



# Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 21, 2018 – 11:46 PM EST

PDB ID : 6BK8  
EMDB ID: : EMD-7109  
Title : S. cerevisiae spliceosomal post-catalytic P complex  
Authors : Liu, S.; Li, X.; Zhou, Z.H.; Zhao, R.  
Deposited on : 2017-11-07  
Resolution : 3.30 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

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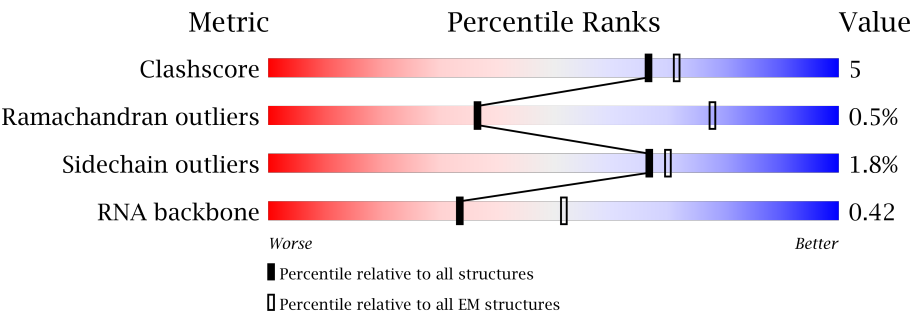
MolProbity : 4.02b-467  
Mogul : 1.7.2 (RC1), CSD as538be (2017)  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030736

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.30 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.




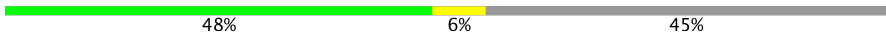














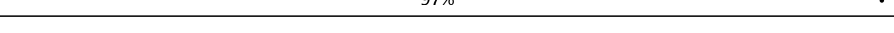
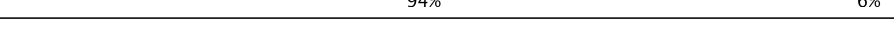







Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026
RNA backbone	3398	335

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	2	1175	<div><div>7% .. 89%</div></div>
2	5	214	<div><div>30% 13% . . 52%</div></div>
3	6	112	<div><div>50% 31% 9% . 9%</div></div>
4	e	34	<div><div>35% 44% 21%</div></div>
5	i	59	<div><div>69% 27% .</div></div>
6	A	2413	<div><div>68% 13% 19%</div></div>
7	B	1008	<div><div>75% 14% . 11%</div></div>
8	D	451	<div><div>65% 14% . 20%</div></div>






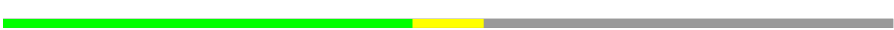






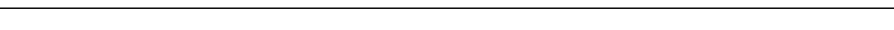
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Mol	Chain	Length	Quality of chain
9	E	379	
10	F	364	
11	G	339	
12	H	175	
13	I	157	
14	K	135	
15	L	577	
16	M	455	
17	N	251	
18	O	382	
19	P	1145	
20	R	215	
21	S	590	
22	T	687	
23	U	859	
24	X	219	
25	Y	16	
26	a	110	
26	q	110	
27	b	86	
27	m	86	
28	c	94	
28	l	94	
29	d	77	
29	n	77	

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Mol	Chain	Length	Quality of chain
30	f	196	
30	k	196	
31	g	101	
31	o	101	
32	h	146	
32	p	146	
33	r	111	
34	s	238	
35	u	503	
35	v	503	
35	w	503	
35	x	503	
36	y	175	

## 2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 82745 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	135	Total	C	N	O	P	0	0
			2848	1272	472	969	135		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	103	Total	C	N	O	P	0	0
			2173	973	367	730	103		

- Molecule 3 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	6	102	Total	C	N	O	P	0	0
			2170	972	386	710	102		

- Molecule 4 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	e	34	Total	C	N	O	P	0	0
			707	319	107	247	34		

- Molecule 5 is a RNA chain called RNA (59-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	i	59	Total	C	N	O	P	0	0
			1239	558	202	420	59		

- Molecule 6 is a protein called Pre-mRNA-splicing factor Prp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	A	1960	Total	C	N	O	S	0	0
			16159	10381	2786	2933	59		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	B	899	Total	C	N	O	S	0	0
			7179	4638	1191	1321	29		

- Molecule 8 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	D	359	Total	C	N	O	S	0	0
			2826	1786	497	533	10		

- Molecule 9 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	E	186	Total	C	N	O	S	0	0
			1494	939	276	273	6		

- Molecule 10 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	F	199	Total	C	N	O	S	0	0
			1576	991	277	293	15		

- Molecule 11 is a protein called Pre-mRNA-splicing factor CWC2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	G	255	Total	C	N	O	S	0	0
			2048	1297	362	378	11		

- Molecule 12 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	H	70	Total	C	N	O	S	0	0
			570	357	113	99	1		

- Molecule 13 is a protein called Pre-mRNA-splicing factor BUD31.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	I	156	Total	C	N	O	S	0	0
			1283	803	239	231	10		

- Molecule 14 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	K	82	Total	C	N	O	S	0	0
			550	332	106	111	1		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CWC22.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	L	412	Total	C	N	O	S	0	0
			3353	2160	556	620	17		

- Molecule 16 is a protein called Pre-mRNA-processing factor Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	M	326	Total	C	N	O	S	0	0
			2607	1649	465	485	8		

- Molecule 17 is a protein called Pre-mRNA-splicing factor Prp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	N	167	Total	C	N	O	S	0	0
			1326	856	233	233	4		

- Molecule 18 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	O	229	Total	C	N	O	S	0	0
			1935	1211	347	368	9		

- Molecule 19 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	P	653	Total	C	N	O	S	0	0
			3872	2393	736	740	3		

- Molecule 20 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	R	101	Total	C	N	O	S	0	0
			813	499	150	163	1		

- Molecule 21 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	238	Total	C	N	O	S	0	0
			1948	1218	355	368	7		

- Molecule 22 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	T	483	Total	C	N	O	S	0	0
			3370	2113	624	625	8		

- Molecule 23 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	U	637	Total	C	N	O	S	0	0
			3625	2226	689	703	7		

- Molecule 24 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
24	X	219	Total	C	N	O	0	0
			1095	657	219	219		

- Molecule 25 is a protein called Unknown protein fragment.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	16	Total	C	N	O	0	0
			80	48	16	16		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
26	q	93	Total	C	N	O	S	0	0
			726	468	136	118	4		

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

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



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

Mol	Chain	Residues	Atoms					AltConf	Trace
28	c	75	Total	C	N	O	S	0	0
			575	379	92	101	3		
28	l	75	Total	C	N	O	S	0	0
			575	379	92	101	3		

- Molecule 29 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	d	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
29	n	69	Total	C	N	O	S	0	0
			526	336	93	95	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	f	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
30	k	78	Total	C	N	O	S	0	0
			610	389	109	109	3		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
31	o	78	Total	C	N	O	S	0	0
			600	384	104	110	2		

- Molecule 32 is a protein called Small nuclear ribonucleoprotein Sm D1.

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

- Molecule 33 is a protein called Lea1.

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

- Molecule 34 is a protein called Msl1.

Mol	Chain	Residues	Atoms				AltConf	Trace
34	s	164	Total	C	N	O	0	0
			816	488	164	164		

- Molecule 35 is a protein called Pre-mRNA-processing factor Prp19.

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

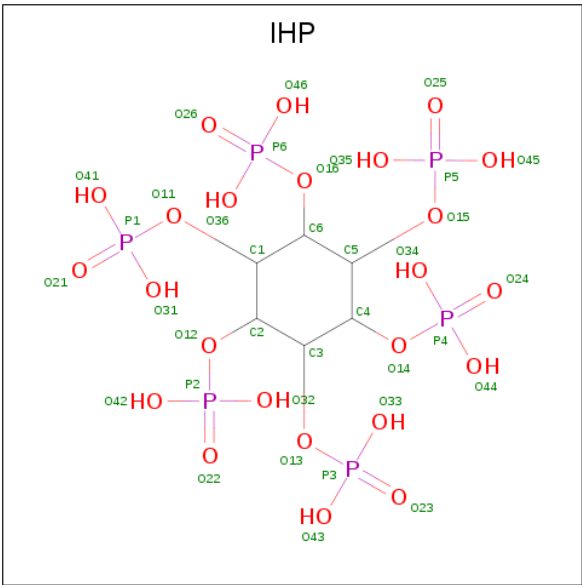
- Molecule 36 is a protein called Pre-mRNA-splicing factor SNT309.

Mol	Chain	Residues	Atoms				AltConf	Trace
36	y	110	Total	C	N	O	0	0
			548	328	110	110		

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

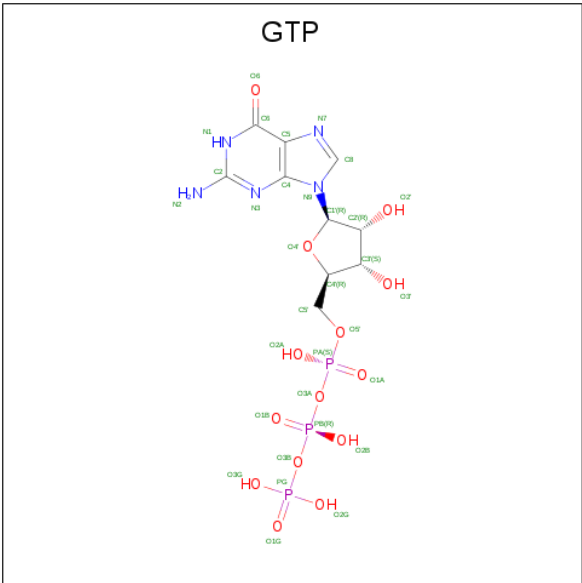
Mol	Chain	Residues	Atoms		AltConf
37	B	1	Total	Mg	0
			1	1	
37	6	4	Total	Mg	0
			4	4	

- Molecule 38 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: C<sub>6</sub>H<sub>18</sub>O<sub>24</sub>P<sub>6</sub>).



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

- Molecule 39 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula:  $C_{10}H_{16}N_5O_{14}P_3$ ).



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

- Molecule 40 is ZINC ION (three-letter code: ZN) (formula:  $Zn$ ).

Mol	Chain	Residues	Atoms		AltConf
40	G	1	Total 1	Zn 1	0
40	I	3	Total 3	Zn 3	0
40	F	2	Total 2	Zn 2	0
40	O	1	Total 1	Zn 1	0

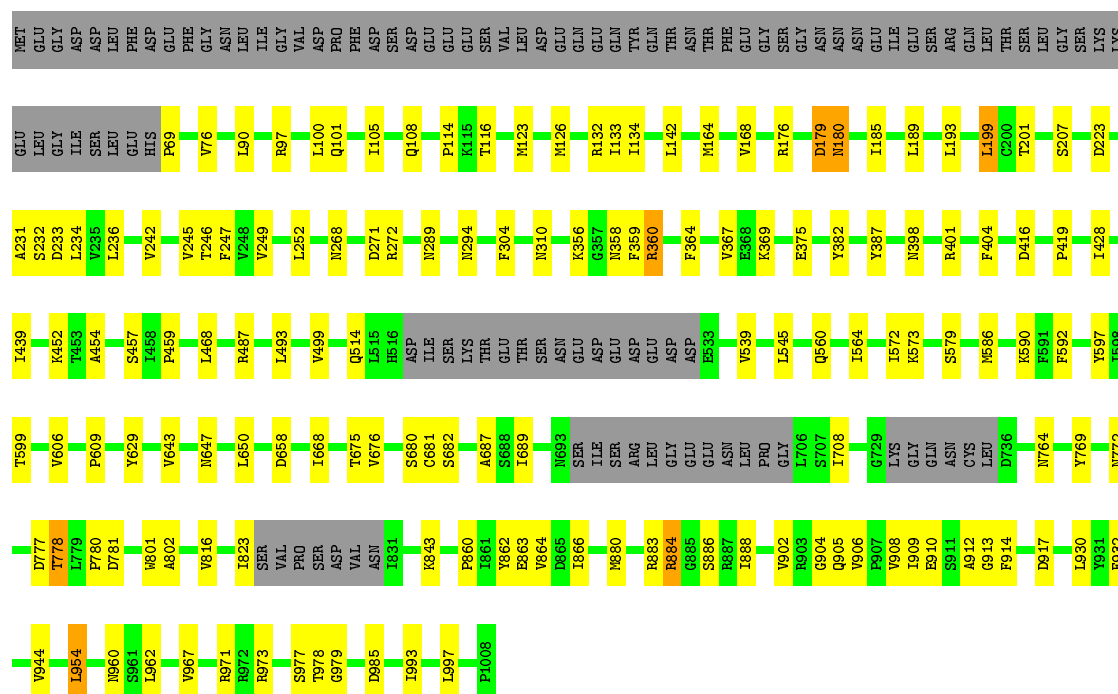
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according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

[illegible]



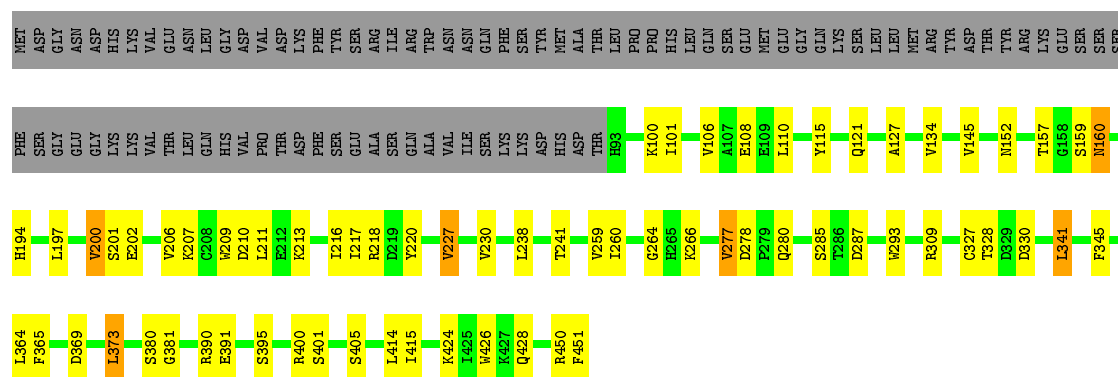
- Molecule 7: Pre-mRNA-splicing factor SNU114

