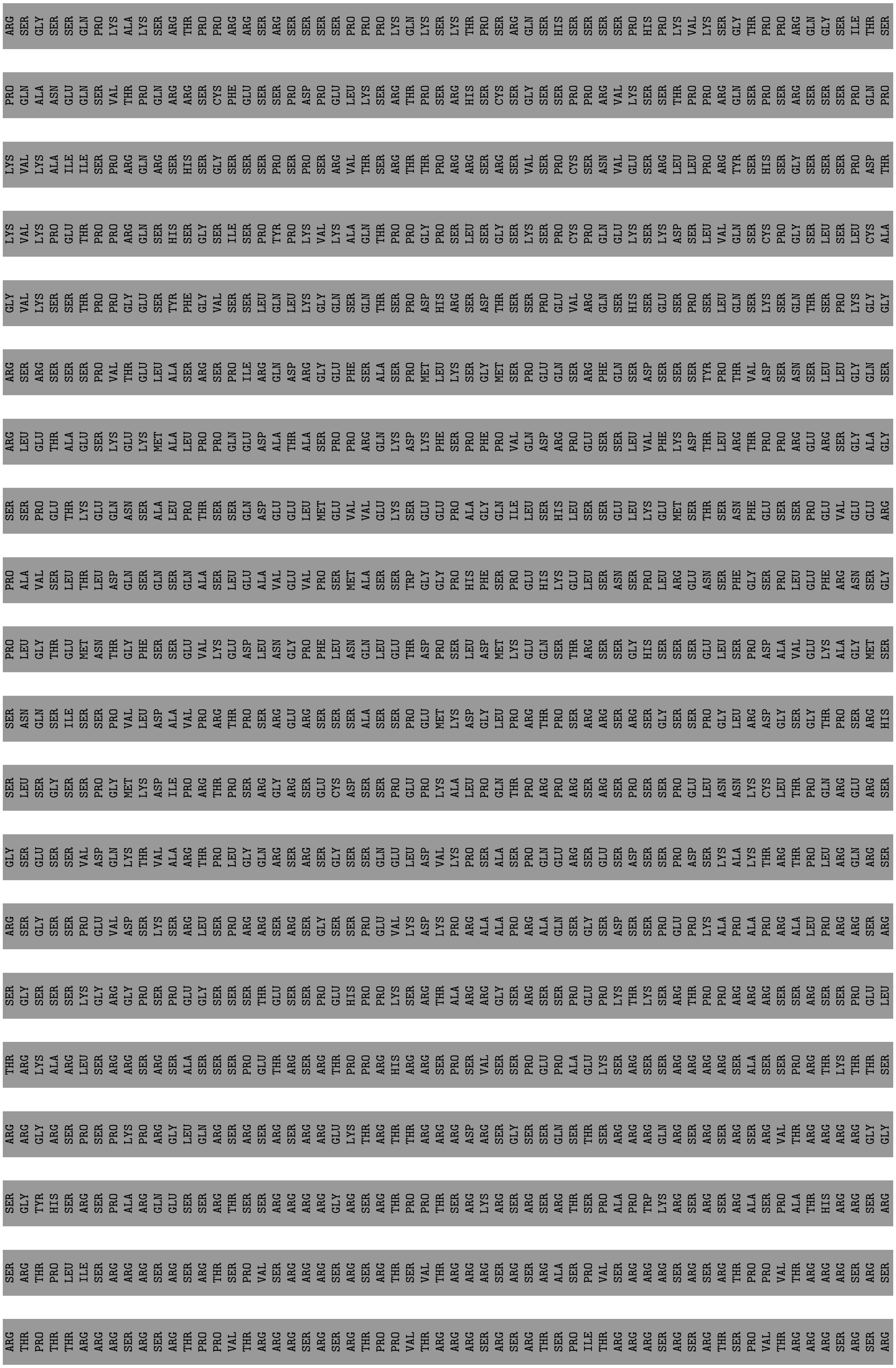


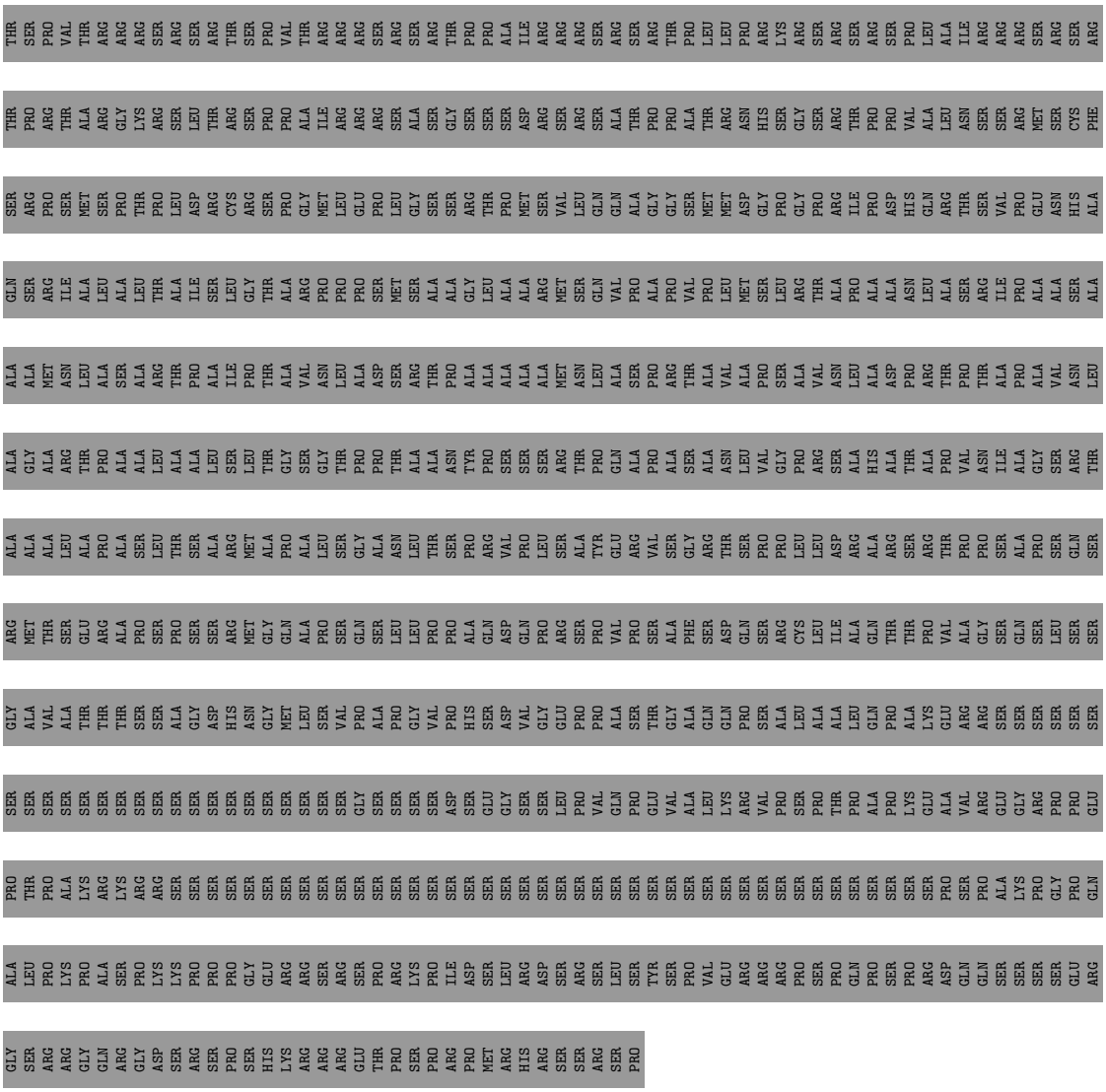


• Molecule 21: Serine/arginine repetitive matrix protein 2

Chain U: 99%

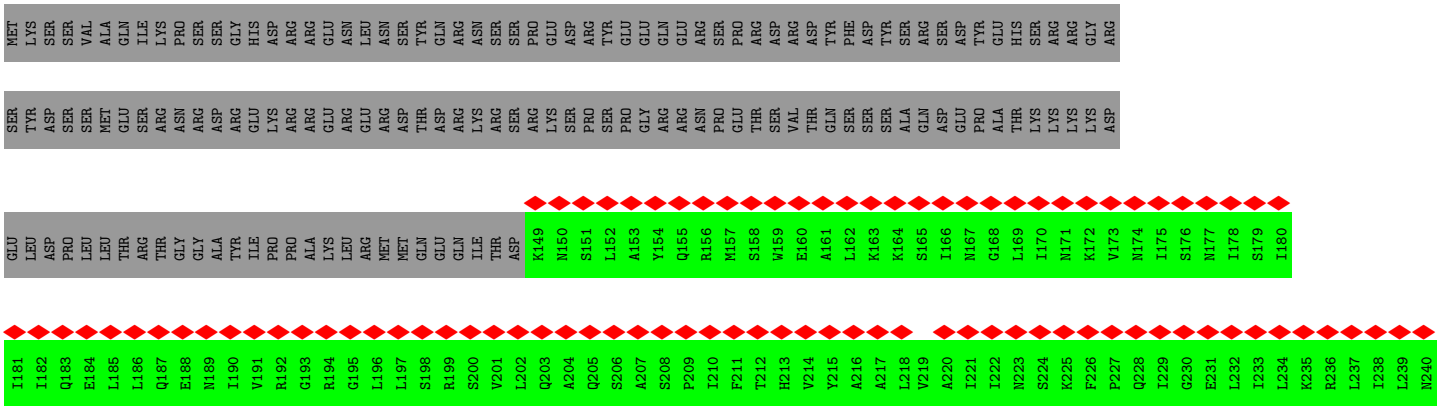


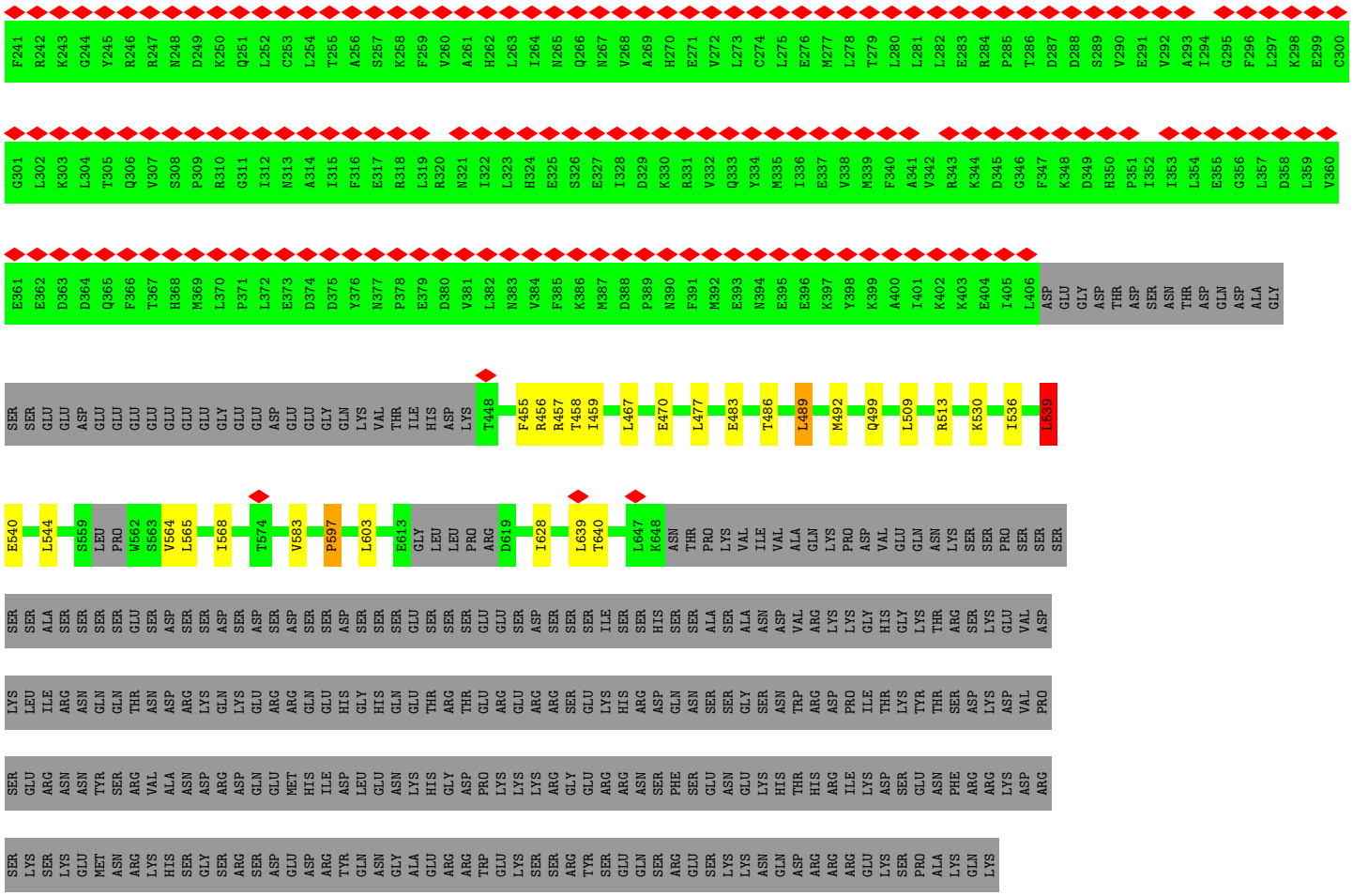

ARG SER GLY SER SER GLN PRO LYS ALA LYS SER ARG THR PRO PRO ARG ARG SER ARG SER SER SER SER PRO PRO PRO LYS GLN LYS SER LYS THR PRO SER ARG GLN SER HIS SER SER SER SER PRO HIS PRO LYS VAL LYS SER GLY THR PRO PRO ARG GLN GLY SER ILE THR SER
PRO GLN ALA ASN GLU GLN SER VAL THR PRO GLN ARG ARG SER CYS PHE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



• Molecule 22: Pre-mRNA-splicing factor CWC22 homolog

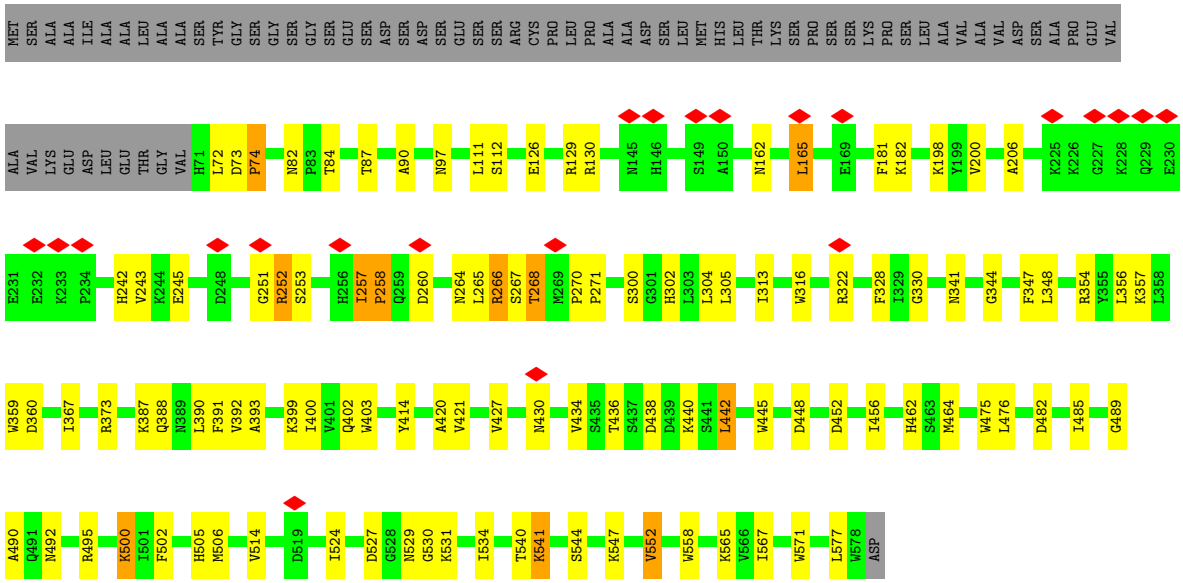
Chain V:





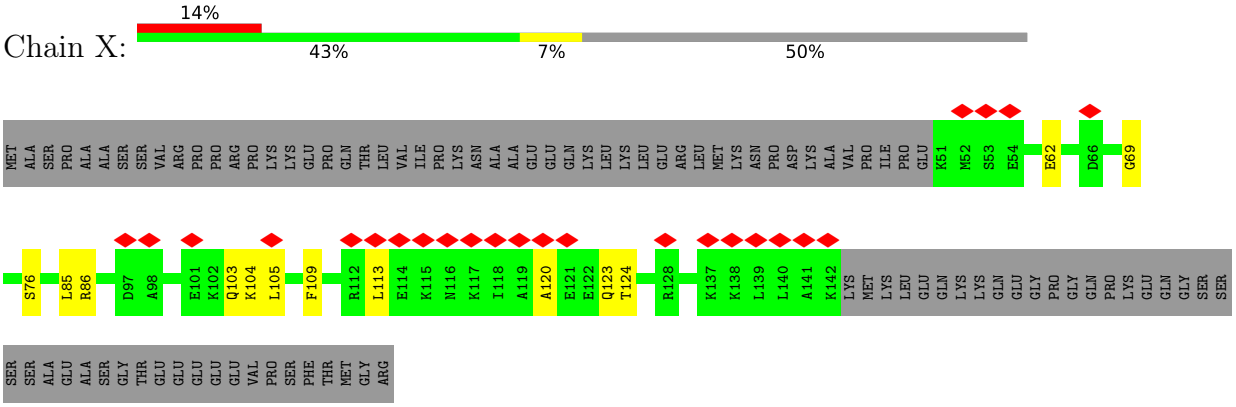
• Molecule 23: Pre-mRNA-processing factor 17

Chain W:



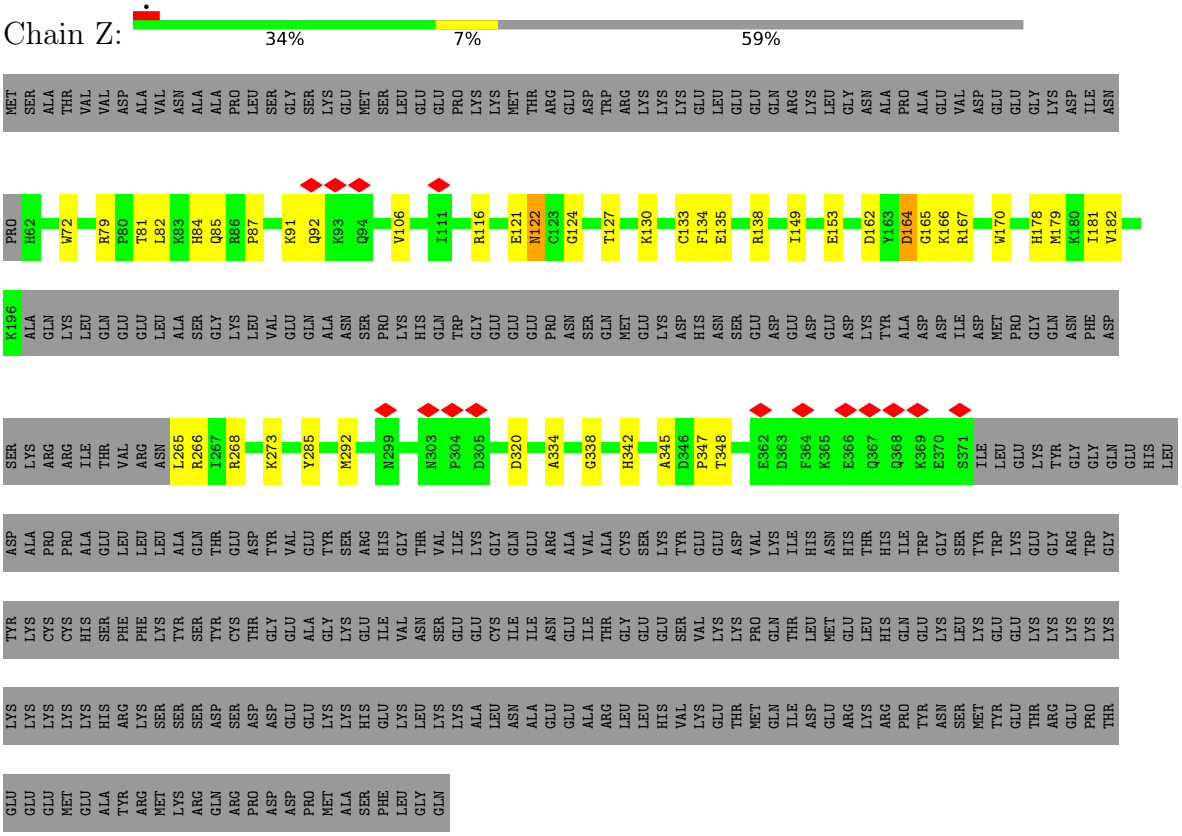
• Molecule 24: PRKR-interacting protein 1

Chain X:



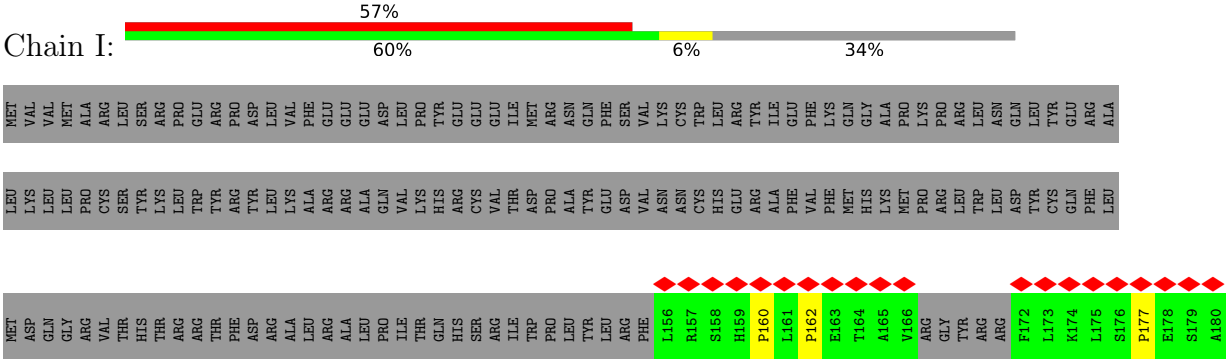
• Molecule 25: Pre-mRNA-splicing factor SLU7

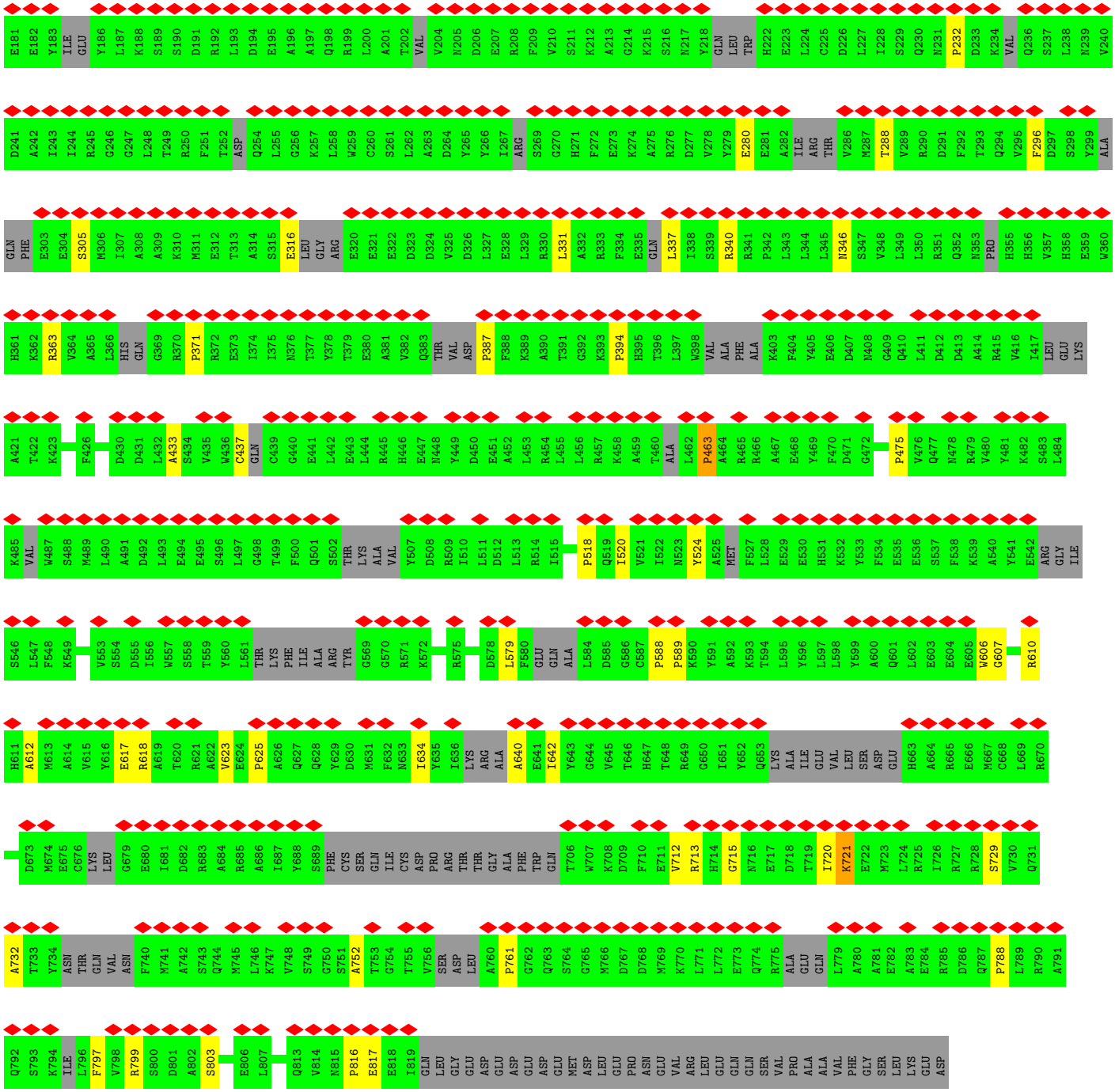
Chain Z:



• Molecule 26: Pre-mRNA-splicing factor SYF1

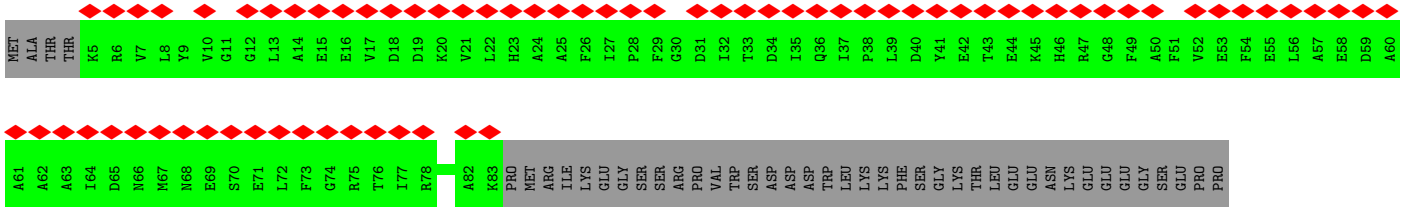
Chain I:

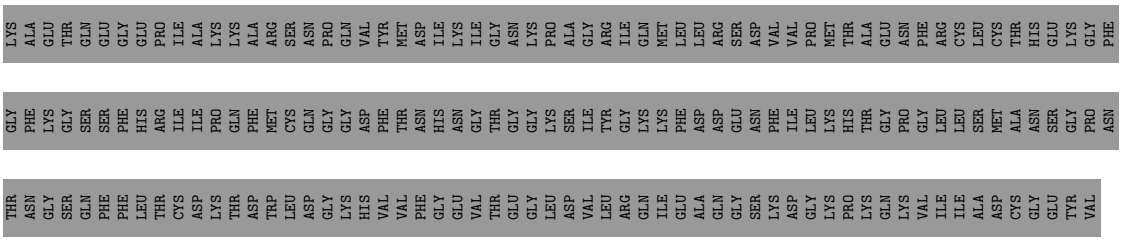




• Molecule 27: Peptidyl-prolyl cis-trans isomerase E

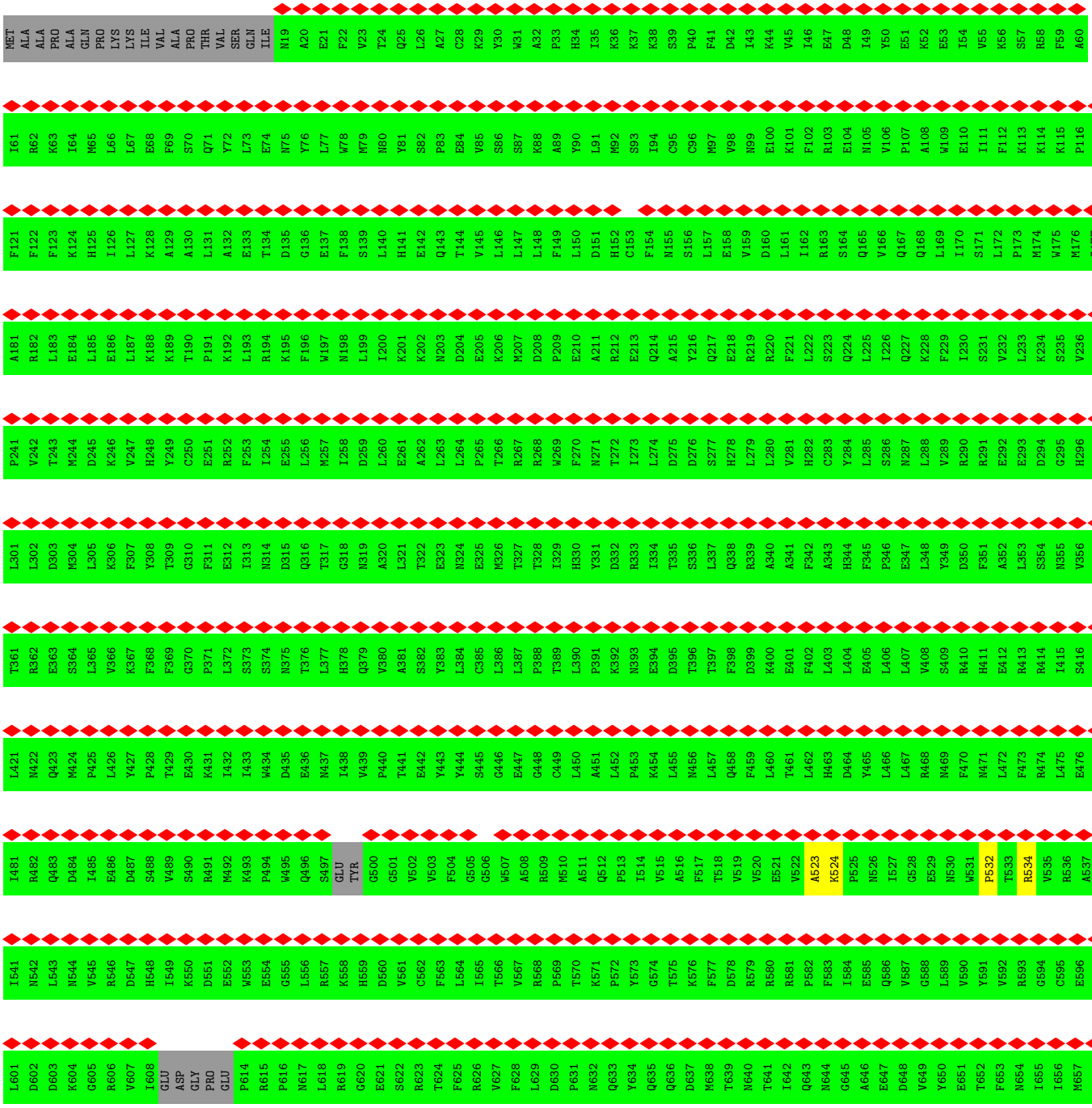
Chain y:

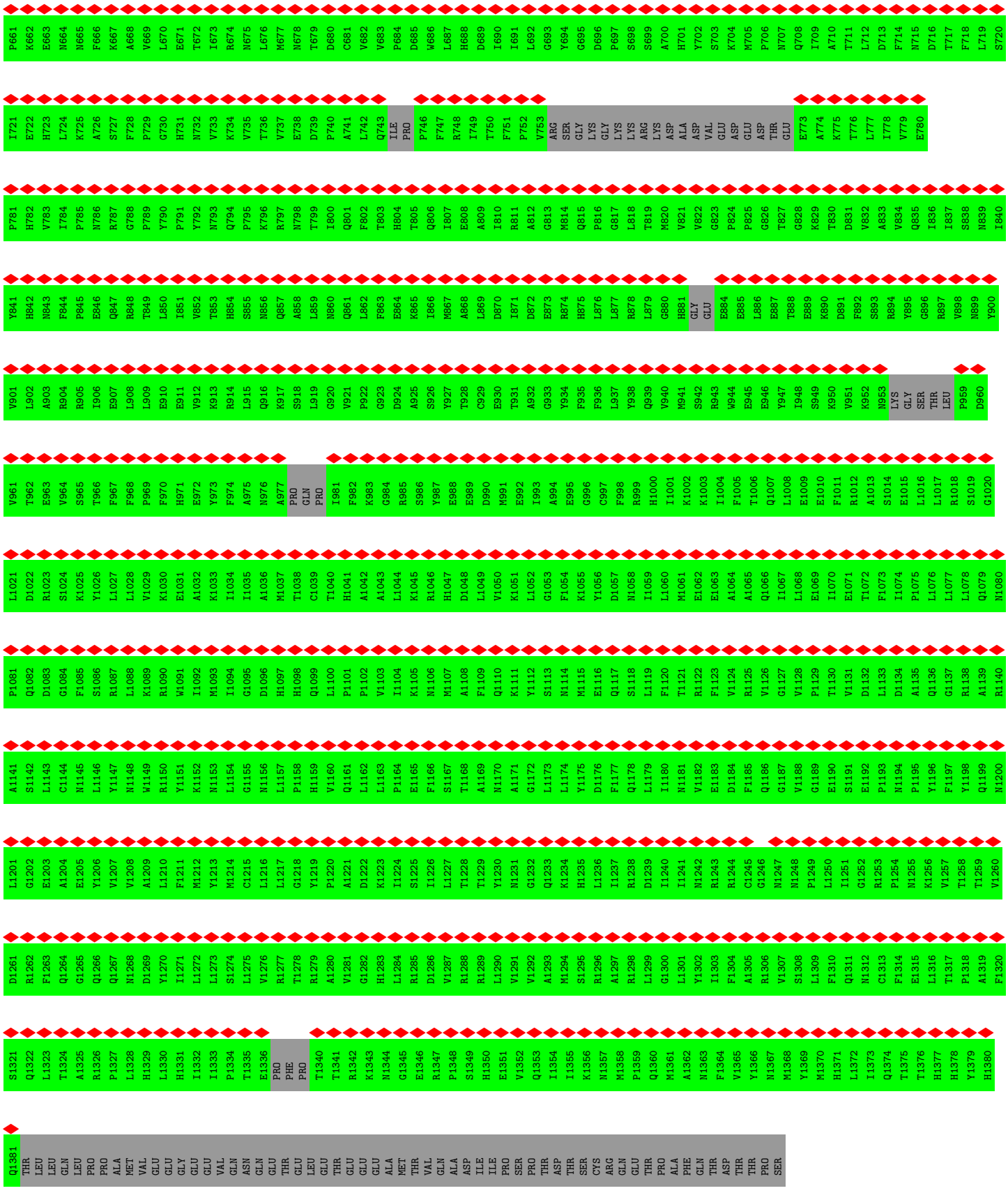


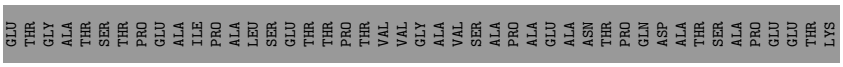


• Molecule 28: RNA helicase aquarius

Chain Q:

