



Full wwPDB EM Validation Report ⓘ

Mar 20, 2026 – 10:37 AM UTC

PDB ID : 5YZG / pdb_00005yzg
EMDB ID : EMD-6864
Title : The Cryo-EM Structure of Human Catalytic Step I Spliceosome (C complex)
at 4.1 angstrom resolution
Authors : Zhan, X.; Yan, C.; Zhang, X.; Lei, J.; Shi, Y.
Deposited on : 2017-12-14
Resolution : 4.10 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

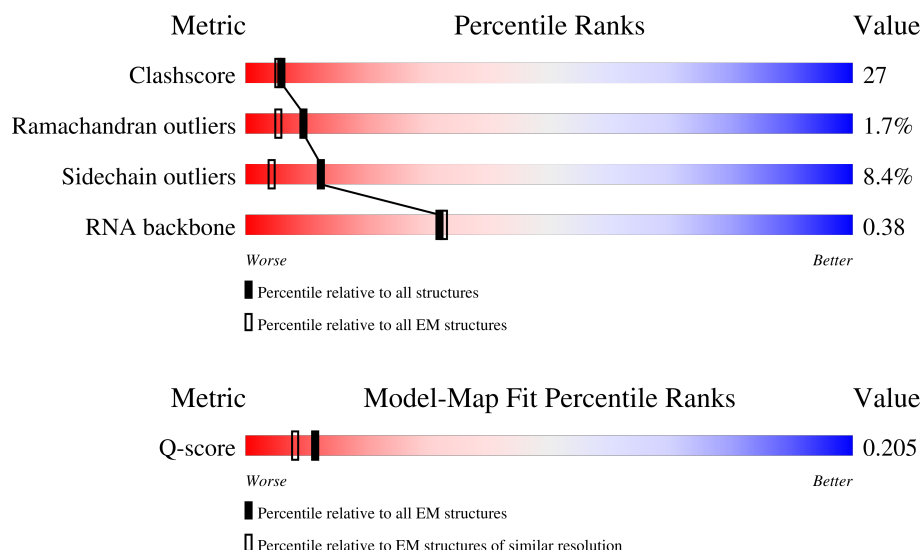
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	A	2335	
2	B	117	
3	C	972	

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Mol	Chain	Length	Quality of chain
4	D	2136	
5	E	357	
6	F	107	
7	G	275	
8	H	188	
9	I	855	
10	J	848	
11	K	225	
12	L	802	
13	y	307	
14	M	243	
15	N	144	
16	O	420	
17	P	229	
18	R	536	
19	S	166	
20	T	514	
21	Q	1485	
22	U	2752	
23	V	908	
24	W	579	
25	X	425	
26	Y	323	
27	Z	1227	
28	q	504	

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Mol	Chain	Length	Quality of chain
28	r	504	
28	s	504	
28	t	504	
29	u	411	
30	v	148	
31	w	174	
32	x	703	
33	a	126	
33	h	126	
34	b	229	
34	i	229	
35	c	119	
35	j	119	
36	d	118	
36	k	118	
37	f	86	
37	m	86	
38	e	92	
38	l	92	
39	g	76	
39	n	76	
40	o	255	
41	p	225	
42	1	301	
43	2	646	

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Mol	Chain	Length	Quality of chain
44	3	754	
45	4	37	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
46	IHP	A	3000	-	-	X	-
50	ZN	N	202	-	-	X	-
50	ZN	Y	400	-	-	X	-

2 Entry composition

There are 51 unique types of molecules in this entry. The entry contains 103906 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Pre-mRNA-processing-splicing factor 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2253	Total	C	N	O	S	0	0
			17519	11136	3147	3166	70		

- Molecule 2 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	84	Total	C	N	O	P	0	0
			1768	792	295	597	84		

- Molecule 3 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	862	Total	C	N	O	S	0	0
			6795	4344	1138	1281	32		

- Molecule 4 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms				AltConf	Trace
4	D	1908	Total	C	N	O	0	0
			7632	3816	1908	1908		

- Molecule 5 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	299	Total	C	N	O	S	0	0
			2338	1470	410	445	13		

- Molecule 6 is a RNA chain called U6 snRNA.

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

- Molecule 7 is a RNA chain called Pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	88	Total	C	N	O	P	0	0
			1641	727	238	589	87		

- Molecule 8 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	139	Total	C	N	O	P	0	0
			2946	1317	507	983	139		

- Molecule 9 is a protein called Pre-mRNA-splicing factor SYF1.

Mol	Chain	Residues	Atoms				AltConf	Trace
9	I	559	Total	C	N	O	0	0
			2757	1639	559	559		

- Molecule 10 is a protein called Crooked neck-like protein 1.

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

- Molecule 11 is a protein called Pre-mRNA-splicing factor SPF27.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	152	Total	C	N	O	S	0	0
			979	611	177	189	2		

- Molecule 12 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	419	Total	C	N	O	S	0	0
			2885	1809	534	537	5		

- Molecule 13 is a protein called Pre-mRNA-splicing factor ISY1 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	y	112	Total	C	N	O	S	0	0
			704	440	130	133	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	M	91	Total	C	N	O	S	0	0
			775	482	146	145	2		

- Molecule 15 is a protein called Protein BUD31 homolog.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	283	Total	C	N	O	S	0	0
			2277	1430	403	424	20		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	96	Total	C	N	O	S	0	0
			829	508	162	157	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	245	Total	C	N	O	P S	0	0
			1962	1231	353	364	2 12		

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

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

- Molecule 20 is a protein called Pleiotropic regulator 1.

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

- Molecule 21 is a protein called Intron-binding protein aquarius.

Mol	Chain	Residues	Atoms				AltConf	Trace
21	Q	1322	Total	C	N	O	0	0
			5288	2644	1322	1322		

- Molecule 22 is a protein called Serine/arginine repetitive matrix protein 2.

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

- Molecule 23 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	V	452	Total	C	N	O	S	0	0
			3410	2194	590	611	15		

- Molecule 24 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	W	440	Total	C	N	O	S	0	0
			2310	1296	487	523	4		

- Molecule 25 is a protein called Pre-mRNA-splicing factor CWC25 homolog.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	X	71	Total	C	N	O	0	0
			480	297	95	88		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
X	145	GLN	LYS	conflict	UNP Q9NXE8
X	149	PRO	LYS	conflict	UNP Q9NXE8

- Molecule 26 is a protein called Coiled-coil domain-containing protein 94.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Y	204	Total	C	N	O	S	0	0
			1426	898	259	261	8		

- Molecule 27 is a protein called Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16.

Mol	Chain	Residues	Atoms				AltConf	Trace
27	Z	635	Total	C	N	O	0	0
			2540	1270	635	635		

- Molecule 28 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	q	132	Total	C	N	O	S	0	0
			918	581	156	178	3		
28	r	131	Total	C	N	O	S	0	0
			901	572	149	177	3		
28	s	374	Total	C	N	O		1	0
			1497	749	374	374			
28	t	67	Total	C	N	O	S	0	0
			476	300	83	92	1		

- Molecule 29 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	u	390	Total	C	N	O	S	0	0
			3126	1974	545	588	19		

- Molecule 30 is a protein called Protein mago nashi homolog 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	v	144	Total	C	N	O	S	0	0
			1196	772	200	221	3		

- Molecule 31 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	w	91	Total	C	N	O	S	0	0
			730	463	122	142	3		

- Molecule 32 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				AltConf	Trace
32	x	25	Total	C	N	O	0	0
			216	136	39	41		

- Molecule 33 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	h	80	Total	C	N	O	S	0	0
			621	388	110	117	6		
33	a	77	Total	C	N	O	S	0	0
			609	381	108	115	5		

- Molecule 34 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	i	86	Total	C	N	O	S	0	0
			690	434	126	123	7		
34	b	83	Total	C	N	O	S	0	0
			675	426	123	119	7		

- Molecule 35 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	j	82	Total	C	N	O	S	0	0
			649	413	113	119	4		
35	c	81	Total	C	N	O	S	0	0
			641	409	112	116	4		

- Molecule 36 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
36	k	85	Total	C	N	O	S	0	0
			688	432	125	126	5		
36	d	97	Total	C	N	O	S	0	0
			768	482	141	140	5		

- Molecule 37 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	m	74	Total	C	N	O	S	0	0
			576	373	95	103	5		
37	f	74	Total	C	N	O	S	0	0
			576	373	95	103	5		

- Molecule 38 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
38	l	79	Total	C	N	O	S	0	0
			652	412	116	119	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
38	e	79	Total	C	N	O	S	0	0
			652	412	116	119	5		

- Molecule 39 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
39	n	68	Total	C	N	O	S	0	0
			533	339	95	93	6		
39	g	74	Total	C	N	O	S	0	0
			569	358	102	103	6		

- Molecule 40 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
40	o	162	Total	C	N	O	S	0	0
			1277	817	219	238	3		

- Molecule 41 is a protein called U2 small nuclear ribonucleoprotein B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
41	p	94	Total	C	N	O	S	0	0
			760	488	135	132	5		

- Molecule 42 is a protein called Peptidyl-prolyl cis-trans isomerase E.