Chain B:  75% 14% • 11%



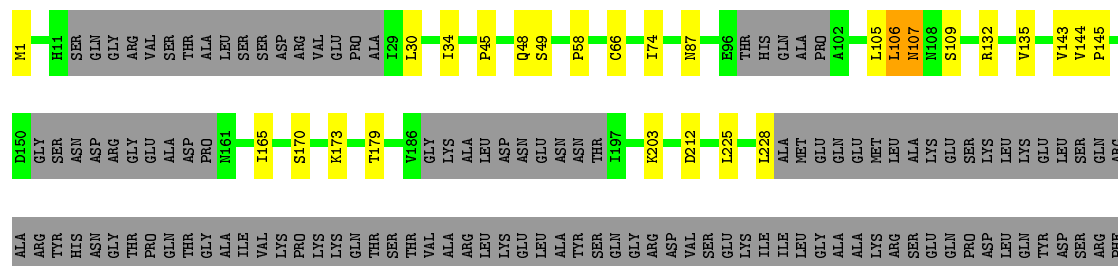
- Molecule 8: Pre-mRNA-splicing factor PRP46

Chain D:  65% 14% • 20%



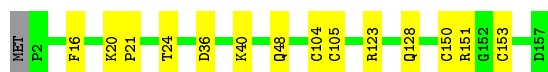
- Molecule 9: Pre-mRNA-processing protein 45

Chain E:  42% 7% 51%



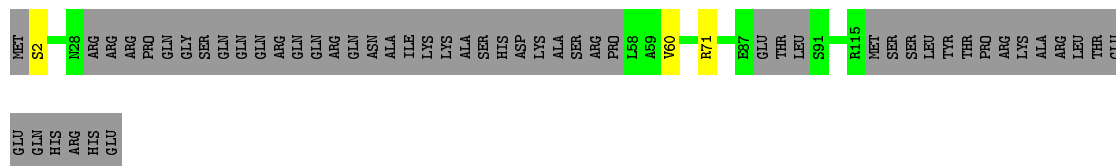






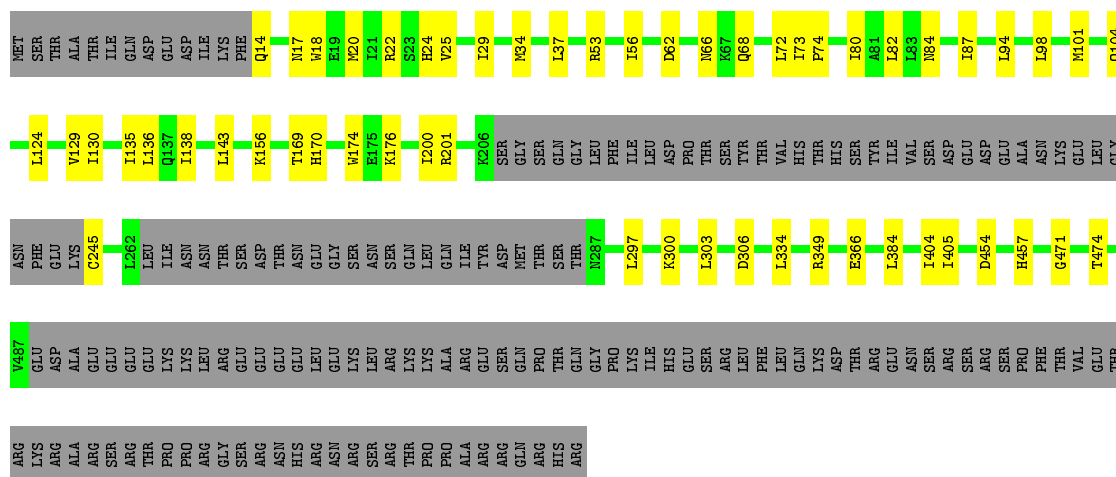
- Molecule 14: Pre-mRNA-splicing factor CWC21

Chain K:  59% . 39%



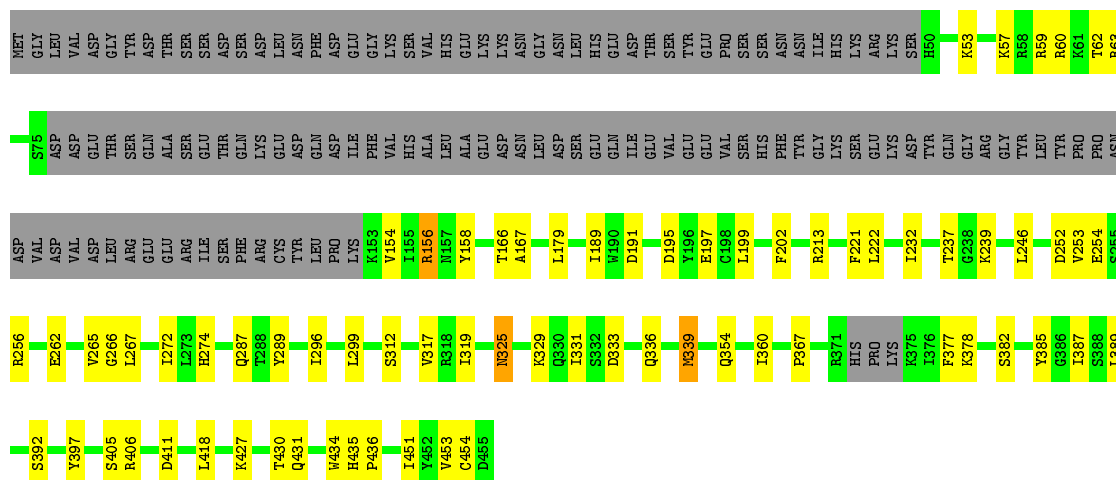
- Molecule 15: Pre-mRNA-splicing factor CWC22

Chain L:  62% 10% 29%



- Molecule 16: Pre-mRNA-processing factor Prp17

Chain M:  56% 15% 28%



- Molecule 17: Pre-mRNA-splicing factor Prp18

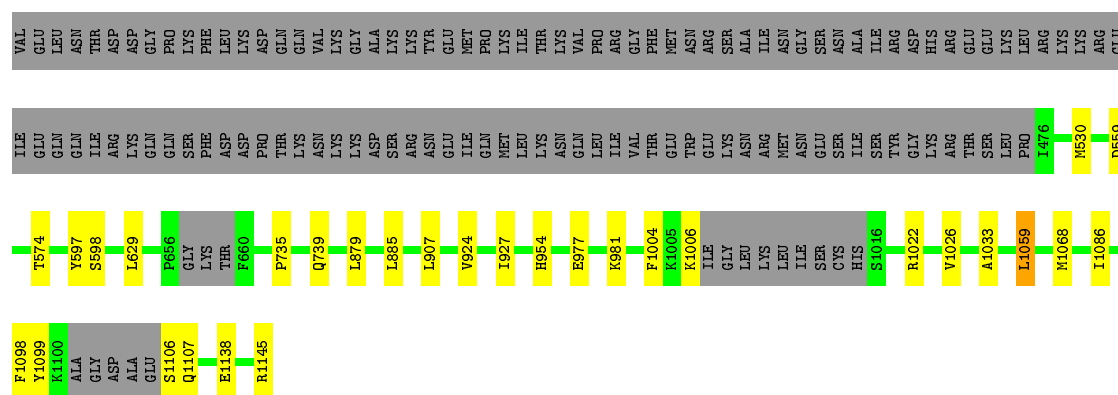
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- Chain O:  49% 11% 40%

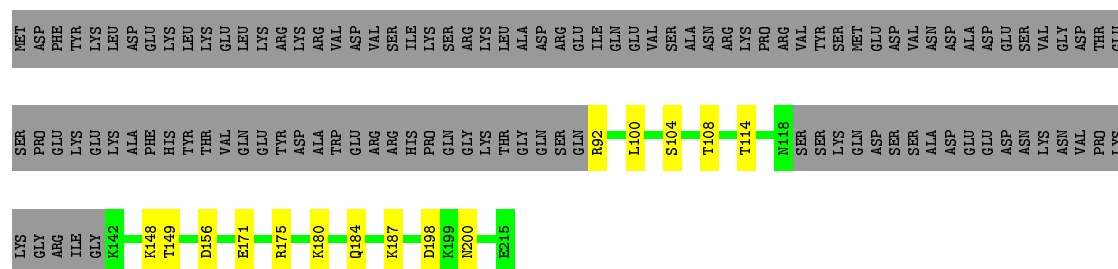
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	LEU	LEU	E260	LYS	GLY	ASN
	LYS	ASP	S261	ASN	LYS	ASN
	LEU	LEU	T262	GLY	SER	ARG
	TYR		Y266	THR	ASP	ASN
	GLY		L158 L159		Y72 L73	ASN
						GLU
			L278		G78	ASN
			D282		LYS	ARG
			E283		ALA	THR
			K284		LYS	ILE
	R289			L197	GLY	ASN
	R290			LYS	ALA	ARG
				GLY	LYS	ASN
	T293			ASP	D86	LYS
	G294			LYS	I87	ARG
				SER	N90	GLN
	L299			GLN		LEU
				THR		GLN
	K322			ASP	K94	GLN
	E323			GLU	I95	ALA
	K324			THR		LYS
	V325			LEU	I99	GLU
	Q326			TRP		LYS
	H327			ASP	F103	ASN
	V328			THR		GLU
				T213	I106	N90
	N332				ARG	
	E347			E217	PRO	I33
	LYS			K220	GLN	P34
	GLN				LYS	R35
	PRO			K225	MET	Y36
	LYS			D226	SER	I37
	ILE			S227	VAL	R38
	VAL			VAL	ASP	N39
	SER			GLY	GLY	R45
	ILE			SER	HIS	ASP
	GLY			LEU	SER	THR
	ASP			LYS	LEU	PRO
	LEU			LYS	SER	LYS
	GLU			ASP	F121	GLN
	ALA			ALA		GLU
	ARG			ASP	M124	GLY
	LYS			ASN		LYS
	VAL			SER	P139	LYS
	ASP			GLN		PRO
	GLY				M142	GLY
	THR			L241	GLN	ASN
					LYS	ASP
	LYS			T246	LEU	ASP
	GLN				VAL	THR
	SER			R249	PRO	SER
	GLU			E250	ASP	THR
	GLU			D251	LEU	THR
	GLN				ASN	ALA
	ARG			T252	SER	GLU

- Chain P:  54% 1% 43%

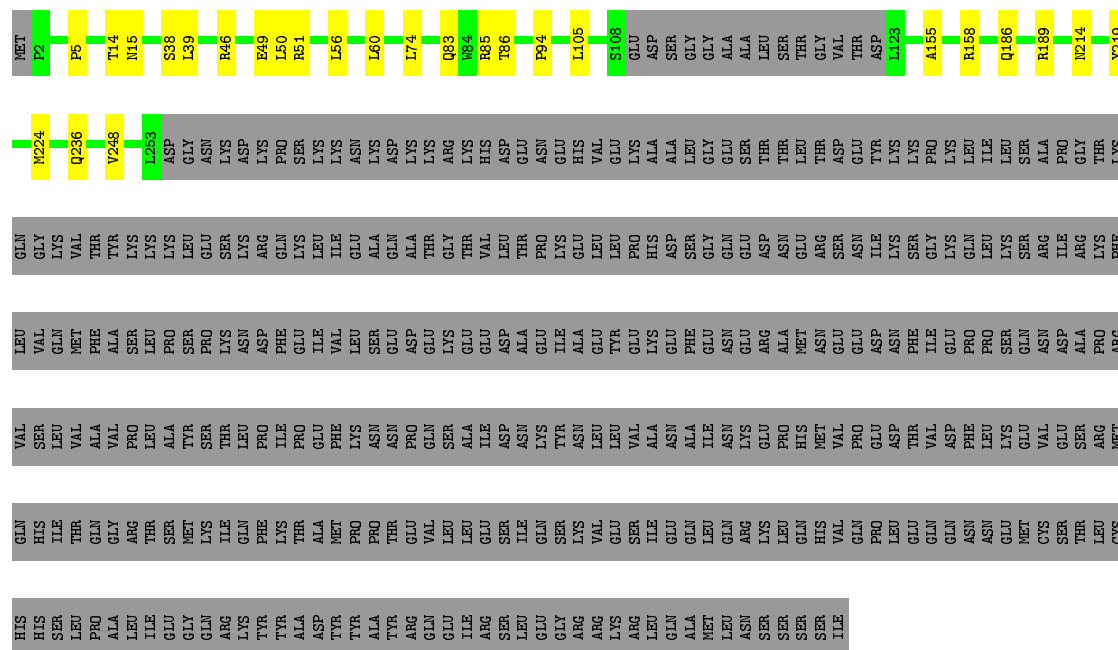
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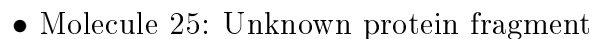
- Molecule 20: Pre-mRNA-splicing factor SYF2



- Molecule 21: Pre-mRNA-splicing factor CEF1




- Molecule 22: Pre-mRNA-splicing factor CLF1

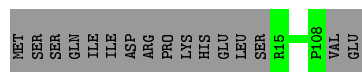


Chain Y:  94% 6%




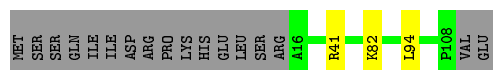
- Molecule 26: Small nuclear ribonucleoprotein Sm D2

Chain a:  85% 15%




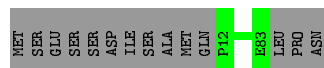
- Molecule 26: Small nuclear ribonucleoprotein Sm D2

Chain q:  82% 15%




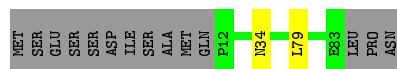
- Molecule 27: Small nuclear ribonucleoprotein F

Chain b:  84% 16%




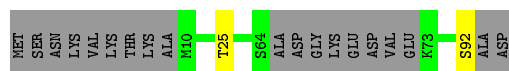
- Molecule 27: Small nuclear ribonucleoprotein F

Chain m:  81% 16%



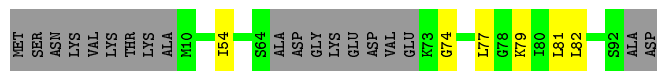
- Molecule 28: Small nuclear ribonucleoprotein E

