



Full wwPDB EM Validation Report ⓘ

Jul 3, 2025 – 02:49 am BST

PDB ID : 6EXN / pdb_00006exn
EMDB ID : EMD-3979
Title : Post-catalytic P complex spliceosome with 3' splice site docked
Authors : Wilkinson, M.E.; Fica, S.M.; Galej, W.P.; Norman, C.M.; Newman, A.J.; Nagai, K.
Deposited on : 2017-11-08
Resolution : 3.70 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.dev118
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0rc1
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.44

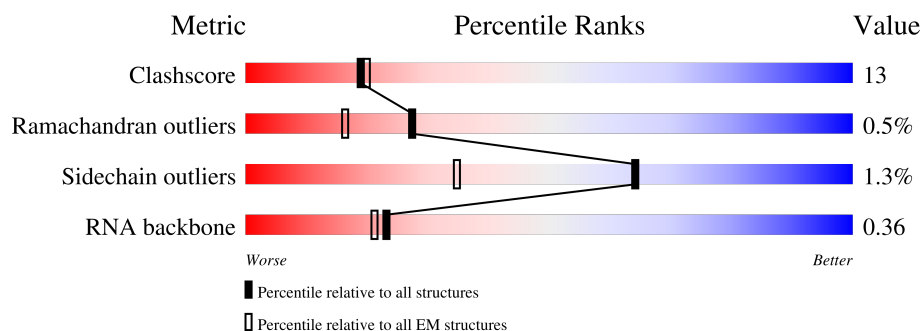
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.70 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	2	1175	<div> <div>9%</div> <div>6%</div> <div>88%</div> </div>
2	5	179	<div> <div>48%</div> <div>43%</div> <div>42%</div> <div>9%</div> </div>
3	6	112	<div> <div>12%</div> <div>40%</div> <div>38%</div> <div>12%</div> <div>9%</div> </div>
4	A	2413	<div> <div>9%</div> <div>60%</div> <div>20%</div> <div>19%</div> </div>
5	C	1008	<div> <div>15%</div> <div>63%</div> <div>24%</div> <div>13%</div> </div>
6	D	278	<div> <div>17%</div> <div>32%</div> <div>65%</div> </div>
7	E	39	<div> <div>44%</div> <div>13%</div> <div>28%</div> <div>41%</div> <div>18%</div> </div>

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Mol	Chain	Length	Quality of chain
8	H	577	
9	I	95	
10	J	451	
11	K	379	
12	L	157	
13	M	339	
14	N	364	
15	O	590	
16	P	175	
17	R	135	
18	S	687	
19	T	859	
20	V	1145	
21	W	238	
22	X	95	
23	Y	111	
24	a	251	
25	b	196	
25	k	196	
26	c	382	
27	d	101	
27	n	101	
28	e	94	
28	p	94	
29	f	86	

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Mol	Chain	Length	Quality of chain
29	q	86	
30	g	77	
30	r	77	
31	h	146	
31	l	146	
32	j	110	
32	m	110	
33	o	455	
34	s	175	
35	t	503	
35	u	503	
35	v	503	
35	w	503	
36	y	215	

2 Entry composition [i](#)

There are 40 unique types of molecules in this entry. The entry contains 80677 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	136	Total	C	N	O	P	0	0
			2868	1282	476	974	136		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	5	171	Total	C	N	O	P	0	0
			3626	1623	630	1203	170		

- 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 protein called Pre-mRNA-splicing factor Prp8.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	1945	Total	C	N	O	S	0	0
			16046	10308	2764	2915	59		

- Molecule 5 is a protein called Pre-mRNA-splicing factor SNU114.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	C	880	Total	C	N	O	S	0	0
			6999	4522	1169	1280	28		

- Molecule 6 is a protein called Pre-mRNA-splicing factor CWC16.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	97	Total	C	N	O	S	0	0
			579	347	108	123	1		

- Molecule 7 is a RNA chain called Ligated exons: UBC4 mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	E	32	Total	C	N	O	P	0	0
			586	258	86	210	32		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	411	Total	C	N	O	S	0	0
			2689	1685	477	521	6		

- Molecule 9 is a RNA chain called Intron lariat: UBC4 RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	39	Total	C	N	O	P	0	0
			804	360	136	269	39		

- Molecule 10 is a protein called Pre-mRNA-splicing factor PRP46.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	342	Total	C	N	O	S	0	0
			2691	1699	475	507	10		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	80	THR	ALA	conflict	UNP Q12417

- Molecule 11 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	170	Total	C	N	O	S	0	0
			1355	847	249	254	5		

- Molecule 12 is a protein called Pre-mRNA-splicing factor BUD31.

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

- Molecule 13 is a protein called Pre-mRNA-splicing factor CWC2.

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

- Molecule 14 is a protein called Pre-mRNA-splicing factor SLT11.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	242	Total	C	N	O	S	0	0
			1917	1217	335	350	15		

- Molecule 15 is a protein called Pre-mRNA-splicing factor CEF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	320	Total	C	N	O	S	0	0
			2350	1457	437	449	7		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
O	125	VAL	ALA	conflict	UNP Q03654
O	285	PRO	SER	conflict	UNP Q03654
O	341	GLU	ASP	conflict	UNP Q03654
O	342	PRO	SER	conflict	UNP Q03654
O	417	SER	PRO	conflict	UNP Q03654
O	425	PRO	ARG	conflict	UNP Q03654

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC15.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	73	Total	C	N	O	S	0	0
			600	378	119	102	1		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
P	49	LYS	ARG	conflict	UNP Q03772
P	58	ASN	SER	conflict	UNP Q03772
P	66	VAL	ALA	conflict	UNP Q03772
P	68	VAL	MET	conflict	UNP Q03772

- Molecule 17 is a protein called Pre-mRNA-splicing factor CWC21.

Mol	Chain	Residues	Atoms				AltConf	Trace
17	R	73	Total	C	N	O	0	0
			423	252	82	89		

- Molecule 18 is a protein called Pre-mRNA-splicing factor CLF1.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	472	Total	C	N	O	S	0	0
			3189	1989	599	593	8		

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	561	LYS	GLU	conflict	UNP Q12309
S	615	MET	LEU	conflict	UNP Q12309
S	649	ASP	ASN	conflict	UNP Q12309
S	659	VAL	ILE	conflict	UNP Q12309

- Molecule 19 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
19	T	594	Total	C	N	O	0	0
			2957	1769	594	594		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
T	695	ILE	THR	conflict	UNP Q04048

- Molecule 20 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP22.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	638	Total	C	N	O	S	0	0
			5059	3217	854	959	29		

- Molecule 21 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	149	Total	C	N	O	S	0	0
			1211	756	223	228	4		

- Molecule 22 is a protein called Unassigned structure.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	95	Total	C	N	O	0	0
			475	285	95	95		

- Molecule 23 is a protein called U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Y	87	Total	C	N	O	S	0	0
			704	451	123	127	3		

- Molecule 24 is a protein called Pre-mRNA-splicing factor Prp18.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	a	171	Total	C	N	O	S	0	0
			1372	878	244	246	4		

- Molecule 25 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	b	80	Total	C	N	O	S	0	0
			631	403	114	111	3		
25	k	70	Total	C	N	O	S	0	0
			563	360	98	102	3		

- Molecule 26 is a protein called Pre-mRNA-splicing factor SLU7.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	c	204	Total	C	N	O	S	0	0
			1709	1072	315	314	8		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	d	82	Total	C	N	O	S	0	0
			625	399	109	115	2		
27	n	82	Total	C	N	O	S	0	0
			632	402	109	119	2		

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

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

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Mol	Chain	Residues	Atoms					AltConf	Trace
28	p	77	Total	C	N	O	S	0	0
			602	396	95	108	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
29	f	72	Total	C	N	O	S	0	0
			573	368	101	103	1		
29	q	73	Total	C	N	O	S	0	0
			585	376	102	106	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	g	69	Total	C	N	O	S	0	0
			529	337	93	97	2		
30	r	75	Total	C	N	O	S	0	0
			577	363	100	112	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
31	h	82	Total	C	N	O	S	0	0
			644	409	110	123	2		
31	l	87	Total	C	N	O	S	0	0
			679	435	118	123	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
32	j	94	Total	C	N	O	S	0	0
			741	477	141	119	4		
32	m	92	Total	C	N	O	S	0	0
			752	481	136	131	4		

- Molecule 33 is a protein called Pre-mRNA-processing factor Prp17.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	o	322	Total	C	N	O	S	0	0
			2599	1655	462	474	8		

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

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

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

Mol	Chain	Residues	Atoms				AltConf	Trace
35	t	117	Total	C	N	O	0	0
			583	349	117	117		
35	u	116	Total	C	N	O	0	0
			578	346	116	116		
35	v	118	Total	C	N	O	0	0
			588	352	118	118		
35	w	114	Total	C	N	O	0	0
			568	340	114	114		

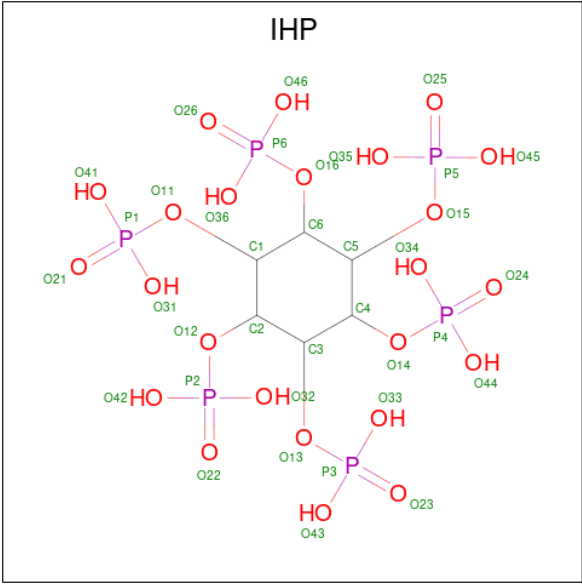
- Molecule 36 is a protein called Pre-mRNA-splicing factor SYF2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	y	88	Total	C	N	O	S	0	0
			719	444	132	142	1		

- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

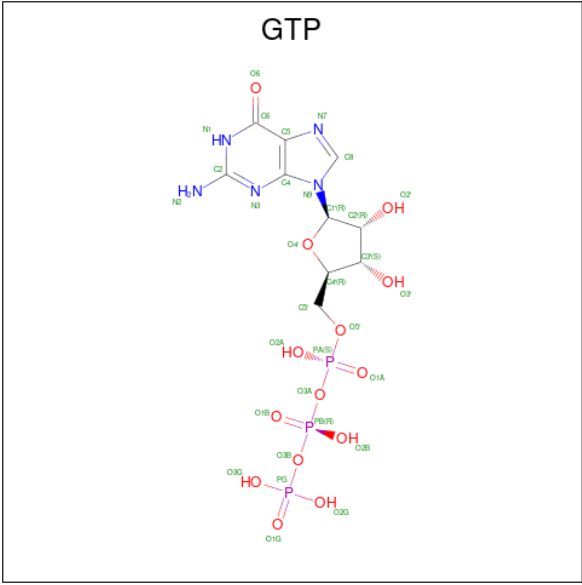
Mol	Chain	Residues	Atoms		AltConf
37	6	1	Total	Mg	0
			1	1	

- Molecule 38 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

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

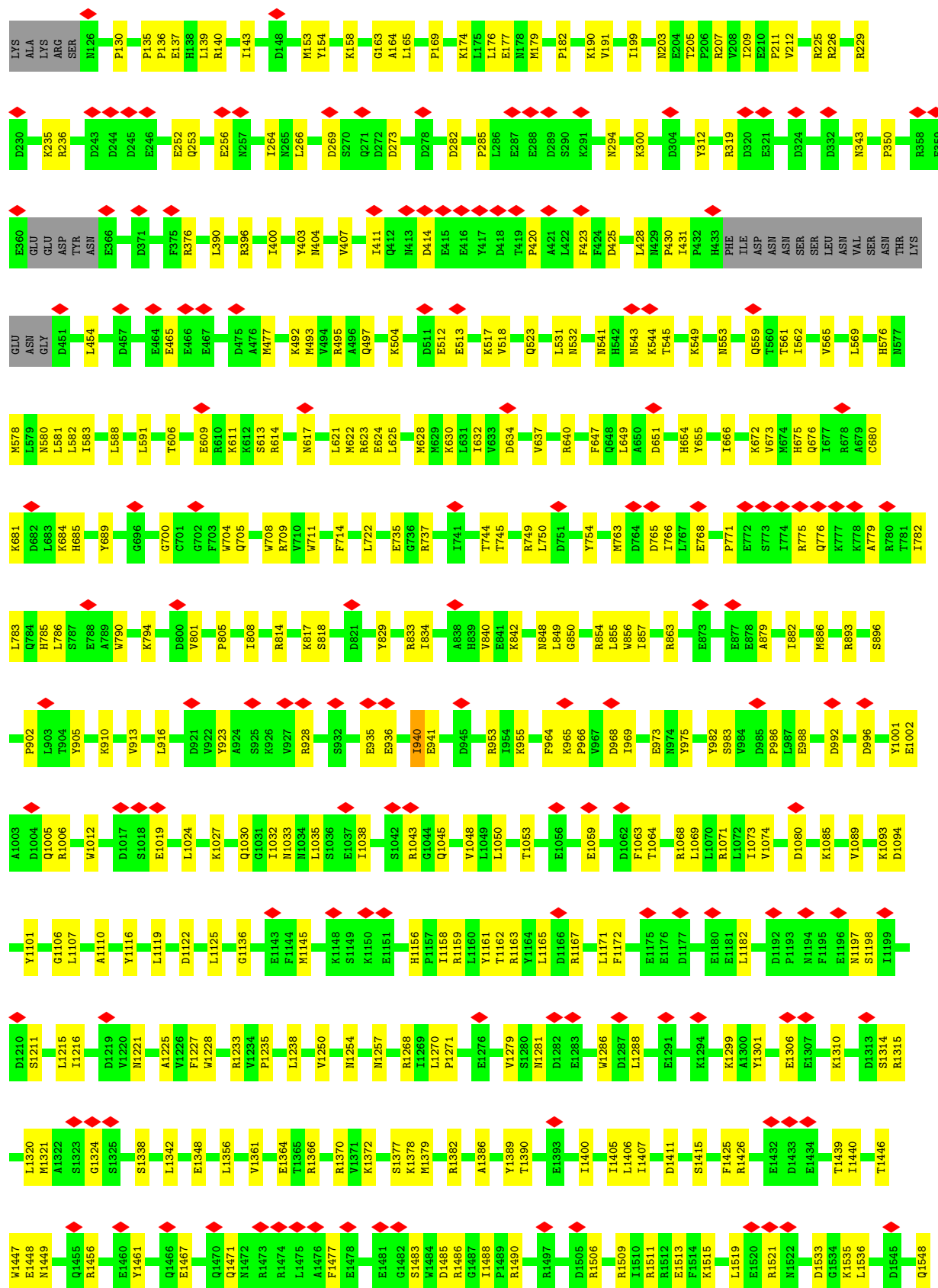


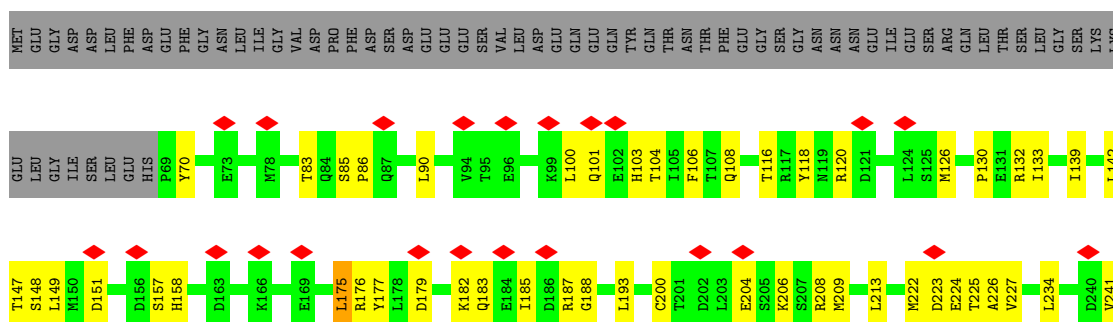
Mol	Chain	Residues	Atoms					AltConf
39	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

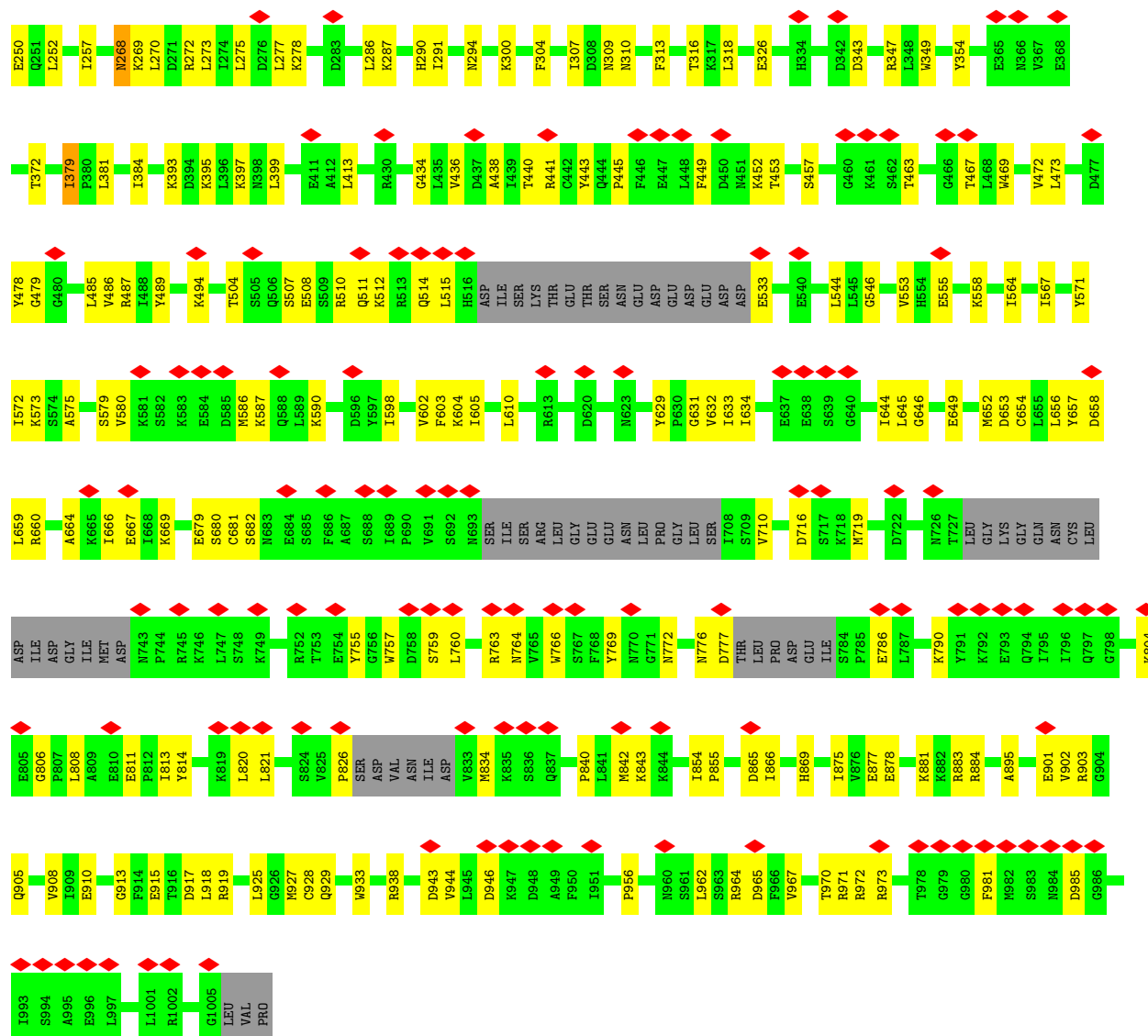
- Molecule 40 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

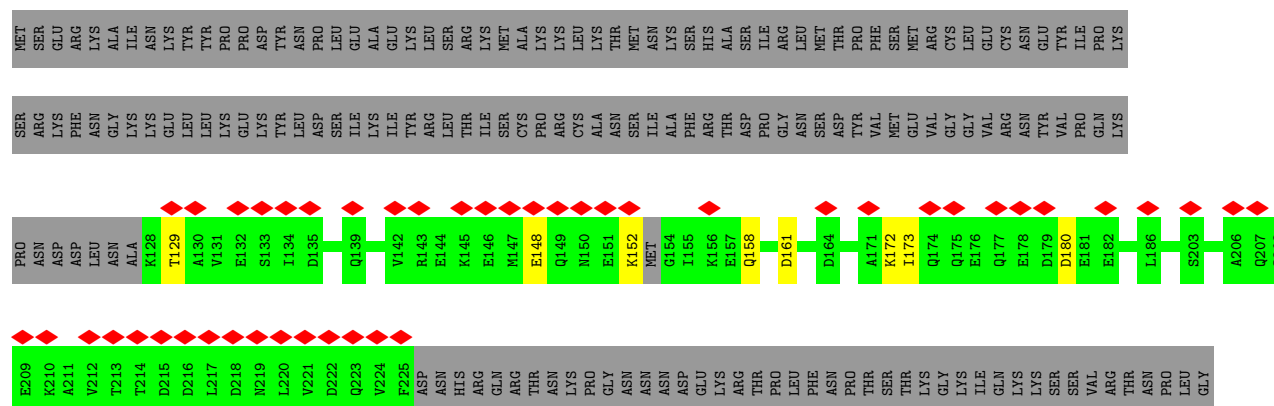




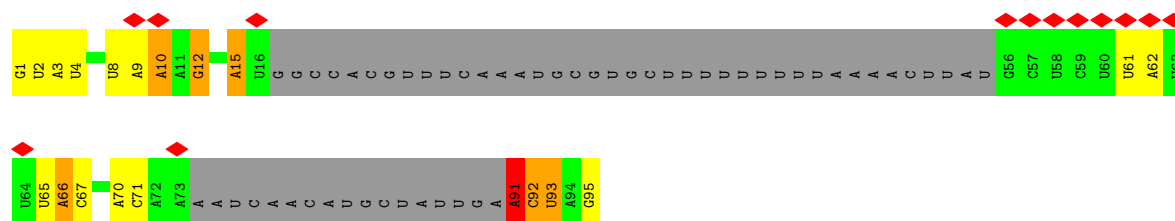




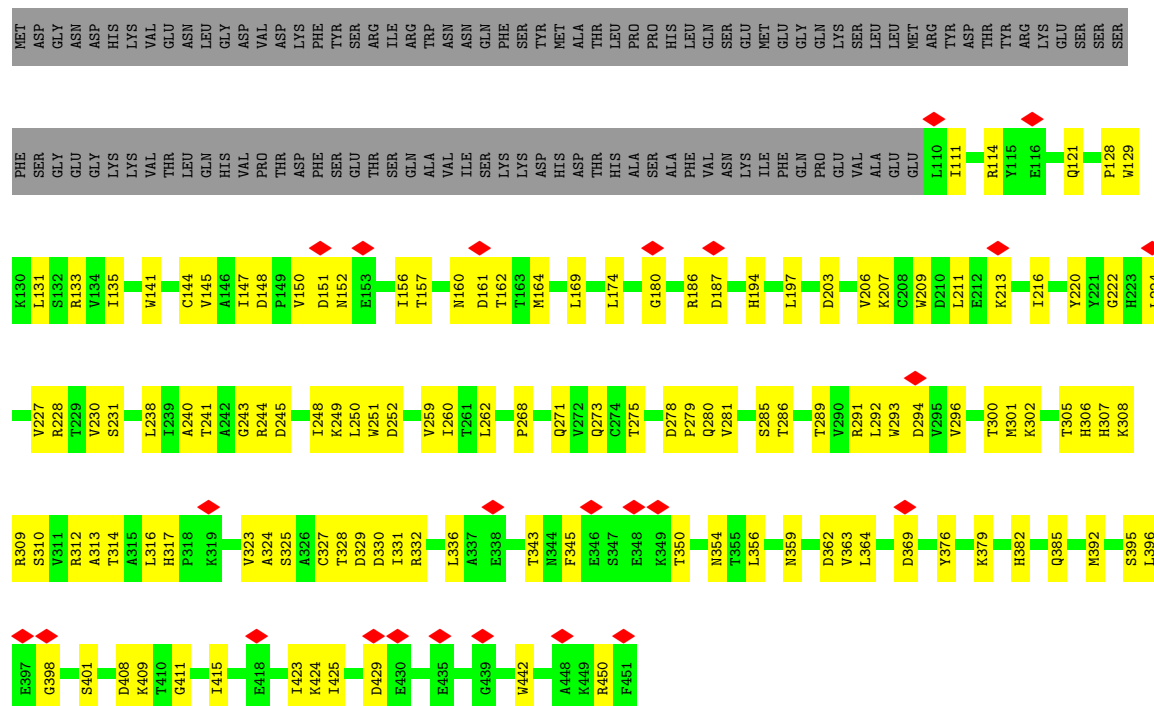
• Molecule 6: Pre-mRNA-splicing factor CWC16



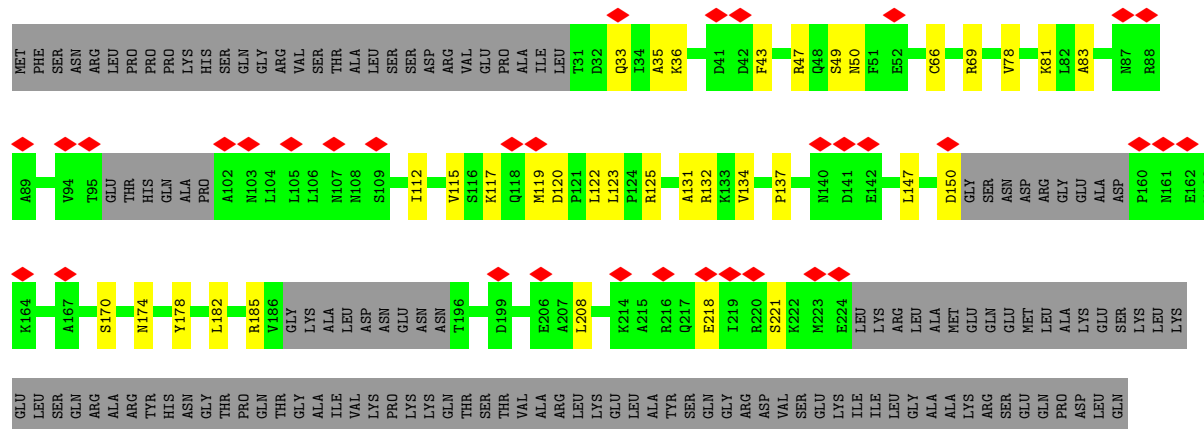
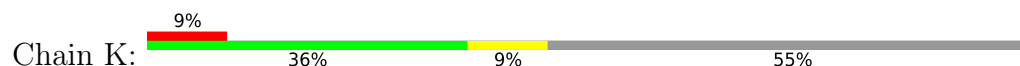




• Molecule 10: Pre-mRNA-splicing factor PRP46

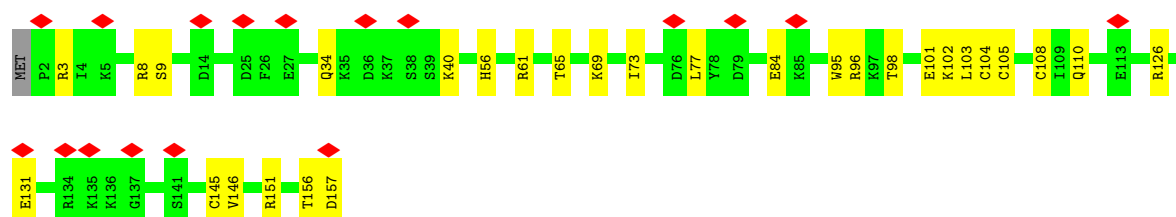
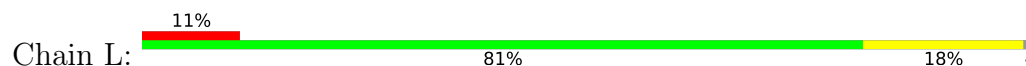


• Molecule 11: Pre-mRNA-processing protein 45

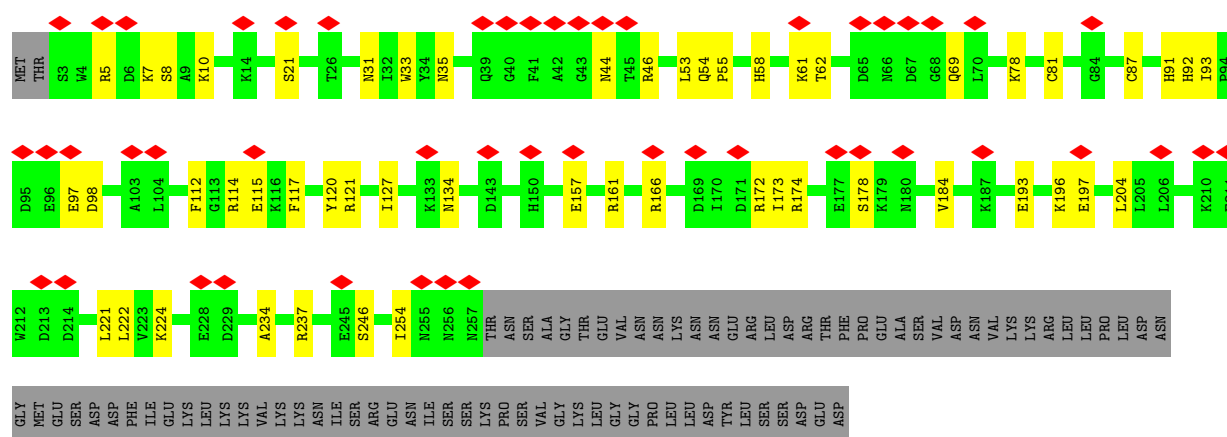


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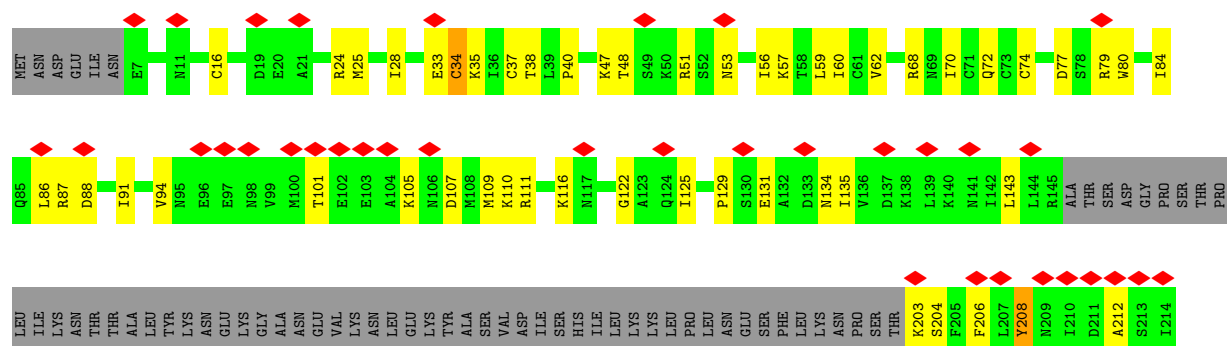
- Molecule 12: Pre-mRNA-splicing factor BUD31

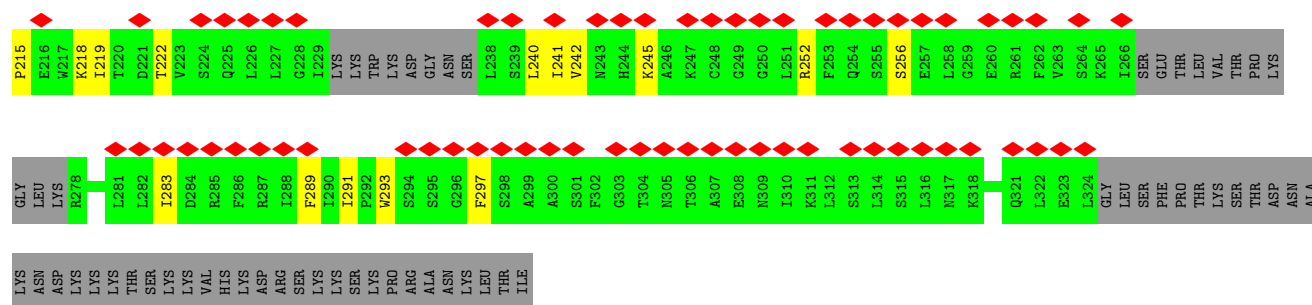


- Molecule 13: Pre-mRNA-splicing factor CWC2

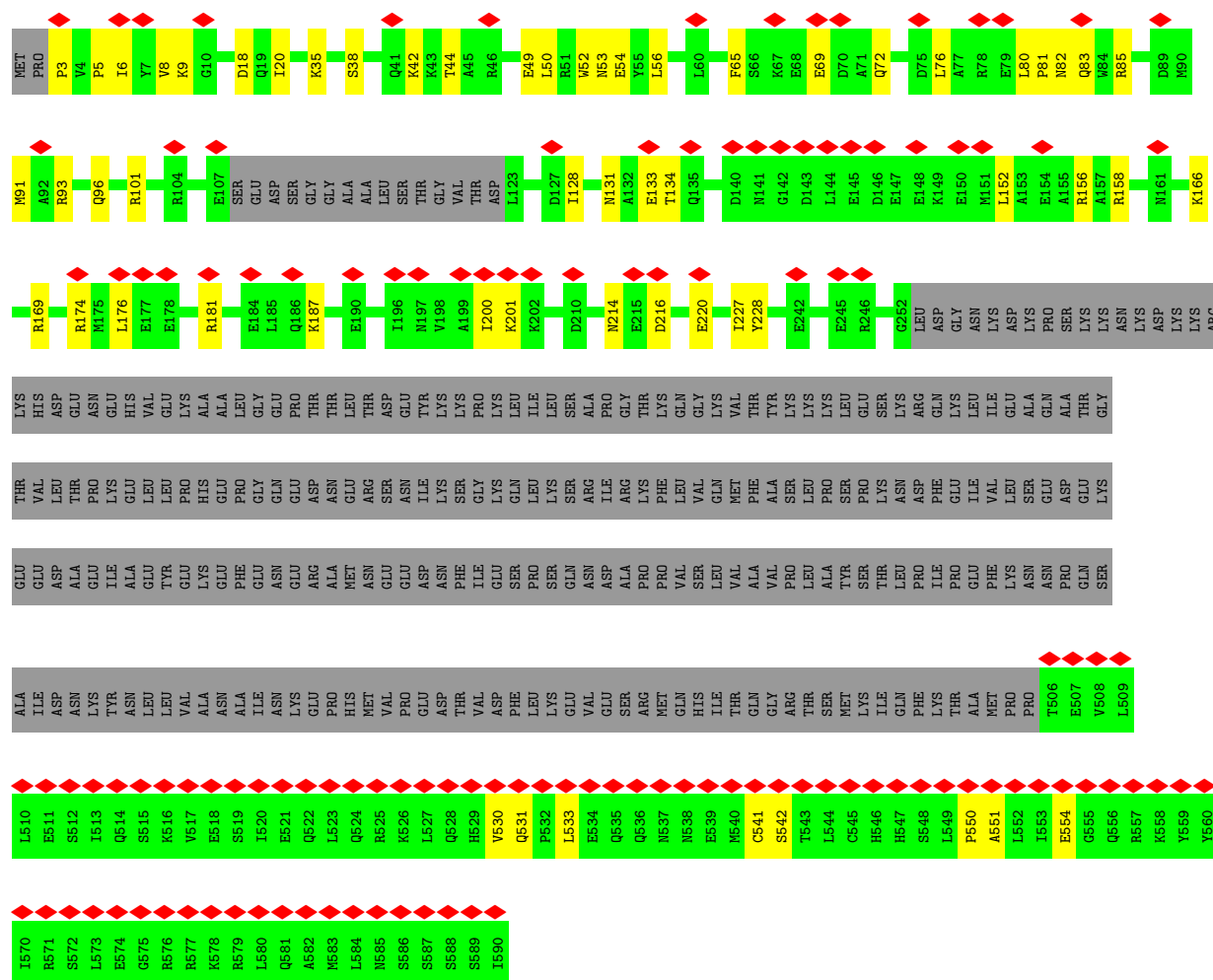
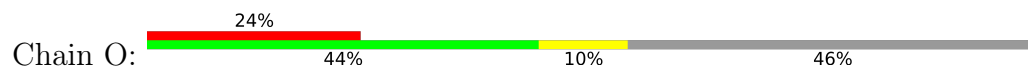


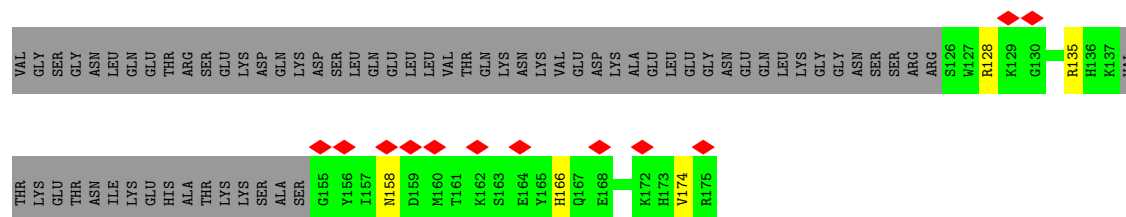
- Molecule 14: Pre-mRNA-splicing factor SLT11