Mol	Chain	Residues	Atoms				AltConf	Trace
42	1	243	Total	C	N	O	0	0
			972	486	243	243		

- Molecule 43 is a protein called Peptidylprolyl isomerase domain and WD repeat-containing protein 1.

Mol	Chain	Residues	Atoms				AltConf	Trace
43	2	416	Total	C	N	O	0	0
			1664	832	416	416		

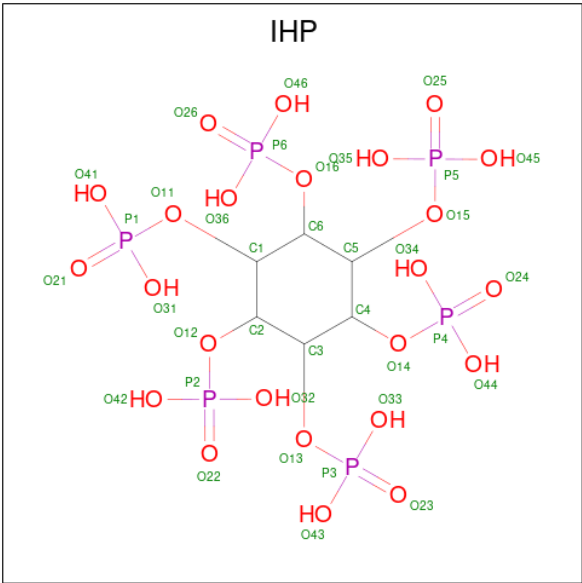
- Molecule 44 is a protein called Peptidyl-prolyl cis-trans isomerase G.

Mol	Chain	Residues	Atoms				AltConf	Trace
44	3	171	Total	C	N	O	0	0
			684	342	171	171		

- Molecule 45 is a protein called UNKNOWN.

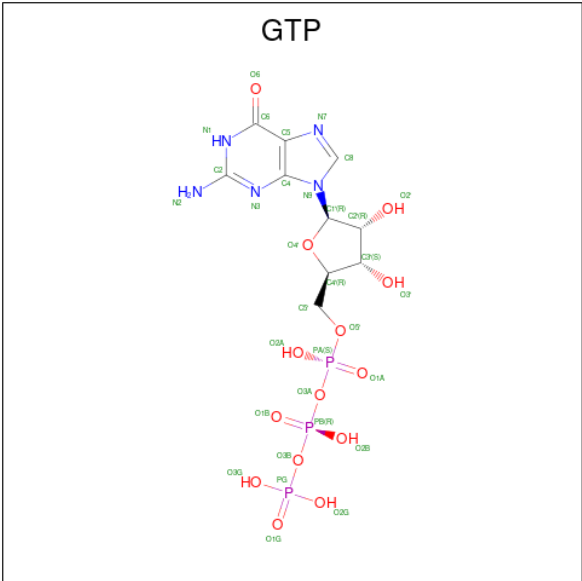
Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
45	4	37	184	110	37	37	0	0

- Molecule 46 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: C₆H₁₈O₂₄P₆).



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

- Molecule 47 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).

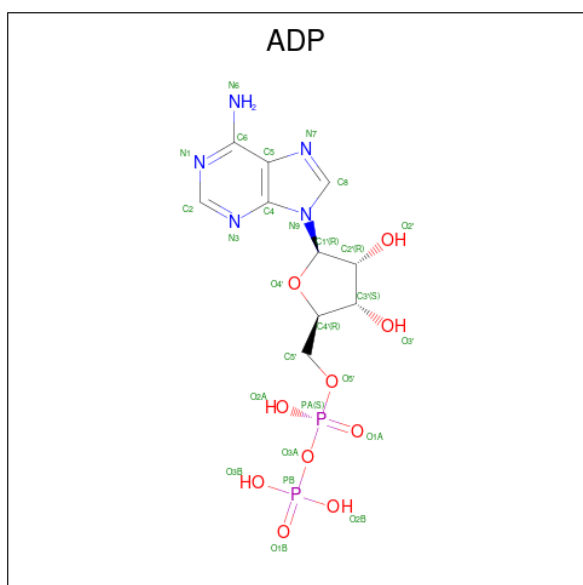


Mol	Chain	Residues	Atoms					AltConf
47	C	1	Total	C	N	O	P	0
			32	10	5	14	3	

- Molecule 48 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
48	C	1	Total	Mg	0
			1	1	
48	F	5	Total	Mg	0
			5	5	
48	u	1	Total	Mg	0
			1	1	

- Molecule 49 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					AltConf
49	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
49	D	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 50 is ZINC ION (CCD ID: ZN) (formula: Zn).

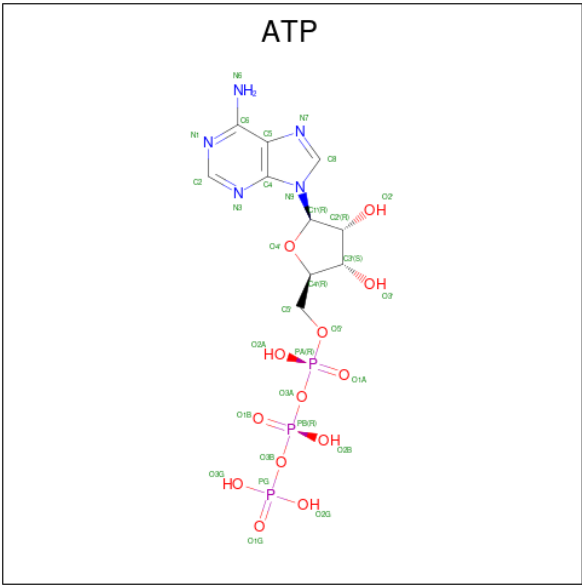
Mol	Chain	Residues	Atoms		AltConf
50	N	3	Total	Zn	0
			3	3	

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Mol	Chain	Residues	Atoms		AltConf
50	O	3	Total	Zn	0
			3	3	
50	Y	1	Total	Zn	0
			1	1	