Chain c:  78% 20%




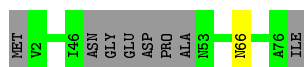
- Molecule 28: Small nuclear ribonucleoprotein E

Chain l:  73% 6% 20%



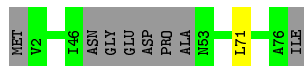
- Molecule 29: Small nuclear ribonucleoprotein G

Chain d:  88% 10%



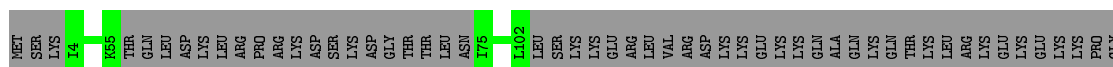
- Molecule 29: Small nuclear ribonucleoprotein G

Chain n: 88% 10%



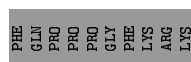
- Molecule 30: Small nuclear ribonucleoprotein-associated protein B

Chain f: 41% 59%



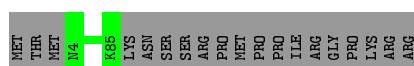
- Molecule 30: Small nuclear ribonucleoprotein-associated protein B

Chain k: 38% 60%



- Molecule 31: Small nuclear ribonucleoprotein Sm D3

Chain g: 81% 19%



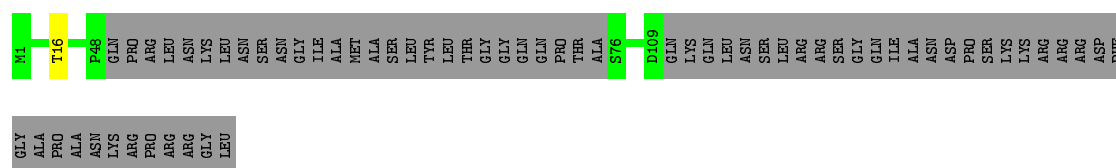
- Molecule 31: Small nuclear ribonucleoprotein Sm D3

Chain o: 74% 23%



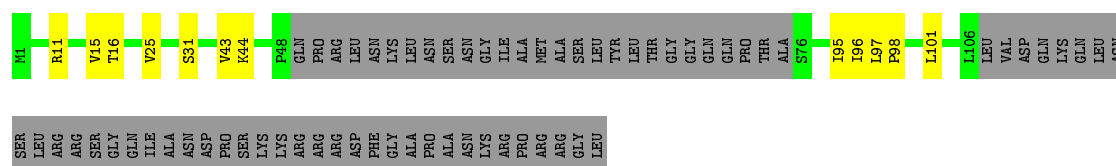
- Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain h:  55% . 44%



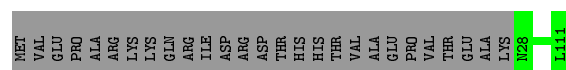
- Molecule 32: Small nuclear ribonucleoprotein Sm D1

Chain p:  46% 8% 46%



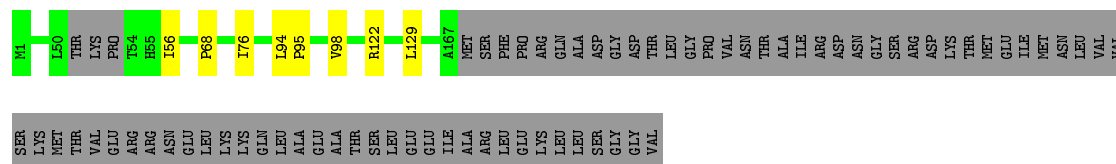
- Molecule 33: Lea1

Chain r:  76% 24%




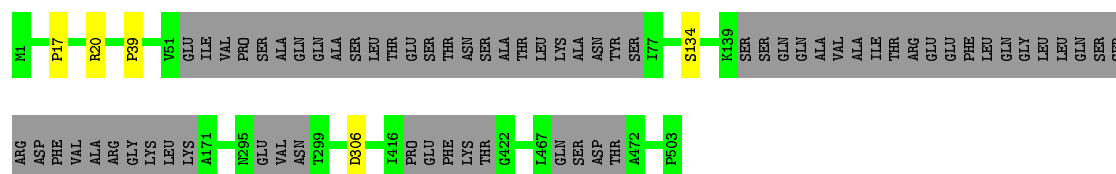
- Molecule 34: Msl1

Chain s:  66% . 31%



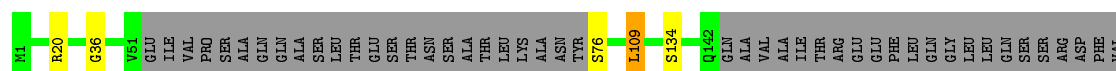
- Molecule 35: Pre-mRNA-processing factor Prp19

Chain u:  85% • 14%

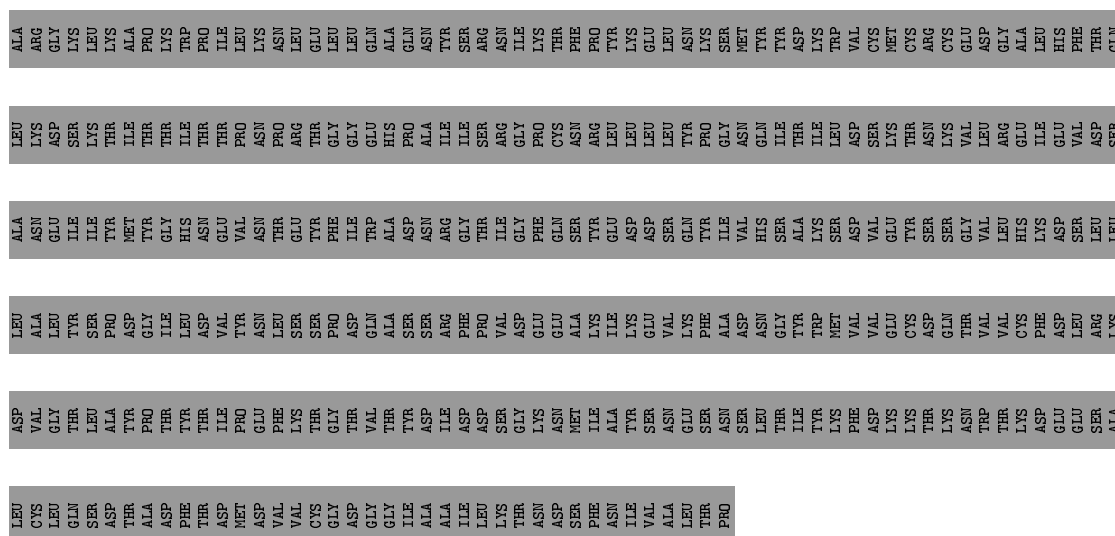


- Molecule 35: Pre-mRNA-processing factor Prp19

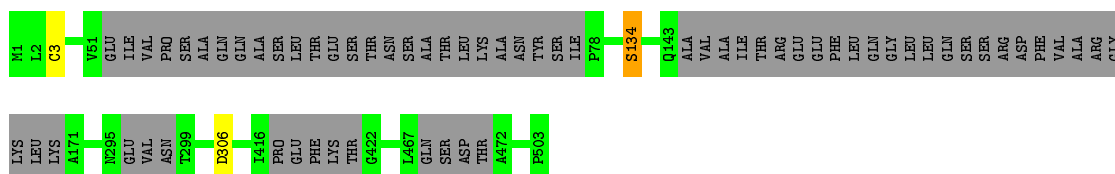
Chain v:  22% 77%



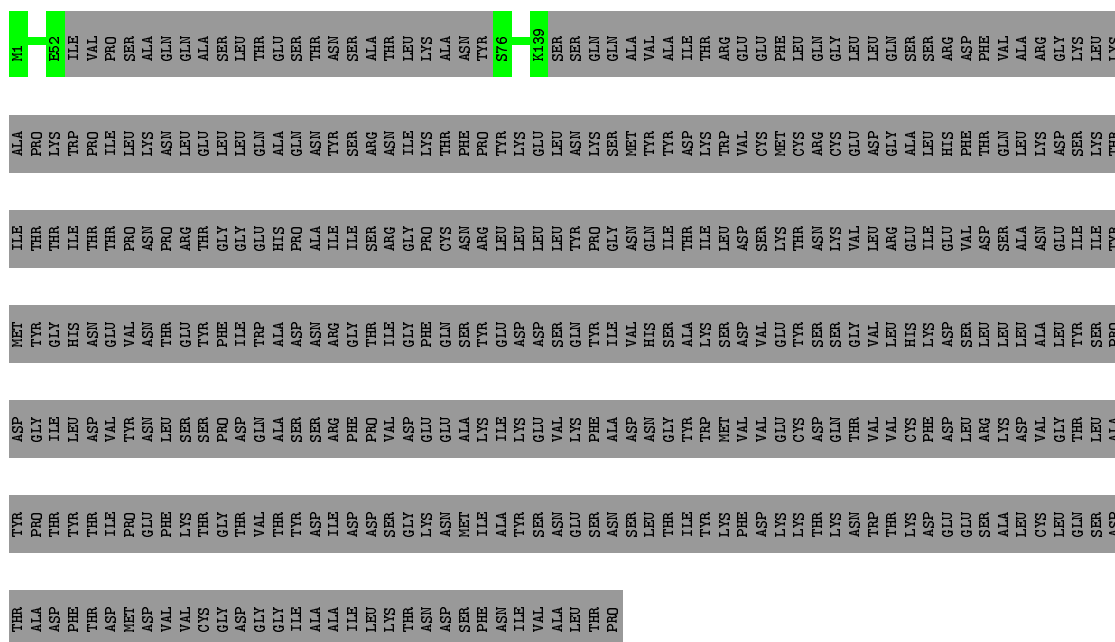




- Molecule 35: Pre-mRNA-processing factor Prp19



- Molecule 35: Pre-mRNA-processing factor Prp19



- Molecule 36: Pre-mRNA-splicing factor SNT309

Chain y:



## 4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	212219	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	2.0	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 2$	RMSZ	# $ Z  > 2$
1	2	0.50	1/3167 (0.0%)	0.92	8/4911 (0.2%)
10	F	0.43	0/1598	0.67	2/2151 (0.1%)
11	G	0.47	0/2094	0.62	2/2815 (0.1%)
12	H	0.41	0/584	0.76	1/781 (0.1%)
13	I	0.49	0/1307	0.59	0/1748
14	K	0.35	0/552	0.56	0/746
15	L	0.38	0/3406	0.63	1/4592 (0.0%)
16	M	0.37	0/2678	0.61	1/3619 (0.0%)
17	N	0.39	0/1354	0.59	0/1838
18	O	0.36	0/1967	0.62	2/2624 (0.1%)
19	P	0.29	0/3918	0.48	2/5386 (0.0%)
2	5	0.88	0/2422	1.16	21/3762 (0.6%)
20	R	0.39	0/817	0.57	1/1083 (0.1%)
21	S	0.46	0/1978	0.63	1/2655 (0.0%)
22	T	0.45	0/3411	0.55	1/4632 (0.0%)
23	U	0.27	0/3625	0.45	0/4963
26	a	0.36	0/753	0.57	0/1013
26	q	0.38	0/738	0.61	0/995
27	b	0.41	0/585	0.57	0/791
27	m	0.40	0/585	0.61	0/791
28	c	0.42	0/585	0.61	0/795
28	l	0.40	0/585	0.56	0/795
29	d	0.50	0/532	0.61	0/715
29	n	0.36	0/529	0.50	0/711
3	6	0.89	0/2427	1.13	15/3778 (0.4%)
30	f	0.36	0/636	0.63	0/856
30	k	0.35	0/614	0.57	0/826
31	g	0.35	0/634	0.56	0/859
31	o	0.37	0/607	0.53	0/820
32	h	0.38	0/649	0.54	0/880
32	p	0.40	0/623	0.65	0/844
33	r	0.33	0/415	0.55	0/577

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >2	RMSZ	# Z  >2
34	s	0.31	0/814	0.53	0/1134
35	u	0.47	0/2150	0.68	2/2989 (0.1%)
35	v	0.59	0/586	0.89	3/816 (0.4%)
35	w	0.47	0/2165	0.71	3/3010 (0.1%)
35	x	0.58	0/576	0.79	0/802
36	y	0.58	0/546	0.80	0/760
4	e	0.82	4/787 (0.5%)	1.48	17/1219 (1.4%)
5	i	0.59	0/1379	1.10	3/2131 (0.1%)
6	A	0.52	0/16570	0.68	8/22456 (0.0%)
7	B	0.49	0/7331	0.70	8/9926 (0.1%)
8	D	0.56	1/2889 (0.0%)	0.71	2/3924 (0.1%)
9	E	0.44	0/1517	0.63	0/2043
All	All	0.49	6/83685 (0.0%)	0.72	104/115562 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
10	F	0	1
11	G	0	2
15	L	0	1
18	O	0	1
30	k	0	1
35	u	0	1
35	v	0	1
35	w	0	2
36	y	0	2
6	A	0	6
7	B	0	9
8	D	0	2
9	E	0	3
All	All	0	32

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	e	9	U	C1'-N1	7.04	1.59	1.48
4	e	-13	U	C1'-N1	6.81	1.58	1.48
4	e	-11	U	C1'-N1	6.04	1.57	1.48
4	e	-2	A	N9-C4	-6.00	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	227	VAL	CB-CG1	-5.37	1.41	1.52
1	2	21	G	N7-C5	-5.24	1.36	1.39