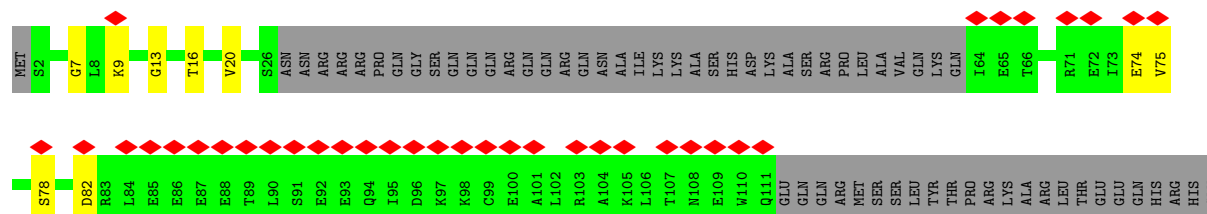


• Molecule 15: Pre-mRNA-splicing factor CEF1

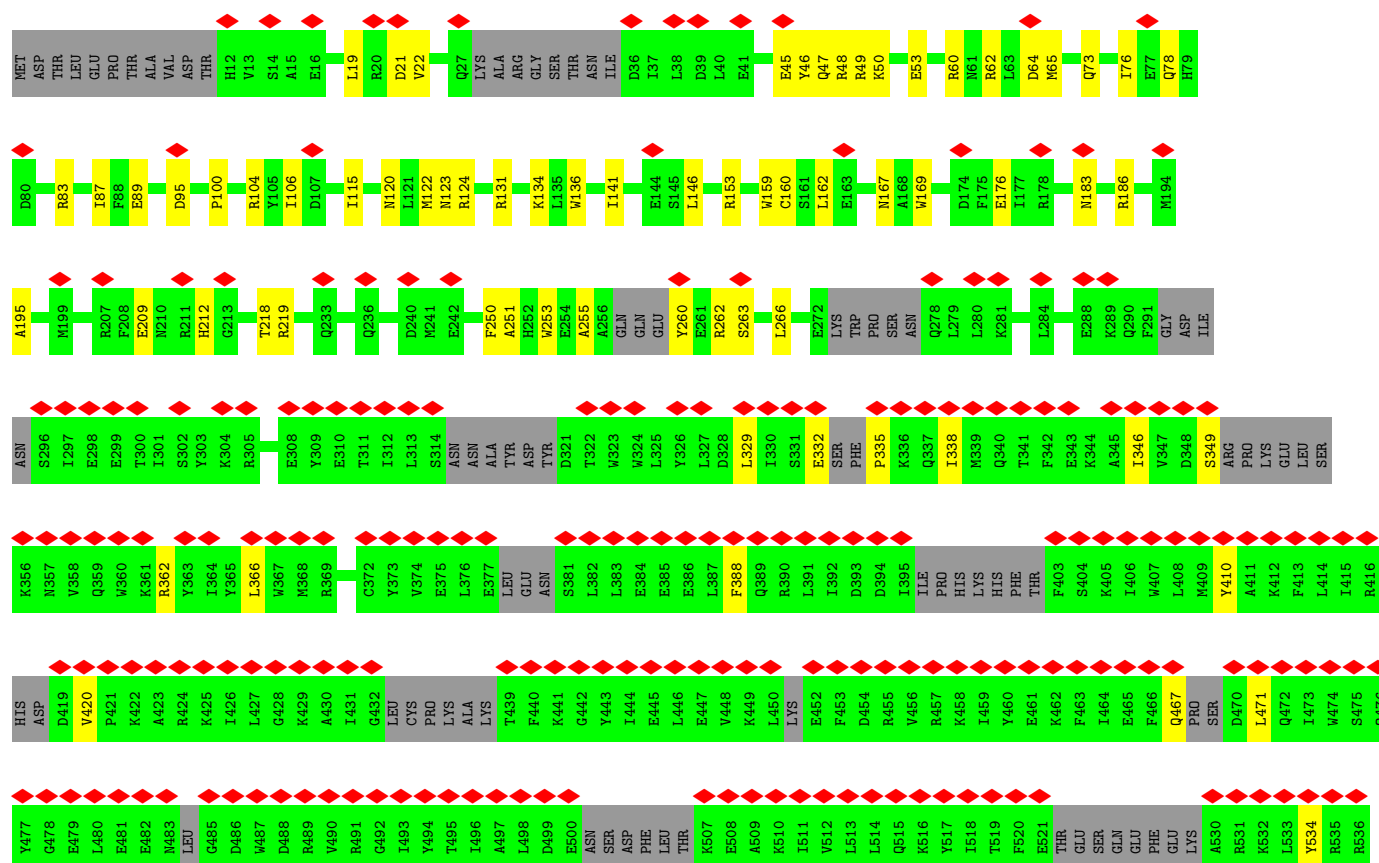


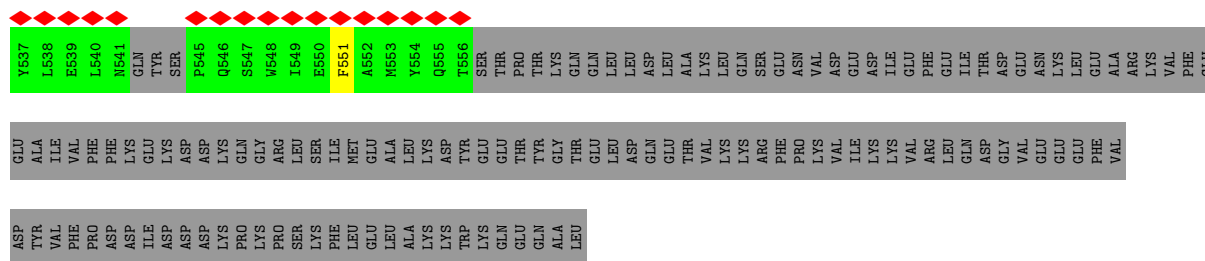


• Molecule 17: Pre-mRNA-splicing factor CWC21

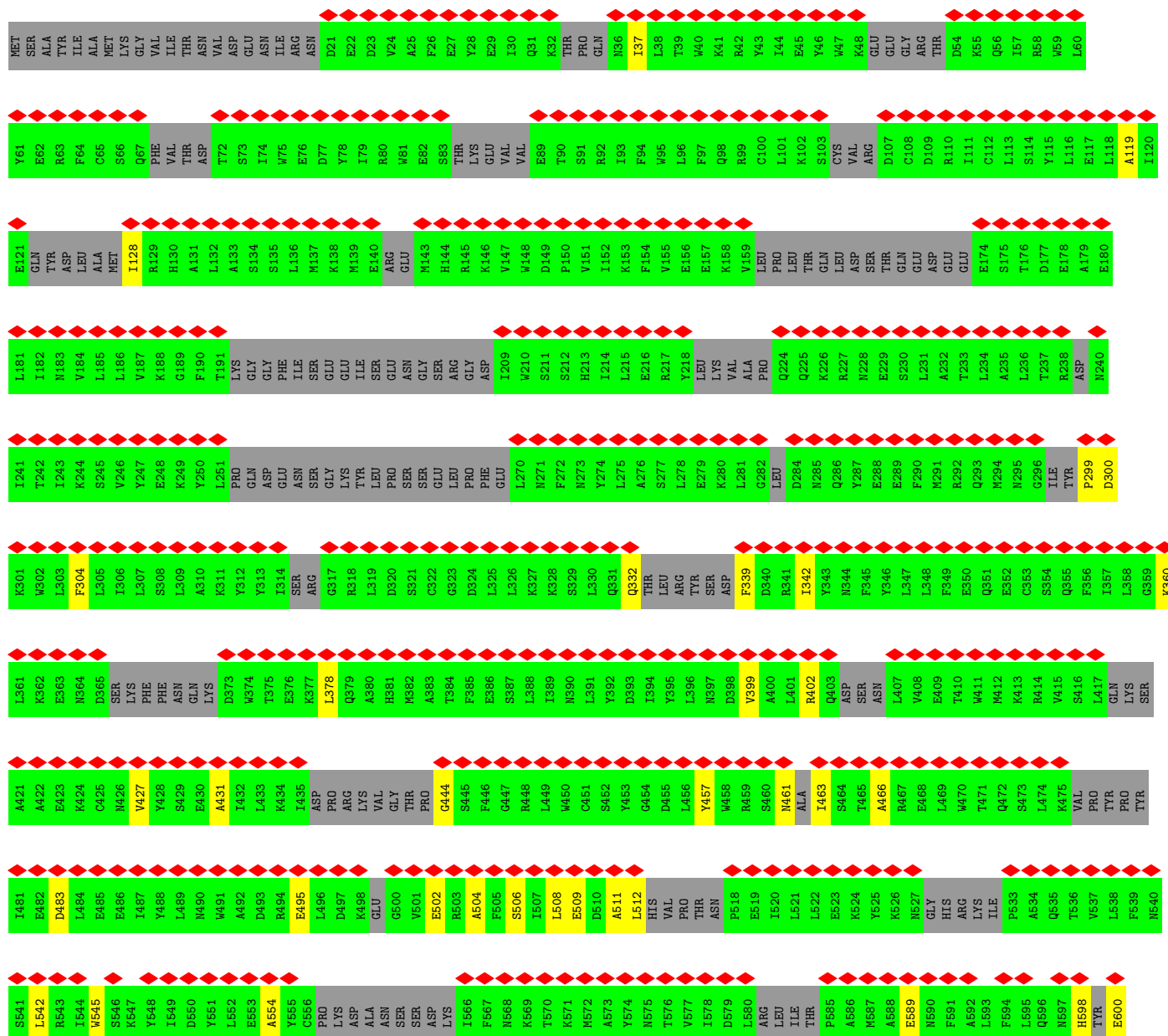


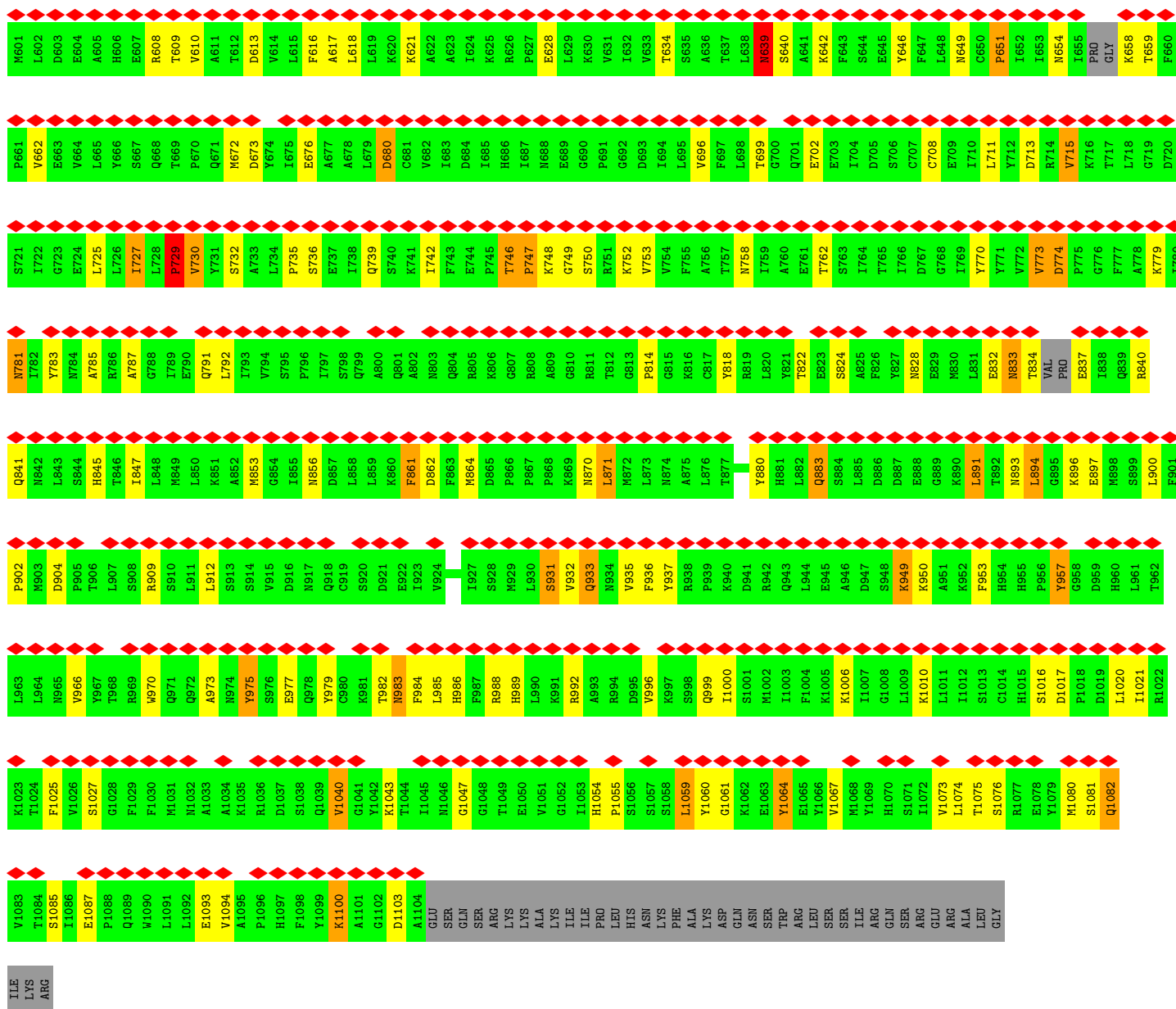
• Molecule 18: Pre-mRNA-splicing factor CLF1



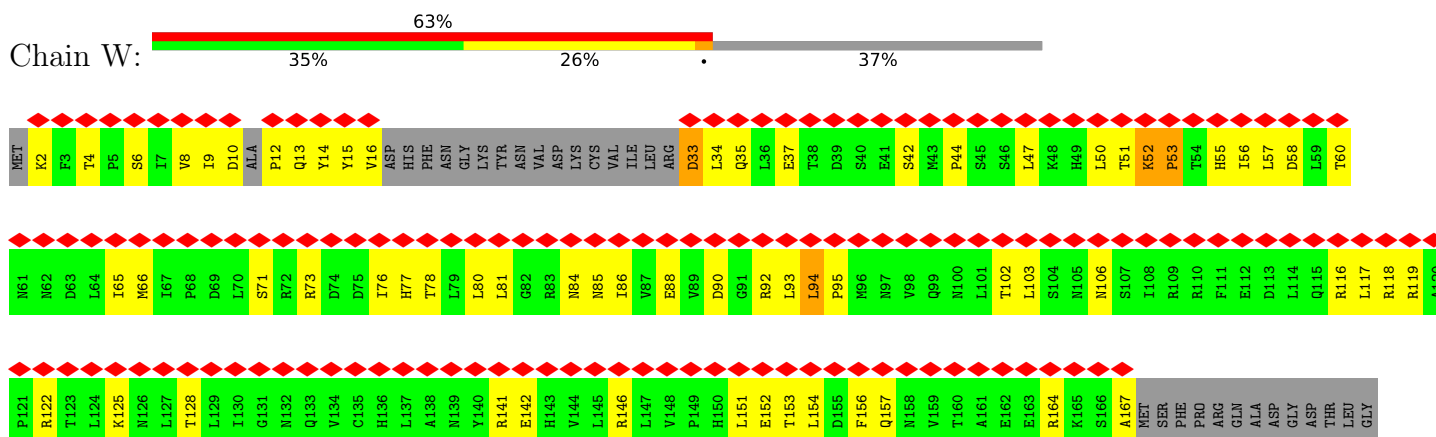


• Molecule 19: Pre-mRNA-splicing factor SYF1



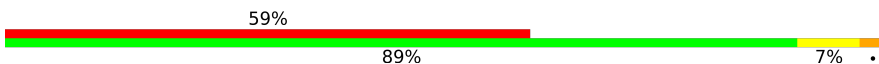


• Molecule 21: U2 small nuclear ribonucleoprotein A'



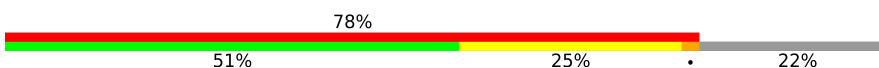
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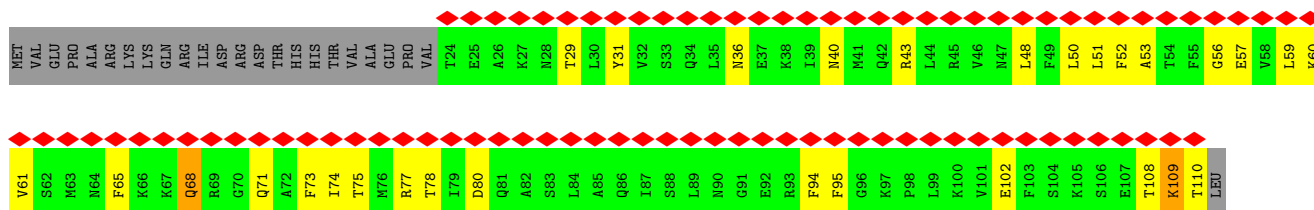
• Molecule 22: Unassigned structure

Chain X: 



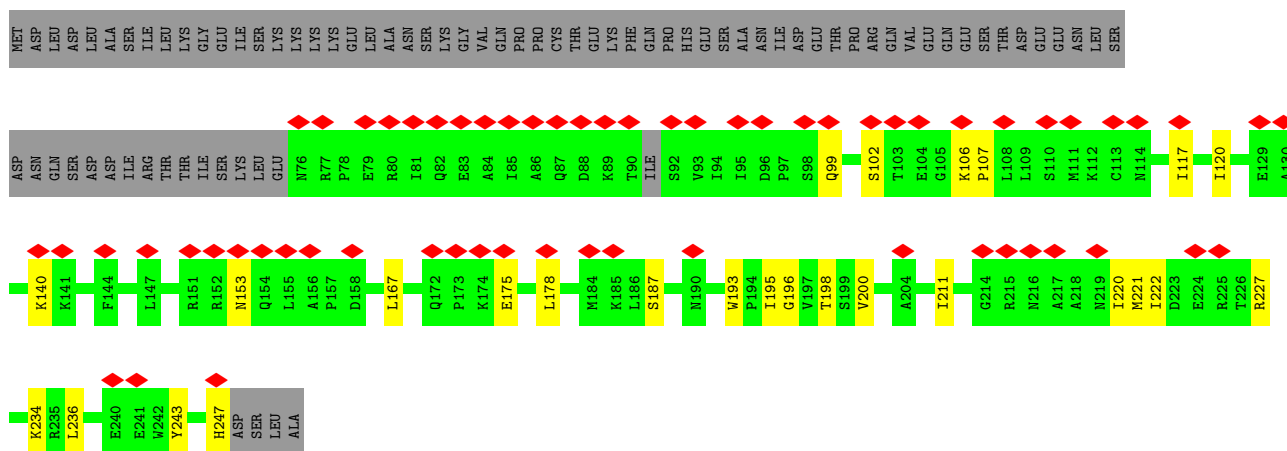
• Molecule 23: U2 small nuclear ribonucleoprotein B"

Chain Y: 



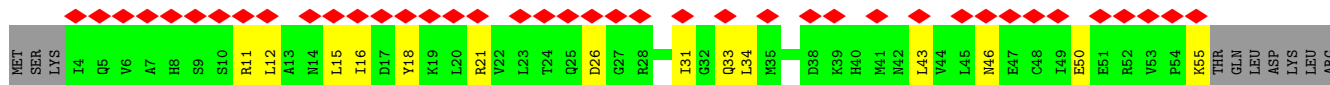
• Molecule 24: Pre-mRNA-splicing factor Prp18

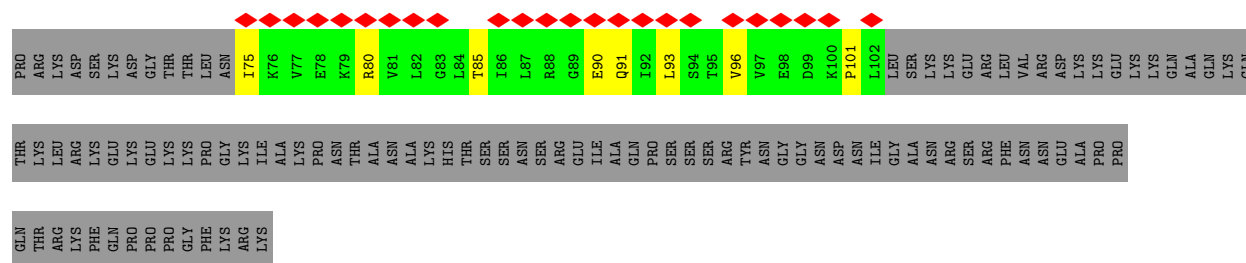
Chain a: 



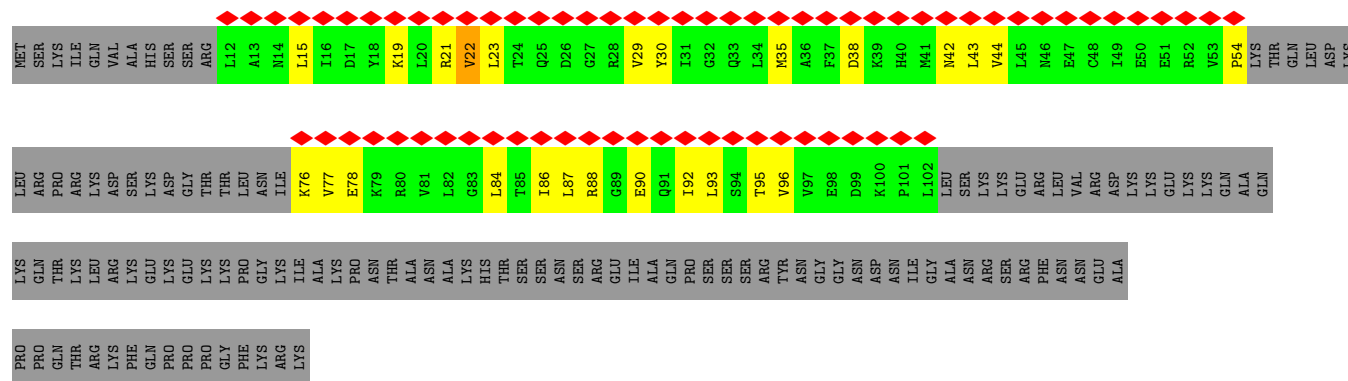
• Molecule 25: Small nuclear ribonucleoprotein-associated protein B

Chain b: 

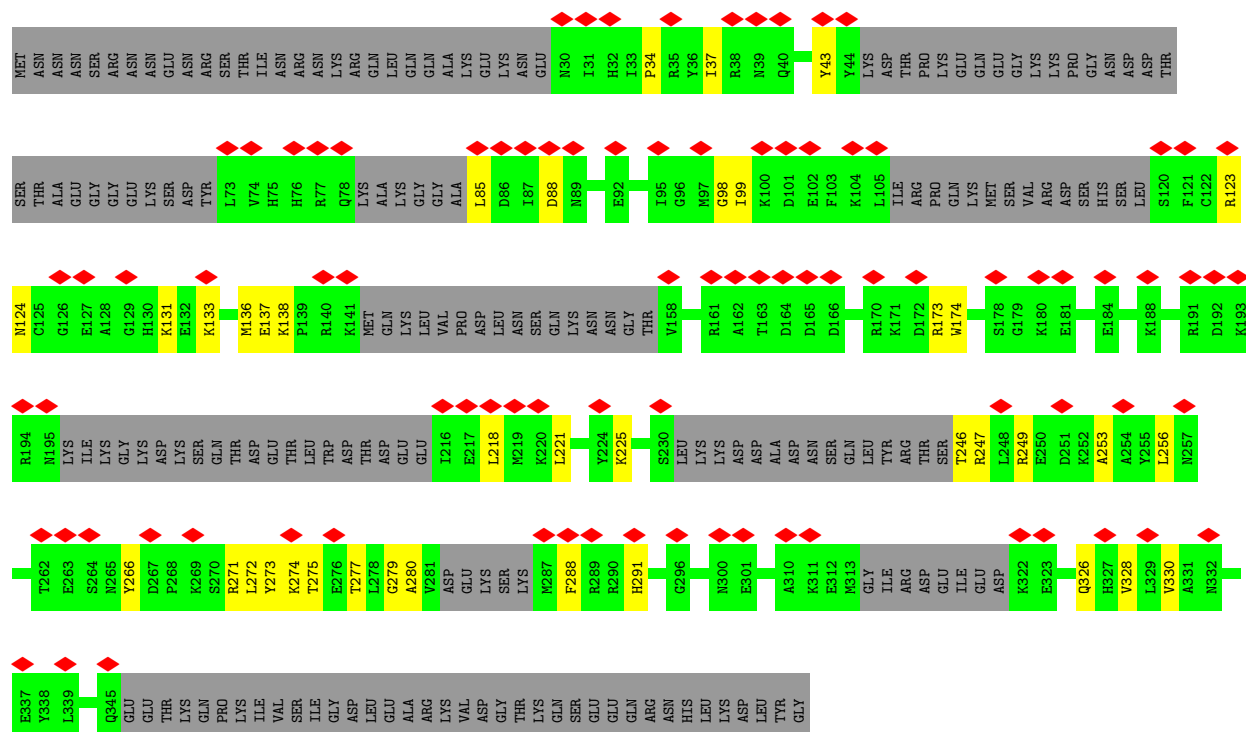




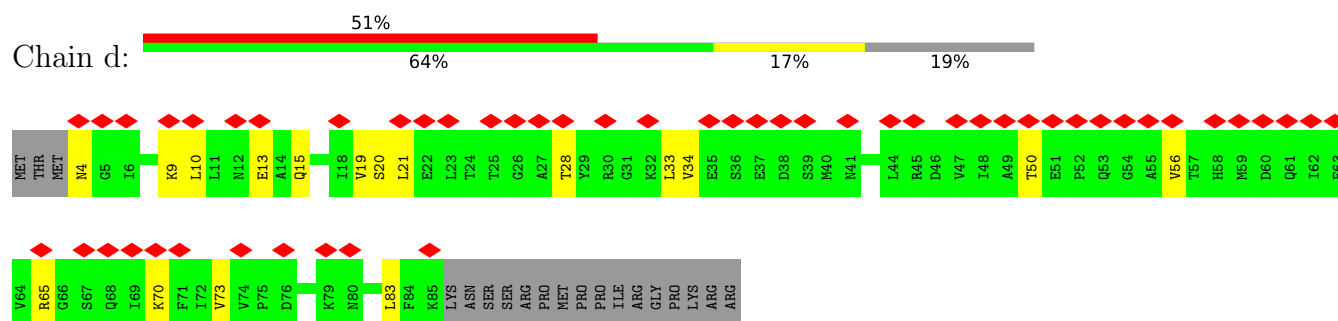
• Molecule 25: Small nuclear ribonucleoprotein-associated protein B



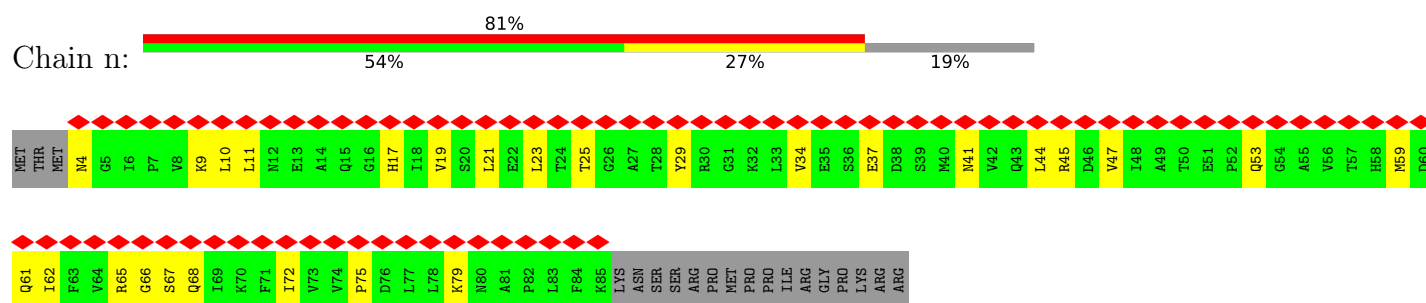
• Molecule 26: Pre-mRNA-splicing factor SLU7



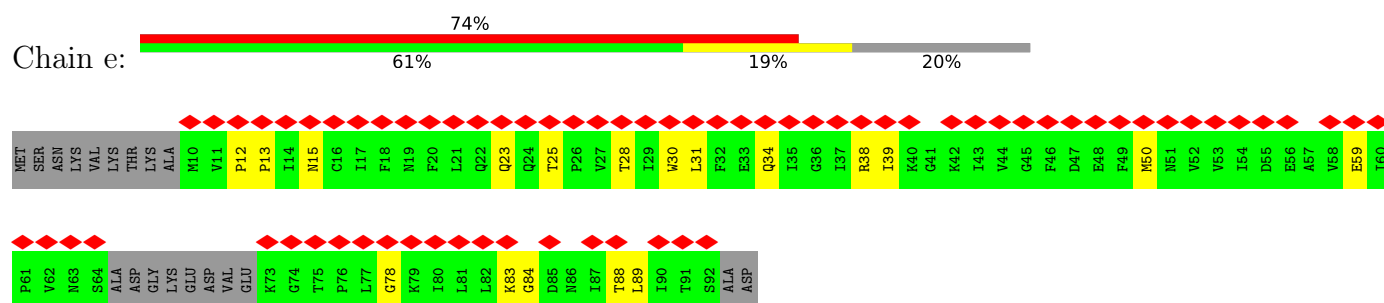
- Molecule 27: Small nuclear ribonucleoprotein Sm D3



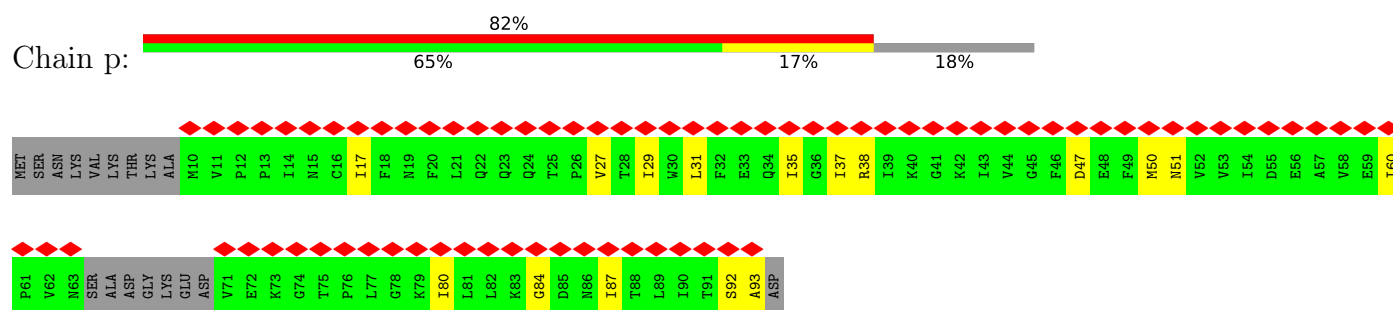
- Molecule 27: Small nuclear ribonucleoprotein Sm D3



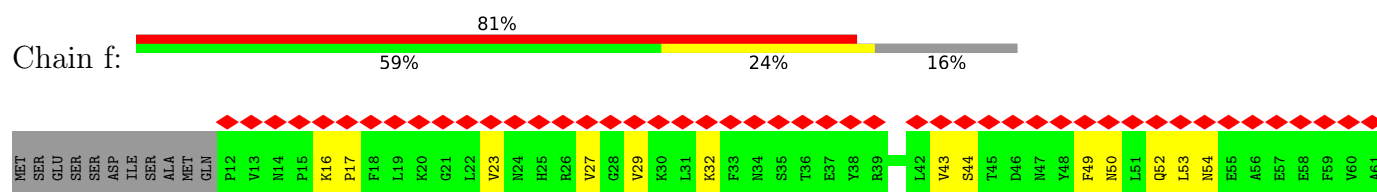
- Molecule 28: Small nuclear ribonucleoprotein E



- Molecule 28: Small nuclear ribonucleoprotein E

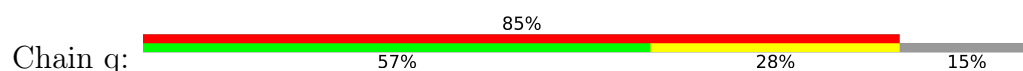


- Molecule 29: Small nuclear ribonucleoprotein F

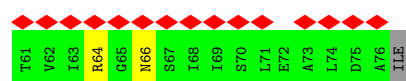
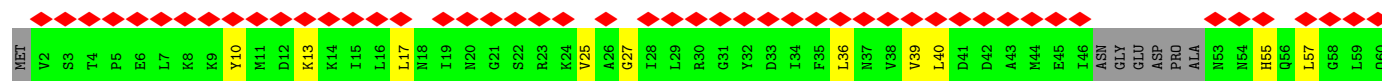
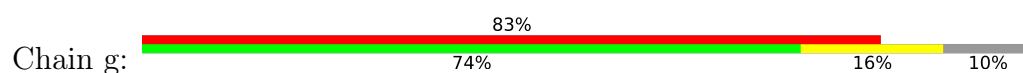




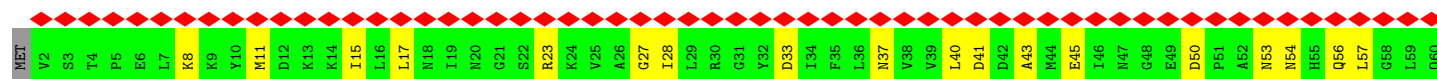
• Molecule 29: Small nuclear ribonucleoprotein F



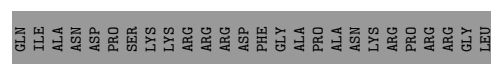
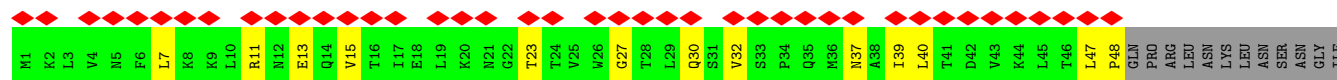
• Molecule 30: Small nuclear ribonucleoprotein G



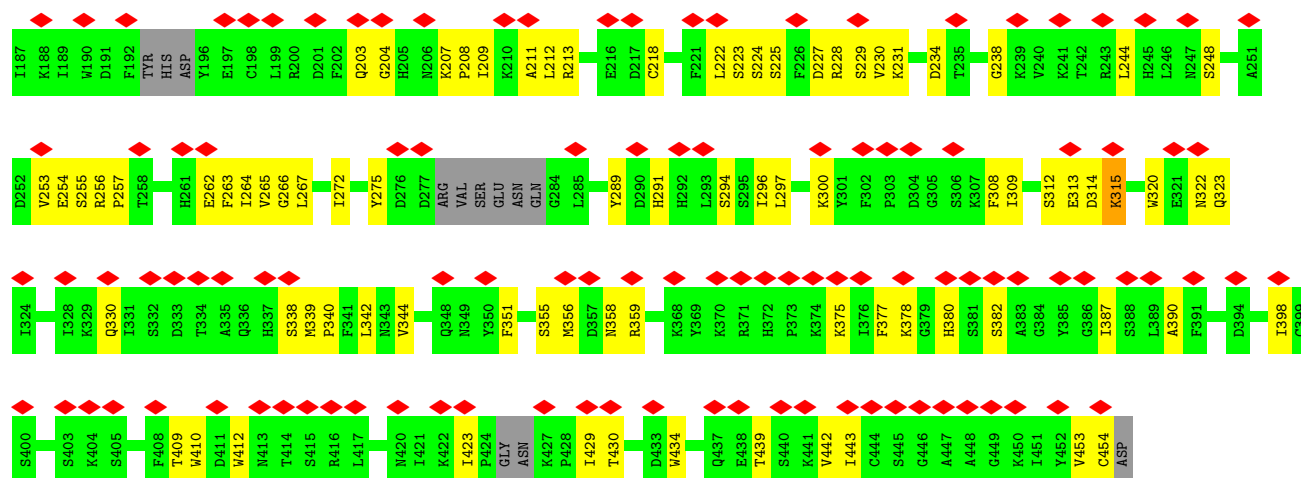
• Molecule 30: Small nuclear ribonucleoprotein G



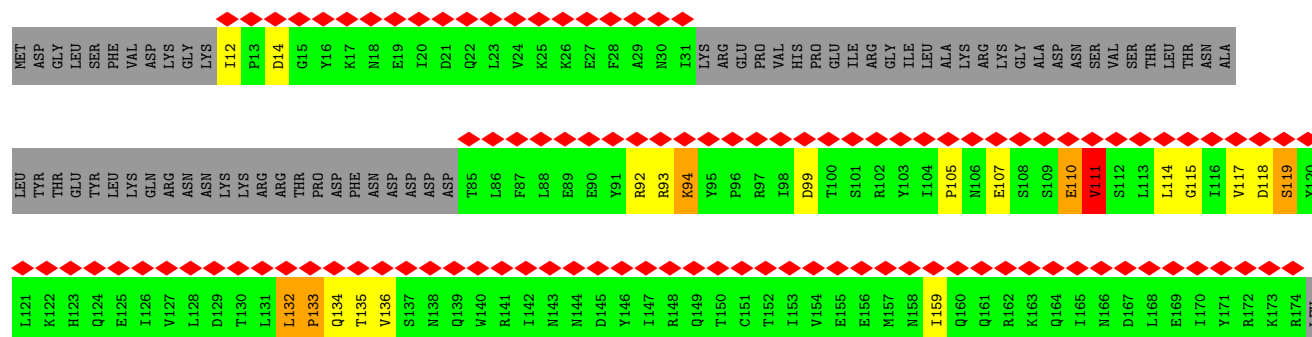
• Molecule 31: Small nuclear ribonucleoprotein Sm D1



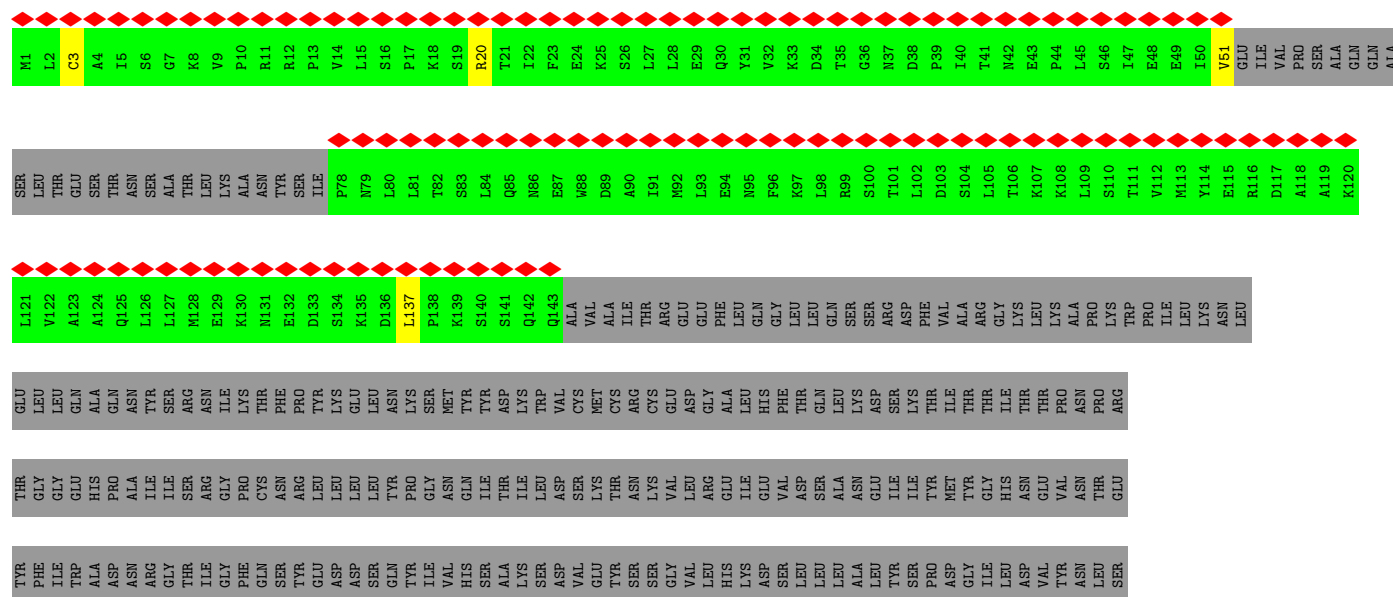
• Molecule 31: Small nuclear ribonucleoprotein Sm D1