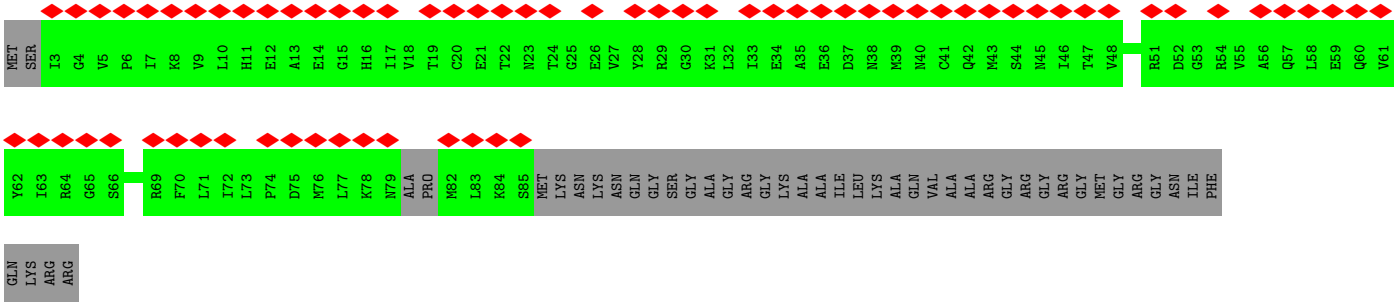



P661 K662 E663 N664 N665 F666 K667 A668 V669 L670 E671 T672 I673 R674 N675 L676 M677 N678 T679 D680 C681 V682 V683 P684 D685 W686 L687 H688 D689 I690 I691 L692 G693 Y694 G695 D696 P697 S698 S699 A700 H701 Y702 S703 K704 M705 P706 N707 Q708 I709 A710 T711 L712 D713 F714 N715 D716 T717 F718 L719 S720
I721 E722 H723 L724 K725 A726 S727 F728 P729 G730 H731 N732 V733 K734 V735 T736 V737 E738 D739 P740 A741 L742 Q743 ILE PRO P746 F747 R748 I749 T750 F751 P752 V753 ARG SER GLY LYS GLY LYS LYS ARG LYS ASP ALA ASP VAL GLU ASP GLU ASP THR GLU E773 A774 K775 T776 L777 I778 V779 E780
P781 H782 V783 I784 P785 N786 R787 G788 P789 Y790 P791 Y792 N793 Q794 P795 K796 R797 N798 T799 I800 Q801 F802 T803 H804 T805 Q806 I807 E808 A809 I810 R811 A812 G813 M814 Q815 P816 G817 L818 T819 M820 V821 V822 G823 P824 P825 G826 T827 G828 K829 T830 D831 V832 A833 V834 Q835 I836 I837 S838 N839 I840
Y841 H842 N843 F844 P845 E846 Q847 R848 T849 L850 I851 V852 T853 H854 S855 N856 Q857 A858 L859 N860 Q861 L862 F863 E864 K865 I866 M867 A868 L869 D870 I871 D872 E873 R874 H875 L876 L877 R878 L879 G880 H881 GLY GLU E884 E885 L886 E887 T888 E889 K890 D891 F892 S893 R894 Y895 G896 R897 V898 N899 Y900
V901 L902 A903 R904 R905 I906 E907 L908 L909 E910 E911 V912 K913 R914 L915 Q916 K917 S918 L919 G920 V921 P922 G923 D924 A925 S926 Y927 T928 C929 E930 T931 A932 G933 Y934 F935 F936 L937 Y938 Q939 V940 M941 S942 R943 W944 E945 E946 Y947 I948 S949 K950 V951 K952 N953 LYS GLY SER THR LEU P959 D960
V961 T962 E963 V964 S965 T966 F967 F968 P969 F970 H971 E972 Y973 F974 A975 N976 A977 PRO GLN PRO I981 P982 K983 G984 R985 S986 Y987 E988 E989 D990 M991 E992 I993 A994 E995 G996 C997 F998 R999 H1000 I1001 K1002 K1003 I1004 F1005 T1006 Q1007 L1008 E1009 E1010 F1011 R1012 A1013 S1014 E1015 L1016 L1017 R1018 S1019 G1020
L1021 D1022 R1023 S1024 K1025 Y1026 L1027 L1028 V1029 K1030 E1031 A1032 K1033 I1034 I1035 A1036 M1037 T1038 C1039 T1040 H1041 A1042 A1043 L1044 K1045 R1046 H1047 D1048 L1049 V1050 K1051 L1052 G1053 F1054 K1055 Y1056 D1057 N1058 I1059 L1060 M1061 E1062 E1063 A1064 A1065 Q1066 I1067 L1068 E1069 I1070 E1071 T1072 F1073 I1074 P1075 L1076 L1077 L1078 Q1079 N1080
P1081 Q1082 D1083 G1084 F1085 S1086 R1087 L1088 K1089 R1090 W1091 I1092 M1093 I1094 G1095 D1096 H1097 H1098 Q1099 L1100 P1101 P1102 V1103 I1104 K1105 N1106 M1107 A1108 F1109 Q1110 K1111 Y1112 S1113 N1114 M1115 E1116 Q1117 S1118 L1119 F1120 I1121 R1122 F1123 V1124 R1125 V1126 Q1127 V1128 P1129 T1130 V1131 D1132 L1133 D1134 A1135 Q1136 G1137 R1138 A1139 R1140
A1141 S1142 L1143 C1144 N1145 L1146 Y1147 N1148 W1149 R1150 Y1151 K1152 N1153 L1154 G1155 N1156 L1157 P1158 H1159 V1160 Q1161 L1162 L1163 P1164 E1165 F1166 S1167 T1168 A1169 N1170 A1171 G1172 L1173 L1174 Y1175 D1176 F1177 Q1178 L1179 I1180 N1181 V1182 E1183 D1184 F1185 Q1186 G1187 V1188 G1189 E1190 S1191 E1192 P1193 N1194 P1195 Y1196 F1197 Y1198 Q1199 N1200
L1201 G1202 E1203 A1204 E1205 Y1206 V1207 V1208 A1209 L1210 F1211 M1212 Y1213 M1214 C1215 L1216 L1217 G1218 Y1219 P1220 A1221 D1222 K1223 I1224 S1225 I1226 L1227 T1228 T1229 Y1230 N1231 G1232 Q1233 K1234 H1235 L1236 I1237 R1238 D1239 I1240 I1241 N1242 R1243 R1244 C1245 G1246 N1247 N1248 P1249 L1250 I1251 G1252 R1253 P1254 N1255 K1256 V1257 T1258 T1259 V1260
D1261 R1262 F1263 Q1264 G1265 Q1266 Q1267 N1268 D1269 Y1270 I1271 I1272 L1273 S1274 L1275 V1276 R1277 T1278 R1279 A1280 V1281 G1282 H1283 L1284 R1285 D1286 V1287 R1288 R1289 L1290 V1291 V1292 A1293 M1294 S1295 R1296 A1297 R1298 L1299 G1300 L1301 Y1302 I1303 F1304 A1305 R1306 V1307 S1308 L1309 F1310 Q1311 N1312 C1313 F1314 E1315 L1316 T1317 P1318 A1319 F1320
S1321 Q1322 L1323 T1324 A1325 R1326 P1327 L1328 H1329 L1330 H1331 I1332 I1333 P1334 T1335 E1336 PRO PHE PRO T1340 T1341 R1342 K1343 N1344 G1345 E1346 R1347 P1348 S1349 H1350 E1351 V1352 Q1353 I1354 I1355 K1356 N1357 M1358 P1359 Q1360 M1361 A1362 N1363 F1364 V1365 Y1366 N1367 M1368 Y1369 M1370 H1371 L1372 I1373 Q1374 T1375 T1376 H1377 H1378 Y1379 H1380
Q1381 THR LEU LEU GLN LEU PRO PRO ALA MET VAL GLU GLU GLY GLU GLU VAL GLN ASN GLN GLU THR GLU LEU GLU THR GLU GLU GLU ALA MET THR VAL GLN ALA ASP ILE ILE PRO SER PRO THR ASP THR SER CYS ARG GLN GLU THR PRO ALA PHE GLN THR ASP THR THR PRO SER



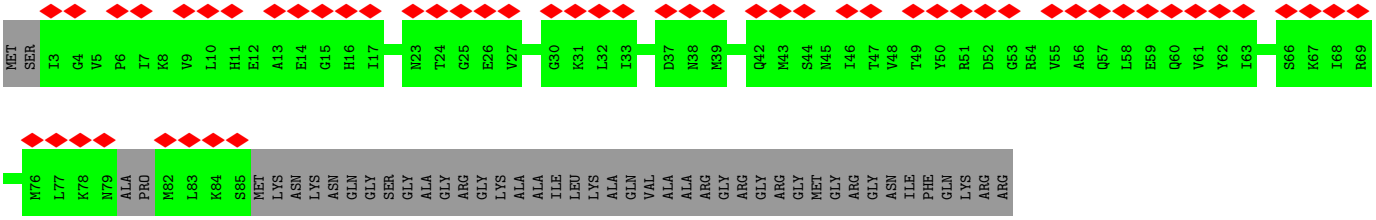
• Molecule 29: Small nuclear ribonucleoprotein Sm D3

Chain h:



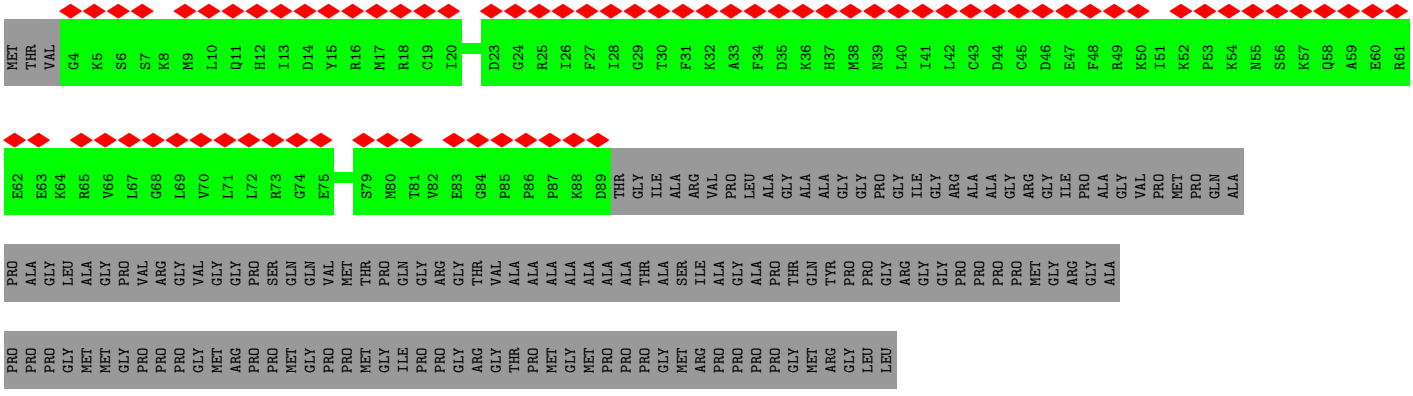
• Molecule 29: Small nuclear ribonucleoprotein Sm D3

Chain a:



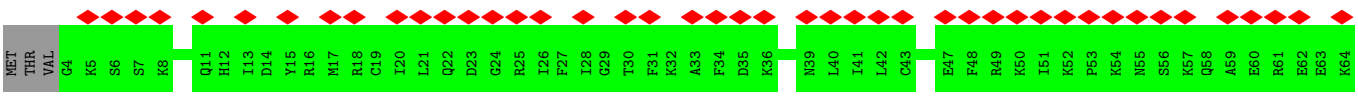
• Molecule 30: Small nuclear ribonucleoprotein-associated protein

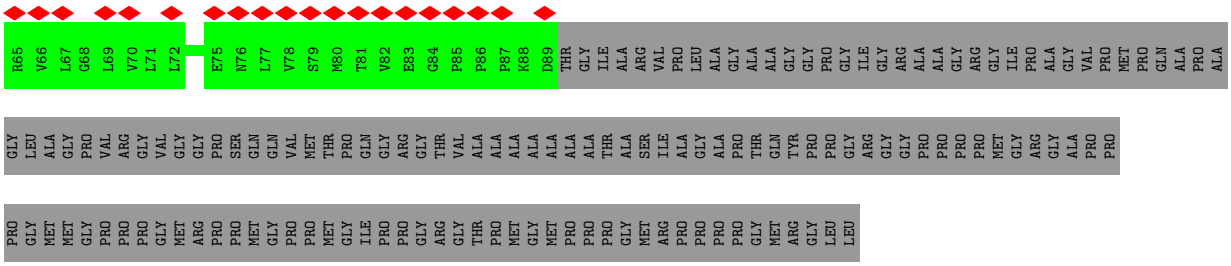
Chain i:



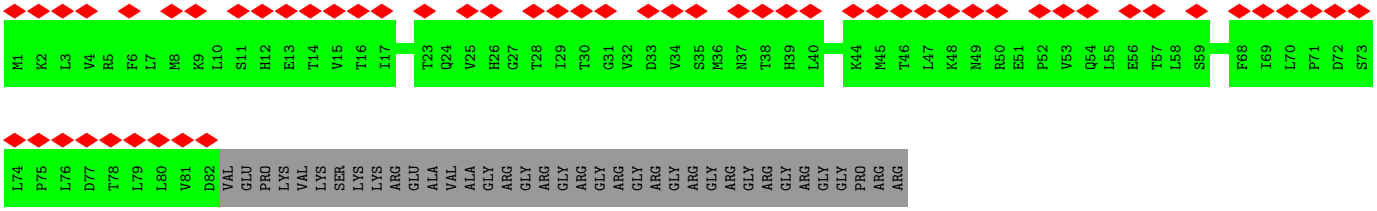
• Molecule 30: Small nuclear ribonucleoprotein-associated protein

Chain b:

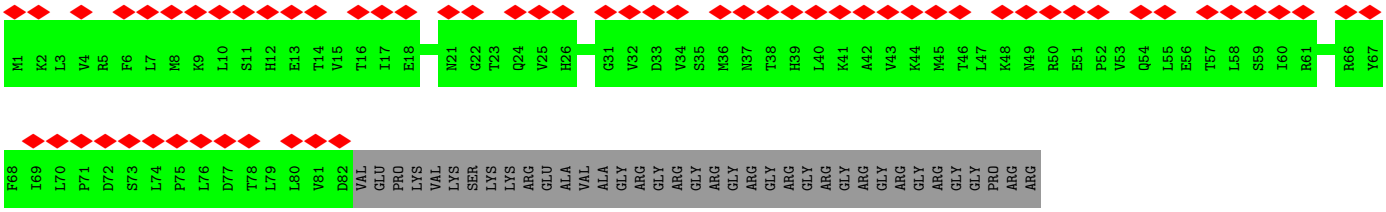




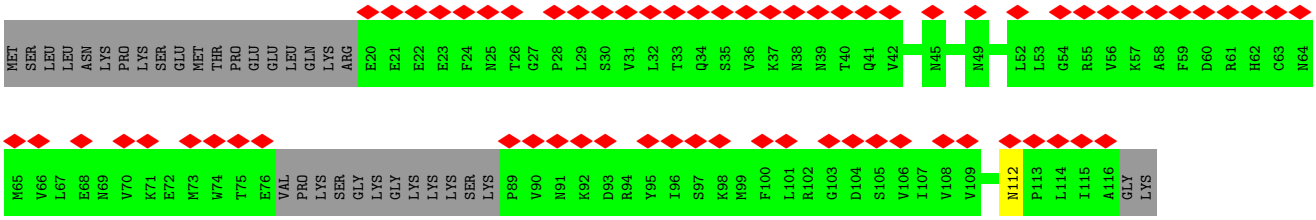
• Molecule 31: Small nuclear ribonucleoprotein Sm D1



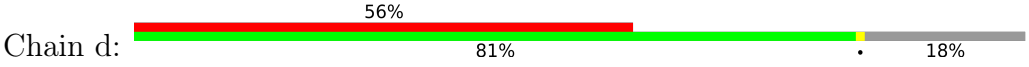
• Molecule 31: Small nuclear ribonucleoprotein Sm D1

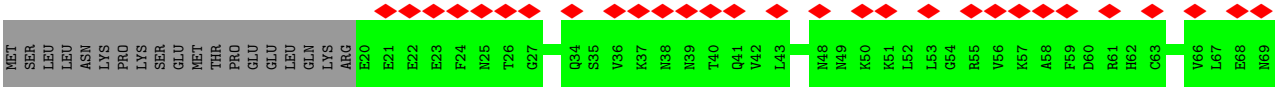


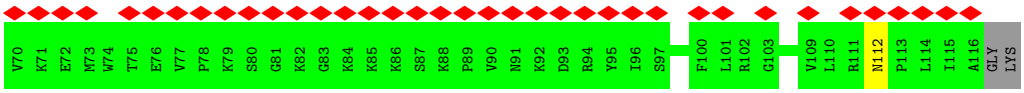
• Molecule 32: Small nuclear ribonucleoprotein Sm D2



• Molecule 32: Small nuclear ribonucleoprotein Sm D2

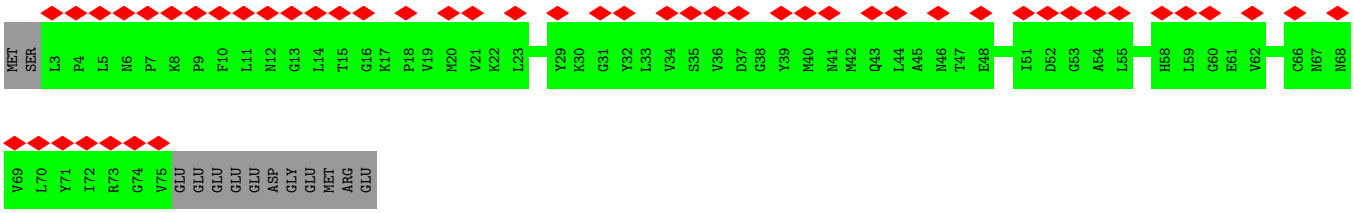






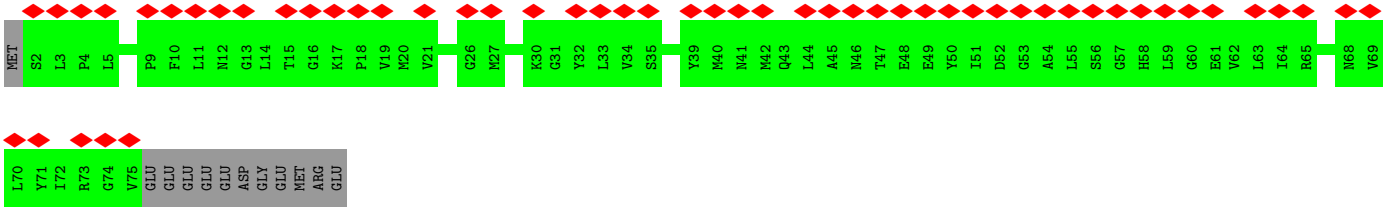
• Molecule 33: Small nuclear ribonucleoprotein F

Chain m:



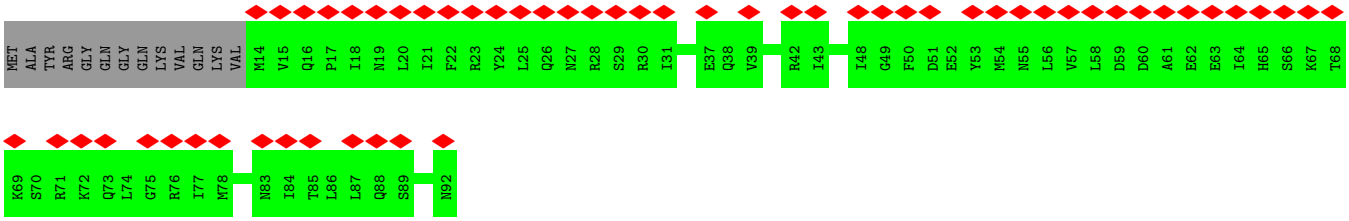
• Molecule 33: Small nuclear ribonucleoprotein F

Chain f:



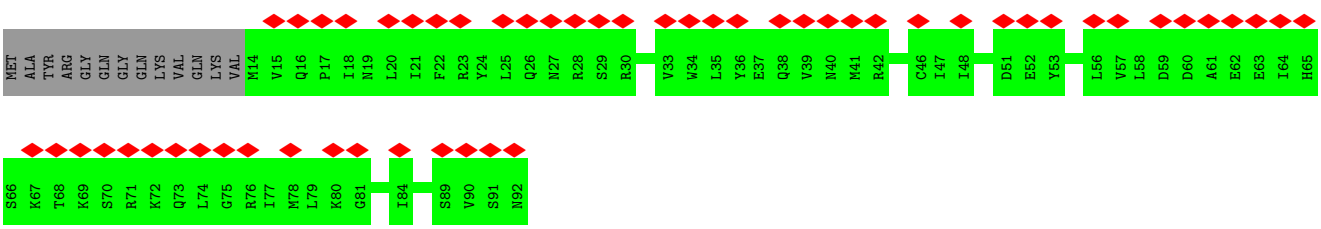
• Molecule 34: Small nuclear ribonucleoprotein E

Chain l:



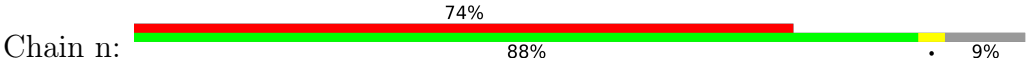
• Molecule 34: Small nuclear ribonucleoprotein E

Chain e:



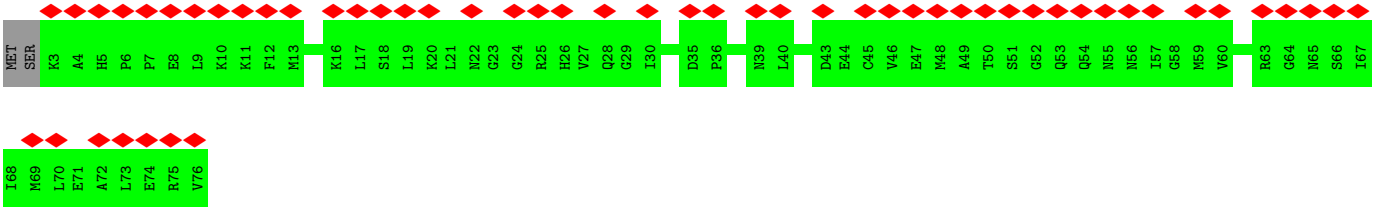
• Molecule 35: Small nuclear ribonucleoprotein G

Chain n:



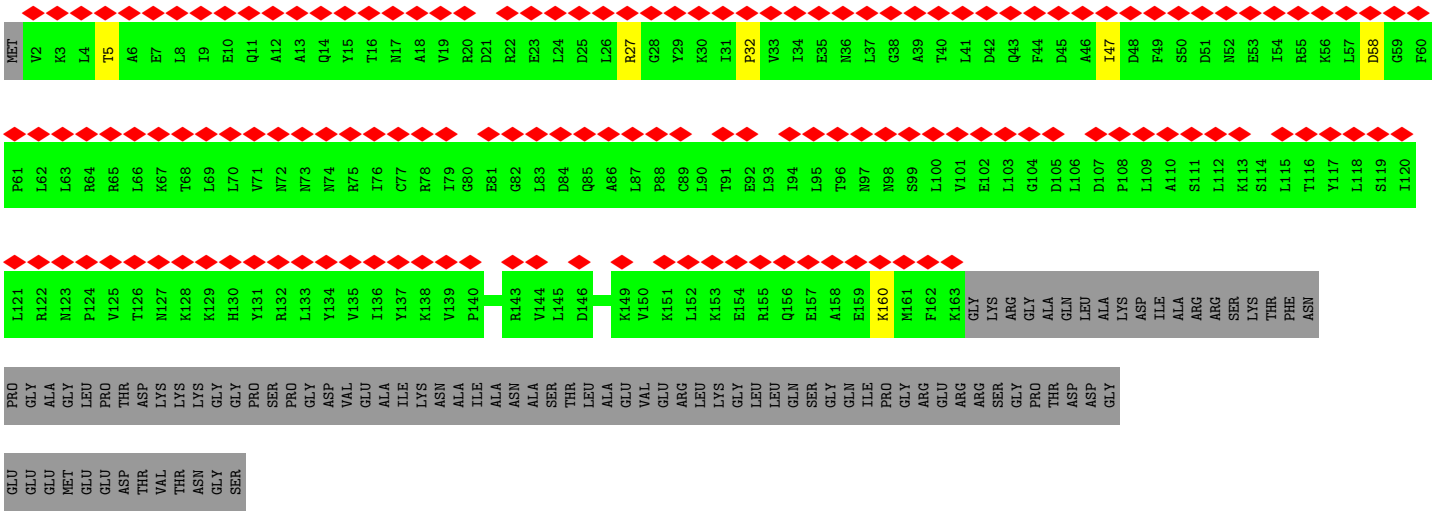
• Molecule 35: Small nuclear ribonucleoprotein G

Chain g:



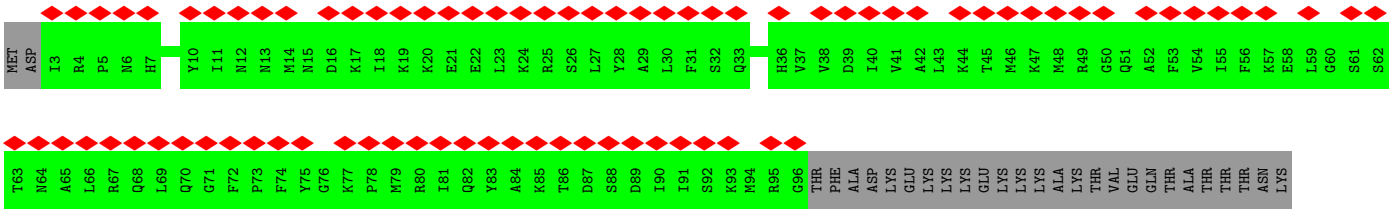
• Molecule 36: U2 small nuclear ribonucleoprotein A'

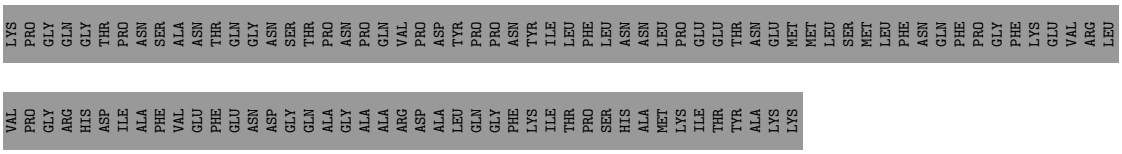
Chain o:



• Molecule 37: U2 small nuclear ribonucleoprotein B"

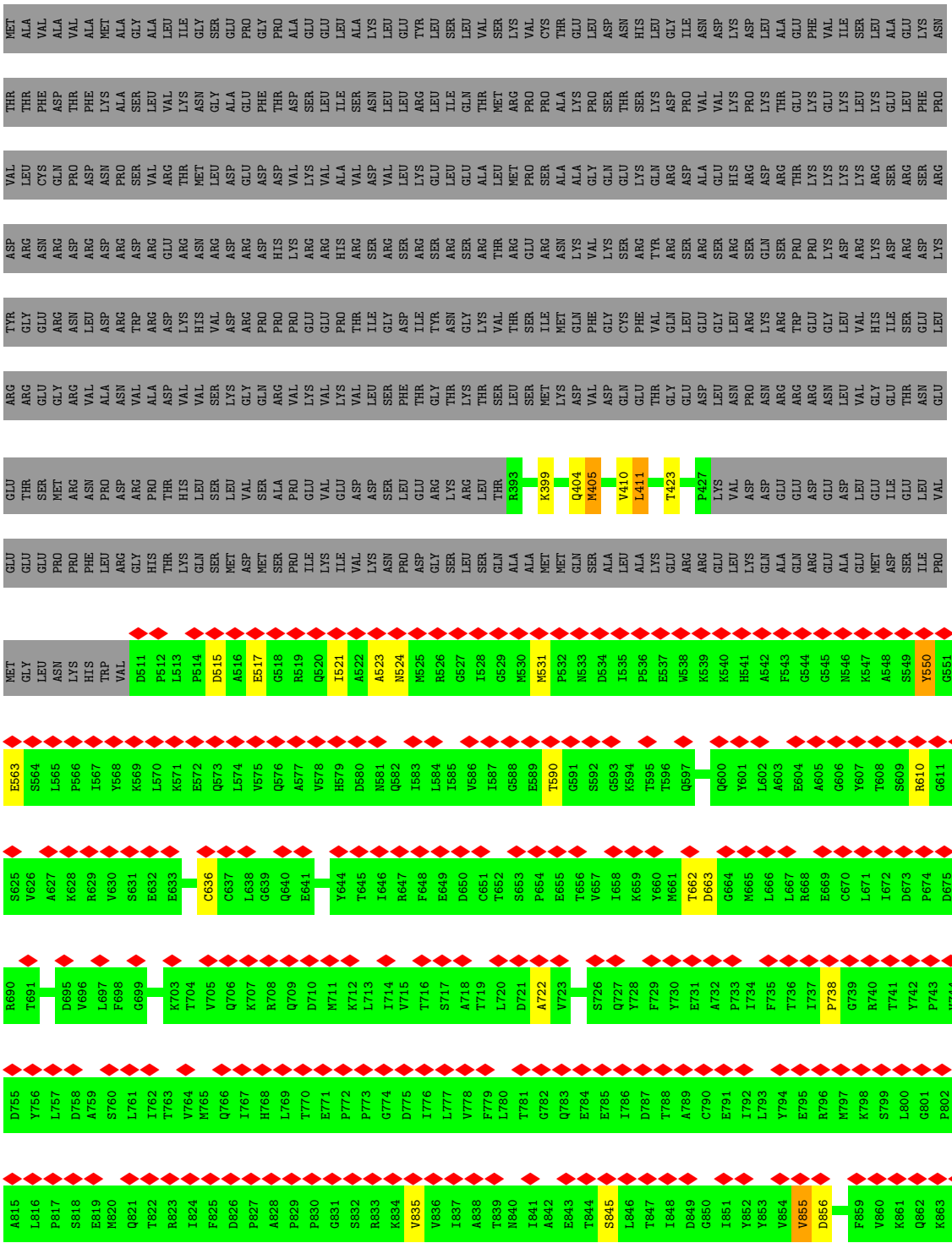
Chain p:

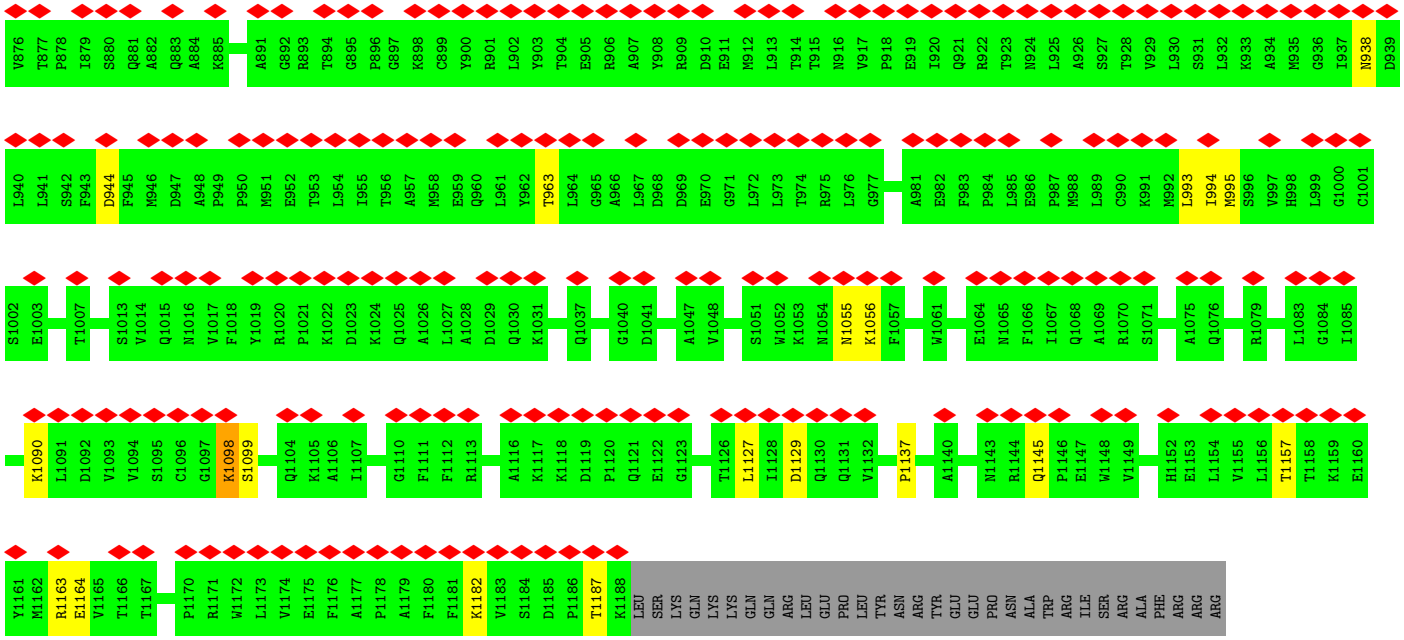




• Molecule 38: ATP-dependent RNA helicase DHX8

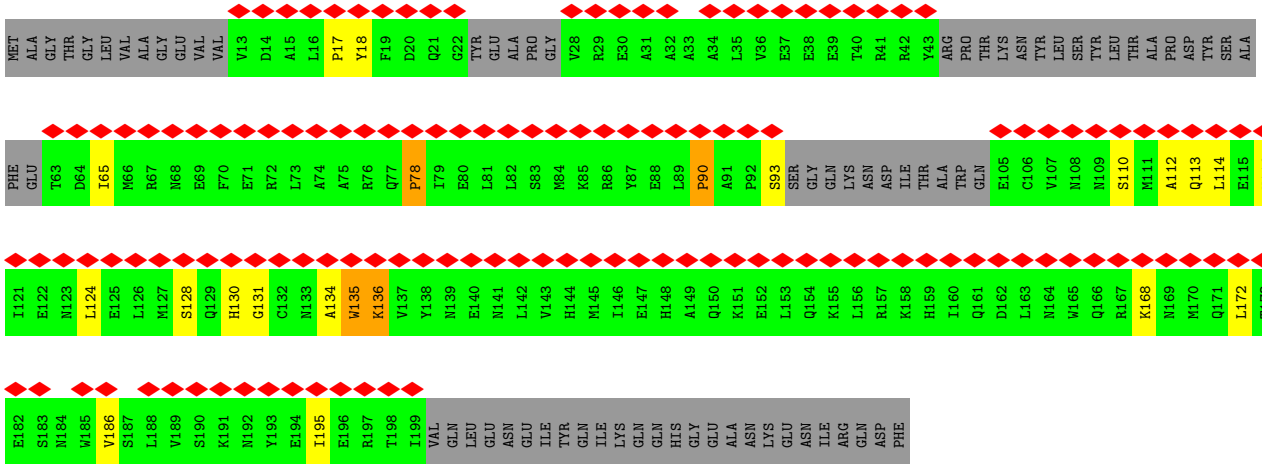
Chain Y:





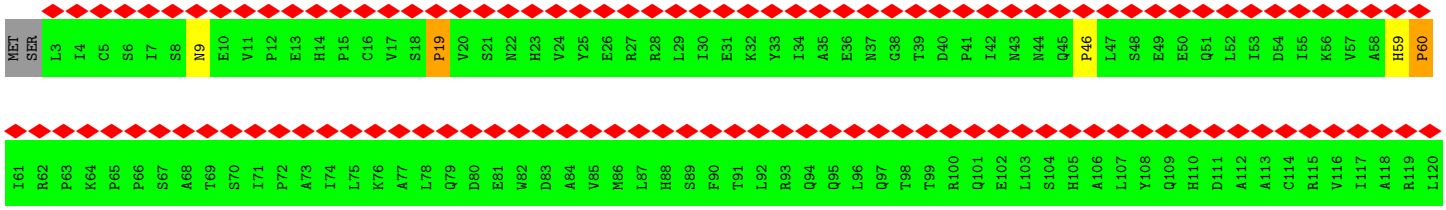
• Molecule 39: Pre-mRNA-splicing factor SPF27