All (104) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	954	LEU	CA-CB-CG	9.20	136.46	115.30
4	e	11	U	C2-N1-C1'	9.14	128.67	117.70
4	e	11	U	N1-C2-O2	8.22	128.55	122.80
35	w	134	SER	CA-C-O	-7.91	103.49	120.10
4	e	2	U	N1-C2-O2	7.86	128.30	122.80
7	B	193	LEU	CA-CB-CG	7.84	133.32	115.30
4	e	11	U	N3-C2-O2	-7.70	116.81	122.20
4	e	2	U	N3-C2-O2	-7.63	116.86	122.20
6	A	355	LEU	CA-CB-CG	7.48	132.50	115.30
18	O	73	LEU	CA-CB-CG	7.35	132.21	115.30
4	e	2	U	C2-N1-C1'	7.31	126.47	117.70
2	5	60	U	N1-C2-O2	7.30	127.91	122.80
8	D	341	LEU	CA-CB-CG	7.12	131.69	115.30
7	B	781	ASP	CB-CG-OD1	7.11	124.70	118.30
2	5	79	C	C2-N1-C1'	7.06	126.57	118.80
2	5	99	U	C5-C6-N1	7.04	126.22	122.70
4	e	-12	U	C2-N1-C1'	7.03	126.13	117.70
7	B	142	LEU	CA-CB-CG	6.99	131.37	115.30
21	S	224	MET	CA-CB-CG	6.97	125.15	113.30
11	G	151	LEU	CA-CB-CG	6.95	131.28	115.30
6	A	852	LEU	CB-CG-CD1	-6.84	99.38	111.00
2	5	60	U	N3-C2-O2	-6.83	117.42	122.20
2	5	60	U	C2-N1-C1'	6.76	125.81	117.70
4	e	17	U	P-O3'-C3'	6.75	127.80	119.70
4	e	4	U	C2-N1-C1'	6.66	125.69	117.70
3	6	67	C	C5-C6-N1	6.46	124.23	121.00
12	H	9	LEU	CA-CB-CG	6.46	130.16	115.30
2	5	97	U	C5-C6-N1	6.45	125.93	122.70
3	6	54	U	O4'-C1'-N1	6.45	113.36	108.20
7	B	236	LEU	CA-CB-CG	6.44	130.11	115.30
7	B	884	ARG	CA-CB-CG	6.43	127.55	113.40
7	B	199	LEU	CA-CB-CG	6.40	130.01	115.30
6	A	1634	LEU	CA-CB-CG	6.39	130.00	115.30
5	i	508	G	P-O3'-C3'	6.38	127.36	119.70
1	2	10	U	C2-N1-C1'	6.34	125.31	117.70
4	e	-12	U	N3-C2-O2	-6.29	117.80	122.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	2	11	U	N1-C2-O2	6.22	127.16	122.80
3	6	89	U	N3-C2-O2	-6.19	117.87	122.20
4	e	4	U	N3-C2-O2	-6.18	117.87	122.20
2	5	90	C	C6-N1-C2	-6.16	117.84	120.30
2	5	79	C	C6-N1-C2	-6.11	117.86	120.30
2	5	90	C	C5-C6-N1	6.09	124.04	121.00
2	5	125	C	C2-N1-C1'	6.06	125.47	118.80
4	e	-12	U	N1-C2-O2	6.05	127.03	122.80
4	e	11	U	C5-C6-N1	6.04	125.72	122.70
35	w	134	SER	O-C-N	6.00	132.30	122.70
6	A	593	LEU	CA-CB-CG	5.99	129.07	115.30
16	M	367	PRO	N-CA-CB	5.96	110.46	103.30
4	e	4	U	N1-C2-O2	5.94	126.96	122.80
3	6	80	U	C5-C6-N1	5.93	125.66	122.70
1	2	41	C	N1-C2-O2	5.92	122.45	118.90
15	L	303	LEU	CA-CB-CG	5.92	128.93	115.30
35	u	39	PRO	N-CA-CB	5.91	110.39	103.30
3	6	66	C	C6-N1-C2	-5.91	117.94	120.30
4	e	6	U	C2-N1-C1'	5.88	124.76	117.70
6	A	786	LEU	CA-CB-CG	5.80	128.64	115.30
3	6	14	C	P-O3'-C3'	5.79	126.64	119.70
2	5	90	C	C2-N1-C1'	5.77	125.14	118.80
3	6	64	U	C5-C6-N1	5.70	125.55	122.70
2	5	99	U	N1-C2-O2	5.69	126.78	122.80
7	B	962	LEU	CA-CB-CG	5.69	128.38	115.30
35	v	134	SER	CA-C-O	-5.69	108.16	120.10
1	2	41	C	P-O3'-C3'	5.67	126.50	119.70
4	e	17	U	OP1-P-O3'	5.66	117.66	105.20
10	F	94	VAL	C-N-CA	5.66	135.85	121.70
1	2	11	U	C5-C6-N1	5.66	125.53	122.70
4	e	11	U	C6-N1-C1'	-5.65	113.29	121.20
22	T	159	TRP	CA-CB-CG	5.63	124.40	113.70
2	5	112	C	C6-N1-C2	-5.63	118.05	120.30
3	6	43	C	N1-C2-O2	5.59	122.26	118.90
6	A	127	LEU	CA-CB-CG	5.59	128.15	115.30
3	6	48	C	C6-N1-C2	-5.57	118.07	120.30
2	5	78	A	OP1-P-O3'	5.52	117.35	105.20
2	5	125	C	C5-C6-N1	5.50	123.75	121.00
2	5	111	C	C6-N1-C2	-5.49	118.11	120.30
19	P	954	HIS	C-N-CA	5.48	135.40	121.70
10	F	37	CYS	CA-CB-SG	5.46	123.82	114.00
2	5	99	U	C2-N1-C1'	5.45	124.24	117.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	6	56	A	P-O3'-C3'	5.44	126.23	119.70
2	5	99	U	N3-C2-O2	-5.41	118.41	122.20
6	A	407	VAL	CG1-CB-CG2	-5.41	102.25	110.90
3	6	89	U	N1-C2-O2	5.38	126.57	122.80
5	i	1111	U	C2-N1-C1'	5.37	124.14	117.70
3	6	64	U	P-O3'-C3'	5.34	126.11	119.70
3	6	67	C	C6-N1-C2	-5.34	118.16	120.30
35	v	76	SER	N-CA-CB	5.33	118.49	110.50
18	O	226	ASP	CB-CG-OD1	5.30	123.07	118.30
1	2	41	C	C5-C6-N1	5.27	123.64	121.00
1	2	21	G	C8-N9-C1'	-5.22	120.21	127.00
6	A	582	LEU	CA-CB-CG	5.22	127.30	115.30
11	G	221	LEU	CA-CB-CG	5.20	127.25	115.30
19	P	1059	LEU	CA-CB-CG	5.17	127.19	115.30
35	v	134	SER	O-C-N	5.17	130.96	122.70
1	2	11	U	N3-C2-O2	-5.12	118.62	122.20
35	w	306	ASP	CB-CA-C	-5.12	100.17	110.40
3	6	89	U	C2-N1-C1'	5.09	123.81	117.70
35	u	306	ASP	CB-CA-C	-5.09	100.22	110.40
2	5	97	U	O5'-P-OP1	-5.07	101.14	105.70
5	i	1111	U	N3-C2-O2	-5.07	118.65	122.20
8	D	373	LEU	CA-CB-CG	5.06	126.94	115.30
2	5	101	C	N1-C2-O2	5.03	121.92	118.90
3	6	61	C	C6-N1-C2	-5.02	118.29	120.30
2	5	78	A	P-O3'-C3'	5.01	125.72	119.70
20	R	100	LEU	CA-CB-CG	5.01	126.83	115.30

There are no chirality outliers.

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	A	1325	SER	Peptide
6	A	1474	ARG	Peptide
6	A	405	ASN	Peptide
6	A	542	HIS	Peptide
6	A	774	ILE	Peptide
6	A	775	ARG	Peptide
7	B	114	PRO	Peptide
7	B	179	ASP	Peptide
7	B	572	ILE	Peptide
7	B	597	TYR	Peptide
7	B	682	SER	Peptide