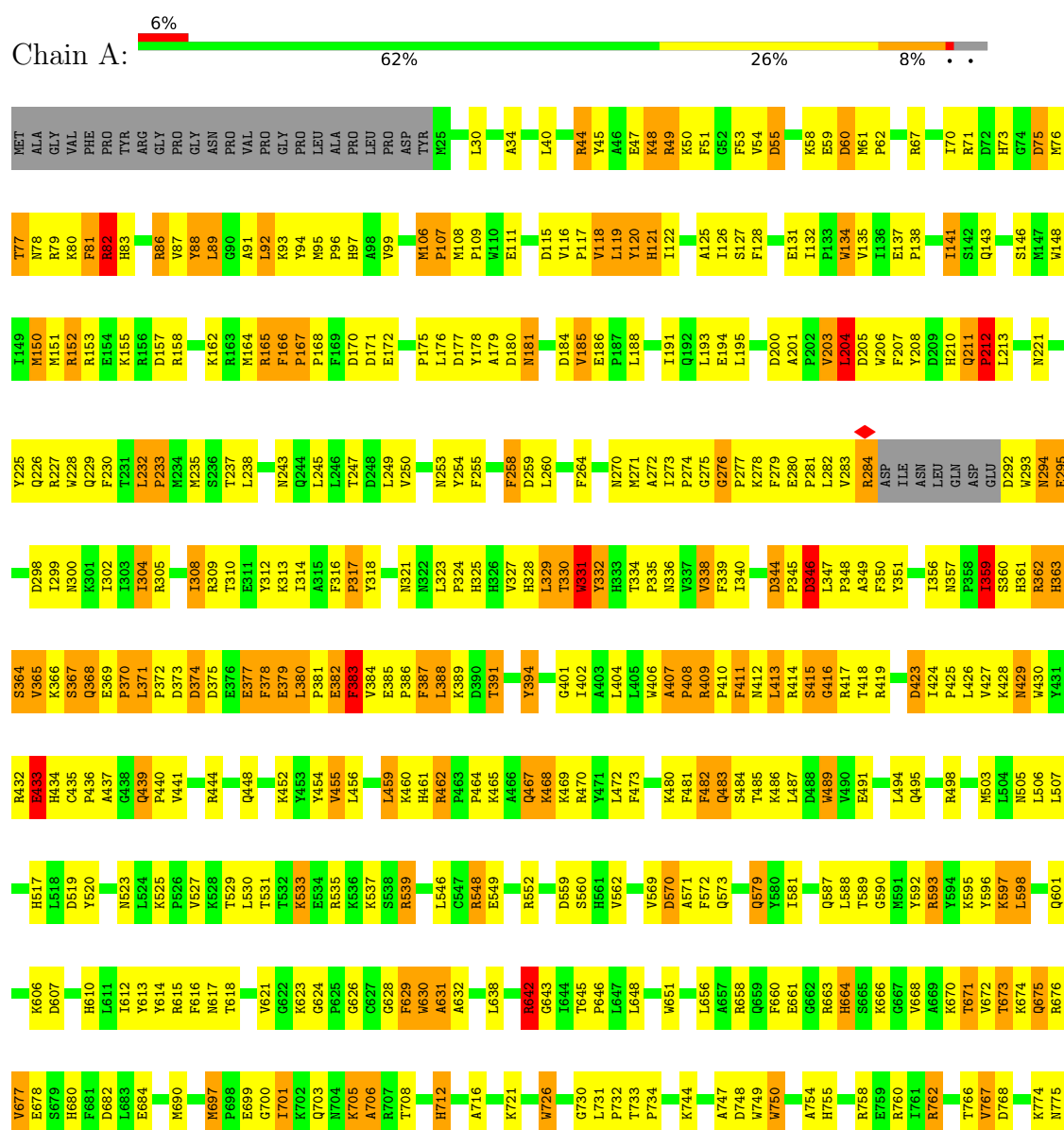
- Molecule 51 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



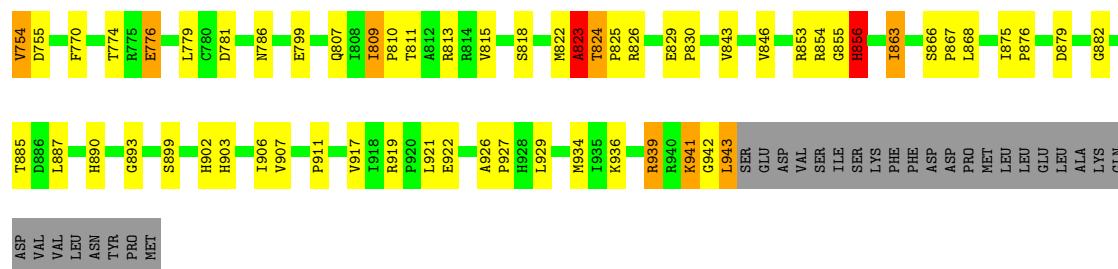
3 Residue-property plots

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

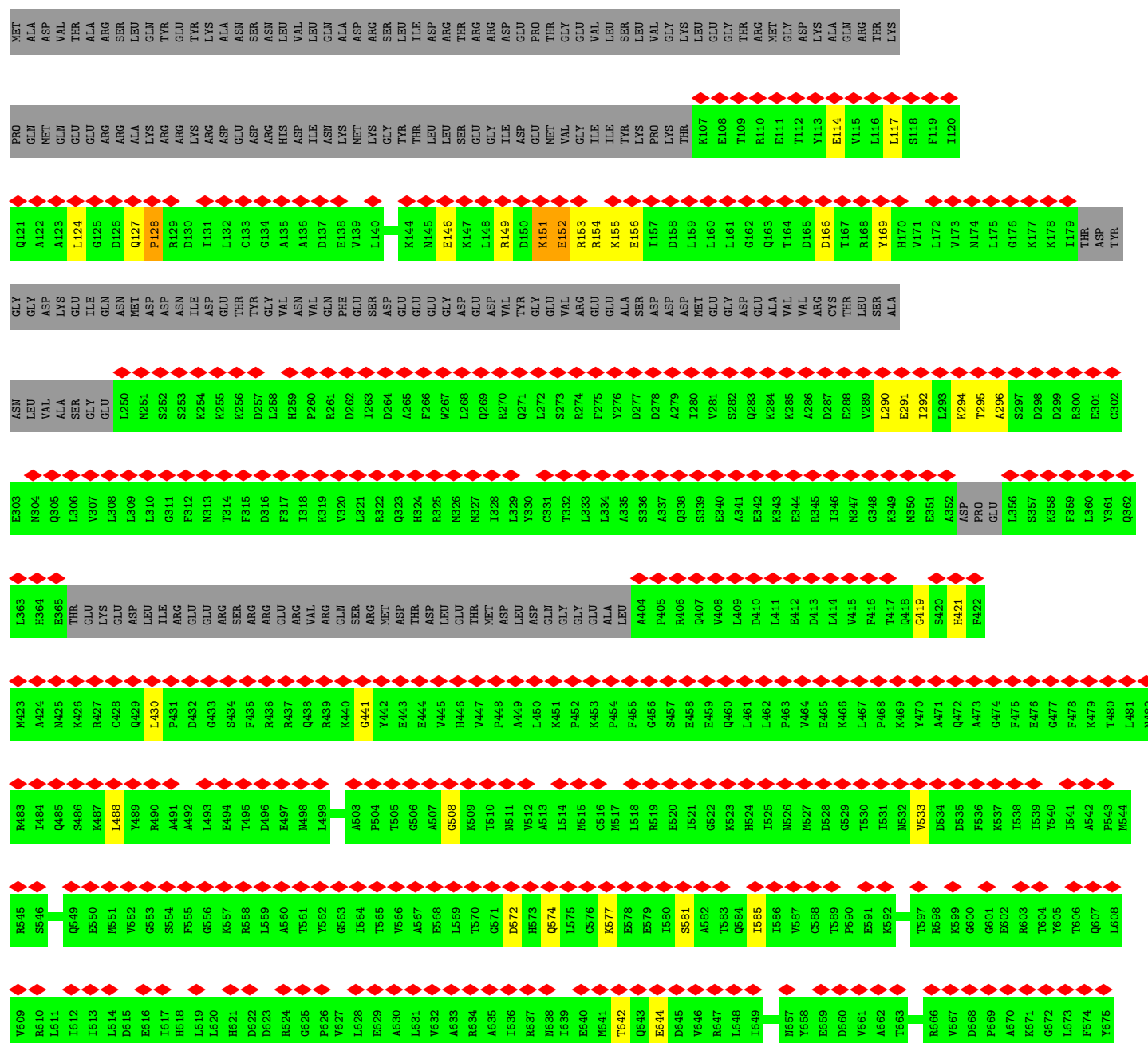
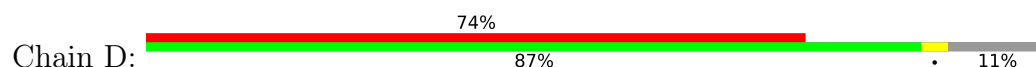
• Molecule 1: Pre-mRNA-processing-splicing factor 8