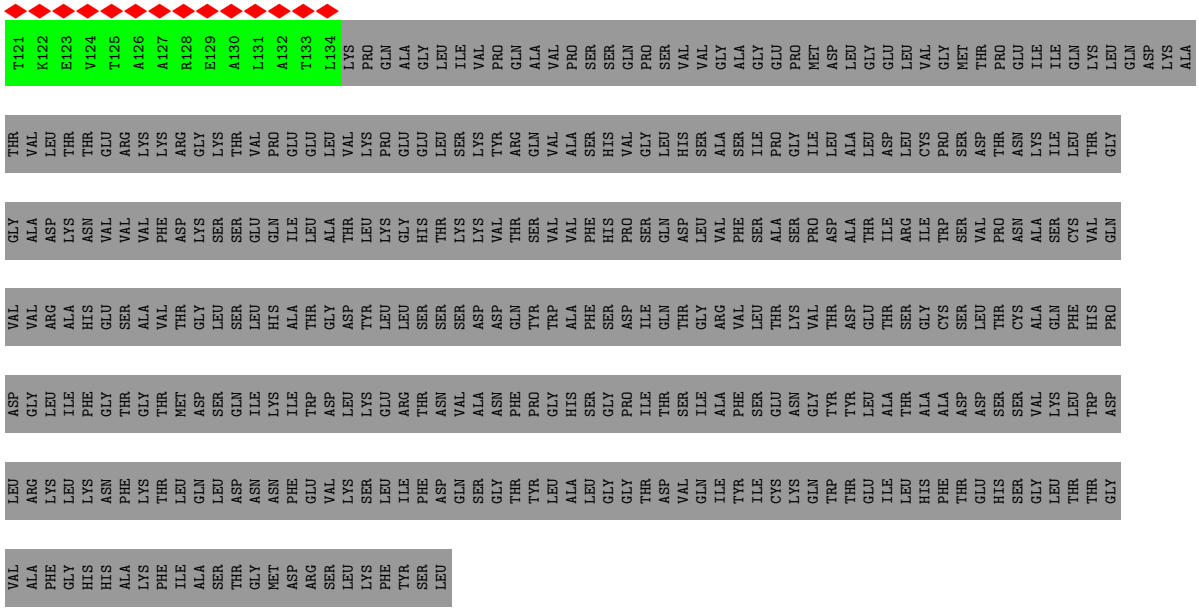
Chain K:



• Molecule 40: Pre-mRNA-processing factor 19

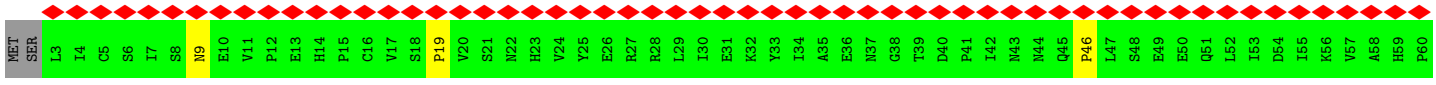
Chain q:

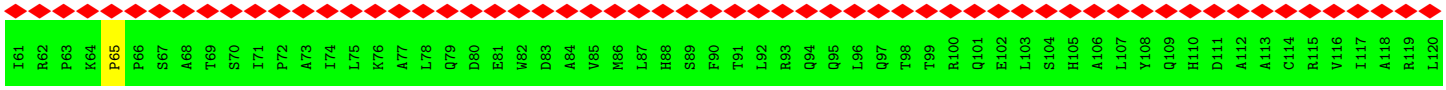


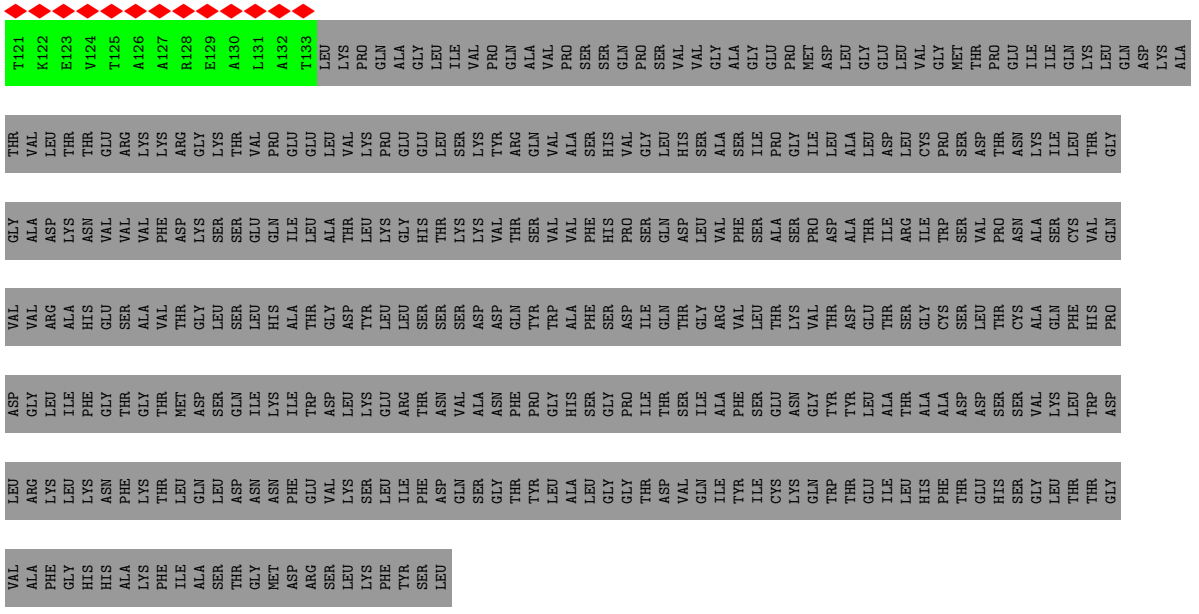


• Molecule 40: Pre-mRNA-processing factor 19

Chain r:

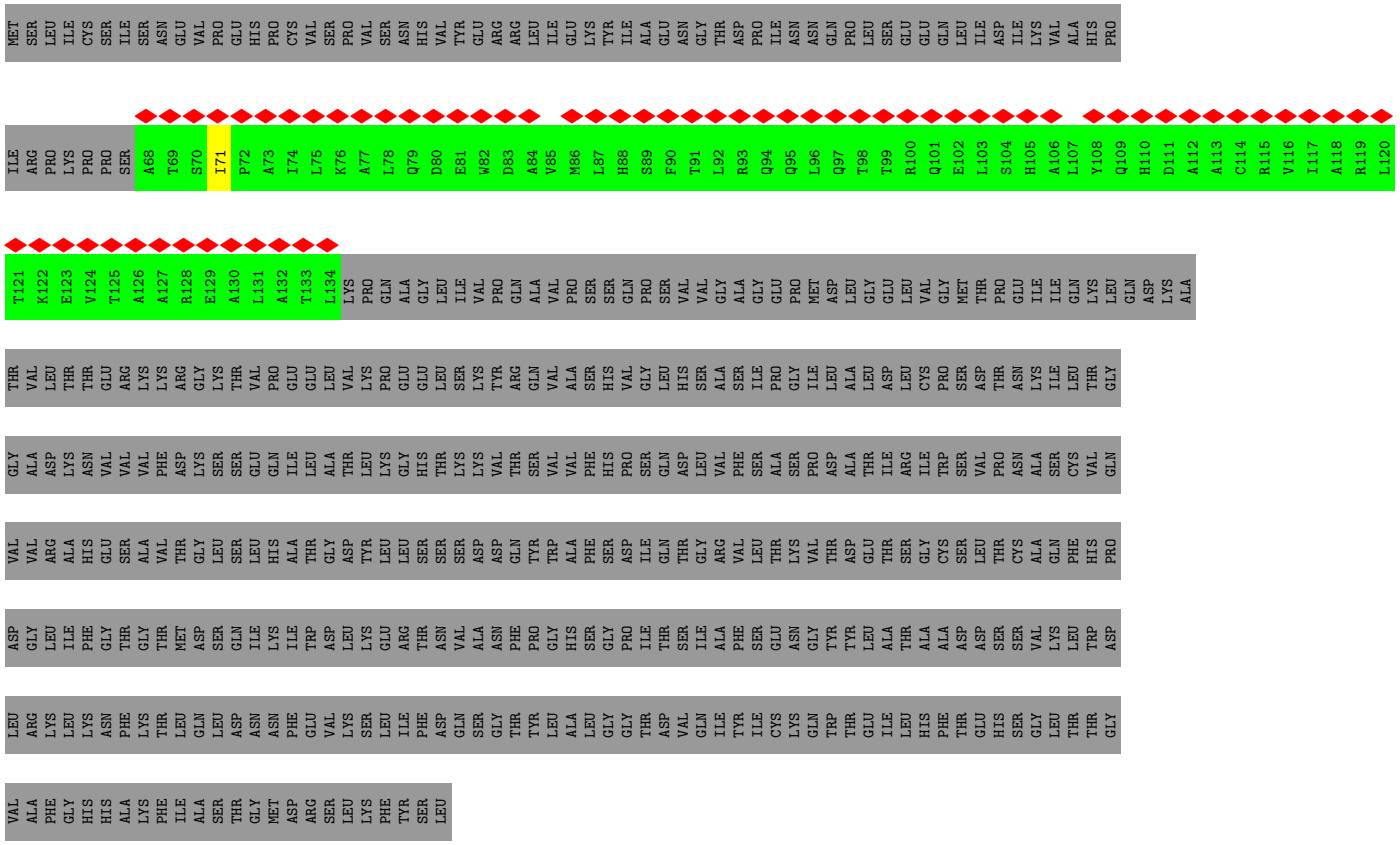






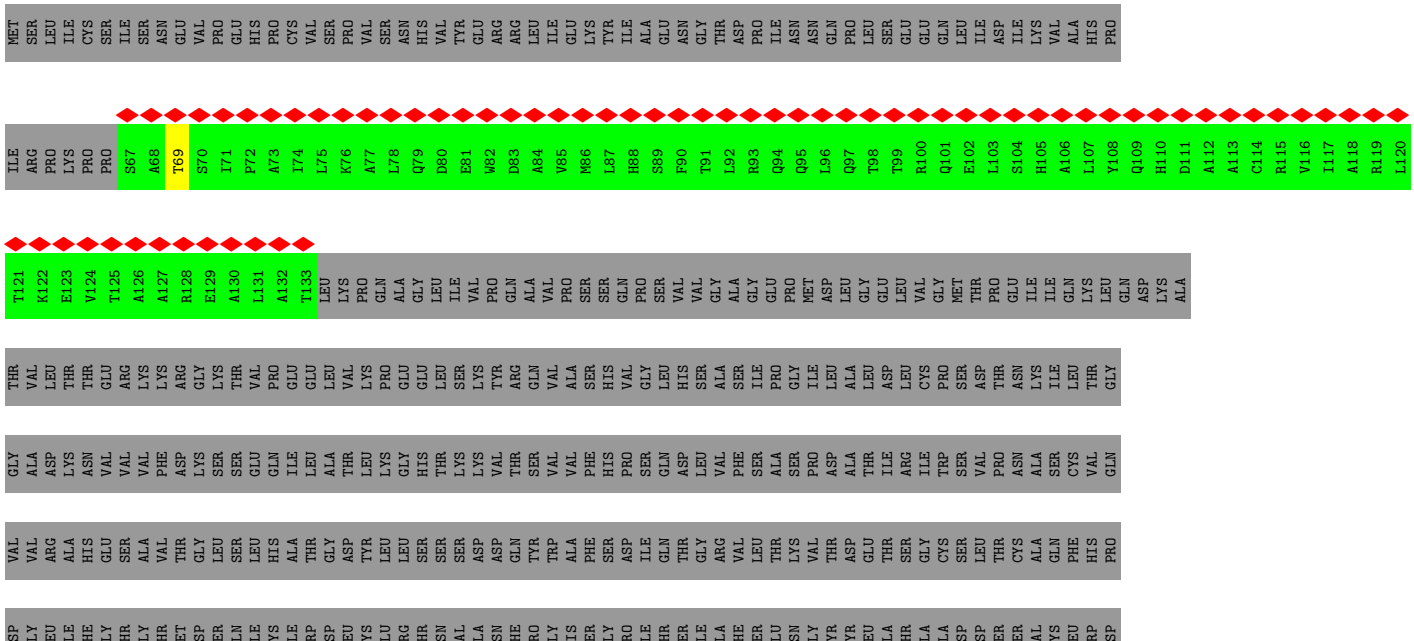
• Molecule 40: Pre-mRNA-processing factor 19

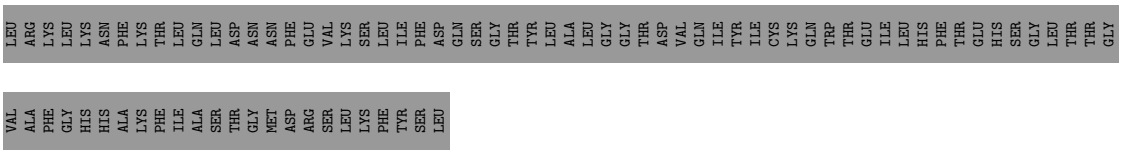
Chain s:



• Molecule 40: Pre-mRNA-processing factor 19

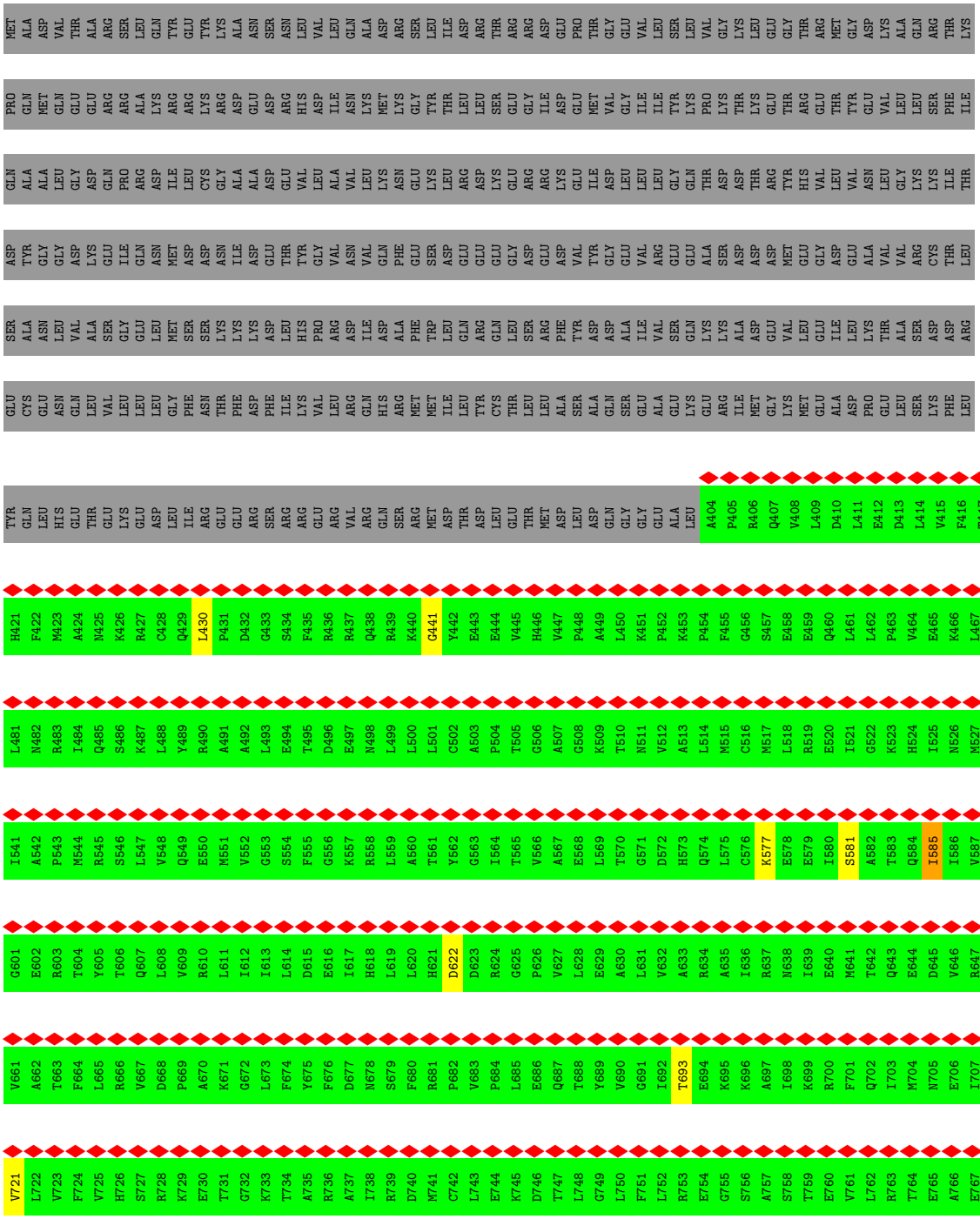
Chain t:



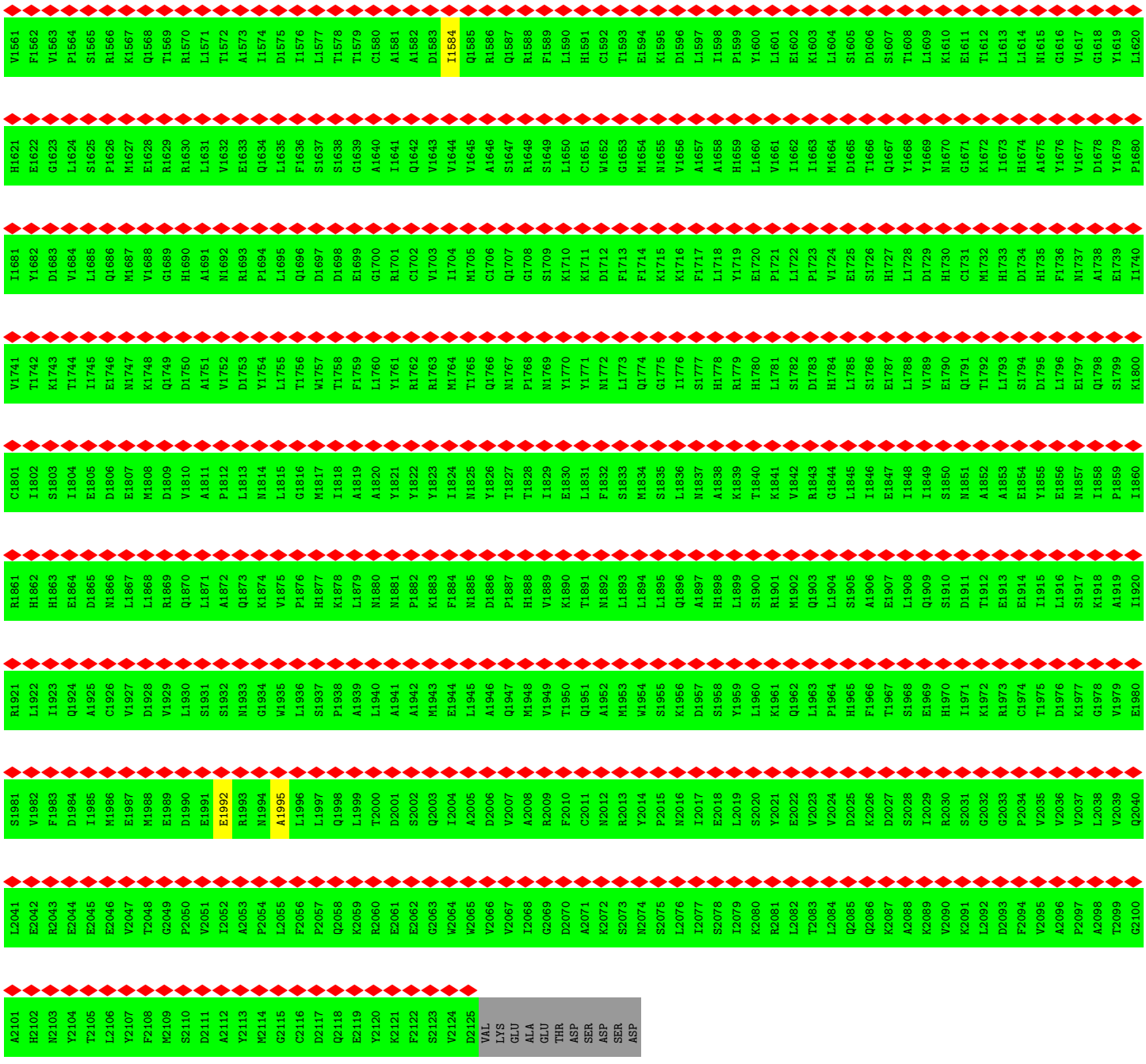


• Molecule 41: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain D:



G781 F782 A783 I784 H785 H786 A787 G788 M789 T790 R791 V792 D793 R794 T795 L796 V797 E798 D799 L800 F801 A802 D803 K804 H805 I806 Q807 V808 L809 V810 S811 T812 A813 T814 L815 A816 W817 G818 V819 N820 L821 P822 A823 H824 T825 V826 I827 I828 K829 G830 T831 Q832 V833 Y834 S835 P836 E837 K838 G839 R840
W841 T842 E843 L844 G845 A846 L847 D848 I849 L850 Q851 M852 L853 G854 R855 A856 G857 R858 P859 D860 Y861 D862 T863 K864 G865 E866 G867 I868 L869 I870 T871 S872 H873 G874 E875 L876 Q877 Y878 Y879 L880 S881 L882 L883 N884 Q885 Q886 L887 P888 I889 E890 S891 Q892 M893 V894 S895 K896 L897 P898 D899 M900
L901 N902 A903 E904 I905 V906 L907 G908 N909 V910 Q911 N912 A913 K914 D915 A916 V917 N918 W919 L920 G921 Y922 A923 Y924 L925 Y926 I927 R928 M929 L930 R931 S932 P933 T934 L935 Y936 G937 I938 S939 H940 D941 D942 L943 K944 G945 D946 P947 L948 L949 D950 Q951 R952 R953 L954 D955 L956 V957 H958 T959 A960
A961 L962 N963 L964 D965 K966 N967 N968 L969 V970 K971 Y972 D973 K974 K975 T976 G977 N978 F979 Q980 V981 T982 E983 L984 G985 R986 I987 A988 S989 H990 Y991 Y992 I993 T994 N995 D996 T997 V998 Q999 T1000 Y1001 N1002 Q1003 L1004 L1005 K1006 P1007 T1008 L1009 S1010 E1011 I1012 E1013 L1014 F1015 R1016 V1017 F1018 S1019 L1020
S1021 S1022 E1023 F1024 K1025 N1026 I1027 T1028 V1029 R1030 E1031 E1032 E1033 K1034 L1035 E1036 L1037 Q1038 K1039 L1040 L1041 E1042 R1043 V1044 P1045 I1046 P1047 V1048 K1049 E1050 S1051 I1052 E1053 E1054 P1055 S1056 A1057 K1058 I1059 N1060 V1061 L1062 L1063 Q1064 A1065 F1066 I1067 S1068 Q1069 L1070 K1071 L1072 E1073 G1074 F1075 A1076 L1077 M1078 A1079 D1080
M1081 V1082 Y1083 V1084 T1085 Q1086 S1087 A1088 G1089 R1090 L1091 M1092 R1093 A1094 I1095 F1096 E1097 I1098 V1099 L1100 N1101 R1102 G1103 W1104 A1105 Q1106 L1107 T1108 D1109 K1110 T1111 L1112 N1113 L1114 C1115 K1116 M1117 I1118 D1119 K1120 R1121 M1122 W1123 Q1124 S1125 M1126 C1127 P1128 L1129 R1130 Q1131 F1132 R1133 K1134 L1135 P1136 E1137 E1138 V1139 V1140
K1141 K1142 I1143 E1144 K1145 K1146 N1147 F1148 P1149 F1150 E1151 R1152 L1153 Y1154 D1155 L1156 N1157 H1158 N1159 E1160 I1161 G1162 E1163 L1164 I1165 R1166 M1167 P1168 K1169 M1170 G1171 K1172 T1173 I1174 H1175 K1176 Y1177 V1178 H1179 L1180 F1181 P1182 K1183 L1184 E1185 L1186 S1187 V1188 H1189 L1190 Q1191 P1192 I1193 T1194 R1195 S1196 T1197 L1198 K1199 V1200
E1201 L1202 T1203 I1204 T1205 P1206 D1207 F1208 Q1209 W1210 D1211 E1212 K1213 V1214 H1215 G1216 S1217 S1218 E1219 A1220 F1221 W1222 I1223 L1224 V1225 E1226 D1227 V1228 D1229 S1230 E1231 V1232 I1233 L1234 H1235 H1236 E1237 Y1238 F1239 L1240 L1241 K1242 A1243 K1244 Y1245 A1246 Q1247 D1248 E1249 H1250 L1251 I1252 T1253 F1254 F1255 V1256 P1257 V1258 F1259 E1260
P1261 L1262 P1263 P1264 Q1265 Y1266 F1267 I1268 R1269 V1270 V1271 S1272 D1273 R1274 W1275 L1276 S1277 C1278 E1279 T1280 Q1281 L1282 P1283 V1284 S1285 F1286 R1287 H1288 L1289 I1290 L1291 P1292 E1293 K1294 Y1295 P1296 P1297 P1298 T1299 E1300 L1301 L1302 D1303 L1304 Q1305 P1306 L1307 P1308 V1309 S1310 A1311 L1312 R1313 N1314 S1315 A1316 F1317 E1318 S1319 L1320
Y1321 Q1322 D1323 K1324 F1325 P1326 F1327 F1328 N1329 P1330 I1331 Q1332 T1333 Q1334 V1335 F1336 N1337 T1338 V1339 Y1340 N1341 S1342 D1343 D1344 N1345 V1346 F1347 V1348 G1349 A1350 P1351 T1352 G1353 S1354 G1355 K1356 T1357 I1358 C1359 A1360 E1361 F1362 A1363 I1364 L1365 R1366 M1367 L1368 L1369 Q1370 S1371 S1372 E1373 G1374 R1375 C1376 V1377 Y1378 I1379 T1380
P1381 M1382 E1383 A1384 L1385 A1386 E1387 Q1388 V1389 Y1390 M1391 D1392 W1393 Y1394 E1395 K1396 F1397 Q1398 D1399 R1400 L1401 N1402 K1403 K1404 V1405 V1406 L1407 L1408 T1409 G1410 E1411 T1412 S1413 T1414 D1415 L1416 K1417 L1418 L1419 G1420 K1421 G1422 N1423 I1424 I1425 I1426 S1427 T1428 P1429 E1430 K1431 W1432 D1433 I1434 L1435 S1436 R1437 R1438 W1439 K1440
Q1441 R1442 K1443 N1444 V1445 Q1446 N1447 I1448 N1449 L1450 F1451 V1452 V1453 D1454 E1455 V1456 H1457 L1458 I1459 G1460 G1461 E1462 N1463 G1464 P1465 V1466 L1467 E1468 V1469 I1470 C1471 S1472 R1473 M1474 R1475 Y1476 I1477 S1478 S1479 Q1480 I1481 E1482 R1483 P1484 I1485 R1486 I1487 V1488 A1489 L1490 S1491 S1492 S1493 L1494 S1495 N1496 A1497 K1498 D1499 V1500
A1501 H1502 W1503 L1504 G1505 C1506 S1507 A1508 T1509 S1510 T1511 F1512 N1513 F1514 H1515 P1516 N1517 V1518 R1519 P1520 V1521 P1522 L1523 E1524 L1525 H1526 I1527 Q1528 G1529 F1530 N1531 I1532 S1533 H1534 T1535 Q1536 T1537 R1538 L1539 L1540 S1541 M1542 A1543 K1544 P1545 V1546 Y1547 H1548 A1549 I1550 T1551 K1552 H1553 S1554 P1555 K1556 K1557 P1558 V1559 I1560


V1561 F1562 V1563 P1564 S1565 R1566 K1567 Q1568 T1569 R1570 L1571 T1572 A1573 I1574 D1575 I1576 L1577 T1578 T1579 C1580 A1581 A1582 D1583 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590 H1591 C1592 T1593 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1605 D1606 S1607 T1608 L1609 K1610 E1611 T1612 L1613 L1614 N1615 G1616 V1617 G1618 Y1619 L1620
H1621 E1622 G1623 L1624 S1625 P1626 M1627 E1628 R1629 R1630 L1631 V1632 E1633 Q1634 L1635 F1636 S1637 S1638 G1639 A1640 I1641 Q1642 V1643 V1644 V1645 A1646 S1647 R1648 S1649 L1650 C1651 W1652 G1653 M1654 N1655 V1656 A1657 A1658 H1659 L1660 V1661 I1662 I1663 M1664 D1665 T1666 Q1667 Y1668 Y1669 N1670 G1671 K1672 I1673 H1674 A1675 Y1676 V1677 D1678 Y1679 P1680
I1681 Y1682 D1683 V1684 L1685 Q1686 M1687 V1688 G1689 H1690 A1691 N1692 R1693 P1694 L1695 Q1696 D1697 D1698 E1699 G1700 R1701 C1702 V1703 I1704 M1705 C1706 Q1707 G1708 S1709 K1710 K1711 D1712 F1713 F1714 K1715 K1716 F1717 L1718 Y1719 E1720 P1721 L1722 P1723 V1724 E1725 S1726 H1727 L1728 D1729 H1730 C1731 M1732 H1733 D1734 H1735 F1736 N1737 A1738 E1739 I1740
V1741 T1742 K1743 T1744 I1745 E1746 N1747 K1748 Q1749 D1750 A1751 V1752 D1753 Y1754 L1755 T1756 W1757 T1758 F1759 L1760 Y1761 R1762 R1763 M1764 T1765 Q1766 N1767 P1768 N1769 Y1770 Y1771 N1772 L1773 Q1774 G1775 I1776 S1777 H1778 R1779 H1780 L1781 S1782 D1783 H1784 L1785 S1786 E1787 L1788 V1789 E1790 Q1791 T1792 L1793 S1794 D1795 L1796 E1797 Q1798 S1799 K1800
C1801 I1802 S1803 I1804 E1805 D1806 E1807 M1808 D1809 V1810 A1811 P1812 L1813 N1814 L1815 G1816 M1817 I1818 A1819 A1820 Y1821 Y1822 Y1823 I1824 N1825 Y1826 T1827 T1828 I1829 E1830 L1831 F1832 S1833 M1834 S1835 L1836 N1837 A1838 K1839 T1840 K1841 V1842 R1843 G1844 L1845 I1846 E1847 I1848 I1849 S1850 N1851 A1852 A1853 E1854 Y1855 E1856 N1857 I1858 P1859 I1860
R1861 H1862 H1863 E1864 D1865 N1866 L1867 L1868 R1869 Q1870 L1871 A1872 Q1873 K1874 V1875 P1876 H1877 K1878 L1879 N1880 N1881 P1882 K1883 F1884 N1885 D1886 P1887 H1888 V1889 K1890 T1691 N1892 L1893 L1894 L1895 Q1896 A1897 H1698 L1899 S1900 T1901 M1902 Q1903 L1904 S1905 A1906 E1907 L1908 Q1909 S1910 D1911 T1912 E1913 E1914 I1915 L1916 S1917 K1918 A1919 I1920
R1921 L1922 I1923 Q1924 A1925 C1926 V1927 D1928 V1929 L1930 S1931 S1932 N1933 G1934 W1935 L1936 S1937 P1938 A1939 L1940 A1941 A1942 M1943 E1944 L1945 A1946 Q1947 M1948 V1949 T1950 Q1951 A1952 M1953 W1954 S1955 K1956 D1957 S1958 Y1959 L1960 K1961 Q1962 L1963 P1964 H1965 F1966 T1967 S1968 E1969 H1970 I1971 K1972 R1973 C1974 T1975 D1976 K1977 G1978 V1979 E1980
S1981 V1982 F1983 D1984 I1985 M1986 E1987 M1988 E1989 D1990 E1991 E1992 R1993 N1994 A1995 L1996 L1997 Q1998 L1999 T2000 D2001 S2002 Q2003 I2004 A2005 D2006 V2007 A2008 R2009 F2010 C2011 N2012 R2013 Y2014 P2015 N2016 I2017 E2018 L2019 S2020 Y2021 E2022 V2023 V2024 D2025 K2026 D2027 S2028 I2029 R2030 S2031 G2032 G2033 P2034 V2035 V2036 V2037 L2038 V2039 Q2040
L2041 E2042 R2043 E2044 E2045 E2046 V2047 T2048 G2049 P2050 V2051 I2052 A2053 P2054 L2055 F2056 P2057 Q2058 K2059 R2060 E2061 E2062 G2063 W2064 W2065 V2066 V2067 I2068 G2069 D2070 A2071 K2072 S2073 N2074 S2075 L2076 I2077 S2078 I2079 K2080 R2081 L2082 T2083 L2084 Q2085 Q2086 K2087 A2088 K2089 V2090 K2091 L2092 D2093 F2094 V2095 A2096 P2097 A2098 T2099 G2100
A2101 H2102 N2103 Y2104 T2105 L2106 Y2107 F2108 M2109 S2110 D2111 A2112 Y2113 M2114 G2115 C2116 D2117 Q2118 E2119 Y2120 K2121 F2122 S2123 V2124 D2125 VAL LYS GLU ALA GLU THR ASP SER ASP SER ASP

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	143320	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.552	Depositor
Minimum map value	-0.288	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.03	Depositor
Map size (Å)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.338, 1.338, 1.338	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	v	0.30	0/710	0.65	0/987
2	w	0.30	0/444	0.78	2/614 (0.3%)
3	u	0.32	0/1906	0.69	0/2653
4	x	0.34	0/123	0.70	0/170
5	A	0.53	0/18287	0.65	7/24842 (0.0%)
6	B	0.77	1/2274 (0.0%)	1.17	25/3535 (0.7%)
7	C	2.14	9/7225 (0.1%)	0.78	12/9818 (0.1%)
8	E	0.34	0/2420	0.64	0/3281
9	F	0.95	0/2323	1.23	19/3619 (0.5%)
10	G	0.57	0/1716	1.23	21/2656 (0.8%)
11	H	0.95	24/3305 (0.7%)	1.55	96/5130 (1.9%)
12	J	0.46	0/3870	0.61	13/5252 (0.2%)
13	L	0.41	0/3091	0.59	7/4178 (0.2%)
14	M	0.41	0/1119	0.63	1/1497 (0.1%)
15	N	1.19	6/1210 (0.5%)	0.87	2/1622 (0.1%)
16	O	0.47	0/2344	0.62	1/3163 (0.0%)
17	P	0.46	0/943	0.61	0/1255
18	R	0.47	0/2091	0.66	1/2809 (0.0%)
19	S	0.35	0/1268	0.59	1/1714 (0.1%)
20	T	0.65	1/2526 (0.0%)	0.82	3/3443 (0.1%)
21	U	0.34	0/196	0.63	0/265
22	V	0.31	0/2784	0.54	3/3791 (0.1%)
23	W	0.40	0/4230	0.69	3/5713 (0.1%)
24	X	0.32	0/714	0.53	2/959 (0.2%)
25	Z	0.37	0/2049	0.61	1/2757 (0.0%)
26	I	0.38	0/2749	0.56	16/3773 (0.4%)
27	y	0.25	0/389	0.62	0/540
28	Q	0.22	0/6565	0.42	0/9143
29	a	0.48	0/397	0.62	0/549
29	h	0.47	0/396	0.61	0/547
30	b	0.51	0/423	0.72	0/587
30	i	0.50	0/423	0.73	0/587

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
31	c	0.57	0/405	0.73	0/563
31	j	0.57	0/405	0.73	0/563
32	d	0.68	0/479	0.85	0/666
32	k	0.70	0/420	0.85	0/583
33	f	0.75	0/360	0.81	0/497
33	m	0.76	0/355	0.81	0/490
34	e	0.65	0/390	0.80	0/542
34	l	0.62	0/390	0.80	0/542
35	g	0.54	0/362	0.71	0/501
35	n	0.50	0/337	0.70	0/465
36	o	0.64	0/803	1.49	4/1119 (0.4%)
37	p	0.61	0/463	1.25	0/643
38	Y	0.46	0/2917	0.92	0/3670
39	K	0.40	1/753 (0.1%)	0.55	3/1046 (0.3%)
40	q	0.35	0/658	0.58	3/919 (0.3%)
40	r	0.33	0/653	0.56	2/912 (0.2%)
40	s	0.27	0/334	0.37	0/466
40	t	0.31	0/334	0.38	0/466
41	D	0.33	0/8529	0.59	0/11891
All	All	0.76	42/99857 (0.0%)	0.77	248/137993 (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
5	A	0	6
7	C	0	7
8	E	0	1
11	H	0	1
12	J	0	3
14	M	0	1
16	O	0	1
17	P	0	1
18	R	0	2
20	T	0	3
23	W	0	3
25	Z	0	2
32	d	0	1
32	k	0	1
38	Y	0	15