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Mol	Chain	Res	Type	Group
7	B	769	TYR	Peptide
7	B	777	ASP	Peptide
7	B	977	SER	Peptide
7	B	978	THR	Peptide
8	D	277	VAL	Peptide
8	D	341	LEU	Peptide
9	E	106	LEU	Peptide
9	E	107	ASN	Peptide
9	E	143	VAL	Peptide
10	F	120	LEU	Peptide
11	G	206	LEU	Peptide
11	G	23	PRO	Peptide
15	L	300	LYS	Peptide
18	O	322	LYS	Peptide
30	k	84	LEU	Peptide
35	u	134	SER	Mainchain
35	v	109	LEU	Mainchain
35	w	134	SER	Mainchain
35	w	3	CYS	Mainchain
36	y	111	VAL	Peptide
36	y	132	LEU	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2848	0	1445	11	0
2	5	2173	0	1102	11	0
3	6	2170	0	1095	14	0
4	e	707	0	354	0	0
5	i	1239	0	624	0	0
6	A	16159	0	16162	181	0
7	B	7179	0	7361	76	0
8	D	2826	0	2816	47	0
9	E	1494	0	1540	22	0
10	F	1576	0	1607	13	0
11	G	2048	0	2011	17	0
12	H	570	0	556	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
13	I	1283	0	1301	10	0
14	K	550	0	454	2	0
15	L	3353	0	3421	30	0
16	M	2607	0	2512	41	0
17	N	1326	0	1367	13	0
18	O	1935	0	1894	35	0
19	P	3872	0	2618	16	0
20	R	813	0	837	11	0
21	S	1948	0	1979	20	0
22	T	3370	0	2727	22	0
23	U	3625	0	2248	15	0
24	X	1095	0	231	9	0
25	Y	80	0	18	1	0
26	a	741	0	778	0	0
26	q	726	0	754	0	0
27	b	573	0	572	0	0
27	m	573	0	572	0	0
28	c	575	0	597	0	0
28	l	575	0	597	0	0
29	d	529	0	557	0	0
29	n	526	0	555	0	0
30	f	631	0	670	0	0
30	k	610	0	638	0	0
31	g	625	0	647	0	0
31	o	600	0	623	0	0
32	h	644	0	686	0	0
32	p	618	0	660	0	0
33	r	416	0	182	0	0
34	s	816	0	341	0	0
35	u	2156	0	938	0	0
35	v	588	0	250	0	0
35	w	2171	0	945	0	0
35	x	578	0	246	0	0
36	y	548	0	219	0	0
37	6	4	0	0	0	0
37	B	1	0	0	0	0
38	A	36	0	6	3	0
39	B	32	0	12	0	0
40	F	2	0	0	0	0
40	G	1	0	0	0	0
40	I	3	0	0	0	0
40	O	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	82745	0	70325	520	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (520) 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)
9:E:212:ASP:OD2	24:X:1024:UNK:O	1.57	1.22
13:I:150:CYS:SG	13:I:153:CYS:HB3	2.11	0.90
19:P:598:SER:O	19:P:629:LEU:HA	1.75	0.87
1:2:1108:A:N6	20:R:108:THR:CB	107.65	0.84
11:G:81:CYS:SG	11:G:91:HIS:HE1	2.01	0.83
9:E:212:ASP:CG	24:X:1024:UNK:O	2.22	0.78
6:A:517:LYS:NZ	38:A:3001:IHP:O45	2.20	0.74
9:E:212:ASP:OD2	24:X:1024:UNK:C	2.36	0.74
2:5:48:G:H1	2:5:67:U:H3	1.37	0.72
8:D:217:ILE:HG22	8:D:218:ARG:HG3	1.70	0.72
23:U:729:TYR:CD2	23:U:748:PHE:HD1	2.09	0.71
8:D:127:ALA:HB3	8:D:428:GLN:HE21	1.56	0.70
8:D:197:LEU:HB3	8:D:209:TRP:HB2	1.73	0.70
6:A:936:GLU:HG2	6:A:986:PRO:HB3	1.75	0.68
8:D:280:GLN:NE2	9:E:66:CYS:SG	2.67	0.67
3:6:90:U:OP2	22:T:104:ARG:NH2	2.28	0.66
8:D:259:VAL:HG12	8:D:260:ILE:HG13	1.76	0.66
15:L:143:LEU:HD23	15:L:176:LYS:HD3	1.78	0.66
7:B:778:THR:HG23	7:B:780:PRO:HD3	1.77	0.66
6:A:141:LYS:HZ3	13:I:48:GLN:HB3	1.61	0.65
1:2:31:A:H4'	21:S:5:PRO:HB3	1.78	0.65
16:M:158:TYR:HB2	16:M:451:ILE:HB	1.80	0.64
16:M:333:ASP:HB2	16:M:336:GLN:HB2	1.80	0.63
20:R:156:ASP:OD2	22:T:119:ARG:NH2	2.31	0.63
7:B:126:MET:HB3	7:B:132:ARG:HG2	1.80	0.63
7:B:105:ILE:O	7:B:180:ASN:ND2	2.30	0.63
7:B:971:ARG:NH1	7:B:985:ASP:O	2.31	0.63
6:A:1071:ARG:HB2	24:X:1025:UNK:CB	2.28	0.63
11:G:212:TRP:O	11:G:215:ARG:NH2	2.32	0.63
8:D:159:SER:OG	8:D:160:ASN:N	2.31	0.62
24:X:2305:UNK:O	24:X:2306:UNK:CB	2.47	0.62
24:X:3402:UNK:O	24:X:3403:UNK:CB	2.45	0.62
6:A:294:ASN:HD21	6:A:299:LYS:HB2	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1851:PHE:O	6:A:1881:THR:HA	2.00	0.61
6:A:1011:ASN:ND2	6:A:1143:GLU:O	2.29	0.61
6:A:319:ARG:NH1	6:A:321:GLU:OE1	2.32	0.61
23:U:716:ALA:HB1	23:U:725:THR:HG22	1.82	0.61
6:A:1073:ILE:HG13	6:A:1074:VAL:HG13	1.82	0.61
17:N:151:ARG:HH11	18:O:220:LYS:HE3	1.66	0.61
9:E:34:ILE:O	22:T:123:ASN:ND2	2.33	0.61
13:I:151:ARG:O	16:M:63:ARG:NH1	2.34	0.61
20:R:187:LYS:NZ	20:R:198:ASP:OD1	2.34	0.61
6:A:1910:LYS:HB3	6:A:1943:PRO:HG2	1.84	0.60
10:F:13:CYS:HB3	10:F:16:CYS:SG	2.40	0.60
6:A:898:ILE:HA	6:A:1006:ARG:HH12	1.66	0.60
1:2:1108:A:H62	20:R:108:THR:CB	107.12	0.59
17:N:205:ARG:H	17:N:208:HIS:HD2	1.48	0.59
15:L:366:GLU:HG2	15:L:404:ILE:HD13	1.82	0.59
7:B:468:LEU:HB3	7:B:579:SER:HB3	1.84	0.59
6:A:1090:ILE:O	6:A:1096:SER:HA	2.03	0.59
6:A:1666:CYS:SG	18:O:249:ARG:NH1	2.75	0.59
20:R:171:GLU:OE2	20:R:175:ARG:NH2	2.35	0.59
6:A:1004:ASP:OD2	6:A:1506:ARG:NH1	2.36	0.59
6:A:1232:SER:OG	12:H:135:ARG:NH2	2.35	0.59
16:M:360:ILE:HB	16:M:377:PHE:HB2	1.84	0.59
2:5:75:A:H4'	2:5:76:U:H5'	1.85	0.59
8:D:121:GLN:NE2	9:E:49:SER:O	2.35	0.59
6:A:1051:GLU:OE2	6:A:1204:ARG:NH2	2.36	0.59
6:A:1405:ILE:HG23	6:A:1439:THR:HG21	1.85	0.58
6:A:835:LYS:HD2	12:H:173:HIS:HE1	1.69	0.58
7:B:234:LEU:HD21	7:B:439:ILE:HG23	1.86	0.58
13:I:104:CYS:SG	13:I:105:CYS:N	2.76	0.58
15:L:94:LEU:O	15:L:98:LEU:HB2	2.03	0.58
6:A:366:GLU:O	6:A:372:ARG:NH2	2.35	0.58
16:M:266:GLY:HA3	16:M:296:ILE:HD11	1.86	0.58
8:D:391:GLU:HB3	8:D:400:ARG:HB3	1.84	0.58
6:A:808:ILE:HD13	9:E:165:ILE:HD11	1.86	0.58
21:S:189:ARG:NH1	22:T:36:ASP:O	2.37	0.57
22:T:233:GLN:HG3	22:T:274:TRP:HE1	1.69	0.57
2:5:97:U:OP1	6:A:839:HIS:NE2	2.36	0.57
23:U:729:TYR:CD2	23:U:748:PHE:CD1	2.92	0.57
6:A:1211:SER:O	6:A:1257:ASN:ND2	2.36	0.57
6:A:228:LYS:NZ	6:A:692:ASN:OD1	2.33	0.57
6:A:1771:THR:HA	6:A:1789:ASN:HD22	1.70	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:2081:ASP:OD1	6:A:2086:GLN:NE2	2.36	0.57
7:B:514:GLN:NE2	7:B:586:MET:O	2.38	0.57
9:E:132:ARG:NH2	10:F:33:GLU:OE1	2.37	0.57
18:O:282:ASP:OD2	18:O:289:ARG:NH2	2.38	0.57
13:I:21:PRO:O	13:I:24:THR:HB	2.05	0.56
19:P:907:LEU:HD22	19:P:927:ILE:HG12	1.87	0.56
11:G:55:PRO:HB3	11:G:93:ILE:HD11	1.88	0.56
22:T:51:ARG:HH22	22:T:83:ARG:HD3	1.69	0.56
7:B:233:ASP:OD1	7:B:487:ARG:NH2	2.34	0.56
6:A:992:ASP:OD2	6:A:1085:LYS:NZ	2.39	0.56
7:B:90:LEU:HD12	8:D:211:LEU:HD22	1.88	0.56
8:D:414:LEU:HB3	8:D:426:TRP:HB2	1.88	0.56
7:B:242:VAL:HG21	7:B:272:ARG:HE	1.70	0.56
6:A:1842:GLU:O	6:A:1849:LYS:NZ	2.38	0.56
16:M:262:GLU:OE1	16:M:274:HIS:NE2	2.39	0.56
6:A:1789:ASN:ND2	18:O:182:TYR:OH	2.34	0.56
10:F:25:MET:HB3	10:F:46:PHE:HB3	1.88	0.56
12:H:8:GLN:O	12:H:10:GLU:N	2.39	0.56
15:L:334:LEU:HD21	15:L:384:LEU:HG	1.88	0.56
6:A:1889:LEU:HD12	6:A:1989:PHE:HB2	1.87	0.55
6:A:380:ARG:NH1	7:B:917:ASP:OD1	2.39	0.55
17:N:140:LYS:NZ	18:O:226:ASP:OD1	2.38	0.55
6:A:1848:ILE:HG23	6:A:1930:PRO:HA	1.88	0.55
15:L:14:GLN:OE1	15:L:245:CYS:N	2.39	0.55
6:A:1393:GLU:OE1	18:O:36:TYR:OH	2.18	0.55
6:A:1578:ALA:O	6:A:1824:GLN:NE2	2.40	0.55
8:D:285:SER:OG	8:D:287:ASP:OD1	2.24	0.55
21:S:51:ARG:HG3	21:S:56:LEU:HD23	1.89	0.55
6:A:1682:THR:OG1	6:A:1702:THR:OG1	2.24	0.55
7:B:176:ARG:NH2	7:B:179:ASP:OD2	2.36	0.55
6:A:1323:SER:O	6:A:1370:ARG:NH1	2.39	0.55
6:A:1876:ASN:HD21	6:A:1895:HIS:HD2	1.55	0.55
19:P:1138:GLU:OE1	19:P:1145:ARG:NH1	2.40	0.55
6:A:341:ALA:HA	6:A:355:LEU:HD21	1.88	0.55
6:A:255:ILE:HG23	6:A:640:ARG:HG2	1.88	0.55
8:D:395:SER:HB2	12:H:158:ASN:HD22	1.72	0.55
6:A:144:ASN:HB3	13:I:36:ASP:HB2	1.89	0.55
16:M:339:MET:N	16:M:339:MET:SD	2.80	0.55
22:T:89:GLU:OE2	22:T:124:ARG:NH2	2.39	0.55
8:D:345:PHE:O	8:D:450:ARG:NH1	2.33	0.54
6:A:1142:ASN:HD21	6:A:1147:PHE:HA	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:18:TRP:HE1	15:L:22:ARG:HH21	1.55	0.54
6:A:216:GLN:NE2	6:A:280:LEU:O	2.35	0.54
8:D:309:ARG:HH11	8:D:328:THR:HG21	1.72	0.54
6:A:266:LEU:HD12	6:A:267:PRO:HD2	1.89	0.54
7:B:245:VAL:HG12	7:B:249:VAL:HG11	1.89	0.54
6:A:1841:ALA:HB2	18:O:299:LEU:HD22	1.89	0.54
7:B:232:SER:O	7:B:452:LYS:NZ	2.38	0.54
13:I:150:CYS:SG	13:I:153:CYS:CB	2.85	0.54
6:A:1684:GLU:HB2	6:A:1700:ASP:HA	1.89	0.54
6:A:613:SER:OG	6:A:613:SER:O	2.24	0.54
7:B:133:ILE:HD13	7:B:560:GLN:HB3	1.88	0.54
2:5:94:C:O2'	6:A:1378:LYS:NZ	2.40	0.54
15:L:25:VAL:HG21	15:L:56:ILE:HG22	1.89	0.54
20:R:180:LYS:O	20:R:184:GLN:NE2	2.40	0.54
7:B:499:VAL:HG12	7:B:579:SER:HB2	1.89	0.54
1:2:1107:C:N3	20:R:104:SER:HA	116.37	0.54
6:A:2002:TYR:HB2	18:O:299:LEU:HD12	1.90	0.54
16:M:253:VAL:HG23	16:M:265:VAL:HG22	1.89	0.54
23:U:436:ASP:O	23:U:441:GLY:N	2.39	0.53
2:5:43:G:C4	7:B:97:ARG:HD2	2.43	0.53
7:B:76:VAL:HG12	8:D:134:VAL:HB	1.90	0.53
3:6:84:C:O2'	12:H:3:THR:O	2.21	0.53
3:6:61:C:H5'	6:A:748:GLN:HE21	1.74	0.53
6:A:1701:ILE:HB	6:A:1734:PHE:HB2	1.90	0.53
6:A:391:TYR:OH	7:B:912:ALA:O	2.26	0.53
6:A:460:PRO:HG2	7:B:375:GLU:HG2	1.89	0.53
6:A:835:LYS:HD2	12:H:173:HIS:CE1	2.43	0.53
22:T:45:GLU:OE2	22:T:48:ARG:NH1	2.41	0.53
7:B:398:ASN:OD1	7:B:401:ARG:NH1	2.42	0.53
23:U:774:PRO:HG3	23:U:808:GLU:HA	1.90	0.53
6:A:204:GLU:OE2	6:A:284:ARG:NH1	2.42	0.53
6:A:1647:GLN:O	6:A:1650:ARG:NH1	2.40	0.53
6:A:1804:THR:HG21	18:O:259:ILE:HA	1.90	0.53
6:A:1035:LEU:HD12	6:A:1038:ILE:HD12	1.91	0.53
7:B:866:ILE:HB	7:B:902:VAL:HB	1.91	0.53
16:M:392:SER:HB3	16:M:397:TYR:HB2	1.90	0.53
19:P:735:PRO:O	19:P:739:GLN:N	2.40	0.53
7:B:189:LEU:HD21	7:B:650:LEU:HD21	1.91	0.53
22:T:176:GLU:HG3	22:T:188:ILE:HD11	1.91	0.53
6:A:320:ASP:OD1	6:A:508:GLN:NE2	2.37	0.52
6:A:856:TRP:HA	12:H:170:LEU:HD21	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:680:CYS:SG	6:A:711:TRP:NE1	2.83	0.52
6:A:1197:ASN:O	6:A:1224:ARG:NH2	2.42	0.52
6:A:190:LYS:HD3	6:A:559:GLN:HE21	1.74	0.52
6:A:1579:SER:HA	6:A:1824:GLN:HE22	1.73	0.52
19:P:1106:SER:OG	19:P:1107:GLN:N	2.42	0.52
8:D:210:ASP:OD2	8:D:213:LYS:NZ	2.43	0.52
8:D:451:PHE:OXT	9:E:48:GLN:NE2	2.42	0.52
10:F:106:ASN:O	10:F:109:MET:N	2.35	0.52
6:A:1952:PRO:O	18:O:266:TYR:OH	2.21	0.52
2:5:43:G:H2'	2:5:45:A:H5''	1.91	0.51
16:M:166:THR:O	16:M:431:GLN:NE2	2.43	0.51
6:A:233:HIS:HE1	18:O:174:TRP:HA	1.75	0.51
7:B:493:LEU:HD21	7:B:539:VAL:HG21	1.92	0.51
23:U:780:LEU:O	23:U:784:PHE:HB2	2.11	0.51
6:A:2056:ARG:HD2	18:O:325:VAL:HG12	1.92	0.51
9:E:45:PRO:HG2	9:E:48:GLN:HB2	1.93	0.51
8:D:206:VAL:HB	8:D:220:TYR:HB2	1.92	0.51
16:M:256:ARG:HH11	16:M:262:GLU:HG3	1.75	0.51
3:6:39:G:N1	11:G:120:TYR:O	2.43	0.51
18:O:35:ARG:O	18:O:39:ASN:ND2	2.43	0.51
8:D:145:VAL:HG23	8:D:157:THR:HB	1.93	0.51
21:S:248:VAL:HG11	22:T:43:LEU:HD22	1.93	0.51
6:A:1420:THR:HG22	7:B:954:LEU:HD21	1.93	0.50
6:A:595:TYR:O	6:A:630:LYS:NZ	2.44	0.50
11:G:151:LEU:HD11	11:G:159:ARG:HE	1.76	0.50
21:S:46:ARG:NH1	21:S:49:GLU:OE1	2.45	0.50
3:6:58:C:C2'	3:6:59:A:H5'	2.40	0.50
7:B:680:SER:OG	7:B:681:CYS:N	2.43	0.50
6:A:744:THR:O	6:A:749:ARG:NH2	2.40	0.50
6:A:770:MET:O	8:D:309:ARG:NH2	2.44	0.50
7:B:454:ALA:HB1	7:B:459:PRO:HB3	1.93	0.50
23:U:742:VAL:HG21	23:U:772:LEU:HG	1.93	0.50
11:G:23:PRO:O	11:G:37:TRP:NE1	2.40	0.50
6:A:1712:SER:OG	6:A:1713:LYS:N	2.44	0.50
11:G:92:HIS:NE2	11:G:98:ASP:OD2	2.34	0.50
6:A:982:TYR:HB2	6:A:1106:GLY:HA3	1.93	0.50
16:M:202:PHE:HZ	16:M:221:PHE:HZ	1.59	0.50
1:2:1108:A:H62	20:R:108:THR:CA	107.39	0.50
2:5:50:G:H1	2:5:65:U:H3	1.58	0.50
6:A:1837:SER:O	6:A:2080:LYS:NZ	2.45	0.50
6:A:456:GLU:HG3	7:B:356:LYS:HG2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1048:VAL:HG22	6:A:1250:VAL:HG22	1.93	0.50
7:B:883:ARG:HD2	7:B:914:PHE:HD1	1.77	0.50
6:A:1347:ARG:NE	6:A:1445:THR:O	2.44	0.49
11:G:139:VAL:HG13	11:G:221:LEU:HD13	1.94	0.49
15:L:129:VAL:HG12	15:L:130:ILE:HG12	1.93	0.49
15:L:73:ILE:HG13	15:L:74:PRO:HD3	1.93	0.49
16:M:317:VAL:HB	16:M:331:ILE:HB	1.94	0.49
6:A:1878:CYS:HA	6:A:1892:LYS:O	2.12	0.49
8:D:309:ARG:HD2	8:D:328:THR:HG21	1.94	0.49
16:M:179:LEU:HB3	16:M:189:ILE:HD12	1.94	0.49
7:B:708:ILE:HG23	7:B:823:ILE:HG22	1.94	0.49
7:B:944:VAL:HG13	7:B:967:VAL:HG21	1.94	0.49
9:E:170:SER:OG	9:E:173:LYS:O	2.30	0.49
15:L:156:LYS:HG2	15:L:200:ILE:HD11	1.95	0.49
15:L:62:ASP:O	15:L:66:ASN:ND2	2.45	0.49
6:A:905:TYR:OH	6:A:1002:GLU:OE2	2.30	0.49
7:B:862:TYR:HD2	7:B:930:LEU:HD23	1.77	0.49
9:E:225:LEU:HD13	9:E:228:LEU:HD12	1.94	0.49
3:6:38:U:H5'	11:G:121:ARG:HH12	1.78	0.49
8:D:115:TYR:HD2	22:T:235:LEU:HD23	1.76	0.49
16:M:354:GLN:HB2	16:M:389:LEU:HD23	1.94	0.49
17:N:155:LEU:HB3	17:N:160:LEU:HD12	1.93	0.49
10:F:214:ILE:HG13	10:F:218:LYS:HD3	1.94	0.49
18:O:324:LYS:HA	18:O:327:HIS:HD2	1.78	0.49
7:B:100:LEU:HD22	7:B:108:GLN:HE21	1.77	0.49
18:O:261:SER:OG	18:O:262:THR:N	2.40	0.49
19:P:559:ASP:HA	19:P:574:THR:HA	1.95	0.49
6:A:342:LEU:HD13	6:A:392:ASN:HD21	1.78	0.49
21:S:60:LEU:HD22	21:S:94:PRO:HG3	1.94	0.49
6:A:1216:ILE:HD12	6:A:1254:ASN:HB3	1.94	0.48
6:A:461:LEU:HD13	7:B:404:PHE:HE1	1.78	0.48
15:L:143:LEU:O	15:L:176:LYS:NZ	2.41	0.48
6:A:1574:PHE:HD2	18:O:33:ILE:HG22	1.77	0.48
11:G:176:VAL:HG12	11:G:179:LYS:H	1.77	0.48
6:A:1668:ILE:HD11	18:O:256:LEU:HD22	1.95	0.48
1:2:38:U:OP1	16:M:329:LYS:NZ	2.38	0.48
6:A:1722:ASP:OD1	6:A:1722:ASP:N	2.47	0.48
16:M:272:ILE:HB	16:M:289:TYR:HB2	1.94	0.48
15:L:454:ASP:HB3	15:L:457:HIS:HD2	1.78	0.48
23:U:36:ASN:O	23:U:38:LEU:N	2.47	0.48
23:U:686:ILE:HG13	23:U:689:ARG:HH21	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:B:231:ALA:O	7:B:487:ARG:NH1	2.46	0.48
7:B:246:THR:OG1	7:B:247:PHE:N	2.46	0.48
6:A:1667:GLN:NE2	18:O:251:ASP:O	2.46	0.48
18:O:293:THR:OG1	18:O:294:GLY:N	2.43	0.48
6:A:901:PRO:HB2	6:A:955:LYS:HE2	1.96	0.48
16:M:154:VAL:HA	16:M:454:CYS:HA	1.95	0.48
6:A:1674:ASP:O	6:A:1677:GLN:N	2.44	0.48
6:A:1922:ARG:HD2	18:O:246:THR:HG23	1.96	0.48
8:D:327:CYS:HB3	8:D:330:ASP:HB3	1.96	0.48
16:M:213:ARG:HG3	16:M:254:GLU:HA	1.96	0.48
23:U:663:LYS:HB2	23:U:708:LEU:HD21	1.95	0.48
15:L:20:MET:O	15:L:24:HIS:HB2	2.13	0.47
3:6:23:G:O6	16:M:53:LYS:NZ	2.40	0.47
3:6:63:G:H2'	3:6:64:U:C6	2.49	0.47
18:O:124:ASN:HD22	18:O:139:PRO:HA	1.78	0.47
6:A:978:ILE:N	12:H:173:HIS:O	2.43	0.47
16:M:385:TYR:O	21:S:186:GLN:NE2	2.48	0.47
1:2:5:A:H5'	20:R:114:THR:HG21	1.95	0.47
2:5:99:U:O2'	3:6:73:A:N6	2.36	0.47
7:B:689:ILE:HD13	7:B:993:ILE:HD12	1.96	0.47
6:A:1039:TRP:O	6:A:1273:GLN:NE2	2.47	0.47
10:F:67:GLN:NE2	10:F:116:LYS:O	2.48	0.47
15:L:101:MET:HA	15:L:104:GLN:HG2	1.96	0.47
16:M:405:SER:OG	16:M:427:LYS:O	2.32	0.47