• Molecule 34: Pre-mRNA-splicing factor SNT309



• Molecule 35: Pre-mRNA-processing factor Prp19



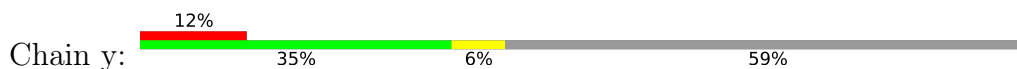


- Molecule 35: Pre-mRNA-processing factor Prp19

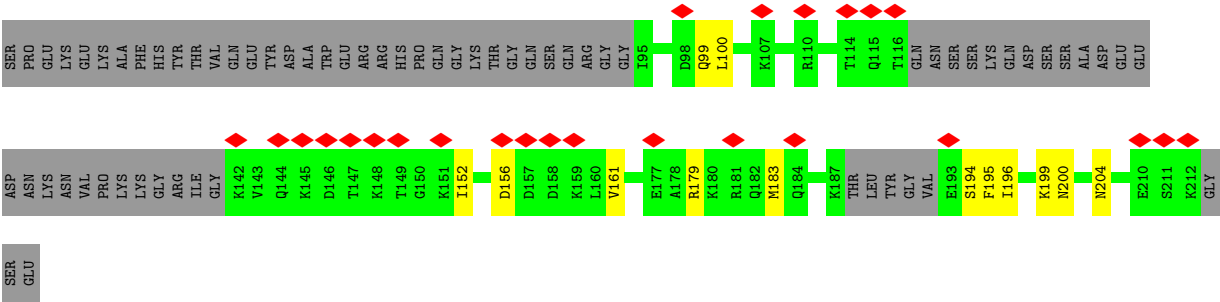


CYS	THR	SER	TRP	THR	GLU	L121	SER	M1
GLY	GLY	PRO	PHE	GLY	LEU	V122	THR	L2
ASP	THR	ASP	ILE	GLY	LEU	A123	GLU	C3
GLY	VAL	GLN	TRP	GLU	GLN	A124	SER	A4
ILE	THR	SER	ASP	HIS	GLN	Q125	THR	I5
ALA	ASP	SER	ASN	ALA	ASN	L126	ASN	S6
ALA	ILE	ARG	ARG	ILE	TYR	L127	SER	G7
LEU	ASP	PHE	GLY	ILE	SER	M128	ALA	X8
ILE	ASP	PRO	THR	ARG	ARG	E129	THR	Y9
LYS	GLY	ILE	GLY	ILE	LYS	K130	LYS	P10
ASN	PHE	PRO	CYS	PRO	THR	N131	ALA	R11
ASP	GLN	GLN	THR	THR	THR	E132	ASN	I12
SER	ASN	SER	ASN	PHE	PHE	D133	TYR	P13
PHE	ILE	ALA	SER	ARG	PRO	S134	SER	V14
ASN	ALA	ILE	TYR	LEU	TYR	X135	ILE	L15
ASN	VAL	LYS	GLN	LEU	ASN	D136	L80	S16
VAL	SER	VAL	ASN	LEU	LEU	L137	N79	P17
VAL	GLU	LYS	TYR	TYR	LYS	P138	L81	K18
THR	SER	PHE	ILE	GLY	ASN	K139	T82	S19
PRO	ASN	ASP	VAL	ASN	MET	SER	S83	R20
	LEU	ASN	HIS	GLN	TYR	SER	L84	T21
	THR	GLY	SER	ILE	TYR	SER	Q85	I22
	ILE	TYR	ALA	THR	ASP	GLN	N86	F23
	THR	TRP	LYS	ILE	LYS	GLN	E87	E24
	LYS	MET	SER	LEU	TRP	ALA	W88	X25
	PHE	VAL	ASP	ASP	CYS	VAL	D89	S26
	ASP	VAL	VAL	LYS	MET	ALA	ARG	L27
	LYS	GLY	GLU	THR	CYS	THR	I91	L28
	LYS	CYS	TYR	THR	ARG	GLY	N92	E29
	THR	ASP	SER	ASN	GLU	ALA	L93	X31
	LYS	GLN	SER	LYS	LEU	GLN	E94	V32
	ASP	PHE	ASP	ILE	LEU	GLY	N95	K33
	GLU	ASP	SER	GLU	HIS	LEU	F96	D34
	THR	LEU	LEU	VAL	PHE	THR	L98	T35
	ALA	LYS	LEU	ASP	GLN	SER	R99	G36
	LYS	ASP	LEU	ALA	ALA	LYS	ASP	N37
	CYS	VAL	ALA	ASN	LEU	ARG	S100	D38
	GLN	GLY	LEU	GLU	ASP	SER	T101	P39
	THR	THR	TYR	ILE	ILE	PHE	L102	I40
	SER	LEU	PRO	ILE	TYR	VAL	D103	T41
	ASP	ALA	GLY	ASP	MET	ALA	ARG	N42
	THR	PRO	ILE	THR	TYR	GLY	LYS	E43
	PHE	THR	LEU	GLY	HIS	THR	L105	P44
	THR	TYR	LEU	ILE	THR	ILE	T106	L45
	ASP	THR	ASP	ASP	ASN	THR	K107	S46
	ASP	ILE	VAL	GLU	GLU	THR	L108	E48
	MET	PRO	VAL	THR	PRO	PRO	L109	E49
	ASP	GLU	ASN	ASN	ASN	LYS	S110	M13
	VAL	PHE	LEU	THR	PRO	TRP	T111	I50
	VAL	LYS	SER	GLU	ARG	ILE	V112	Y51
						LEU	M113	E115
							Y114	R116
							E115	D117
							R116	A118
							D117	A119
							A118	K120

- Molecule 36: Pre-mRNA-splicing factor SYF2



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	48617	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 ($e^-/\text{\AA}^2$)	47	Depositor
Minimum defocus (nm)	200	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.174	Depositor
Minimum map value	-0.094	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size (Å)	537.6, 537.6, 537.6	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.12, 1.12, 1.12	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: IHP, GTP, MG, 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 > 5$	RMSZ	# $ Z > 5$
1	2	0.35	0/3190	0.64	0/4946
2	5	0.25	0/4049	0.48	1/6300 (0.0%)
3	6	0.27	0/2427	0.47	0/3778
4	A	0.32	0/16452	0.57	0/22294
5	C	0.31	0/7147	0.57	0/9673
6	D	0.17	0/577	0.36	0/787
7	E	0.35	0/651	0.68	0/1008
8	H	0.39	0/2716	1.05	2/3702 (0.1%)
9	I	0.24	0/895	0.50	2/1384 (0.1%)
10	J	0.35	0/2750	0.57	2/3735 (0.1%)
11	K	0.26	0/1375	0.53	0/1854
12	L	0.27	0/1307	0.50	0/1748
13	M	0.26	0/2094	0.51	0/2815
14	N	0.25	0/1945	0.55	0/2617
15	O	0.47	0/2378	0.86	6/3212 (0.2%)
16	P	0.24	0/616	0.47	0/822
17	R	0.43	0/423	1.13	0/577
18	S	0.35	0/3221	0.97	1/4379 (0.0%)
19	T	0.48	1/2918 (0.0%)	1.32	6/4015 (0.1%)
20	V	0.83	2/5157 (0.0%)	1.62	49/6973 (0.7%)
21	W	0.36	0/1228	0.91	2/1663 (0.1%)
23	Y	0.27	0/713	0.71	1/952 (0.1%)
24	a	0.25	0/1400	0.57	0/1897
25	b	0.21	0/636	0.54	0/856
25	k	0.32	0/567	0.68	0/762
26	c	0.25	0/1737	0.60	0/2315
27	d	0.20	0/634	0.54	0/859
27	n	0.28	0/641	0.64	0/868
28	e	0.22	0/585	0.55	0/795
28	p	0.28	0/612	0.61	0/830
29	f	0.25	0/585	0.65	2/791 (0.3%)
29	q	0.32	0/597	0.73	0/807

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	g	0.19	0/532	0.56	0/715
30	r	0.30	0/582	0.71	0/785
31	h	0.19	0/649	0.51	0/880
31	l	0.32	0/685	0.96	8/926 (0.9%)
32	j	0.20	0/753	0.57	0/1013
32	m	0.31	0/764	0.78	2/1026 (0.2%)
33	o	0.25	0/2671	0.57	0/3605
34	s	0.98	1/546 (0.2%)	1.45	11/760 (1.4%)
35	t	0.79	0/581	1.30	2/809 (0.2%)
35	u	0.96	1/576 (0.2%)	1.34	3/802 (0.4%)
35	v	1.02	2/586 (0.3%)	1.56	7/816 (0.9%)
35	w	0.78	0/566	1.25	3/788 (0.4%)
36	y	0.24	0/721	0.49	0/954
All	All	0.40	7/82435 (0.0%)	0.80	110/113893 (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
14	N	0	1
18	S	0	1
20	V	0	23
21	W	0	3
22	X	0	3
26	c	0	2
30	r	0	1
34	s	0	2
35	t	0	1
35	v	0	1
35	w	0	1
All	All	0	39

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	493	ILE	CA-CB	8.29	1.63	1.54
35	v	109	LEU	C-N	7.98	1.44	1.33
19	T	612	ILE	C-N	5.78	1.41	1.34
35	v	134	SER	C-O	-5.66	1.17	1.24
34	s	133	PRO	CA-C	5.64	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	V	563	THR	N-CA	5.14	1.52	1.46
35	u	77	ILE	C-N	5.08	1.40	1.33

All (110) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	V	493	ILE	N-CA-CB	19.36	131.72	110.62
20	V	493	ILE	CB-CA-C	-15.33	92.65	111.81
8	H	87	ILE	CA-C-N	14.34	134.48	118.85
8	H	87	ILE	C-N-CA	14.34	134.48	118.85
35	v	134	SER	CA-C-O	-11.55	108.17	120.42
20	V	833	ASN	O-C-N	10.76	135.75	123.27
35	v	137	LEU	CA-C-N	10.19	130.36	119.05
35	v	137	LEU	C-N-CA	10.19	130.36	119.05
34	s	132	LEU	CA-C-N	10.07	132.42	119.84
34	s	132	LEU	C-N-CA	10.07	132.42	119.84
15	O	551	ALA	N-CA-C	9.91	122.16	111.36
20	V	512	LYS	N-CA-C	9.06	121.15	111.28
35	u	137	LEU	CA-C-N	8.98	128.71	119.19
35	u	137	LEU	C-N-CA	8.98	128.71	119.19
20	V	493	ILE	N-CA-C	-8.96	101.61	110.30
20	V	493	ILE	CA-CB-CG1	8.81	125.37	110.40
20	V	833	ASN	CA-C-N	-8.67	106.10	121.70
20	V	833	ASN	C-N-CA	-8.67	106.10	121.70
20	V	975	TYR	N-CA-C	8.47	120.97	108.60
35	v	110	SER	N-CA-C	8.45	120.49	111.28
35	t	137	LEU	CA-C-N	8.23	127.82	118.85
35	t	137	LEU	C-N-CA	8.23	127.82	118.85
20	V	894	LEU	CB-CA-C	-7.96	98.38	110.88
34	s	135	THR	CA-C-O	-7.84	112.16	120.55
35	v	134	SER	O-C-N	7.72	130.96	122.15
15	O	541	CYS	N-CA-C	7.72	119.48	111.14
20	V	522	GLU	CB-CG-CD	7.67	125.64	112.60
20	V	750	SER	N-CA-C	7.67	118.69	107.88
19	T	612	ILE	CA-C-N	-7.54	111.20	119.19
19	T	612	ILE	C-N-CA	-7.54	111.20	119.19
20	V	477	SER	N-CA-CB	-7.44	97.91	110.49
20	V	559	ASP	CA-CB-CG	7.39	120.00	112.60
31	l	47	LEU	CA-C-N	7.28	128.94	119.84
31	l	47	LEU	C-N-CA	7.28	128.94	119.84
19	T	602	MET	N-CA-C	7.28	119.21	111.28
31	l	43	VAL	N-CA-C	7.12	118.08	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	T	612	ILE	CA-C-O	-6.95	114.03	118.69
18	S	420	VAL	O-C-N	6.91	124.84	120.42
20	V	616	PHE	CA-CB-CG	6.84	120.64	113.80
35	u	134	SER	CA-C-O	-6.84	112.11	119.97
20	V	746	THR	CA-C-N	6.73	128.25	119.84
20	V	746	THR	C-N-CA	6.73	128.25	119.84
19	T	611	THR	N-CA-C	-6.69	103.99	111.28
15	O	531	GLN	CA-C-N	6.66	128.16	119.84
15	O	531	GLN	C-N-CA	6.66	128.16	119.84
20	V	729	PRO	CA-C-N	6.61	132.06	121.95
20	V	729	PRO	C-N-CA	6.61	132.06	121.95
35	w	39	PRO	N-CA-CB	6.58	110.50	103.39
20	V	591	ASP	CA-CB-CG	6.47	119.07	112.60
19	T	304	PHE	N-CA-C	-6.30	104.41	111.28
9	I	91	A	P-O3'-C3'	6.27	129.60	120.20
20	V	1017	ASP	CA-CB-CG	6.13	118.73	112.60
35	w	137	LEU	CA-C-N	6.12	125.68	119.19
35	w	137	LEU	C-N-CA	6.12	125.68	119.19
23	Y	68	GLN	N-CA-C	-6.04	104.08	112.30
20	V	506	GLY	CA-C-N	6.03	133.06	121.54
20	V	506	GLY	C-N-CA	6.03	133.06	121.54
31	l	51	ARG	N-CA-C	-5.85	103.16	111.24
31	l	49	GLN	CA-C-N	5.84	127.14	119.84
31	l	49	GLN	C-N-CA	5.84	127.14	119.84
15	O	542	SER	N-CA-C	5.83	117.43	111.14
32	m	66	ASN	N-CA-C	-5.83	101.66	110.28
10	J	161	ASP	CA-C-N	5.79	132.60	121.54
10	J	161	ASP	C-N-CA	5.79	132.60	121.54
20	V	640	SER	N-CA-C	5.79	119.44	112.38
20	V	781	ASN	CA-CB-CG	5.77	118.37	112.60
34	s	132	LEU	N-CA-C	5.75	122.53	109.81
34	s	159	ILE	CA-C-O	5.70	127.38	121.05
20	V	506	GLY	O-C-N	5.69	130.09	122.70
20	V	894	LEU	N-CA-CB	5.68	118.25	110.01
15	O	568	GLN	N-CA-C	-5.66	105.11	111.28
20	V	496	VAL	CA-C-N	5.66	127.80	120.44
20	V	496	VAL	C-N-CA	5.66	127.80	120.44
20	V	562	TYR	CA-C-N	5.66	132.34	121.54
20	V	562	TYR	C-N-CA	5.66	132.34	121.54
20	V	787	ALA	N-CA-C	-5.63	108.21	114.62
34	s	117	VAL	CA-C-O	5.63	124.02	119.29
34	s	135	THR	O-C-N	5.62	128.97	122.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	V	1021	ILE	CA-C-N	5.60	127.72	120.44
20	V	1021	ILE	C-N-CA	5.60	127.72	120.44
32	m	96	LEU	N-CA-C	5.58	117.49	108.34
34	s	132	LEU	CA-C-O	5.57	127.80	120.16
31	l	97	LEU	CA-C-N	5.51	125.44	119.76
31	l	97	LEU	C-N-CA	5.51	125.44	119.76
20	V	651	PRO	CA-C-N	5.45	130.64	122.58
20	V	651	PRO	C-N-CA	5.45	130.64	122.58
20	V	883	GLN	OE1-CD-NE2	-5.39	117.21	122.60
20	V	856	ASN	CA-CB-CG	-5.38	107.22	112.60
21	W	52	LYS	N-CA-C	5.35	121.64	109.81
20	V	680	ASP	CA-CB-CG	-5.32	107.28	112.60
20	V	936	PHE	CA-CB-CG	5.28	119.08	113.80
20	V	983	ASN	CA-CB-CG	5.25	117.84	112.60
20	V	639	ASN	N-CA-C	5.22	121.92	110.80
34	s	134	GLN	N-CA-C	-5.20	104.87	111.11
20	V	535	GLN	OE1-CD-NE2	-5.17	117.43	122.60
20	V	730	VAL	CB-CA-C	-5.14	103.88	111.80
20	V	573	ASP	N-CA-C	-5.14	108.03	114.56
20	V	1025	PHE	CA-CB-CG	-5.14	108.66	113.80
20	V	1054	HIS	CB-CG-CD2	-5.13	124.52	131.20
20	V	538	ARG	NE-CZ-NH2	5.11	123.79	119.20
2	5	174	G	P-O3'-C3'	5.10	127.86	120.20
9	I	91	A	C2'-C3'-O3'	5.10	117.15	109.50
20	V	715	VAL	CA-C-O	-5.09	115.45	120.85
34	s	110	GLU	N-CA-C	5.09	117.81	110.28
35	v	109	LEU	CA-C-N	5.07	127.08	120.28
35	v	109	LEU	C-N-CA	5.07	127.08	120.28
21	W	55	HIS	N-CA-C	-5.04	107.81	114.31
29	f	23	VAL	CA-C-N	5.04	129.56	122.46
29	f	23	VAL	C-N-CA	5.04	129.56	122.46
34	s	111	VAL	N-CA-C	5.04	119.81	109.34

There are no chirality outliers.

All (39) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
14	N	208	TYR	Peptide
18	S	212	HIS	Peptide
20	V	1027	SER	Peptide
20	V	1064	TYR	Peptide
20	V	1080	MET	Peptide

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Mol	Chain	Res	Type	Group
20	V	1100	LYS	Peptide
20	V	489	ARG	Sidechain
20	V	493	ILE	Peptide
20	V	497	ARG	Sidechain
20	V	506	GLY	Peptide
20	V	526	SER	Peptide
20	V	537	ARG	Sidechain
20	V	562	TYR	Peptide
20	V	575	ARG	Sidechain
20	V	672	MET	Peptide
20	V	729	PRO	Peptide
20	V	746	THR	Peptide
20	V	749	GLY	Peptide
20	V	770	TYR	Sidechain
20	V	818	TYR	Sidechain
20	V	861	PHE	Peptide
20	V	880	TYR	Sidechain
20	V	933	GLN	Peptide
20	V	957	TYR	Sidechain
20	V	975	TYR	Sidechain
21	W	93	LEU	Peptide
21	W	94	LEU	Peptide
21	W	95	PRO	Peptide
22	X	25	UNK	Mainchain
22	X	26	UNK	Mainchain
22	X	27	UNK	Mainchain
26	c	88	ASP	Peptide
26	c	98	GLY	Peptide
30	r	50	ASP	Peptide
34	s	111	VAL	Peptide
34	s	132	LEU	Peptide
35	t	3	CYS	Mainchain
35	v	109	LEU	Mainchain
35	w	134	SER	Mainchain

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	2	2868	0	1455	90	0
2	5	3626	0	1834	56	0
3	6	2170	0	1095	41	0
4	A	16046	0	16046	391	0
5	C	6999	0	7168	187	0
6	D	579	0	376	8	0
7	E	586	0	294	73	0
8	H	2689	0	2087	26	0
9	I	804	0	404	14	0
10	J	2691	0	2690	92	0
11	K	1355	0	1383	30	0
12	L	1283	0	1301	23	0
13	M	2048	0	2011	44	0
14	N	1917	0	1974	49	0
15	O	2350	0	2134	52	0
16	P	600	0	589	17	0
17	R	423	0	286	24	0
18	S	3189	0	2485	85	0
19	T	2957	0	1259	26	0
20	V	5059	0	5064	226	0
21	W	1211	0	1230	189	0
22	X	475	0	106	20	0
23	Y	704	0	735	107	0
24	a	1372	0	1413	18	0
25	b	631	0	670	19	0
25	k	563	0	600	76	0
26	c	1709	0	1681	39	0
27	d	625	0	647	16	0
27	n	632	0	653	27	0
28	e	575	0	597	15	0
28	p	602	0	631	12	0
29	f	573	0	572	19	0
29	q	585	0	587	15	0
30	g	529	0	557	10	0
30	r	577	0	595	16	0
31	h	644	0	686	14	0
31	l	679	0	732	133	0
32	j	741	0	778	23	0
32	m	752	0	786	43	0
33	o	2599	0	2553	70	0
34	s	548	0	219	10	0
35	t	583	0	249	2	0
35	u	578	0	246	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	v	588	0	250	5	0
35	w	568	0	242	1	0
36	y	719	0	750	11	0
37	6	1	0	0	0	0
38	A	36	0	6	2	0
39	C	32	0	12	3	0
40	L	3	0	0	0	0
40	M	1	0	0	0	0
40	N	2	0	0	0	0
40	c	1	0	0	0	0
All	All	80677	0	70718	1898	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 13.