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
41	D	0	1
All	All	0	49

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	172	PHE	CE1-CZ	84.80	2.98	1.37
7	C	172	PHE	CE2-CZ	79.82	2.89	1.37
7	C	172	PHE	CD1-CE1	78.14	2.95	1.39
7	C	172	PHE	CD2-CE2	76.95	2.93	1.39
7	C	172	PHE	CG-CD1	47.98	2.10	1.38
7	C	172	PHE	CG-CD2	47.86	2.10	1.38
7	C	104	LEU	CB-CG	38.63	2.64	1.52
15	N	137	CYS	CB-SG	-12.16	1.61	1.82
15	N	142	CYS	CB-SG	-8.15	1.68	1.82
15	N	102	CYS	CB-SG	-8.14	1.68	1.82
11	H	142	C	C1'-N1	7.52	1.60	1.48
11	H	77	C	C1'-N1	7.33	1.59	1.48
11	H	69	U	C1'-N1	7.03	1.59	1.48
11	H	54	U	C1'-N1	7.01	1.59	1.48
11	H	91	U	C1'-N1	6.99	1.59	1.48
11	H	60	U	C1'-N1	6.91	1.59	1.48
6	B	103	G	C1'-N9	-6.89	1.37	1.46
11	H	74	U	C1'-N1	6.88	1.59	1.48
11	H	89	U	C1'-N1	6.87	1.59	1.48
11	H	72	U	C1'-N1	6.86	1.59	1.48
11	H	150	U	C1'-N1	6.79	1.58	1.48
11	H	55	U	C1'-N1	6.79	1.58	1.48
11	H	92	U	C1'-N1	6.76	1.58	1.48
11	H	182	U	C1'-N1	6.75	1.58	1.48
11	H	58	U	C1'-N1	6.73	1.58	1.48
15	N	117	CYS	CB-SG	-6.55	1.71	1.82
11	H	73	C	C1'-N1	6.41	1.58	1.48
15	N	139	CYS	CB-SG	-6.37	1.71	1.82
11	H	78	C	C1'-N1	6.36	1.58	1.48
11	H	151	C	C1'-N1	6.35	1.58	1.48
11	H	141	C	C1'-N1	6.34	1.58	1.48
11	H	184	C	C1'-N1	6.29	1.58	1.48
11	H	84	C	C1'-N1	6.24	1.58	1.48
11	H	67	C	C1'-N1	6.24	1.58	1.48
11	H	148	C	C1'-N1	6.24	1.58	1.48
11	H	71	C	C1'-N1	6.22	1.58	1.48

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	H	70	C	C1'-N1	6.18	1.58	1.48
7	C	104	LEU	CG-CD1	6.12	1.74	1.51
7	C	104	LEU	CG-CD2	6.00	1.74	1.51
15	N	101	CYS	CB-SG	-5.92	1.72	1.81
20	T	306	CYS	CB-SG	-5.56	1.72	1.81
39	K	186	VAL	CA-CB	-5.14	1.44	1.54

All (248) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	104	LEU	CA-CB-CG	18.46	157.76	115.30
7	C	104	LEU	CB-CG-CD1	16.32	138.75	111.00
7	C	104	LEU	CB-CG-CD2	15.04	136.56	111.00
11	H	167	U	C5-C4-O4	11.93	133.06	125.90
7	C	172	PHE	CD1-CG-CD2	9.95	131.24	118.30
6	B	23	C	N1-C2-O2	9.93	124.86	118.90
7	C	172	PHE	CB-CG-CD2	-9.29	114.30	120.80
7	C	104	LEU	CD1-CG-CD2	-9.28	82.65	110.50
7	C	172	PHE	CB-CG-CD1	-9.20	114.36	120.80
20	T	342	GLU	C-N-CD	-9.10	100.57	120.60
10	G	163	C	N1-C2-O2	9.09	124.35	118.90
10	G	-6	C	N1-C2-O2	8.96	124.28	118.90
11	H	162	U	N3-C2-O2	-8.82	116.02	122.20
6	B	23	C	C2-N1-C1'	8.81	128.49	118.80
10	G	17	U	N1-C2-O2	8.68	128.87	122.80
10	G	-6	C	C2-N1-C1'	8.50	128.15	118.80
10	G	163	C	N3-C2-O2	-8.42	116.01	121.90
6	B	23	C	N3-C2-O2	-8.14	116.20	121.90
20	T	402	ASP	CB-CG-OD1	8.02	125.52	118.30
10	G	17	U	N3-C2-O2	-8.02	116.59	122.20
9	F	60	C	C6-N1-C2	-7.98	117.11	120.30
11	H	167	U	N3-C4-O4	-7.97	113.82	119.40
10	G	17	U	C2-N1-C1'	7.95	127.24	117.70
11	H	39	U	C2'-C3'-O3'	7.91	126.90	109.50
10	G	163	C	C2-N1-C1'	7.59	127.15	118.80
10	G	163	C	C6-N1-C2	-7.49	117.31	120.30
6	B	36	C	N1-C2-O2	7.42	123.35	118.90
6	B	55	C	C6-N1-C2	-7.41	117.33	120.30
11	H	69	U	OP2-P-O3'	7.34	121.34	105.20
11	H	167	U	N1-C2-O2	7.32	127.92	122.80
11	H	77	C	OP2-P-O3'	7.28	121.21	105.20
11	H	70	C	OP2-P-O3'	7.27	121.20	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	83	A	OP2-P-O3'	7.27	121.19	105.20
11	H	141	C	OP2-P-O3'	7.27	121.19	105.20
11	H	54	U	OP2-P-O3'	7.26	121.18	105.20
11	H	92	U	OP2-P-O3'	7.26	121.16	105.20
11	H	149	A	OP2-P-O3'	7.26	121.16	105.20
11	H	148	C	OP2-P-O3'	7.25	121.16	105.20
11	H	59	A	OP2-P-O3'	7.23	121.11	105.20
11	H	81	G	OP2-P-O3'	7.23	121.10	105.20
11	H	180	G	OP2-P-O3'	7.22	121.08	105.20
11	H	67	C	OP2-P-O3'	7.22	121.08	105.20
11	H	78	C	OP2-P-O3'	7.22	121.08	105.20
11	H	80	A	OP2-P-O3'	7.22	121.08	105.20
11	H	89	U	OP2-P-O3'	7.22	121.08	105.20
11	H	74	U	OP2-P-O3'	7.21	121.05	105.20
11	H	88	A	OP2-P-O3'	7.20	121.04	105.20
11	H	55	U	OP2-P-O3'	7.20	121.03	105.20
11	H	181	G	OP2-P-O3'	7.20	121.03	105.20
11	H	182	U	OP2-P-O3'	7.19	121.03	105.20
11	H	90	A	OP2-P-O3'	7.19	121.02	105.20
6	B	36	C	C2-N1-C1'	7.19	126.71	118.80
11	H	183	G	OP2-P-O3'	7.19	121.01	105.20
11	H	91	U	OP2-P-O3'	7.18	121.00	105.20
11	H	57	A	OP2-P-O3'	7.18	121.00	105.20
11	H	150	U	OP2-P-O3'	7.18	121.00	105.20
11	H	71	C	OP2-P-O3'	7.17	120.98	105.20
11	H	93	A	OP2-P-O3'	7.17	120.98	105.20
11	H	58	U	OP2-P-O3'	7.16	120.95	105.20
11	H	72	U	OP2-P-O3'	7.16	120.95	105.20
11	H	68	G	OP2-P-O3'	7.16	120.95	105.20
11	H	84	C	OP2-P-O3'	7.16	120.95	105.20
11	H	56	A	OP2-P-O3'	7.16	120.94	105.20
11	H	73	C	OP2-P-O3'	7.15	120.94	105.20
11	H	79	G	OP2-P-O3'	7.15	120.92	105.20
24	X	85	LEU	CA-CB-CG	7.13	131.69	115.30
11	H	82	G	OP2-P-O3'	7.07	120.76	105.20
11	H	167	U	N3-C2-O2	-7.05	117.27	122.20
11	H	54	U	O3'-P-O5'	-6.86	90.97	104.00
11	H	82	G	O3'-P-O5'	-6.86	90.97	104.00
6	B	104	C	C2'-C3'-O3'	-6.85	94.44	109.50
11	H	84	C	O3'-P-O5'	-6.84	91.00	104.00
11	H	150	U	O3'-P-O5'	-6.84	91.00	104.00
11	H	88	A	O3'-P-O5'	-6.84	91.00	104.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	93	A	O3'-P-O5'	-6.83	91.03	104.00
11	H	78	C	O3'-P-O5'	-6.82	91.04	104.00
11	H	73	C	O3'-P-O5'	-6.82	91.05	104.00
5	A	1109	LEU	CA-CB-CG	6.81	130.97	115.30
11	H	55	U	O3'-P-O5'	-6.81	91.06	104.00
11	H	83	A	O3'-P-O5'	-6.81	91.06	104.00
11	H	67	C	O3'-P-O5'	-6.81	91.07	104.00
11	H	181	G	O3'-P-O5'	-6.80	91.07	104.00
11	H	92	U	O3'-P-O5'	-6.80	91.08	104.00
11	H	141	C	O3'-P-O5'	-6.79	91.09	104.00
11	H	74	U	O3'-P-O5'	-6.79	91.10	104.00
6	B	40	U	N1-C2-O2	6.79	127.55	122.80
10	G	137	C	C2'-C3'-O3'	6.79	124.56	113.70
11	H	80	A	O3'-P-O5'	-6.79	91.11	104.00
11	H	180	G	O3'-P-O5'	-6.78	91.12	104.00
11	H	59	A	O3'-P-O5'	-6.78	91.12	104.00
11	H	56	A	O3'-P-O5'	-6.78	91.13	104.00
11	H	79	G	O3'-P-O5'	-6.77	91.13	104.00
11	H	57	A	O3'-P-O5'	-6.77	91.14	104.00
10	G	-6	C	N3-C2-O2	-6.75	117.17	121.90
11	H	69	U	O3'-P-O5'	-6.75	91.17	104.00
11	H	148	C	O3'-P-O5'	-6.75	91.17	104.00
11	H	182	U	O3'-P-O5'	-6.75	91.18	104.00
11	H	149	A	O3'-P-O5'	-6.74	91.19	104.00
11	H	89	U	O3'-P-O5'	-6.74	91.20	104.00
11	H	72	U	O3'-P-O5'	-6.74	91.20	104.00
11	H	91	U	O3'-P-O5'	-6.73	91.21	104.00
11	H	183	G	O3'-P-O5'	-6.73	91.21	104.00
11	H	58	U	O3'-P-O5'	-6.73	91.22	104.00
11	H	70	C	O3'-P-O5'	-6.72	91.22	104.00
11	H	71	C	O3'-P-O5'	-6.72	91.23	104.00
11	H	68	G	O3'-P-O5'	-6.72	91.24	104.00
11	H	81	G	O3'-P-O5'	-6.71	91.24	104.00
11	H	90	A	O3'-P-O5'	-6.71	91.24	104.00
11	H	155	C	P-O3'-C3'	6.71	127.75	119.70
6	B	20	G	O4'-C1'-N9	6.70	113.56	108.20
9	F	60	C	C5-C6-N1	6.69	124.35	121.00
11	H	77	C	O3'-P-O5'	-6.69	91.28	104.00
16	O	193	LEU	CA-CB-CG	6.69	130.68	115.30
40	q	46	PRO	N-CA-CB	6.64	111.27	103.30
9	F	61	C	C6-N1-C2	-6.58	117.67	120.30
39	K	90	PRO	N-CA-CB	6.58	111.19	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	29	A	P-O3'-C3'	6.53	127.53	119.70
6	B	43	U	N1-C2-O2	6.50	127.35	122.80
40	r	46	PRO	N-CA-CB	6.49	111.08	103.30
2	w	114	LYS	N-CA-C	-6.42	93.67	111.00
40	q	60	PRO	N-CA-CB	6.40	110.98	103.30
10	G	-6	C	C6-N1-C1'	-6.38	113.14	120.80
5	A	422	LEU	CB-CG-CD2	-6.37	100.17	111.00
39	K	78	PRO	N-CA-CB	6.37	110.94	103.30
10	G	131	U	C2'-C3'-O3'	-6.36	95.51	109.50
36	o	5	THR	N-CA-CB	-6.30	98.34	110.30
26	I	589	PRO	N-CA-CB	6.29	110.85	103.30
6	B	36	C	C6-N1-C2	-6.26	117.80	120.30
26	I	475	PRO	N-CA-CB	6.25	110.80	103.30
7	C	172	PHE	CD1-CE1-CZ	-6.21	112.65	120.10
6	B	36	C	C5-C6-N1	6.21	124.10	121.00
7	C	105	MET	CA-CB-CG	6.20	123.83	113.30
6	B	43	U	N3-C2-O2	-6.18	117.88	122.20
13	L	558	PRO	N-CA-CB	6.16	110.70	103.30
9	F	38	G	C6-C5-N7	-6.16	126.71	130.40
6	B	23	C	C6-N1-C1'	-6.15	113.42	120.80
12	J	637	PRO	N-CA-CB	6.15	110.68	103.30
11	H	165	A	O4'-C1'-N9	-6.14	103.29	108.20
26	I	162	PRO	N-CA-CB	6.10	110.62	103.30
26	I	232	PRO	N-CA-CB	6.10	110.61	103.30
26	I	371	PRO	N-CA-CB	6.09	110.61	103.30
10	G	13	C	C5-C6-N1	6.09	124.04	121.00
26	I	394	PRO	N-CA-CB	6.08	110.59	103.30
10	G	16	G	P-O3'-C3'	6.07	126.98	119.70
26	I	788	PRO	N-CA-CB	6.06	110.57	103.30
26	I	177	PRO	N-CA-CB	6.06	110.57	103.30
15	N	119	CYS	CA-CB-SG	6.05	124.89	114.00
26	I	816	PRO	N-CA-CB	6.04	110.55	103.30
13	L	546	PRO	N-CA-CB	6.03	110.54	103.30
12	J	670	PRO	N-CA-CB	6.02	110.53	103.30
12	J	220	LEU	CA-CB-CG	6.01	129.13	115.30
5	A	1405	LEU	CA-CB-CG	6.00	129.09	115.30
12	J	523	PRO	N-CA-CB	6.00	110.49	103.30
11	H	162	U	N1-C2-O2	5.99	126.99	122.80
11	H	104	U	C2'-C3'-O3'	5.97	123.25	113.70
13	L	594	PRO	N-CA-CB	5.96	110.46	103.30
13	L	563	PRO	N-CA-CB	5.96	110.45	103.30
26	I	160	PRO	N-CA-CB	5.96	110.45	103.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	H	172	C	P-O3'-C3'	5.95	126.84	119.70
6	B	36	C	N3-C2-O2	-5.93	117.75	121.90
40	r	19	PRO	N-CA-CB	5.92	110.41	103.30
12	J	604	PRO	N-CA-CB	5.91	110.39	103.30
26	I	518	PRO	N-CA-CB	5.89	110.37	103.30
26	I	387	PRO	N-CA-CB	5.88	110.35	103.30
11	H	14	C	N1-C2-O2	5.87	122.42	118.90
6	B	55	C	N3-C2-O2	-5.86	117.80	121.90
22	V	539	LEU	CA-CB-CG	5.85	128.75	115.30
40	q	19	PRO	N-CA-CB	5.84	110.31	103.30
12	J	675	PRO	N-CA-CB	5.83	110.30	103.30
13	L	548	PRO	N-CA-CB	5.82	110.29	103.30
36	o	27	ARG	CB-CA-C	-5.82	98.76	110.40
6	B	40	U	N3-C2-O2	-5.80	118.14	122.20
9	F	25	C	P-O3'-C3'	5.79	126.65	119.70
12	J	551	PRO	N-CA-CB	5.77	110.23	103.30
9	F	38	G	N3-C4-N9	5.77	129.46	126.00
22	V	489	LEU	CA-CB-CG	5.76	128.54	115.30
12	J	488	PRO	N-CA-CB	5.75	110.20	103.30
12	J	566	PRO	N-CA-CB	5.74	110.19	103.30
13	L	564	PRO	N-CA-CB	5.74	110.19	103.30
9	F	60	C	N3-C2-O2	-5.71	117.90	121.90
13	L	620	PRO	N-CA-CB	5.70	110.14	103.30
6	B	40	U	C2-N1-C1'	5.70	124.54	117.70
26	I	588	PRO	N-CA-CB	5.69	110.12	103.30
9	F	26	U	C6-N1-C2	-5.68	117.59	121.00
11	H	156	U	P-O3'-C3'	-5.68	112.88	119.70
6	B	52	U	N3-C2-O2	-5.65	118.25	122.20
7	C	93	ILE	CG1-CB-CG2	-5.64	98.99	111.40
25	Z	82	LEU	CA-CB-CG	5.64	128.28	115.30
12	J	205	LEU	C-N-CA	5.63	135.76	121.70
9	F	60	C	N1-C2-O2	5.59	122.26	118.90
12	J	522	PRO	N-CA-CB	5.59	110.01	103.30
23	W	251	GLY	N-CA-C	-5.59	99.12	113.10
36	o	58	ASP	N-CA-CB	-5.56	100.58	110.60
26	I	463	PRO	N-CA-CB	5.55	109.96	103.30
23	W	165	LEU	CA-CB-CG	5.53	128.03	115.30
5	A	1889	LEU	CA-CB-CG	5.53	128.02	115.30
9	F	37	C	O4'-C1'-N1	5.53	112.62	108.20
6	B	23	C	C6-N1-C2	-5.51	118.10	120.30
10	G	6	A	N7-C8-N9	5.51	116.55	113.80
39	K	93	SER	N-CA-CB	-5.50	102.25	110.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	20	G	C4-N9-C1'	5.47	133.61	126.50
26	I	761	PRO	N-CA-CB	5.46	109.86	103.30
14	M	186	LEU	CB-CG-CD1	-5.45	101.74	111.00
7	C	943	LEU	CA-CB-CG	5.41	127.73	115.30
10	G	17	U	C5-C6-N1	5.37	125.39	122.70
10	G	18	A	C6-N1-C2	5.37	121.82	118.60
36	o	47	ILE	N-CA-CB	5.36	123.13	110.80
26	I	625	PRO	N-CA-CB	5.36	109.73	103.30
12	J	187	VAL	C-N-CA	5.36	135.09	121.70
9	F	31	U	N3-C2-O2	-5.35	118.46	122.20
9	F	31	U	N1-C2-O2	5.34	126.54	122.80
5	A	623	LYS	N-CA-C	-5.34	96.58	111.00
11	H	156	U	OP2-P-O3'	5.31	116.87	105.20
6	B	58	U	N3-C2-O2	-5.30	118.49	122.20
20	T	401	PRO	C-N-CA	5.30	134.96	121.70
6	B	56	C	N1-C2-O2	5.30	122.08	118.90
9	F	89	U	N3-C2-O2	-5.30	118.49	122.20
9	F	26	U	N3-C2-O2	-5.29	118.50	122.20
10	G	5	G	C4-N9-C1'	5.28	133.36	126.50
7	C	298	LEU	CA-CB-CG	5.25	127.38	115.30
10	G	1	G	C2'-C3'-O3'	5.24	122.09	113.70
5	A	1763	LEU	CA-CB-CG	5.22	127.31	115.30
11	H	157	G	O4'-C1'-N9	-5.22	104.03	108.20
2	w	115	GLY	N-CA-C	5.20	126.11	113.10
11	H	162	U	C2-N3-C4	-5.18	123.89	127.00
24	X	85	LEU	CB-CG-CD1	-5.18	102.19	111.00
9	F	60	C	C2-N1-C1'	5.17	124.49	118.80
15	N	101	CYS	CA-CB-SG	-5.17	104.69	114.00
11	H	157	G	P-O5'-C5'	-5.16	112.64	120.90
6	B	21	A	OP2-P-O3'	5.16	116.54	105.20
12	J	195	LEU	CA-CB-CG	5.16	127.16	115.30
11	H	160	A	C4'-C3'-C2'	-5.14	97.46	102.60
5	A	1090	ARG	NE-CZ-NH2	-5.14	117.73	120.30
11	H	13	C	N3-C2-O2	-5.13	118.31	121.90
10	G	-12	G	P-O3'-C3'	5.12	125.85	119.70
6	B	55	C	N1-C2-O2	5.12	121.97	118.90
9	F	26	U	P-O3'-C3'	5.12	125.84	119.70
9	F	38	G	C4-N9-C1'	5.11	133.15	126.50
18	R	275	LEU	CA-CB-CG	5.11	127.04	115.30
11	H	160	A	P-O5'-C5'	-5.10	112.74	120.90
11	H	156	U	C4'-C3'-C2'	5.10	107.70	102.60
11	H	29	A	OP1-P-O3'	5.09	116.39	105.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	467	LEU	CA-CB-CG	5.08	126.98	115.30
11	H	176	G	OP1-P-OP2	-5.06	112.01	119.60
9	F	52	U	N3-C2-O2	-5.04	118.67	122.20
19	S	106	ASP	CB-CG-OD1	5.04	122.84	118.30
23	W	442	LEU	CA-CB-CG	5.02	126.84	115.30
9	F	89	U	N1-C2-O2	5.00	126.30	122.80

There are no chirality outliers.

All (49) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	1070	ASP	Peptide
5	A	1091	TYR	Peptide
5	A	1209	HIS	Peptide
5	A	1502	PHE	Peptide
5	A	851	SER	Peptide
5	A	941	LYS	Peptide
7	C	103	THR	Peptide
7	C	167	TYR	Peptide
7	C	439	PRO	Peptide
7	C	456	GLY	Peptide
7	C	534	VAL	Peptide
7	C	560	VAL	Peptide
7	C	93	ILE	Peptide
41	D	430	LEU	Peptide
8	E	192	ASN	Peptide
11	H	40	C	Sidechain
12	J	205	LEU	Peptide
12	J	240	THR	Peptide
12	J	241	VAL	Peptide
14	M	124	PHE	Peptide
16	O	133	PRO	Peptide
17	P	204	GLN	Peptide
18	R	183	GLN	Peptide
18	R	185	GLY	Peptide
20	T	185	MET	Peptide
20	T	400	PHE	Peptide
20	T	457	GLY	Peptide
23	W	198	LYS	Peptide
23	W	242	HIS	Peptide
23	W	245	GLU	Peptide
38	Y	1098	LYS	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
38	Y	1127	LEU	Peptide
38	Y	1163	ARG	Peptide
38	Y	1187	THR	Peptide
38	Y	515	ASP	Peptide
38	Y	550	TYR	Peptide
38	Y	563	GLU	Peptide
38	Y	636	CYS	Peptide
38	Y	662	THR	Peptide
38	Y	811	PRO	Peptide
38	Y	855	VAL	Peptide
38	Y	868	LYS	Peptide
38	Y	938	ASN	Peptide
38	Y	963	THR	Peptide
38	Y	993	LEU	Peptide
25	Z	135	GLU	Peptide
25	Z	92	GLN	Peptide
32	d	112	ASN	Peptide
32	k	112	ASN	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	v	711	0	299	0	0
2	w	445	0	203	0	0
3	u	1907	0	845	0	0
4	x	124	0	51	0	0
5	A	17837	0	17053	235	0
6	B	2040	0	1034	51	0
7	C	7066	0	7084	130	0
8	E	2366	0	2303	65	0
9	F	2075	0	1048	27	0
10	G	1549	0	784	51	0
11	H	2966	0	1505	227	0
12	J	3829	0	2907	38	0
13	L	3064	0	2521	40	0
14	M	1098	0	1082	25	0
15	N	1184	0	1189	41	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	O	2296	0	2284	36	0
17	P	929	0	910	6	0
18	R	2073	0	2119	36	0
19	S	1236	0	1210	23	0
20	T	2461	0	2420	69	0
21	U	193	0	196	4	0
22	V	2765	0	1955	17	0
23	W	4122	0	4031	109	0
24	X	701	0	631	30	0
25	Z	1999	0	1951	35	0
26	I	2782	0	1245	52	0
27	y	390	0	190	0	0
28	Q	6562	0	2836	5	0
29	a	399	0	173	0	0
29	h	398	0	172	0	0
30	b	424	0	179	0	0
30	i	424	0	179	0	0
31	c	406	0	170	0	0
31	j	406	0	170	0	0
32	d	480	0	200	0	0
32	k	422	0	175	0	0
33	f	361	0	158	0	0
33	m	356	0	156	0	0
34	e	391	0	163	0	0
34	l	391	0	163	0	0
35	g	363	0	160	0	0
35	n	339	0	145	0	0
36	o	804	0	350	0	0
37	p	464	0	205	0	0
38	Y	2917	0	857	9	0
39	K	757	0	338	19	0
40	q	659	0	296	0	0
40	r	654	0	294	0	0
40	s	335	0	168	0	0
40	t	335	0	168	0	0
41	D	8530	0	3747	8	0
42	A	36	0	6	3	0
43	C	32	0	12	2	0
44	C	1	0	0	0	0
44	F	6	0	0	0	0
44	Q	2	0	0	0	0
45	N	3	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
45	O	3	0	0	0	0
45	Z	1	0	0	0	0
46	Q	31	0	12	0	0
All	All	97900	0	70702	1177	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 (1177) 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)
7:C:104:LEU:CG	7:C:104:LEU:CD1	1.74	1.61
12:J:466:ARG:CB	26:I:607:GLY:HA2	1.44	1.47
8:E:56:GLN:NE2	8:E:97:GLY:HA2	1.35	1.40
7:C:172:PHE:CD1	7:C:172:PHE:CG	2.10	1.39
7:C:172:PHE:CG	7:C:172:PHE:CD2	2.10	1.39
23:W:257:ILE:HD12	23:W:258:PRO:CD	1.51	1.36
23:W:257:ILE:CD1	23:W:258:PRO:HD2	1.54	1.34
11:H:150:U:O3'	24:X:124:THR:HG22	1.31	1.27
26:I:331:LEU:CB	26:I:340:ARG:CB	2.12	1.26
39:K:113:GLN:O	39:K:117:GLN:CB	1.87	1.22
23:W:258:PRO:CG	23:W:265:LEU:HD22	1.74	1.16
20:T:342:GLU:CB	20:T:343:PRO:HD2	1.63	1.15
23:W:258:PRO:HG3	23:W:265:LEU:CD2	1.74	1.15
20:T:399:LYS:HB2	20:T:406:ILE:HD11	1.14	1.13
12:J:427:LYS:NZ	26:I:579:LEU:CB	2.12	1.13
26:I:612:ALA:CB	26:I:623:VAL:CB	2.26	1.12
12:J:484:VAL:CB	26:I:642:ILE:CB	2.28	1.12
39:K:112:ALA:O	39:K:116:HIS:CB	1.98	1.11
7:C:104:LEU:CD1	7:C:104:LEU:CD2	2.30	1.10
26:I:296:PHE:HA	26:I:305:SER:CB	1.80	1.10
26:I:346:ASN:CB	28:Q:524:LYS:CB	2.30	1.10
11:H:150:U:H5"	24:X:124:THR:CB	1.81	1.10
12:J:466:ARG:CB	26:I:607:GLY:CA	2.30	1.09
12:J:427:LYS:CE	26:I:579:LEU:CB	2.30	1.09
10:G:138:A:C2	11:H:39:U:O2	2.07	1.08
26:I:612:ALA:HB2	26:I:623:VAL:CB	1.84	1.07
11:H:150:U:H5"	24:X:124:THR:HB	1.31	1.07
23:W:257:ILE:HD12	23:W:258:PRO:N	1.67	1.07
11:H:156:U:H6	11:H:156:U:H5"	1.09	1.07
11:H:150:U:H5"	24:X:124:THR:CG2	1.84	1.06