6:A:1967:ALA:HB2	6:A:2016:LYS:HB2	1.96	0.47
11:G:109:LEU:HD13	11:G:113:GLY:HA2	1.96	0.47
2:5:78:A:O2'	2:5:79:C:O5'	2.27	0.47
6:A:517:LYS:HG3	6:A:518:VAL:HG23	1.97	0.47
19:P:879:LEU:HD23	19:P:885:LEU:HB2	1.97	0.47
21:S:39:LEU:HD11	21:S:155:ALA:HA	1.97	0.47
6:A:1925:PRO:HD2	6:A:1928:GLU:HB3	1.97	0.47
10:F:91:ILE:HB	10:F:99:VAL:HG11	1.97	0.47
21:S:38:SER:OG	21:S:158:ARG:NH1	2.48	0.47
6:A:2053:SER:OG	6:A:2056:ARG:NH1	2.48	0.47
6:A:467:GLU:O	7:B:387:TYR:OH	2.25	0.47
15:L:98:LEU:HA	15:L:101:MET:HG2	1.97	0.47
6:A:1676:LEU:HD11	6:A:1797:LEU:HD13	1.97	0.46
6:A:1910:LYS:HG3	6:A:1940:MET:HE2	1.96	0.46
9:E:135:VAL:HG21	21:S:219:TYR:CE1	2.51	0.46
9:E:135:VAL:HG21	21:S:219:TYR:HE1	1.80	0.46
6:A:1485:ASP:O	6:A:1490:ARG:NH2	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:L:29:ILE:HG21	15:L:82:LEU:HD13	12.90	0.46
6:A:143:ILE:HD11	6:A:574:GLN:HE21	1.80	0.46
6:A:905:TYR:HB3	6:A:908:ASP:HB2	1.97	0.46
6:A:757:GLU:HG2	8:D:202:GLU:CD	2.35	0.46
7:B:223:ASP:OD1	7:B:223:ASP:N	2.47	0.46
7:B:675:THR:HG22	7:B:909:ILE:HD12	1.97	0.46
23:U:713:ILE:HD12	23:U:729:TYR:CE1	2.51	0.46
6:A:1759:TYR:HB3	6:A:1767:TYR:HE2	1.81	0.46
6:A:1142:ASN:ND2	6:A:1146:GLN:O	2.49	0.46
6:A:1451:PHE:O	6:A:1455:GLN:NE2	2.49	0.46
6:A:1347:ARG:NH1	6:A:1450:GLU:OE1	2.49	0.46
6:A:1446:THR:OG1	6:A:1449:ASN:ND2	2.49	0.46
6:A:1869:ASN:OD1	6:A:1869:ASN:N	2.45	0.46
7:B:599:THR:OG1	7:B:647:ASN:ND2	2.49	0.46
8:D:238:LEU:HD21	9:E:74:ILE:HD13	1.98	0.46
22:T:119:ARG:NH1	22:T:143:GLU:OE2	2.49	0.46
6:A:252:GLU:HG3	6:A:253:GLN:HG3	1.97	0.46
7:B:69:PRO:O	8:D:390:ARG:NH1	2.48	0.46
10:F:13:CYS:HB2	10:F:71:CYS:SG	2.56	0.46
7:B:539:VAL:HG13	7:B:564:ILE:HG23	1.98	0.45
15:L:34:MET:HA	15:L:37:LEU:HD12	1.97	0.45
15:L:68:GLN:HA	15:L:72:LEU:HD23	1.98	0.45
6:A:759:ARG:HH12	12:H:7:PRO:HB3	1.82	0.45
8:D:218:ARG:NH2	12:H:34:HIS:O	2.49	0.45
15:L:170:HIS:CE1	15:L:174:TRP:HE1	2.34	0.45
16:M:167:ALA:HA	16:M:431:GLN:HG2	1.98	0.45
16:M:191:ASP:HB3	16:M:199:LEU:HD11	1.97	0.45
18:O:217:GLU:HA	18:O:220:LYS:HE2	1.98	0.45
19:P:1086:ILE:HA	19:P:1086:ILE:HD12	1.82	0.45
2:5:77:A:H61	7:B:101:GLN:NE2	2.14	0.45
8:D:201:SER:OG	8:D:202:GLU:N	2.49	0.45
16:M:213:ARG:HB2	16:M:222:LEU:HD12	1.99	0.45
6:A:454:LEU:HD13	7:B:359:PHE:HE2	1.81	0.45
7:B:886:SER:HB3	7:B:906:VAL:HG23	1.98	0.45
8:D:330:ASP:OD1	8:D:450:ARG:NH2	2.37	0.45
16:M:319:ILE:HB	16:M:329:LYS:HB3	1.98	0.45
7:B:457:SER:HB3	7:B:592:PHE:HA	1.98	0.45
6:A:775:ARG:HE	6:A:776:GLN:H	1.65	0.45
8:D:207:LYS:HD3	8:D:216:ILE:HD13	1.98	0.45
11:G:119:ASP:N	11:G:119:ASP:OD1	2.49	0.45
17:N:93:VAL:O	17:N:171:GLN:NE2	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:968:ASP:OD1	21:S:46:ARG:NH2	2.49	0.45
6:A:332:ASP:OD1	6:A:332:ASP:N	2.49	0.45
6:A:1383:PHE:HB3	6:A:1388:PHE:HE2	1.81	0.45
15:L:53:ARG:HA	15:L:56:ILE:HG12	1.99	0.45
16:M:411:ASP:HB2	16:M:418:LEU:HD11	1.99	0.45
7:B:164:MET:HG3	7:B:168:VAL:HG23	1.98	0.45
7:B:271:ASP:OD1	7:B:271:ASP:N	2.50	0.45
8:D:380:SER:OG	8:D:381:GLY:N	2.50	0.45
11:G:207:PRO:HA	11:G:212:TRP:CG	2.52	0.45
15:L:404:ILE:HG13	15:L:405:ILE:HG23	1.99	0.45
17:N:118:HIS:HD2	18:O:225:LYS:HE3	1.82	0.45
22:T:235:LEU:HD22	22:T:237:ILE:HD11	1.99	0.45
8:D:200:VAL:HG23	8:D:206:VAL:HG22	2.00	0.44
16:M:287:GLN:HE21	16:M:325:ASN:HB2	1.81	0.44
6:A:1904:ARG:O	6:A:1906:SER:N	2.41	0.44
6:A:400:ILE:HA	6:A:401:PRO:HD3	1.86	0.44
20:R:148:LYS:HD2	20:R:149:THR:HG23	1.99	0.44
3:6:5:G:O6	3:6:21:U:O2	2.34	0.44
6:A:1068:ARG:HA	24:X:1025:UNK:CB	2.47	0.44
6:A:1087:ASN:HD21	21:S:86:THR:H	1.65	0.44
19:P:924:VAL:HG21	19:P:1004:PHE:HE2	1.83	0.44
22:T:148:ASN:HB3	22:T:151:ILE:HD13	2.00	0.44
6:A:764:ASP:O	6:A:768:GLU:HG2	2.18	0.44
7:B:802:ALA:HB2	7:B:843:LYS:HA	2.00	0.44
17:N:159:LEU:HD21	17:N:229:TRP:HH2	1.82	0.44
6:A:1892:LYS:HG2	6:A:1916:GLU:HG2	1.98	0.44
6:A:1932:GLN:OE1	18:O:290:ARG:NH2	2.49	0.44
7:B:675:THR:OG1	7:B:676:VAL:N	2.51	0.44
12:H:6:ARG:HA	12:H:7:PRO:HD3	1.75	0.44
6:A:347:PRO:HG3	14:K:2:SER:HB3	2.00	0.44
19:P:1099:TYR:HB3	24:X:3369:UNK:HA	2.00	0.44
6:A:1287:ASP:OD1	6:A:1287:ASP:N	2.36	0.44
15:L:306:ASP:OD1	15:L:349:ARG:NE	2.51	0.44
16:M:195:ASP:HB3	16:M:197:GLU:HG3	1.98	0.44
9:E:144:VAL:HA	9:E:145:PRO:HD3	1.92	0.43
23:U:709:TRP:NE1	23:U:732:CYS:SG	2.89	0.43
6:A:1279:VAL:O	6:A:1299:LYS:NZ	2.51	0.43
7:B:993:ILE:HD11	7:B:997:LEU:HD22	2.00	0.43
10:F:104:ALA:HB1	10:F:109:MET:HG3	1.99	0.43
11:G:102:LEU:HB3	11:G:106:THR:HG23	2.00	0.43
11:G:153:PRO:HB3	11:G:175:TYR:HE2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:P:1098:PHE:HD2	19:P:1099:TYR:HD1	1.66	0.43
1:2:30:A:H62	21:S:38:SER:HB3	1.81	0.43
6:A:621:LEU:HD23	6:A:722:LEU:HD21	2.00	0.43
8:D:327:CYS:SG	8:D:328:THR:N	2.88	0.43
7:B:367:VAL:HG11	7:B:369:LYS:HE2	2.00	0.43
9:E:105:LEU:HD21	9:E:109:SER:HA	2.01	0.43
16:M:382:SER:HB3	16:M:387:ILE:HD13	2.00	0.43
8:D:390:ARG:O	8:D:424:LYS:NZ	2.52	0.43
9:E:179:THR:H	20:R:200:ASN:HD21	1.66	0.43
6:A:1882:LEU:HB3	6:A:1889:LEU:HD23	2.00	0.43
17:N:226:THR:HA	17:N:229:TRP:CD1	2.53	0.43
18:O:36:TYR:CD1	18:O:37:ILE:HG13	2.54	0.43
6:A:1094:ASP:OD1	6:A:1094:ASP:N	2.42	0.43
6:A:1750:ARG:HD2	18:O:99:ILE:HG12	2.01	0.43
8:D:277:VAL:HG12	8:D:278:ASP:H	1.84	0.43
3:6:19:C:H2'	3:6:20:G:C8	2.54	0.43
6:A:1270:LEU:HD22	6:A:1271:PRO:HD2	1.99	0.43
6:A:495:ARG:NH2	6:A:497:GLN:HE21	2.17	0.43
7:B:863:GLU:HG2	7:B:905:GLN:HG2	2.01	0.43
15:L:135:ILE:HA	15:L:138:ILE:HG12	2.01	0.43
16:M:222:LEU:HD23	16:M:232:ILE:HG12	2.01	0.43
16:M:296:ILE:HA	16:M:312:SER:HA	2.01	0.43
17:N:114:ASN:O	17:N:118:HIS:ND1	2.52	0.43
22:T:222:TYR:HB3	22:T:250:PHE:CD2	2.54	0.43
23:U:437:PRO:HA	23:U:441:GLY:HA3	1.99	0.43
6:A:383:TYR:CZ	7:B:913:GLY:HA3	2.53	0.43
7:B:801:TRP:CD1	7:B:843:LYS:HD3	2.53	0.43
8:D:264:GLY:HA3	8:D:293:TRP:HH2	1.84	0.43
17:N:183:TYR:CZ	17:N:234:LYS:HB2	2.54	0.43
21:S:74:LEU:HG	21:S:105:LEU:HD13	2.01	0.43
6:A:665:GLY:HA2	6:A:667:TYR:CE2	2.54	0.42
15:L:82:LEU:HD22	15:L:87:ILE:HG13	14.13	0.42
16:M:246:LEU:HD13	16:M:267:LEU:HD11	2.01	0.42
6:A:468:LEU:HD11	7:B:382:TYR:HB3	2.02	0.42
8:D:197:LEU:HD23	8:D:209:TRP:CD1	2.53	0.42
13:I:16:PHE:O	13:I:20:LYS:N	2.52	0.42
16:M:252:ASP:HB3	16:M:299:LEU:HD23	2.02	0.42
16:M:59:ARG:O	16:M:62:THR:OG1	2.31	0.42
3:6:26:A:O2'	13:I:123:ARG:NH2	2.50	0.42
6:A:1161:TYR:CD1	6:A:1170:MET:HG2	2.55	0.42
6:A:1286:TRP:CD1	6:A:1448:GLU:HB2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:145:ALA:HB2	11:G:221:LEU:HB3	2.01	0.42
6:A:1902:GLN:HG2	17:N:211:ILE:HD11	2.02	0.42
8:D:106:VAL:HG12	8:D:108:GLU:H	1.84	0.42
19:P:907:LEU:HD13	19:P:927:ILE:HG23	2.02	0.42
6:A:231:ARG:HH22	6:A:648:GLN:HE21	1.66	0.42
6:A:326:ASN:ND2	6:A:405:ASN:O	2.41	0.42
6:A:194:HIS:HD2	6:A:557:PHE:HE1	1.66	0.42
7:B:860:PRO:HG2	7:B:908:VAL:HG11	2.00	0.42
6:A:2079:ILE:HB	18:O:328:VAL:HG21	2.01	0.42
6:A:1068:ARG:NE	24:X:1024:UNK:CB	2.83	0.42
6:A:688:TYR:HE2	38:A:3001:IHP:O32	2.02	0.42
6:A:594:ASP:N	6:A:594:ASP:OD1	2.53	0.42
7:B:360:ARG:HD2	7:B:364:PHE:HD1	1.83	0.42
7:B:862:TYR:CD1	7:B:932:PHE:HB2	2.55	0.42
10:F:107:ASP:HA	10:F:110:LYS:HG2	2.02	0.42
6:A:1894:ILE:HG23	6:A:1898:VAL:HG21	2.02	0.42
8:D:100:LYS:HG3	8:D:101:ILE:HG13	2.01	0.42
19:P:977:GLU:O	19:P:981:LYS:CB	2.68	0.42
21:S:14:THR:OG1	21:S:15:ASN:N	2.53	0.42
6:A:1727:LEU:HD22	6:A:1728:ILE:H	1.84	0.42
6:A:778:LYS:O	6:A:782:ILE:HG12	2.20	0.42
6:A:876:PRO:HG2	9:E:203:LYS:HG3	2.02	0.42
17:N:170:LEU:HD13	17:N:237:ILE:HG12	2.01	0.42
6:A:1433:ASP:OD1	6:A:1433:ASP:N	2.52	0.42
6:A:143:ILE:HD13	6:A:143:ILE:HA	1.87	0.42
23:U:780:LEU:O	23:U:784:PHE:CB	2.68	0.42
6:A:1161:TYR:HD1	6:A:1170:MET:HG2	1.85	0.42
6:A:1855:THR:HG22	6:A:1937:ARG:HD2	2.02	0.42
6:A:282:ASP:HB2	6:A:285:PRO:HA	2.01	0.42
7:B:416:ASP:HB2	7:B:419:PRO:HD2	2.01	0.42
7:B:864:VAL:HB	7:B:904:GLY:O	2.20	0.42
23:U:729:TYR:O	23:U:732:CYS:HB3	2.20	0.42
7:B:772:ASN:HB3	7:B:816:VAL:H	1.85	0.41
7:B:973:ARG:HA	7:B:973:ARG:HD2	1.85	0.41
16:M:435:HIS:HD2	16:M:436:PRO:HD2	1.85	0.41
3:6:73:A:OP1	6:A:732:ARG:NE	2.41	0.41
6:A:1674:ASP:O	6:A:1676:LEU:N	2.53	0.41
6:A:896:SER:HA	6:A:897:PRO:HD3	1.89	0.41
7:B:201:THR:HG22	7:B:207:SER:HB3	2.01	0.41
16:M:387:ILE:HG13	16:M:430:THR:HG22	2.02	0.41
6:A:1368:GLN:NE2	6:A:1389:TYR:OH	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:365:PHE:HE1	8:D:373:LEU:HB2	1.85	0.41
16:M:392:SER:HA	16:M:434:TRP:CE2	2.55	0.41
18:O:261:SER:HG	18:O:262:THR:H	1.68	0.41
6:A:1562:PHE:HE2	18:O:87:ILE:HG22	1.85	0.41
6:A:1834:PHE:O	6:A:1839:ASN:ND2	2.50	0.41
6:A:878:GLU:OE1	6:A:1237:SER:OG	2.36	0.41
7:B:134:ILE:HD11	7:B:234:LEU:HD23	2.01	0.41
8:D:277:VAL:HG21	9:E:58:PRO:HB2	2.02	0.41
8:D:345:PHE:HE2	8:D:364:LEU:HD13	1.85	0.41
10:F:11:ASN:N	10:F:11:ASN:OD1	2.53	0.41
10:F:51:ARG:HA	10:F:51:ARG:HD3	1.76	0.41
15:L:80:ILE:HB	15:L:124:LEU:HD21	2.01	0.41
15:L:297:LEU:HD13	15:L:297:LEU:HA	1.89	0.41
18:O:103:PHE:HB3	18:O:159:LEU:HB3	2.02	0.41
2:5:82:A:O3'	6:A:709:ARG:NH2	2.54	0.41
7:B:606:VAL:HG22	7:B:643:VAL:HG12	2.02	0.41
3:6:79:A:OP1	3:6:81:G:O2'	2.33	0.41
6:A:966:PRO:HD2	21:S:50:LEU:HD21	2.02	0.41
1:2:4:A:H2'	1:2:5:A:C8	2.55	0.41
7:B:123:MET:HB2	7:B:199:LEU:HD23	2.03	0.41
7:B:883:ARG:NH1	7:B:910:GLU:O	2.52	0.41
10:F:77:ASP:OD1	10:F:87:ARG:NH1	2.49	0.41
19:P:1022:ARG:O	19:P:1026:VAL:HG23	2.21	0.41
22:T:240:ASP:N	22:T:240:ASP:OD1	2.51	0.41
6:A:1675:VAL:H	6:A:1675:VAL:HG23	1.59	0.41
7:B:687:ALA:HB1	14:K:60:VAL:HB	2.02	0.41
8:D:405:SER:HA	8:D:415:ILE:O	2.21	0.41
15:L:471:GLY:O	15:L:474:THR:OG1	2.34	0.41
16:M:156:ARG:HE	16:M:453:VAL:HG11	1.85	0.41
18:O:332:ASN:N	18:O:332:ASN:OD1	2.54	0.41
6:A:1130:ARG:HA	6:A:1130:ARG:HD2	1.87	0.41
6:A:180:PRO:O	6:A:181:HIS:ND1	2.44	0.41
6:A:688:TYR:CE2	38:A:3001:IHP:O32	2.74	0.41
7:B:176:ARG:HH12	7:B:185:ILE:HA	1.86	0.41
11:G:19:PRO:O	13:I:40:LYS:NZ	2.48	0.41
6:A:1087:ASN:HD22	21:S:83:GLN:HB3	1.85	0.41
6:A:1567:PHE:O	18:O:90:ASN:HB3	2.21	0.41
9:E:30:LEU:HD21	22:T:151:ILE:HG13	2.02	0.41
19:P:530:MET:H	19:P:597:TYR:HA	1.86	0.41
22:T:54:TYR:HD1	22:T:67:GLN:HE21	1.69	0.41
1:2:41:C:H6	1:2:41:C:H2'	1.72	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:A:1607:THR:HG22	6:A:1641:LEU:HD13	2.03	0.41
6:A:835:LYS:HE2	6:A:835:LYS:HB3	1.91	0.41
6:A:902:PRO:HD2	6:A:905:TYR:HD1	1.85	0.41
7:B:304:PHE:HD2	7:B:310:ASN:HB3	1.85	0.41
22:T:73:GLN:O	22:T:77:GLU:HG2	2.21	0.41
6:A:1156:HIS:CD2	6:A:1158:ILE:H	2.39	0.40
16:M:57:LYS:HG2	16:M:60:ARG:NH1	2.35	0.40
18:O:94:LYS:HA	18:O:94:LYS:HD3	1.84	0.40
6:A:1370:ARG:HD2	6:A:1370:ARG:HA	1.82	0.40
6:A:1718:HIS:NE2	18:O:95:ILE:HD11	2.36	0.40
6:A:242:PHE:HE1	6:A:638:GLN:HE21	1.68	0.40
6:A:319:ARG:HD2	6:A:319:ARG:HH11	1.76	0.40
7:B:252:LEU:HD23	7:B:252:LEU:HA	1.94	0.40
7:B:609:PRO:HA	7:B:668:ILE:HG22	2.04	0.40
8:D:110:LEU:HD11	22:T:194:MET:HB3	2.04	0.40
8:D:365:PHE:CE1	8:D:373:LEU:HB2	2.56	0.40
9:E:1:MET:HG3	25:Y:13:UNK:CB	2.52	0.40
15:L:17:ASN:HA	15:L:20:MET:HG2	2.03	0.40
17:N:159:LEU:HD21	17:N:229:TRP:CH2	2.55	0.40
21:S:214:ASN:ND2	22:T:48:ARG:HB2	2.37	0.40
22:T:170:ASN:HA	22:T:173:VAL:HG22	2.02	0.40
1:2:4:A:H2'	1:2:5:A:H8	1.86	0.40
6:A:291:LYS:HE2	6:A:292:LYS:HE3	2.04	0.40
15:L:136:LEU:HD22	15:L:169:THR:HG21	2.03	0.40
6:A:860:GLU:OE2	6:A:863:ARG:NH2	2.51	0.40
7:B:629:TYR:OH	7:B:658:ASP:OD2	2.29	0.40
7:B:880:MET:HG3	7:B:888:ILE:HD11	2.04	0.40
16:M:237:THR:HG21	16:M:239:LYS:HE2	2.03	0.40
19:P:1033:ALA:HA	19:P:1068:MET:HA	2.03	0.40
6:A:522:TYR:O	6:A:526:LEU:HB2	2.22	0.40
6:A:797:ILE:HA	6:A:798:PRO:HD3	1.89	0.40
6:A:902:PRO:HD2	6:A:905:TYR:CD1	2.57	0.40
6:A:964:PHE:O	21:S:85:ARG:NH2	2.44	0.40
8:D:230:VAL:HG22	8:D:241:THR:HG22	2.02	0.40
8:D:369:ASP:HA	8:D:401:SER:HB2	2.04	0.40
6:A:1544:THR:HG22	18:O:36:TYR:O	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	A	1954/2413 (81%)	1813 (93%)	126 (6%)	15 (1%)	22	57
7	B	889/1008 (88%)	830 (93%)	55 (6%)	4 (0%)	38	71
8	D	357/451 (79%)	329 (92%)	28 (8%)	0	100	100
9	E	176/379 (46%)	164 (93%)	11 (6%)	1 (1%)	28	63
10	F	193/364 (53%)	173 (90%)	19 (10%)	1 (0%)	32	66
11	G	253/339 (75%)	229 (90%)	23 (9%)	1 (0%)	38	71
12	H	64/175 (37%)	55 (86%)	8 (12%)	1 (2%)	11	43
13	I	154/157 (98%)	140 (91%)	14 (9%)	0	100	100
14	K	76/135 (56%)	72 (95%)	4 (5%)	0	100	100
15	L	406/577 (70%)	380 (94%)	26 (6%)	0	100	100
16	M	320/455 (70%)	302 (94%)	18 (6%)	0	100	100
17	N	163/251 (65%)	157 (96%)	6 (4%)	0	100	100
18	O	215/382 (56%)	196 (91%)	19 (9%)	0	100	100
19	P	645/1145 (56%)	610 (95%)	35 (5%)	0	100	100
20	R	97/215 (45%)	94 (97%)	3 (3%)	0	100	100
21	S	234/590 (40%)	223 (95%)	11 (5%)	0	100	100
22	T	451/687 (66%)	442 (98%)	9 (2%)	0	100	100
23	U	587/859 (68%)	555 (94%)	30 (5%)	2 (0%)	44	76
26	a	92/110 (84%)	83 (90%)	9 (10%)	0	100	100
26	q	91/110 (83%)	84 (92%)	7 (8%)	0	100	100
27	b	70/86 (81%)	61 (87%)	9 (13%)	0	100	100
27	m	70/86 (81%)	65 (93%)	5 (7%)	0	100	100
28	c	71/94 (76%)	62 (87%)	9 (13%)	0	100	100
28	l	71/94 (76%)	66 (93%)	4 (6%)	1 (1%)	13	46
29	d	65/77 (84%)	63 (97%)	2 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	n	65/77 (84%)	57 (88%)	8 (12%)	0	100	100
30	f	76/196 (39%)	74 (97%)	2 (3%)	0	100	100
30	k	74/196 (38%)	66 (89%)	7 (10%)	1 (1%)	13	46
31	g	80/101 (79%)	73 (91%)	7 (9%)	0	100	100
31	o	74/101 (73%)	70 (95%)	4 (5%)	0	100	100
32	h	78/146 (53%)	71 (91%)	7 (9%)	0	100	100
32	p	75/146 (51%)	65 (87%)	8 (11%)	2 (3%)	6	32
33	r	82/111 (74%)	76 (93%)	6 (7%)	0	100	100
34	s	160/238 (67%)	117 (73%)	35 (22%)	8 (5%)	2	17
35	u	423/503 (84%)	413 (98%)	8 (2%)	2 (0%)	32	66
35	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	6	33
35	w	426/503 (85%)	417 (98%)	9 (2%)	0	100	100
35	x	112/503 (22%)	104 (93%)	8 (7%)	0	100	100
36	y	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	2	14
All	All	9709/14738 (66%)	9051 (93%)	610 (6%)	48 (0%)	37	66