All (1898) 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)
20:V:621:LYS:HE2	20:V:861:PHE:CE1	1.29	1.64
19:T:589:GLU:CB	22:X:216:UNK:CB	1.77	1.63
21:W:15:TYR:CZ	25:k:19:LYS:CE	1.81	1.57
21:W:50:LEU:HD12	21:W:73:ARG:CZ	1.31	1.56
21:W:35:GLN:HE22	23:Y:57:GLU:CG	1.11	1.55
20:V:566:PHE:CE2	20:V:996:VAL:HG23	1.41	1.53
25:k:29:VAL:HG21	31:l:67:LEU:CB	1.36	1.51
4:A:1592:HIS:CE1	7:E:3:A:H5'	1.41	1.51
31:l:70:GLY:CA	31:l:80:ALA:CB	1.89	1.50
20:V:785:ALA:CA	20:V:871:LEU:HD11	1.26	1.50
25:k:23:LEU:HD13	31:l:67:LEU:CD2	1.04	1.48
21:W:35:GLN:HE22	23:Y:57:GLU:CB	1.25	1.47
20:V:646:TYR:CE1	20:V:864:MET:HB2	1.49	1.47
20:V:566:PHE:CD1	20:V:999:GLN:HB3	1.50	1.45
4:A:928:ARG:NH1	7:E:4:U:H5'	1.18	1.44
31:l:70:GLY:HA2	31:l:80:ALA:CB	1.44	1.43
21:W:156:PHE:CE2	23:Y:51:LEU:HB2	1.54	1.41
20:V:646:TYR:CD1	20:V:864:MET:HB2	1.52	1.40
31:l:70:GLY:CA	31:l:80:ALA:HB1	1.47	1.40
25:k:23:LEU:CD1	31:l:67:LEU:CD2	1.99	1.39
21:W:50:LEU:CD1	21:W:73:ARG:NH2	1.86	1.39
20:V:785:ALA:HA	20:V:871:LEU:CD1	1.50	1.38
21:W:35:GLN:NE2	23:Y:57:GLU:HG2	1.30	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:1165:C:H4'	21:W:118:ARG:NH1	1.35	1.38
4:A:1592:HIS:CE1	7:E:3:A:C5'	2.05	1.38
21:W:35:GLN:NE2	23:Y:57:GLU:CG	1.79	1.38
21:W:50:LEU:HD13	21:W:73:ARG:NH2	1.37	1.35
20:V:646:TYR:CD1	20:V:864:MET:CB	2.11	1.32
20:V:566:PHE:CD1	20:V:999:GLN:CB	2.13	1.31
20:V:646:TYR:CE1	20:V:864:MET:CB	2.11	1.31
1:2:1107:C:N3	23:Y:31:TYR:CE1	1.72	1.30
20:V:586:ARG:CZ	20:V:902:PRO:HA	1.62	1.30
20:V:507:GLU:OE1	20:V:658:LYS:N	1.60	1.29
20:V:646:TYR:CE1	20:V:864:MET:CA	2.16	1.29
21:W:141:ARG:NH2	21:W:157:GLN:NE2	1.79	1.29
18:S:251:ALA:HA	18:S:263:SER:CB	1.62	1.28
21:W:15:TYR:CZ	25:k:19:LYS:HE3	1.47	1.28
20:V:785:ALA:O	20:V:870:ASN:ND2	1.65	1.27
21:W:50:LEU:CD1	21:W:73:ARG:CZ	2.12	1.26
21:W:15:TYR:OH	25:k:19:LYS:CE	1.71	1.26
18:S:467:GLN:CA	18:S:471:LEU:HA	1.65	1.26
31:l:64:SER:O	31:l:67:LEU:HG	1.12	1.26
20:V:621:LYS:CE	20:V:861:PHE:CE1	2.18	1.25
31:l:27:GLY:HA3	31:l:43:VAL:CG2	1.66	1.25
18:S:346:ILE:CA	18:S:366:LEU:CB	2.15	1.24
32:m:46:ILE:CD1	32:m:67:MET:HE1	1.67	1.24
21:W:141:ARG:NH2	21:W:157:GLN:HE21	1.35	1.24
21:W:156:PHE:CE2	23:Y:51:LEU:HD13	1.71	1.24
21:W:15:TYR:CE1	25:k:19:LYS:HE3	1.73	1.22
4:A:928:ARG:HH12	7:E:4:U:C5'	1.52	1.22
6:D:129:THR:CB	20:V:824:SER:HB3	1.68	1.22
20:V:610:VAL:N	20:V:837:GLU:OE1	1.70	1.21
25:k:23:LEU:HD13	31:l:67:LEU:HD23	1.21	1.21
21:W:35:GLN:NE2	23:Y:57:GLU:CB	1.93	1.20
25:k:29:VAL:CG2	31:l:67:LEU:CB	2.19	1.20
4:A:928:ARG:NH1	7:E:4:U:C5'	2.02	1.20
32:m:26:PHE:CZ	32:m:61:PHE:CE1	2.28	1.20
15:O:550:PRO:O	15:O:554:GLU:O	1.59	1.19
18:S:346:ILE:CB	18:S:366:LEU:CB	2.21	1.18
19:T:461:ASN:O	19:T:463:ILE:CB	1.90	1.18
7:E:16:A:OP2	20:V:1073:VAL:HG13	1.42	1.18
21:W:14:TYR:OH	23:Y:57:GLU:CD	1.86	1.18
5:C:763:ARG:HH22	17:R:82:ASP:N	1.40	1.17
20:V:785:ALA:CA	20:V:871:LEU:CD1	2.00	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:444:GLY:HA2	19:T:483:ASP:CB	1.76	1.15
31:l:70:GLY:CA	31:l:80:ALA:HB2	1.65	1.15
1:2:1165:C:C4'	21:W:118:ARG:HH22	1.58	1.15
31:l:49:GLN:HB3	31:l:50:PRO:CD	1.75	1.15
21:W:15:TYR:CZ	25:k:19:LYS:HE2	1.52	1.15
1:2:1150:U:O2'	27:n:53:GLN:HG2	1.43	1.14
7:E:15:C:H5''	20:V:1075:THR:HB	1.22	1.14
21:W:156:PHE:HE2	23:Y:51:LEU:CB	1.62	1.13
7:E:15:C:H5''	20:V:1075:THR:CB	1.78	1.13
21:W:14:TYR:OH	23:Y:57:GLU:CG	1.96	1.12
31:l:70:GLY:HA3	31:l:80:ALA:CB	1.63	1.12
1:2:1165:C:C4'	21:W:118:ARG:HH12	1.61	1.11
25:k:23:LEU:HD13	31:l:67:LEU:HD21	1.20	1.11
25:k:29:VAL:HG21	31:l:67:LEU:HB3	1.18	1.11
31:l:49:GLN:CB	31:l:50:PRO:HD2	1.77	1.11
1:2:1165:C:H4'	21:W:118:ARG:CZ	1.81	1.11
21:W:156:PHE:CE2	23:Y:51:LEU:CB	2.32	1.11
25:k:29:VAL:CG2	31:l:67:LEU:HB2	1.76	1.11
31:l:27:GLY:CA	31:l:43:VAL:HG22	1.80	1.10
21:W:78:THR:CG2	23:Y:50:LEU:HD21	1.81	1.10
31:l:64:SER:HA	31:l:67:LEU:HD23	1.11	1.10
1:2:1107:C:C4'	23:Y:68:GLN:NE2	2.15	1.10
18:S:346:ILE:C	18:S:366:LEU:CB	2.25	1.10
3:6:29:U:OP2	14:N:51:ARG:NH1	1.83	1.10
20:V:566:PHE:CD2	20:V:996:VAL:HG23	1.87	1.10
5:C:763:ARG:HH22	17:R:82:ASP:CA	1.64	1.10
5:C:763:ARG:NH1	17:R:78:SER:O	1.82	1.10
21:W:15:TYR:CE2	25:k:19:LYS:HE2	1.87	1.09
20:V:566:PHE:CE2	20:V:996:VAL:CG2	2.34	1.09
1:2:1098:C:OP1	23:Y:43:ARG:HD2	1.52	1.09
21:W:153:THR:CG2	23:Y:43:ARG:HH21	1.65	1.09
20:V:566:PHE:HA	20:V:999:GLN:HG3	1.26	1.08
1:2:1166:G:H4'	21:W:119:ARG:HD3	1.09	1.08
1:2:1166:G:H4'	21:W:119:ARG:CD	1.84	1.07
31:l:64:SER:O	31:l:67:LEU:CG	2.01	1.07
32:m:46:ILE:HD13	32:m:67:MET:HE1	1.36	1.07
4:A:1592:HIS:HE1	7:E:3:A:C5'	1.49	1.07
31:l:7:LEU:HD11	32:m:95:PHE:CE2	1.90	1.07
25:k:29:VAL:HG22	31:l:67:LEU:HD22	1.30	1.07
20:V:566:PHE:CE1	20:V:999:GLN:HB3	1.90	1.06
21:W:37:GLU:OE2	23:Y:56:GLY:HA2	1.56	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:l:49:GLN:CB	31:l:50:PRO:CD	2.33	1.06
5:C:763:ARG:NH2	17:R:82:ASP:CA	2.18	1.05
18:S:251:ALA:CA	18:S:263:SER:CB	2.35	1.05
1:2:1107:C:N3	23:Y:31:TYR:HE1	0.94	1.05
20:V:586:ARG:HD3	20:V:902:PRO:HG3	1.35	1.05
5:C:883:ARG:NH1	5:C:917:ASP:OD2	1.88	1.04
15:O:566:TYR:O	15:O:569:GLU:CB	2.04	1.04
20:V:646:TYR:CE1	20:V:864:MET:N	2.25	1.04
25:k:23:LEU:HD13	31:l:67:LEU:HD22	1.08	1.04
5:C:760:LEU:HD13	17:R:74:GLU:CB	1.55	1.04
21:W:78:THR:HG21	23:Y:50:LEU:HD21	1.38	1.03
20:V:618:LEU:HD13	20:V:853:MET:SD	1.96	1.03
4:A:992:ASP:OD2	4:A:1085:LYS:NZ	1.91	1.03
7:E:16:A:OP2	20:V:1073:VAL:CG1	2.05	1.03
18:S:467:GLN:HA	18:S:471:LEU:HA	1.03	1.02
32:m:46:ILE:HD11	32:m:67:MET:HE1	1.36	1.02
18:S:467:GLN:CB	18:S:471:LEU:O	2.07	1.02
1:2:1107:C:C5'	23:Y:68:GLN:NE2	2.23	1.01
1:2:1165:C:C4'	21:W:118:ARG:NH2	2.23	1.01
13:M:5:ARG:NH1	13:M:97:GLU:OE2	1.94	1.01
21:W:35:GLN:NE2	23:Y:57:GLU:HB2	1.68	1.01
21:W:156:PHE:CE2	23:Y:51:LEU:CD1	2.43	1.01
25:k:29:VAL:HG21	31:l:67:LEU:HB2	1.03	1.01
1:2:1107:C:C4'	23:Y:68:GLN:HE22	1.70	1.01
31:l:49:GLN:HB2	31:l:50:PRO:HD2	1.41	1.00
32:m:26:PHE:CZ	32:m:61:PHE:CD1	2.48	1.00
1:2:1107:C:H4'	23:Y:68:GLN:NE2	1.41	1.00
20:V:621:LYS:HE2	20:V:861:PHE:CD1	1.96	1.00
20:V:642:LYS:CD	20:V:832:GLU:OE1	1.98	0.99
21:W:153:THR:CG2	23:Y:43:ARG:NH2	2.25	0.99
21:W:142:GLU:O	21:W:146:ARG:HG2	1.63	0.99
18:S:467:GLN:CA	18:S:471:LEU:CA	2.37	0.98
25:k:29:VAL:CG2	31:l:67:LEU:HB3	1.90	0.98
7:E:15:C:C5'	20:V:1075:THR:HG21	1.94	0.98
18:S:346:ILE:O	18:S:366:LEU:CB	2.11	0.98
20:V:646:TYR:CZ	20:V:864:MET:HB2	1.99	0.98
21:W:84:ASN:O	21:W:86:ILE:N	1.96	0.98
4:A:1592:HIS:CE1	7:E:3:A:H5''	1.96	0.97
20:V:646:TYR:CD1	20:V:864:MET:CG	2.47	0.97
25:k:23:LEU:CD1	31:l:67:LEU:HD21	1.81	0.97
23:Y:75:THR:OG1	23:Y:108:THR:HG21	1.64	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:467:GLN:HA	18:S:471:LEU:CA	1.90	0.97
32:m:41:ARG:HG2	32:m:41:ARG:HH21	1.30	0.97
1:2:1107:C:C5'	23:Y:68:GLN:HE22	1.77	0.97
21:W:156:PHE:CZ	23:Y:51:LEU:HB2	1.99	0.97
31:l:64:SER:HA	31:l:67:LEU:CD2	1.95	0.96
20:V:512:LYS:HA	20:V:516:ILE:HD13	1.44	0.96
21:W:15:TYR:OH	25:k:19:LYS:HE2	1.41	0.96
1:2:1150:U:HO2'	27:n:53:GLN:HG2	1.17	0.96
20:V:735:PRO:HG3	20:V:937:TYR:CE1	2.00	0.95
18:S:349:SER:O	18:S:362:ARG:CB	2.14	0.95
20:V:642:LYS:O	20:V:864:MET:CE	2.15	0.94
1:2:1166:G:C4'	21:W:119:ARG:HD3	1.96	0.94
20:V:566:PHE:CA	20:V:999:GLN:HG3	1.97	0.94
21:W:33:ASP:HB2	21:W:56:ILE:HB	1.47	0.94
21:W:35:GLN:HE22	23:Y:57:GLU:HB2	1.24	0.94
25:k:23:LEU:HD22	31:l:67:LEU:HD21	1.48	0.94
32:m:26:PHE:HZ	32:m:61:PHE:CD1	1.85	0.94
1:2:1165:C:C1'	21:W:118:ARG:NH2	2.31	0.94
20:V:507:GLU:OE2	20:V:659:THR:HG22	1.66	0.94
18:S:346:ILE:HA	18:S:366:LEU:CB	1.96	0.94
21:W:35:GLN:HE21	23:Y:57:GLU:HG2	1.18	0.93
20:V:646:TYR:CE1	20:V:864:MET:HA	2.02	0.93
35:t:20:ARG:CB	35:u:52:GLU:O	2.16	0.93
20:V:646:TYR:CG	20:V:864:MET:HB2	2.05	0.92
31:l:68:THR:HB	31:l:82:LEU:HD21	1.51	0.92
31:l:27:GLY:HA3	31:l:43:VAL:HG22	0.94	0.92
19:T:495:GLU:CB	19:T:504:ALA:HB2	2.00	0.92
25:k:29:VAL:HG22	31:l:67:LEU:CD2	1.98	0.92
25:k:23:LEU:CD2	31:l:67:LEU:HD21	1.99	0.92
1:2:1165:C:O4'	21:W:118:ARG:NH2	2.02	0.91
20:V:566:PHE:HE2	20:V:996:VAL:HG23	1.25	0.91
10:J:306:HIS:HB3	10:J:332:ARG:HH11	1.35	0.91
21:W:156:PHE:CZ	23:Y:51:LEU:HD13	2.06	0.90
31:l:7:LEU:CD1	32:m:95:PHE:CE2	2.54	0.90
1:2:1165:C:C4'	21:W:118:ARG:NH1	2.25	0.90
4:A:928:ARG:HH11	7:E:4:U:H5'	1.11	0.90
20:V:642:LYS:O	20:V:864:MET:HE1	1.71	0.90
34:s:114:LEU:O	34:s:118:ASP:N	2.04	0.90
32:m:46:ILE:CD1	32:m:67:MET:CE	2.49	0.90
32:m:46:ILE:HD11	32:m:67:MET:CE	2.02	0.90
21:W:14:TYR:OH	23:Y:57:GLU:HG2	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:621:LYS:HE2	20:V:861:PHE:HE1	1.22	0.89
21:W:156:PHE:HD2	23:Y:94:PHE:CD1	1.90	0.89
33:o:256:ARG:NH1	33:o:322:ASN:OD1	2.05	0.89
20:V:735:PRO:CG	20:V:937:TYR:CE1	2.56	0.89
21:W:50:LEU:HD12	21:W:73:ARG:NH1	1.86	0.89
20:V:791:GLN:HB2	20:V:1074:LEU:HD22	1.55	0.89
20:V:783:TYR:HE2	20:V:871:LEU:CD1	1.86	0.89
31:l:47:LEU:HB2	31:l:65:LEU:CD1	2.03	0.89
18:S:467:GLN:CB	18:S:471:LEU:HA	2.03	0.89
20:V:646:TYR:CB	20:V:864:MET:SD	2.61	0.89
25:k:96:VAL:HG11	31:l:82:LEU:HD22	1.53	0.89
19:T:444:GLY:CA	19:T:483:ASP:CB	2.50	0.89
10:J:222:GLY:O	10:J:249:LYS:NZ	2.06	0.88
25:k:23:LEU:CG	31:l:67:LEU:HD21	2.03	0.88
1:2:1165:C:H4'	21:W:118:ARG:NH2	1.87	0.88
18:S:332:GLU:CB	18:S:338:ILE:CB	2.51	0.88
21:W:153:THR:HG22	23:Y:43:ARG:NH2	1.87	0.88
20:V:586:ARG:CZ	20:V:902:PRO:CA	2.48	0.88
20:V:586:ARG:NH1	20:V:902:PRO:HA	1.88	0.88
23:Y:109:LYS:O	23:Y:110:THR:O	1.92	0.88
18:S:346:ILE:CB	18:S:366:LEU:CA	2.52	0.88
5:C:964:ARG:HH12	5:C:985:ASP:HB3	1.39	0.87
20:V:646:TYR:HE1	20:V:864:MET:CA	1.79	0.87
18:S:467:GLN:CB	18:S:471:LEU:CA	2.52	0.87
20:V:586:ARG:CD	20:V:902:PRO:HG3	2.04	0.87
20:V:646:TYR:HB2	20:V:864:MET:SD	2.14	0.87
21:W:156:PHE:CE2	23:Y:51:LEU:CG	2.58	0.87
21:W:156:PHE:HE2	23:Y:51:LEU:CG	1.87	0.87
31:l:64:SER:CA	31:l:67:LEU:HD23	2.01	0.87
20:V:642:LYS:C	20:V:864:MET:HE1	1.99	0.87
1:2:1107:C:C2	23:Y:31:TYR:HE1	1.91	0.87
21:W:35:GLN:CD	23:Y:57:GLU:HB2	1.99	0.87
1:2:1107:C:H4'	23:Y:68:GLN:HE22	1.20	0.87
20:V:783:TYR:CE2	20:V:871:LEU:HG	2.10	0.86
20:V:783:TYR:HE2	20:V:871:LEU:HG	1.40	0.86
7:E:15:C:C4'	20:V:1075:THR:HG21	2.04	0.86
4:A:896:SER:OG	4:A:1006:ARG:NH1	2.09	0.86
31:l:7:LEU:HD11	32:m:95:PHE:CZ	2.09	0.86
4:A:1156:HIS:O	4:A:1159:ARG:NH1	2.09	0.86
21:W:15:TYR:CE2	25:k:19:LYS:CE	2.52	0.86
21:W:58:ASP:OD2	23:Y:57:GLU:OE1	1.94	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:5:50:G:H1	2:5:65:U:H3	1.19	0.85
5:C:763:ARG:NH2	17:R:82:ASP:CB	2.38	0.85
5:C:763:ARG:NH2	17:R:82:ASP:HA	1.89	0.85
1:2:1165:C:O2'	21:W:118:ARG:CZ	2.23	0.85
21:W:15:TYR:OH	25:k:19:LYS:HE3	1.51	0.85
25:k:15:LEU:HD11	31:l:84:TYR:CZ	2.12	0.85
4:A:1521:ARG:HG3	7:E:5:C:C1'	2.07	0.85
20:V:566:PHE:CD1	20:V:999:GLN:CG	2.59	0.84
34:s:99:ASP:CB	35:v:81:LEU:HA	2.07	0.84
25:k:96:VAL:HG12	31:l:85:ILE:HG12	1.60	0.84
1:2:1098:C:OP1	23:Y:43:ARG:CD	2.24	0.84
7:E:15:C:C5'	20:V:1075:THR:CG2	2.55	0.84
31:l:67:LEU:HD12	31:l:68:THR:N	1.91	0.84
5:C:452:LYS:HZ2	5:C:487:ARG:NH1	1.75	0.84
20:V:566:PHE:HD1	20:V:999:GLN:CG	1.89	0.84
10:J:111:ILE:HG12	10:J:114:ARG:HH11	1.42	0.84
21:W:50:LEU:HB2	21:W:73:ARG:HH12	1.43	0.84
20:V:783:TYR:HE2	20:V:871:LEU:CG	1.90	0.83
32:m:54:ILE:HG12	32:m:74:GLU:HG2	1.56	0.83
31:l:70:GLY:HA2	31:l:80:ALA:HB1	0.85	0.83
4:A:1053:THR:OG1	4:A:1167:ARG:NH1	2.12	0.83
13:M:114:ARG:NH2	13:M:193:GLU:OE2	2.12	0.83
5:C:972:ARG:NH1	5:C:981:PHE:O	2.11	0.82
4:A:928:ARG:HH12	7:E:4:U:C4'	1.91	0.82
20:V:618:LEU:HD22	20:V:853:MET:HE1	1.61	0.82
1:2:3:G:H1	3:6:102:U:H3	1.27	0.82
21:W:141:ARG:HH21	21:W:157:GLN:NE2	1.78	0.82
8:H:302:SER:O	8:H:312:LYS:NZ	2.11	0.82
21:W:84:ASN:C	21:W:86:ILE:H	1.87	0.82
1:2:1150:U:O2'	27:n:53:GLN:CG	2.25	0.81
4:A:902:PRO:O	4:A:955:LYS:NZ	2.14	0.81
4:A:1592:HIS:HE1	7:E:3:A:H5'	0.67	0.81
12:L:131:GLU:OE2	33:o:50:HIS:N	2.13	0.81
25:k:21:ARG:NH1	31:l:67:LEU:O	2.13	0.81
21:W:156:PHE:HE2	23:Y:51:LEU:HB2	1.02	0.81
31:l:70:GLY:HA3	31:l:80:ALA:HB2	1.33	0.81
4:A:1286:TRP:NE1	4:A:1348:GLU:OE2	2.13	0.81
20:V:642:LYS:HD2	20:V:832:GLU:OE1	1.78	0.81
1:2:1108:A:N6	23:Y:73:PHE:CE1	2.49	0.81
18:S:329:LEU:HA	18:S:338:ILE:CB	2.10	0.81
21:W:78:THR:HG23	23:Y:50:LEU:HD21	1.60	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:343:ASP:HB3	5:C:347:ARG:HH12	1.46	0.81
7:E:5:C:OP2	7:E:6:C:OP2	1.98	0.81
7:E:12:C:O2'	7:E:13:U:OP1	1.99	0.81
4:A:269:ASP:H	26:c:138:LYS:HZ3	1.25	0.81
13:M:46:ARG:HH12	13:M:222:LEU:HB2	1.45	0.81
21:W:78:THR:CG2	23:Y:50:LEU:CD2	2.57	0.81
4:A:928:ARG:HH12	7:E:4:U:H5'	1.00	0.80
4:A:1928:GLU:OE1	24:a:234:LYS:NZ	2.13	0.80
21:W:33:ASP:CB	21:W:56:ILE:HB	2.10	0.80
2:5:94:C:O2'	4:A:1378:LYS:NZ	2.14	0.80
1:2:1165:C:C1'	21:W:118:ARG:HH22	1.93	0.80
20:V:621:LYS:NZ	20:V:861:PHE:CZ	2.49	0.80
5:C:393:LYS:NZ	5:C:413:LEU:O	2.14	0.80
7:E:15:C:H3'	20:V:1075:THR:HG22	1.63	0.80
2:5:84:A:OP2	4:A:532:ASN:ND2	2.13	0.80
31:l:68:THR:C	31:l:70:GLY:H	1.88	0.80
4:A:1477:PHE:HZ	7:E:11:A:O3'	1.64	0.79
5:C:187:ARG:NH1	5:C:654:CYS:SG	2.56	0.79
5:C:146:LYS:NZ	39:C:2501:GTP:O2G	2.16	0.79
18:S:467:GLN:CB	18:S:471:LEU:C	2.56	0.79
4:A:1592:HIS:NE2	7:E:3:A:C5'	2.46	0.79
21:W:84:ASN:HB2	21:W:86:ILE:CD1	2.12	0.79
7:E:2:G:O2'	7:E:3:A:OP1	1.99	0.79
7:E:15:C:H4'	20:V:1075:THR:HG21	1.64	0.79
7:E:16:A:C2	20:V:933:GLN:NE2	2.49	0.79
20:V:791:GLN:CB	20:V:1074:LEU:HD22	2.13	0.79
1:2:1098:C:OP2	23:Y:40:ASN:ND2	2.15	0.78
1:2:1165:C:H4'	21:W:118:ARG:HH12	0.81	0.78
7:E:15:C:H5''	20:V:1075:THR:CG2	2.13	0.78
14:N:116:LYS:NZ	15:O:220:GLU:O	2.16	0.78
14:N:16:CYS:SG	14:N:74:CYS:HB3	2.22	0.78
20:V:646:TYR:CD1	20:V:864:MET:HG3	2.16	0.78
21:W:84:ASN:O	21:W:106:ASN:OD1	2.01	0.78
18:S:534:TYR:HA	18:S:551:PHE:CB	2.13	0.78
21:W:14:TYR:OH	23:Y:57:GLU:OE2	1.88	0.78
21:W:156:PHE:CZ	23:Y:51:LEU:CB	2.64	0.78
18:S:219:ARG:NH1	22:X:107:UNK:CA	2.46	0.78
25:k:23:LEU:HD11	31:l:64:SER:CB	2.14	0.78
31:l:67:LEU:CD1	31:l:68:THR:HG23	2.13	0.78
21:W:141:ARG:CZ	21:W:157:GLN:HE21	1.97	0.78
32:j:78:GLU:OE1	32:j:87:ARG:NH1	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:T:457:TYR:CB	19:T:466:ALA:HB2	2.13	0.78
4:A:414:ASP:OD1	26:c:123:ARG:NH1	2.16	0.77
31:l:60:ILE:HG22	31:l:61:ALA:N	1.98	0.77
4:A:941:GLU:CD	22:X:61:UNK:CB	2.58	0.77
16:P:10:GLU:OE2	18:S:62:ARG:NH1	2.16	0.77
20:V:791:GLN:HG3	20:V:1074:LEU:CB	2.15	0.77
21:W:156:PHE:CD2	23:Y:94:PHE:CD1	2.73	0.77
20:V:512:LYS:HD2	20:V:634:THR:HG22	1.66	0.77
20:V:646:TYR:HE1	20:V:864:MET:N	1.72	0.77
1:2:1166:G:H5'	21:W:119:ARG:HH11	1.49	0.77
20:V:512:LYS:HD2	20:V:634:THR:CG2	2.14	0.77
1:2:1098:C:P	23:Y:40:ASN:ND2	2.58	0.77
21:W:37:GLU:OE2	23:Y:56:GLY:CA	2.32	0.77
20:V:566:PHE:HA	20:V:999:GLN:CG	2.13	0.77
21:W:78:THR:HG21	23:Y:50:LEU:CD2	2.14	0.76
21:W:128:THR:HG21	21:W:156:PHE:HE1	1.48	0.76
4:A:923:TYR:OH	4:A:936:GLU:OE2	2.01	0.76
4:A:1592:HIS:NE2	7:E:3:A:H5''	2.01	0.76
21:W:50:LEU:HD13	21:W:73:ARG:HH22	1.45	0.76
31:l:49:GLN:HB3	31:l:50:PRO:HD3	1.66	0.76
4:A:1279:VAL:O	4:A:1299:LYS:NZ	2.18	0.76
20:V:642:LYS:O	20:V:864:MET:HE3	1.86	0.75
5:C:120:ARG:HH11	5:C:158:HIS:HE1	1.32	0.75
20:V:783:TYR:CE2	20:V:871:LEU:CD1	2.69	0.75
31:l:47:LEU:HB2	31:l:65:LEU:HD12	1.67	0.75
1:2:1107:C:C6	23:Y:71:GLN:OE1	2.39	0.75
1:2:1107:C:H5''	23:Y:68:GLN:CD	2.11	0.75
7:E:17:U:H5'	20:V:779:LYS:HD2	1.67	0.75
25:k:54:PRO:HB3	31:l:66:TYR:CE1	2.22	0.75
15:O:181:ARG:HH11	18:S:49:ARG:HH21	1.34	0.75
20:V:507:GLU:CD	20:V:658:LYS:N	2.44	0.74
1:2:1108:A:C5	23:Y:73:PHE:CZ	2.41	0.74
20:V:610:VAL:HG11	20:V:841:GLN:HE22	1.52	0.74
31:l:21:ASN:HB2	31:l:61:ALA:HB2	1.69	0.74
31:l:67:LEU:HD11	31:l:68:THR:HG23	1.68	0.74
4:A:1647:GLN:OE1	4:A:1650:ARG:NH1	2.20	0.74
21:W:156:PHE:CZ	23:Y:51:LEU:CD1	2.68	0.74
1:2:31:A:H8	22:X:68:UNK:CB	2.00	0.74
4:A:1477:PHE:CE2	7:E:11:A:H5''	2.21	0.74
7:E:15:C:C3'	20:V:1075:THR:HG22	2.17	0.74
18:S:219:ARG:NH1	22:X:107:UNK:CB	2.50	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:445:LYS:NZ	8:H:447:ASP:OD1	2.21	0.74
20:V:566:PHE:HD1	20:V:999:GLN:CB	1.93	0.74
20:V:566:PHE:CB	20:V:999:GLN:HG3	2.18	0.74
5:C:763:ARG:NH2	17:R:82:ASP:N	2.26	0.73
1:2:1167:U:H5'	21:W:92:ARG:NH2	2.03	0.73
3:6:31:G:O6	14:N:47:LYS:NZ	2.21	0.73
15:O:49:GLU:OE2	15:O:53:ASN:ND2	2.20	0.73
18:S:332:GLU:CB	18:S:335:PRO:HA	2.18	0.73
21:W:156:PHE:HZ	23:Y:51:LEU:HA	1.54	0.73
3:6:38:U:O2	13:M:196:LYS:NZ	2.20	0.72
10:J:150:VAL:O	10:J:409:LYS:NZ	2.22	0.72
20:V:646:TYR:CG	20:V:864:MET:SD	2.82	0.72
20:V:883:GLN:HE22	20:V:909:ARG:HH21	1.37	0.72
2:5:154:G:OP1	31:h:11:ARG:NH1	2.23	0.72
4:A:1747:ASP:OD2	4:A:1750:ARG:NH2	2.22	0.72
4:A:1910:LYS:HE3	4:A:1937:ARG:HH12	1.54	0.72
25:k:54:PRO:CB	31:l:66:TYR:CE1	2.72	0.72
31:l:68:THR:CB	31:l:82:LEU:HD21	2.19	0.72
2:5:102:C:OP1	4:A:675:HIS:NE2	2.22	0.72
7:E:15:C:C5'	20:V:1075:THR:CB	2.61	0.72
21:W:84:ASN:HB2	21:W:86:ILE:HD12	1.72	0.72
7:E:15:C:C4'	20:V:1075:THR:CG2	2.67	0.72
21:W:13:GLN:HG2	21:W:34:LEU:CD2	2.19	0.72
25:k:23:LEU:CD1	31:l:67:LEU:HD22	1.92	0.72
21:W:14:TYR:CE1	21:W:33:ASP:OD2	2.43	0.72
8:H:416:GLN:OE1	22:X:1:UNK:CB	2.38	0.72
20:V:676:GLU:OE1	22:X:26:UNK:O	2.08	0.72
3:6:70:U:OP2	4:A:737:ARG:NH1	2.20	0.71
20:V:566:PHE:CD2	20:V:996:VAL:CG2	2.65	0.71
35:v:20:ARG:CB	35:w:51:VAL:CB	2.68	0.71
7:E:10:U:O2'	7:E:11:A:O4'	2.07	0.71
20:V:1059:LEU:HA	20:V:1064:TYR:CE1	2.25	0.71
4:A:376:ARG:NE	5:C:910:GLU:OE2	2.19	0.71
21:W:156:PHE:HD2	23:Y:94:PHE:HD1	1.38	0.71
31:l:94:GLN:HB2	32:m:94:LEU:HD11	1.71	0.71
7:E:9:C:H4'	7:E:10:U:OP2	1.91	0.71
4:A:928:ARG:HH12	7:E:4:U:H4'	1.55	0.71
4:A:1904:ARG:NH1	4:A:1907:GLN:OE1	2.23	0.71
21:W:141:ARG:HH22	21:W:157:GLN:HE21	1.36	0.71
32:m:75:LEU:HD13	32:m:88:GLU:HB3	1.73	0.71
4:A:684:LYS:NZ	38:A:2500:IHP:O23	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:10:ASP:C	21:W:12:PRO:HD3	2.16	0.70
1:2:1107:C:C5'	23:Y:68:GLN:CD	2.50	0.70
6:D:129:THR:CB	20:V:824:SER:CB	2.60	0.70
7:E:6:C:O2'	7:E:7:A:OP2	2.07	0.70
18:S:219:ARG:NH1	22:X:107:UNK:N	2.40	0.70
4:A:617:ASN:O	4:A:621:LEU:HB2	1.90	0.70
4:A:1125:LEU:O	4:A:1233:ARG:NH1	2.25	0.70
10:J:194:HIS:O	16:P:40:ARG:NH1	2.24	0.70
18:S:534:TYR:CB	18:S:551:PHE:CB	2.69	0.70
32:m:80:LYS:HE2	32:m:85:ILE:HG23	1.74	0.70
20:V:610:VAL:HG23	20:V:837:GLU:HG2	1.74	0.70
5:C:208:ARG:NH1	5:C:440:THR:OG1	2.25	0.70
10:J:306:HIS:HB3	10:J:332:ARG:NH1	2.06	0.70
20:V:566:PHE:HE2	20:V:996:VAL:CG2	1.91	0.70
20:V:791:GLN:HG3	20:V:1074:LEU:HB2	1.74	0.70
31:l:60:ILE:O	31:l:61:ALA:C	2.35	0.70
7:E:2:G:H4'	7:E:3:A:OP2	1.91	0.69
20:V:646:TYR:CD1	20:V:864:MET:CA	2.64	0.69
1:2:31:A:C8	22:X:68:UNK:CB	2.75	0.69
13:M:46:ARG:NH1	13:M:221:LEU:O	2.24	0.69
18:S:106:ILE:HD13	18:S:122:MET:HE3	1.73	0.69
32:m:46:ILE:HD13	32:m:67:MET:CE	2.18	0.69
20:V:618:LEU:HD13	20:V:853:MET:CE	2.23	0.69
20:V:676:GLU:OE1	22:X:26:UNK:C	2.38	0.69
21:W:141:ARG:NH2	21:W:157:GLN:HE22	1.89	0.69
20:V:610:VAL:HG21	20:V:841:GLN:NE2	2.08	0.69
21:W:50:LEU:HD13	21:W:73:ARG:HH21	1.49	0.69
21:W:142:GLU:O	21:W:146:ARG:CG	2.40	0.69
32:m:26:PHE:CE2	32:m:61:PHE:CE1	2.79	0.69
4:A:1005:GLN:OE1	4:A:1506:ARG:NH1	2.24	0.69
7:E:18:G:H5'	20:V:732:SER:HB3	1.75	0.69
2:5:6:G:H1'	25:b:11:ARG:HH12	1.57	0.69
4:A:1477:PHE:CZ	7:E:11:A:H5''	2.27	0.69
4:A:2080:LYS:HZ2	4:A:2093:VAL:HG13	1.57	0.69
21:W:15:TYR:CE1	25:k:19:LYS:CE	2.49	0.69
21:W:128:THR:HG21	21:W:156:PHE:CE1	2.27	0.69
4:A:269:ASP:H	26:c:138:LYS:NZ	1.91	0.69
4:A:996:ASP:OD2	4:A:1511:ARG:NE	2.19	0.69
21:W:13:GLN:HG2	21:W:34:LEU:HD23	1.74	0.69
9:I:8:U:OP1	15:O:201:LYS:NZ	2.26	0.69
9:I:15:A:OP1	13:M:174:ARG:NH1	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:621:LYS:CE	20:V:861:PHE:CZ	2.77	0.68
31:l:64:SER:OG	31:l:67:LEU:HD21	1.93	0.68
5:C:307:ILE:HG13	5:C:349:TRP:HB3	1.74	0.68
5:C:918:LEU:HD12	5:C:928:CYS:HB2	1.76	0.68
12:L:104:CYS:SG	12:L:108:CYS:HB2	2.33	0.68
32:j:102:ILE:HG22	32:j:103:VAL:HG23	1.75	0.68
4:A:1406:LEU:N	8:H:308:GLU:OE2	2.19	0.68
21:W:77:HIS:CE1	25:k:76:LYS:HD2	2.28	0.68
21:W:156:PHE:CD2	23:Y:94:PHE:CE1	2.82	0.68
32:m:41:ARG:HG2	32:m:41:ARG:NH2	2.02	0.68
21:W:15:TYR:OH	25:k:19:LYS:CD	2.40	0.67
31:l:64:SER:CA	31:l:67:LEU:CD2	2.68	0.67
4:A:794:LYS:HB3	4:A:854:ARG:NH1	2.09	0.67
20:V:966:VAL:HG21	20:V:985:LEU:HD21	1.75	0.67
31:l:45:LEU:HD12	31:l:65:LEU:CD2	2.25	0.67
1:2:1165:C:O2'	21:W:118:ARG:NH2	2.28	0.67
5:C:176:ARG:HH12	5:C:188:GLY:HA2	1.59	0.67
20:V:566:PHE:CG	20:V:999:GLN:CB	2.76	0.67
25:k:23:LEU:HD11	31:l:64:SER:HB2	1.77	0.67
5:C:759:SER:OG	17:R:78:SER:CB	2.43	0.67
5:C:760:LEU:HD12	17:R:75:VAL:CA	1.46	0.67
20:V:609:THR:C	20:V:837:GLU:OE1	2.38	0.67
31:l:60:ILE:O	31:l:62:MET:N	2.27	0.67
21:W:35:GLN:HE22	23:Y:57:GLU:CD	1.99	0.66
25:k:54:PRO:CB	31:l:66:TYR:CD1	2.79	0.66
4:A:1922:ARG:NH1	26:c:246:THR:O	2.28	0.66
25:k:15:LEU:HD11	31:l:84:TYR:CE1	2.29	0.66
4:A:403:TYR:OH	5:C:915:GLU:OE2	2.13	0.66
21:W:156:PHE:HZ	23:Y:51:LEU:CA	2.09	0.66
20:V:785:ALA:CA	20:V:871:LEU:HD13	2.12	0.66
21:W:153:THR:HG22	23:Y:43:ARG:HH22	1.60	0.66
21:W:153:THR:HG21	23:Y:43:ARG:HH21	1.60	0.66
1:2:144:G:H4'	21:W:122:ARG:HH12	1.60	0.66
1:2:1166:G:H5'	21:W:119:ARG:NH1	2.11	0.66
31:l:10:LEU:HD13	31:l:97:LEU:HD21	1.78	0.66
5:C:764:ASN:HB3	5:C:776:ASN:HB2	1.78	0.66
7:E:15:C:H5'	20:V:1075:THR:HG21	1.76	0.66
20:V:883:GLN:HE22	20:V:909:ARG:NH2	1.92	0.66
21:W:15:TYR:HH	25:k:19:LYS:HE3	1.59	0.66
31:l:70:GLY:C	31:l:80:ALA:HB2	2.21	0.66
18:S:47:GLN:HE21	18:S:78:GLN:HE21	1.43	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:W:35:GLN:OE1	23:Y:57:GLU:HB2	1.94	0.66
4:A:783:LEU:O	4:A:786:LEU:HB3	1.96	0.66
31:l:47:LEU:HB2	31:l:65:LEU:HD11	1.78	0.66
29:q:37:GLU:HB2	29:q:59:PHE:HB2	1.77	0.66
18:S:534:TYR:CA	18:S:551:PHE:CB	2.74	0.65
10:J:180:GLY:O	10:J:207:LYS:NZ	2.29	0.65
3:6:71:G:N2	3:6:74:U:OP2	2.28	0.65
21:W:153:THR:HG23	23:Y:43:ARG:HH21	1.58	0.65
32:m:26:PHE:HZ	32:m:61:PHE:CE1	1.98	0.65
11:K:35:ALA:H	18:S:123:ASN:HD21	1.44	0.65
18:S:346:ILE:CB	18:S:366:LEU:C	2.70	0.65
19:T:339:PHE:HA	19:T:399:VAL:CB	2.26	0.65
21:W:141:ARG:CZ	21:W:157:GLN:NE2	2.57	0.65
31:l:61:ALA:O	31:l:64:SER:N	2.29	0.65
5:C:970:THR:HG22	5:C:973:ARG:HH11	1.61	0.65
20:V:566:PHE:CD1	20:V:999:GLN:HB2	2.27	0.65
21:W:4:THR:HG22	21:W:6:SER:H	1.61	0.65
5:C:604:LYS:NZ	5:C:973:ARG:HH12	1.93	0.65
20:V:735:PRO:CG	20:V:937:TYR:HE1	2.10	0.65
5:C:452:LYS:NZ	5:C:487:ARG:NH1	2.44	0.64
21:W:50:LEU:HB2	21:W:73:ARG:NH1	2.10	0.64
31:l:36:MET:SD	32:m:97:ARG:NH1	2.71	0.64
31:l:68:THR:O	31:l:70:GLY:N	2.29	0.64
4:A:404:ASN:ND2	5:C:927:MET:SD	2.70	0.64
5:C:268:ASN:HD21	5:C:316:THR:HG23	1.62	0.64
7:E:18:G:C5'	20:V:732:SER:HB3	2.28	0.64
20:V:489:ARG:HE	20:V:519:TYR:HB3	1.60	0.64
20:V:725:LEU:HD11	20:V:753:VAL:HG23	1.78	0.64
3:6:50:G:O2'	9:I:3:A:N6	2.31	0.64
20:V:642:LYS:HD3	20:V:832:GLU:OE1	1.94	0.64
25:k:54:PRO:HB2	31:l:66:TYR:CD1	2.32	0.64
1:2:1165:C:C2'	21:W:118:ARG:NH2	2.60	0.64
15:O:6:ILE:HG22	15:O:9:LYS:HE2	1.79	0.64
20:V:736:SER:OG	20:V:988:ARG:NE	2.26	0.64
25:k:86:ILE:HG22	27:n:72:ILE:H	1.62	0.64
28:p:29:ILE:HD11	28:p:87:ILE:HG23	1.79	0.64
34:s:107:GLU:CB	34:s:110:GLU:CB	2.76	0.64
11:K:132:ARG:HD3	14:N:111:ARG:HE	1.62	0.64
20:V:894:LEU:H	20:V:894:LEU:HD12	1.63	0.64
31:l:46:THR:HG23	31:l:79:ILE:HG12	1.80	0.64
27:n:65:ARG:NH1	30:r:65:GLY:O	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:893:ARG:NH1	4:A:1136:GLY:O	2.31	0.64
1:2:1107:C:C5	23:Y:31:TYR:OH	2.28	0.64
1:2:112:A:N6	29:q:47:ASN:O	2.31	0.63
3:6:5:G:H1	3:6:21:U:H3	1.46	0.63
20:V:957:TYR:CE2	20:V:1064:TYR:HA	2.33	0.63
31:l:16:THR:HG22	31:l:26:TRP:HD1	1.63	0.63
24:a:106:LYS:NZ	24:a:153:ASN:OD1	2.29	0.63
10:J:197:LEU:HB3	10:J:209:TRP:HB2	1.80	0.63
1:2:1165:C:C4'	21:W:118:ARG:CZ	2.58	0.63
21:W:51:THR:HG22	21:W:53:PRO:HD3	1.81	0.63
20:V:512:LYS:HA	20:V:516:ILE:CD1	2.25	0.63
29:f:74:ARG:HH12	32:j:64:HIS:HA	1.63	0.63
21:W:50:LEU:HD12	21:W:73:ARG:NE	2.03	0.63
1:2:1108:A:C5	23:Y:73:PHE:HZ	2.12	0.63
31:l:45:LEU:N	31:l:45:LEU:HD23	2.13	0.63
4:A:611:LYS:HG2	4:A:614:ARG:HH12	1.64	0.62
4:A:1701:ILE:HB	4:A:1734:PHE:HB2	1.79	0.62
10:J:250:LEU:HD12	10:J:260:ILE:HB	1.80	0.62
31:l:67:LEU:HD12	31:l:67:LEU:C	2.24	0.62
20:V:586:ARG:HD3	20:V:902:PRO:CG	2.21	0.62
23:Y:59:LEU:HD23	23:Y:60:LYS:HG2	1.82	0.62
31:l:68:THR:C	31:l:70:GLY:N	2.57	0.62
5:C:452:LYS:NZ	5:C:487:ARG:HH11	1.98	0.62
25:k:29:VAL:CG2	31:l:67:LEU:CD2	2.76	0.62
20:V:646:TYR:CD1	20:V:864:MET:HA	2.30	0.62
4:A:1647:GLN:O	4:A:1650:ARG:NH1	2.32	0.62
18:S:46:TYR:HD1	18:S:49:ARG:HH11	1.44	0.62
10:J:133:ARG:NH1	10:J:169:LEU:O	2.31	0.62
4:A:1941:LEU:HD11	4:A:1958:PRO:HB3	1.81	0.62
28:e:83:LYS:NZ	29:f:49:PHE:O	2.33	0.62
4:A:630:LYS:NZ	4:A:634:ASP:OD2	2.22	0.62
5:C:139:ILE:HD12	5:C:252:LEU:HD22	1.82	0.62
21:W:56:ILE:HG12	21:W:78:THR:HB	1.80	0.62
2:5:22:G:H1	2:5:149:U:H3	1.48	0.61
5:C:759:SER:C	17:R:78:SER:CB	2.73	0.61
7:E:15:C:C3'	20:V:1075:THR:CG2	2.77	0.61
20:V:785:ALA:HA	20:V:871:LEU:HD11	0.63	0.61
4:A:1032:ILE:HG12	4:A:1171:LEU:HD22	1.81	0.61
20:V:957:TYR:CD2	20:V:1085:SER:HB2	2.35	0.61
25:k:23:LEU:CD1	31:l:64:SER:CB	2.77	0.61
25:k:23:LEU:CD1	31:l:67:LEU:HD23	1.98	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:k:96:VAL:HG11	31:l:82:LEU:CD2	2.29	0.61
31:l:51:ARG:HA	31:l:62:MET:HE1	1.81	0.61
15:O:228:TYR:H	18:S:120:ASN:HD21	1.48	0.61
20:V:791:GLN:CG	20:V:1074:LEU:HD22	2.29	0.61
20:V:783:TYR:HE2	20:V:871:LEU:HD12	1.66	0.61
33:o:169:LYS:HZ2	33:o:213:ARG:HB2	1.66	0.61
10:J:152:ASN:HD21	10:J:409:LYS:HB3	1.64	0.61
21:W:84:ASN:CB	21:W:86:ILE:HG13	2.30	0.61
13:M:81:CYS:SG	13:M:91:HIS:HE1	2.23	0.61
25:k:96:VAL:CG1	31:l:85:ILE:HG12	2.28	0.61
31:l:68:THR:CG2	31:l:82:LEU:HD21	2.31	0.61
4:A:1790:TRP:CD1	4:A:1795:LYS:HZ1	2.19	0.61
5:C:343:ASP:O	5:C:347:ARG:NH1	2.34	0.61
8:H:392:LEU:HB3	8:H:398:LEU:HD23	1.83	0.61
21:W:37:GLU:CD	23:Y:56:GLY:HA2	2.24	0.61
21:W:16:VAL:O	21:W:16:VAL:HG12	2.00	0.61
3:6:72:C:H41	4:A:617:ASN:HD22	1.47	0.61
5:C:604:LYS:HZ2	5:C:973:ARG:HH12	1.49	0.61
5:C:808:LEU:O	5:C:971:ARG:NH2	2.34	0.61
7:E:17:U:H1'	20:V:779:LYS:O	2.01	0.61
20:V:791:GLN:HG2	20:V:792:LEU:H	1.65	0.61
1:2:16:U:O2'	36:y:179:ARG:NH2	2.34	0.60
5:C:343:ASP:HB3	5:C:347:ARG:NH1	2.14	0.60
14:N:252:ARG:NH2	14:N:297:PHE:O	2.34	0.60
20:V:566:PHE:CG	20:V:999:GLN:HB2	2.36	0.60
21:W:156:PHE:CE2	23:Y:51:LEU:HD22	2.37	0.60
29:q:74:ARG:HG3	29:q:76:ASN:H	1.66	0.60
3:6:61:C:OP2	3:6:80:U:O2'	2.12	0.60
4:A:982:TYR:HB2	4:A:1106:GLY:HA3	1.83	0.60
5:C:176:ARG:NH1	5:C:188:GLY:HA2	2.15	0.60
5:C:604:LYS:NZ	5:C:973:ARG:NH1	2.50	0.60
10:J:327:CYS:SG	10:J:328:THR:N	2.75	0.60
20:V:566:PHE:HD1	20:V:999:GLN:CD	2.09	0.60
24:a:187:SER:HA	24:a:220:ILE:HD11	1.83	0.60
4:A:140:ARG:NH1	4:A:256:GLU:OE1	2.35	0.60
4:A:1715:SER:HB2	4:A:1719:GLU:HG3	1.83	0.60
20:V:621:LYS:NZ	20:V:861:PHE:CE1	2.69	0.60
23:Y:59:LEU:O	23:Y:60:LYS:HD3	2.01	0.60
20:V:646:TYR:CG	20:V:864:MET:CG	2.85	0.60
5:C:175:LEU:HD13	5:C:177:TYR:HB2	1.82	0.60
5:C:760:LEU:N	17:R:78:SER:CB	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:586:ARG:CD	20:V:902:PRO:CG	2.79	0.60
33:o:63:ARG:HH11	33:o:70:GLY:N	1.98	0.60
5:C:763:ARG:HH21	17:R:82:ASP:HA	1.64	0.60
5:C:866:ILE:O	5:C:901:GLU:HA	2.02	0.60
10:J:280:GLN:NE2	11:K:66:CYS:SG	2.74	0.60
18:S:251:ALA:HA	18:S:263:SER:CA	2.31	0.60
23:Y:78:THR:HG22	23:Y:80:ASP:H	1.66	0.60
25:k:54:PRO:HB2	31:l:66:TYR:CE1	2.35	0.60
1:2:1138:G:P	23:Y:65:PHE:CE1	2.95	0.59
5:C:101:GLN:O	5:C:182:LYS:NZ	2.25	0.59
19:T:502:GLU:O	19:T:506:SER:N	2.33	0.59
21:W:84:ASN:C	21:W:86:ILE:N	2.51	0.59
32:j:57:ARG:HB3	32:j:70:GLU:HB2	1.84	0.59
7:E:15:C:H3'	20:V:1075:THR:CG2	2.30	0.59
15:O:38:SER:O	15:O:158:ARG:NH1	2.35	0.59
18:S:219:ARG:CZ	22:X:107:UNK:CB	2.80	0.59
23:Y:75:THR:OG1	23:Y:108:THR:CG2	2.45	0.59
32:j:46:ILE:HG12	32:j:104:VAL:HG22	1.85	0.59
21:W:50:LEU:CD1	21:W:73:ARG:HH22	2.04	0.59
4:A:1591:THR:HG22	4:A:1593:ALA:H	1.66	0.59
4:A:1912:LYS:NZ	4:A:1916:GLU:OE2	2.24	0.59
5:C:133:ILE:HG12	5:C:209:MET:HB3	1.84	0.59
28:p:17:ILE:HD11	28:p:50:MET:HE2	1.84	0.59
3:6:77:G:HO2'	7:E:-2:A:HO2'	1.49	0.59
4:A:1650:ARG:NH2	4:A:1942:ASP:OD2	2.34	0.59
4:A:1681:VAL:O	26:c:249:ARG:NH2	2.35	0.59
1:2:1150:U:HO2'	27:n:53:GLN:CG	2.03	0.59
1:2:1165:C:H1'	21:W:118:ARG:NH2	2.18	0.59
3:6:90:U:OP2	18:S:104:ARG:NH2	2.36	0.59
4:A:411:ILE:HB	5:C:278:LYS:HD3	1.84	0.59
25:k:21:ARG:HD3	31:l:67:LEU:O	2.03	0.59
4:A:209:ILE:HG22	4:A:211:PRO:HD2	1.85	0.59
4:A:1915:GLU:OE2	24:a:196:GLY:N	2.36	0.59
8:H:300:LEU:HD22	8:H:347:LEU:HD11	1.85	0.59
15:O:181:ARG:HH11	18:S:49:ARG:NH2	1.99	0.59
21:W:141:ARG:HH22	21:W:157:GLN:NE2	1.91	0.59
31:l:7:LEU:CD1	32:m:95:PHE:CZ	2.82	0.59
29:q:39:ARG:HE	29:q:84:LEU:HD22	1.66	0.59
10:J:306:HIS:O	10:J:332:ARG:NH1	2.36	0.59
12:L:61:ARG:HH12	12:L:102:LYS:HA	1.68	0.59
20:V:932:VAL:HG12	20:V:933:GLN:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:d:50:THR:HG22	27:d:56:VAL:HG12	1.84	0.59
4:A:1844:PHE:HB2	4:A:1885:LYS:HD3	1.85	0.58
18:S:251:ALA:O	18:S:263:SER:CB	2.51	0.58
21:W:15:TYR:CZ	25:k:19:LYS:NZ	2.65	0.58
21:W:146:ARG:HD3	21:W:167:ALA:HB2	1.85	0.58
27:d:15:GLN:NE2	27:d:34:VAL:O	2.35	0.58
2:5:167:A:N1	32:j:63:ARG:NH1	2.49	0.58
2:5:170:U:H5'	2:5:171:U:H5'	1.84	0.58
5:C:766:TRP:NE1	5:C:776:ASN:OD1	2.37	0.58
8:H:335:LEU:HD23	8:H:381:GLN:HB3	1.85	0.58
12:L:104:CYS:SG	12:L:105:CYS:N	2.76	0.58
31:l:96:ILE:N	31:l:96:ILE:HD12	2.18	0.58
1:2:1107:C:O5'	23:Y:68:GLN:NE2	2.33	0.58
4:A:1615:ASN:HB2	4:A:1641:LEU:HD21	1.85	0.58
4:A:1712:SER:O	4:A:1789:ASN:ND2	2.35	0.58
20:V:586:ARG:HD2	20:V:902:PRO:HB3	1.85	0.58
21:W:156:PHE:HE2	23:Y:51:LEU:CD2	2.15	0.58
25:k:96:VAL:HG21	31:l:82:LEU:HD23	1.84	0.58
4:A:1080:ASP:OD1	15:O:82:ASN:ND2	2.37	0.58
1:2:1107:C:H5''	23:Y:68:GLN:NE2	2.14	0.58
4:A:1477:PHE:CZ	7:E:11:A:O3'	2.52	0.58
1:2:18:U:OP1	36:y:199:LYS:NZ	2.33	0.58
4:A:2083:ILE:HD11	26:c:330:VAL:HG11	1.85	0.58
4:A:1116:TYR:O	4:A:1119:LEU:HB3	2.03	0.58
20:V:646:TYR:CZ	20:V:864:MET:N	2.71	0.58
4:A:842:LYS:HG2	4:A:1321:MET:HG3	1.86	0.58
2:5:171:U:H1'	25:b:90:GLU:HB2	1.86	0.58
4:A:425:ASP:H	4:A:428:LEU:HD12	1.68	0.58
25:b:21:ARG:HB2	25:b:96:VAL:HB	1.86	0.58
31:l:82:LEU:N	31:l:82:LEU:HD12	2.18	0.58
4:A:1864:LYS:O	33:o:330:GLN:NE2	2.37	0.58
32:m:49:ARG:NH1	29:q:77:ASN:OD1	2.37	0.58
33:o:209:ILE:HA	33:o:225:SER:HA	1.85	0.58
4:A:1063:PHE:HB2	15:O:83:GLN:HE21	1.68	0.57
11:K:112:ILE:HD13	14:N:25:MET:HE3	1.85	0.57
14:N:68:ARG:O	14:N:87:ARG:NH2	2.37	0.57
21:W:60:THR:HG21	23:Y:53:ALA:O	2.03	0.57
33:o:63:ARG:HH11	33:o:70:GLY:H	1.51	0.57
20:V:617:ALA:HB1	20:V:861:PHE:CE2	2.39	0.57
20:V:702:GLU:CD	20:V:702:GLU:H	2.12	0.57
31:l:44:LYS:HB3	31:l:81:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:34:CYS:HB2	14:N:60:ILE:HA	1.87	0.57
31:l:25:VAL:HG13	31:l:43:VAL:HG11	1.87	0.57
1:2:1166:G:C5'	21:W:119:ARG:HD3	2.35	0.57
3:6:41:A:N1	13:M:31:ASN:ND2	2.52	0.57
4:A:1585:MET:HB3	4:A:1598:LEU:HD11	1.86	0.57
4:A:1879:ILE:HB	4:A:1892:LYS:HB3	1.85	0.57
4:A:1993:ASP:OD1	4:A:1993:ASP:N	2.38	0.57
20:V:610:VAL:HG23	20:V:837:GLU:CG	2.34	0.57
31:l:45:LEU:HD12	31:l:65:LEU:HD21	1.86	0.57
18:S:349:SER:C	18:S:362:ARG:CB	2.77	0.57
10:J:231:SER:HB3	10:J:240:ALA:HB3	1.86	0.57
18:S:251:ALA:C	18:S:263:SER:CB	2.78	0.57
22:X:25:UNK:O	22:X:26:UNK:C	2.51	0.57
31:h:13:GLU:HB3	31:h:98:PRO:HG2	1.87	0.57
33:o:248:SER:HB3	33:o:267:LEU:HD12	1.85	0.57
12:L:151:ARG:HG3	33:o:71:SER:HA	1.87	0.57
20:V:489:ARG:HG2	20:V:519:TYR:CE2	2.40	0.57
20:V:833:ASN:ND2	20:V:834:THR:O	2.35	0.57
25:k:88:ARG:HG2	25:k:90:GLU:H	1.70	0.57
4:A:854:ARG:NH2	4:A:1094:ASP:OD2	2.37	0.57
4:A:1864:LYS:NZ	33:o:330:GLN:O	2.30	0.57
10:J:309:ARG:HH11	10:J:328:THR:HG21	1.68	0.57
4:A:176:LEU:O	4:A:708:TRP:NE1	2.33	0.57
18:S:89:GLU:OE1	18:S:124:ARG:NH2	2.38	0.57
20:V:586:ARG:NE	20:V:902:PRO:HA	2.15	0.57
31:h:7:LEU:HB3	31:h:32:VAL:HG21	1.87	0.57
31:l:44:LYS:HA	31:l:81:SER:HA	1.86	0.57
4:A:745:THR:OG1	10:J:203:ASP:OD1	2.21	0.56
4:A:1163:ARG:NH2	4:A:1165:LEU:O	2.38	0.56
4:A:1703:MET:HB2	4:A:1732:MET:HB2	1.87	0.56
21:W:35:GLN:HG2	23:Y:77:ARG:NH1	2.19	0.56
31:l:47:LEU:HD13	31:l:62:MET:HG2	1.85	0.56
1:2:1107:C:C5	23:Y:71:GLN:OE1	2.59	0.56
1:2:1149:G:N2	27:n:53:GLN:O	2.38	0.56
4:A:1832:GLU:HG3	26:c:272:LEU:HD22	1.87	0.56
5:C:287:LYS:NZ	5:C:291:ILE:HD11	2.19	0.56
5:C:944:VAL:HG13	5:C:967:VAL:HG21	1.86	0.56
10:J:292:LEU:HD12	10:J:302:LYS:HB3	1.87	0.56
21:W:151:LEU:O	21:W:164:ARG:NH2	2.38	0.56
22:X:26:UNK:O	22:X:27:UNK:C	2.52	0.56
5:C:494:LYS:HG2	5:C:555:GLU:HG2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:241:THR:OG1	10:J:251:TRP:NE1	2.32	0.56
14:N:208:TYR:HB2	14:N:289:PHE:HB2	1.87	0.56
20:V:566:PHE:HB2	20:V:992:ARG:HH12	1.70	0.56
21:W:156:PHE:CZ	23:Y:51:LEU:CA	2.87	0.56
10:J:408:ASP:HB3	10:J:411:GLY:H	1.70	0.56
14:N:87:ARG:HH12	14:N:122:GLY:C	2.13	0.56
20:V:949:LYS:HE2	20:V:984:PHE:O	2.06	0.56
31:l:10:LEU:HD13	31:l:97:LEU:CD2	2.35	0.56
4:A:680:CYS:SG	4:A:711:TRP:NE1	2.79	0.56
4:A:1446:THR:OG1	4:A:1449:ASN:ND2	2.37	0.56
4:A:1485:ASP:O	4:A:1490:ARG:NH1	2.39	0.56
4:A:1859:ARG:NH1	4:A:1969:MET:HE2	2.20	0.56
5:C:270:LEU:HD11	5:C:313:PHE:HB3	1.87	0.56
10:J:238:LEU:HD12	10:J:250:LEU:HB3	1.88	0.56
15:O:152:LEU:HD11	15:O:156:ARG:HH21	1.71	0.56
19:T:542:LEU:O	19:T:545:TRP:N	2.39	0.56
20:V:957:TYR:CE2	20:V:1085:SER:HA	2.41	0.56
23:Y:29:THR:OG1	23:Y:108:THR:HG22	2.05	0.56
25:k:88:ARG:NH1	27:n:66:GLY:O	2.36	0.56
4:A:158:LYS:NZ	13:M:35:ASN:HD21	2.04	0.56
4:A:794:LYS:HB3	4:A:854:ARG:HH12	1.70	0.56
4:A:1754:ALA:O	4:A:1758:ASP:HB2	2.05	0.56
13:M:172:ARG:NH1	14:N:212:ALA:O	2.38	0.56
30:r:54:ASN:HB3	30:r:57:LEU:HD21	1.86	0.56
4:A:829:TYR:OH	4:A:833:ARG:NH2	2.39	0.56
25:b:26:ASP:OD2	27:d:70:LYS:NZ	2.21	0.56
1:2:3:G:N2	3:6:102:U:O2	2.36	0.56
8:H:380:ASP:OD1	8:H:383:ARG:NH2	2.39	0.56
13:M:157:GLU:OE2	13:M:161:ARG:NE	2.38	0.56
5:C:646:GLY:HA3	5:C:652:MET:HE3	1.88	0.55
14:N:62:VAL:HG22	14:N:72:GLN:HE22	1.71	0.55
20:V:791:GLN:HG3	20:V:1074:LEU:HB3	1.88	0.55
27:d:65:ARG:NH1	30:g:36:LEU:HB3	2.21	0.55
28:e:30:TRP:HB2	28:e:89:LEU:HD13	1.89	0.55
4:A:744:THR:O	4:A:749:ARG:NH2	2.39	0.55
4:A:1324:GLY:O	7:E:2:G:N2	2.39	0.55
18:S:251:ALA:CB	18:S:263:SER:CB	2.84	0.55
32:m:38:MET:SD	32:m:61:PHE:HD2	2.29	0.55
1:2:114:U:H5'	1:2:115:U:H5'	1.88	0.55
5:C:100:LEU:HD12	5:C:108:GLN:HE21	1.71	0.55
5:C:820:LEU:HD21	5:C:842:MET:HE1	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:E:12:C:C1'	7:E:13:U:P	2.94	0.55
10:J:206:VAL:HB	10:J:220:TYR:HB2	1.89	0.55
31:l:67:LEU:HD12	31:l:68:THR:HG23	1.85	0.55
11:K:134:VAL:HG22	14:N:111:ARG:HD3	1.86	0.55
15:O:96:GLN:HB3	15:O:134:THR:HG21	1.88	0.55
31:l:82:LEU:HD13	31:l:85:ILE:HD11	1.88	0.55
27:n:21:LEU:HD12	27:n:44:LEU:HD22	1.88	0.55
5:C:865:ASP:HB3	5:C:929:GLN:HB2	1.87	0.55
20:V:783:TYR:CE2	20:V:871:LEU:CG	2.77	0.55
4:A:1601:ILE:HD11	9:I:93:U:H5'	1.87	0.55
5:C:120:ARG:HH11	5:C:158:HIS:CE1	2.18	0.55
2:5:143:U:H2'	2:5:144:G:H8	1.71	0.55
20:V:646:TYR:HD1	20:V:864:MET:HG3	1.71	0.55
33:o:183:ASN:HA	33:o:208:PRO:HB3	1.88	0.55
30:r:17:LEU:HD23	30:r:71:LEU:HB3	1.89	0.55
34:s:114:LEU:O	34:s:118:ASP:CA	2.54	0.55
21:W:156:PHE:HB3	23:Y:94:PHE:CD1	2.41	0.55
31:l:45:LEU:HD21	31:l:82:LEU:HD13	1.88	0.55
1:2:1167:U:C5'	21:W:92:ARG:NH2	2.70	0.55
4:A:236:ARG:NH1	4:A:655:TYR:HB2	2.22	0.55
20:V:735:PRO:HG2	20:V:937:TYR:CZ	2.42	0.55
25:k:92:ILE:HG23	31:l:88:ARG:HD3	1.87	0.55
1:2:25:A:H5'	1:2:26:G:H5''	1.89	0.55
4:A:1378:LYS:HD2	7:E:-6:A:OP1	2.06	0.55
4:A:1407:ILE:HG21	4:A:1426:ARG:HH11	1.72	0.55
4:A:1991:ILE:HG21	4:A:2008:LEU:HD22	1.89	0.55
5:C:763:ARG:NH1	17:R:78:SER:C	2.63	0.55
10:J:133:ARG:HD2	10:J:425:ILE:HD12	1.88	0.55
15:O:174:ARG:HH12	18:S:53:GLU:CD	2.15	0.55
22:X:27:UNK:O	22:X:28:UNK:C	2.52	0.55
2:5:93:G:H4'	17:R:13:GLY:HA2	1.90	0.54
4:A:430:PRO:HG3	8:H:198:PHE:CB	2.37	0.54
4:A:814:ARG:HH12	10:J:401:SER:HB3	1.72	0.54
4:A:1563:LYS:HD3	4:A:1781:TYR:HD1	1.71	0.54
5:C:710:VAL:HB	5:C:820:LEU:HD23	1.89	0.54
13:M:161:ARG:HH11	14:N:241:ILE:HG23	1.72	0.54
19:T:299:PRO:O	19:T:300:ASP:C	2.49	0.54
21:W:34:LEU:CD1	21:W:50:LEU:HD22	2.37	0.54
33:o:443:ILE:HG12	33:o:453:VAL:HG22	1.88	0.54
10:J:180:GLY:HA3	10:J:216:ILE:HD11	1.89	0.54
10:J:354:ASN:ND2	10:J:369:ASP:OD1	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:7:LYS:NZ	13:M:10:LYS:HE3	2.22	0.54
21:W:12:PRO:HB2	21:W:35:GLN:HB3	1.89	0.54
3:6:33:C:OP1	14:N:57:LYS:NZ	2.34	0.54
5:C:309:ASN:HB3	5:C:438:ALA:HA	1.89	0.54
5:C:772:ASN:ND2	5:C:813:ILE:O	2.41	0.54
5:C:866:ILE:HB	5:C:902:VAL:HB	1.88	0.54
10:J:156:ILE:HG21	10:J:197:LEU:HD11	1.89	0.54
20:V:953:PHE:CE2	20:V:966:VAL:HG23	2.42	0.54
2:5:173:U:O2'	29:f:74:ARG:NH2	2.40	0.54
4:A:282:ASP:HB2	4:A:285:PRO:HA	1.89	0.54
4:A:312:TYR:O	4:A:319:ARG:NH2	2.40	0.54
8:H:323:LYS:HZ1	8:H:358:TRP:CG	2.25	0.54
25:b:21:ARG:HG2	25:b:31:ILE:HG22	1.88	0.54
4:A:1749:SER:OG	4:A:1785:ASP:OD2	2.19	0.54
18:S:65:MET:HE3	18:S:95:ASP:HB2	1.90	0.54
26:c:131:LYS:HD2	26:c:133:LYS:NZ	2.21	0.54
27:d:19:VAL:HG21	27:d:33:LEU:HD12	1.88	0.54
4:A:1197:ASN:ND2	4:A:1221:ASN:OD1	2.41	0.54
4:A:1790:TRP:CG	4:A:1795:LYS:HZ1	2.26	0.54
4:A:1859:ARG:HH12	4:A:1969:MET:HE2	1.72	0.54
5:C:469:TRP:NE1	5:C:590:LYS:O	2.41	0.54
5:C:510:ARG:O	5:C:514:GLN:N	2.40	0.54
10:J:291:ARG:HH11	10:J:300:THR:HG21	1.72	0.54
10:J:395:SER:OG	16:P:158:ASN:ND2	2.34	0.54
12:L:40:LYS:HE3	13:M:21:SER:HB3	1.89	0.54
20:V:586:ARG:NE	20:V:902:PRO:CA	2.70	0.54
20:V:773:VAL:HG12	20:V:774:ASP:H	1.73	0.54
1:2:1148:U:H4'	25:k:78:GLU:OE2	2.08	0.54
5:C:90:LEU:HD12	10:J:211:LEU:HD22	1.90	0.54
27:n:4:ASN:HD21	27:n:9:LYS:HD3	1.73	0.54
2:5:85:U:OP1	4:A:672:LYS:NZ	2.41	0.54
20:V:735:PRO:HG2	20:V:937:TYR:CE1	2.38	0.54
25:b:93:LEU:HA	31:h:91:THR:HG21	1.89	0.54
31:l:95:ILE:HG23	32:m:95:PHE:HB3	1.89	0.54
20:V:511:GLY:O	20:V:515:GLN:HB2	2.08	0.54
27:d:20:SER:HB2	27:d:73:VAL:HB	1.89	0.54
3:6:79:A:OP1	3:6:81:G:H4'	2.07	0.54
4:A:2011:LEU:HD23	4:A:2055:MET:HG3	1.89	0.54
5:C:183:GLN:HE21	5:C:657:TYR:HB3	1.72	0.54
5:C:680:SER:OG	5:C:814:TYR:O	2.25	0.54
10:J:281:VAL:HB	10:J:293:TRP:HB2	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:255:ALA:HA	18:S:260:TYR:HA	1.89	0.54
21:W:35:GLN:NE2	23:Y:57:GLU:CD	2.60	0.54
1:2:113:U:H1'	30:r:66:ASN:HB2	1.90	0.53
2:5:167:A:N6	29:f:50:ASN:OD1	2.41	0.53
2:5:174:G:H22	32:j:49:ARG:HH12	1.56	0.53
4:A:1566:GLY:O	4:A:1820:ARG:NH2	2.41	0.53
5:C:869:HIS:HD2	5:C:925:LEU:HB3	1.72	0.53
18:S:262:ARG:CB	22:X:107:UNK:CB	2.85	0.53
20:V:610:VAL:HG11	20:V:841:GLN:NE2	2.20	0.53
21:W:84:ASN:N	21:W:106:ASN:OD1	2.37	0.53
32:j:26:PHE:HA	32:j:31:MET:HB2	1.89	0.53
25:k:21:ARG:HD3	31:l:68:THR:HA	1.90	0.53
25:k:84:LEU:HD22	27:n:79:LYS:HB3	1.90	0.53
33:o:291:HIS:HB2	33:o:320:TRP:HZ2	1.73	0.53
4:A:1182:LEU:HD13	16:P:128:ARG:HH12	1.72	0.53
5:C:287:LYS:HZ2	5:C:291:ILE:HD11	1.72	0.53
29:q:30:LYS:HA	29:q:37:GLU:HG2	1.89	0.53
4:A:685:HIS:NE2	38:A:2500:IHP:O33	2.40	0.53
5:C:145:GLY:O	5:C:149:LEU:N	2.39	0.53
25:k:22:VAL:HG13	25:k:30:TYR:HB2	1.89	0.53
2:5:116:U:H2'	2:5:117:G:H8	1.73	0.53
4:A:833:ARG:HG3	4:A:840:VAL:HG22	1.89	0.53
10:J:135:ILE:HB	10:J:423:ILE:HB	1.89	0.53
25:b:12:LEU:HD12	25:b:15:LEU:HD11	1.90	0.53
31:l:10:LEU:CD1	31:l:97:LEU:HD21	2.37	0.53
4:A:1521:ARG:NH1	7:E:5:C:Cl'	2.71	0.53
4:A:1856:ASN:ND2	4:A:1966:SER:O	2.41	0.53
5:C:478:TYR:OH	5:C:546:GLY:O	2.25	0.53
20:V:834:THR:OG1	20:V:840:ARG:NH2	2.42	0.53
21:W:156:PHE:CE2	23:Y:51:LEU:CD2	2.91	0.53
33:o:315:LYS:HA	33:o:338:SER:HA	1.90	0.53
1:2:24:U:H4'	4:A:850:GLY:HA3	1.91	0.53
4:A:1722:ASP:OD2	4:A:1795:LYS:NZ	2.42	0.53
18:S:131:ARG:HH22	18:S:162:LEU:HB3	1.74	0.53
20:V:715:VAL:HG21	20:V:725:LEU:CB	2.39	0.53
21:W:33:ASP:HB2	21:W:56:ILE:CB	2.32	0.53
32:j:45:ILE:HA	32:j:54:ILE:O	2.09	0.53
33:o:169:LYS:NZ	33:o:213:ARG:HD3	2.23	0.53
34:s:92:ARG:CB	35:v:96:PHE:CB	2.87	0.53
36:y:194:SER:O	36:y:204:ASN:ND2	2.41	0.53
1:2:15:C:O2	1:2:18:U:N3	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:6:30:G:H1'	12:L:146:VAL:HG21	1.89	0.53
10:J:186:ARG:HH12	10:J:228:ARG:NH1	2.06	0.53
20:V:566:PHE:CD2	20:V:996:VAL:CB	2.91	0.53
32:m:104:VAL:HB	29:q:72:PHE:HB3	1.91	0.53
27:n:41:ASN:OD1	27:n:66:GLY:N	2.41	0.53
3:6:91:A:OP2	18:S:100:PRO:HB3	2.09	0.53
15:O:214:ASN:HD21	18:S:48:ARG:HB2	1.74	0.53
31:l:84:TYR:CD1	31:l:84:TYR:C	2.86	0.53
1:2:17:U:OP2	3:6:88:U:O2'	2.25	0.52
5:C:629:TYR:OH	5:C:658:ASP:OD2	2.14	0.52
10:J:244:ARG:HA	10:J:268:PRO:HB3	1.91	0.52
10:J:323:VAL:HG23	10:J:336:LEU:HD11	1.91	0.52
11:K:132:ARG:NH1	14:N:40:PRO:HD3	2.24	0.52
20:V:489:ARG:NE	20:V:519:TYR:HB3	2.24	0.52
20:V:783:TYR:CE2	20:V:871:LEU:HD12	2.39	0.52
4:A:543:ASN:ND2	4:A:545:THR:O	2.42	0.52
4:A:654:HIS:HD2	4:A:704:TRP:HA	1.74	0.52
12:L:73:ILE:HG23	12:L:77:LEU:HB3	1.91	0.52
21:W:84:ASN:CB	21:W:86:ILE:CD1	2.85	0.52
27:n:65:ARG:HH21	27:n:67:SER:HB3	1.74	0.52
2:5:101:C:H5'	4:A:672:LYS:HG3	1.91	0.52
4:A:407:VAL:O	5:C:272:ARG:NH2	2.40	0.52
4:A:1653:LEU:O	4:A:1657:ILE:N	2.42	0.52
14:N:109:MET:HE1	15:O:220:GLU:H	1.74	0.52
27:n:23:LEU:HD23	27:n:25:THR:H	1.74	0.52
21:W:77:HIS:NE2	25:k:76:LYS:HD2	2.24	0.52
21:W:156:PHE:CZ	23:Y:51:LEU:HA	2.41	0.52
36:y:179:ARG:NH1	36:y:183:MET:HG2	2.24	0.52
5:C:200:CYS:HB3	5:C:436:VAL:HG21	1.92	0.52
15:O:96:GLN:NE2	15:O:131:ASN:OD1	2.40	0.52
21:W:84:ASN:HB3	21:W:86:ILE:HG13	1.91	0.52
21:W:156:PHE:HE2	23:Y:51:LEU:HD22	1.75	0.52
23:Y:109:LYS:C	23:Y:110:THR:O	2.52	0.52
25:b:91:GLN:HG3	27:d:70:LYS:HA	1.92	0.52
9:I:12:G:N2	13:M:178:SER:O	2.42	0.52
20:V:646:TYR:HE1	20:V:864:MET:HA	1.51	0.52
20:V:646:TYR:CE2	20:V:864:MET:HB2	2.44	0.52
2:5:43:G:O2'	5:C:108:GLN:OE1	2.28	0.52
4:A:855:LEU:HD13	16:P:166:HIS:HE1	1.74	0.52
4:A:975:TYR:OH	4:A:1321:MET:SD	2.67	0.52
6:D:173:ILE:HA	15:O:5:PRO:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:121:GLN:NE2	11:K:49:SER:O	2.42	0.52
14:N:94:VAL:HG11	14:N:135:ILE:HG13	1.90	0.52
28:p:38:ARG:HB2	28:p:60:ILE:HB	1.92	0.52
4:A:252:GLU:HG2	4:A:253:GLN:HG3	1.92	0.52
4:A:953:ARG:NH1	15:O:128:ILE:HD12	2.25	0.52
4:A:1033:ASN:HD22	4:A:1288:LEU:HB3	1.75	0.52
5:C:452:LYS:NZ	5:C:489:TYR:OH	2.35	0.52
31:h:103:LEU:HD13	32:j:59:LYS:HG2	1.91	0.52
2:5:74:U:O2'	2:5:77:A:N3	2.41	0.52
4:A:212:VAL:HG11	4:A:285:PRO:HG3	1.91	0.52
4:A:235:LYS:HE3	26:c:173:ARG:HH11	1.73	0.52
7:E:17:U:C1'	20:V:779:LYS:O	2.58	0.52
13:M:54:GLN:HB2	13:M:58:HIS:HD2	1.75	0.52
18:S:332:GLU:CB	18:S:335:PRO:CA	2.87	0.52
19:T:119:ALA:HB1	19:T:128:ILE:CA	2.39	0.52
19:T:598:HIS:O	19:T:600:GLU:N	2.43	0.52
21:W:156:PHE:CD2	23:Y:94:PHE:HD1	2.17	0.52
32:m:72:VAL:HB	32:m:91:ILE:HB	1.90	0.52
10:J:248:ILE:HB	10:J:262:LEU:HB2	1.92	0.52
14:N:37:CYS:HA	14:N:110:LYS:HB3	1.92	0.52
19:T:427:VAL:O	19:T:431:ALA:N	2.32	0.52
21:W:90:ASP:OD1	21:W:116:ARG:NE	2.40	0.52
33:o:272:ILE:HD12	33:o:320:TRP:HZ3	1.75	0.52
28:p:35:ILE:HA	30:r:23:ARG:HH21	1.75	0.52
4:A:376:ARG:NH1	5:C:956:PRO:HB2	2.25	0.51
4:A:1073:ILE:HG13	4:A:1074:VAL:HG13	1.92	0.51
5:C:118:TYR:HE1	5:C:157:SER:HB3	1.74	0.51
10:J:121:GLN:HE22	11:K:50:ASN:HA	1.75	0.51
19:T:339:PHE:CA	19:T:399:VAL:CB	2.88	0.51
31:l:45:LEU:HD12	31:l:65:LEU:HD23	1.92	0.51
29:q:32:LYS:HA	29:q:79:LEU:HD12	1.92	0.51
2:5:21:G:H2'	2:5:22:G:H8	1.76	0.51
4:A:182:PRO:HB3	4:A:264:ILE:HD12	1.92	0.51
18:S:183:ASN:OD1	18:S:186:ARG:NH2	2.43	0.51
4:A:190:LYS:HG2	4:A:561:THR:HG22	1.92	0.51
4:A:1590:LEU:HD13	4:A:1594:GLN:HB3	1.92	0.51
8:H:377:TYR:HB3	8:H:381:GLN:HB2	1.91	0.51
18:S:73:GLN:HA	18:S:76:ILE:HD12	1.92	0.51
28:e:12:PRO:HD2	28:e:15:ASN:HB2	1.92	0.51
32:m:72:VAL:HG21	32:m:94:LEU:HB3	1.93	0.51
33:o:222:LEU:HD11	33:o:255:SER:HB3	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:965:LYS:HE2	15:O:133:GLU:OE2	2.11	0.51
28:e:23:GLN:HB3	28:e:25:THR:HG23	1.92	0.51
33:o:263:PHE:HD2	33:o:275:TYR:HB2	1.75	0.51
20:V:565:ARG:HH22	20:V:931:SER:HB3	1.75	0.51
20:V:566:PHE:CD1	20:V:999:GLN:HG3	2.45	0.51