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:104:LEU:CB	7:C:104:LEU:HG	1.86	1.06
8:E:56:GLN:HE22	8:E:97:GLY:CA	1.67	1.05
11:H:151:C:OP1	24:X:123:GLN:HB2	1.55	1.03
20:T:342:GLU:HB3	20:T:343:PRO:CD	1.88	1.03
8:E:60:MET:HG3	8:E:353:MET:SD	1.99	1.03
7:C:104:LEU:HD11	7:C:104:LEU:HD21	1.40	1.01
8:E:56:GLN:NE2	8:E:97:GLY:CA	2.23	0.99
5:A:1976:TRP:O	5:A:1980:GLU:HG3	1.62	0.99
11:H:106:G:H4'	11:H:107:A:OP1	1.62	0.99
23:W:257:ILE:HD12	23:W:258:PRO:HD2	1.05	0.98
24:X:120:ALA:O	24:X:124:THR:HG23	1.64	0.97
38:Y:405:MET:HE3	38:Y:411:LEU:HD23	1.46	0.97
11:H:151:C:P	24:X:124:THR:HG22	2.05	0.96
8:E:60:MET:HB3	8:E:353:MET:HB2	1.45	0.96
11:H:156:U:H5"	11:H:156:U:C6	2.02	0.94
5:A:1673:SER:CB	25:Z:164:ASP:OD1	2.15	0.94
5:A:1945:VAL:HG11	5:A:1990:ASP:CG	1.86	0.94
11:H:150:U:C5'	24:X:124:THR:HB	1.97	0.93
11:H:150:U:OP1	24:X:124:THR:HB	1.69	0.93
23:W:257:ILE:HD13	23:W:258:PRO:HD2	1.51	0.92
8:E:54:SER:N	8:E:96:TYR:HE1	1.66	0.92
11:H:108:G:H2'	11:H:109:C:H6	1.31	0.92
16:O:72:GLN:HG3	16:O:82:GLN:HE22	1.35	0.92
11:H:106:G:H5'	11:H:106:G:H8	1.36	0.90
20:T:342:GLU:CB	20:T:343:PRO:CD	2.47	0.90
13:L:65:ARG:NH2	26:I:799:ARG:O	2.04	0.90
8:E:56:GLN:HE22	8:E:97:GLY:HA2	1.07	0.90
10:G:138:A:N1	11:H:39:U:O2	2.05	0.89
11:H:100:U:H5'	11:H:100:U:C6	2.07	0.89
10:G:129:G:O3'	23:W:541:LYS:HE3	1.72	0.88
20:T:399:LYS:CB	20:T:406:ILE:HD11	2.02	0.88
5:A:1673:SER:HB2	25:Z:164:ASP:OD1	1.74	0.88
20:T:342:GLU:HB3	20:T:343:PRO:HD2	0.91	0.88
26:I:612:ALA:HB1	26:I:623:VAL:CB	2.04	0.87
11:H:154:C:O2	11:H:176:G:N2	2.07	0.87
11:H:156:U:H6	11:H:156:U:C5'	1.89	0.86
11:H:166:G:N2	11:H:166:G:OP2	2.08	0.86
8:E:56:GLN:HE21	8:E:97:GLY:HA2	1.36	0.86
26:I:280:GLU:C	26:I:288:THR:CB	2.43	0.86
7:C:104:LEU:HB3	7:C:172:PHE:CE1	2.11	0.85
39:K:131:GLY:O	39:K:135:TRP:CB	2.24	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:Y:405:MET:CE	38:Y:411:LEU:HD23	2.06	0.85
38:Y:405:MET:CE	38:Y:411:LEU:CD2	2.54	0.85
8:E:54:SER:N	8:E:96:TYR:CE1	2.44	0.85
7:C:104:LEU:CD1	7:C:104:LEU:HD21	2.03	0.84
26:I:280:GLU:O	26:I:288:THR:CB	2.25	0.84
11:H:41:U:H5"	11:H:41:U:H6	1.43	0.83
11:H:98:G:H4'	11:H:98:G:OP2	1.78	0.83
11:H:152:G:N2	11:H:153:A:N7	2.26	0.83
12:J:427:LYS:HE2	26:I:579:LEU:CB	2.09	0.83
6:B:80:U:H2'	6:B:80:U:OP1	1.79	0.83
11:H:150:U:C3'	24:X:124:THR:HG22	2.10	0.81
11:H:152:G:H5"	11:H:153:A:OP2	1.80	0.81
39:K:114:LEU:O	39:K:118:ALA:N	2.13	0.81
11:H:106:G:H5'	11:H:106:G:C8	2.16	0.81
5:A:1831:LYS:HG2	10:G:2:U:OP2	1.80	0.80
11:H:151:C:OP2	24:X:124:THR:HA	1.80	0.80
23:W:265:LEU:HD23	23:W:300:SER:CB	2.12	0.80
10:G:126:C:H4'	10:G:127:U:OP1	1.82	0.79
11:H:108:G:H2'	11:H:109:C:C6	2.17	0.79
10:G:130:A:O2'	10:G:131:U:OP2	1.99	0.79
23:W:252:ARG:HH11	23:W:252:ARG:HG2	1.46	0.79
11:H:153:A:H2'	11:H:154:C:H5'	1.65	0.78
10:G:138:A:H2	11:H:39:U:O2	1.65	0.78
5:A:1980:GLU:OE1	25:Z:347:PRO:HD2	1.84	0.78
8:E:61:LEU:HG	8:E:62:LEU:N	1.97	0.78
11:H:150:U:OP1	24:X:124:THR:CB	2.32	0.78
38:Y:405:MET:HE3	38:Y:411:LEU:CD2	2.14	0.78
10:G:142:U:O2'	10:G:143:U:OP1	2.01	0.77
28:Q:523:ALA:HB3	28:Q:534:ARG:H	1.48	0.77
5:A:1979:VAL:HA	5:A:1982:GLN:OE1	1.83	0.77
20:T:342:GLU:OE2	20:T:342:GLU:HA	1.82	0.77
11:H:107:A:N3	11:H:107:A:H3'	2.00	0.77
11:H:177:A:H5"	11:H:178:A:OP1	1.84	0.77
12:J:427:LYS:HZ1	26:I:579:LEU:CB	1.95	0.77
20:T:399:LYS:HB2	20:T:406:ILE:CD1	2.07	0.76
11:H:150:U:H5"	24:X:124:THR:HG21	1.66	0.76
6:B:75:G:N7	6:B:76:A:C8	2.54	0.76
11:H:143:A:H3'	11:H:143:A:N3	2.00	0.76
12:J:427:LYS:HZ3	26:I:579:LEU:CB	1.95	0.76
16:O:72:GLN:HG3	16:O:82:GLN:NE2	2.01	0.76
5:A:1945:VAL:CG1	5:A:1990:ASP:CG	2.55	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:474:LEU:HA	7:C:498:SER:O	1.86	0.75
6:B:72:U:H1'	6:B:74:U:H1'	1.68	0.75
6:B:81:U:O2'	6:B:82:A:OP2	2.02	0.75
10:G:129:G:H4'	23:W:541:LYS:CD	2.16	0.75
20:T:346:ILE:HD12	20:T:356:LEU:HD12	1.66	0.75
7:C:104:LEU:CG	7:C:104:LEU:CB	2.64	0.75
26:I:720:ILE:O	26:I:721:LYS:CB	2.34	0.74
12:J:493:ALA:HB1	12:J:499:ARG:CB	2.18	0.74
11:H:153:A:C2'	11:H:154:C:H5'	2.17	0.74
23:W:258:PRO:HB2	23:W:265:LEU:HD13	1.69	0.74
11:H:150:U:P	24:X:124:THR:HB	2.28	0.74
15:N:38:GLU:OE2	15:N:38:GLU:HA	1.87	0.74
11:H:151:C:OP1	24:X:123:GLN:CB	2.36	0.73
11:H:41:U:H2'	11:H:42:G:C8	2.23	0.73
12:J:463:GLY:O	26:I:610:ARG:CB	2.37	0.73
5:A:1945:VAL:CG1	5:A:1990:ASP:OD2	2.37	0.73
23:W:541:LYS:HB2	23:W:541:LYS:HZ2	1.54	0.73
11:H:179:C:H2'	11:H:180:G:H8	1.53	0.72
7:C:104:LEU:HB2	7:C:172:PHE:CD1	2.25	0.72
11:H:153:A:H2'	11:H:154:C:C5'	2.19	0.72
5:A:1673:SER:HB3	25:Z:164:ASP:OD1	1.88	0.72
11:H:150:U:O3'	24:X:124:THR:CG2	2.24	0.72
6:B:74:U:O4	6:B:75:G:O6	2.07	0.71
7:C:104:LEU:HB2	7:C:172:PHE:CG	2.25	0.71
11:H:39:U:C5'	11:H:39:U:H6	2.03	0.71
39:K:130:HIS:O	39:K:134:ALA:HB3	1.90	0.71
8:E:56:GLN:HE22	8:E:97:GLY:C	1.93	0.71
11:H:151:C:P	24:X:124:THR:CG2	2.78	0.71
5:A:1946:ASN:HD22	5:A:1986:LEU:HD11	1.54	0.71
11:H:105:G:N3	11:H:105:G:H2'	2.05	0.71
10:G:138:A:N1	11:H:39:U:C2	2.58	0.71
11:H:151:C:OP1	24:X:120:ALA:O	2.09	0.71
6:B:96:A:C6	6:B:97:G:C5	2.78	0.71
39:K:135:TRP:O	39:K:136:LYS:CB	2.38	0.71
7:C:104:LEU:HG	7:C:172:PHE:CE2	2.26	0.70
11:H:152:G:OP2	24:X:123:GLN:NE2	2.19	0.70
6:B:78:U:H6	6:B:78:U:H3'	1.57	0.70
23:W:252:ARG:HG3	23:W:253:SER:N	2.05	0.70
28:Q:523:ALA:HB3	28:Q:534:ARG:N	2.07	0.70
11:H:154:C:H2'	11:H:155:C:C6	2.26	0.70
23:W:258:PRO:HD2	23:W:266:ARG:HH12	1.56	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1935:ARG:HH21	25:Z:348:THR:HG21	1.56	0.69
13:L:65:ARG:CZ	26:I:799:ARG:O	2.40	0.69
11:H:153:A:N6	11:H:177:A:C2	2.60	0.69
5:A:671:THR:O	5:A:676:ARG:NH1	2.26	0.69
11:H:97:G:H4'	11:H:99:A:OP1	1.91	0.69
11:H:150:U:H3	11:H:181:G:H1	1.41	0.68
23:W:257:ILE:CD1	23:W:258:PRO:CD	2.33	0.68
20:T:356:LEU:HD22	20:T:366:VAL:HB	1.74	0.68
11:H:150:U:C5'	24:X:124:THR:CG2	2.69	0.68
10:G:137:C:C5'	10:G:137:C:H6	2.06	0.68
12:J:512:GLU:CB	26:I:640:ALA:N	2.57	0.68
13:L:65:ARG:NH2	26:I:799:ARG:HA	2.09	0.68
11:H:152:G:O3'	11:H:153:A:O4'	2.11	0.67
11:H:143:A:H2'	11:H:144:C:H6	1.59	0.67
13:L:28:LYS:HE2	13:L:50:TRP:HE1	1.60	0.67
23:W:265:LEU:HD23	23:W:300:SER:HB2	1.76	0.67
20:T:329:HIS:ND1	20:T:349:SER:OG	2.27	0.67
26:I:337:LEU:CB	26:I:363:ARG:O	2.43	0.67
23:W:266:ARG:HD3	23:W:266:ARG:N	2.10	0.67
11:H:108:G:O2'	11:H:109:C:H5'	1.95	0.67
11:H:151:C:O2	11:H:152:G:C8	2.48	0.67
39:K:113:GLN:O	39:K:117:GLN:N	2.27	0.67
5:A:663:ARG:NH1	9:F:64:U:OP2	2.28	0.66
7:C:623:GLU:H	7:C:941:LYS:HZ2	1.41	0.66
6:B:96:A:O2'	6:B:97:G:H5'	1.95	0.66
20:T:270:VAL:HB	20:T:284:TYR:HB2	1.77	0.66
11:H:67:C:H42	11:H:85:A:H61	1.44	0.66
13:L:65:ARG:NE	26:I:799:ARG:O	2.29	0.66
11:H:151:C:H2'	11:H:152:G:H8	1.59	0.66
23:W:541:LYS:HB2	23:W:541:LYS:NZ	2.10	0.66
11:H:151:C:C2	11:H:152:G:C8	2.84	0.66
6:B:96:A:C6	6:B:97:G:C6	2.84	0.66
5:A:761:ILE:HD12	5:A:775:ASN:HD22	1.61	0.66
20:T:314:ILE:HD11	20:T:326:LEU:HD21	1.78	0.65
11:H:153:A:C3'	11:H:154:C:H5'	2.25	0.65
26:I:296:PHE:CA	26:I:305:SER:CB	2.66	0.65
11:H:75:A:H61	11:H:77:C:H42	1.43	0.65
23:W:445:TRP:HE1	23:W:452:ASP:HB3	1.62	0.65
5:A:1594:CYS:SG	25:Z:268:ARG:NH2	2.68	0.65
23:W:252:ARG:HH11	23:W:252:ARG:CG	2.10	0.65
5:A:188:LEU:HD22	5:A:567:GLY:HA2	1.79	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:E:56:GLN:HG2	8:E:57:ALA:N	2.11	0.65
5:A:1699:THR:HA	5:A:1717:ASN:HD22	1.62	0.65
5:A:44:ARG:HH22	8:E:286:LYS:HB2	1.60	0.65
16:O:78:LYS:O	16:O:97:ARG:NH2	2.29	0.65
5:A:1945:VAL:HG13	5:A:1990:ASP:OD2	1.97	0.65
5:A:1437:ARG:NH1	5:A:1455:TRP:O	2.30	0.64
7:C:817:TYR:O	7:C:821:LEU:HB2	1.97	0.64
11:H:98:G:N3	11:H:98:G:H3'	2.13	0.64
23:W:258:PRO:HB2	23:W:265:LEU:CD1	2.26	0.64
11:H:153:A:H3'	11:H:154:C:H5'	1.79	0.64
20:T:282:ARG:HB2	20:T:320:LYS:HD3	1.79	0.64
10:G:129:G:C4'	23:W:541:LYS:HE3	2.28	0.64
20:T:314:ILE:HD12	20:T:324:HIS:HB2	1.78	0.64
7:C:829:GLU:HB2	7:C:907:VAL:HG22	1.80	0.64
14:M:239:ARG:HD3	26:I:817:GLU:CB	2.28	0.64
23:W:313:ILE:HB	23:W:328:PHE:HB2	1.80	0.63
11:H:147:G:H2'	11:H:148:C:H6	1.62	0.63
20:T:458:SER:OG	20:T:459:LEU:N	2.32	0.63
23:W:258:PRO:HG3	23:W:265:LEU:HD22	0.82	0.63
5:A:270:ASN:HD21	21:U:8:PRO:HB3	1.63	0.63
7:C:224:GLY:HA3	7:C:438:ILE:HD12	1.81	0.63
10:G:137:C:H2'	10:G:138:A:C8	2.34	0.63
16:O:50:ARG:NH1	16:O:122:GLU:OE1	2.32	0.63
41:D:1992:GLU:HA	41:D:1995:ALA:HB3	1.80	0.63
5:A:200:ASP:OD1	5:A:240:ARG:NH2	2.32	0.63
11:H:154:C:H2'	11:H:155:C:H6	1.62	0.63
5:A:1986:LEU:HD23	5:A:1986:LEU:C	2.19	0.62
5:A:1615:HIS:HB3	5:A:1618:LYS:HB3	1.82	0.62
5:A:1667:ARG:HH12	5:A:1674:HIS:HA	1.64	0.62
12:J:512:GLU:CB	26:I:640:ALA:HA	2.30	0.62
23:W:485:ILE:HB	23:W:502:PHE:HB2	1.80	0.62
14:M:178:GLU:OE2	14:M:181:ARG:NH2	2.32	0.62
5:A:1476:GLN:OE1	22:V:457:ARG:NH1	2.32	0.62
11:H:112:G:H2'	11:H:113:G:H8	1.64	0.62
11:H:157:G:H8	11:H:157:G:H5"	1.65	0.62
5:A:907:PRO:HG2	5:A:1032:ARG:HH21	1.65	0.62
39:K:134:ALA:O	39:K:136:LYS:N	2.33	0.62
8:E:61:LEU:HG	8:E:62:LEU:H	1.64	0.62
11:H:18:U:OP2	14:M:221:LYS:NZ	2.32	0.62
11:H:151:C:OP2	24:X:124:THR:CA	2.48	0.62
11:H:152:G:C2	11:H:153:A:C5	2.87	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:443:VAL:HG12	5:A:610:HIS:HB3	1.81	0.62
6:B:74:U:N3	6:B:75:G:C6	2.68	0.62
11:H:143:A:H2'	11:H:144:C:C6	2.35	0.62
8:E:217:ILE:HB	8:E:231:MET:HB2	1.81	0.62
11:H:156:U:C6	11:H:156:U:C5'	2.72	0.62
5:A:974:ASN:HB2	5:A:1178:TYR:HB3	1.81	0.62
42:A:3000:IHP:O24	25:Z:167:ARG:NH2	2.29	0.62
19:S:72:ARG:HD3	23:W:90:ALA:HB3	1.81	0.62
5:A:1809:ILE:HB	5:A:1818:PHE:HB2	1.81	0.61
23:W:265:LEU:CD2	23:W:300:SER:HB2	2.29	0.61
9:F:46:G:OP1	13:L:169:ARG:NH1	2.32	0.61
13:L:65:ARG:HG2	26:I:803:SER:CB	2.30	0.61
13:L:764:PRO:O	13:L:765:ARG:CB	2.48	0.61
11:H:142:C:C2'	11:H:143:A:H5'	2.30	0.61
11:H:166:G:H2'	11:H:166:G:N3	2.15	0.61
23:W:341:ASN:OD1	23:W:388:GLN:NE2	2.32	0.61
5:A:274:PRO:HG3	21:U:1:MET:HB3	1.83	0.61
7:C:737:PRO:HB3	7:C:775:ARG:HB3	1.82	0.61
19:S:131:ARG:NH1	19:S:132:VAL:O	2.34	0.61
12:J:466:ARG:CB	26:I:606:TRP:O	2.47	0.61
16:O:234:LEU:HB2	16:O:272:ILE:HB	1.81	0.61
5:A:419:ARG:NH2	5:A:423:ASP:O	2.33	0.61
15:N:101:CYS:SG	15:N:102:CYS:N	2.73	0.61
15:N:120:ARG:HH11	15:N:142:CYS:CB	2.13	0.61
23:W:258:PRO:CD	23:W:266:ARG:HH12	2.12	0.61
11:H:153:A:N6	11:H:177:A:H2	1.98	0.61
39:K:124:LEU:O	39:K:128:SER:N	2.27	0.61
7:C:172:PHE:CE2	7:C:172:PHE:CZ	2.89	0.61
8:E:90:ILE:HB	8:E:105:LEU:HB2	1.81	0.61
9:F:29:A:N6	10:G:17:U:OP2	2.34	0.60
11:H:151:C:P	24:X:124:THR:N	2.74	0.60
20:T:210:ILE:HG12	20:T:221:THR:HG22	1.83	0.60
20:T:349:SER:OG	20:T:351:ASP:OD1	2.17	0.60
5:A:1248:LEU:O	5:A:1298:ARG:NH1	2.34	0.60
11:H:108:G:O5'	11:H:108:G:H8	1.84	0.60
23:W:391:PHE:O	23:W:402:GLN:HA	2.01	0.60
10:G:130:A:O2'	10:G:131:U:P	2.60	0.60
23:W:565:LYS:HD2	23:W:577:LEU:HD21	1.83	0.60
25:Z:124:GLY:HA3	25:Z:149:ILE:HG23	1.83	0.60
22:V:628:ILE:HG12	22:V:640:THR:HB	1.84	0.60
5:A:43:LYS:O	5:A:49:ARG:NH1	2.33	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:L:155:ALA:O	13:L:159:LEU:HB2	2.00	0.60
7:C:684:LYS:HB3	7:C:795:VAL:HB	1.82	0.60
5:A:506:LEU:O	5:A:510:ARG:HB2	2.02	0.60
7:C:449:ILE:HG13	7:C:465:MET:HB3	1.84	0.60
8:E:144:VAL:HG12	8:E:145:LYS:HG3	1.84	0.60
10:G:138:A:O5'	10:G:138:A:H8	1.83	0.59
14:M:239:ARG:HG2	26:I:817:GLU:CB	2.32	0.59
20:T:347:THR:HG22	20:T:357:TRP:HE1	1.66	0.59
39:K:112:ALA:O	39:K:116:HIS:N	2.35	0.59
23:W:436:THR:HG21	23:W:464:MET:HB2	1.85	0.59
5:A:975:VAL:HB	5:A:1099:PHE:HB2	1.83	0.59
5:A:1946:ASN:ND2	5:A:1986:LEU:HD21	2.17	0.59
8:E:274:VAL:HG12	8:E:275:LYS:HG3	1.83	0.59
15:N:40:LYS:CG	15:N:41:ARG:H	2.15	0.59
7:C:277:LYS:NZ	7:C:864:PRO:O	2.36	0.59
10:G:134:U:C5'	10:G:135:G:OP2	2.51	0.59
11:H:104:U:H6	11:H:104:U:H3'	1.66	0.59
5:A:1860:GLN:HG2	5:A:1883:VAL:HB	1.85	0.59
10:G:134:U:C5	10:G:135:G:N2	2.71	0.59
5:A:1136:ARG:HA	5:A:1139:ARG:HE	1.67	0.58
6:B:96:A:N6	6:B:97:G:C6	2.71	0.58
10:G:137:C:C5'	10:G:137:C:C6	2.85	0.58
23:W:265:LEU:HD21	23:W:302:HIS:HB2	1.84	0.58
16:O:197:ASN:HB3	16:O:200:ASP:HB2	1.84	0.58
19:S:72:ARG:NH2	23:W:73:ASP:O	2.35	0.58
20:T:345:ILE:HD11	20:T:359:LEU:HD13	1.85	0.58
23:W:304:LEU:HB3	23:W:316:TRP:HB2	1.85	0.58
15:N:118:ILE:HD13	15:N:132:ILE:CG2	2.32	0.58
7:C:245:HIS:O	7:C:249:GLU:HB2	2.03	0.58
9:F:49:G:OP1	13:L:33:ARG:NH1	2.37	0.58
5:A:650:ARG:HH21	5:A:651:TRP:HE1	1.51	0.58
5:A:1784:ASN:HD22	5:A:1897:LEU:HD12	1.69	0.58
7:C:343:LEU:HD13	7:C:373:ILE:HD11	1.85	0.58
15:N:118:ILE:HD13	15:N:132:ILE:HG23	1.86	0.58
20:T:261:LEU:HB2	20:T:273:TRP:HB2	1.85	0.58
6:B:13:C:C2	6:B:65:G:C2	2.92	0.57
7:C:221:ILE:HG23	7:C:495:ARG:HB2	1.84	0.57
10:G:129:G:H4'	23:W:541:LYS:HD2	1.86	0.57
11:H:105:G:N1	11:H:107:A:H5'	2.19	0.57
6:B:96:A:C5	6:B:97:G:N7	2.73	0.57
7:C:104:LEU:CB	7:C:172:PHE:CE1	2.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:13:ASN:HA	19:S:25:LEU:O	2.03	0.57
20:T:250:ARG:NH1	20:T:266:GLU:OE2	2.36	0.57
13:L:65:ARG:NH2	26:I:799:ARG:CA	2.67	0.57
19:S:26:GLU:OE1	19:S:131:ARG:NH2	2.37	0.57
20:T:356:LEU:CD2	20:T:366:VAL:HB	2.34	0.57
5:A:1781:ASP:HB3	5:A:1808:PHE:HB3	1.86	0.57
6:B:40:U:H3	10:G:-1:G:H22	1.52	0.57
6:B:87:A:H2'	6:B:87:A:N3	2.19	0.57
13:L:263:ASP:OD2	14:M:199:ARG:NH2	2.33	0.57
5:A:617:ASN:HB2	5:A:622:GLY:O	2.04	0.57
10:G:127:U:P	23:W:547:LYS:NZ	2.78	0.57
5:A:474:ARG:HD2	6:B:14:U:H5'	1.86	0.57
5:A:1072:LEU:HD22	5:A:1087:LEU:HD22	1.86	0.57
7:C:846:VAL:HG22	7:C:887:LEU:HD11	1.86	0.57
11:H:152:G:N2	11:H:153:A:C5	2.73	0.57
11:H:154:C:O2'	11:H:155:C:H5'	2.04	0.57
16:O:72:GLN:CG	16:O:82:GLN:NE2	2.67	0.57
23:W:347:PHE:HD2	23:W:359:TRP:HB2	1.68	0.57
39:K:113:GLN:O	39:K:117:GLN:CA	2.53	0.57
6:B:96:A:C2'	6:B:97:G:H5'	2.34	0.57
11:H:169:C:O5'	11:H:169:C:H6	1.88	0.57
19:S:102:ASN:ND2	19:S:108:ASN:OD1	2.29	0.57
20:T:318:ARG:HD3	20:T:319:THR:HG23	1.87	0.57
25:Z:121:GLU:HB2	25:Z:130:LYS:HD3	1.87	0.57
5:A:798:GLY:HA3	18:R:281:ASN:HD22	1.70	0.57
20:T:272:CYS:HB3	20:T:282:ARG:HG2	1.86	0.57
6:B:78:U:H3'	6:B:78:U:C6	2.40	0.56
11:H:77:C:H2'	11:H:78:C:H6	1.70	0.56
11:H:179:C:H2'	11:H:180:G:C8	2.38	0.56
23:W:258:PRO:CB	23:W:265:LEU:HD13	2.35	0.56
5:A:1193:GLU:HB3	5:A:1231:ARG:HB3	1.86	0.56
5:A:1386:TRP:HB3	38:Y:410:VAL:HG21	1.88	0.56
7:C:172:PHE:CD2	7:C:172:PHE:CE2	2.93	0.56
8:E:239:THR:O	8:E:290:ARG:NH1	2.37	0.56
10:G:136:U:OP2	10:G:136:U:H6	1.88	0.56
11:H:71:C:C2	11:H:72:U:C5	2.94	0.56
11:H:77:C:C2	11:H:78:C:C5	2.93	0.56
11:H:141:C:C2	11:H:142:C:C5	2.94	0.56
11:H:149:A:H2'	11:H:150:U:H6	1.71	0.56
20:T:311:THR:HG22	20:T:327:SER:HB3	1.88	0.56
11:H:181:G:H2'	11:H:182:U:H6	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:27:CYS:SG	16:O:83:THR:OG1	2.63	0.56
6:B:96:A:C4	6:B:97:G:C8	2.93	0.56
11:H:73:C:C2	11:H:74:U:C5	2.94	0.56
11:H:183:G:H2'	11:H:184:C:H6	1.71	0.56
20:T:312:ALA:HB3	20:T:326:LEU:HD12	1.87	0.56
8:E:94:ASN:HB2	8:E:99:CYS:HA	1.88	0.56
11:H:72:U:C2	11:H:73:C:C5	2.94	0.56
11:H:83:A:H2'	11:H:84:C:H6	1.71	0.56
12:J:466:ARG:CA	26:I:607:GLY:HA2	2.29	0.56
5:A:409:ARG:HH11	6:B:25:C:H2'	1.71	0.56
7:C:104:LEU:CB	7:C:172:PHE:CZ	2.89	0.56
11:H:70:C:C2	11:H:71:C:C5	2.93	0.56
11:H:70:C:H2'	11:H:71:C:H6	1.70	0.56
12:J:344:GLN:HG2	14:M:132:LEU:HD21	1.87	0.56
5:A:788:GLN:HG2	5:A:1024:HIS:HB3	1.88	0.56
11:H:57:A:H2'	11:H:58:U:H6	1.70	0.56
11:H:69:U:C2	11:H:70:C:C5	2.94	0.56
11:H:73:C:H2'	11:H:74:U:H6	1.70	0.56
15:N:120:ARG:NH1	15:N:142:CYS:HB3	2.20	0.56
23:W:330:GLY:O	23:W:357:LYS:NZ	2.37	0.56
11:H:152:G:N2	11:H:153:A:C8	2.73	0.56
5:A:112:GLN:HE21	5:A:189:GLU:HA	1.71	0.56
8:E:60:MET:HB3	8:E:353:MET:CB	2.27	0.56
11:H:91:U:C2	11:H:92:U:C5	2.94	0.56
23:W:531:LYS:HG2	23:W:547:LYS:HA	1.88	0.56
25:Z:285:TYR:HD1	25:Z:292:MET:HG2	1.71	0.56
11:H:54:U:C2	11:H:55:U:C5	2.94	0.55
11:H:68:G:H2'	11:H:69:U:H6	1.71	0.55
11:H:150:U:H2'	11:H:151:C:H6	1.71	0.55
16:O:223:LEU:HD22	16:O:285:GLU:HG2	1.86	0.55
18:R:94:GLY:O	19:S:141:ARG:NH1	2.38	0.55
18:R:106:GLN:HG2	18:R:110:LYS:HD3	1.88	0.55
5:A:1986:LEU:HD23	5:A:1986:LEU:O	2.07	0.55
11:H:141:C:H2'	11:H:142:C:H6	1.71	0.55
13:L:59:LYS:HA	14:M:243:VAL:H	1.71	0.55
7:C:813:ARG:NH2	7:C:817:TYR:OH	2.40	0.55
11:H:91:U:H2'	11:H:92:U:H6	1.71	0.55
11:H:150:U:C2	11:H:151:C:C5	2.94	0.55
11:H:183:G:C4	11:H:184:C:C5	2.94	0.55
15:N:40:LYS:CG	15:N:41:ARG:N	2.70	0.55
18:R:91:ASP:OD1	18:R:91:ASP:N	2.39	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1980:GLU:OE1	25:Z:347:PRO:HG2	2.06	0.55
6:B:20:G:H1'	6:B:21:A:H5"	1.89	0.55
6:B:74:U:H5'	6:B:75:G:O5'	2.07	0.55
7:C:488:VAL:HG13	7:C:609:LYS:HE2	1.87	0.55
5:A:1431:ALA:O	5:A:1434:LYS:NZ	2.40	0.55
11:H:40:C:H2'	11:H:41:U:C6	2.40	0.55
11:H:90:A:H2'	11:H:91:U:H6	1.71	0.55
11:H:147:G:C4	11:H:148:C:C5	2.94	0.55
11:H:69:U:H2'	11:H:70:C:H6	1.71	0.55
11:H:88:A:H2'	11:H:89:U:H6	1.70	0.55
5:A:608:LEU:HD13	5:A:632:ALA:HB1	1.87	0.55
5:A:1773:SER:O	5:A:1813:ARG:NH1	2.37	0.55
11:H:54:U:H2'	11:H:55:U:H6	1.71	0.55
11:H:71:C:H2'	11:H:72:U:H6	1.70	0.55
11:H:90:A:C4	11:H:91:U:C5	2.95	0.55
18:R:145:GLU:OE1	18:R:148:ARG:NH2	2.40	0.55
5:A:1593:LEU:HD12	5:A:1664:ILE:HD11	1.89	0.55
7:C:172:PHE:CD1	7:C:172:PHE:CE1	2.95	0.55
8:E:196:VAL:HA	8:E:212:GLY:HA2	1.88	0.55
11:H:149:A:C4	11:H:150:U:C5	2.95	0.55
5:A:293:TRP:HB2	5:A:1136:ARG:HH22	1.71	0.55
5:A:1491:LYS:O	5:A:1710:ASN:ND2	2.40	0.55
5:A:1816:GLN:HE21	5:A:1916:LEU:HD21	1.71	0.55
7:C:312:SER:OG	43:C:1500:GTP:N7	2.40	0.55
11:H:59:A:H2'	11:H:60:U:H6	1.70	0.55
11:H:171:U:H6	11:H:171:U:H5'	1.72	0.55
5:A:909:TYR:HB2	5:A:1033:GLY:HA3	1.89	0.54
5:A:1476:GLN:NE2	25:Z:85:GLN:OE1	2.37	0.54
6:B:85:C:H3'	6:B:85:C:OP1	2.07	0.54
7:C:169:ASP:HB2	7:C:174:GLU:HB3	1.89	0.54
10:G:137:C:H6	10:G:137:C:O5'	1.90	0.54
11:H:68:G:C4	11:H:69:U:C5	2.95	0.54
11:H:181:G:C4	11:H:182:U:C5	2.95	0.54
14:M:226:TYR:O	14:M:230:THR:N	2.39	0.54
26:I:280:GLU:CB	26:I:288:THR:CB	2.85	0.54
7:C:561:LYS:NZ	7:C:614:TYR:O	2.36	0.54
11:H:72:U:H2'	11:H:73:C:H6	1.71	0.54
16:O:239:LEU:O	16:O:296:ARG:NH1	2.34	0.54
23:W:268:THR:HG22	23:W:270:PRO:HD2	1.88	0.54
5:A:680:HIS:NE2	5:A:684:GLU:OE2	2.40	0.54
6:B:100:C:H2'	6:B:101:U:C6	2.42	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:172:PHE:CD1	7:C:172:PHE:HA	2.43	0.54
15:N:97:TYR:HA	15:N:120:ARG:HH22	1.72	0.54
23:W:505:HIS:HB2	23:W:527:ASP:HB3	1.88	0.54
10:G:129:G:C3'	23:W:541:LYS:HE3	2.37	0.54
11:H:57:A:C4	11:H:58:U:C5	2.95	0.54
11:H:153:A:C3'	11:H:154:C:C5'	2.86	0.54
16:O:173:CYS:HB3	23:W:206:ALA:HB3	1.89	0.54
5:A:942:PRO:HD3	5:A:1091:TYR:HA	1.88	0.54
11:H:83:A:C4	11:H:84:C:C5	2.95	0.54
11:H:88:A:C4	11:H:89:U:C5	2.95	0.54
41:D:1048:VAL:O	41:D:1050:GLU:N	2.40	0.54
5:A:1980:GLU:OE1	25:Z:347:PRO:CD	2.54	0.54
7:C:143:THR:HG23	7:C:168:THR:HB	1.89	0.54
12:J:214:ILE:HG23	12:J:219:GLU:HB2	1.89	0.54
5:A:361:HIS:NE2	7:C:283:ASP:OD2	2.40	0.54
7:C:104:LEU:CB	7:C:172:PHE:CD1	2.91	0.54
8:E:208:ILE:HG23	8:E:220:TRP:HB2	1.89	0.54
11:H:59:A:C4	11:H:60:U:C5	2.95	0.54
20:T:185:MET:SD	20:T:442:ARG:NH1	2.80	0.54
5:A:1433:ASP:OD1	5:A:1439:ARG:NH2	2.40	0.54
8:E:304:SER:H	8:E:330:ILE:HB	1.72	0.54
22:V:483:GLU:O	22:V:486:THR:OG1	2.24	0.54
5:A:58:LYS:NZ	5:A:479:THR:O	2.34	0.54
5:A:1210:LYS:HG3	22:V:509:LEU:HD13	1.90	0.54
5:A:1945:VAL:HG11	5:A:1990:ASP:OD2	2.02	0.54
20:T:346:ILE:CD1	20:T:356:LEU:HD12	2.36	0.54
5:A:1904:ASP:OD1	24:X:86:ARG:NH2	2.40	0.53
6:B:79:C:H2'	6:B:79:C:O2	2.07	0.53
23:W:442:LEU:HB2	23:W:456:ILE:HB	1.89	0.53
5:A:266:SER:OG	5:A:271:MET:O	2.23	0.53
5:A:579:GLN:HG3	5:A:629:PHE:H	1.74	0.53
5:A:781:ARG:HH21	11:H:24:A:H5"	1.73	0.53
7:C:718:PHE:HB3	7:C:724:TRP:HB3	1.91	0.53
8:E:171:SER:OG	8:E:173:ASP:OD1	2.27	0.53
25:Z:179:MET:O	25:Z:182:VAL:HB	2.08	0.53
25:Z:342:HIS:HB3	25:Z:345:ALA:HB3	1.91	0.53
5:A:1132:LYS:HA	5:A:1139:ARG:HH12	1.73	0.53
5:A:1889:LEU:HB2	5:A:2013:GLY:HA3	1.90	0.53
23:W:257:ILE:HD12	23:W:257:ILE:C	2.25	0.53
5:A:48:LYS:HG3	5:A:49:ARG:HD2	1.90	0.53
5:A:1807:ILE:HB	5:A:1820:LYS:HB3	1.90	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1942:ALA:CB	5:A:1983:LEU:HD22	2.37	0.53
6:B:78:U:O2'	6:B:79:C:OP1	2.21	0.53
7:C:704:VAL:HG23	7:C:705:VAL:HG22	1.91	0.53
16:O:88:LEU:O	18:R:183:GLN:NE2	2.42	0.53
25:Z:273:LYS:HB3	25:Z:292:MET:HG3	1.90	0.53
5:A:725:PRO:HB2	18:R:272:GLY:HA3	1.90	0.53
12:J:343:GLU:HG3	12:J:369:PHE:HZ	1.73	0.53
7:C:501:ILE:O	7:C:543:ARG:HA	2.09	0.53
20:T:346:ILE:HD12	20:T:356:LEU:CD1	2.38	0.53
22:V:603:LEU:HD12	22:V:639:LEU:HD13	1.91	0.53
6:B:13:C:C2	6:B:65:G:N2	2.77	0.53
19:S:11:PRO:O	19:S:29:TRP:NE1	2.31	0.53
5:A:79:ARG:O	5:A:82:ARG:HB2	2.09	0.53
5:A:829:PRO:O	5:A:882:LYS:NZ	2.38	0.53
7:C:104:LEU:CB	7:C:172:PHE:CE2	2.92	0.53
9:F:28:A:H1'	15:N:40:LYS:O	2.09	0.53
5:A:65:HIS:HD2	15:N:46:LEU:HD22	1.73	0.53
20:T:210:ILE:HG13	20:T:480:ALA:HB2	1.91	0.53
7:C:259:LYS:HG2	43:C:1500:GTP:C6	2.43	0.52
11:H:147:G:H2'	11:H:148:C:C6	2.43	0.52
8:E:160:ALA:HB2	8:E:166:LEU:H	1.72	0.52
11:H:153:A:H3'	11:H:154:C:C5'	2.38	0.52
6:B:96:A:N6	6:B:97:G:O6	2.42	0.52
23:W:265:LEU:HD23	23:W:300:SER:OG	2.08	0.52
25:Z:127:THR:OG1	25:Z:153:GLU:OE1	2.26	0.52
6:B:71:C:H5"	6:B:72:U:C6	2.45	0.52
23:W:392:VAL:HG22	23:W:402:GLN:HG2	1.92	0.52
19:S:41:GLU:OE2	19:S:44:ARG:NH2	2.41	0.52
23:W:427:VAL:HG23	23:W:490:ALA:HB1	1.91	0.52
11:H:39:U:H6	11:H:39:U:H5"	1.72	0.52
20:T:353:THR:HG22	20:T:369:THR:HG22	1.91	0.52
18:R:61:GLY:HA2	19:S:136:ILE:HB	1.90	0.52
25:Z:87:PRO:HB2	25:Z:91:LYS:HD3	1.91	0.52
5:A:57:GLN:NE2	5:A:59:GLU:OE2	2.37	0.52
9:F:14:C:H2'	9:F:15:A:H8	1.73	0.52
10:G:136:U:OP2	10:G:136:U:C6	2.62	0.52
10:G:137:C:C6	10:G:137:C:H5"	2.45	0.52
11:H:108:G:C4	11:H:109:C:C5	2.98	0.52
12:J:355:ARG:HH21	14:M:139:THR:HG23	1.75	0.52
5:A:855:ARG:HD2	5:A:1523:ARG:HH12	1.75	0.52
5:A:2090:ILE:HA	5:A:2223:CYS:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:75:G:C8	6:B:76:A:C8	2.97	0.52
7:C:172:PHE:CE1	7:C:172:PHE:CZ	2.98	0.52
7:C:508:LYS:HE3	7:C:510:LEU:HD21	1.91	0.52
22:V:456:ARG:HG3	22:V:492:MET:HG3	1.92	0.52
23:W:265:LEU:HG	23:W:300:SER:HB2	1.90	0.52
8:E:326:HIS:HD1	8:E:346:SER:HG	1.56	0.51
9:F:22:A:H5"	15:N:115:THR:OG1	2.10	0.51
13:L:526:ARG:CB	13:L:594:PRO:CB	2.88	0.51
23:W:354:ARG:NH1	23:W:373:ARG:O	2.44	0.51
39:K:114:LEU:O	39:K:118:ALA:HB2	2.10	0.51
6:B:99:C:H2'	6:B:100:C:C6	2.45	0.51
11:H:143:A:N3	11:H:143:A:C3'	2.73	0.51
11:H:150:U:O5'	24:X:124:THR:HB	2.10	0.51
5:A:1921:ASP:HB3	5:A:1966:HIS:CD2	2.44	0.51
6:B:46:U:O2	21:U:11:ARG:NH2	2.43	0.51
8:E:80:THR:HA	8:E:93:TRP:O	2.11	0.51
20:T:307:SER:OG	20:T:308:ARG:N	2.44	0.51
23:W:265:LEU:CG	23:W:300:SER:HB2	2.40	0.51
8:E:259:VAL:HB	8:E:277:PHE:HB2	1.92	0.51
13:L:696:LEU:HA	39:K:110:SER:CB	2.40	0.51
23:W:500:LYS:HA	23:W:540:THR:HG21	1.93	0.51
5:A:71:ARG:NH1	15:N:34:THR:HG22	2.26	0.51
5:A:658:ARG:NH1	9:F:67:G:OP1	2.35	0.51
8:E:91:LEU:HD22	8:E:101:ASN:HD21	1.74	0.51
11:H:105:G:N3	11:H:105:G:C2'	2.72	0.51
12:J:466:ARG:CB	26:I:610:ARG:CB	2.89	0.51
5:A:1776:ILE:HB	5:A:1858:PRO:HA	1.92	0.51
10:G:127:U:P	23:W:547:LYS:HZ3	2.33	0.51
11:H:108:G:C4	11:H:109:C:C6	2.98	0.51
23:W:266:ARG:N	23:W:266:ARG:CD	2.73	0.51
26:I:729:SER:O	26:I:732:ALA:HB3	2.09	0.51
10:G:130:A:HO2'	10:G:131:U:P	2.34	0.51
5:A:584:HIS:HE1	42:A:3000:IHP:O22	1.93	0.51
7:C:734:ALA:HB2	7:C:767:VAL:HG22	1.93	0.51
7:C:926:ALA:HA	7:C:929:LEU:HG	1.92	0.51
20:T:477:LEU:HB3	20:T:489:TYR:HB2	1.92	0.51
5:A:552:ARG:NH1	5:A:589:THR:O	2.44	0.51
5:A:711:GLN:HE22	11:H:18:U:H3'	1.76	0.51
12:J:512:GLU:CB	26:I:640:ALA:CA	2.88	0.51
18:R:52:PRO:HB3	18:R:57:ASP:HB3	1.93	0.51
5:A:109:PRO:HG3	5:A:630:TRP:HE1	1.76	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:78:U:C6	6:B:78:U:C3'	2.94	0.50
7:C:445:ALA:HA	7:C:448:LYS:HB3	1.93	0.50
23:W:267:SER:O	23:W:268:THR:O	2.28	0.50
7:C:448:LYS:O	7:C:452:THR:HB	2.11	0.50
7:C:622:GLU:OE1	7:C:941:LYS:NZ	2.38	0.50
15:N:18:ILE:HG21	15:N:70:ILE:HD11	1.93	0.50
15:N:120:ARG:NH1	15:N:142:CYS:CB	2.75	0.50
23:W:552:VAL:HG13	23:W:571:TRP:CD1	2.46	0.50
25:Z:122:ASN:O	25:Z:138:ARG:NH2	2.44	0.50
5:A:329:LEU:HD12	7:C:177:ARG:HD2	1.92	0.50
5:A:425:PRO:HG3	6:B:26:A:H5'	1.93	0.50
7:C:104:LEU:CB	7:C:172:PHE:CD2	2.94	0.50
20:T:427:LEU:HB3	20:T:439:TRP:HB2	1.93	0.50
23:W:252:ARG:HD2	23:W:257:ILE:HG22	1.94	0.50
5:A:108:MET:O	5:A:110:TRP:N	2.44	0.50
5:A:663:ARG:NH2	9:F:65:G:N7	2.58	0.50
6:B:74:U:N3	6:B:75:G:C5	2.80	0.50
12:J:294:HIS:CD2	13:L:227:THR:HG1	2.29	0.50
13:L:48:ALA:O	13:L:52:GLU:CB	2.60	0.50
20:T:289:SER:OG	20:T:308:ARG:NE	2.36	0.50
23:W:387:LYS:HD3	23:W:390:LEU:HD12	1.93	0.50
23:W:534:ILE:HB	23:W:544:SER:HB3	1.94	0.50
23:W:541:LYS:NZ	23:W:541:LYS:CB	2.73	0.50
11:H:100:U:H4'	11:H:101:U:H5'	1.93	0.50
16:O:176:GLY:HA2	23:W:206:ALA:HB2	1.94	0.50
16:O:283:ALA:O	16:O:287:SER:HB3	2.11	0.50
5:A:658:ARG:NH2	9:F:65:G:OP2	2.43	0.50
7:C:725:ASP:O	7:C:729:ALA:N	2.43	0.50
10:G:129:G:H4'	23:W:541:LYS:CE	2.41	0.50
20:T:213:GLU:HG3	20:T:218:TRP:CE2	2.47	0.50
8:E:69:VAL:HG11	8:E:351:LEU:HD21	1.94	0.50
10:G:129:G:C4'	23:W:541:LYS:CE	2.90	0.50
11:H:168:A:H3'	11:H:169:C:C5	2.47	0.50
5:A:1318:THR:HB	5:A:1324:GLY:HA3	1.94	0.50
5:A:1676:ILE:HD13	5:A:1706:ASP:HB2	1.93	0.50
7:C:129:ILE:HG22	7:C:199:LEU:HB3	1.93	0.50
8:E:258:THR:HG22	8:E:260:ARG:HG3	1.94	0.50
5:A:160:HIS:HE1	25:Z:170:TRP:HA	1.77	0.50
5:A:161:PHE:CE2	5:A:626:GLY:HA2	2.47	0.50
5:A:1137:ASP:O	5:A:1141:ARG:NH1	2.43	0.50
13:L:65:ARG:NH2	26:I:799:ARG:C	2.64	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:530:LYS:NZ	22:V:564:VAL:O	2.45	0.50
5:A:380:LEU:HD12	5:A:384:VAL:HG21	1.92	0.49
5:A:1949:ARG:NH2	24:X:62:GLU:OE1	2.45	0.49
7:C:168:THR:HG23	7:C:184:THR:HB	1.93	0.49
12:J:427:LYS:HE3	26:I:579:LEU:CB	2.36	0.49
12:J:466:ARG:CB	26:I:606:TRP:C	2.80	0.49
5:A:224:THR:N	6:B:12:U:OP1	2.39	0.49
5:A:409:ARG:HE	5:A:413:LEU:HD21	1.77	0.49
7:C:485:ASP:OD1	7:C:485:ASP:N	2.44	0.49
9:F:78:A:OP2	13:L:170:LYS:NZ	2.38	0.49
9:F:85:U:H5'	14:M:193:ARG:HD2	1.94	0.49
11:H:110:A:H2'	11:H:111:G:C2	2.46	0.49
23:W:252:ARG:CG	23:W:252:ARG:NH1	2.73	0.49
39:K:114:LEU:O	39:K:118:ALA:CB	2.60	0.49
7:C:137:HIS:HB3	7:C:140:HIS:CD2	2.47	0.49
7:C:834:VAL:HG21	7:C:883:PHE:HE2	1.78	0.49
18:R:151:LEU:HD22	20:T:323:VAL:HG11	1.92	0.49
5:A:1275:ARG:HD2	5:A:1375:TRP:CE2	2.47	0.49
7:C:171:LEU:HD11	7:C:182:LYS:HD2	1.94	0.49
7:C:774:THR:HA	7:C:784:ILE:HD12	1.94	0.49
5:A:1275:ARG:NH1	5:A:1373:GLN:O	2.39	0.49
5:A:1984:LYS:HG2	5:A:1988:LEU:HD12	1.94	0.49
6:B:79:C:C6	6:B:79:C:C5'	2.95	0.49
9:F:21:U:H1'	15:N:121:VAL:CG2	2.42	0.49
9:F:21:U:O4'	15:N:121:VAL:HG23	2.12	0.49
16:O:26:THR:HG22	16:O:155:PRO:HB3	1.93	0.49
5:A:1972:THR:OG1	5:A:1975:GLU:OE1	2.24	0.49
7:C:476:CYS:HB2	7:C:565:ILE:HB	1.95	0.49
7:C:747:ASP:HB3	7:C:791:ILE:HB	1.94	0.49
10:G:126:C:O3'	23:W:547:LYS:NZ	2.46	0.49
15:N:119:CYS:SG	15:N:139:CYS:HB3	2.53	0.49
23:W:531:LYS:HD3	23:W:547:LYS:HG2	1.93	0.49
16:O:56:ARG:HG2	16:O:67:LYS:HB3	1.95	0.49
28:Q:523:ALA:O	28:Q:532:PRO:HA	2.13	0.49
5:A:118:VAL:HG21	5:A:487:LEU:HD12	1.94	0.49
5:A:1576:ILE:O	5:A:1746:ARG:NH1	2.38	0.49
5:A:1894:GLN:NE2	24:X:69:GLY:O	2.46	0.49
14:M:239:ARG:CG	26:I:817:GLU:CB	2.91	0.49
16:O:34:ILE:HB	18:R:197:ILE:HG12	1.94	0.49
5:A:379:GLU:HG2	7:C:355:LYS:HB3	1.92	0.49
5:A:1215:ASN:HB3	5:A:1224:ARG:HD2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:44:A:O2'	10:G:-5:G:N2	2.43	0.49
14:M:210:TYR:HB3	14:M:219:ASN:HD22	1.78	0.49
17:P:13:ARG:NH1	20:T:329:HIS:O	2.45	0.49
18:R:132:LEU:HA	20:T:399:LYS:HE3	1.95	0.49
20:T:342:GLU:CG	20:T:343:PRO:CD	2.91	0.49
12:J:221:ASN:ND2	13:L:211:ASN:OD1	2.46	0.48
13:L:65:ARG:HE	26:I:803:SER:CB	2.26	0.48
18:R:107:SER:OG	18:R:109:ASP:OD1	2.28	0.48
20:T:339:GLN:NE2	20:T:342:GLU:O	2.45	0.48
5:A:1066:GLN:CG	38:Y:423:THR:O	2.61	0.48
5:A:1615:HIS:HD2	5:A:1616:PRO:HD2	1.78	0.48
7:C:135:CYS:HB2	7:C:242:LEU:HD13	1.95	0.48
7:C:137:HIS:HB2	7:C:239:THR:HG23	1.94	0.48
11:H:107:A:N3	11:H:107:A:C3'	2.74	0.48
20:T:422:ASN:HB3	20:T:424:ASP:H	1.78	0.48
5:A:699:GLU:OE1	18:R:235:ARG:NH2	2.46	0.48
13:L:784:LEU:CB	39:K:195:ILE:CB	2.90	0.48
18:R:74:LEU:HD23	18:R:75:ASP:H	1.76	0.48
5:A:1610:GLN:NE2	5:A:1612:GLU:OE2	2.46	0.48
23:W:258:PRO:CB	23:W:265:LEU:CD1	2.91	0.48
6:B:96:A:C2	6:B:97:G:C4	3.02	0.48
5:A:768:ASP:OD1	6:B:40:U:O2'	2.27	0.48
5:A:854:SER:OG	5:A:855:ARG:N	2.47	0.48
8:E:233:GLY:O	8:E:260:ARG:NH1	2.46	0.48
8:E:92:LEU:HD12	8:E:103:ALA:HB3	1.93	0.48
10:G:136:U:H2'	10:G:137:C:C5	2.49	0.48
20:T:394:ASN:OD1	20:T:396:LYS:NZ	2.47	0.48
5:A:1865:ARG:NH1	10:G:147:C:OP1	2.47	0.48
11:H:101:U:H4'	11:H:102:U:OP1	2.14	0.48
13:L:59:LYS:HG2	14:M:243:VAL:HA	1.96	0.48
16:O:276:THR:HG23	16:O:279:ALA:H	1.78	0.48
8:E:260:ARG:HG2	8:E:276:ILE:HG12	1.96	0.48
11:H:151:C:OP2	24:X:124:THR:N	2.46	0.48
13:L:74:LEU:HD23	13:L:77:LEU:HD12	1.94	0.48
5:A:325:HIS:HD2	5:A:326:HIS:HD2	1.60	0.47
5:A:522:PHE:O	5:A:548:ARG:NH2	2.38	0.47
5:A:1768:TYR:CZ	5:A:2012:LEU:HD11	2.49	0.47
7:C:226:VAL:HA	7:C:254:THR:O	2.14	0.47
5:A:211:GLN:OE1	5:A:214:ARG:NH1	2.47	0.47
5:A:1214:TRP:CE2	5:A:1230:LEU:HD11	2.49	0.47
5:A:1219:GLU:O	5:A:1222:LYS:NZ	2.42	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1560:ILE:HG21	5:A:1573:LEU:HD13	1.95	0.47
20:T:248:THR:HB	20:T:266:GLU:HG3	1.95	0.47
28:Q:523:ALA:CB	28:Q:534:ARG:O	2.63	0.47
5:A:356:ILE:HD13	7:C:867:PRO:HD3	1.96	0.47
5:A:1831:LYS:HG2	10:G:2:U:P	2.53	0.47
5:A:1962:THR:HG22	5:A:1969:PRO:HA	1.96	0.47
7:C:440:SER:O	7:C:443:VAL:N	2.47	0.47
11:H:44:U:H2'	11:H:45:C:C6	2.48	0.47
12:J:323:LEU:HD22	14:M:179:ILE:HG22	1.96	0.47
14:M:237:LEU:HD11	18:R:264:LEU:HD22	1.95	0.47
19:S:18:THR:HG22	19:S:159:ILE:HG12	1.96	0.47
7:C:506:PRO:HA	7:C:526:THR:HA	1.96	0.47
7:C:938:ARG:HE	7:C:945:GLU:HA	1.80	0.47
8:E:167:VAL:HB	8:E:179:TRP:HB2	1.96	0.47
11:H:42:G:H8	11:H:42:G:O5'	1.98	0.47
11:H:151:C:C2	11:H:152:G:N7	2.82	0.47
18:R:185:GLY:O	18:R:187:ALA:N	2.47	0.47
23:W:258:PRO:HD2	23:W:266:ARG:NH1	2.28	0.47
5:A:1775:GLN:HG2	5:A:1859:LYS:HD2	1.97	0.47
6:B:93:U:H4'	6:B:94:U:H5"	1.97	0.47
10:G:138:A:H2'	10:G:139:U:C6	2.49	0.47
14:M:221:LYS:HE3	18:R:249:PRO:HB3	1.96	0.47
5:A:1251:SER:O	5:A:1298:ARG:NH2	2.33	0.47
16:O:123:ARG:NH1	18:R:222:PRO:O	2.46	0.47
5:A:62:PRO:HG3	15:N:53:HIS:CD2	2.50	0.47
5:A:425:PRO:HB2	5:A:428:LYS:HB2	1.97	0.47
10:G:129:G:H4'	23:W:541:LYS:HE3	1.95	0.47
11:H:153:A:C8	11:H:154:C:H5'	2.50	0.47
16:O:27:CYS:SG	16:O:66:LYS:NZ	2.81	0.47
20:T:416:ILE:HA	20:T:431:ALA:HA	1.95	0.47
22:V:565:LEU:HG	22:V:568:ILE:HD12	1.95	0.47
9:F:25:C:N4	16:O:39:GLU:OE1	2.47	0.47
10:G:145:U:HO2'	10:G:146:C:P	2.38	0.47
11:H:98:G:N3	11:H:98:G:C3'	2.78	0.47
11:H:141:C:H2'	11:H:142:C:C6	2.50	0.47
11:H:183:G:H2'	11:H:184:C:C6	2.50	0.47
20:T:342:GLU:CG	20:T:343:PRO:HD2	2.37	0.47
8:E:60:MET:CG	8:E:353:MET:SD	2.89	0.47
11:H:91:U:H2'	11:H:92:U:C6	2.50	0.47
11:H:149:A:H2'	11:H:150:U:C6	2.50	0.47
25:Z:133:CYS:SG	25:Z:134:PHE:N	2.88	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:143:GLN:NE2	5:A:207:PHE:O	2.45	0.47
5:A:668:VAL:HB	9:F:68:C:H5"	1.96	0.47
5:A:1763:LEU:HG	5:A:1862:ILE:HD13	1.96	0.47
7:C:205:THR:HB	7:C:215:VAL:HG22	1.97	0.47
11:H:41:U:H5"	11:H:41:U:C6	2.35	0.47
16:O:22:ILE:HG23	23:W:112:SER:HB3	1.97	0.47
22:V:470:GLU:OE2	22:V:513:ARG:NH1	2.47	0.47
5:A:1350:ILE:HD12	22:V:470:GLU:HG3	1.97	0.46
5:A:1806:ALA:HA	5:A:1820:LYS:O	2.14	0.46
9:F:82:A:N6	11:H:19:G:OP1	2.48	0.46
10:G:134:U:H5"	10:G:135:G:OP2	2.15	0.46
11:H:38:A:H2'	11:H:39:U:H5"	1.97	0.46
11:H:72:U:H2'	11:H:73:C:C6	2.50	0.46
19:S:52:LYS:HE3	19:S:156:ASP:HA	1.97	0.46
22:V:536:ILE:H	22:V:536:ILE:HG13	1.49	0.46
7:C:448:LYS:O	7:C:452:THR:CB	2.63	0.46
7:C:692:LEU:HD12	7:C:786:ASN:HA	1.96	0.46
13:L:48:ALA:O	13:L:52:GLU:HB3	2.15	0.46
25:Z:334:ALA:O	25:Z:338:GLY:N	2.44	0.46
12:J:466:ARG:CB	26:I:607:GLY:N	2.75	0.46
14:M:239:ARG:CD	26:I:817:GLU:CB	2.92	0.46
23:W:524:ILE:HD11	23:W:558:TRP:HE3	1.79	0.46
5:A:856:LEU:HD23	5:A:860:GLN:HB3	1.97	0.46
7:C:156:GLU:OE2	7:C:167:TYR:OH	2.33	0.46
8:E:326:HIS:CE1	8:E:346:SER:HG	2.32	0.46
11:H:57:A:H2'	11:H:58:U:C6	2.50	0.46
11:H:150:U:H2'	11:H:151:C:C6	2.49	0.46
18:R:127:ALA:HB2	20:T:442:ARG:HD3	1.97	0.46
5:A:103:LEU:HD11	5:A:554:THR:HG22	1.97	0.46
11:H:41:U:H6	11:H:41:U:C5'	2.20	0.46
11:H:90:A:H2'	11:H:91:U:C6	2.50	0.46
11:H:182:U:H2'	11:H:183:G:H8	1.81	0.46
12:J:193:GLN:O	12:J:196:ARG:HB3	2.16	0.46
12:J:221:ASN:HD22	12:J:221:ASN:HA	1.54	0.46
23:W:400:ILE:HD12	23:W:445:TRP:CZ3	2.51	0.46
23:W:506:MET:H	23:W:527:ASP:HB2	1.81	0.46
5:A:976:MET:HG2	5:A:1187:PHE:HB3	1.97	0.46
5:A:1045:GLY:HA3	5:A:1090:ARG:NH2	2.29	0.46
5:A:542:ASN:O	5:A:546:LEU:HB2	2.15	0.46
5:A:944:ASP:HA	5:A:1437:ARG:HE	1.81	0.46
5:A:1312:PRO:HG2	5:A:1314:VAL:HG12	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:698:GLU:O	7:C:702:ASN:N	2.49	0.46
8:E:338:ASP:OD1	8:E:338:ASP:N	2.49	0.46
9:F:21:U:OP1	15:N:116:ASN:ND2	2.49	0.46
11:H:70:C:H2'	11:H:71:C:C6	2.49	0.46
11:H:104:U:H4'	11:H:105:G:C4'	2.45	0.46
11:H:108:G:H8	11:H:108:G:P	2.39	0.46
11:H:181:G:H2'	11:H:182:U:C6	2.50	0.46
22:V:539:LEU:HD12	22:V:544:LEU:HD23	1.98	0.46
23:W:400:ILE:HD11	23:W:421:VAL:HG11	1.98	0.46
5:A:320:TYR:OH	7:C:634:GLU:OE2	2.30	0.46
5:A:852:VAL:O	5:A:854:SER:N	2.49	0.46
5:A:1418:ARG:HE	5:A:1464:LEU:HD23	1.80	0.46
8:E:98:ASP:HB3	8:E:100:ASP:OD1	2.16	0.46
11:H:81:G:H2'	11:H:82:G:H8	1.80	0.46
11:H:142:C:H2'	11:H:143:A:H5'	1.98	0.46
14:M:209:ASP:HB2	18:R:263:PRO:HG3	1.98	0.46
41:D:1349:GLY:HA2	41:D:1491:SER:O	2.16	0.46
7:C:935:ILE:O	7:C:939:ARG:N	2.46	0.46
11:H:68:G:H2'	11:H:69:U:C6	2.50	0.46
11:H:69:U:H2'	11:H:70:C:C6	2.49	0.46
11:H:78:C:H2'	11:H:79:G:H8	1.81	0.46
13:L:140:ASP:OD1	13:L:140:ASP:N	2.49	0.46
23:W:434:VAL:HG21	23:W:476:LEU:HD11	1.98	0.46
11:H:152:G:O2'	11:H:153:A:H1'	2.16	0.46
16:O:236:VAL:O	16:O:269:CYS:HA	2.16	0.46
11:H:56:A:H2'	11:H:57:A:H8	1.81	0.45
11:H:104:U:H3'	11:H:104:U:C6	2.49	0.45
26:I:712:VAL:O	26:I:715:GLY:N	2.49	0.45
5:A:359:ILE:HA	7:C:864:PRO:HB3	1.97	0.45
5:A:603:ARG:O	5:A:606:LYS:HB2	2.16	0.45
5:A:1242:ASN:OD1	5:A:1245:ARG:NH2	2.42	0.45
11:H:54:U:H2'	11:H:55:U:C6	2.50	0.45
11:H:71:C:H2'	11:H:72:U:C6	2.50	0.45
5:A:696:MET:HB2	5:A:696:MET:HE3	1.81	0.45
5:A:1382:SER:HA	5:A:1415:GLY:HA2	1.98	0.45
5:A:1945:VAL:HG11	5:A:1990:ASP:CB	2.46	0.45
7:C:104:LEU:CB	7:C:172:PHE:CG	2.97	0.45
7:C:227:LEU:HB3	7:C:255:VAL:HG22	1.98	0.45
9:F:1:G:O2'	15:N:99:ASN:ND2	2.50	0.45
10:G:137:C:C5	10:G:137:C:OP2	2.69	0.45
11:H:102:U:OP2	11:H:102:U:H3'	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:H:171:U:H2'	11:H:172:C:O4'	2.16	0.45
41:D:441:GLY:O	41:D:693:THR:N	2.36	0.45
5:A:2121:ARG:O	5:A:2154:HIS:HA	2.15	0.45
7:C:87:GLN:HE21	20:T:239:LYS:HB3	1.81	0.45
11:H:88:A:H2'	11:H:89:U:C6	2.50	0.45
11:H:92:U:H2'	11:H:93:A:H8	1.82	0.45
18:R:303:GLU:OE2	18:R:307:GLN:NE2	2.49	0.45
8:E:75:HIS:NE2	8:E:121:GLY:O	2.46	0.45
11:H:58:U:H2'	11:H:59:A:H8	1.82	0.45
11:H:74:U:H2'	11:H:75:A:H8	1.81	0.45
11:H:79:G:H2'	11:H:80:A:H8	1.81	0.45
11:H:82:G:H2'	11:H:83:A:H8	1.81	0.45
16:O:280:ALA:HB1	16:O:302:TRP:HH2	1.81	0.45
5:A:338:VAL:HG12	7:C:262:ARG:HH21	1.82	0.45
6:B:96:A:N1	6:B:97:G:C5	2.84	0.45
9:F:22:A:OP2	23:W:130:ARG:NH2	2.50	0.45
10:G:139:U:O4	10:G:140:A:N6	2.50	0.45
11:H:73:C:H2'	11:H:74:U:C6	2.50	0.45
11:H:148:C:H2'	11:H:149:A:H8	1.82	0.45
13:L:28:LYS:NZ	18:R:273:ARG:HH22	2.15	0.45
15:N:118:ILE:CD1	15:N:132:ILE:HG23	2.46	0.45
16:O:68:THR:HA	16:O:83:THR:HG22	1.99	0.45
18:R:94:GLY:HA3	19:S:141:ARG:HD3	1.97	0.45
5:A:1908:LYS:HE3	23:W:448:ASP:HB3	1.98	0.45
7:C:566:THR:OG1	7:C:567:GLU:N	2.50	0.45
7:C:604:LEU:HD23	7:C:607:LEU:HD12	1.98	0.45
8:E:95:VAL:HB	8:E:96:TYR:HD2	1.81	0.45
11:H:89:U:H2'	11:H:90:A:H8	1.82	0.45
11:H:100:U:C6	11:H:100:U:C5'	2.93	0.45
5:A:1980:GLU:OE1	25:Z:347:PRO:CG	2.64	0.45
7:C:158:ARG:HB2	7:C:165:LEU:HB3	1.99	0.45
10:G:120:G:O4'	26:I:316:GLU:O	2.34	0.45
11:H:80:A:H2'	11:H:81:G:H8	1.81	0.45
15:N:118:ILE:H	15:N:118:ILE:HG13	1.62	0.45
16:O:233:THR:HA	16:O:272:ILE:O	2.17	0.45
6:B:69:A:N6	6:B:70:A:N3	2.64	0.45
7:C:94:ILE:H	7:C:94:ILE:HG13	1.45	0.45
7:C:887:LEU:HD23	7:C:897:SER:HB2	1.98	0.45
11:H:67:C:H2'	11:H:68:G:H8	1.81	0.45
19:S:72:ARG:HH22	23:W:74:PRO:HA	1.82	0.45
20:T:373:LYS:HD2	20:T:392:PRO:HB2	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:221:ILE:O	7:C:495:ARG:NH1	2.50	0.45
12:J:466:ARG:HA	26:I:606:TRP:C	2.37	0.45
13:L:52:GLU:OE2	13:L:134:THR:OG1	2.34	0.45
13:L:717:MET:O	13:L:721:LEU:N	2.48	0.45
20:T:418:THR:HG21	20:T:468:CYS:H	1.81	0.45
23:W:257:ILE:HG23	23:W:257:ILE:O	2.17	0.45
23:W:267:SER:O	23:W:268:THR:C	2.56	0.45
23:W:514:VAL:HA	23:W:524:ILE:O	2.16	0.45
39:K:112:ALA:O	39:K:116:HIS:CA	2.62	0.45
5:A:1986:LEU:C	5:A:1986:LEU:CD2	2.85	0.44
11:H:106:G:C4'	11:H:107:A:OP1	2.45	0.44
22:V:499:GLN:HG2	25:Z:72:TRP:CG	2.52	0.44
41:D:721:VAL:HA	41:D:825:THR:O	2.17	0.44
8:E:355:GLU:H	23:W:82:ASN:ND2	2.16	0.44
11:H:84:C:H2'	11:H:85:A:H8	1.82	0.44
11:H:93:A:H2'	11:H:94:A:H8	1.82	0.44
17:P:204:GLN:O	17:P:206:LYS:N	2.50	0.44
23:W:420:ALA:O	23:W:438:ASP:N	2.46	0.44
5:A:417:ARG:NH1	6:B:58:U:O3'	2.44	0.44
6:B:20:G:H8	6:B:21:A:H2'	1.81	0.44
7:C:63:LYS:HE3	7:C:65:TYR:HE1	1.82	0.44
9:F:23:U:OP1	15:N:115:THR:HG21	2.17	0.44
11:H:180:G:H2'	11:H:181:G:H8	1.81	0.44
13:L:699:ASN:CB	39:K:114:LEU:CB	2.95	0.44
7:C:112:THR:HG23	7:C:154:HIS:CD2	2.53	0.44
11:H:55:U:H2'	11:H:56:A:H8	1.82	0.44
11:H:59:A:H2'	11:H:60:U:C6	2.50	0.44
11:H:170:C:C6	11:H:170:C:OP2	2.70	0.44
12:J:251:TRP:CE3	12:J:252:GLU:HG3	2.53	0.44
18:R:64:PHE:H	18:R:71:GLN:HE22	1.65	0.44
20:T:405:PHE:O	20:T:405:PHE:CD1	2.70	0.44
23:W:181:PHE:HD1	23:W:200:VAL:HG12	1.83	0.44
23:W:264:ASN:ND2	23:W:267:SER:HB2	2.32	0.44
38:Y:405:MET:CE	38:Y:411:LEU:HD21	2.43	0.44
5:A:348:PRO:HB3	5:A:394:TYR:CZ	2.52	0.44
5:A:1497:THR:OG1	5:A:1499:GLU:OE1	2.26	0.44
42:A:3000:IHP:H3	42:A:3000:IHP:O32	2.17	0.44
11:H:153:A:C2'	11:H:154:C:C5'	2.86	0.44
13:L:55:ASP:HB3	13:L:58:ILE:HG13	2.00	0.44
14:M:162:PRO:HA	14:M:167:LEU:HD12	1.98	0.44
18:R:105:GLY:HA3	18:R:225:PRO:HG2	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:294:LEU:HD12	20:T:303:LEU:HD11	2.00	0.44
23:W:462:HIS:CE1	23:W:482:ASP:HB3	2.52	0.44
5:A:89:LEU:O	5:A:92:LEU:HB3	2.18	0.44
5:A:121:HIS:HD2	18:R:207:MET:HG3	1.82	0.44
5:A:721:LYS:O	5:A:781:ARG:NH1	2.51	0.44
5:A:1214:TRP:NE1	5:A:1276:GLU:OE1	2.50	0.44
11:H:83:A:H2'	11:H:84:C:C6	2.49	0.44
19:S:58:LYS:HE2	19:S:144:MET:HG2	2.00	0.44
5:A:620:PRO:HG2	25:Z:134:PHE:HE2	1.83	0.44
5:A:1494:TYR:HB3	5:A:1744:ARG:HD3	2.00	0.44
5:A:2008:ARG:O	5:A:2012:LEU:HB2	2.18	0.44
7:C:82:GLN:HE21	20:T:238:LEU:H	1.66	0.44
7:C:311:SER:HB3	7:C:316:ILE:HB	2.00	0.44
11:H:77:C:H2'	11:H:78:C:C6	2.50	0.44
11:H:143:A:OP2	11:H:143:A:C2	2.71	0.44
18:R:136:ASP:HB3	18:R:138:GLU:H	1.82	0.44
8:E:299:LYS:HE3	8:E:320:LEU:HD13	1.99	0.44
8:E:346:SER:OG	8:E:348:ASP:OD1	2.36	0.44
11:H:169:C:O5'	11:H:169:C:C6	2.70	0.44
15:N:118:ILE:CD1	15:N:132:ILE:CG2	2.95	0.44
9:F:21:U:C1'	15:N:121:VAL:CG2	2.96	0.44
9:F:28:A:C1'	15:N:40:LYS:O	2.66	0.44
11:H:108:G:C5	11:H:109:C:C5	3.06	0.44
11:H:114:A:C8	11:H:114:A:OP2	2.70	0.44
11:H:153:A:H2'	11:H:154:C:H5"	2.00	0.44
12:J:232:GLU:OE2	12:J:267:ARG:NH2	2.44	0.44
12:J:338:GLU:OE2	14:M:164:SER:OG	2.28	0.44
5:A:787:GLU:OE2	5:A:790:ARG:NH2	2.43	0.43
5:A:1286:ASP:OD1	5:A:1354:ARG:NH2	2.51	0.43
11:H:150:U:C4'	24:X:124:THR:HG22	2.48	0.43
11:H:154:C:O2'	11:H:155:C:C5'	2.66	0.43
20:T:354:ILE:HD11	20:T:389:SER:CB	2.48	0.43
5:A:106:MET:HA	5:A:107:PRO:HD3	1.84	0.43
5:A:1199:LYS:HD3	5:A:1206:GLU:HG3	2.00	0.43
8:E:336:HIS:CD2	8:E:337:PRO:HD2	2.52	0.43
9:F:21:U:C1'	15:N:121:VAL:HG23	2.48	0.43
13:L:703:MET:O	13:L:707:ALA:HB3	2.18	0.43
20:T:289:SER:OG	20:T:290:ALA:N	2.51	0.43
26:I:433:ALA:O	26:I:437:CYS:N	2.50	0.43
7:C:101:LYS:HG2	7:C:172:PHE:HE2	1.83	0.43
7:C:107:GLN:HG3	7:C:108:THR:H	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:G:143:U:H2'	10:G:145:U:C5	2.53	0.43
20:T:297:HIS:HB2	20:T:302:VAL:HG12	2.00	0.43
5:A:1070:ASP:OD1	5:A:1073:SER:OG	2.28	0.43
7:C:747:ASP:OD1	7:C:747:ASP:N	2.50	0.43
11:H:178:A:N3	11:H:178:A:H2'	2.33	0.43
16:O:133:PRO:HB2	16:O:136:MET:HB3	2.00	0.43
20:T:345:ILE:O	20:T:357:TRP:HD1	2.01	0.43
7:C:134:LEU:HD23	7:C:226:VAL:HB	2.00	0.43
7:C:296:GLU:HB2	7:C:299:ILE:HD11	2.01	0.43
10:G:134:U:H3'	10:G:135:G:H21	1.84	0.43
11:H:104:U:C6	11:H:104:U:C3'	3.01	0.43
11:H:157:G:H2'	11:H:158:G:O4'	2.18	0.43
11:H:166:G:OP2	11:H:166:G:C2	2.72	0.43
7:C:264:ILE:HG12	7:C:378:TYR:CE1	2.53	0.43
9:F:17:C:H2'	9:F:18:A:H8	1.84	0.43
11:H:142:C:O2'	11:H:143:A:H5'	2.18	0.43
12:J:228:ARG:NE	12:J:252:GLU:OE2	2.51	0.43
6:B:74:U:O2	6:B:74:U:H2'	2.18	0.43
12:J:213:LYS:HA	13:L:243:ARG:HA	2.01	0.43
15:N:133:GLU:OE2	15:N:140:ARG:NH2	2.36	0.43
16:O:76:LYS:HG2	23:W:111:LEU:HD22	2.00	0.43
18:R:119:LEU:HD21	18:R:230:MET:HB3	2.01	0.43
19:S:72:ARG:HG3	23:W:72:LEU:HD13	2.00	0.43
5:A:624:GLY:HA2	5:A:625:PRO:HD3	1.69	0.43
5:A:1130:ASN:HB3	5:A:1132:LYS:HE3	2.00	0.43
5:A:1803:ILE:HG13	5:A:1804:ASN:H	1.84	0.43
7:C:242:LEU:HD23	7:C:242:LEU:HA	1.87	0.43
7:C:255:VAL:HG21	7:C:285:VAL:HG11	2.00	0.43
13:L:53:TRP:HD1	13:L:54:LEU:HD12	1.84	0.43
15:N:37:HIS:CG	15:N:37:HIS:O	2.70	0.43
16:O:196:GLN:HE22	16:O:209:VAL:HG23	1.83	0.43
23:W:360:ASP:HB2	23:W:367:ILE:HD11	2.01	0.43
23:W:452:ASP:OD1	23:W:452:ASP:N	2.52	0.43
13:L:227:THR:O	13:L:227:THR:OG1	2.37	0.43
19:S:55:ARG:HH21	19:S:57:ILE:HD11	1.82	0.43
5:A:893:GLU:OE2	5:A:1018:ASN:ND2	2.52	0.43
7:C:669:THR:HG22	7:C:690:GLU:HG3	2.01	0.43
8:E:59:ILE:HD12	8:E:59:ILE:HA	1.87	0.43
8:E:178:LEU:HB2	8:E:188:GLN:HB3	2.01	0.43
8:E:310:TYR:HE1	8:E:322:LYS:HG3	1.84	0.43
13:L:65:ARG:CG	26:I:803:SER:CB	2.97	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:125:SER:HB3	18:R:239:VAL:HG22	2.00	0.43
16:O:235:TYR:HD2	16:O:301:LYS:HB2	1.84	0.43
23:W:348:LEU:HD11	23:W:356:LEU:HD21	2.00	0.43
5:A:549:GLU:HB3	5:A:591:MET:HG2	2.00	0.42
8:E:277:PHE:HE1	8:E:317:ARG:HG2	1.83	0.42
11:H:43:U:H2'	11:H:44:U:C6	2.53	0.42
15:N:118:ILE:HD13	15:N:132:ILE:HG21	2.01	0.42
15:N:120:ARG:HA	15:N:120:ARG:HD2	1.43	0.42
7:C:80:ILE:HG22	7:C:82:GLN:HG2	2.01	0.42
7:C:924:GLN:HG3	7:C:932:GLU:HG3	2.01	0.42
8:E:307:ARG:NE	8:E:326:HIS:O	2.42	0.42
10:G:119:G:H4'	10:G:120:G:OP1	2.19	0.42
15:N:40:LYS:HE2	15:N:40:LYS:HB2	1.26	0.42
23:W:258:PRO:CG	23:W:266:ARG:NH1	2.82	0.42
5:A:25:MET:SD	8:E:215:ASN:ND2	2.91	0.42
11:H:106:G:C8	11:H:106:G:C5'	2.96	0.42
22:V:455:PHE:O	22:V:459:ILE:HG12	2.19	0.42
5:A:167:PRO:HA	5:A:168:PRO:HD3	1.90	0.42
5:A:1891:LEU:HD22	5:A:1937:ILE:HD12	2.01	0.42
7:C:160:ARG:NH1	7:C:410:LEU:HD22	2.34	0.42
7:C:711:ARG:NH2	7:C:730:ARG:O	2.37	0.42
11:H:39:U:H2'	11:H:40:C:C6	2.55	0.42
18:R:177:ILE:HG13	18:R:197:ILE:HB	2.01	0.42
23:W:399:LYS:HA	23:W:414:TYR:O	2.19	0.42
23:W:530:GLY:HA2	23:W:552:VAL:HA	2.01	0.42
38:Y:399:LYS:HB2	38:Y:399:LYS:HE3	1.59	0.42
5:A:523:ASN:OD1	5:A:552:ARG:NH2	2.53	0.42
6:B:74:U:C4	6:B:75:G:C6	3.07	0.42
8:E:181:ILE:HG13	8:E:182:ARG:HG3	2.00	0.42
11:H:112:G:H2'	11:H:113:G:C8	2.50	0.42
16:O:31:ASN:O	18:R:195:ARG:NH1	2.52	0.42
17:P:54:VAL:HG13	17:P:59:PHE:HZ	1.83	0.42
22:V:540:GLU:O	22:V:544:LEU:N	2.45	0.42
25:Z:265:LEU:HB3	25:Z:266:ARG:H	1.71	0.42
5:A:569:VAL:HG12	5:A:573:GLN:HB2	2.02	0.42
5:A:793:ASN:HD22	7:C:60:HIS:CD2	2.38	0.42
5:A:1017:ILE:HD11	5:A:1031:ILE:HD11	2.02	0.42
7:C:277:LYS:HD2	7:C:865:GLY:HA3	2.00	0.42
7:C:442:LYS:HG2	7:C:468:CYS:HB2	2.02	0.42
11:H:155:C:H2'	11:H:156:U:H5"	2.02	0.42
15:N:22:LEU:HD23	15:N:22:LEU:HA	1.82	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:121:VAL:HA	15:N:122:PRO:HD3	1.88	0.42
23:W:258:PRO:CG	23:W:265:LEU:HD13	2.49	0.42
25:Z:84:HIS:ND1	25:Z:85:GLN:OE1	2.53	0.42
5:A:1260:VAL:HG21	5:A:1325:LEU:HB3	2.01	0.42
7:C:264:ILE:HG21	7:C:381:LEU:HD12	2.01	0.42
8:E:96:TYR:N	8:E:96:TYR:CD2	2.88	0.42
13:L:83:ARG:HA	13:L:83:ARG:HD3	1.87	0.42
5:A:67:ARG:HD2	15:N:33:GLU:OE2	2.20	0.42
5:A:451:LEU:HD23	5:A:451:LEU:HA	1.89	0.42
5:A:1275:ARG:NH2	5:A:1464:LEU:O	2.43	0.42
8:E:60:MET:C	8:E:60:MET:SD	2.96	0.42
8:E:95:VAL:C	8:E:96:TYR:CD2	2.93	0.42
12:J:287:MET:HB3	14:M:186:LEU:HD11	2.00	0.42
12:J:311:GLN:HG3	14:M:131:GLN:HG2	2.02	0.42
15:N:22:LEU:HD11	15:N:60:ILE:HD11	2.02	0.42
18:R:113:TYR:OH	20:T:402:ASP:O	2.33	0.42
26:I:712:VAL:O	26:I:713:ARG:C	2.57	0.42
5:A:156:ARG:HD3	25:Z:153:GLU:HG2	2.02	0.42
5:A:723:ASN:ND2	5:A:788:GLN:OE1	2.52	0.42
10:G:137:C:OP2	10:G:137:C:H5	2.02	0.42
14:M:176:THR:HA	14:M:179:ILE:HG12	2.02	0.42
38:Y:411:LEU:HD23	38:Y:411:LEU:HA	1.84	0.42
5:A:546:LEU:HD22	5:A:648:LEU:HD11	2.02	0.42
5:A:1507:SER:HB2	5:A:1511:GLU:HG3	2.01	0.42
6:B:63:A:H2'	6:B:64:G:C8	2.55	0.42
9:F:22:A:C8	15:N:121:VAL:HG21	2.54	0.42
10:G:142:U:HO2'	10:G:143:U:P	2.38	0.42
15:N:102:CYS:HB3	15:N:104:ARG:H	1.84	0.42
18:R:175:GLN:NE2	18:R:176:TYR:O	2.52	0.42
19:S:102:ASN:H	19:S:126:HIS:CE1	2.38	0.42
20:T:371:HIS:NE2	20:T:389:SER:OG	2.35	0.42
22:V:459:ILE:HD12	22:V:489:LEU:HD23	2.00	0.42
25:Z:79:ARG:O	25:Z:81:THR:N	2.53	0.42
5:A:533:LYS:NZ	10:G:5:G:OP2	2.34	0.41
5:A:1772:PHE:HB3	25:Z:320:ASP:HB2	2.01	0.41
6:B:78:U:HO2'	6:B:79:C:P	2.37	0.41
7:C:62:ASP:OD1	7:C:62:ASP:N	2.33	0.41
7:C:131:ASN:HB3	7:C:222:SER:HA	2.01	0.41
8:E:81:LEU:HB2	8:E:93:TRP:HB2	2.02	0.41
8:E:161:ARG:HH22	8:E:243:LEU:HD12	1.85	0.41
12:J:242:ILE:HD13	12:J:275:ASN:ND2	2.35	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:314:ILE:CD1	20:T:326:LEU:HD21	2.47	0.41
20:T:329:HIS:ND1	20:T:349:SER:CB	2.82	0.41
23:W:475:TRP:CD1	23:W:489:GLY:HA2	2.55	0.41
5:A:1807:ILE:HG12	5:A:1841:THR:HG23	2.02	0.41
7:C:623:GLU:H	7:C:941:LYS:NZ	2.14	0.41
8:E:340:PRO:HB2	8:E:356:ILE:HB	2.01	0.41
10:G:21:A:N6	16:O:91:GLY:O	2.43	0.41
13:L:262:LYS:HE3	13:L:266:HIS:CE1	2.55	0.41
19:S:20:MET:HG3	19:S:142:VAL:HG22	2.02	0.41
21:U:23:LEU:HD12	22:V:477:LEU:HD13	2.02	0.41
23:W:305:LEU:HD21	23:W:313:ILE:HG23	2.02	0.41
26:I:296:PHE:CB	26:I:305:SER:O	2.68	0.41
5:A:99:VAL:HG13	5:A:554:THR:HG21	2.02	0.41
5:A:531:THR:HG23	5:A:534:GLU:H	1.84	0.41
5:A:620:PRO:HG2	25:Z:134:PHE:CE2	2.55	0.41
5:A:762:ARG:NH2	17:P:227:TYR:OH	2.53	0.41
5:A:1490:PHE:O	5:A:1493:THR:OG1	2.35	0.41
5:A:1976:TRP:HA	5:A:1979:VAL:HG22	2.03	0.41
13:L:699:ASN:HA	39:K:114:LEU:CB	2.50	0.41
14:M:212:ASN:HB3	14:M:215:ASN:H	1.85	0.41
23:W:126:GLU:HB3	23:W:130:ARG:NH1	2.35	0.41
5:A:866:LEU:HD12	5:A:913:PRO:HB2	2.02	0.41
5:A:1174:PHE:HE2	5:A:1176:SER:HB2	1.85	0.41
11:H:113:G:C2'	11:H:114:A:H5'	2.50	0.41
19:S:24:VAL:HB	19:S:134:GLN:HB3	2.02	0.41
5:A:506:LEU:O	5:A:510:ARG:CB	2.68	0.41
5:A:955:TRP:HE1	5:A:976:MET:HE3	1.85	0.41
8:E:294:SER:HB3	8:E:299:LYS:HB2	2.02	0.41
11:H:43:U:OP2	11:H:43:U:C6	2.74	0.41
11:H:151:C:OP1	24:X:124:THR:N	2.54	0.41
5:A:764:GLY:HA2	5:A:1245:ARG:NH1	2.36	0.41
7:C:441:PRO:O	7:C:445:ALA:HB2	2.20	0.41
11:H:157:G:H5"	11:H:157:G:C8	2.50	0.41
39:K:18:TYR:CB	39:K:168:LYS:HA	2.50	0.41
5:A:555:LYS:NZ	5:A:559:ASP:OD2	2.43	0.41
6:B:70:A:H5"	6:B:70:A:H8	1.85	0.41
23:W:84:THR:O	23:W:87:THR:OG1	2.35	0.41
10:G:163:C:H2'	10:G:164:A:O4'	2.20	0.41
11:H:37:U:H2'	11:H:38:A:H8	1.85	0.41
15:N:120:ARG:HH11	15:N:142:CYS:HB2	1.86	0.41
16:O:240:GLY:H	16:O:268:GLN:HB3	1.86	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:707:ARG:HG2	17:P:9:PHE:CZ	2.56	0.41
5:A:835:ASP:OD1	5:A:921:TYR:OH	2.33	0.41
5:A:1088:PHE:HD1	5:A:1097:ILE:HG12	1.85	0.41
5:A:1590:VAL:HG22	5:A:1664:ILE:HD12	2.03	0.41
5:A:2332:ASP:O	5:A:2334:TYR:N	2.54	0.41
7:C:87:GLN:HA	7:C:88:PRO:HD2	1.97	0.41
7:C:743:ASN:HB3	7:C:770:PHE:CZ	2.56	0.41
11:H:152:G:H2'	11:H:153:A:C1'	2.51	0.41
16:O:110:SER:OG	16:O:113:ASN:ND2	2.53	0.41
23:W:97:ASN:OD1	23:W:97:ASN:N	2.54	0.41
23:W:304:LEU:HD11	23:W:567:ILE:HG21	2.02	0.41
23:W:387:LYS:NZ	23:W:430:ASN:OD1	2.49	0.41
23:W:393:ALA:HB3	23:W:403:TRP:HZ3	1.86	0.41
25:Z:178:HIS:O	25:Z:181:ILE:HB	2.21	0.41
41:D:538:ILE:O	41:D:585:ILE:HA	2.21	0.41
41:D:577:LYS:O	41:D:581:SER:N	2.54	0.41
5:A:192:GLN:H	5:A:192:GLN:HG2	1.69	0.41
5:A:1790:ILE:HD13	24:X:76:SER:HB2	2.03	0.41
7:C:618:THR:HB	7:C:630:LEU:HB2	2.03	0.41
7:C:637:LEU:HD23	7:C:637:LEU:HA	1.94	0.41
7:C:833:PHE:HB2	7:C:902:HIS:ND1	2.36	0.41
9:F:17:C:H2'	9:F:18:A:C8	2.56	0.41
11:H:102:U:OP2	11:H:102:U:H2'	2.21	0.41
20:T:366:VAL:HG21	20:T:402:ASP:HA	2.03	0.41
23:W:341:ASN:HB3	23:W:344:GLY:H	1.86	0.41
5:A:913:PRO:HA	5:A:916:LYS:HD3	2.04	0.40
5:A:1244:VAL:HG11	5:A:1291:CYS:HB3	2.03	0.40
5:A:1820:LYS:HD3	5:A:1914:MET:HE1	2.02	0.40
5:A:1946:ASN:HD22	5:A:1986:LEU:HD21	1.83	0.40
7:C:101:LYS:HG2	7:C:172:PHE:CE2	2.56	0.40
7:C:112:THR:H	7:C:155:PRO:HD2	1.87	0.40
7:C:169:ASP:OD1	7:C:169:ASP:N	2.54	0.40
7:C:843:VAL:HG13	7:C:871:ILE:HD11	2.03	0.40
11:H:152:G:H2'	11:H:152:G:N3	2.36	0.40
11:H:153:A:C8	11:H:154:C:O4'	2.74	0.40
12:J:493:ALA:CB	12:J:499:ARG:CB	2.96	0.40
16:O:230:THR:H	16:O:277:ARG:NH1	2.18	0.40
19:S:136:ILE:HA	19:S:139:VAL:HG12	2.03	0.40
20:T:193:PRO:HD2	20:T:495:ALA:HB1	2.03	0.40
20:T:483:ASP:OD1	20:T:485:THR:OG1	2.34	0.40
25:Z:106:VAL:HG12	25:Z:153:GLU:HG3	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Z:162:ASP:HB2	25:Z:165:GLY:H	1.85	0.40
5:A:1591:MET:HE3	5:A:1595:GLN:HG3	2.03	0.40
6:B:85:C:H3'	6:B:85:C:P	2.61	0.40
7:C:706:GLN:HG3	7:C:707:ILE:H	1.86	0.40
8:E:253:ASN:HB3	8:E:259:VAL:HG13	2.02	0.40
8:E:295:PRO:HG3	8:E:337:PRO:HA	2.03	0.40
16:O:64:ARG:HD2	16:O:163:HIS:CE1	2.56	0.40
17:P:66:ARG:HH22	20:T:217:GLN:HE22	1.68	0.40
19:S:25:LEU:HA	19:S:132:VAL:HA	2.03	0.40
23:W:162:ASN:HB3	23:W:165:LEU:HG	2.03	0.40
5:A:155:LYS:HZ3	5:A:624:GLY:H	1.69	0.40
5:A:1241:HIS:HB2	5:A:1287:LEU:HD21	2.02	0.40
5:A:1590:VAL:HG11	5:A:1614:ILE:HD11	2.04	0.40
7:C:104:LEU:HG	7:C:172:PHE:CD2	2.56	0.40
7:C:231:ALA:O	7:C:277:LYS:HE3	2.21	0.40
7:C:263:LEU:HD23	7:C:267:LEU:HD12	2.02	0.40
11:H:149:A:C6	11:H:150:U:C4	3.09	0.40
11:H:183:G:C6	11:H:184:C:N4	2.89	0.40
15:N:70:ILE:HG12	15:N:74:LEU:HD23	2.03	0.40
20:T:314:ILE:O	20:T:323:VAL:N	2.54	0.40
5:A:1803:ILE:O	5:A:1824:THR:HG22	2.22	0.40
7:C:104:LEU:CG	7:C:172:PHE:CE2	3.01	0.40
7:C:506:PRO:HG2	7:C:568:PRO:HG3	2.03	0.40
11:H:57:A:C6	11:H:58:U:C4	3.10	0.40
13:L:176:LEU:HD22	23:W:440:LYS:HE3	2.04	0.40
18:R:91:ASP:HB3	18:R:97:LYS:HE3	2.02	0.40
19:S:142:VAL:HG13	19:S:157:VAL:HG11	2.04	0.40
20:T:438:LEU:HB2	20:T:448:GLN:HB3	2.03	0.40
26:I:729:SER:HA	26:I:732:ALA:HB3	2.04	0.40
41:D:420:SER:CB	41:D:622:ASP:HA	2.52	0.40
5:A:156:ARG:NH1	25:Z:153:GLU:OE2	2.55	0.40
5:A:796:LYS:HD3	18:R:279:HIS:HE1	1.87	0.40
5:A:1330:MET:HG3	5:A:1367:ASN:OD1	2.21	0.40
5:A:1403:LEU:HD23	5:A:1403:LEU:HA	1.92	0.40
7:C:104:LEU:HB3	7:C:172:PHE:CZ	2.56	0.40
8:E:95:VAL:C	8:E:96:TYR:HD2	2.25	0.40
8:E:95:VAL:HG23	8:E:96:TYR:H	1.85	0.40
8:E:282:HIS:NE2	8:E:289:LEU:HD12	2.36	0.40
20:T:320:LYS:HB2	20:T:320:LYS:HE3	1.85	0.40
26:I:520:ILE:O	26:I:524:TYR:N	2.54	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
1	v	142/148 (96%)	138 (97%)	4 (3%)	0	100 100
2	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	14 50
3	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	19 57
4	x	23/703 (3%)	22 (96%)	1 (4%)	0	100 100
5	A	2247/2335 (96%)	2091 (93%)	147 (6%)	9 (0%)	34 72
7	C	892/972 (92%)	798 (90%)	90 (10%)	4 (0%)	34 72
8	E	301/357 (84%)	273 (91%)	28 (9%)	0	100 100
12	J	530/848 (62%)	491 (93%)	32 (6%)	7 (1%)	12 45
13	L	436/802 (54%)	405 (93%)	27 (6%)	4 (1%)	17 55
14	M	128/243 (53%)	124 (97%)	3 (2%)	1 (1%)	19 57
15	N	141/144 (98%)	126 (89%)	13 (9%)	2 (1%)	11 43
16	O	283/420 (67%)	260 (92%)	22 (8%)	1 (0%)	34 72
17	P	104/229 (45%)	86 (83%)	15 (14%)	3 (3%)	4 24
18	R	255/536 (48%)	229 (90%)	24 (9%)	2 (1%)	19 57
19	S	157/166 (95%)	148 (94%)	9 (6%)	0	100 100
20	T	311/514 (60%)	281 (90%)	23 (7%)	7 (2%)	6 30
21	U	24/2752 (1%)	23 (96%)	1 (4%)	0	100 100
22	V	444/908 (49%)	429 (97%)	14 (3%)	1 (0%)	47 82
23	W	506/579 (87%)	441 (87%)	60 (12%)	5 (1%)	15 53
24	X	90/184 (49%)	84 (93%)	6 (7%)	0	100 100
25	Z	238/586 (41%)	214 (90%)	24 (10%)	0	100 100
26	I	498/855 (58%)	481 (97%)	10 (2%)	7 (1%)	11 43
27	y	77/301 (26%)	75 (97%)	2 (3%)	0	100 100
28	Q	1308/1485 (88%)	1282 (98%)	26 (2%)	0	100 100
29	a	77/126 (61%)	76 (99%)	1 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
30	b	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
30	i	84/231 (36%)	82 (98%)	2 (2%)	0	100	100
31	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
31	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
32	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
32	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
33	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
33	m	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
34	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
34	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
35	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
35	n	65/76 (86%)	59 (91%)	4 (6%)	2 (3%)	4	23
36	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	12	45
37	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
38	Y	709/1220 (58%)	616 (87%)	61 (9%)	32 (4%)	2	14
39	K	144/225 (64%)	129 (90%)	8 (6%)	7 (5%)	2	13
40	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	4	23
40	r	129/504 (26%)	119 (92%)	8 (6%)	2 (2%)	9	40
40	s	65/504 (13%)	62 (95%)	2 (3%)	1 (2%)	10	42
40	t	65/504 (13%)	64 (98%)	0	1 (2%)	10	42
41	D	1720/2136 (80%)	1633 (95%)	84 (5%)	3 (0%)	47	82
All	All	13914/24425 (57%)	12995 (93%)	808 (6%)	111 (1%)	24	57