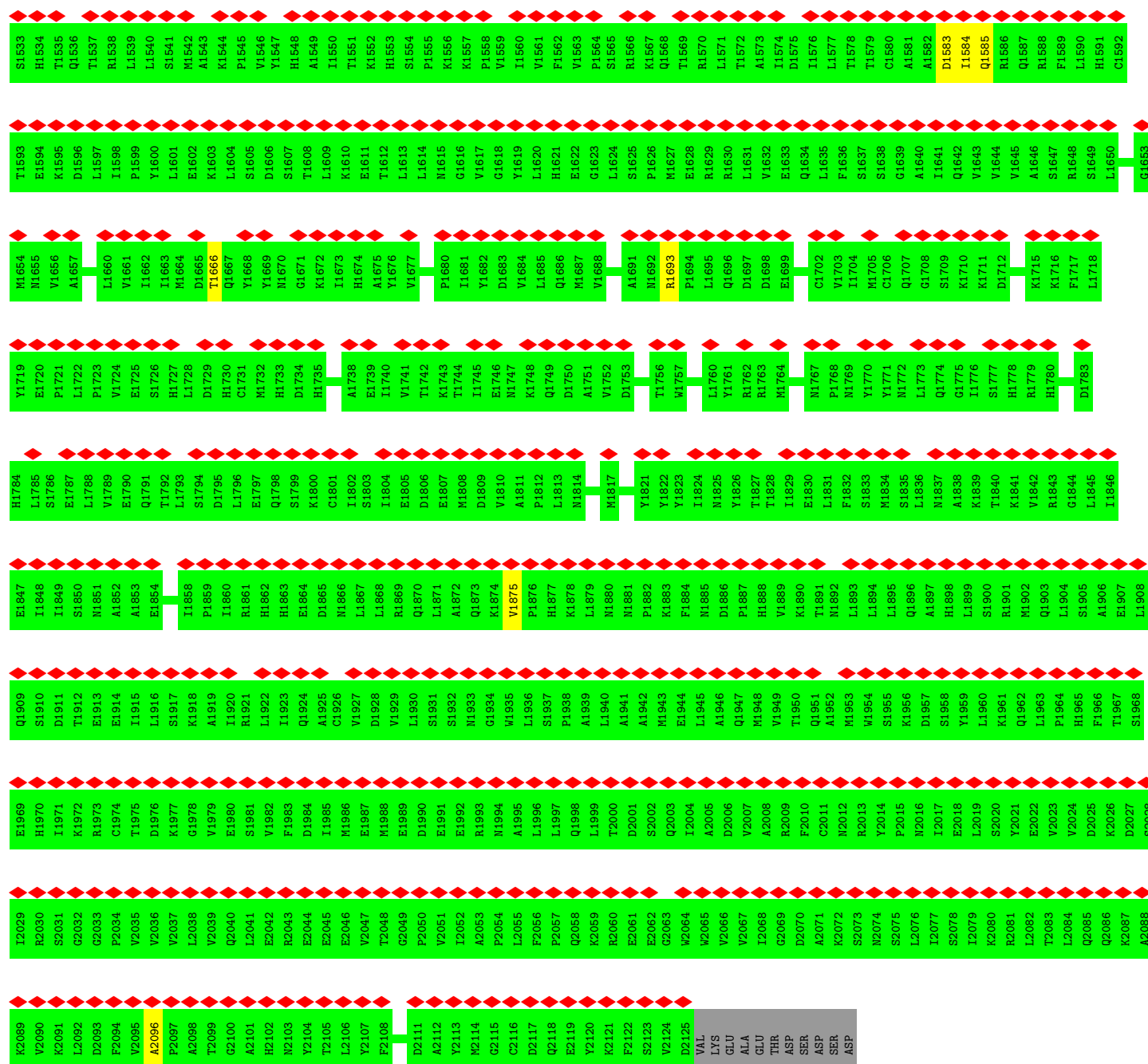




● Molecule 4: U5 small nuclear ribonucleoprotein 200 kDa helicase

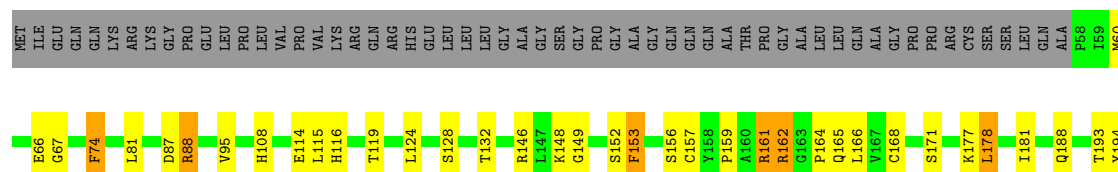




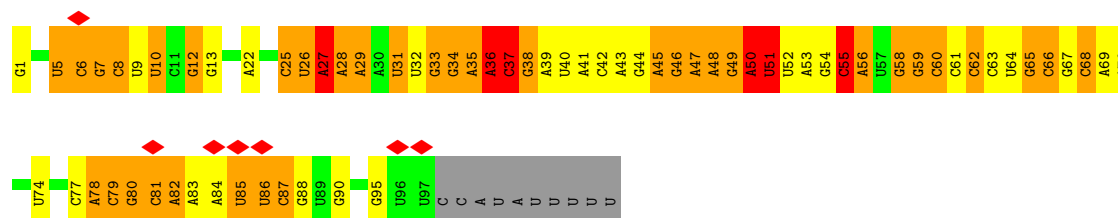
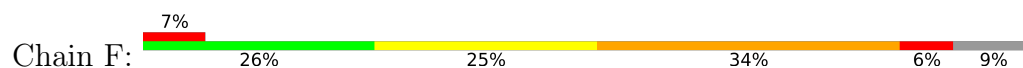