29:f:53:LEU:HB2	29:f:71:ILE:HD11	1.93	0.51
25:k:43:LEU:O	25:k:87:LEU:N	2.38	0.51
31:l:64:SER:O	31:l:67:LEU:CD2	2.58	0.51
4:A:137:GLU:HG3	12:L:34:GLN:HE21	1.76	0.51
4:A:169:PRO:HD3	4:A:622:MET:HE1	1.92	0.51
4:A:771:PRO:HA	10:J:309:ARG:HH22	1.75	0.51
4:A:1386:ALA:O	4:A:1390:THR:OG1	2.27	0.51
5:C:132:ARG:NH2	27:d:13:GLU:O	2.44	0.51
5:C:760:LEU:CB	17:R:75:VAL:HA	2.27	0.51
28:e:28:THR:HG21	30:g:57:LEU:HD12	1.91	0.51
31:h:23:THR:HA	31:h:48:PRO:HD3	1.93	0.51
4:A:1281:ASN:ND2	4:A:1301:TYR:OH	2.44	0.51
4:A:1548:GLN:HE21	8:H:294:LYS:NZ	2.09	0.51
4:A:1853:ASP:HB3	4:A:1880:PHE:HB3	1.91	0.51
13:M:120:TYR:OH	13:M:134:ASN:ND2	2.44	0.51
14:N:107:ASP:HB3	14:N:111:ARG:HH12	1.76	0.51
21:W:58:ASP:HA	21:W:80:LEU:HB2	1.92	0.51
31:l:52:LEU:HG	31:l:52:LEU:O	2.10	0.51
4:A:1632:ILE:HG21	4:A:1645:LEU:HD13	1.92	0.51
4:A:1962:ARG:O	4:A:2013:ARG:NH2	2.43	0.51
15:O:18:ASP:OD2	15:O:56:LEU:HD21	2.11	0.51
20:V:957:TYR:CD1	20:V:1064:TYR:CE1	2.99	0.51
1:2:114:U:H3	27:n:41:ASN:HD21	1.59	0.51
1:2:1098:C:P	23:Y:40:ASN:HD22	2.31	0.51
4:A:625:LEU:HD21	4:A:714:PHE:HE2	1.75	0.51
5:C:224:GLU:O	5:C:227:VAL:HB	2.11	0.51
5:C:572:ILE:HG22	5:C:573:LYS:HG3	1.93	0.51
14:N:88:ASP:OD2	14:N:101:THR:OG1	2.24	0.51
18:S:346:ILE:CB	18:S:366:LEU:HA	2.40	0.51
20:V:511:GLY:O	20:V:515:GLN:HG2	2.10	0.51
33:o:149:TYR:N	33:o:439:THR:O	2.44	0.51
1:2:1167:U:H5'	21:W:92:ARG:CZ	2.41	0.51
4:A:591:LEU:HD11	4:A:613:SER:HB2	1.92	0.51
4:A:1848:ILE:HD13	4:A:1928:GLU:HA	1.93	0.51
10:J:314:THR:HA	10:J:324:ALA:O	2.11	0.51
11:K:218:GLU:O	11:K:221:SER:OG	2.28	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:h:93:ARG:HD3	32:j:48:LEU:HD21	1.93	0.51
4:A:1320:LEU:HB3	4:A:1370:ARG:HH11	1.75	0.50
18:S:115:ILE:HD12	36:y:161:VAL:HG22	1.91	0.50
19:T:332:GLN:O	19:T:402:ARG:CB	2.59	0.50
4:A:174:LYS:NZ	4:A:205:THR:HG22	2.26	0.50
4:A:621:LEU:HD22	4:A:722:LEU:HD11	1.93	0.50
21:W:14:TYR:HH	23:Y:57:GLU:CD	1.75	0.50
21:W:78:THR:HG23	23:Y:50:LEU:CD2	2.32	0.50
30:g:27:GLY:HA3	30:g:40:LEU:HD13	1.92	0.50
31:l:64:SER:C	31:l:67:LEU:HG	2.15	0.50
33:o:375:LYS:NZ	33:o:412:TRP:HE3	2.08	0.50
3:6:65:U:OP2	16:P:12:ARG:HD3	2.10	0.50
4:A:1563:LYS:HZ2	26:c:85:LEU:N	2.09	0.50
4:A:1845:ASN:ND2	26:c:291:HIS:O	2.36	0.50
5:C:206:LYS:NZ	27:d:15:GLN:HB3	2.26	0.50
7:E:2:G:HO2'	7:E:3:A:P	2.32	0.50
18:S:219:ARG:NH1	22:X:107:UNK:HA	2.26	0.50
25:k:29:VAL:HG11	31:l:67:LEU:HB2	1.93	0.50
25:k:29:VAL:CG1	31:l:67:LEU:HB2	2.42	0.50
33:o:300:LYS:HD2	33:o:344:VAL:HG23	1.93	0.50
6:D:148:GLU:O	6:D:152:LYS:N	2.43	0.50
28:e:34:GLN:HA	29:f:32:LYS:NZ	2.25	0.50
31:l:51:ARG:HA	31:l:62:MET:CE	2.41	0.50
31:l:61:ALA:O	31:l:62:MET:C	2.54	0.50
33:o:339:MET:SD	33:o:355:SER:OG	2.69	0.50
5:C:580:VAL:HG21	5:C:586:MET:HB3	1.93	0.50
5:C:679:GLU:OE2	5:C:808:LEU:HB2	2.12	0.50
18:S:19:LEU:HA	18:S:22:VAL:HG12	1.93	0.50
18:S:153:ARG:NE	18:S:176:GLU:OE2	2.44	0.50
26:c:218:LEU:HD23	26:c:221:LEU:HD12	1.92	0.50
27:d:4:ASN:HB3	27:d:9:LYS:HE3	1.93	0.50
30:r:8:LYS:HD2	30:r:11:MET:HG3	1.92	0.50
4:A:154:TYR:O	4:A:158:LYS:N	2.38	0.50
13:M:254:ILE:HD12	14:N:143:LEU:HD12	1.94	0.50
20:V:610:VAL:HG23	20:V:837:GLU:CD	2.36	0.50
30:r:33:ASP:OD1	30:r:37:ASN:N	2.38	0.50
34:s:114:LEU:O	34:s:118:ASP:CB	2.60	0.50
5:C:486:VAL:HG21	5:C:564:ILE:HD12	1.94	0.50
7:E:3:A:O2'	7:E:4:U:O5'	2.20	0.50
12:L:157:ASP:OXT	33:o:63:ARG:NH2	2.45	0.50
25:b:50:GLU:HB3	25:b:80:ARG:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:256:ARG:HH21	33:o:264:ILE:HD11	1.76	0.50
24:a:243:TYR:O	24:a:247:HIS:ND1	2.45	0.50
4:A:158:LYS:HZ1	13:M:35:ASN:HD21	1.59	0.50
4:A:1945:GLU:HG2	26:c:271:ARG:HH12	1.77	0.50
5:C:510:ARG:NH1	5:C:533:GLU:O	2.45	0.50
10:J:273:GLN:HE21	10:J:316:LEU:HG	1.77	0.50
14:N:70:ILE:HD13	14:N:84:ILE:HD11	1.94	0.50
31:h:95:ILE:HB	32:j:95:PHE:HB3	1.94	0.50
32:j:66:ASN:OD1	32:j:98:GLY:N	2.44	0.50
33:o:211:ALA:H	33:o:224:SER:HG	1.58	0.50
28:p:84:GLY:HA2	28:p:87:ILE:HD12	1.94	0.50
3:6:34:A:N6	13:M:112:PHE:O	2.37	0.49
4:A:1068:ARG:HG3	11:K:208:LEU:HB3	1.93	0.49
4:A:1182:LEU:HD13	16:P:128:ARG:NH1	2.27	0.49
4:A:1663:PHE:O	4:A:1666:CYS:HB2	2.11	0.49
5:C:915:GLU:OE2	5:C:919:ARG:NH2	2.45	0.49
13:M:161:ARG:NH2	14:N:242:VAL:O	2.45	0.49
33:o:55:GLU:HA	33:o:58:ARG:HG2	1.94	0.49
34:s:93:ARG:O	34:s:94:LYS:CB	2.59	0.49
4:A:1071:ARG:NH2	4:A:1080:ASP:OD1	2.45	0.49
4:A:1257:ASN:CG	4:A:1268:ARG:HH11	2.20	0.49
4:A:1925:PRO:O	4:A:1929:GLN:N	2.45	0.49
5:C:840:PRO:HA	5:C:843:LYS:HG2	1.93	0.49
19:T:332:GLN:CB	19:T:342:ILE:CB	2.91	0.49
20:V:646:TYR:CD2	20:V:864:MET:HB2	2.46	0.49
20:V:791:GLN:HG2	20:V:792:LEU:N	2.27	0.49
23:Y:36:ASN:ND2	23:Y:95:PHE:O	2.40	0.49
26:c:275:THR:OG1	26:c:277:THR:O	2.30	0.49
4:A:1033:ASN:HB2	4:A:1288:LEU:HD23	1.93	0.49
4:A:2079:ILE:HD12	26:c:330:VAL:HB	1.93	0.49
6:D:180:ASP:OD1	15:O:42:LYS:NZ	2.35	0.49
7:E:3:A:C1'	7:E:4:U:P	3.00	0.49
11:K:43:PHE:HE1	11:K:147:LEU:HB3	1.77	0.49
11:K:132:ARG:NH2	14:N:33:GLU:OE2	2.44	0.49
25:b:55:LYS:HA	25:b:75:ILE:HD13	1.94	0.49
31:h:47:LEU:HD22	31:h:77:ASP:HB2	1.94	0.49
4:A:817:LYS:HD2	10:J:396:LEU:HD23	1.93	0.49
4:A:936:GLU:HB3	4:A:986:PRO:HB3	1.94	0.49
4:A:1867:GLU:OE2	15:O:169:ARG:HB3	2.11	0.49
4:A:1910:LYS:HE3	4:A:1937:ARG:NH1	2.24	0.49
27:n:45:ARG:HG2	27:n:61:GLN:HE22	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:o:294:SER:OG	33:o:314:ASP:N	2.42	0.49
33:o:300:LYS:HG3	33:o:342:LEU:HG	1.94	0.49
4:A:1893:ILE:HD12	4:A:1978:VAL:HA	1.94	0.49
10:J:227:VAL:HA	10:J:243:GLY:HA3	1.94	0.49
14:N:48:THR:HG23	14:N:56:ILE:HD13	1.94	0.49
19:T:360:LYS:CB	19:T:378:LEU:CB	2.91	0.49
2:5:82:A:O3'	4:A:709:ARG:NH2	2.45	0.49
5:C:755:TYR:HB2	5:C:757:TRP:CD1	2.48	0.49
21:W:50:LEU:CB	21:W:73:ARG:HH12	2.18	0.49
3:6:65:U:OP1	16:P:16:LYS:NZ	2.38	0.49
4:A:1488:ILE:HG12	4:A:1536:LEU:HD22	1.93	0.49
5:C:453:THR:O	5:C:457:SER:OG	2.28	0.49
11:K:174:ASN:ND2	11:K:178:TYR:O	2.41	0.49
18:S:167:ASN:ND2	36:y:99:GLN:OE1	2.45	0.49
20:V:900:LEU:HD21	20:V:1006:LYS:HE3	1.95	0.49
21:W:84:ASN:HB2	21:W:86:ILE:CG1	2.42	0.49
35:t:51:VAL:CB	35:u:20:ARG:CB	2.91	0.49
3:6:59:A:O2'	7:E:2:G:OP2	2.31	0.49
15:O:9:LYS:HD2	15:O:44:THR:HG22	1.95	0.49
20:V:513:THR:CG2	20:V:544:VAL:HG21	2.43	0.49
32:m:38:MET:SD	32:m:61:PHE:CD2	3.06	0.49
33:o:230:VAL:HB	33:o:244:LEU:HB2	1.93	0.49
3:6:38:U:H4'	13:M:121:ARG:NH1	2.28	0.49
4:A:1509:ARG:NH1	4:A:1533:ASP:OD2	2.46	0.49
13:M:92:HIS:HE1	13:M:98:ASP:OD2	1.96	0.49
23:Y:61:VAL:HG22	23:Y:74:ILE:HG12	1.95	0.49
29:q:19:LEU:HD23	29:q:45:THR:HG21	1.94	0.49
2:5:109:A:O2'	16:P:32:PRO:O	2.27	0.49
5:C:649:GLU:OE2	5:C:913:GLY:N	2.45	0.49
19:T:119:ALA:HB1	19:T:128:ILE:HA	1.94	0.49
20:V:715:VAL:HG21	20:V:725:LEU:HB3	1.95	0.49
20:V:791:GLN:CG	20:V:792:LEU:H	2.26	0.49
32:m:34:ILE:HG12	32:m:61:PHE:HB3	1.93	0.49
33:o:256:ARG:HD2	33:o:262:GLU:HB3	1.95	0.49
2:5:96:U:OP2	4:A:1370:ARG:NH1	2.45	0.48
2:5:108:C:O2'	16:P:34:HIS:N	2.43	0.48
3:6:54:U:O3'	15:O:35:LYS:NZ	2.38	0.48
4:A:226:ARG:HH21	26:c:138:LYS:H	1.60	0.48
4:A:1400:ILE:HG21	4:A:1440:ILE:HD12	1.94	0.48
4:A:1609:TRP:HE3	4:A:1823:LEU:HD13	1.77	0.48
7:E:11:A:O2'	7:E:12:C:OP2	2.25	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:129:TRP:O	10:J:385:GLN:NE2	2.45	0.48
20:V:891:LEU:H	20:V:891:LEU:HD22	1.77	0.48
21:W:2:LYS:HG3	21:W:42:SER:HB2	1.95	0.48
1:2:1108:A:C4	23:Y:73:PHE:CZ	2.92	0.48
3:6:39:G:N7	13:M:127:ILE:N	2.53	0.48
4:A:842:LYS:NZ	4:A:1324:GLY:HA2	2.28	0.48
5:C:508:GLU:O	5:C:511:GLN:HB3	2.13	0.48
2:5:79:C:H2'	2:5:114:G:H21	1.77	0.48
4:A:425:ASP:HB3	4:A:428:LEU:HG	1.93	0.48
4:A:495:ARG:NH1	4:A:497:GLN:HE21	2.11	0.48
5:C:326:GLU:HB2	5:C:434:GLY:HA3	1.95	0.48
15:O:156:ARG:NH1	18:S:21:ASP:HB2	2.28	0.48
15:O:181:ARG:NH1	18:S:49:ARG:HH21	2.06	0.48
4:A:140:ARG:HD3	4:A:252:GLU:HB3	1.94	0.48
4:A:236:ARG:HH11	4:A:655:TYR:HB2	1.76	0.48
4:A:294:ASN:HB2	4:A:300:LYS:HB2	1.95	0.48
5:C:632:VAL:HA	5:C:645:LEU:O	2.13	0.48
4:A:1664:ASP:OD1	26:c:247:ARG:NH1	2.46	0.48
10:J:289:THR:HG22	10:J:305:THR:HG22	1.95	0.48
20:V:586:ARG:CD	20:V:902:PRO:CB	2.91	0.48
28:p:47:ASP:OD1	28:p:51:ASN:N	2.46	0.48
36:y:196:ILE:H	36:y:200:ASN:HD22	1.62	0.48
2:5:116:U:H2'	2:5:117:G:C8	2.48	0.48
4:A:583:ILE:HG23	4:A:588:LEU:HB2	1.95	0.48
5:C:381:LEU:HA	5:C:384:ILE:HD12	1.94	0.48
7:E:16:A:OP2	20:V:1075:THR:CG2	2.61	0.48
10:J:343:THR:HG23	11:K:47:ARG:HB3	1.95	0.48
25:k:23:LEU:CG	31:l:67:LEU:CD2	2.74	0.48
4:A:273:ASP:OD2	26:c:138:LYS:NZ	2.43	0.48
4:A:1320:LEU:HD11	4:A:1366:ARG:HB3	1.95	0.48
27:d:21:LEU:O	27:d:28:THR:HA	2.13	0.48
4:A:916:LEU:HD22	4:A:940:ILE:HG13	1.95	0.48
13:M:78:LYS:HE3	13:M:197:GLU:OE2	2.14	0.48
32:m:36:ASP:HA	32:m:39:VAL:HG12	1.95	0.48
4:A:512:GLU:HG3	4:A:513:GLU:HG2	1.95	0.48
4:A:623:ARG:NH1	4:A:624:GLU:OE2	2.47	0.48
4:A:966:PRO:HD2	15:O:50:LEU:HD11	1.95	0.48
4:A:973:GLU:OE2	4:A:975:TYR:HA	2.14	0.48
5:C:148:SER:HA	5:C:151:ASP:OD2	2.14	0.48
21:W:156:PHE:HB3	23:Y:94:PHE:HD1	1.77	0.48
5:C:604:LYS:HZ1	5:C:973:ARG:NH1	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:415:PRO:HB2	22:X:1:UNK:CB	2.44	0.48
13:M:8:SER:HA	13:M:61:LYS:H	1.78	0.48
20:V:715:VAL:HG11	20:V:725:LEU:HB3	1.96	0.48
21:W:156:PHE:N	21:W:156:PHE:CD1	2.82	0.48
24:a:221:MET:HG3	24:a:227:ARG:HG3	1.95	0.48
32:m:41:ARG:NH2	32:m:41:ARG:CG	2.72	0.48
10:J:359:ASN:HB3	10:J:363:VAL:H	1.78	0.47
13:M:246:SER:HA	14:N:86:LEU:HD21	1.97	0.47
25:b:96:VAL:HG11	31:h:82:LEU:HD13	1.94	0.47
2:5:85:U:H2'	2:5:86:G:H8	1.79	0.47
4:A:1268:ARG:HH12	4:A:1270:LEU:HD22	1.78	0.47
7:E:17:U:H5'	20:V:779:LYS:CD	2.40	0.47
13:M:55:PRO:HG2	13:M:166:ARG:HB3	1.96	0.47
20:V:511:GLY:O	20:V:515:GLN:CG	2.63	0.47
25:k:21:ARG:CD	31:l:68:THR:HA	2.43	0.47
29:q:31:LEU:HD22	29:q:36:THR:HB	1.95	0.47
3:6:81:G:H2'	3:6:82:A:H8	1.79	0.47
4:A:776:GLN:HE22	18:S:64:ASP:HA	1.79	0.47
4:A:1379:MET:HE3	7:E:-5:G:OP1	2.14	0.47
4:A:2056:ARG:NH1	26:c:326:GLN:HE21	2.12	0.47
10:J:224:LEU:HD23	16:P:12:ARG:HG3	1.95	0.47
12:L:8:ARG:NH1	12:L:9:SER:HB3	2.28	0.47
20:V:565:ARG:O	20:V:992:ARG:NH2	2.39	0.47
24:a:175:GLU:HG2	24:a:178:LEU:HD12	1.96	0.47
32:m:102:ILE:HG22	32:m:103:VAL:HG23	1.96	0.47
31:h:27:GLY:HA3	31:h:40:LEU:HD22	1.97	0.47
35:v:108:LYS:C	35:v:110:SER:N	2.70	0.47
1:2:144:G:H4'	21:W:122:ARG:NH1	2.29	0.47
4:A:1486:ARG:HH11	8:H:383:ARG:NH2	2.12	0.47
5:C:242:VAL:HG23	5:C:277:LEU:HD11	1.96	0.47
13:M:53:LEU:HD22	13:M:55:PRO:HG3	1.96	0.47
21:W:35:GLN:HG2	23:Y:77:ARG:HH12	1.80	0.47
21:W:156:PHE:N	21:W:156:PHE:HD1	2.13	0.47
26:c:279:GLY:H	26:c:291:HIS:CD2	2.32	0.47
33:o:212:LEU:HD23	33:o:223:SER:HA	1.95	0.47
4:A:745:THR:OG1	4:A:745:THR:O	2.29	0.47
14:N:215:PRO:HD2	14:N:218:LYS:HD3	1.96	0.47
29:f:50:ASN:ND2	29:f:75:CYS:SG	2.87	0.47
33:o:387:ILE:HG23	33:o:430:THR:HA	1.96	0.47
1:2:1165:C:C3'	21:W:118:ARG:NH1	2.77	0.47
3:6:89:U:H4'	3:6:90:U:OP1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:203:ASN:HD22	4:A:559:GLN:HE22	1.63	0.47
5:C:182:LYS:HA	5:C:185:ILE:HD12	1.97	0.47
5:C:970:THR:CG2	5:C:973:ARG:HH11	2.28	0.47
20:V:957:TYR:CD2	20:V:1064:TYR:CD1	3.02	0.47
25:b:34:LEU:HD11	25:b:43:LEU:HD22	1.97	0.47
28:e:30:TRP:H	28:e:89:LEU:HB2	1.80	0.47
29:f:29:VAL:HG11	29:f:73:ILE:HG21	1.97	0.47
20:V:739:GLN:O	20:V:742:ILE:HG22	2.15	0.47
26:c:266:TYR:HD1	26:c:273:TYR:HB3	1.80	0.47
32:j:45:ILE:HB	32:j:105:LEU:HG	1.96	0.47
32:j:49:ARG:HB2	32:j:100:SER:HB3	1.97	0.47
30:r:43:ALA:N	30:r:56:GLN:O	2.42	0.47
4:A:1535:LYS:HE3	7:E:9:C:OP1	2.15	0.47
12:L:98:THR:HA	12:L:101:GLU:OE2	2.15	0.47
21:W:125:LYS:HD2	21:W:152:GLU:HG2	1.95	0.47
31:l:96:ILE:N	31:l:96:ILE:CD1	2.78	0.47
33:o:207:LYS:HB2	33:o:227:ASP:HB2	1.97	0.47
33:o:359:ARG:HG2	33:o:378:LYS:HA	1.96	0.47
34:s:99:ASP:CB	35:v:81:LEU:CA	2.89	0.47
2:5:147:C:H2'	2:5:148:G:C8	2.50	0.47
2:5:147:C:H2'	2:5:148:G:H8	1.79	0.47
4:A:611:LYS:HA	4:A:614:ARG:NH1	2.30	0.47
4:A:768:GLU:OE2	10:J:310:SER:N	2.49	0.47
4:A:2080:LYS:NZ	4:A:2093:VAL:HG13	2.28	0.47
5:C:273:LEU:HD21	5:C:287:LYS:HG2	1.97	0.47
11:K:170:SER:O	11:K:185:ARG:NH1	2.47	0.47
15:O:91:MET:HB3	15:O:93:ARG:HD2	1.97	0.47
20:V:610:VAL:HG23	20:V:837:GLU:OE1	2.14	0.47
32:m:76:TRP:CE2	32:m:87:ARG:HB3	2.50	0.47
34:s:115:GLY:O	34:s:119:SER:CB	2.63	0.47
1:2:1166:G:H5'	21:W:119:ARG:HD3	1.96	0.46
2:5:48:G:H1	2:5:67:U:H3	1.63	0.46
4:A:191:VAL:HG11	4:A:562:ILE:HG12	1.97	0.46
8:H:451:PRO:HB2	8:H:454:GLY:HA3	1.97	0.46
10:J:362:ASP:OD2	10:J:379:LYS:HE3	2.15	0.46
4:A:965:LYS:N	4:A:988:GLU:OE2	2.47	0.46
10:J:131:LEU:HD11	10:J:424:LYS:HD3	1.96	0.46
12:L:95:TRP:HE1	12:L:103:LEU:HB3	1.79	0.46
14:N:204:SER:OG	14:N:293:TRP:O	2.33	0.46
15:O:530:VAL:O	15:O:533:LEU:N	2.48	0.46
18:S:346:ILE:CB	18:S:366:LEU:O	2.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:646:TYR:HB2	20:V:864:MET:CE	2.44	0.46
21:W:92:ARG:HD3	21:W:119:ARG:HE	1.80	0.46
4:A:1652:HIS:HD2	24:a:198:THR:HB	1.80	0.46
4:A:2080:LYS:NZ	4:A:2093:VAL:HG22	2.31	0.46
13:M:173:ILE:HG12	13:M:184:VAL:HG13	1.96	0.46
3:6:53:A:N7	3:6:58:C:N4	2.63	0.46
4:A:1461:TYR:HD2	20:V:302:LEU:HD21	1.81	0.46
5:C:463:THR:HG23	5:C:590:LYS:NZ	2.30	0.46
19:T:463:ILE:O	19:T:466:ALA:HB3	2.15	0.46
20:V:480:ARG:HE	20:V:551:GLU:CD	2.23	0.46
33:o:174:THR:HB	33:o:176:HIS:HD2	1.80	0.46
5:C:397:LYS:HD3	5:C:413:LEU:HD21	1.98	0.46
5:C:943:ASP:HB2	5:C:946:ASP:HB2	1.97	0.46
9:I:10:A:N3	13:M:44:ASN:ND2	2.63	0.46
10:J:296:VAL:HG21	11:K:69:ARG:NH1	2.31	0.46
15:O:176:LEU:HD21	33:o:315:LYS:NZ	2.31	0.46
20:V:566:PHE:CD2	20:V:996:VAL:HA	2.50	0.46
29:f:27:VAL:HA	29:f:82:ARG:O	2.15	0.46
25:k:44:VAL:HG11	27:n:10:LEU:HD13	1.98	0.46
34:s:12:ILE:C	34:s:14:ASP:H	2.24	0.46
3:6:52:G:H5''	15:O:166:LYS:HD2	1.97	0.46
4:A:1705:SER:OG	4:A:1707:HIS:O	2.28	0.46
7:E:-1:G:H5''	7:E:1:A:OP2	2.16	0.46
15:O:550:PRO:O	15:O:554:GLU:C	2.52	0.46
29:f:76:ASN:ND2	32:j:99:ASP:O	2.41	0.46
2:5:169:U:H1'	30:g:66:ASN:HB2	1.97	0.46
4:A:863:ARG:O	4:A:1101:TYR:OH	2.29	0.46
10:J:275:THR:OG1	10:J:279:PRO:O	2.29	0.46
14:N:203:LYS:HD3	14:N:256:SER:HA	1.98	0.46
21:W:71:SER:HA	21:W:94:LEU:HD13	1.98	0.46
26:c:131:LYS:HD2	26:c:133:LYS:HZ2	1.80	0.46
28:e:88:THR:HG22	28:e:89:LEU:HD12	1.97	0.46
32:m:26:PHE:CE1	32:m:61:PHE:CD1	3.02	0.46
4:A:164:ALA:HB1	4:A:199:ILE:HB	1.97	0.46
4:A:1048:VAL:HG22	4:A:1250:VAL:HG22	1.97	0.46
4:A:1562:PHE:O	4:A:1565:THR:OG1	2.31	0.46
4:A:1608:LEU:HD21	4:A:1648:ILE:HD11	1.97	0.46
9:I:65:U:H2'	9:I:66:A:H8	1.80	0.46
10:J:244:ARG:NH1	16:P:8:GLN:OE1	2.48	0.46
33:o:358:ASN:HD22	33:o:382:SER:H	1.64	0.46
33:o:423:ILE:HB	33:o:429:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:p:92:SER:OG	28:p:93:ALA:N	2.49	0.46
10:J:252:ASP:OD2	11:K:78:VAL:HG21	2.16	0.46
11:K:119:MET:HE2	14:N:28:ILE:HG23	1.98	0.46
2:5:103:A:OP2	4:A:675:HIS:HE1	1.99	0.46
2:5:107:C:O2'	10:J:213:LYS:NZ	2.44	0.46
3:6:21:U:H2'	3:6:22:G:C8	2.52	0.46
4:A:229:ARG:HB2	26:c:136:MET:HE1	1.98	0.46
4:A:1406:LEU:HB3	4:A:1425:PHE:HB3	1.98	0.46
9:I:61:U:H2'	9:I:62:A:C8	2.51	0.46
10:J:111:ILE:HG12	10:J:114:ARG:NH1	2.21	0.46
31:l:10:LEU:HD22	31:l:97:LEU:HD22	1.98	0.46
4:A:928:ARG:HH11	7:E:4:U:C5'	2.01	0.45
20:V:525:PHE:CG	20:V:526:SER:N	2.84	0.45
28:e:34:GLN:HA	29:f:32:LYS:HZ2	1.81	0.45
32:m:55:ILE:HG23	32:m:73:LYS:HB3	1.96	0.45
4:A:1211:SER:O	4:A:1257:ASN:ND2	2.50	0.45
4:A:1361:VAL:HG11	17:R:16:THR:HG22	1.98	0.45
10:J:259:VAL:O	11:K:81:LYS:NZ	2.47	0.45
21:W:80:LEU:HA	21:W:102:THR:HG22	1.97	0.45
33:o:207:LYS:NZ	33:o:228:ARG:HH22	2.13	0.45
1:2:31:A:H1'	22:X:68:UNK:CB	2.47	0.45
4:A:681:LYS:O	4:A:684:LYS:HB3	2.16	0.45
14:N:77:ASP:OD2	14:N:80:TRP:N	2.45	0.45
18:S:115:ILE:HD13	18:S:146:LEU:HD21	1.97	0.45
23:Y:48:LEU:HD22	23:Y:52:PHE:HE2	1.82	0.45
28:e:13:PRO:HG3	30:g:39:VAL:HG23	1.97	0.45
30:g:17:LEU:HB2	30:g:25:VAL:HB	1.99	0.45
1:2:1150:U:O2'	27:n:53:GLN:CD	2.59	0.45
4:A:576:HIS:O	4:A:580:ASN:HB2	2.16	0.45
5:C:257:ILE:HG21	5:C:300:LYS:NZ	2.31	0.45
5:C:759:SER:CB	17:R:78:SER:CB	2.94	0.45
11:K:115:VAL:HG21	14:N:24:ARG:HH11	1.81	0.45
19:T:444:GLY:CA	19:T:483:ASP:CA	2.95	0.45
20:V:642:LYS:C	20:V:864:MET:CE	2.77	0.45
26:c:124:ASN:ND2	26:c:137:GLU:O	2.49	0.45
33:o:272:ILE:HD11	33:o:296:ILE:HG21	1.98	0.45
4:A:139:LEU:HD22	4:A:562:ILE:HG21	1.99	0.45
4:A:1668:ILE:HD13	4:A:1801:SER:HB3	1.98	0.45
4:A:1690:LYS:NZ	4:A:1735:ASP:OD1	2.50	0.45
10:J:169:LEU:HD21	10:J:415:ILE:HD11	1.97	0.45
18:S:160:CYS:HB3	18:S:169:TRP:CH2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:511:GLY:O	20:V:515:GLN:CB	2.65	0.45
33:o:161:HIS:CD2	33:o:185:HIS:HB2	2.52	0.45
30:r:45:GLU:HB3	30:r:53:ASN:HB2	1.97	0.45
4:A:350:PRO:HA	4:A:523:GLN:HG3	1.97	0.45
4:A:856:TRP:CD1	16:P:174:VAL:HG11	2.52	0.45
4:A:1050:LEU:HD11	4:A:1227:PHE:HD1	1.82	0.45
4:A:1315:ARG:NE	4:A:1338:SER:OG	2.49	0.45
12:L:3:ARG:HH11	12:L:84:GLU:CD	2.21	0.45
20:V:791:GLN:CG	20:V:1074:LEU:CD2	2.95	0.45
21:W:88:GLU:OE2	21:W:116:ARG:NH1	2.50	0.45
28:p:27:VAL:HA	28:p:92:SER:HA	1.98	0.45
1:2:42:U:H2'	1:2:43:G:H8	1.81	0.45
2:5:67:U:H2'	2:5:68:A:C8	2.52	0.45
4:A:207:ARG:HB3	4:A:493:MET:HB3	1.99	0.45
5:C:130:PRO:HB3	5:C:558:LYS:HD2	1.98	0.45
6:D:158:GLN:HA	6:D:161:ASP:OD2	2.16	0.45
10:J:271:GLN:HG2	10:J:314:THR:H	1.80	0.45
27:n:34:VAL:HG21	27:n:45:ARG:HD3	1.97	0.45
33:o:165:THR:H	33:o:182:GLY:HA2	1.82	0.45
33:o:256:ARG:HH22	33:o:323:GLN:H	1.64	0.45
4:A:651:ASP:OD2	4:A:700:GLY:N	2.49	0.45
4:A:750:LEU:O	4:A:754:TYR:CB	2.65	0.45
4:A:1122:ASP:OD1	4:A:1161:TYR:OH	2.28	0.45
4:A:1590:LEU:HD12	4:A:1591:THR:H	1.82	0.45
4:A:1618:ASN:N	4:A:1744:ASP:OD2	2.32	0.45
5:C:445:PRO:O	5:C:449:PHE:HB3	2.16	0.45
5:C:777:ASP:HB2	5:C:821:LEU:HA	1.97	0.45
5:C:806:GLY:HA3	5:C:813:ILE:HD11	1.98	0.45
8:H:355:HIS:CD2	8:H:357:SER:H	2.35	0.45
10:J:308:LYS:NZ	11:K:150:ASP:HB3	2.32	0.45
18:S:250:PHE:CE2	18:S:266:LEU:CB	3.00	0.45
25:k:35:MET:HB2	25:k:44:VAL:HG23	1.98	0.45
31:l:15:VAL:HG11	31:l:95:ILE:HD11	1.98	0.45
3:6:92:C:OP1	18:S:134:LYS:NZ	2.43	0.45
4:A:135:PRO:HB3	12:L:56:HIS:CD2	2.52	0.45
4:A:396:ARG:NE	5:C:667:GLU:OE2	2.50	0.45
4:A:975:TYR:H	4:A:1314:SER:HB3	1.82	0.45
4:A:1216:ILE:HG13	4:A:1254:ASN:HB3	1.99	0.45
5:C:250:GLU:OE2	5:C:903:ARG:NH2	2.45	0.45
5:C:806:GLY:N	5:C:811:GLU:O	2.44	0.45
7:E:5:C:P	7:E:5:C:H3'	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:91:A:H4'	9:I:92:C:H5'	1.99	0.45
10:J:147:ILE:HD11	10:J:169:LEU:HD11	1.98	0.45
15:O:20:ILE:HD11	15:O:152:LEU:HD23	1.98	0.45
20:V:989:HIS:CD2	20:V:989:HIS:C	2.95	0.45
21:W:77:HIS:NE2	25:k:76:LYS:CD	2.79	0.45
24:a:120:ILE:HG21	24:a:236:LEU:HB3	1.98	0.45
27:d:65:ARG:HD2	30:g:36:LEU:HD23	1.99	0.45
29:f:80:TYR:HE2	29:f:82:ARG:HD2	1.82	0.45
28:p:31:LEU:HD12	28:p:37:ILE:HG23	1.97	0.45
2:5:40:C:N4	4:A:541:ASN:O	2.49	0.45
4:A:814:ARG:NH1	10:J:398:GLY:O	2.49	0.45
4:A:1198:SER:HB2	4:A:1215:LEU:HD13	1.99	0.45
5:C:786:GLU:O	5:C:790:LYS:HB2	2.16	0.45
11:K:117:LYS:HE3	14:N:28:ILE:HD11	1.99	0.45
24:a:117:ILE:HG13	24:a:167:LEU:HD21	1.99	0.45
2:5:50:G:H2'	2:5:51:G:H8	1.82	0.44
4:A:765:ASP:OD1	10:J:312:ARG:NH2	2.35	0.44
4:A:1035:LEU:HB2	4:A:1038:ILE:HB	1.98	0.44
4:A:1647:GLN:NE2	9:I:92:C:O5'	2.50	0.44
20:V:785:ALA:HB1	20:V:871:LEU:HD13	1.37	0.44
27:n:44:LEU:HB3	27:n:62:ILE:HG22	1.99	0.44
33:o:308:PHE:HD2	33:o:320:TRP:HB2	1.82	0.44
2:5:96:U:OP1	4:A:1370:ARG:NH2	2.48	0.44
4:A:882:ILE:HD11	4:A:1238:LEU:HD11	1.98	0.44
4:A:1377:SER:OG	4:A:1382:ARG:NH1	2.46	0.44
5:C:826:PRO:HD2	5:C:834:MET:HE1	2.00	0.44
7:E:5:C:OP2	7:E:5:C:H3'	2.16	0.44
10:J:111:ILE:HD12	18:S:195:ALA:HA	2.00	0.44
14:N:222:THR:HG21	14:N:283:ILE:HG12	2.00	0.44
15:O:76:LEU:O	15:O:80:LEU:N	2.42	0.44
20:V:783:TYR:CD2	20:V:871:LEU:HG	2.51	0.44
21:W:50:LEU:CB	21:W:73:ARG:NH1	2.80	0.44
28:e:31:LEU:HD11	28:e:39:ILE:HG12	2.00	0.44
27:n:21:LEU:O	27:n:29:TYR:N	2.45	0.44
29:q:58:GLU:HB3	29:q:65:HIS:HB3	1.98	0.44
4:A:1182:LEU:HG	4:A:1225:ALA:HB1	1.98	0.44
4:A:1895:HIS:CD2	4:A:1897:SER:H	2.35	0.44
5:C:304:PHE:HD1	5:C:310:ASN:HB3	1.83	0.44
7:E:17:U:C4'	20:V:779:LYS:HB3	2.47	0.44
10:J:309:ARG:HH11	10:J:328:THR:CG2	2.31	0.44
15:O:65:PHE:CD2	15:O:101:ARG:HG2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:209:GLU:HB3	18:S:218:THR:HG22	1.99	0.44
21:W:9:ILE:O	21:W:12:PRO:HD2	2.18	0.44
28:e:78:GLY:H	29:f:82:ARG:HH11	1.65	0.44
32:m:75:LEU:CD1	32:m:88:GLU:HB3	2.44	0.44
33:o:309:ILE:HD13	33:o:351:PHE:HE1	1.81	0.44
2:5:81:A:H4'	2:5:82:A:OP2	2.18	0.44
4:A:910:LYS:HA	4:A:913:VAL:HG12	1.99	0.44
4:A:1306:GLU:HG2	4:A:1310:LYS:HE3	2.00	0.44
4:A:1904:ARG:H	9:I:1:G:H5''	1.82	0.44
13:M:204:LEU:HG	13:M:221:LEU:HD11	1.99	0.44
23:Y:29:THR:OG1	23:Y:108:THR:CG2	2.66	0.44
32:j:45:ILE:HG12	32:j:55:ILE:HG12	1.99	0.44
4:A:225:ARG:HE	26:c:136:MET:HG2	1.82	0.44
4:A:569:LEU:HD21	4:A:637:VAL:HG21	2.00	0.44
4:A:1515:LYS:HB3	4:A:1519:LEU:HD12	2.00	0.44
4:A:1667:GLN:O	4:A:1671:GLY:N	2.50	0.44
5:C:226:ALA:HB2	5:C:598:ILE:HG13	2.00	0.44
5:C:286:LEU:HD13	8:H:182:GLN:CB	2.47	0.44
10:J:156:ILE:HD11	10:J:164:MET:HB3	2.00	0.44
12:L:126:ARG:N	12:L:157:ASP:OD2	2.49	0.44
20:V:484:PRO:HD3	20:V:658:LYS:HE2	1.42	0.44
33:o:390:ALA:HB1	33:o:434:TRP:HD1	1.82	0.44
5:C:133:ILE:HA	5:C:209:MET:O	2.18	0.44
14:N:206:PHE:HD2	14:N:291:ILE:HD12	1.83	0.44
15:O:200:ILE:HG21	18:S:45:GLU:HG3	1.99	0.44
15:O:214:ASN:ND2	18:S:48:ARG:HB2	2.33	0.44
20:V:735:PRO:HG2	20:V:937:TYR:OH	2.18	0.44
33:o:300:LYS:HB2	33:o:309:ILE:HB	1.99	0.44
1:2:23:U:OP1	4:A:790:TRP:NE1	2.48	0.44
4:A:1651:ALA:HB2	24:a:200:VAL:HG12	1.98	0.44
4:A:1708:GLU:OE2	4:A:1728:ILE:HD11	2.17	0.44
4:A:1885:LYS:O	4:A:2001:SER:OG	2.34	0.44
4:A:1935:VAL:HG22	4:A:1958:PRO:HA	2.00	0.44
5:C:544:LEU:HG	5:C:553:VAL:HG21	1.99	0.44
31:l:66:TYR:CD1	31:l:66:TYR:O	2.70	0.44
33:o:204:GLY:O	33:o:231:LYS:NZ	2.32	0.44
2:5:101:C:OP1	4:A:672:LYS:N	2.46	0.44
4:A:420:PRO:HG2	4:A:423:PHE:HB3	2.00	0.44
4:A:2009:THR:HG21	4:A:2083:ILE:HG12	1.99	0.44
4:A:2080:LYS:HZ2	4:A:2093:VAL:HG22	1.83	0.44
5:C:193:LEU:HD12	5:C:213:LEU:HD22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:504:THR:O	5:C:507:SER:OG	2.33	0.44
10:J:144:CYS:HB2	10:J:187:ASP:HA	1.99	0.44
12:L:65:THR:HG23	12:L:69:LYS:HD2	2.00	0.44
13:M:87:CYS:HB3	13:M:91:HIS:NE2	2.32	0.44
21:W:80:LEU:HD13	23:Y:53:ALA:HB1	1.99	0.44
21:W:81:LEU:C	21:W:84:ASN:ND2	2.76	0.44
23:Y:29:THR:HA	23:Y:75:THR:HA	2.00	0.44
2:5:107:C:O3'	10:J:213:LYS:NZ	2.48	0.44
3:6:67:C:H5''	3:6:68:C:OP2	2.18	0.44
4:A:676:GLN:HG2	4:A:714:PHE:HB2	2.00	0.44
4:A:1405:ILE:HG23	4:A:1439:THR:HG21	1.99	0.44
4:A:1747:ASP:OD2	4:A:1750:ARG:HD3	2.17	0.44
5:C:473:LEU:HD12	5:C:485:LEU:HG	1.99	0.44
13:M:117:PHE:HE2	13:M:127:ILE:HD12	1.83	0.44
13:M:234:ALA:HA	13:M:237:ARG:HE	1.81	0.44
19:T:508:LEU:O	19:T:511:ALA:HB3	2.17	0.44
20:V:515:GLN:HB3	20:V:519:TYR:CZ	2.52	0.44
29:f:44:SER:OG	29:f:52:GLN:OE1	2.33	0.44
33:o:442:VAL:O	33:o:454:CYS:N	2.39	0.44
4:A:465:GLU:OE2	5:C:399:LEU:HD11	2.18	0.43
4:A:735:GLU:O	11:K:131:ALA:N	2.42	0.43
4:A:1920:LEU:O	4:A:1923:SER:OG	2.33	0.43
18:S:141:ILE:HD13	18:S:141:ILE:HA	1.87	0.43
21:W:65:ILE:HG23	21:W:66:MET:HG3	1.99	0.43
25:b:85:THR:HG22	27:d:73:VAL:HA	1.99	0.43
25:k:38:ASP:OD1	25:k:42:ASN:N	2.47	0.43
33:o:161:HIS:HB3	33:o:163:GLU:H	1.83	0.43
28:p:38:ARG:O	28:p:60:ILE:N	2.39	0.43
4:A:630:LYS:HG2	4:A:634:ASP:OD2	2.18	0.43
5:C:354:TYR:HB2	5:C:372:THR:HG22	2.00	0.43
5:C:760:LEU:HD23	17:R:78:SER:CB	2.48	0.43
7:E:17:U:H5'	20:V:779:LYS:HB3	1.99	0.43
14:N:33:GLU:HB3	14:N:38:THR:HA	2.00	0.43
14:N:131:GLU:HA	14:N:134:ASN:HD22	1.83	0.43
18:S:346:ILE:HA	18:S:366:LEU:CA	2.46	0.43
21:W:44:PRO:HB3	21:W:47:LEU:HD13	1.99	0.43
30:r:43:ALA:HB3	30:r:56:GLN:H	1.83	0.43
3:6:51:A:N1	9:I:95:G:O2'	2.50	0.43
4:A:966:PRO:HB3	4:A:1089:VAL:HB	2.00	0.43
11:K:120:ASP:OD2	11:K:123:LEU:HG	2.18	0.43
18:S:219:ARG:HE	18:S:253:TRP:HZ3	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:388:PHE:CB	18:S:410:TYR:CB	2.96	0.43
31:l:16:THR:HG22	31:l:26:TRP:CD1	2.50	0.43
32:m:54:ILE:HG23	32:m:72:VAL:HG13	2.01	0.43
27:n:11:LEU:HD11	27:n:72:ILE:HD13	1.99	0.43
35:u:107:LYS:C	35:u:109:LEU:H	2.25	0.43
4:A:902:PRO:HD2	4:A:905:TYR:HB2	1.99	0.43
5:C:514:GLN:NE2	5:C:587:LYS:O	2.51	0.43
6:D:172:LYS:HD3	15:O:3:PRO:HG3	1.99	0.43
8:H:471:LEU:HB3	8:H:473:LEU:HG	2.00	0.43
11:K:137:PRO:HG2	14:N:116:LYS:HB3	2.01	0.43
13:M:115:GLU:HB3	14:N:35:LYS:HE3	2.00	0.43
21:W:84:ASN:HB2	21:W:86:ILE:HG13	1.96	0.43
26:c:280:ALA:HB3	26:c:288:PHE:HB2	1.99	0.43
29:f:43:VAL:HG21	29:f:54:ASN:HD22	1.83	0.43
33:o:380:HIS:CE1	33:o:410:TRP:HE1	2.37	0.43
30:r:28:ILE:O	30:r:41:ASP:N	2.48	0.43
30:r:37:ASN:OD1	30:r:65:GLY:N	2.41	0.43
2:5:115:G:H4'	4:A:492:LYS:NZ	2.33	0.43
3:6:85:C:O2	16:P:3:THR:OG1	2.31	0.43
4:A:1648:ILE:HD13	4:A:1819:ILE:HG12	2.00	0.43
12:L:156:THR:O	33:o:60:ARG:NE	2.50	0.43
14:N:79:ARG:HH12	14:N:129:PRO:HA	1.83	0.43
14:N:91:ILE:HD13	14:N:125:ILE:HD13	2.01	0.43
15:O:69:GLU:HA	15:O:72:GLN:HG2	2.00	0.43
33:o:266:GLY:HA2	33:o:272:ILE:HG12	2.01	0.43
2:5:125:C:OP2	12:L:96:ARG:NH2	2.42	0.43
4:A:165:LEU:HD13	4:A:582:LEU:HD12	1.99	0.43
4:A:177:GLU:OE2	4:A:497:GLN:NE2	2.52	0.43
4:A:1563:LYS:HB2	26:c:85:LEU:HD23	2.00	0.43
5:C:769:TYR:OH	5:C:804:LYS:NZ	2.35	0.43
20:V:957:TYR:CE1	20:V:1064:TYR:CZ	3.06	0.43
21:W:103:LEU:O	21:W:106:ASN:ND2	2.51	0.43
25:b:16:ILE:HG13	25:b:34:LEU:HD22	1.99	0.43
33:o:340:PRO:HG2	33:o:356:MET:HE3	2.00	0.43
2:5:96:U:H3	7:E:-1:G:H1	1.65	0.43
4:A:465:GLU:OE2	5:C:395:LYS:HE2	2.19	0.43
4:A:1630:THR:HG21	4:A:1649:PHE:HB3	2.01	0.43
14:N:105:LYS:N	15:O:216:ASP:OD2	2.41	0.43
20:V:621:LYS:CE	20:V:861:PHE:CD1	2.81	0.43
23:Y:31:TYR:N	23:Y:102:GLU:O	2.49	0.43
32:m:62:ASP:CB	32:m:66:ASN:HB2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:r:15:ILE:HD11	30:r:40:LEU:HD21	2.01	0.43
4:A:495:ARG:CZ	4:A:497:GLN:HE21	2.31	0.43
4:A:1663:PHE:HD2	26:c:247:ARG:HG2	1.84	0.43
4:A:1862:VAL:HB	4:A:1870:VAL:HG12	2.00	0.43
4:A:2063:TYR:OH	6:D:158:GLN:NE2	2.51	0.43
5:C:664:ALA:HB1	5:C:666:ILE:HG12	2.00	0.43
10:J:278:ASP:N	10:J:278:ASP:OD1	2.52	0.43
10:J:331:ILE:HD12	10:J:376:TYR:HE2	1.83	0.43
15:O:174:ARG:NH1	18:S:53:GLU:OE2	2.52	0.43
21:W:15:TYR:OH	25:k:19:LYS:HD2	2.18	0.43
25:b:18:TYR:HA	25:b:101:PRO:HG3	2.00	0.43
25:b:50:GLU:CD	25:b:80:ARG:HH11	2.27	0.43
31:l:33:SER:HB3	31:l:37:ASN:H	1.84	0.43
32:m:26:PHE:CE2	32:m:61:PHE:CZ	3.06	0.43
4:A:1716:LEU:HD11	26:c:99:ILE:HD12	2.01	0.43
5:C:126:MET:HE1	5:C:208:ARG:HA	2.01	0.43
5:C:905:GLN:OE1	5:C:938:ARG:NH2	2.52	0.43
10:J:382:HIS:HD2	10:J:442:TRP:HE3	1.67	0.43
12:L:157:ASP:HB2	33:o:72:TRP:HZ2	1.83	0.43
20:V:932:VAL:HB	20:V:989:HIS:CE1	2.53	0.43
20:V:1100:LYS:HE2	20:V:1103:ASP:OD1	2.19	0.43
27:n:19:VAL:HG21	27:n:72:ILE:HD11	2.01	0.43
2:5:50:G:H2'	2:5:51:G:C8	2.54	0.43
4:A:849:LEU:HD11	4:A:973:GLU:HB2	2.00	0.43
5:C:962:LEU:O	5:C:965:ASP:HB3	2.19	0.43
10:J:330:ASP:N	10:J:330:ASP:OD1	2.52	0.43
15:O:54:GLU:OE2	15:O:85:ARG:NH1	2.46	0.43
19:T:444:GLY:HA3	19:T:483:ASP:CA	2.49	0.43
25:k:95:THR:HG23	31:l:86:ASN:HB3	2.01	0.43
30:r:27:GLY:HA3	30:r:40:LEU:HD13	2.01	0.43
2:5:36:A:OP1	4:A:553:ASN:ND2	2.52	0.42
4:A:805:PRO:HG2	4:A:808:ILE:HD12	2.01	0.42
4:A:886:MET:HG3	4:A:1069:LEU:HD22	2.01	0.42
15:O:187:LYS:HD2	33:o:313:GLU:OE2	2.19	0.42
21:W:154:LEU:O	21:W:157:GLN:HB2	2.19	0.42
28:e:38:ARG:O	28:e:59:GLU:HA	2.19	0.42
31:h:15:VAL:HG12	31:h:98:PRO:HD3	2.00	0.42
32:j:27:LYS:HA	32:j:32:SER:HB3	2.00	0.42
1:2:36:A:H2'	1:2:37:G:C8	2.54	0.42
4:A:565:VAL:HG21	4:A:640:ARG:HG3	2.01	0.42
4:A:1372:LYS:HD2	4:A:1378:LYS:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1626:GLN:HE21	4:A:1631:GLY:HA2	1.83	0.42
5:C:248:VAL:HG22	5:C:933:TRP:HH2	1.83	0.42
5:C:602:VAL:HG12	5:C:908:VAL:HG11	2.01	0.42
8:H:466:PHE:HD1	8:H:469:ILE:HD12	1.83	0.42
9:I:3:A:H5'	9:I:4:U:OP2	2.19	0.42
10:J:285:SER:OG	10:J:286:THR:N	2.53	0.42
18:S:467:GLN:CB	18:S:471:LEU:CB	2.93	0.42
20:V:586:ARG:NH2	20:V:902:PRO:HA	2.21	0.42
20:V:608:ARG:HH21	20:V:613:ASP:CG	2.27	0.42
25:b:33:GLN:HB2	25:b:46:ASN:HB3	2.01	0.42
27:d:10:LEU:HD12	27:d:83:LEU:HD11	2.00	0.42
33:o:229:SER:HA	33:o:244:LEU:O	2.19	0.42
4:A:1043:ARG:HB2	4:A:1045:GLN:HE22	1.85	0.42
10:J:141:TRP:HB2	10:J:160:ASN:ND2	2.34	0.42
13:M:55:PRO:HB3	13:M:93:ILE:HD11	2.01	0.42
14:N:57:LYS:HE2	14:N:59:LEU:HD21	2.01	0.42
15:O:216:ASP:O	18:S:83:ARG:NH2	2.52	0.42
20:V:483:LEU:HD21	20:V:515:GLN:HG3	2.00	0.42
20:V:949:LYS:HD3	20:V:950:LYS:N	2.34	0.42
21:W:57:LEU:HD12	21:W:76:ILE:HD13	2.02	0.42
25:b:26:ASP:CG	27:d:70:LYS:HZ3	2.17	0.42
32:j:62:ASP:OD2	32:j:66:ASN:HB2	2.20	0.42
31:l:61:ALA:O	31:l:63:ALA:N	2.51	0.42
33:o:387:ILE:HG12	33:o:430:THR:HG22	2.02	0.42
2:5:85:U:H2'	2:5:86:G:C8	2.53	0.42
2:5:143:U:H2'	2:5:144:G:C8	2.53	0.42
4:A:964:PHE:HB3	4:A:988:GLU:OE2	2.19	0.42
4:A:1257:ASN:OD1	4:A:1268:ARG:NH1	2.49	0.42
5:C:633:ILE:HG13	5:C:645:LEU:HB2	2.01	0.42
14:N:219:ILE:HG22	14:N:240:LEU:HD11	2.00	0.42
19:T:554:ALA:HA	22:X:205:UNK:HA	1.74	0.42
28:e:78:GLY:N	29:f:82:ARG:HH11	2.16	0.42
1:2:20:G:C2	16:P:6:ARG:HD3	2.55	0.42
1:2:25:A:O5'	4:A:854:ARG:NH2	2.53	0.42
1:2:1108:A:C6	23:Y:73:PHE:CE1	2.62	0.42
3:6:6:C:H2'	3:6:7:G:H8	1.85	0.42
4:A:431:ILE:HG12	5:C:895:ALA:HB1	2.02	0.42
4:A:775:ARG:HB2	4:A:779:ALA:HB2	2.02	0.42
4:A:1891:LEU:HD22	4:A:1974:LEU:HD22	2.01	0.42
4:A:1952:PRO:HG2	26:c:253:ALA:HB2	2.01	0.42
10:J:213:LYS:HE3	16:P:38:LYS:NZ	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:345:PHE:O	10:J:450:ARG:NH2	2.52	0.42
31:h:37:ASN:OD1	31:h:89:GLY:N	2.49	0.42
33:o:297:LEU:H	33:o:312:SER:HA	1.84	0.42
4:A:606:THR:HG1	4:A:609:GLU:H	1.63	0.42
4:A:1001:TYR:HD1	4:A:1506:ARG:HD3	1.84	0.42
4:A:1648:ILE:O	4:A:1818:ARG:NH1	2.46	0.42
5:C:120:ARG:NH1	5:C:158:HIS:HE1	2.08	0.42
20:V:483:LEU:HG	20:V:511:GLY:HA3	2.02	0.42
20:V:617:ALA:HB1	20:V:861:PHE:HE2	1.83	0.42
24:a:140:LYS:HE3	26:c:225:LYS:HG3	2.02	0.42
26:c:34:PRO:HD2	26:c:37:ILE:HD12	2.01	0.42
31:l:67:LEU:HD12	31:l:68:THR:CG2	2.49	0.42
2:5:36:A:H2'	2:5:37:C:C6	2.54	0.42
4:A:319:ARG:HA	4:A:504:LYS:NZ	2.35	0.42
4:A:935:GLU:HG3	15:O:8:VAL:HG12	2.02	0.42
4:A:1854:ASP:OD2	4:A:1940:MET:HB2	2.19	0.42
4:A:1865:THR:HG21	4:A:1871:ALA:HB3	2.01	0.42
5:C:223:ASP:O	5:C:226:ALA:HB3	2.20	0.42
5:C:318:LEU:HD23	5:C:318:LEU:HA	1.91	0.42
5:C:716:ASP:H	5:C:719:MET:HE2	1.84	0.42
10:J:317:HIS:NE2	10:J:362:ASP:OD1	2.34	0.42
13:M:196:LYS:HE2	13:M:224:LYS:HA	2.01	0.42
20:V:489:ARG:O	20:V:489:ARG:HD2	2.20	0.42
20:V:646:TYR:HB3	20:V:864:MET:SD	2.57	0.42
29:f:71:ILE:HD13	29:f:73:ILE:HG13	2.00	0.42
32:j:72:VAL:HB	32:j:91:ILE:HB	2.02	0.42
32:m:72:VAL:HG21	32:m:94:LEU:CB	2.50	0.42
33:o:377:PHE:HB3	33:o:410:TRP:CE2	2.55	0.42
4:A:343:ASN:HD21	17:R:9:LYS:HG2	1.85	0.42
4:A:517:LYS:NZ	4:A:685:HIS:CD2	2.88	0.42
4:A:666:ILE:HG13	4:A:673:VAL:HG21	2.01	0.42
4:A:905:TYR:OH	4:A:1002:GLU:OE2	2.31	0.42
4:A:1030:GLN:HE22	4:A:1288:LEU:HA	1.84	0.42
4:A:1687:HIS:CD2	4:A:1689:ARG:H	2.38	0.42
5:C:83:THR:OG1	10:J:174:LEU:O	2.26	0.42
5:C:760:LEU:HB2	17:R:75:VAL:HA	1.99	0.42
7:E:12:C:HO2'	7:E:13:U:P	2.33	0.42
7:E:16:A:H5'	20:V:792:LEU:HD13	2.02	0.42
19:T:119:ALA:HB1	19:T:128:ILE:CB	2.50	0.42
2:5:104:G:OP2	4:A:531:LEU:HD11	2.19	0.42
4:A:163:GLY:HA3	11:K:122:LEU:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:834:ILE:HD12	4:A:848:ASN:HD22	1.85	0.42
4:A:1548:GLN:HE21	8:H:294:LYS:HZ2	1.66	0.42
4:A:1694:MET:O	4:A:1759:TYR:OH	2.37	0.42
5:C:70:TYR:OH	10:J:392:MET:SD	2.65	0.42
5:C:106:PHE:CG	5:C:479:GLY:HA3	2.55	0.42
5:C:147:THR:HG21	5:C:179:ASP:OD2	2.19	0.42
29:f:16:LYS:HG3	29:f:17:PRO:HD3	2.01	0.42
30:g:10:TYR:HA	30:g:13:LYS:HE3	2.01	0.42
31:l:31:SER:HB2	31:l:39:ILE:HD11	2.01	0.42
32:m:49:ARG:HA	32:m:102:ILE:HD11	2.01	0.42
4:A:518:VAL:HG21	4:A:689:TYR:CD2	2.54	0.42
4:A:818:SER:HB3	10:J:141:TRP:CZ2	2.55	0.42
4:A:1483:SER:HA	4:A:1486:ARG:HE	1.84	0.42
4:A:1652:HIS:HB3	4:A:1655:GLN:HB3	2.01	0.42
4:A:1753:ARG:HE	26:c:99:ILE:HG12	1.85	0.42
5:C:103:HIS:ND1	5:C:104:THR:HG23	2.35	0.42
5:C:234:LEU:HD12	5:C:443:TYR:HB2	2.02	0.42
5:C:656:LEU:HB3	5:C:660:ARG:NH1	2.35	0.42
26:c:274:LYS:HD3	26:c:288:PHE:CZ	2.54	0.42
25:k:77:VAL:HG22	25:k:78:GLU:HG2	2.01	0.42
1:2:1166:G:H4'	21:W:119:ARG:HD2	1.91	0.41
4:A:199:ILE:HD13	4:A:578:MET:HE1	2.02	0.41
4:A:544:LYS:NZ	4:A:549:LYS:NZ	2.68	0.41
4:A:879:ALA:HB1	11:K:208:LEU:HD21	2.01	0.41
5:C:142:LEU:HD22	5:C:927:MET:HE2	2.01	0.41
5:C:223:ASP:OD2	5:C:631:GLY:HA3	2.20	0.41
5:C:472:VAL:HG22	5:C:486:VAL:HG22	2.01	0.41
5:C:915:GLU:HA	5:C:928:CYS:HB3	2.02	0.41
18:S:250:PHE:CD2	18:S:266:LEU:CB	3.03	0.41
20:V:586:ARG:NE	20:V:902:PRO:HG3	2.33	0.41
21:W:8:VAL:HG23	21:W:9:ILE:HG13	2.00	0.41
25:k:54:PRO:HB2	31:l:66:TYR:HD1	1.81	0.41
33:o:171:LEU:HD22	33:o:218:CYS:HB3	2.01	0.41
33:o:213:ARG:HG2	33:o:254:GLU:HG2	2.02	0.41
33:o:256:ARG:HA	33:o:257:PRO:HD3	1.94	0.41
4:A:1348:GLU:OE2	4:A:1447:TRP:HB2	2.19	0.41
5:C:175:LEU:O	5:C:177:TYR:N	2.53	0.41
5:C:605:ILE:HD13	5:C:656:LEU:HD11	2.01	0.41
8:H:396:GLU:HB3	8:H:440:ARG:NH1	2.34	0.41
10:J:313:ALA:O	10:J:325:SER:HA	2.20	0.41
15:O:227:ILE:HD12	36:y:152:ILE:HD12	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:V:957:TYR:CG	20:V:1064:TYR:CE1	3.08	0.41
24:a:222:ILE:H	24:a:222:ILE:HG13	1.63	0.41
25:k:29:VAL:CB	31:l:67:LEU:HB2	2.45	0.41
27:n:68:GLN:HG3	30:r:69:ILE:HA	2.03	0.41
1:2:1098:C:H4'	21:W:152:GLU:OE1	2.20	0.41
1:2:1165:C:C2'	21:W:118:ARG:CZ	2.98	0.41
1:2:1165:C:C5'	21:W:118:ARG:HH12	2.24	0.41
4:A:136:PRO:HB3	4:A:562:ILE:HG22	2.00	0.41
4:A:264:ILE:HD11	4:A:647:PHE:HA	2.01	0.41
4:A:628:MET:HE1	4:A:711:TRP:HB3	2.02	0.41
4:A:1027:LYS:O	4:A:1145:MET:HE1	2.21	0.41
4:A:1158:ILE:HG12	4:A:1172:PHE:CE1	2.55	0.41
5:C:268:ASN:HD22	5:C:269:LYS:H	1.68	0.41
5:C:634:ILE:HG12	5:C:644:ILE:HG12	2.02	0.41
5:C:964:ARG:NH1	5:C:985:ASP:HB3	2.19	0.41
10:J:291:ARG:HD3	10:J:300:THR:HG21	2.02	0.41
20:V:957:TYR:CE2	20:V:1085:SER:CA	3.03	0.41
33:o:234:ASP:HB2	33:o:238:GLY:H	1.85	0.41
30:r:70:SER:OG	30:r:71:LEU:N	2.53	0.41
1:2:33:U:H2'	1:2:34:G:H8	1.84	0.41
4:A:857:ILE:HD11	4:A:969:ILE:HD11	2.01	0.41
4:A:1063:PHE:HB2	15:O:83:GLN:NE2	2.35	0.41
4:A:1286:TRP:CD1	4:A:1448:GLU:HB2	2.55	0.41
4:A:1624:LEU:HG	4:A:1633:PHE:HB3	2.02	0.41
5:C:116:THR:HA	5:C:158:HIS:HA	2.01	0.41
5:C:604:LYS:HZ2	5:C:973:ARG:NH1	2.12	0.41
20:V:893:ASN:HA	20:V:896:LYS:HE3	2.03	0.41
30:g:55:HIS:HD2	30:g:57:LEU:HD23	1.85	0.41
33:o:272:ILE:HB	33:o:289:TYR:HB2	2.03	0.41
2:5:159:C:O2'	2:5:161:U:OP2	2.37	0.41
4:A:1165:LEU:HD11	4:A:1513:GLU:OE2	2.19	0.41
4:A:1998:ARG:HD3	4:A:2045:ASP:OD2	2.20	0.41
5:C:379:ILE:HD12	5:C:379:ILE:HA	1.91	0.41
5:C:772:ASN:OD1	5:C:772:ASN:N	2.52	0.41
7:E:9:C:C4'	7:E:10:U:OP2	2.66	0.41
10:J:245:ASP:OD1	10:J:245:ASP:N	2.52	0.41
10:J:307:HIS:NE2	10:J:325:SER:OG	2.38	0.41
19:T:339:PHE:CB	19:T:399:VAL:C	2.94	0.41
20:V:736:SER:HG	20:V:988:ARG:HE	1.62	0.41
21:W:50:LEU:HB3	21:W:73:ARG:HH22	1.85	0.41
21:W:81:LEU:O	21:W:84:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:n:37:GLU:HB2	27:n:41:ASN:HB2	2.02	0.41
4:A:1145:MET:HE3	4:A:1145:MET:HB2	1.70	0.41
4:A:1235:PRO:HD2	4:A:1238:LEU:HD12	2.03	0.41
4:A:1456:ARG:HH12	4:A:1486:ARG:NH1	2.19	0.41
4:A:1666:CYS:O	4:A:1670:ASP:N	2.48	0.41
5:C:512:LYS:O	5:C:515:LEU:HB2	2.20	0.41
5:C:602:VAL:HG11	5:C:908:VAL:HG21	2.03	0.41
10:J:356:LEU:HD22	10:J:364:LEU:HD21	2.02	0.41
18:S:50:LYS:HD3	18:S:50:LYS:HA	1.91	0.41
20:V:791:GLN:CD	20:V:1074:LEU:HD23	2.45	0.41
31:h:30:GLN:HB3	31:h:39:ILE:HB	2.03	0.41
32:m:97:ARG:HG3	32:m:99:ASP:H	1.86	0.41
33:o:169:LYS:HZ2	33:o:213:ARG:HD3	1.86	0.41
33:o:398:ILE:O	33:o:409:THR:HA	2.21	0.41
4:A:343:ASN:HD21	17:R:9:LYS:HA	1.85	0.41
4:A:1364:GLU:OE2	4:A:1389:TYR:OH	2.31	0.41
5:C:290:HIS:CE1	5:C:294:ASN:HD21	2.39	0.41
39:C:2501:GTP:O2A	39:C:2501:GTP:O1B	2.39	0.41
10:J:128:PRO:HG2	10:J:429:ASP:OD2	2.21	0.41
10:J:364:LEU:HB3	10:J:376:TYR:HB2	2.02	0.41
12:L:61:ARG:NH1	12:L:102:LYS:HA	2.35	0.41
32:j:69:LEU:HD12	32:j:94:LEU:HD22	2.03	0.41
27:n:47:VAL:HG13	27:n:59:MET:HB2	2.02	0.41
29:q:60:VAL:N	29:q:63:VAL:O	2.53	0.41
4:A:390:LEU:HB2	5:C:653:ASP:HB3	2.03	0.41
4:A:953:ARG:HH12	15:O:128:ILE:HD12	1.86	0.41
5:C:241:VAL:O	5:C:287:LYS:NZ	2.50	0.41
5:C:603:PHE:HD2	5:C:652:MET:HG3	1.84	0.41
8:H:347:LEU:O	8:H:351:MET:HG2	2.21	0.41
9:I:65:U:H2'	9:I:66:A:C8	2.56	0.41
10:J:145:VAL:HG22	10:J:157:THR:HG22	2.03	0.41
3:6:65:U:H3	3:6:82:A:H61	1.69	0.41
3:6:73:A:N7	3:6:75:A:N6	2.68	0.41
4:A:130:PRO:O	12:L:110:GLN:NE2	2.54	0.41
4:A:153:MET:HE3	4:A:154:TYR:CZ	2.56	0.41
4:A:400:ILE:HD11	5:C:657:TYR:CZ	2.55	0.41
4:A:454:LEU:HD23	4:A:454:LEU:HA	1.92	0.41
4:A:544:LYS:NZ	4:A:549:LYS:HZ2	2.19	0.41
4:A:968:ASP:O	4:A:983:SER:N	2.50	0.41
4:A:1019:GLU:OE2	4:A:1024:LEU:HD13	2.21	0.41
4:A:1348:GLU:HB3	4:A:1446:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1739:ARG:HH12	4:A:1751:TYR:HB2	1.86	0.41
4:A:2000:SER:HB2	4:A:2002:TYR:CE1	2.55	0.41
5:C:472:VAL:HB	5:C:575:ALA:HB3	2.03	0.41
5:C:656:LEU:HD23	5:C:659:LEU:HD12	2.02	0.41
5:C:875:ILE:O	5:C:878:GLU:HB2	2.20	0.41
5:C:877:GLU:O	5:C:881:LYS:N	2.54	0.41
8:H:290:VAL:HG13	26:c:43:TYR:HE2	1.86	0.41
10:J:329:ASP:OD1	10:J:350:THR:N	2.54	0.41
11:K:83:ALA:O	11:K:125:ARG:NH1	2.54	0.41
13:M:62:THR:HG21	13:M:91:HIS:HD2	1.86	0.41
20:V:727:ILE:C	20:V:727:ILE:HD12	2.46	0.41
24:a:211:ILE:H	24:a:211:ILE:HG13	1.79	0.41
32:j:40:THR:HG22	32:j:42:THR:HG23	2.02	0.41
25:k:30:TYR:HE2	25:k:87:LEU:HD13	1.85	0.41
31:l:10:LEU:CD1	31:l:97:LEU:CD2	2.98	0.41
36:y:156:ASP:OD1	36:y:156:ASP:N	2.53	0.41
2:5:67:U:H2'	2:5:68:A:H8	1.85	0.41
4:A:179:MET:HE3	4:A:632:ILE:HG23	2.03	0.41
4:A:1467:GLU:O	4:A:1471:GLN:N	2.44	0.41
5:C:567:ILE:HG22	5:C:571:TYR:HE1	1.86	0.41
5:C:610:LEU:HD12	5:C:669:LYS:HE3	2.03	0.41
13:M:69:GLN:OE1	14:N:53:ASN:ND2	2.54	0.41
17:R:7:GLY:HA2	17:R:20:VAL:HG21	2.03	0.41
19:T:509:GLU:O	19:T:512:LEU:N	2.54	0.41
20:V:609:THR:HA	20:V:837:GLU:OE1	2.20	0.41
20:V:891:LEU:H	20:V:891:LEU:CD2	2.34	0.41
21:W:156:PHE:CD2	23:Y:94:PHE:HE1	2.37	0.41
25:b:12:LEU:HD21	25:b:43:LEU:HD21	2.02	0.41
33:o:186:THR:HG21	33:o:203:GLN:HA	2.03	0.41
28:p:31:LEU:HD23	28:p:31:LEU:HA	1.93	0.41
29:q:26:ARG:HD3	29:q:39:ARG:HH12	1.86	0.41
1:2:25:A:C8	4:A:1093:LYS:HD2	2.56	0.40
2:5:169:U:O4'	30:g:64:ARG:NH2	2.54	0.40
3:6:64:U:O2'	18:S:60:ARG:O	2.38	0.40
4:A:666:ILE:HG23	4:A:673:VAL:HG11	2.03	0.40
4:A:1012:TRP:HB2	4:A:1162:THR:HA	2.03	0.40
4:A:1342:LEU:HD21	4:A:1356:LEU:HD11	2.02	0.40
5:C:681:CYS:SG	5:C:682:SER:N	2.94	0.40
5:C:760:LEU:HD12	17:R:75:VAL:CB	2.30	0.40
10:J:148:ASP:OD2	10:J:151:ASP:HB2	2.21	0.40
11:K:182:LEU:HD21	15:O:52:TRP:HH2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:S:83:ARG:O	18:S:87:ILE:HG12	2.21	0.40
18:S:136:TRP:CZ3	18:S:159:TRP:HB2	2.56	0.40
18:S:219:ARG:HH11	22:X:107:UNK:CA	2.31	0.40
20:V:566:PHE:HD2	20:V:996:VAL:HB	1.85	0.40
21:W:117:LEU:HD23	21:W:117:LEU:HA	1.90	0.40
31:l:47:LEU:HA	31:l:48:PRO:HD2	1.81	0.40
27:n:17:HIS:HB3	27:n:75:PRO:HG3	2.03	0.40
2:5:12:C:H2'	2:5:13:A:C8	2.57	0.40
2:5:21:G:H2'	2:5:22:G:C8	2.54	0.40
2:5:35:A:O2'	2:5:36:A:H8	2.04	0.40
4:A:477:MET:HE3	5:C:275:LEU:HD23	2.02	0.40
4:A:581:LEU:HD22	13:M:33:TRP:HE3	1.86	0.40
4:A:705:GLN:HE22	4:A:709:ARG:HD2	1.86	0.40
4:A:782:ILE:O	4:A:785:HIS:HB2	2.21	0.40
4:A:1107:LEU:HB2	4:A:1110:ALA:HB2	2.03	0.40
4:A:1228:TRP:HE1	16:P:135:ARG:HH11	1.69	0.40
4:A:1659:GLU:OE2	26:c:246:THR:N	2.55	0.40
4:A:1878:CYS:HB2	4:A:1891:LEU:HD11	2.03	0.40
4:A:1915:GLU:OE2	24:a:195:ILE:N	2.53	0.40
5:C:147:THR:OG1	39:C:2501:GTP:O2B	2.31	0.40
5:C:183:GLN:NE2	5:C:654:CYS:O	2.48	0.40
5:C:204:GLU:OE2	5:C:441:ARG:NH1	2.55	0.40
13:M:161:ARG:NH1	14:N:241:ILE:HG23	2.35	0.40
20:V:566:PHE:HB2	20:V:992:ARG:NH1	2.34	0.40
20:V:949:LYS:HG3	20:V:983:ASN:C	2.46	0.40
24:a:99:GLN:HA	24:a:102:SER:HB3	2.03	0.40
28:e:50:MET:HB2	28:e:84:GLY:HA3	2.03	0.40
32:j:56:ALA:HB1	32:j:69:LEU:HB3	2.02	0.40
31:l:44:LYS:HG3	31:l:44:LYS:O	2.20	0.40
4:A:763:MET:HB2	4:A:783:LEU:HD11	2.03	0.40
4:A:1064:THR:HG22	15:O:81:PRO:HD3	2.04	0.40
4:A:1270:LEU:HA	4:A:1271:PRO:HD3	1.91	0.40
4:A:1382:ARG:NH2	4:A:1635:HIS:O	2.43	0.40
4:A:1667:GLN:HB2	26:c:256:LEU:HD13	2.03	0.40
4:A:1908:LEU:HG	24:a:193:TRP:HH2	1.87	0.40
7:E:10:U:O2'	7:E:11:A:OP2	2.39	0.40
8:H:396:GLU:HB3	8:H:440:ARG:HH12	1.87	0.40
11:K:33:GLN:HA	11:K:36:LYS:HD3	2.03	0.40
12:L:145:CYS:SG	12:L:146:VAL:N	2.94	0.40
20:V:586:ARG:CD	20:V:902:PRO:HB3	2.47	0.40
25:k:93:LEU:HA	31:l:91:THR:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:l:45:LEU:HD23	31:l:45:LEU:H	1.82	0.40
33:o:63:ARG:NH1	33:o:68:PRO:O	2.54	0.40
36:y:195:PHE:HB3	36:y:204:ASN:HD22	1.87	0.40
3:6:82:A:H2'	3:6:83:A:H8	1.86	0.40
3:6:92:C:H5'	36:y:100:LEU:HD11	2.04	0.40
4:A:863:ARG:NH1	4:A:1059:GLU:O	2.54	0.40
4:A:1411:ASP:O	4:A:1415:SER:N	2.49	0.40
4:A:1753:ARG:NH2	26:c:174:TRP:O	2.33	0.40
5:C:222:MET:O	5:C:225:THR:HB	2.22	0.40
5:C:854:ILE:HA	5:C:855:PRO:HD3	1.96	0.40
8:H:367:GLU:HG2	8:H:405:ILE:HG12	2.03	0.40
13:M:62:THR:HG21	13:M:91:HIS:CD2	2.57	0.40
20:V:646:TYR:HB2	20:V:864:MET:HE3	2.04	0.40
24:a:107:PRO:HG3	24:a:153:ASN:HD22	1.86	0.40
27:d:15:GLN:HA	27:d:33:LEU:HD22	2.04	0.40
33:o:253:VAL:HG13	33:o:265:VAL:HG22	2.02	0.40
28:p:80:ILE:HG23	29:q:80:TYR:HB2	2.04	0.40
29:q:53:LEU:HB2	29:q:71:ILE:HG22	2.03	0.40
1:2:1108:A:N6	23:Y:73:PHE:CD1	2.88	0.40
4:A:266:LEU:HD22	26:c:138:LYS:HD3	2.02	0.40
4:A:2035:LYS:HB2	4:A:2038:HIS:ND1	2.37	0.40
5:C:85:SER:HA	5:C:86:PRO:HD3	1.91	0.40
5:C:286:LEU:CD1	8:H:182:GLN:CB	2.98	0.40
5:C:467:THR:OG1	5:C:579:SER:O	2.32	0.40
10:J:294:ASP:HB2	10:J:301:MET:HG3	2.04	0.40
13:M:174:ARG:HE	14:N:245:LYS:HG3	1.86	0.40
18:S:255:ALA:HA	18:S:260:TYR:CA	2.51	0.40
20:V:513:THR:HG22	20:V:544:VAL:HG21	2.03	0.40
21:W:84:ASN:O	21:W:106:ASN:CG	2.64	0.40
29:f:68:LEU:HD13	29:f:71:ILE:HG21	2.04	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	
4	A	1935/2413 (80%)	1824 (94%)	111 (6%)	0	100	100
5	C	868/1008 (86%)	812 (94%)	56 (6%)	0	100	100
6	D	93/278 (34%)	91 (98%)	2 (2%)	0	100	100
8	H	403/577 (70%)	380 (94%)	23 (6%)	0	100	100
10	J	340/451 (75%)	318 (94%)	22 (6%)	0	100	100
11	K	162/379 (43%)	155 (96%)	7 (4%)	0	100	100
12	L	154/157 (98%)	150 (97%)	4 (3%)	0	100	100
13	M	253/339 (75%)	238 (94%)	15 (6%)	0	100	100
14	N	234/364 (64%)	223 (95%)	11 (5%)	0	100	100
15	O	314/590 (53%)	293 (93%)	20 (6%)	1 (0%)	37	67
16	P	67/175 (38%)	64 (96%)	3 (4%)	0	100	100
17	R	69/135 (51%)	66 (96%)	3 (4%)	0	100	100
18	S	436/687 (64%)	427 (98%)	9 (2%)	0	100	100
19	T	516/859 (60%)	509 (99%)	6 (1%)	1 (0%)	44	72
20	V	630/1145 (55%)	549 (87%)	59 (9%)	22 (4%)	3	25
21	W	143/238 (60%)	122 (85%)	18 (13%)	3 (2%)	5	33
23	Y	85/111 (77%)	79 (93%)	6 (7%)	0	100	100
24	a	167/251 (66%)	148 (89%)	19 (11%)	0	100	100
25	b	76/196 (39%)	68 (90%)	8 (10%)	0	100	100
25	k	66/196 (34%)	59 (89%)	7 (11%)	0	100	100
26	c	186/382 (49%)	157 (84%)	29 (16%)	0	100	100
27	d	80/101 (79%)	74 (92%)	6 (8%)	0	100	100
27	n	80/101 (79%)	76 (95%)	4 (5%)	0	100	100
28	e	71/94 (76%)	66 (93%)	5 (7%)	0	100	100
28	p	73/94 (78%)	70 (96%)	3 (4%)	0	100	100
29	f	70/86 (81%)	57 (81%)	13 (19%)	0	100	100
29	q	71/86 (83%)	68 (96%)	3 (4%)	0	100	100
30	g	65/77 (84%)	61 (94%)	4 (6%)	0	100	100
30	r	73/77 (95%)	62 (85%)	11 (15%)	0	100	100
31	h	78/146 (53%)	70 (90%)	8 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	l	81/146 (56%)	74 (91%)	2 (2%)	5 (6%)	1	15
32	j	92/110 (84%)	86 (94%)	6 (6%)	0	100	100
32	m	90/110 (82%)	86 (96%)	4 (4%)	0	100	100
33	o	312/455 (69%)	274 (88%)	38 (12%)	0	100	100
34	s	106/175 (61%)	92 (87%)	8 (8%)	6 (6%)	1	16
35	t	113/503 (22%)	108 (96%)	5 (4%)	0	100	100
35	u	112/503 (22%)	104 (93%)	8 (7%)	0	100	100
35	v	114/503 (23%)	108 (95%)	3 (3%)	3 (3%)	4	29
35	w	110/503 (22%)	105 (96%)	3 (3%)	2 (2%)	7	35
36	y	82/215 (38%)	82 (100%)	0	0	100	100
All	All	9070/15016 (60%)	8455 (93%)	572 (6%)	43 (0%)	27	57