All (111) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	u	383	ASN
15	N	36	PRO
18	R	233	PRO
20	T	343	PRO
20	T	458	SER
23	W	268	THR
26	I	463	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
26	I	721	LYS
26	I	797	PHE
38	Y	531	MET
38	Y	610	ARG
38	Y	855	VAL
38	Y	944	ASP
38	Y	995	MET
38	Y	1090	LYS
38	Y	1098	LYS
38	Y	1099	SER
38	Y	1129	ASP
38	Y	1145	GLN
38	Y	1164	GLU
39	K	78	PRO
39	K	90	PRO
39	K	135	TRP
40	q	59	HIS
40	q	60	PRO
40	s	71	ILE
40	t	69	THR
41	D	957	VAL
41	D	1584	ILE
2	w	115	GLY
3	u	340	GLY
3	u	385	ASP
7	C	94	ILE
12	J	188	GLN
12	J	241	VAL
12	J	709	VAL
13	L	765	ARG
15	N	37	HIS
17	P	205	LYS
18	R	186	VAL
23	W	243	VAL
23	W	258	PRO
26	I	618	ARG
26	I	634	ILE
36	o	160	LYS
38	Y	517	GLU
38	Y	845	SER
38	Y	870	GLY
38	Y	1182	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
39	K	136	LYS
39	K	172	LEU
40	q	9	ASN
12	J	205	LEU
17	P	48	GLN
20	T	186	PRO
20	T	328	GLY
26	I	752	ALA
35	n	6	PRO
38	Y	524	ASN
38	Y	550	TYR
38	Y	806	GLU
38	Y	994	ILE
38	Y	1055	ASN
38	Y	1056	LYS
40	q	19	PRO
40	r	9	ASN
5	A	1092	ILE
5	A	1190	CYS
12	J	604	PRO
13	L	585	TYR
20	T	406	ILE
23	W	74	PRO
26	I	617	GLU
35	n	8	GLU
36	o	32	PRO
38	Y	590	THR
38	Y	663	ASP
38	Y	722	ALA
38	Y	835	VAL
39	K	65	ILE
5	A	56	ALA
5	A	108	MET
5	A	570	ASP
12	J	341	PRO
14	M	125	SER
22	V	597	PRO
38	Y	811	PRO
5	A	109	PRO
5	A	853	LYS
5	A	1503	TRP
13	L	763	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
16	O	20	PHE
17	P	11	PRO
38	Y	523	ALA
38	Y	856	ASP
38	Y	1157	THR
7	C	87	GLN
7	C	441	PRO
13	L	764	PRO
38	Y	738	PRO
38	Y	1137	PRO
39	K	17	PRO
40	r	65	PRO
5	A	852	VAL
12	J	206	LEU
20	T	185	MET
20	T	401	PRO
38	Y	521	ILE
23	W	271	PRO
41	D	585	ILE
7	C	440	SER