- Molecule 5: U5 small nuclear ribonucleoprotein 40 kDa protein

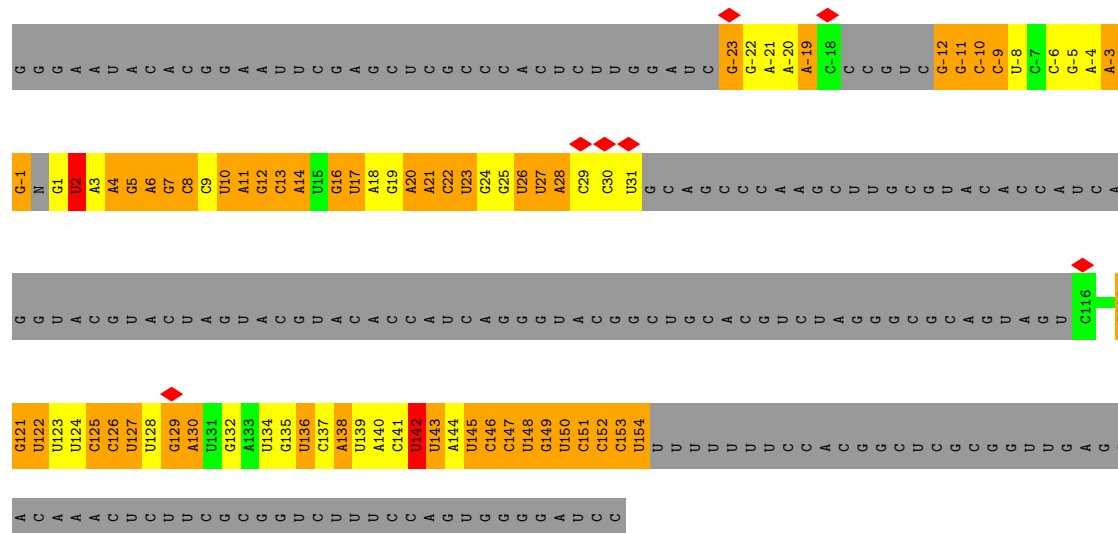
Chain E: 57% 22% 16%



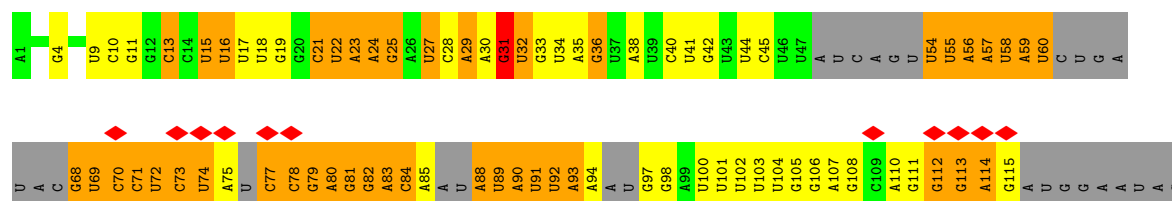
- Molecule 6: U6 snRNA

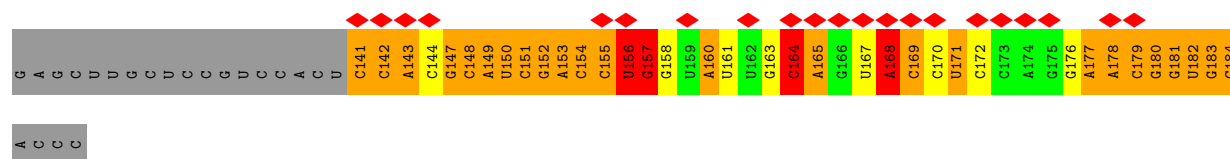


- Molecule 7: Pre-mRNA

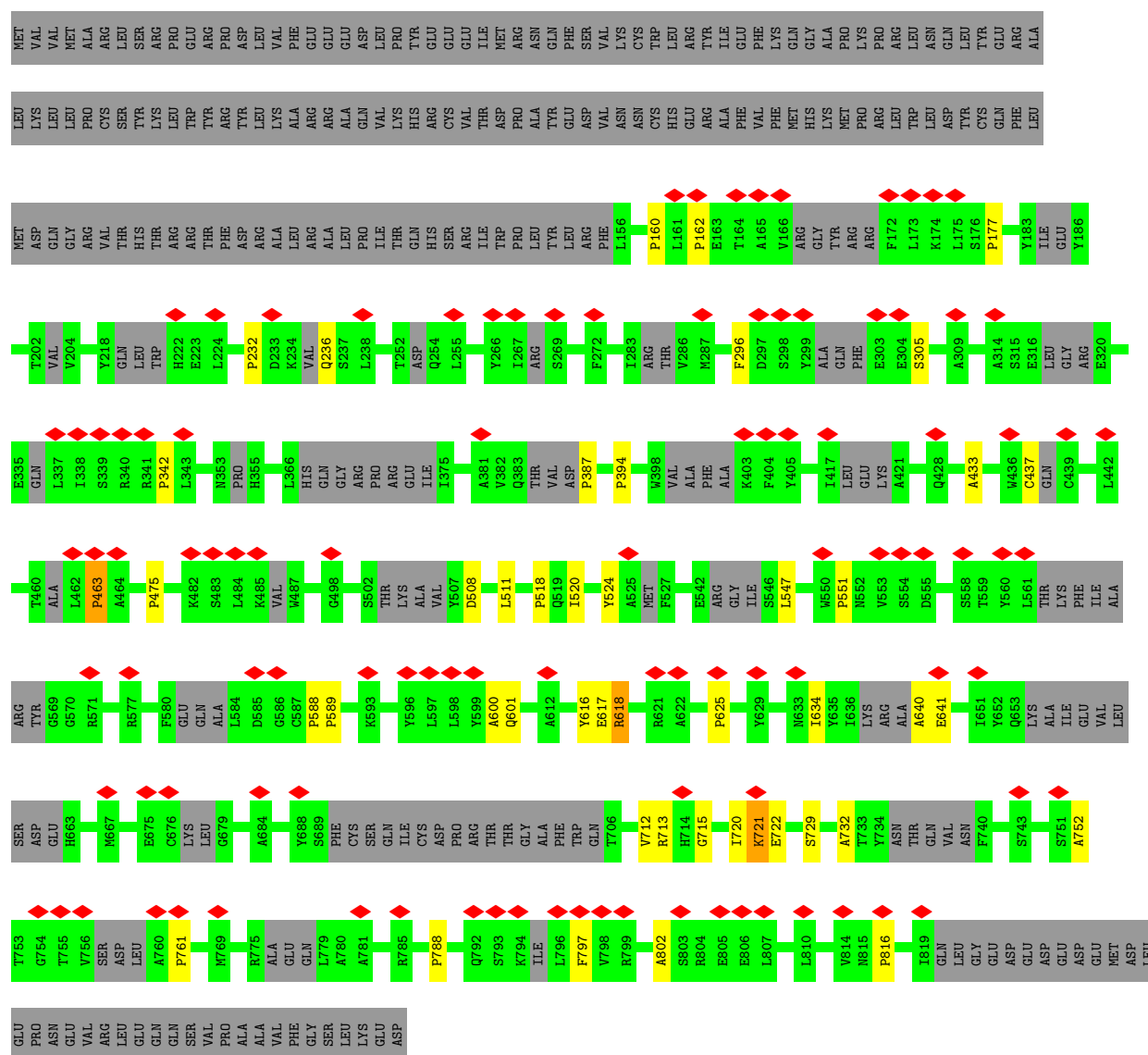


- Molecule 8: U2 snRNA

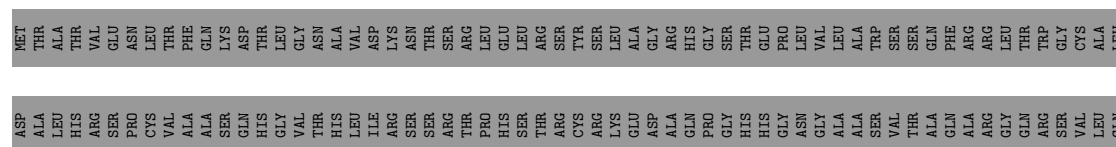


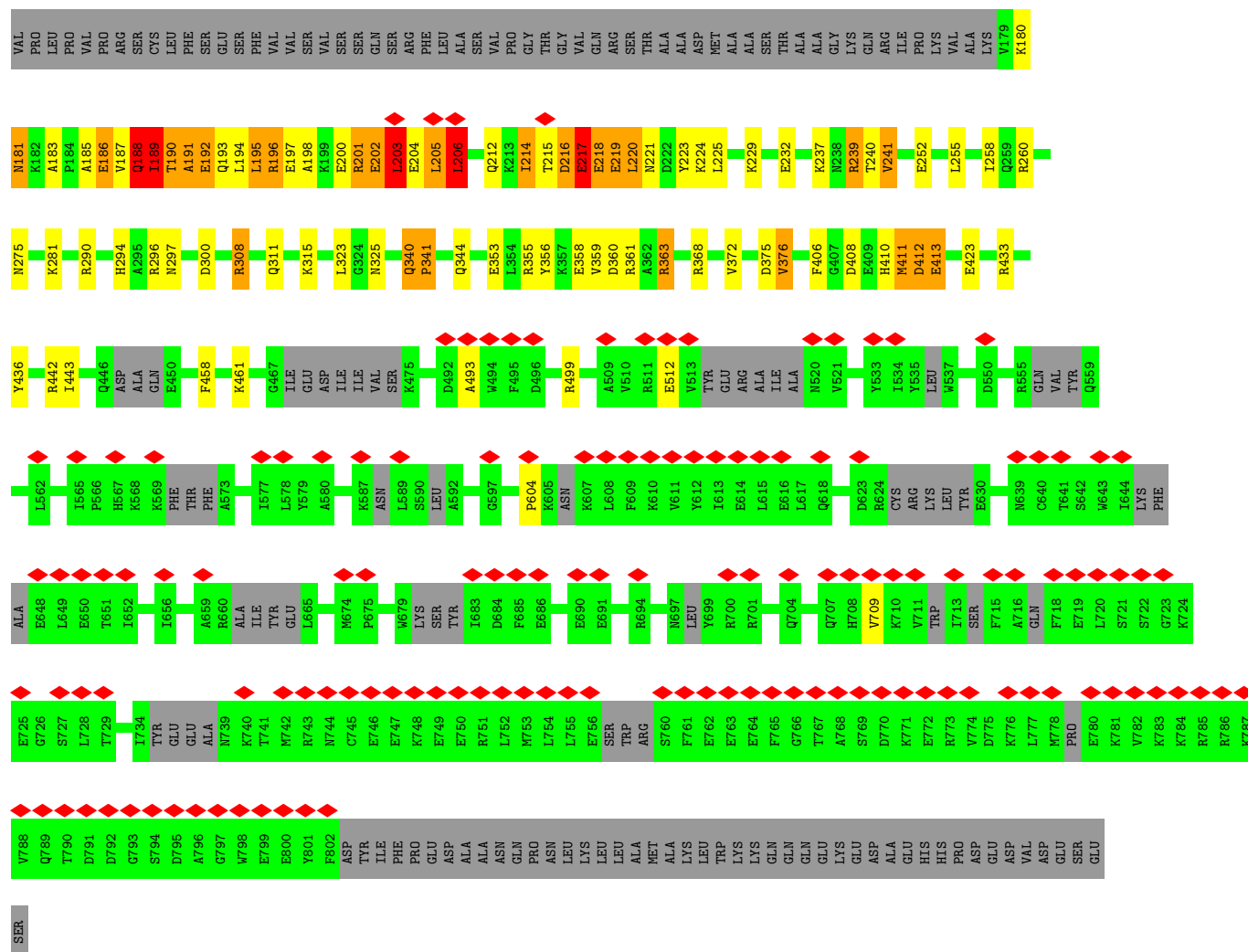


• Molecule 9: Pre-mRNA-splicing factor SYF1

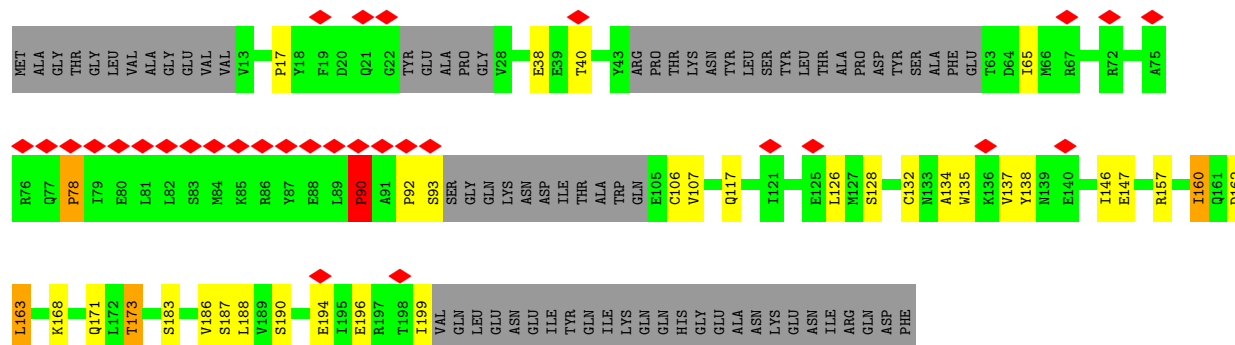