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	V	507	GLU
20	V	729	PRO
20	V	747	PRO
20	V	773	VAL
20	V	774	ASP
20	V	862	ASP
20	V	1060	TYR
21	W	52	LYS
21	W	85	ASN
31	l	49	GLN
31	l	50	PRO
31	l	61	ALA
34	s	94	LYS
34	s	111	VAL
34	s	133	PRO
20	V	528	TYR
20	V	1061	GLY
20	V	1076	SER
20	V	1082	GLN
34	s	105	PRO
34	s	136	VAL
35	v	109	LEU
20	V	639	ASN

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Mol	Chain	Res	Type
20	V	1016	SER
31	l	69	GLY
35	v	20	ARG
20	V	673	ASP
20	V	758	ASN
20	V	973	ALA
34	s	119	SER
35	w	20	ARG
15	O	569	GLU
20	V	1040	VAL
35	w	17	PRO
20	V	1055	PRO
31	l	62	MET
20	V	651	PRO
21	W	53	PRO
20	V	592	PRO
19	T	37	ILE
35	v	36	GLY
20	V	814	PRO
20	V	1047	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	
4	A	1768/2182 (81%)	1762 (100%)	6 (0%)	91	94
5	C	783/910 (86%)	779 (100%)	4 (0%)	86	92
6	D	26/256 (10%)	26 (100%)	0	100	100
8	H	183/538 (34%)	181 (99%)	2 (1%)	70	80
10	J	299/398 (75%)	297 (99%)	2 (1%)	81	88
11	K	152/328 (46%)	152 (100%)	0	100	100
12	L	140/141 (99%)	140 (100%)	0	100	100
13	M	219/296 (74%)	219 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	N	221/332 (67%)	220 (100%)	1 (0%)	86	92
15	O	205/526 (39%)	205 (100%)	0	100	100
16	P	60/152 (40%)	60 (100%)	0	100	100
17	R	22/121 (18%)	22 (100%)	0	100	100
18	S	216/633 (34%)	216 (100%)	0	100	100
20	V	562/1029 (55%)	495 (88%)	67 (12%)	4	21
21	W	142/219 (65%)	141 (99%)	1 (1%)	81	88
23	Y	78/100 (78%)	77 (99%)	1 (1%)	65	77
24	a	151/225 (67%)	151 (100%)	0	100	100
25	b	70/176 (40%)	70 (100%)	0	100	100
25	k	64/176 (36%)	63 (98%)	1 (2%)	58	74
26	c	184/346 (53%)	183 (100%)	1 (0%)	86	92
27	d	69/89 (78%)	69 (100%)	0	100	100
27	n	71/89 (80%)	71 (100%)	0	100	100
28	e	65/83 (78%)	65 (100%)	0	100	100
28	p	69/83 (83%)	69 (100%)	0	100	100
29	f	63/77 (82%)	63 (100%)	0	100	100
29	q	65/77 (84%)	65 (100%)	0	100	100
30	g	58/66 (88%)	58 (100%)	0	100	100
30	r	64/66 (97%)	64 (100%)	0	100	100
31	h	77/129 (60%)	77 (100%)	0	100	100
31	l	78/129 (60%)	75 (96%)	3 (4%)	28	53
32	j	79/103 (77%)	79 (100%)	0	100	100
32	m	85/103 (82%)	85 (100%)	0	100	100
33	o	291/413 (70%)	290 (100%)	1 (0%)	91	94
36	y	81/193 (42%)	81 (100%)	0	100	100
All	All	6760/10784 (63%)	6670 (99%)	90 (1%)	64	77