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	A	1905	LEU
12	H	9	LEU
23	U	37	ILE
34	s	76	ILE
36	y	94	LYS
36	y	111	VAL
36	y	133	PRO
6	A	483	PRO
6	A	775	ARG
6	A	1675	VAL
7	B	778	THR
9	E	107	ASN
34	s	122	ARG
35	v	109	LEU
36	y	105	PRO
36	y	136	VAL
6	A	180	PRO
6	A	401	PRO

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Mol	Chain	Res	Type
6	A	1475	LEU
6	A	1674	ASP
7	B	573	LYS
30	k	81	VAL
34	s	95	PRO
35	v	20	ARG
6	A	543	ASN
6	A	776	GLN
7	B	116	THR
10	F	120	LEU
11	G	120	TYR
23	U	300	ASP
32	p	31	SER
34	s	68	PRO
34	s	94	LEU
34	s	129	LEU
35	u	20	ARG
36	y	119	SER
6	A	406	PRO
6	A	1328	PHE
6	A	1491	ILE
7	B	979	GLY
32	p	98	PRO
35	u	17	PRO
6	A	181	HIS
6	A	484	PHE
28	l	74	GLY
34	s	56	ILE
34	s	98	VAL
35	v	36	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
6	A	1778/2182 (82%)	1741 (98%)	37 (2%)	59 81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	B	809/910 (89%)	797 (98%)	12 (2%)	70	85
8	D	313/397 (79%)	307 (98%)	6 (2%)	62	81
9	E	168/328 (51%)	166 (99%)	2 (1%)	75	87
10	F	183/332 (55%)	183 (100%)	0	100	100
11	G	219/296 (74%)	216 (99%)	3 (1%)	71	85
12	H	58/151 (38%)	53 (91%)	5 (9%)	12	42
13	I	140/141 (99%)	139 (99%)	1 (1%)	87	92
14	K	44/121 (36%)	43 (98%)	1 (2%)	56	79
15	L	379/538 (70%)	377 (100%)	2 (0%)	91	94
16	M	288/413 (70%)	283 (98%)	5 (2%)	66	83
17	N	144/225 (64%)	143 (99%)	1 (1%)	87	92
18	O	210/346 (61%)	208 (99%)	2 (1%)	80	88
19	P	178/1029 (17%)	176 (99%)	2 (1%)	78	88
20	R	90/193 (47%)	89 (99%)	1 (1%)	78	88
21	S	208/525 (40%)	207 (100%)	1 (0%)	91	94
22	T	248/633 (39%)	244 (98%)	4 (2%)	68	84
23	U	131/786 (17%)	126 (96%)	5 (4%)	38	70
26	a	79/103 (77%)	79 (100%)	0	100	100
26	q	77/103 (75%)	74 (96%)	3 (4%)	37	70
27	b	63/77 (82%)	63 (100%)	0	100	100
27	m	63/77 (82%)	61 (97%)	2 (3%)	44	74
28	c	65/83 (78%)	63 (97%)	2 (3%)	45	75
28	l	65/83 (78%)	60 (92%)	5 (8%)	15	47
29	d	58/66 (88%)	57 (98%)	1 (2%)	66	83
29	n	57/66 (86%)	56 (98%)	1 (2%)	64	83
30	f	70/176 (40%)	70 (100%)	0	100	100
30	k	67/176 (38%)	66 (98%)	1 (2%)	70	85
31	g	69/89 (78%)	69 (100%)	0	100	100
31	o	67/89 (75%)	64 (96%)	3 (4%)	32	67
32	h	77/129 (60%)	76 (99%)	1 (1%)	73	86
32	p	73/129 (57%)	63 (86%)	10 (14%)	4	20