• Molecule 10: Crooked neck-like protein 1

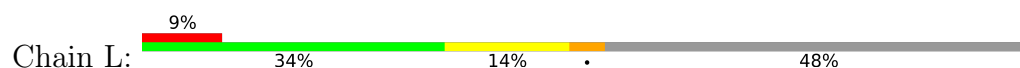


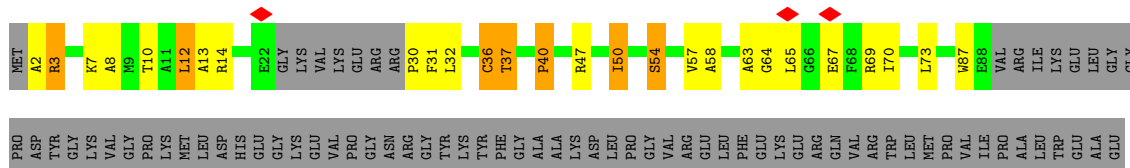


• Molecule 11: Pre-mRNA-splicing factor SPF27

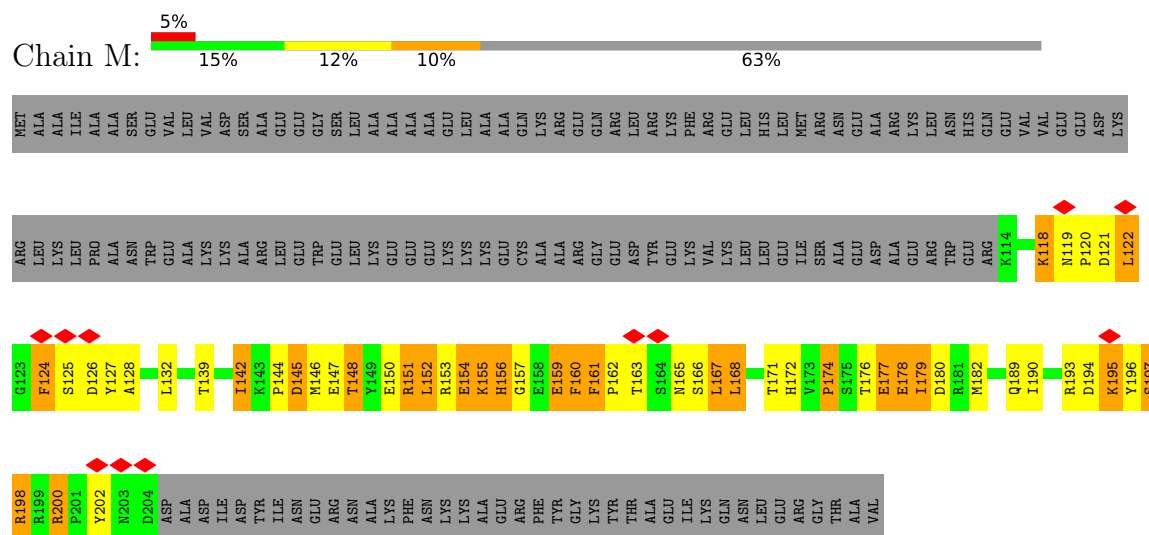


• Molecule 12: Cell division cycle 5-like protein

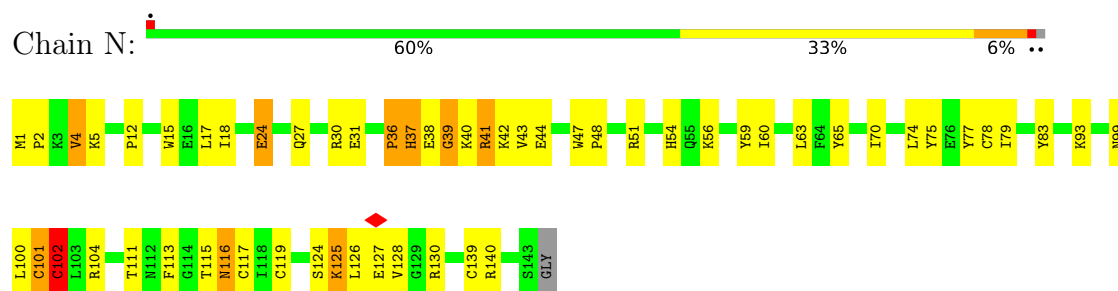




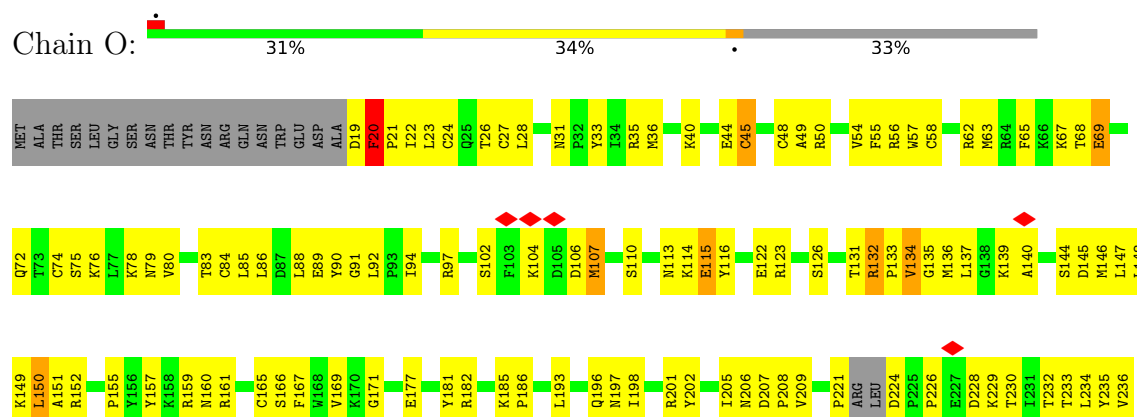
- Molecule 14: Pre-mRNA-splicing factor SYF2



- Molecule 15: Protein BUD31 homolog

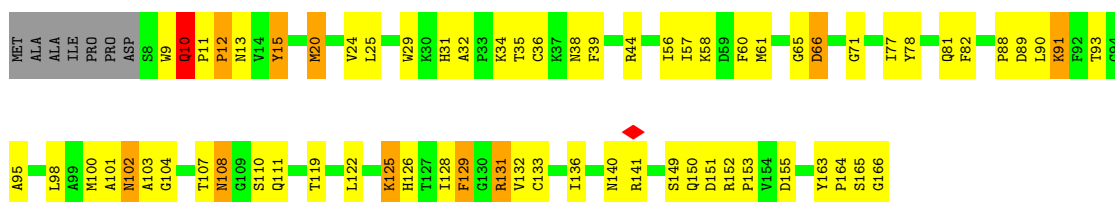


- Molecule 16: Pre-mRNA-splicing factor RBM22