All (90) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	143	ILE
4	A	649	LEU

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Mol	Chain	Res	Type
4	A	766	ILE
4	A	801	VAL
4	A	940	ILE
4	A	1590	LEU
5	C	175	LEU
5	C	268	ASN
5	C	379	ILE
5	C	884	ARG
8	H	384	ILE
8	H	437	LEU
10	J	162	THR
10	J	230	VAL
14	N	34	CYS
20	V	483	LEU
20	V	485	VAL
20	V	486	TYR
20	V	489	ARG
20	V	493	ILE
20	V	497	ARG
20	V	508	THR
20	V	516	ILE
20	V	527	ASN
20	V	534	THR
20	V	538	ARG
20	V	544	VAL
20	V	555	LYS
20	V	556	VAL
20	V	559	ASP
20	V	573	ASP
20	V	574	THR
20	V	580	THR
20	V	587	GLU
20	V	599	VAL
20	V	628	GLU
20	V	639	ASN
20	V	649	ASN
20	V	654	ASN
20	V	662	VAL
20	V	680	ASP
20	V	696	VAL
20	V	699	THR
20	V	708	CYS

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Mol	Chain	Res	Type
20	V	711	LEU
20	V	713	ASP
20	V	727	ILE
20	V	730	VAL
20	V	747	PRO
20	V	748	LYS
20	V	752	LYS
20	V	762	THR
20	V	781	ASN
20	V	822	THR
20	V	828	ASN
20	V	845	HIS
20	V	847	ILE
20	V	871	LEU
20	V	891	LEU
20	V	897	GLU
20	V	904	ASP
20	V	912	LEU
20	V	931	SER
20	V	935	VAL
20	V	949	LYS
20	V	970	TRP
20	V	977	GLU
20	V	979	TYR
20	V	982	THR
20	V	986	HIS
20	V	1000	ILE
20	V	1010	LYS
20	V	1020	LEU
20	V	1040	VAL
20	V	1043	LYS
20	V	1059	LEU
20	V	1067	VAL
20	V	1081	SER
20	V	1082	GLN
20	V	1087	GLU
20	V	1093	GLU
20	V	1094	VAL
21	W	33	ASP
23	Y	109	LYS
26	c	328	VAL
25	k	22	VAL

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Mol	Chain	Res	Type
31	l	45	LEU
31	l	82	LEU
31	l	95	ILE
33	o	315	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (157) such sidechains are listed below:

Mol	Chain	Res	Type
4	A	178	ASN
4	A	203	ASN
4	A	233	HIS
4	A	326	ASN
4	A	343	ASN
4	A	368	ASN
4	A	405	ASN
4	A	487	ASN
4	A	497	GLN
4	A	509	HIS
4	A	541	ASN
4	A	542	HIS
4	A	543	ASN
4	A	553	ASN
4	A	574	GLN
4	A	598	ASN
4	A	617	ASN
4	A	654	HIS
4	A	659	HIS
4	A	685	HIS
4	A	713	ASN
4	A	733	GLN
4	A	776	GLN
4	A	796	ASN
4	A	848	ASN
4	A	948	HIS
4	A	952	ASN
4	A	976	GLN
4	A	1097	HIS
4	A	1115	GLN
4	A	1140	ASN
4	A	1190	ASN
4	A	1281	ASN
4	A	1376	ASN

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Mol	Chain	Res	Type
4	A	1417	GLN
4	A	1449	ASN
4	A	1529	ASN
4	A	1531	HIS
4	A	1548	GLN
4	A	1592	HIS
4	A	1618	ASN
4	A	1635	HIS
4	A	1652	HIS
4	A	1687	HIS
4	A	1763	ASN
4	A	1883	ASN
4	A	1888	HIS
4	A	1895	HIS
4	A	1902	GLN
4	A	1990	ASN
5	C	112	ASN
5	C	119	ASN
5	C	158	HIS
5	C	183	GLN
5	C	268	ASN
5	C	290	HIS
5	C	334	HIS
5	C	403	ASN
5	C	554	HIS
5	C	869	HIS
6	D	158	GLN
8	H	320	ASN
8	H	336	GLN
8	H	355	HIS
8	H	363	ASN
8	H	458	HIS
10	J	121	GLN
10	J	136	ASN
10	J	152	ASN
10	J	214	ASN
10	J	271	GLN
10	J	273	GLN
10	J	280	GLN
10	J	306	HIS
10	J	360	GLN
11	K	107	ASN

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Mol	Chain	Res	Type
12	L	34	GLN
12	L	54	GLN
12	L	56	HIS
12	L	110	GLN
12	L	116	ASN
12	L	147	HIS
13	M	35	ASN
13	M	58	HIS
13	M	134	ASN
13	M	189	GLN
13	M	201	ASN
13	M	227	ASN
14	N	11	ASN
14	N	53	ASN
14	N	54	ASN
14	N	72	GLN
14	N	134	ASN
14	N	243	ASN
15	O	26	GLN
15	O	41	GLN
15	O	83	GLN
15	O	186	GLN
15	O	249	ASN
16	P	171	HIS
18	S	67	GLN
18	S	78	GLN
18	S	117	HIS
18	S	120	ASN
18	S	123	ASN
18	S	210	ASN
18	S	212	HIS
20	V	518	GLN
20	V	585	GLN
20	V	701	GLN
20	V	881	HIS
20	V	883	GLN
20	V	917	ASN
20	V	918	GLN
20	V	972	GLN
20	V	978	GLN
20	V	989	HIS
21	W	35	GLN

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Mol	Chain	Res	Type
21	W	55	HIS
21	W	105	ASN
21	W	157	GLN
23	Y	28	ASN
24	a	87	GLN
24	a	149	GLN
24	a	246	ASN
25	b	8	HIS
25	b	25	GLN
26	c	32	HIS
26	c	89	ASN
26	c	90	ASN
26	c	300	ASN
26	c	326	GLN
26	c	332	ASN
27	d	17	HIS
27	d	41	ASN
29	f	54	ASN
30	g	18	ASN
30	g	20	ASN
30	g	55	HIS
30	g	66	ASN
31	l	78	ASN
31	l	90	ASN
32	m	52	HIS
27	n	4	ASN
27	n	43	GLN
27	n	53	GLN
27	n	68	GLN
33	o	176	HIS
33	o	323	GLN
33	o	325	ASN
33	o	336	GLN
33	o	358	ASN
28	p	86	ASN
29	q	25	HIS
30	r	56	GLN
36	y	200	ASN
36	y	204	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	2	128/1175 (10%)	44 (34%)	3 (2%)
2	5	169/179 (94%)	57 (33%)	6 (3%)
3	6	101/112 (90%)	26 (25%)	3 (2%)
7	E	32/39 (82%)	21 (65%)	4 (12%)
9	I	36/95 (37%)	10 (27%)	2 (5%)
All	All	466/1600 (29%)	158 (33%)	18 (3%)

All (158) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	2	5	A
1	2	6	U
1	2	14	C
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	22	C
1	2	25	A
1	2	30	A
1	2	31	A
1	2	37	G
1	2	106	A
1	2	108	A
1	2	112	A
1	2	113	U
1	2	114	U
1	2	115	U
1	2	116	U
1	2	117	U
1	2	118	U
1	2	119	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

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Mol	Chain	Res	Type
1	2	1104	U
1	2	1106	G
1	2	1107	C
1	2	1108	A
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	9	U
2	5	12	C
2	5	13	A
2	5	14	G
2	5	17	C
2	5	18	A
2	5	20	U
2	5	25	G
2	5	27	G
2	5	28	G
2	5	31	G
2	5	32	G
2	5	33	U
2	5	34	C
2	5	36	A
2	5	39	U
2	5	41	A
2	5	42	A
2	5	43	G
2	5	45	A
2	5	55	U
2	5	56	U
2	5	57	U
2	5	58	U
2	5	61	U
2	5	70	A
2	5	75	A
2	5	76	U
2	5	77	A
2	5	79	C
2	5	80	G

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Mol	Chain	Res	Type
2	5	81	A
2	5	84	A
2	5	95	C
2	5	96	U
2	5	101	C
2	5	104	G
2	5	109	A
2	5	113	G
2	5	126	A
2	5	127	U
2	5	131	A
2	5	135	G
2	5	138	A
2	5	139	A
2	5	141	G
2	5	142	C
2	5	148	G
2	5	151	A
2	5	160	U
2	5	161	U
2	5	168	U
2	5	170	U
2	5	171	U
2	5	173	U
2	5	174	G
2	5	175	G
3	6	12	A
3	6	15	C
3	6	31	G
3	6	35	A
3	6	36	U
3	6	37	U
3	6	49	A
3	6	51	A
3	6	52	G
3	6	54	U
3	6	55	G
3	6	60	G
3	6	62	A
3	6	68	C
3	6	74	U
3	6	79	A

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Mol	Chain	Res	Type
3	6	80	U
3	6	83	A
3	6	85	C
3	6	86	G
3	6	87	U
3	6	90	U
3	6	91	A
3	6	92	C
3	6	93	A
3	6	99	A
7	E	-13	G
7	E	-12	U
7	E	-11	G
7	E	-10	A
7	E	-9	U
7	E	-6	A
7	E	-1	G
7	E	1	A
7	E	2	G
7	E	3	A
7	E	4	U
7	E	5	C
7	E	6	C
7	E	7	A
7	E	8	C
7	E	9	C
7	E	10	U
7	E	11	A
7	E	12	C
7	E	13	U
7	E	16	A
9	I	2	U
9	I	9	A
9	I	10	A
9	I	12	G
9	I	15	A
9	I	67	C
9	I	70	A
9	I	71	C
9	I	92	C
9	I	93	U

All (18) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	2	15	C
1	2	18	U
1	2	1145	U
2	5	17	C
2	5	41	A
2	5	56	U
2	5	130	A
2	5	150	U
2	5	174	G
3	6	36	U
3	6	82	A
3	6	92	C
7	E	-14	A
7	E	1	A
7	E	2	G
7	E	15	C
9	I	66	A
9	I	91	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 8 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	2500	-	36,36,36	0.70	0	54,60,60	0.52	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	GTP	C	2501	-	26,34,34	1.30	1 (3%)	32,54,54	1.67	8 (25%)

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	2500	-	-	5/30/54/54	0/1/1/1
39	GTP	C	2501	-	-	6/18/38/38	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	2501	GTP	C5-C6	-4.64	1.38	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	C	2501	GTP	PA-O3A-PB	-3.62	120.41	132.83
39	C	2501	GTP	PB-O3B-PG	-3.48	120.90	132.83
39	C	2501	GTP	C5-C6-N1	3.40	119.95	113.95
39	C	2501	GTP	C8-N7-C5	2.90	108.51	102.99
39	C	2501	GTP	C2-N1-C6	-2.87	119.80	125.10
39	C	2501	GTP	C3'-C2'-C1'	2.76	105.13	100.98
39	C	2501	GTP	O3G-PG-O3B	2.54	113.16	104.64
39	C	2501	GTP	O6-C6-C5	-2.47	119.55	124.37

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
38	A	2500	IHP	C2-O12-P2-O22
39	C	2501	GTP	C5'-O5'-PA-O1A
39	C	2501	GTP	C5'-O5'-PA-O2A
38	A	2500	IHP	C1-O11-P1-O31
39	C	2501	GTP	PB-O3A-PA-O1A
39	C	2501	GTP	PB-O3A-PA-O2A
38	A	2500	IHP	C3-O13-P3-O23
38	A	2500	IHP	C1-O11-P1-O41