5.3.2 Protein sidechains (i)

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
5	A	1795/2108 (85%)	1780 (99%)	15 (1%)	81 93
7	C	793/866 (92%)	786 (99%)	7 (1%)	78 92
8	E	259/300 (86%)	254 (98%)	5 (2%)	57 84
12	J	241/751 (32%)	239 (99%)	2 (1%)	81 93
13	L	208/709 (29%)	204 (98%)	4 (2%)	57 84
14	M	117/209 (56%)	113 (97%)	4 (3%)	37 72
15	N	130/130 (100%)	124 (95%)	6 (5%)	27 64
16	O	255/361 (71%)	250 (98%)	5 (2%)	55 83

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
17	P	99/203 (49%)	98 (99%)	1 (1%)	76 91
18	R	219/457 (48%)	212 (97%)	7 (3%)	39 74
19	S	129/134 (96%)	129 (100%)	0	100 100
20	T	269/441 (61%)	261 (97%)	8 (3%)	41 75
21	U	21/2432 (1%)	20 (95%)	1 (5%)	25 62
22	V	140/838 (17%)	136 (97%)	4 (3%)	42 76
23	W	447/502 (89%)	434 (97%)	13 (3%)	42 76
24	X	62/157 (40%)	57 (92%)	5 (8%)	11 40
25	Z	214/520 (41%)	210 (98%)	4 (2%)	57 84
38	Y	8/1085 (1%)	5 (62%)	3 (38%)	0 0
All	All	5406/12203 (44%)	5312 (98%)	94 (2%)	62 85

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	258	PHE
5	A	409	ARG
5	A	623	LYS
5	A	642	ARG
5	A	762	ARG
5	A	994	ASN
5	A	1090	ARG
5	A	1341	ARG
5	A	1393	ARG
5	A	1402	ARG
5	A	1543	ASN
5	A	1763	LEU
5	A	1774	ASN
5	A	1984	LYS
5	A	1985	ASP
7	C	105	MET
7	C	158	ARG
7	C	256	CYS
7	C	297	ASN
7	C	308	CYS
7	C	495	ARG
7	C	678	THR
8	E	54	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	E	56	GLN
8	E	59	ILE
8	E	60	MET
8	E	99	CYS
12	J	201	ARG
12	J	221	ASN
13	L	41	LYS
13	L	181	ARG
13	L	227	THR
13	L	240	ARG
14	M	181	ARG
14	M	184	ILE
14	M	212	ASN
14	M	215	ASN
15	N	38	GLU
15	N	40	LYS
15	N	119	CYS
15	N	120	ARG
15	N	121	VAL
15	N	130	ARG
16	O	45	CYS
16	O	73	THR
16	O	75	SER
16	O	147	LEU
16	O	222	ARG
17	P	212	ASN
18	R	74	LEU
18	R	78	ARG
18	R	95	LYS
18	R	212	PHE
18	R	258	LYS
18	R	276	GLN
18	R	312	MET
20	T	327	SER
20	T	339	GLN
20	T	342	GLU
20	T	344	GLN
20	T	356	LEU
20	T	404	SER
20	T	406	ILE
20	T	412	HIS
21	U	23	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	V	458	THR
22	V	539	LEU
22	V	583	VAL
22	V	597	PRO
23	W	129	ARG
23	W	182	LYS
23	W	252	ARG
23	W	257	ILE
23	W	260	ASP
23	W	266	ARG
23	W	322	ARG
23	W	492	ASN
23	W	495	ARG
23	W	500	LYS
23	W	529	ASN
23	W	541	LYS
23	W	552	VAL
24	X	103	GLN
24	X	104	LYS
24	X	105	LEU
24	X	109	PHE
24	X	113	LEU
25	Z	116	ARG
25	Z	122	ASN
25	Z	164	ASP
25	Z	166	LYS
38	Y	404	GLN
38	Y	405	MET
38	Y	411	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (64) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	97	HIS
5	A	160	HIS
5	A	181	ASN
5	A	270	ASN
5	A	294	ASN
5	A	326	HIS
5	A	328	HIS
5	A	579	GLN
5	A	617	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	A	723	ASN
5	A	775	ASN
5	A	994	ASN
5	A	1069	ASN
5	A	1075	GLN
5	A	1460	HIS
5	A	1615	HIS
5	A	1717	ASN
5	A	1774	ASN
5	A	1816	GLN
5	A	1946	ASN
7	C	60	HIS
7	C	82	GLN
7	C	154	HIS
7	C	297	ASN
7	C	548	ASN
7	C	627	HIS
7	C	642	HIS
7	C	924	GLN
8	E	56	GLN
8	E	94	ASN
8	E	101	ASN
8	E	202	ASN
8	E	287	ASN
12	J	221	ASN
12	J	238	ASN
12	J	331	GLN
12	J	347	HIS
13	L	211	ASN
13	L	266	HIS
14	M	212	ASN
15	N	99	ASN
16	O	72	GLN
16	O	82	GLN
16	O	163	HIS
16	O	251	HIS
17	P	29	GLN
17	P	212	ASN
18	R	71	GLN
18	R	175	GLN
18	R	276	GLN
18	R	279	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
19	S	134	GLN
20	T	278	ASN
20	T	339	GLN
20	T	384	HIS
20	T	446	ASN
23	W	82	ASN
23	W	103	GLN
23	W	119	HIS
23	W	462	HIS
23	W	492	ASN
23	W	529	ASN
24	X	103	GLN
24	X	116	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
10	G	82/273 (30%)	44 (53%)	7 (8%)
11	H	133/188 (70%)	45 (33%)	9 (6%)
6	B	96/117 (82%)	46 (47%)	8 (8%)
9	F	96/107 (89%)	33 (34%)	6 (6%)
All	All	407/685 (59%)	168 (41%)	30 (7%)

All (168) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
6	B	9	G
6	B	10	U
6	B	13	C
6	B	19	A
6	B	20	G
6	B	21	A
6	B	22	U
6	B	24	G
6	B	25	C
6	B	26	A
6	B	28	A
6	B	33	U
6	B	36	C
6	B	38	C
6	B	40	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	B	45	C
6	B	47	A
6	B	52	U
6	B	57	G
6	B	66	A
6	B	67	A
6	B	71	C
6	B	72	U
6	B	73	C
6	B	74	U
6	B	75	G
6	B	76	A
6	B	77	G
6	B	78	U
6	B	79	C
6	B	80	U
6	B	81	U
6	B	82	A
6	B	83	A
6	B	84	C
6	B	85	C
6	B	86	C
6	B	87	A
6	B	88	A
6	B	89	U
6	B	90	U
6	B	91	U
6	B	92	U
6	B	94	U
6	B	95	G
6	B	96	A
9	F	6	C
9	F	7	G
9	F	9	U
9	F	10	U
9	F	12	G
9	F	26	U
9	F	27	A
9	F	28	A
9	F	29	A
9	F	33	G
9	F	34	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	F	37	C
9	F	38	G
9	F	46	G
9	F	49	G
9	F	51	U
9	F	54	G
9	F	58	G
9	F	59	G
9	F	60	C
9	F	61	C
9	F	68	C
9	F	69	A
9	F	74	U
9	F	79	C
9	F	81	C
9	F	82	A
9	F	83	A
9	F	84	A
9	F	85	U
9	F	86	U
9	F	87	C
9	F	89	U
10	G	-11	G
10	G	-7	C
10	G	-6	C
10	G	-1	G
10	G	2	U
10	G	5	G
10	G	8	C
10	G	11	A
10	G	13	C
10	G	17	U
10	G	18	A
10	G	21	A
10	G	22	C
10	G	23	U
10	G	25	G
10	G	27	U
10	G	120	G
10	G	123	U
10	G	124	U
10	G	125	C

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	G	126	C
10	G	127	U
10	G	128	U
10	G	129	G
10	G	130	A
10	G	131	U
10	G	134	U
10	G	135	G
10	G	136	U
10	G	137	C
10	G	138	A
10	G	139	U
10	G	140	A
10	G	141	C
10	G	142	U
10	G	143	U
10	G	144	A
10	G	145	U
10	G	146	C
10	G	149	G
10	G	163	C
10	G	164	A
10	G	166	A
10	G	167	G
11	H	14	C
11	H	15	U
11	H	16	U
11	H	17	U
11	H	19	G
11	H	20	G
11	H	24	A
11	H	25	G
11	H	29	A
11	H	30	A
11	H	31	G
11	H	33	G
11	H	38	A
11	H	39	U
11	H	40	C
11	H	41	U
11	H	42	G
11	H	43	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	H	98	G
11	H	99	A
11	H	100	U
11	H	101	U
11	H	102	U
11	H	103	U
11	H	104	U
11	H	105	G
11	H	106	G
11	H	107	A
11	H	111	G
11	H	112	G
11	H	114	A
11	H	115	G
11	H	143	A
11	H	147	G
11	H	152	G
11	H	153	A
11	H	154	C
11	H	156	U
11	H	157	G
11	H	168	A
11	H	170	C
11	H	171	U
11	H	177	A
11	H	178	A
11	H	179	C

All (30) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
6	B	20	G
6	B	21	A
6	B	78	U
6	B	79	C
6	B	80	U
6	B	88	A
6	B	92	U
6	B	95	G
9	F	5	U
9	F	25	C
9	F	26	U

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	F	33	G
9	F	50	A
9	F	58	G
10	G	-12	G
10	G	1	G
10	G	16	G
10	G	21	A
10	G	137	C
10	G	138	A
10	G	142	U
11	H	29	A
11	H	39	U
11	H	40	C
11	H	100	U
11	H	104	U
11	H	105	G
11	H	106	G
11	H	156	U
11	H	168	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
18	SEP	R	232	18	8,9,10	1.47	1 (12%)	8,12,14	2.47	2 (25%)
18	SEP	R	224	18	8,9,10	0.81	0	8,12,14	1.48	1 (12%)

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
18	SEP	R	232	18	-	1/5/8/10	-
18	SEP	R	224	18	-	1/5/8/10	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	R	232	SEP	P-O1P	3.18	1.60	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	R	232	SEP	P-OG-CB	-5.11	104.21	118.30
18	R	232	SEP	OG-CB-CA	4.37	112.39	108.14
18	R	224	SEP	OG-CB-CA	-2.59	105.63	108.14

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	232	SEP	N-CA-CB-OG
18	R	224	SEP	CB-OG-P-O1P

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 19 ligands modelled in this entry, 16 are monoatomic - leaving 3 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	$\#\|Z\|>2$
43	GTP	C	1500	44	26,34,34	1.34	3 (11%)	32,54,54	1.51	7 (21%)
42	IHP	A	3000	-	36,36,36	0.83	0	54,60,60	1.05	2 (3%)
46	ATP	Q	1501	44	26,33,33	1.73	8 (30%)	31,52,52	1.87	10 (32%)

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
43	GTP	C	1500	44	-	4/18/38/38	0/3/3/3
42	IHP	A	3000	-	-	7/30/54/54	0/1/1/1
46	ATP	Q	1501	44	-	4/18/38/38	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	C	1500	GTP	C5-C6	-4.30	1.38	1.47
46	Q	1501	ATP	C2'-C1'	-3.61	1.48	1.53
46	Q	1501	ATP	C4-N3	3.59	1.40	1.35
46	Q	1501	ATP	C6-N6	3.25	1.45	1.34
46	Q	1501	ATP	C2'-C3'	-2.78	1.45	1.53
46	Q	1501	ATP	O2'-C2'	-2.27	1.37	1.43
43	C	1500	GTP	C5-C4	-2.23	1.37	1.43
46	Q	1501	ATP	C3'-C4'	-2.22	1.47	1.53
46	Q	1501	ATP	O3'-C3'	-2.11	1.38	1.43
43	C	1500	GTP	O4'-C4'	-2.08	1.40	1.45
46	Q	1501	ATP	C2-N3	2.08	1.35	1.32

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	Q	1501	ATP	PB-O3B-PG	-5.52	113.89	132.83
46	Q	1501	ATP	N3-C2-N1	-4.26	122.02	128.68
43	C	1500	GTP	C5-C6-N1	3.52	120.18	113.95
43	C	1500	GTP	C8-N7-C5	3.16	109.00	102.99
43	C	1500	GTP	C2-N1-C6	-3.07	119.44	125.10
43	C	1500	GTP	PA-O3A-PB	-3.07	122.28	132.83
46	Q	1501	ATP	PA-O3A-PB	-2.58	123.97	132.83
46	Q	1501	ATP	C1'-N9-C4	-2.51	122.22	126.64
46	Q	1501	ATP	O2G-PG-O1G	-2.39	101.31	110.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
43	C	1500	GTP	O6-C6-C5	-2.38	119.73	124.37
46	Q	1501	ATP	O2A-PA-O1A	-2.36	100.58	112.24
42	A	3000	IHP	O13-C3-C2	2.36	114.24	108.69
46	Q	1501	ATP	O2G-PG-O3B	2.31	112.39	104.64
43	C	1500	GTP	PB-O3B-PG	-2.20	125.28	132.83
46	Q	1501	ATP	O5'-C5'-C4'	2.11	116.25	108.99
42	A	3000	IHP	O44-P4-O34	2.10	115.67	107.64
46	Q	1501	ATP	O2B-PB-O1B	-2.09	101.93	112.24
43	C	1500	GTP	C2'-C3'-C4'	2.07	106.66	102.64
46	Q	1501	ATP	O3G-PG-O3B	2.06	111.56	104.64

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
42	A	3000	IHP	C2-O12-P2-O22
42	A	3000	IHP	C6-O16-P6-O26
43	C	1500	GTP	PB-O3B-PG-O3G
46	Q	1501	ATP	C5'-O5'-PA-O1A
46	Q	1501	ATP	C5'-O5'-PA-O2A
43	C	1500	GTP	C3'-C4'-C5'-O5'
43	C	1500	GTP	O4'-C4'-C5'-O5'
42	A	3000	IHP	C4-O14-P4-O44
42	A	3000	IHP	C6-O16-P6-O36
42	A	3000	IHP	C3-C2-O12-P2
46	Q	1501	ATP	PB-O3A-PA-O2A
42	A	3000	IHP	C2-C1-O11-P1
42	A	3000	IHP	C4-O14-P4-O34
46	Q	1501	ATP	C5'-O5'-PA-O3A
43	C	1500	GTP	PB-O3A-PA-O2A

There are no ring outliers.