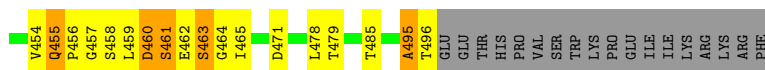
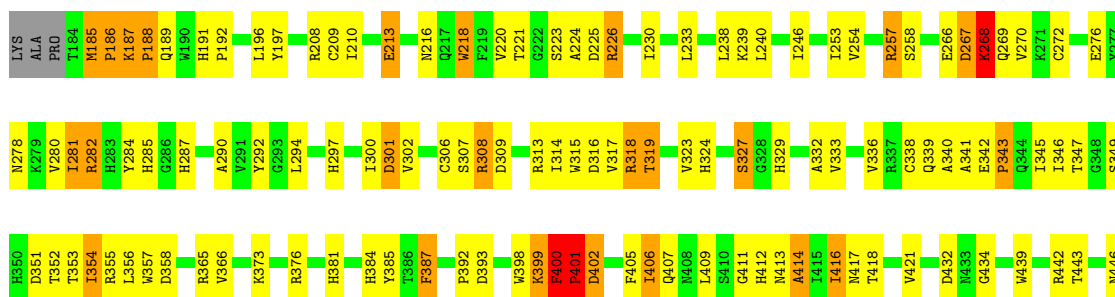
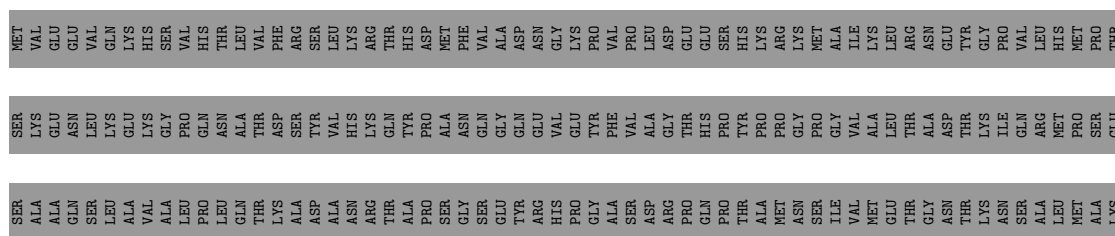
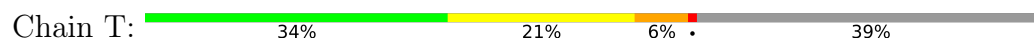




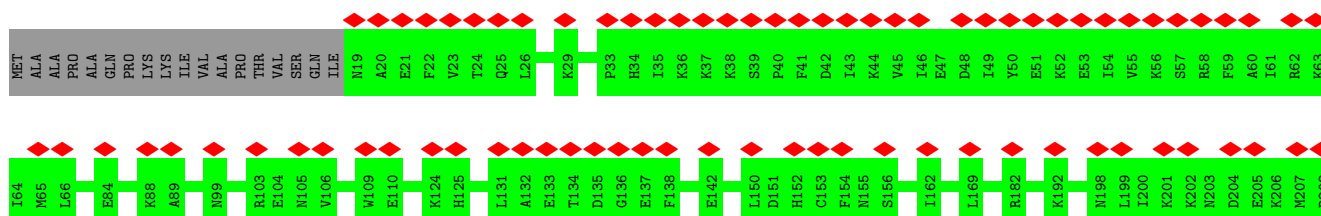
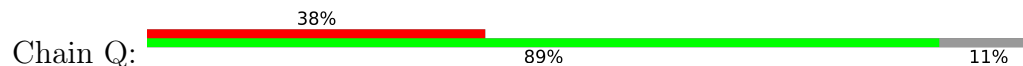
- Molecule 19: Peptidyl-prolyl cis-trans isomerase-like 1



- Molecule 20: Pleiotropic regulator 1



- Molecule 21: Intron-binding protein aquarius





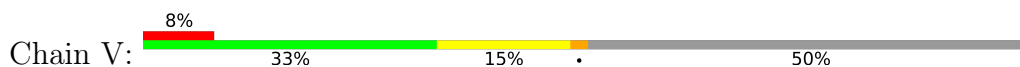
Chain U: 99%



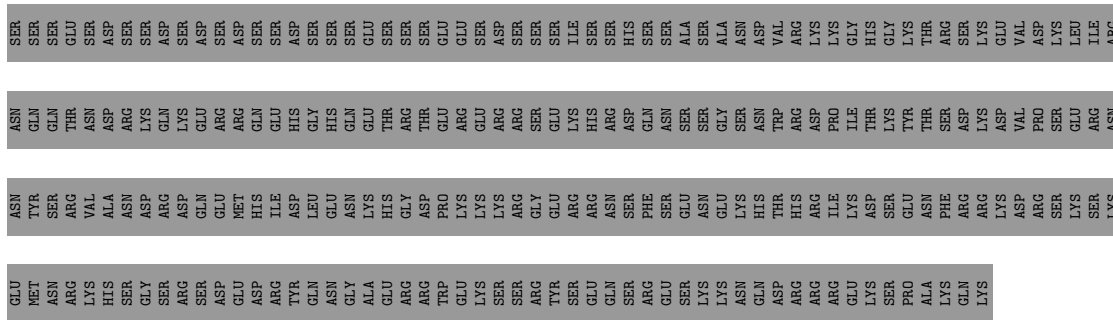


[illegible]