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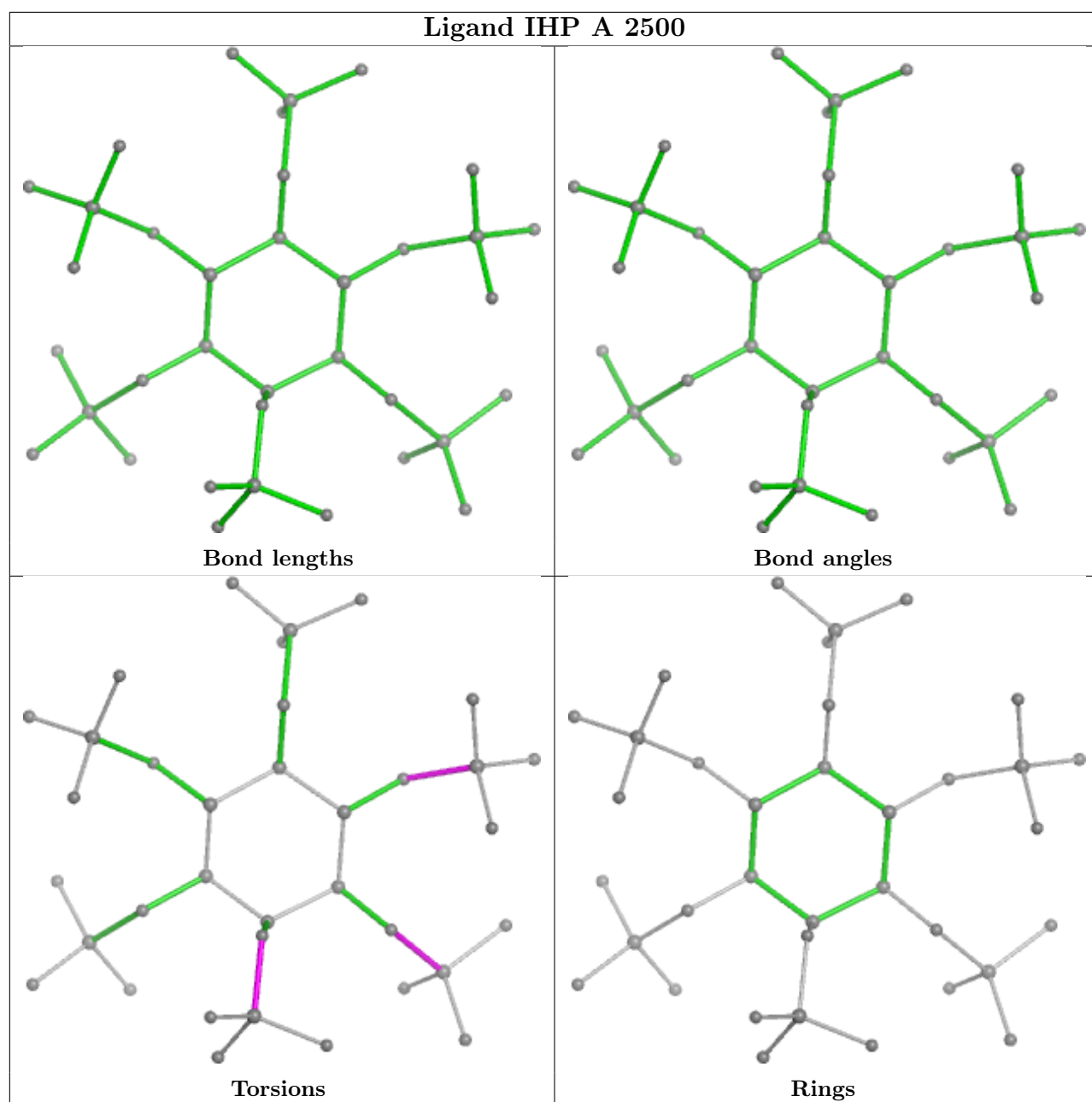
Mol	Chain	Res	Type	Atoms
38	A	2500	IHP	C3-O13-P3-O33
39	C	2501	GTP	C5'-O5'-PA-O3A
39	C	2501	GTP	O4'-C4'-C5'-O5'

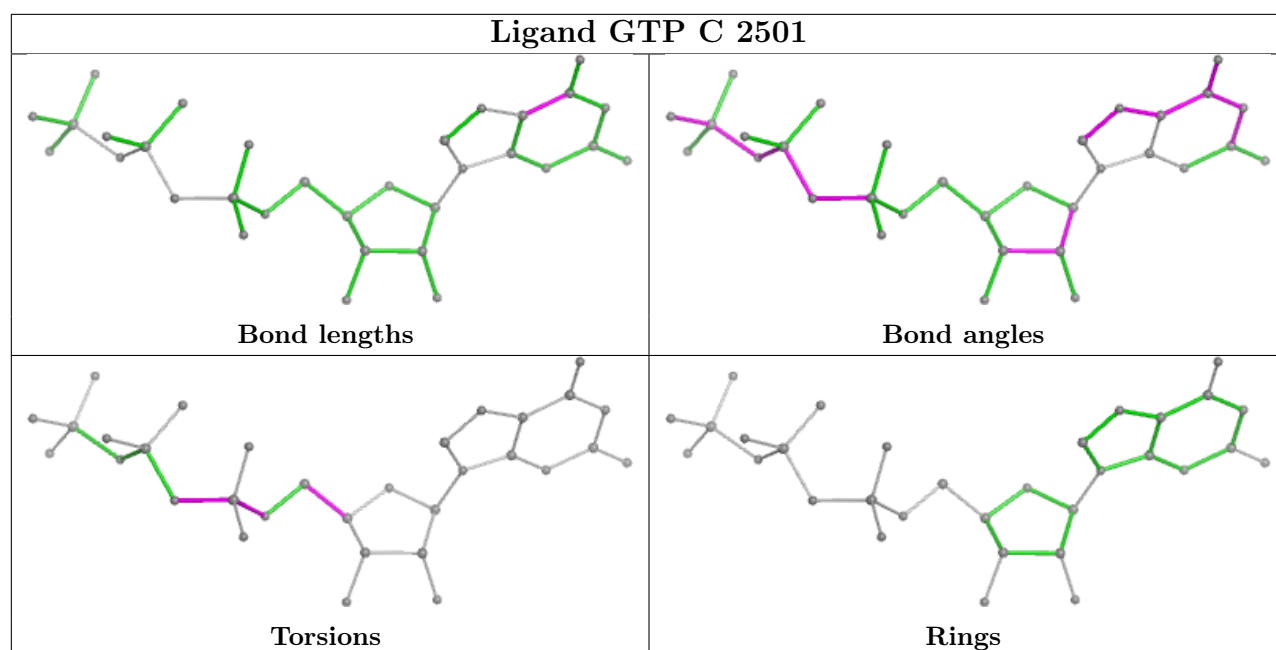
There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
38	A	2500	IHP	2	0
39	C	2501	GTP	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 than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	X	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	X	70:UNK	C	100:UNK	N	122.60
1	X	156:UNK	C	200:UNK	N	74.32
1	X	28:UNK	C	60:UNK	N	43.20
1	X	117:UNK	C	130:UNK	N	9.37
1	X	142:UNK	C	150:UNK	N	9.29

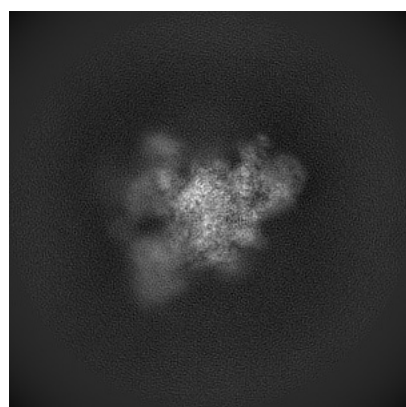
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3979. These allow visual inspection of the internal detail of the map and identification of artifacts.

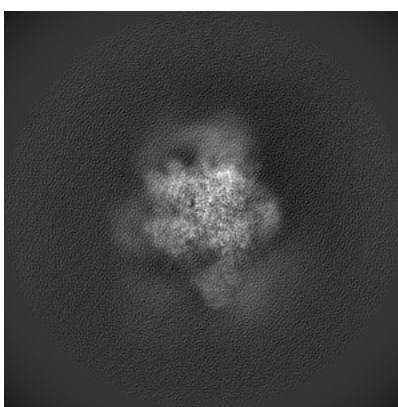
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

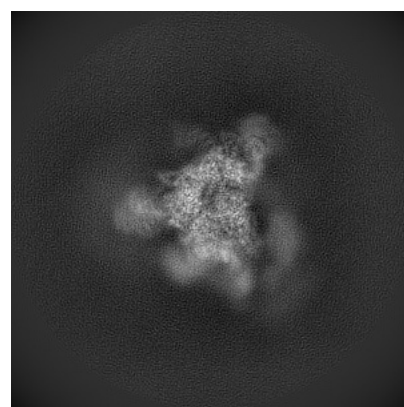
6.1.1 Primary map



X



Y

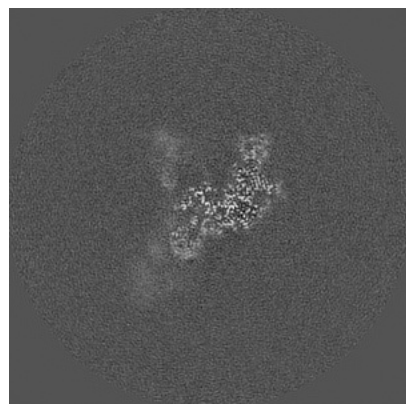


Z

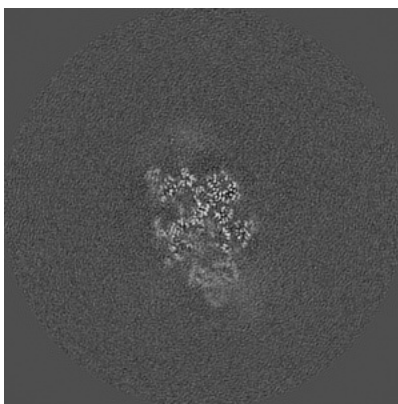
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

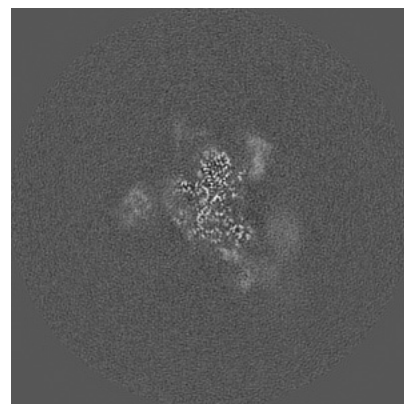
6.2.1 Primary map



X Index: 240



Y Index: 240

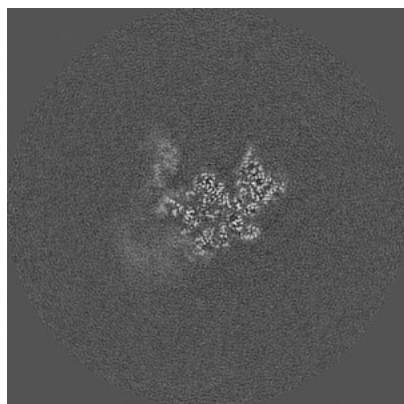


Z Index: 240

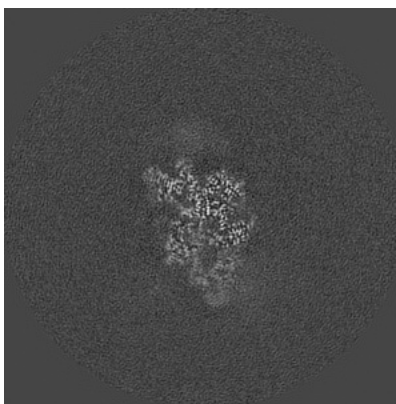
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

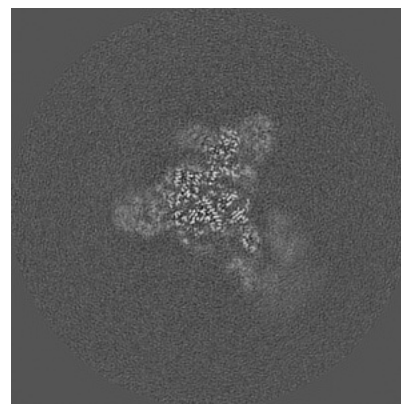
6.3.1 Primary map



X Index: 259



Y Index: 236

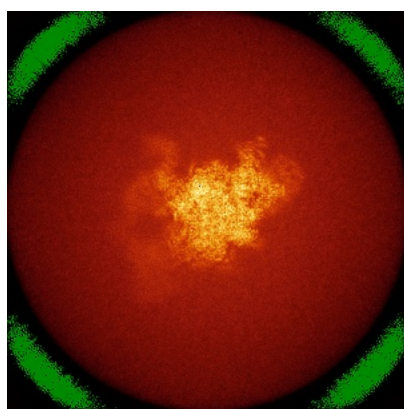


Z Index: 261

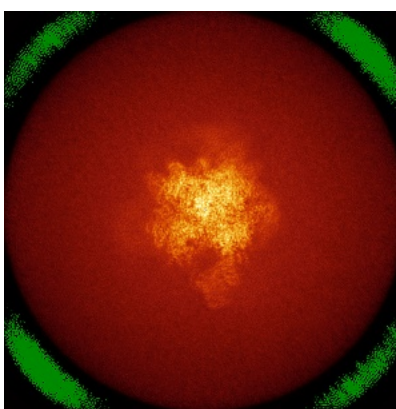
The images above show the largest variance slices of the map in three orthogonal directions.

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

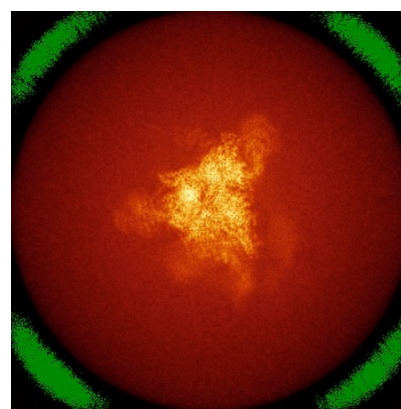
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.04. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

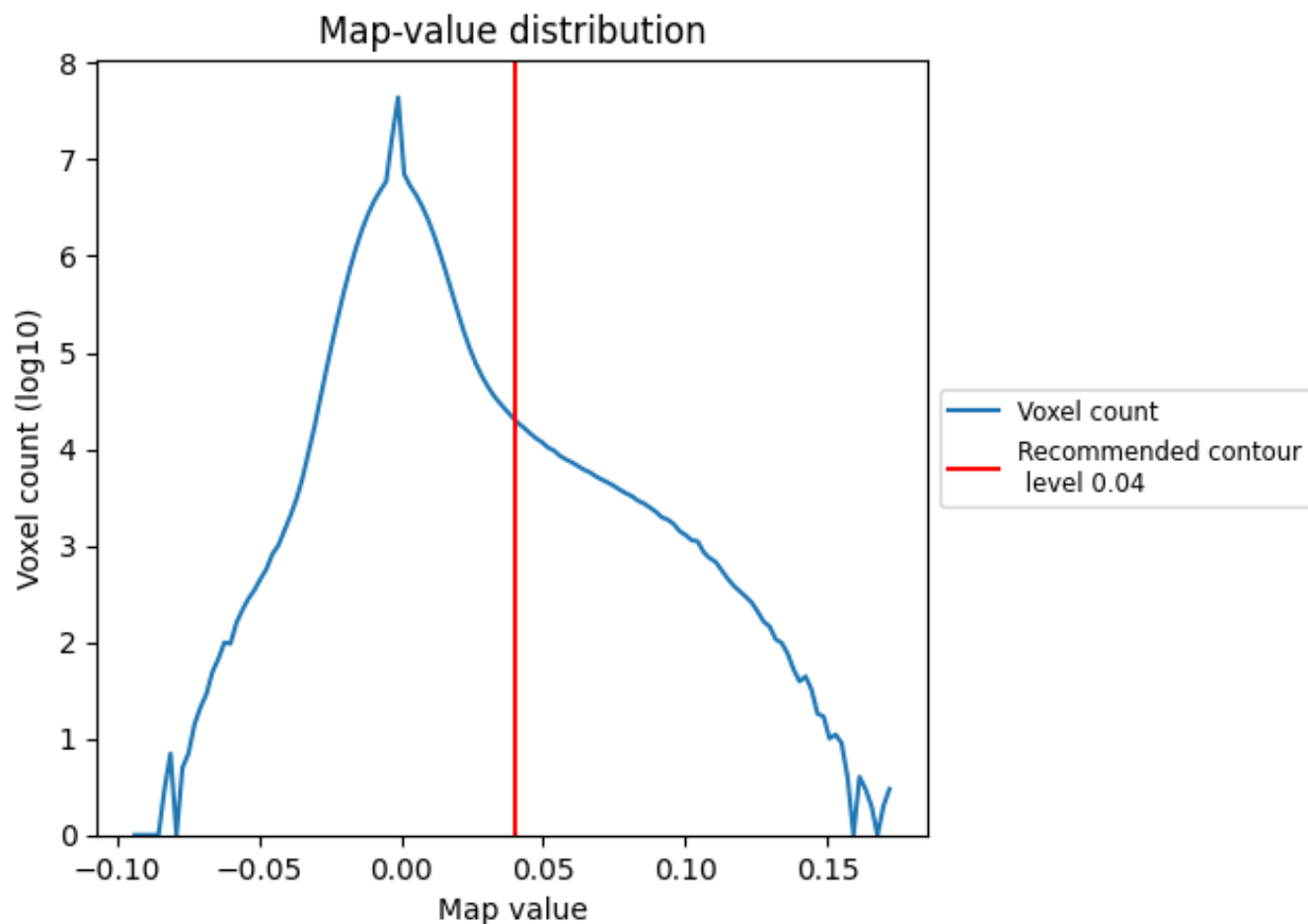
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

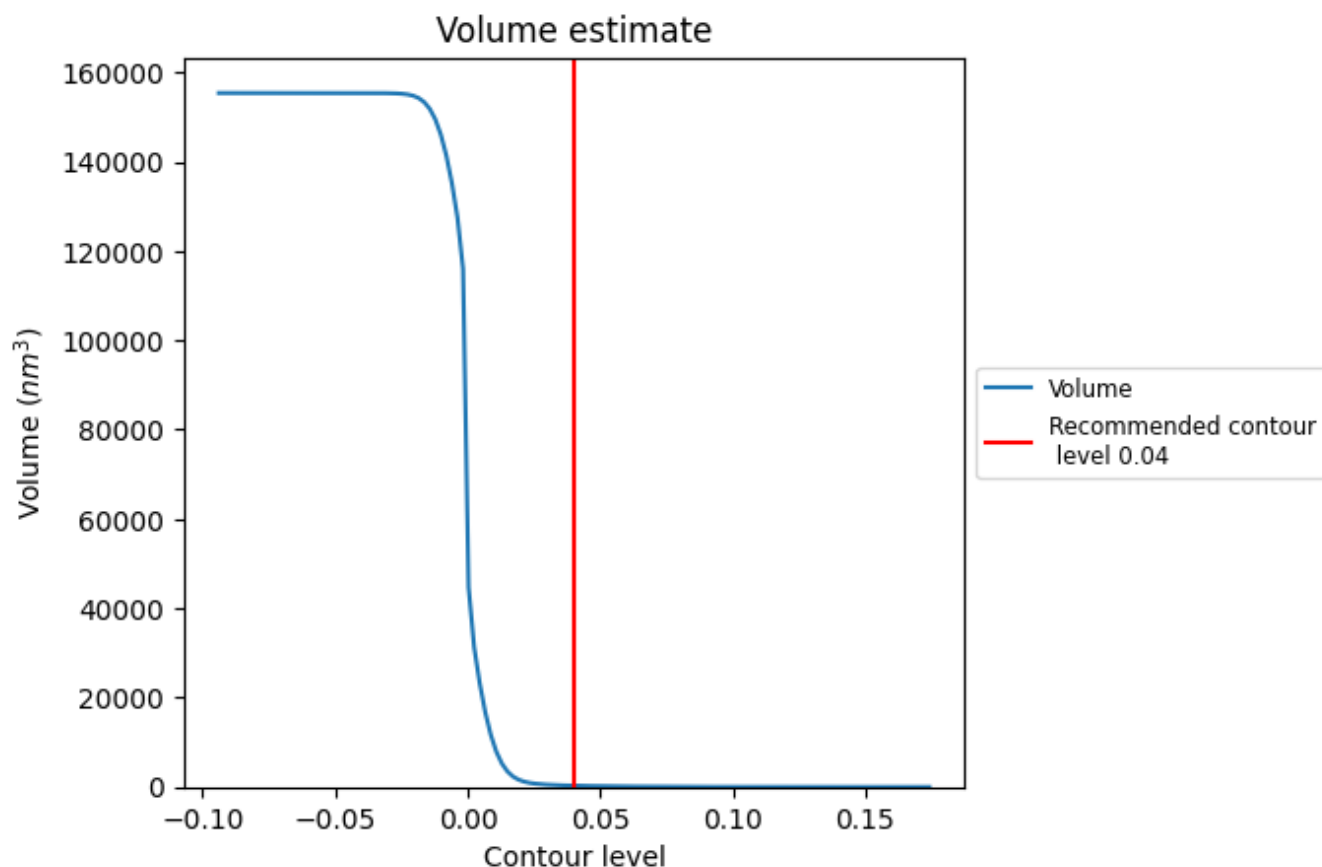
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

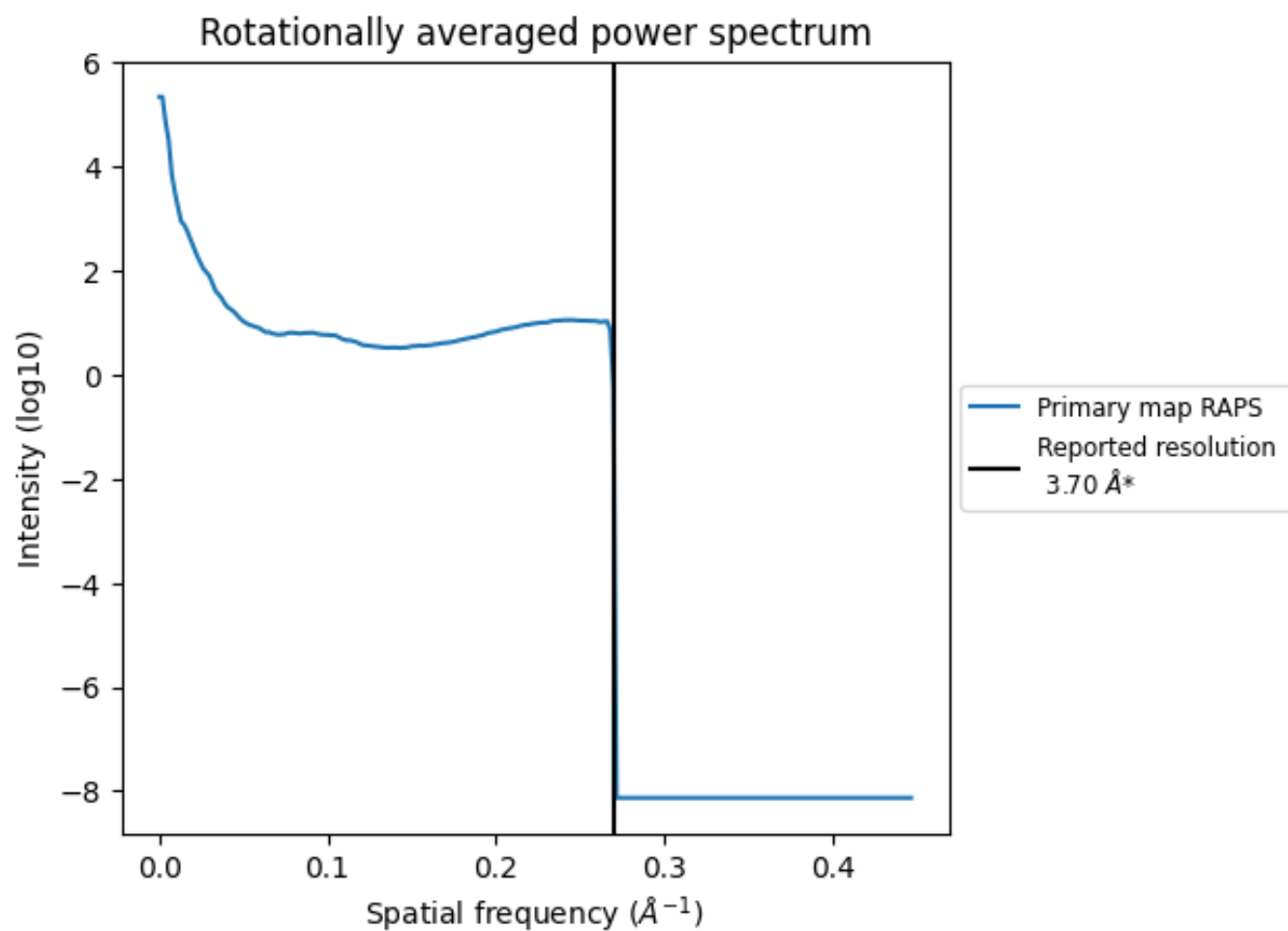
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 287 nm³; this corresponds to an approximate mass of 259 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

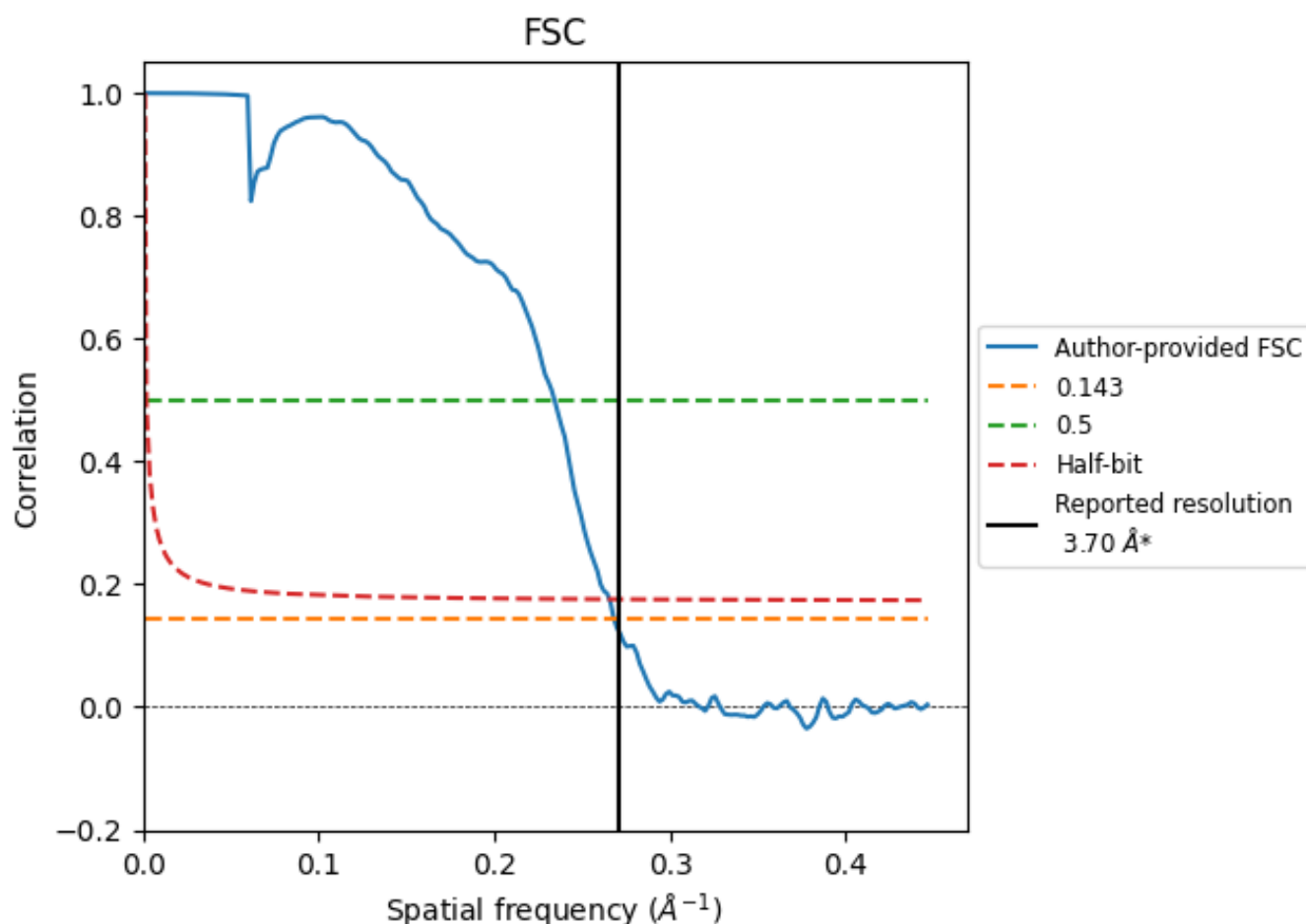


*Reported resolution corresponds to spatial frequency of 0.270 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.270 \AA^{-1}

8.2 Resolution estimates [i](#)

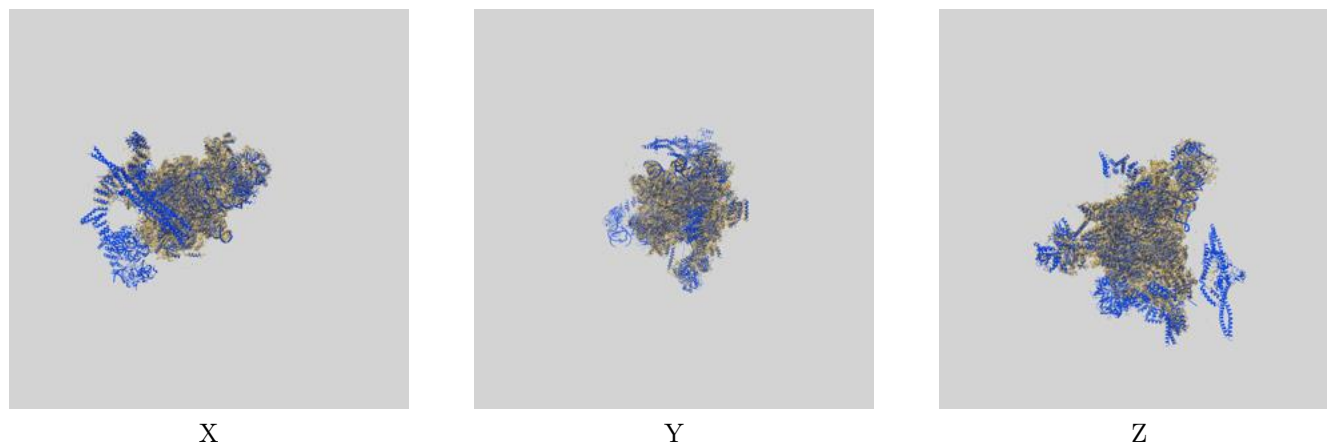
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.70	-	-
Author-provided FSC curve	3.73	4.27	3.77
Unmasked-calculated*	-	-	-

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

9 Map-model fit [i](#)

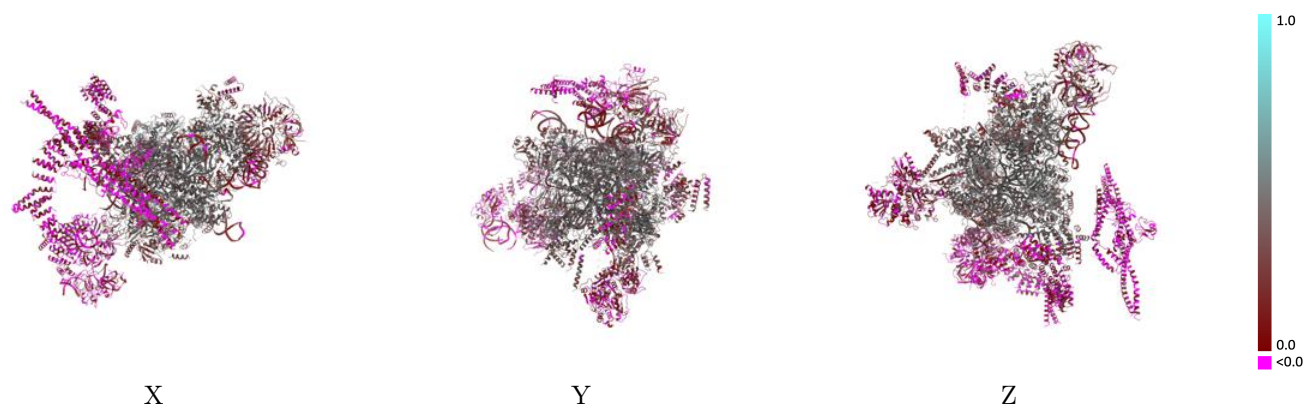
This section contains information regarding the fit between EMDB map EMD-3979 and PDB model 6EXN. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



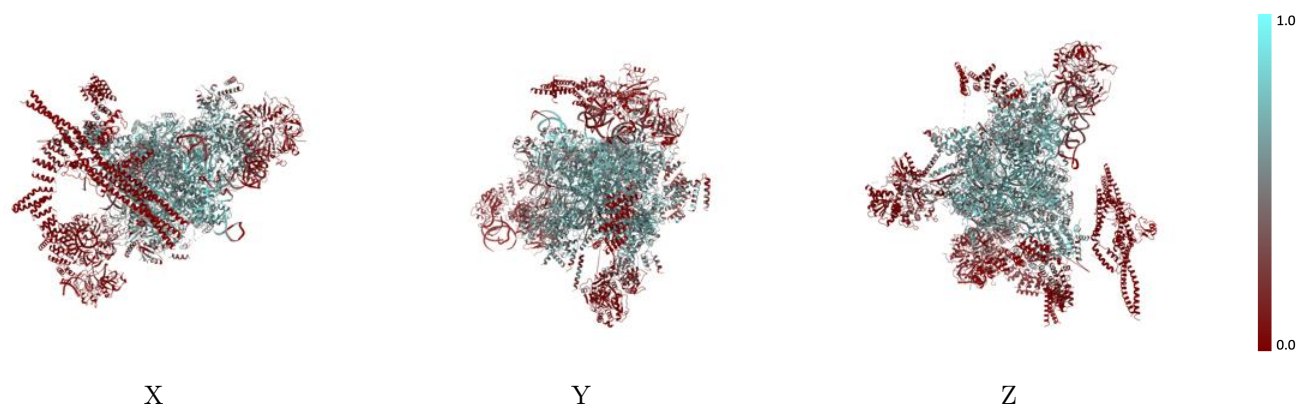
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



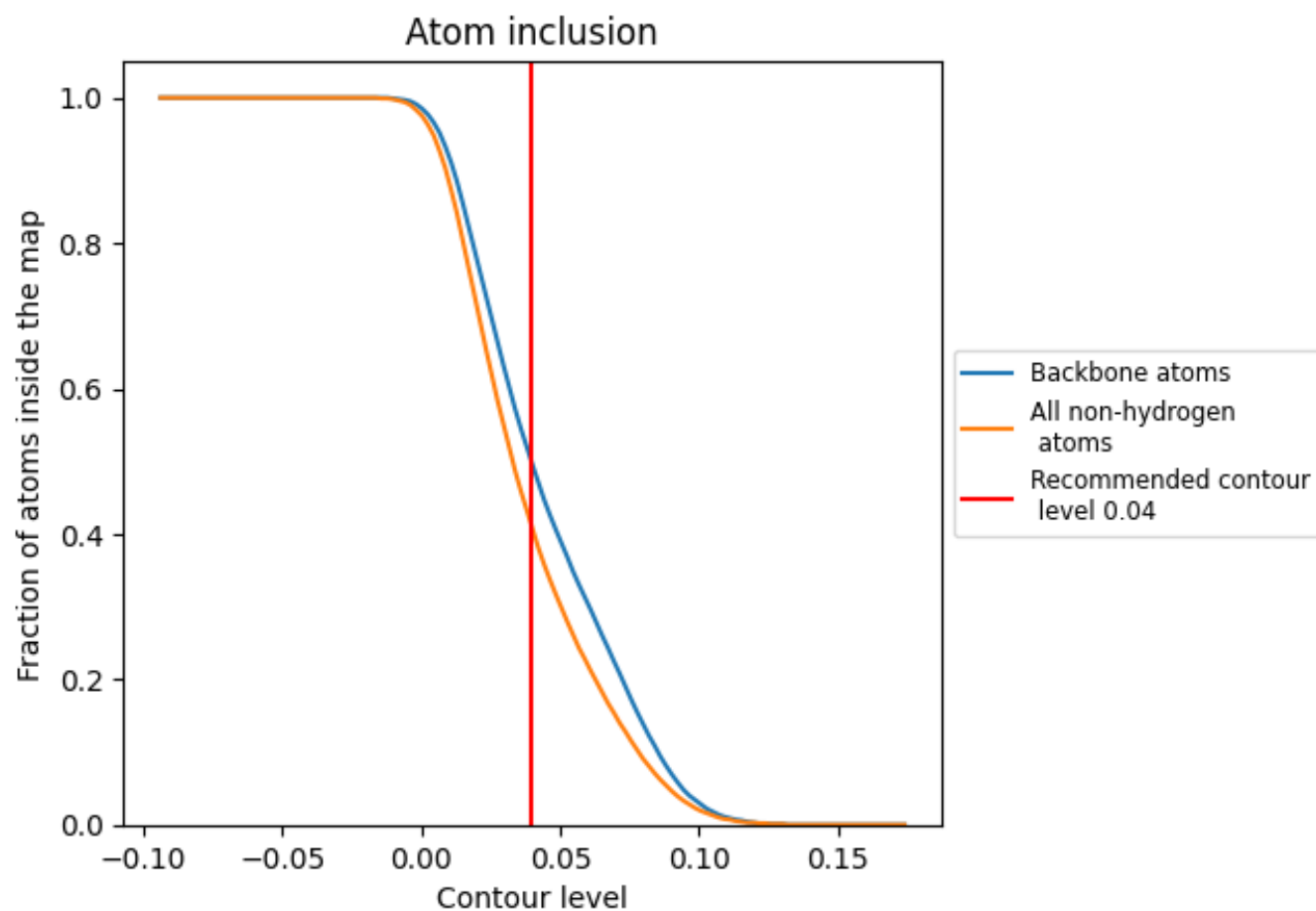
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.04).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 50% of all backbone atoms, 41% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4080	 0.2960
2	 0.1910	 0.1300
5	 0.4610	 0.2840
6	 0.6910	 0.3820
A	 0.6210	 0.4310
C	 0.5850	 0.4150
D	 0.4390	 0.3080
E	 0.4490	 0.3090
H	 0.3720	 0.2960
I	 0.5630	 0.3590
J	 0.6440	 0.4540
K	 0.5550	 0.4100
L	 0.6340	 0.4270
M	 0.5750	 0.3970
N	 0.4620	 0.3610
O	 0.4480	 0.3180
P	 0.5840	 0.4480
R	 0.4380	 0.2970
S	 0.4410	 0.2850
T	 0.1180	 0.0880
V	 0.1130	 0.1090
W	 0.0000	 0.0040
X	 0.3700	 0.2460
Y	 0.0000	 0.0310
a	 0.4740	 0.3540
b	 0.2660	 0.3200
c	 0.4590	 0.3660
d	 0.3300	 0.3480
e	 0.1080	 0.2290
f	 0.0980	 0.2000
g	 0.1460	 0.2540
h	 0.1670	 0.2620
j	 0.1050	 0.1980
k	 0.0020	 0.0530
l	 0.0000	 -0.0180



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Chain	Atom inclusion	Q-score
m	 0.0000	 0.0040
n	 0.0030	 0.0520
o	 0.4440	 0.3500
p	 0.0000	 -0.0040
q	 0.0020	 0.0330
r	 0.0000	 0.0440
s	 0.0070	 0.0320
t	 0.0000	 -0.0120
u	 0.0000	 0.0350
v	 0.0000	 -0.0410
w	 0.0020	 0.0170
y	 0.5370	 0.3950