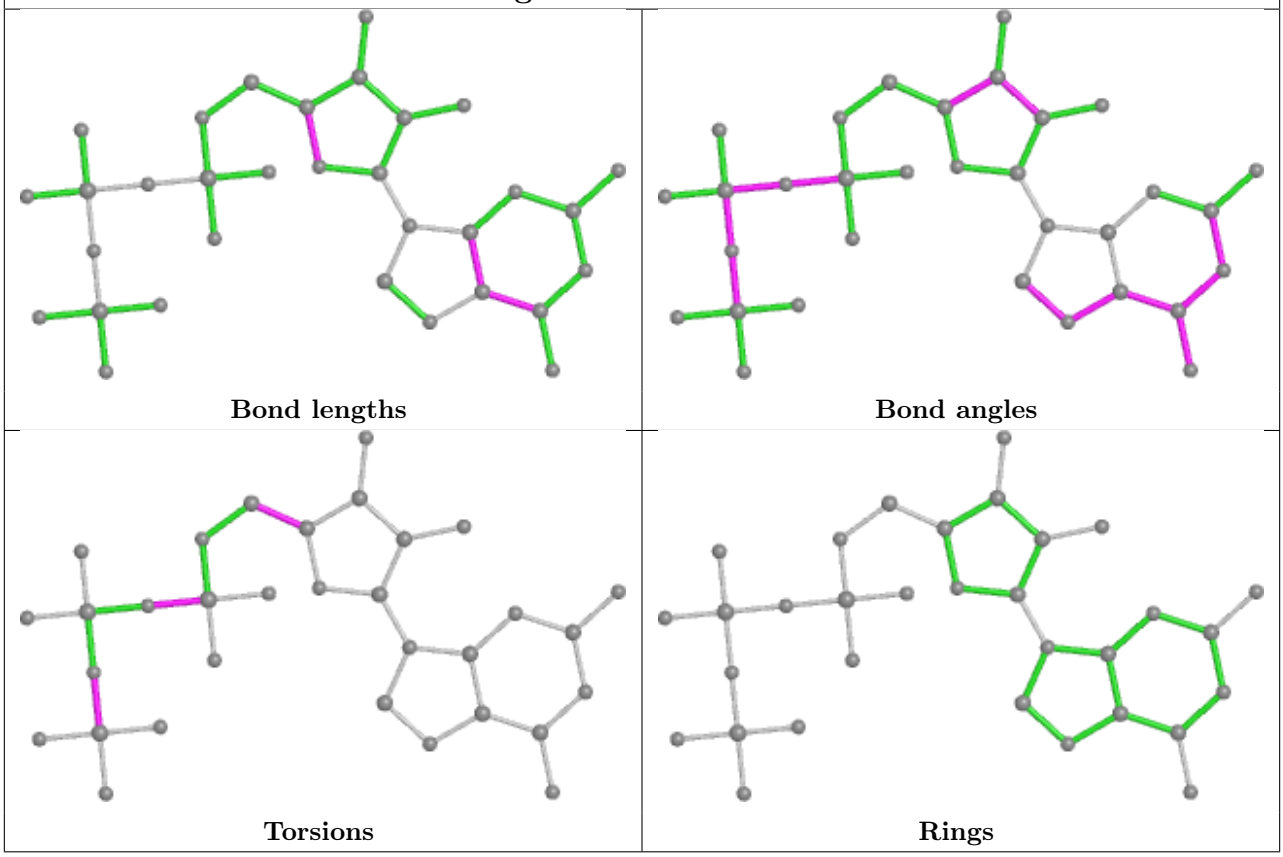
2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
43	C	1500	GTP	2	0
42	A	3000	IHP	3	0

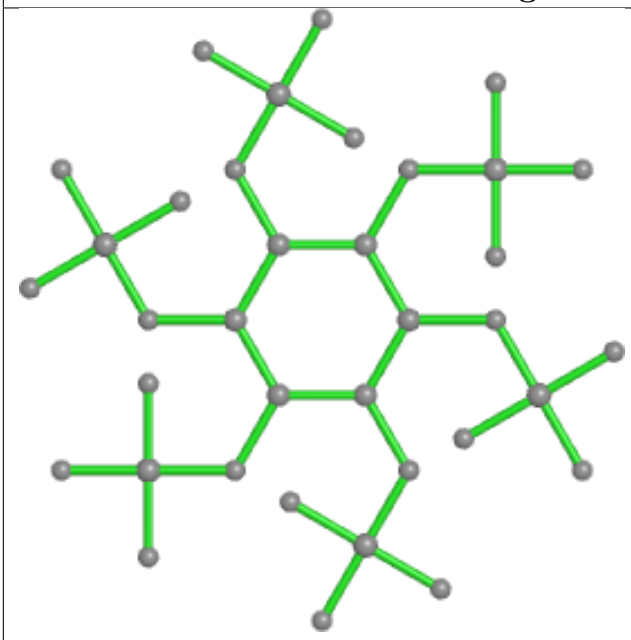
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

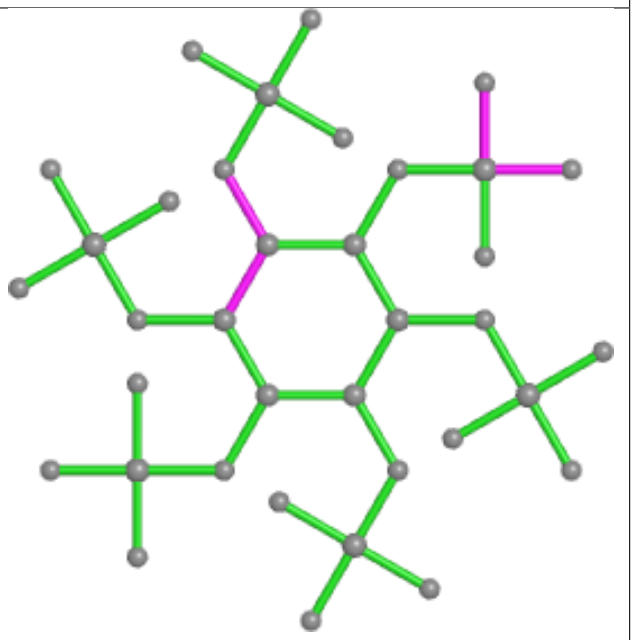
Ligand GTP C 1500



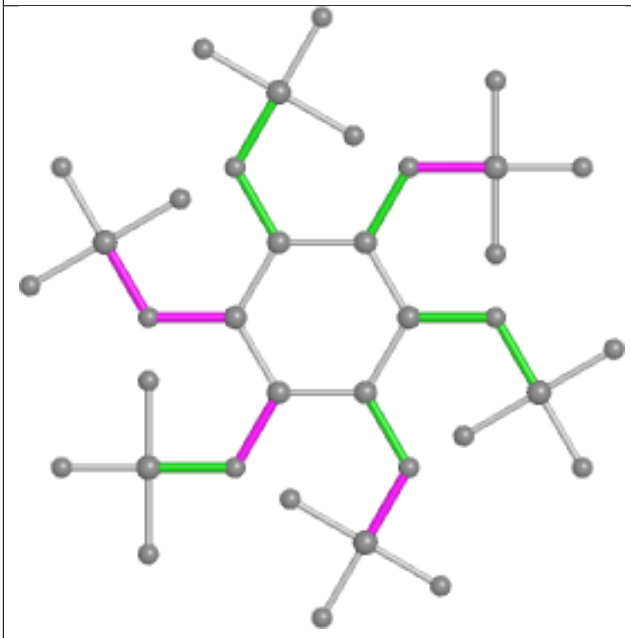
Ligand IHP A 3000



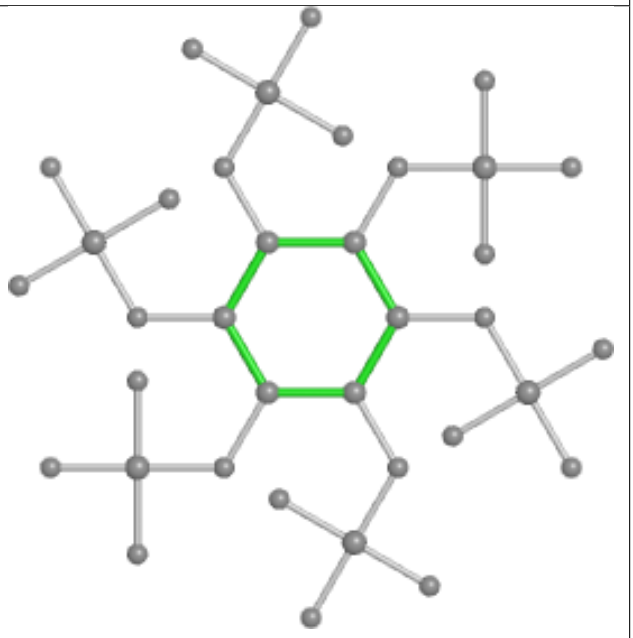
Bond lengths



Bond angles

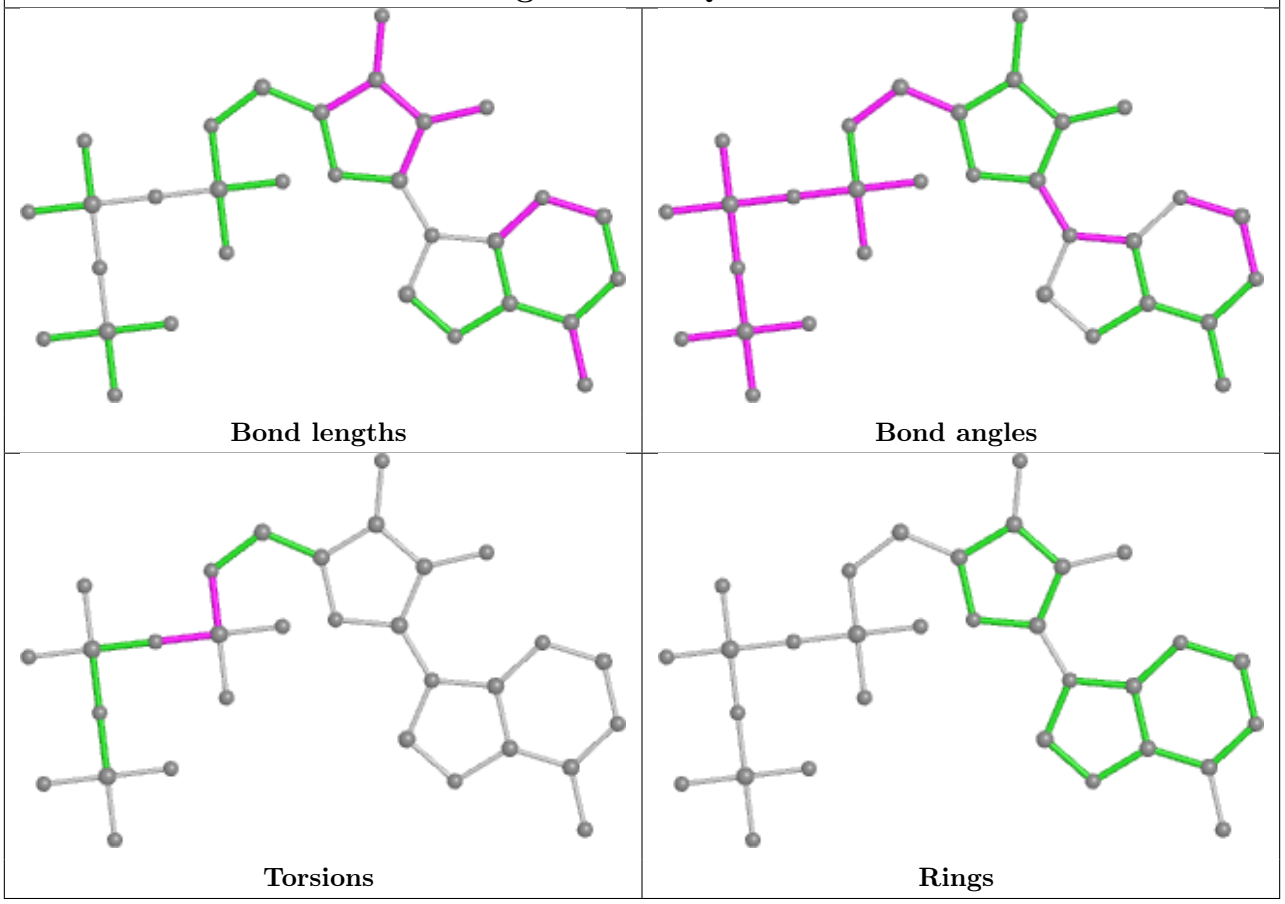


Torsions



Rings

Ligand ATP Q 1501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

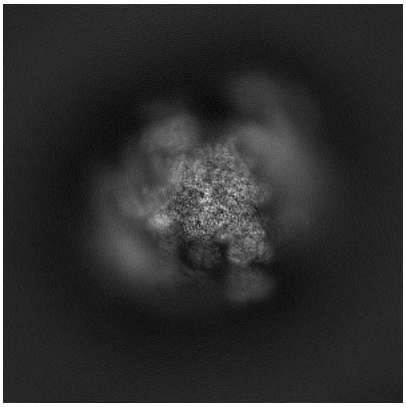
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-9645. These allow visual inspection of the internal detail of the map and identification of artifacts.

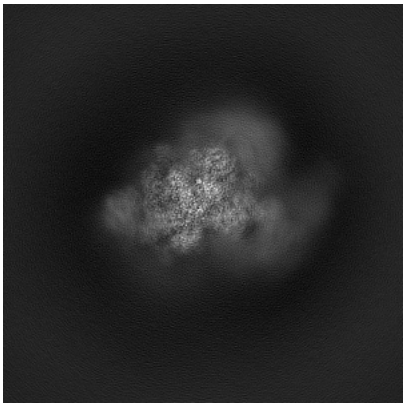
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

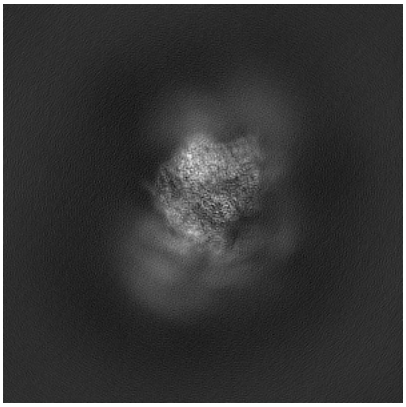
6.1.1 Primary map



X



Y

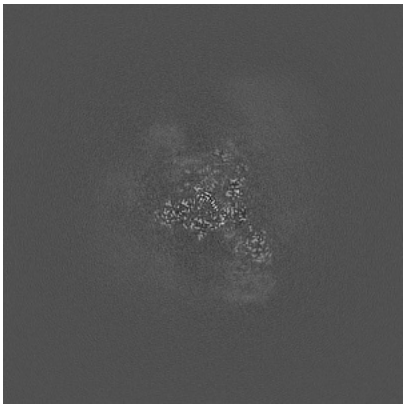


Z

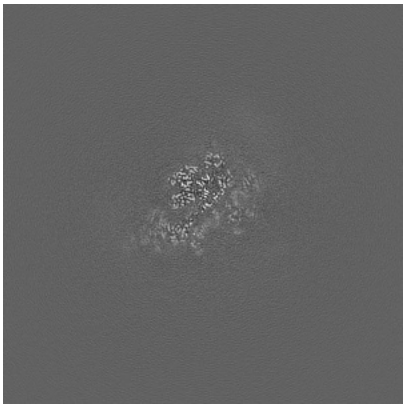
The images above show the map projected in three orthogonal directions.

6.2 Central slices

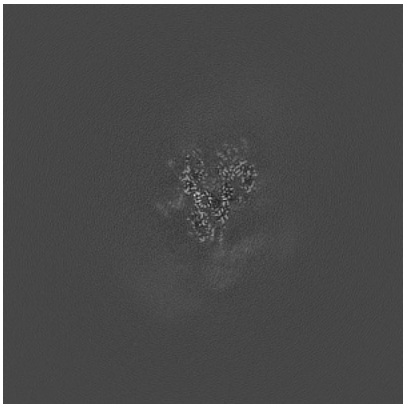
6.2.1 Primary map



X Index: 200



Y Index: 200

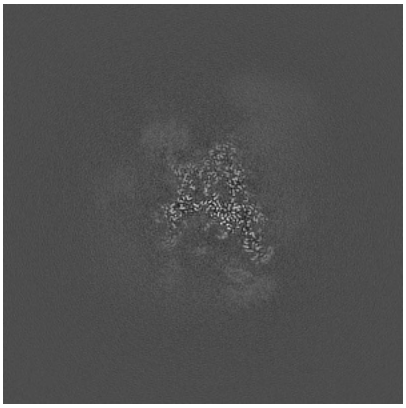


Z Index: 200

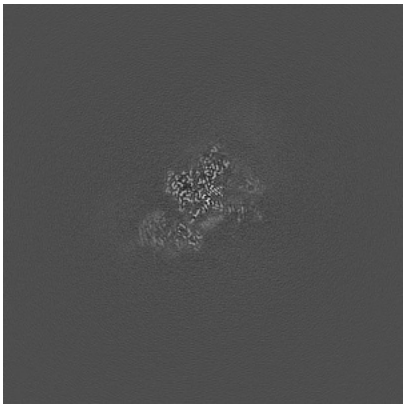
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

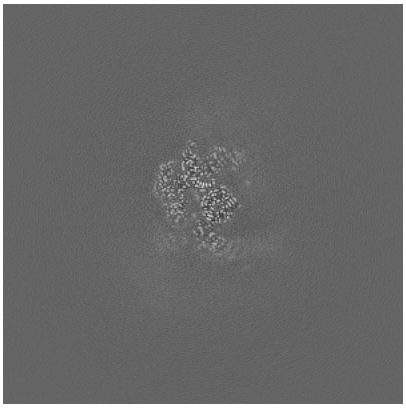
6.3.1 Primary map



X Index: 193



Y Index: 205

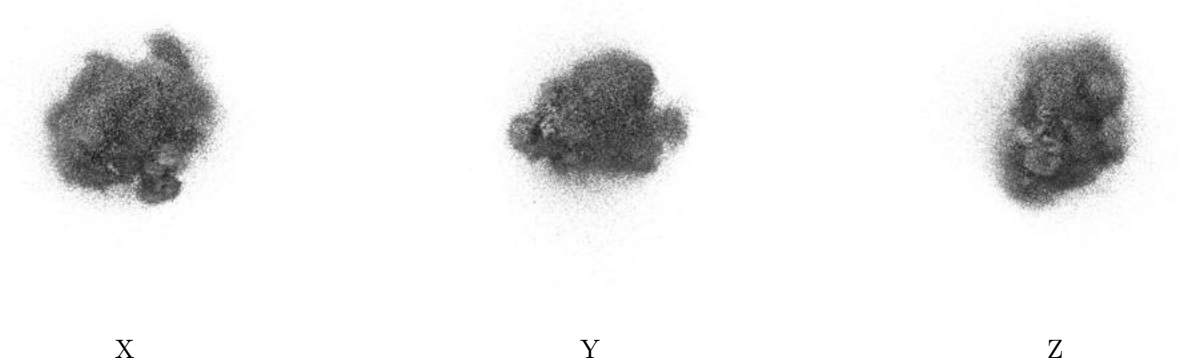


Z Index: 180

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.03. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

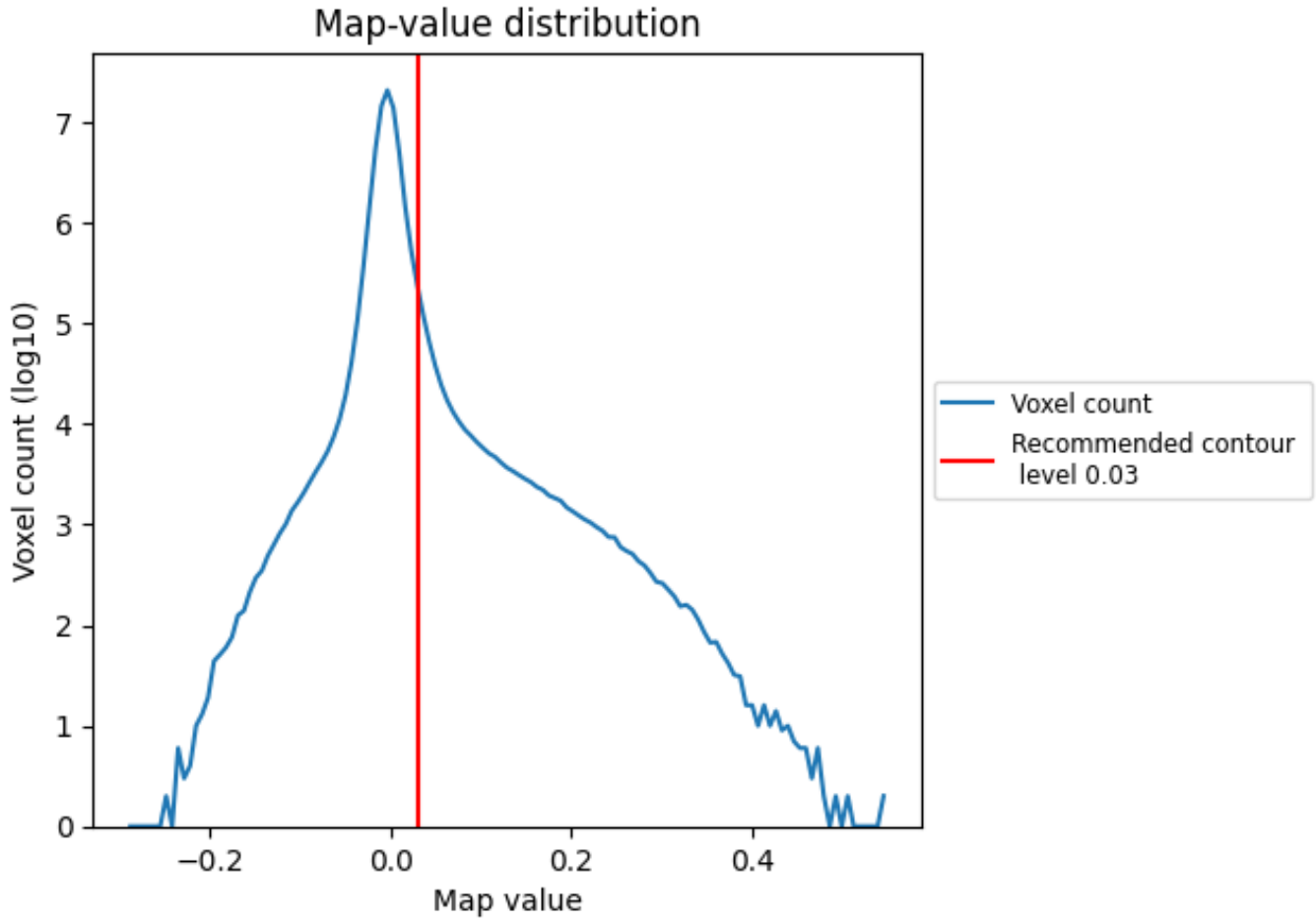
6.5 Mask visualisation (i)

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

7 Map analysis

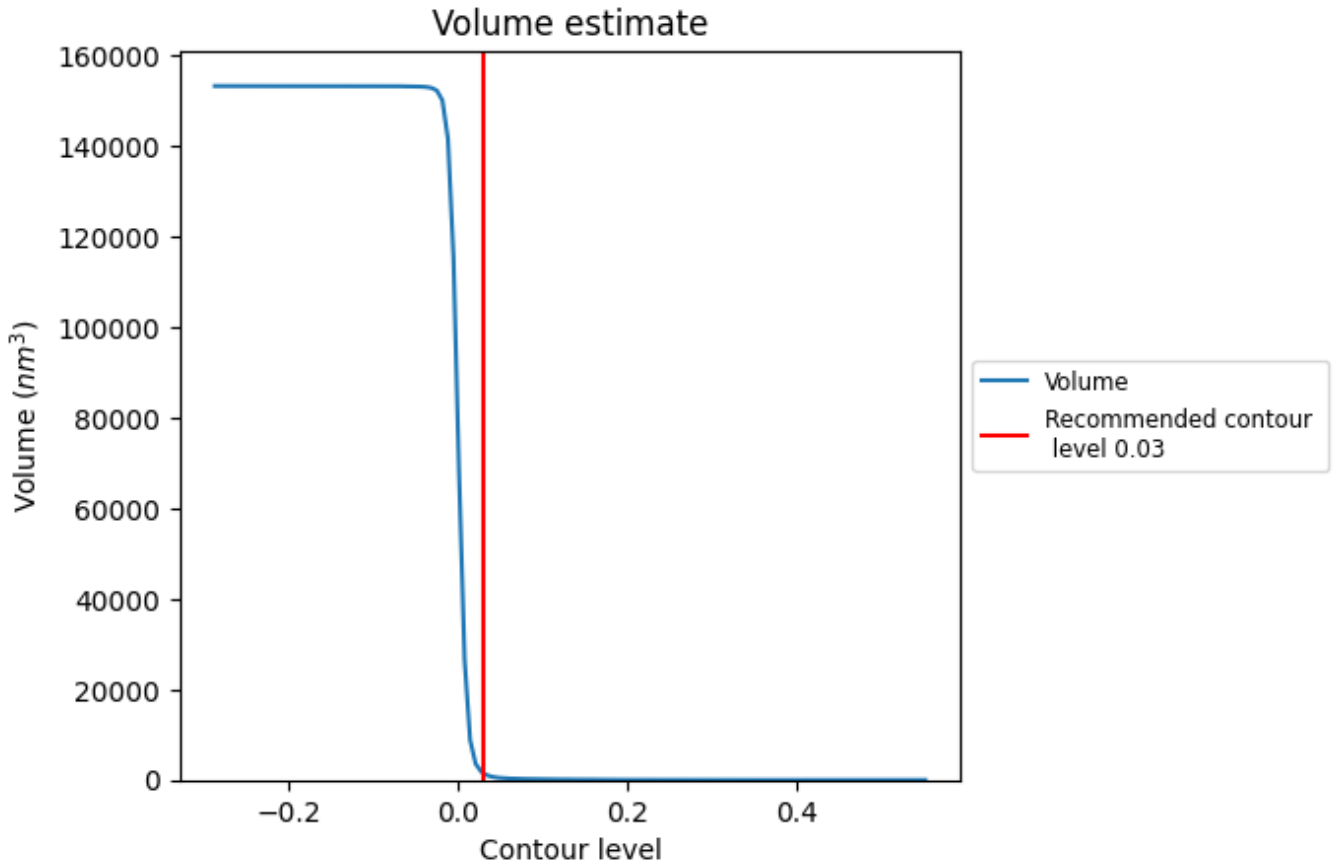
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

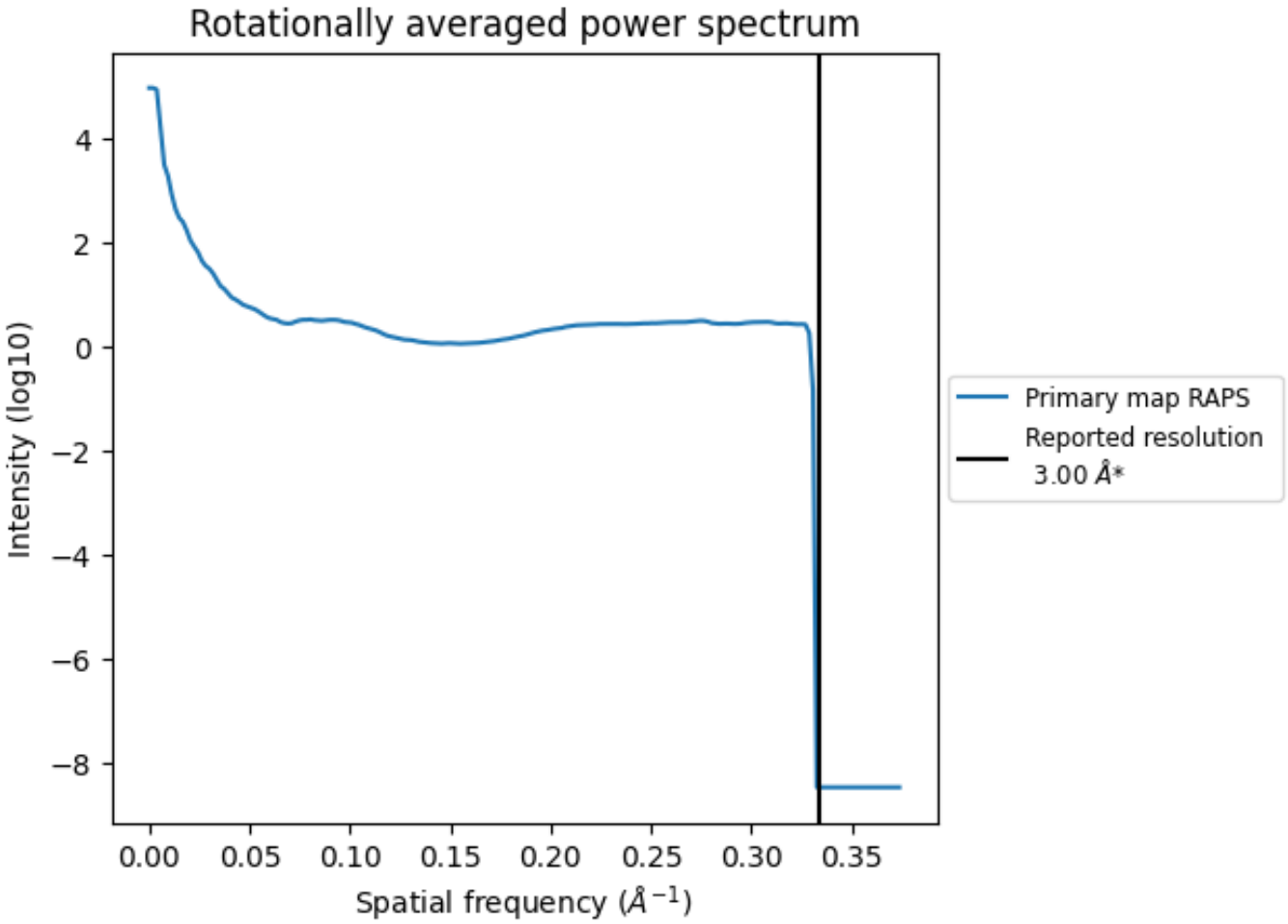
7.2 Volume estimate



The volume at the recommended contour level is 1504 nm^3; this corresponds to an approximate mass of 1358 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 (i)



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

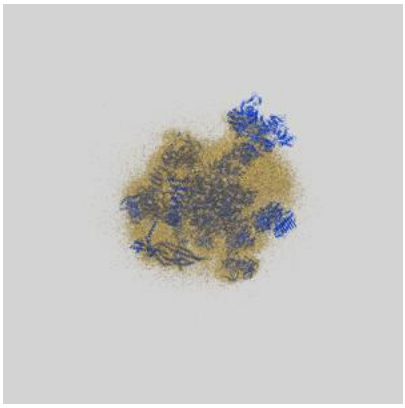
8 Fourier-Shell correlation (i)

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

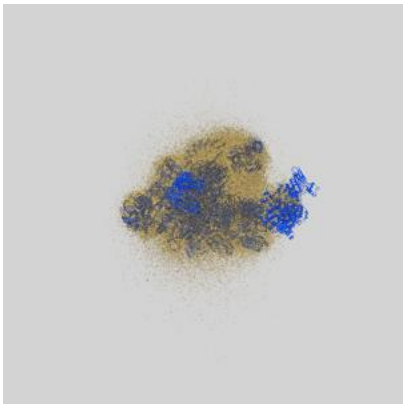
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-9645 and PDB model 6ICZ. Per-residue inclusion information can be found in section 3 on page 14.

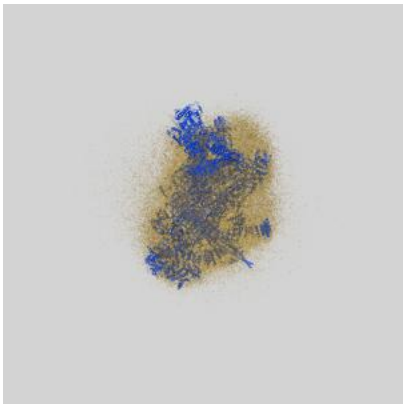
9.1 Map-model overlay



X



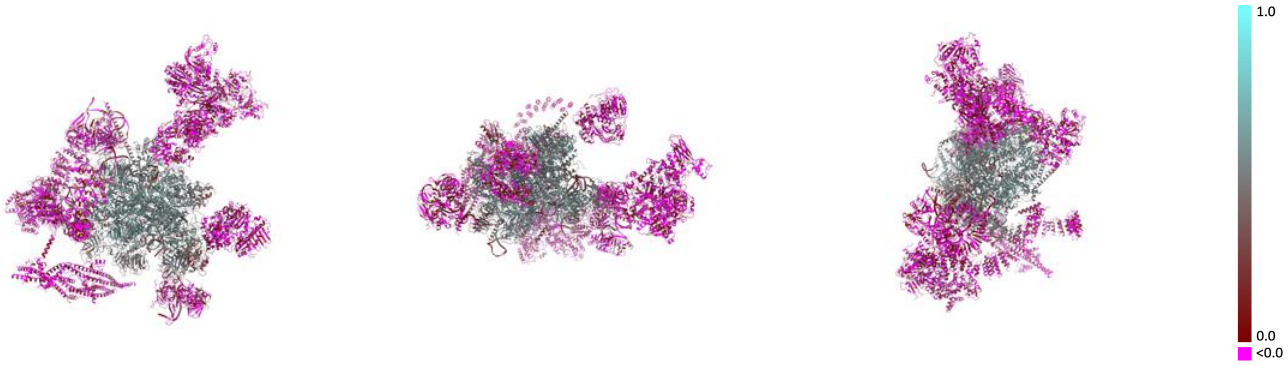
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.03 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.

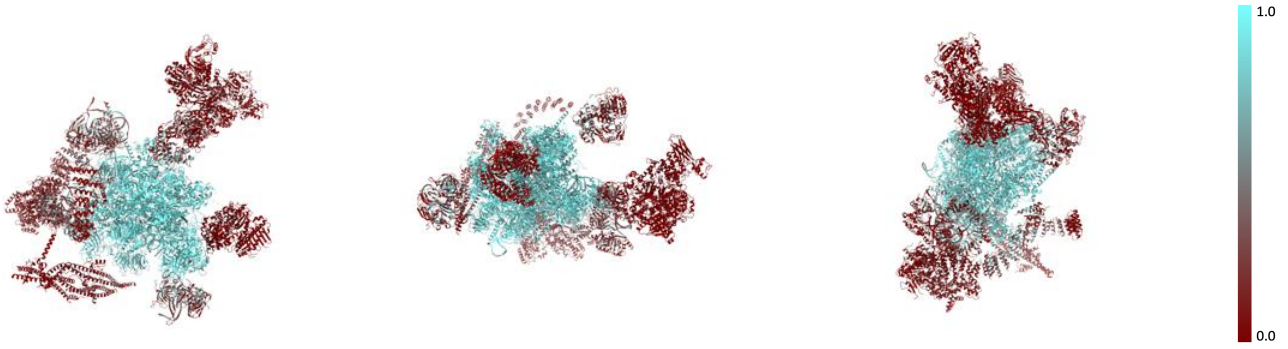
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

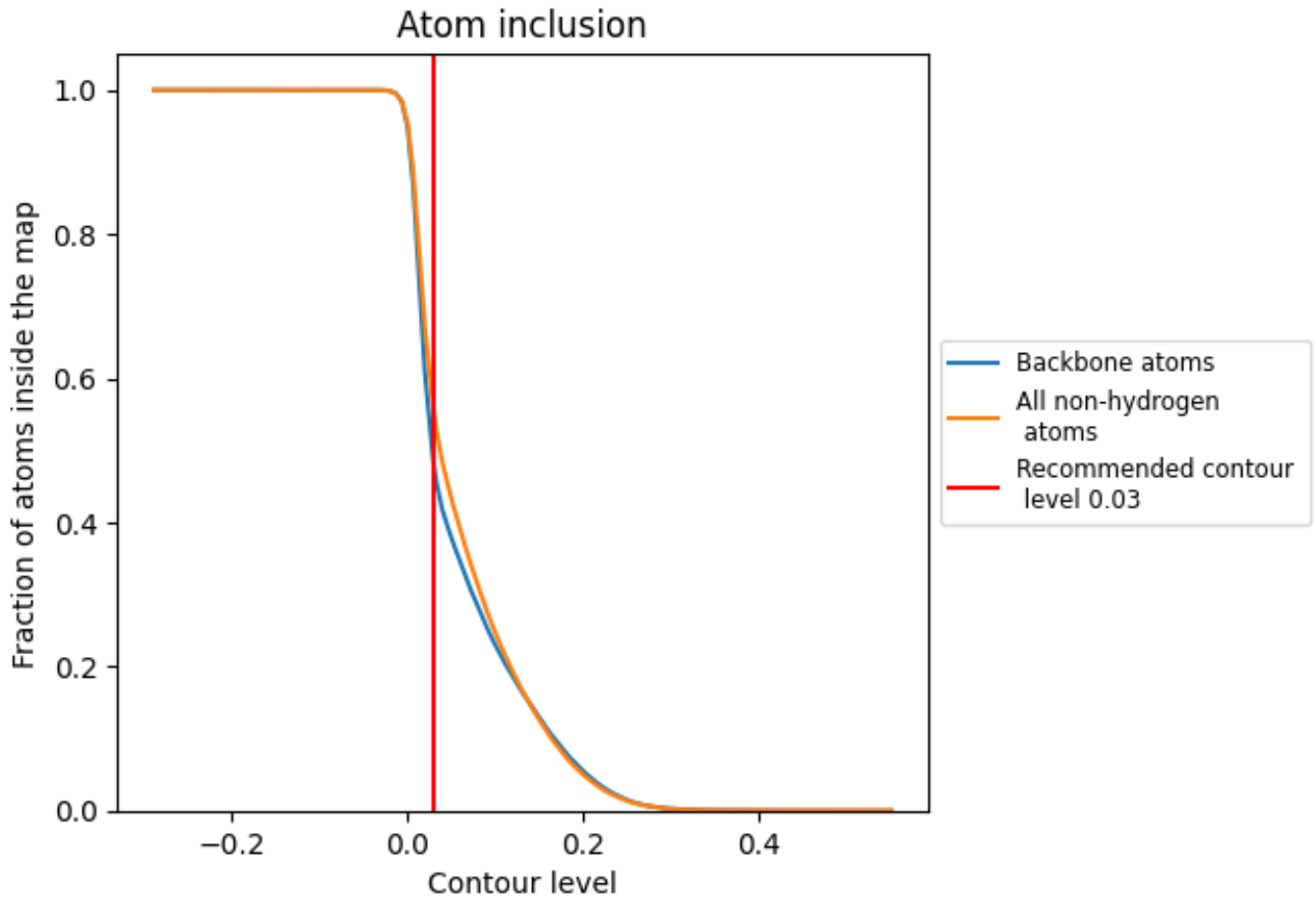
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.03).

9.4 Atom inclusion (i)



At the recommended contour level, 49% of all backbone atoms, 56% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5599	0.2840
A	0.8723	0.5070
B	0.7662	0.3530
C	0.8956	0.4650
D	0.0168	0.0020
E	0.8601	0.4140
F	0.9332	0.4850
G	0.7650	0.3440
H	0.4879	0.1340
I	0.2182	0.0190
J	0.5974	0.3190
K	0.1123	-0.0060
L	0.5997	0.3280
M	0.8731	0.4830
N	0.9349	0.5390
O	0.8165	0.4200
P	0.8335	0.4750
Q	0.0295	0.0020
R	0.8773	0.4780
S	0.8673	0.4200
T	0.9651	0.5840
U	0.8235	0.5200
V	0.4894	0.2780
W	0.8305	0.4190
X	0.5932	0.3250
Y	0.2627	0.0450
Z	0.7968	0.4390
a	0.3459	0.0120
b	0.3255	0.0300
c	0.2931	0.0150
d	0.3208	0.0150
e	0.3223	0.0560
f	0.3019	0.0360
g	0.3003	0.0160
h	0.1985	-0.0100

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
i	0.2028	0.0080
j	0.3645	0.0370
k	0.2938	-0.0060
l	0.3043	0.0530
m	0.3820	0.0410
n	0.2271	-0.0020
o	0.1493	0.0120
p	0.2392	-0.0180
q	0.0425	-0.0060
r	0.0688	0.0010
s	0.1194	0.0440
t	0.0567	-0.0170
u	0.0288	-0.0080
v	0.0014	0.0100
w	0.0000	0.0450
x	0.0000	0.0520
y	0.1872	-0.0070