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	6538/10992 (60%)	6419 (98%)	119 (2%)	67	83

All (119) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	A	334	LYS
6	A	343	ASN
6	A	355	LEU
6	A	396	ARG
6	A	526	LEU
6	A	653	ILE
6	A	705	GLN
6	A	716	ARG
6	A	760	ASN
6	A	848	ASN
6	A	906	LYS
6	A	944	TYR
6	A	1067	ASN
6	A	1105	ARG
6	A	1295	GLN
6	A	1346	PHE
6	A	1426	ARG
6	A	1456	ARG
6	A	1465	ARG
6	A	1466	GLN
6	A	1521	ARG
6	A	1529	ASN
6	A	1553	ILE
6	A	1561	LEU
6	A	1568	ASN
6	A	1695	ASN
6	A	1739	ARG
6	A	1753	ARG
6	A	1782	ASN
6	A	1803	ARG
6	A	1809	ASN
6	A	1903	LYS
6	A	1998	ARG
6	A	2018	ASN
6	A	2027	LEU
6	A	2086	GLN
6	A	2098	MET

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Mol	Chain	Res	Type
7	B	180	ASN
7	B	268	ASN
7	B	289	ASN
7	B	294	ASN
7	B	358	ASN
7	B	360	ARG
7	B	428	ILE
7	B	545	LEU
7	B	590	LYS
7	B	764	ASN
7	B	884	ARG
7	B	960	ASN
8	D	152	ASN
8	D	160	ASN
8	D	194	HIS
8	D	200	VAL
8	D	227	VAL
8	D	266	LYS
9	E	87	ASN
9	E	106	LEU
11	G	44	ASN
11	G	151	LEU
11	G	206	LEU
12	H	8	GLN
12	H	30	LEU
12	H	36	THR
12	H	135	ARG
12	H	157	ILE
13	I	128	GLN
14	K	71	ARG
15	L	84	ASN
15	L	201	ARG
16	M	156	ARG
16	M	325	ASN
16	M	339	MET
16	M	378	LYS
16	M	406	ARG
17	N	177	ASN
18	O	278	LEU
18	O	284	LYS
19	P	1006	LYS
19	P	1059	LEU

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Mol	Chain	Res	Type
20	R	92	ARG
21	S	236	GLN
22	T	61	ASN
22	T	123	ASN
22	T	183	ASN
22	T	201	THR
23	U	663	LYS
23	U	726	ARG
23	U	760	ARG
23	U	777	ASN
23	U	801	LEU
28	c	25	THR
28	c	92	SER
29	d	66	ASN
32	h	16	THR
30	k	19	LYS
28	l	54	ILE
28	l	77	LEU
28	l	79	LYS
28	l	81	LEU
28	l	82	LEU
27	m	34	ASN
27	m	79	LEU
29	n	71	LEU
31	o	20	SER
31	o	43	GLN
31	o	76	ASP
32	p	11	ARG
32	p	15	VAL
32	p	16	THR
32	p	25	VAL
32	p	43	VAL
32	p	44	LYS
32	p	95	ILE
32	p	96	ILE
32	p	97	LEU
32	p	101	LEU
26	q	41	ARG
26	q	82	LYS
26	q	94	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
6	A	310	ASN
6	A	343	ASN
6	A	481	HIS
6	A	648	GLN
6	A	676	GLN
6	A	748	GLN
6	A	974	ASN
6	A	1087	ASN
6	A	1156	HIS
6	A	1368	GLN
6	A	1449	ASN
6	A	1455	GLN
6	A	1529	ASN
6	A	1548	GLN
6	A	1568	ASN
6	A	1687	HIS
6	A	1695	ASN
6	A	1782	ASN
6	A	1809	ASN
6	A	1824	GLN
6	A	1876	ASN
6	A	1895	HIS
7	B	101	GLN
7	B	103	HIS
7	B	180	ASN
7	B	255	GLN
7	B	268	ASN
7	B	289	ASN
7	B	294	ASN
7	B	358	ASN
7	B	511	GLN
7	B	514	GLN
7	B	647	ASN
7	B	764	ASN
7	B	869	HIS
7	B	960	ASN
7	B	1004	ASN
8	D	428	GLN
9	E	87	ASN
9	E	107	ASN
10	F	89	HIS
11	G	39	GLN
11	G	44	ASN

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Mol	Chain	Res	Type
11	G	248	ASN
12	H	8	GLN
12	H	173	HIS
13	I	48	GLN
15	L	14	GLN
15	L	66	ASN
15	L	354	HIS
15	L	390	HIS
15	L	441	ASN
15	L	457	HIS
16	M	219	GLN
16	M	261	HIS
16	M	325	ASN
16	M	380	HIS
17	N	177	ASN
17	N	208	HIS
18	O	39	ASN
18	O	327	HIS
19	P	960	HIS
19	P	986	HIS
19	P	989	HIS
19	P	1082	GLN
19	P	1107	GLN
20	R	184	GLN
20	R	200	ASN
20	R	204	ASN
22	T	61	ASN
22	T	183	ASN
22	T	210	ASN
22	T	277	ASN
23	U	777	ASN
32	h	94	GLN
29	n	53	ASN
32	p	14	GLN
32	p	21	ASN
32	p	86	ASN
32	p	94	GLN

### 5.3.3 RNA ⓘ

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	127/1175 (10%)	44 (34%)	4 (3%)
2	5	100/214 (46%)	25 (25%)	2 (2%)
3	6	101/112 (90%)	28 (27%)	3 (2%)
4	e	33/34 (97%)	19 (57%)	0
5	i	54/59 (91%)	18 (33%)	0
All	All	415/1594 (26%)	134 (32%)	9 (2%)

All (134) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	A
1	2	11	U
1	2	16	U
1	2	17	U
1	2	18	U
1	2	19	U
1	2	20	G
1	2	21	G
1	2	23	U
1	2	24	U
1	2	25	A
1	2	30	A
1	2	31	A
1	2	32	G
1	2	40	U
1	2	41	C
1	2	42	U
1	2	63	U
1	2	64	G
1	2	141	A
1	2	1094	G
1	2	1096	C
1	2	1098	C
1	2	1099	G
1	2	1100	A
1	2	1101	C
1	2	1102	C
1	2	1103	C
1	2	1104	U
1	2	1106	G
1	2	1107	C

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Mol	Chain	Res	Type
1	2	1108	A
1	2	1120	G
1	2	1123	C
1	2	1124	U
1	2	1125	U
1	2	1126	G
1	2	1139	G
1	2	1144	U
1	2	1145	U
1	2	1146	G
1	2	1149	G
1	2	1152	U
1	2	1166	G
2	5	33	U
2	5	42	A
2	5	43	G
2	5	44	A
2	5	45	A
2	5	46	C
2	5	70	A
2	5	75	A
2	5	76	U
2	5	77	A
2	5	79	C
2	5	80	G
2	5	81	A
2	5	82	A
2	5	84	A
2	5	92	U
2	5	96	U
2	5	101	C
2	5	108	C
2	5	113	G
2	5	127	U
2	5	169	U
2	5	170	U
2	5	171	U
2	5	172	U
3	6	12	A
3	6	13	A
3	6	14	C
3	6	15	C

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Mol	Chain	Res	Type
3	6	17	U
3	6	34	A
3	6	36	U
3	6	42	A
3	6	44	A
3	6	53	A
3	6	54	U
3	6	55	G
3	6	57	U
3	6	59	A
3	6	60	G
3	6	62	A
3	6	64	U
3	6	65	U
3	6	66	C
3	6	67	C
3	6	73	A
3	6	74	U
3	6	80	U
3	6	81	G
3	6	85	C
3	6	86	G
3	6	88	U
3	6	99	A
4	e	-12	U
4	e	-11	U
4	e	-9	A
4	e	-4	A
4	e	3	A
4	e	4	U
4	e	5	A
4	e	6	U
4	e	8	U
4	e	9	U
4	e	10	U
4	e	11	U
4	e	13	U
4	e	15	U
4	e	17	U
4	e	18	U
4	e	19	U
4	e	20	A

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Mol	Chain	Res	Type
4	e	21	U
5	i	2	U
5	i	9	U
5	i	505	C
5	i	508	G
5	i	509	U
5	i	511	A
5	i	514	A
5	i	515	A
5	i	516	C
5	i	518	U
5	i	1008	A
5	i	1111	U
5	i	1112	U
5	i	1113	A
5	i	1114	U
5	i	1115	A
5	i	1117	A
5	i	1118	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	41	C
1	2	1123	C
1	2	1124	U
1	2	1145	U
2	5	78	A
2	5	81	A
3	6	14	C
3	6	56	A
3	6	64	U

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 14 ligands modelled in this entry, 12 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	IHP	A	3001	-	36,36,36	0.83	0	54,60,60	1.53	8 (14%)
39	GTP	B	2001	37	27,34,34	1.12	2 (7%)	27,54,54	1.93	6 (22%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
38	IHP	A	3001	-	-	0/30/54/54	0/1/1/1
39	GTP	B	2001	37	-	0/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	B	2001	GTP	O4'-C4'	-2.11	1.40	1.45
39	B	2001	GTP	C6-N1	2.46	1.37	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B	2001	GTP	N3-C2-N1	-5.44	119.52	127.46
39	B	2001	GTP	C1'-N9-C4	-3.49	120.60	126.64
39	B	2001	GTP	C6-C5-C4	-2.81	118.05	120.84
39	B	2001	GTP	N2-C2-N1	2.13	120.64	117.24
38	A	3001	IHP	O15-C5-C4	2.30	114.11	108.68
38	A	3001	IHP	O11-C1-C6	2.31	114.15	108.68
38	A	3001	IHP	O11-C1-C2	2.41	114.38	108.68
39	B	2001	GTP	C6-N1-C2	2.57	119.75	116.06
38	A	3001	IHP	C3-C2-C1	3.16	117.47	110.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	A	3001	IHP	O15-C5-C6	3.29	116.44	108.68
38	A	3001	IHP	C5-C4-C3	3.41	118.02	110.46
38	A	3001	IHP	C5-C6-C1	3.57	118.38	110.46
38	A	3001	IHP	C4-C3-C2	3.61	118.45	110.46
39	B	2001	GTP	C2-N3-C4	4.36	120.25	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A	3001	IHP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
24	X	4
5	i	4

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	i	15:U	O3'	501:A	P	58.05
1	X	3370:UNK	C	3389:UNK	N	35.33
1	X	1031:UNK	C	2287:UNK	N	34.77
1	X	125:UNK	C	1001:UNK	N	25.13
1	X	2322:UNK	C	3364:UNK	N	19.85
1	i	628:U	O3'	1001:A	P	15.34
1	i	518:U	O3'	620:U	P	7.99
1	i	1008:A	O3'	1110:A	P	5.10