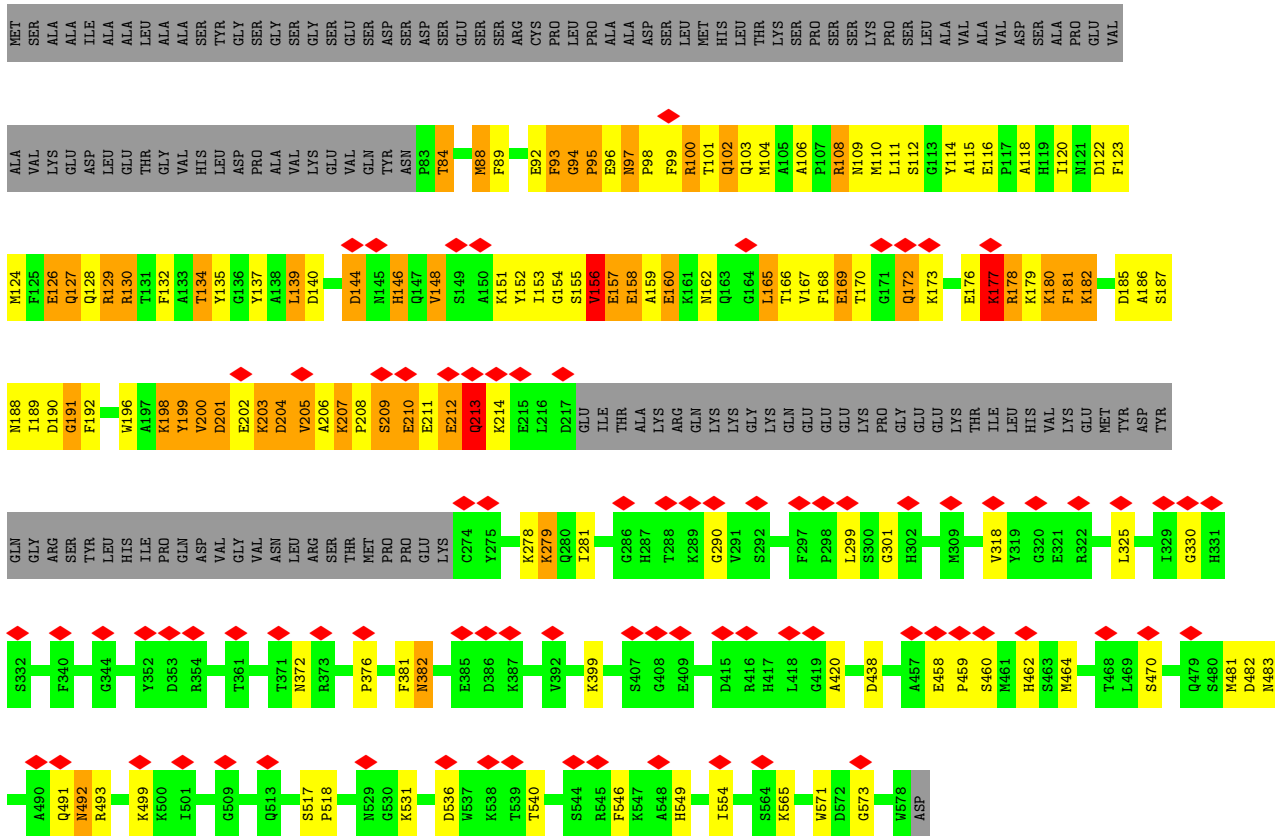
- Molecule 23: Pre-mRNA-splicing factor CWC22 homolog



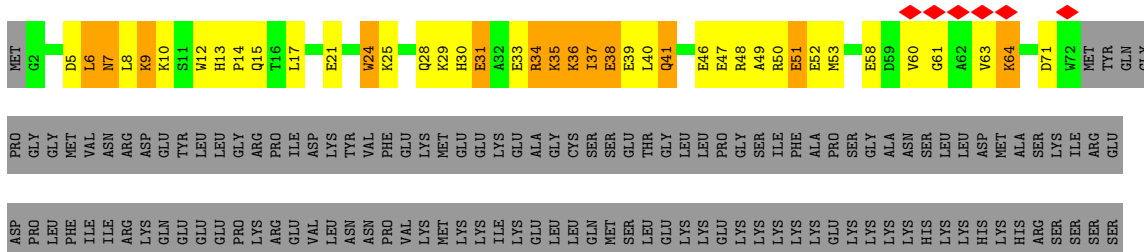
MET	F612	Q532	A462	A400	R192	K298	G193	TYR	SER
	E613	Y533		I401	G193	G311		ASP	TYR
	GLY	D534	S465	K402				ASP	ASP
	LEU	T535	S466	K403	R194			PRO	SER
	LEU	I536	L467	E404	G196	F316		LEU	SER
	PRO	H537	D468	E404	L196	R320		LEU	MET
	ARG		E469	I405	L197			THR	GLU
		E540	E470	I405	S198			ARG	GLN
	D619	T541	E471	L406		E325		ARG	GLN
	N620		C472	ASP				THR	LYS
MET	P621		A473	GLY	L202			GLY	ASN
	R622	N546	H474	GLY		D329		GLY	ARG
	N623	V547	A473	THR	K330			ALA	SER
	T624	A548	K475	ASP	R331			ASP	SER
	R625	K549	L476	THR	R331			TYR	GLY
		M550	L477	ASP	V332			ILE	HIS
	N629	F551	K478	SER	Q333			GLY	ASP
	F630	A552		ASN	Y215			PRO	LYS
	F631	H553		THR	A216			ALA	ARG
			E483	ASP	A217			LEU	GLU
MET	I634	Y566	S484	GLN	L218	F340		ARG	ASN
		T567	Q485	ASP				GLU	LEU
	G637	D568	T486	ALA	V219	R343		MET	ASN
	G638	S559	K487	GLY	A220	K344		ASP	ASP
	L639	LEU	L489	SER				GLN	THR
	T640	PRO	C490	GLY	K225			GLY	ASP
	D641	H622	N491	GLU	E231			ILE	ARG
	E642		M492	GLU	L232			GLN	ARG
	L643	L565	I493	ASP	I233			LYS	ASN
	R644	S571	C496	GLU	K234			ARG	SER
MET	E645	E572	C497	GLU	L235			LYS	PRO
	H646			GLU	R247			SER	TYR
	L647	E573	Q500	GLY				PRO	GLY
	ASN	T574	R501	GLY	K250			GLY	GLN
	THR	T575	T502	GLY	Q251			ARG	GLN
	PRO	T576	Y503	GLY	E362			ARG	GLN
	LYS	S577	E504	GLU	L252			ASN	ARG
	VAL	S578	K505	GLU				PRO	SER
	ILE	S579	K506	ASP	V260			GLU	PRO
	VAL	R580	F507	GLY	L370			THR	ARG
MET	ALA	K584		GLY	A261			GLU	ARG
	GLN	I585	L510	GLN	H262			SER	ASP
	LYS	F586	A511	GLY	L263			VAL	ASP
	PRO	F587	G512	LYS	I264			THR	ASP
	ASP	Q588	R513	VAL				GLN	TYR
	VAL	E589	F514	THR	A269			SER	PHE
	GLY		C515	ILE				ASP	TYR
	GLN	L596		HIS	C274			SER	TYR
	ASN	P597		ASP				ALA	SER
	LYS	Y521	E520	LYS				GLN	ARG
MET	SER	M600	M522	T448	K277			ASP	SER
	PRO	A601	E523	E449	L278			GLY	TYR
	SER	R602	S524		T279			ALA	GLU
	SER	L603	F525	L452	E283			HIS	HIS
	SER		E526		R284			LYS	SER
	SER	E606	G527	F455				ARG	ARG
	SER	T607	G527	R456	D287			LYS	ARG
	SER	L608	F529	R457	D288			LYS	GLY
	ALA	Q609	K530	T458				ASP	ARG
	ALA		E531	T459				ASP	ARG



- Molecule 24: Pre-mRNA-processing factor 17

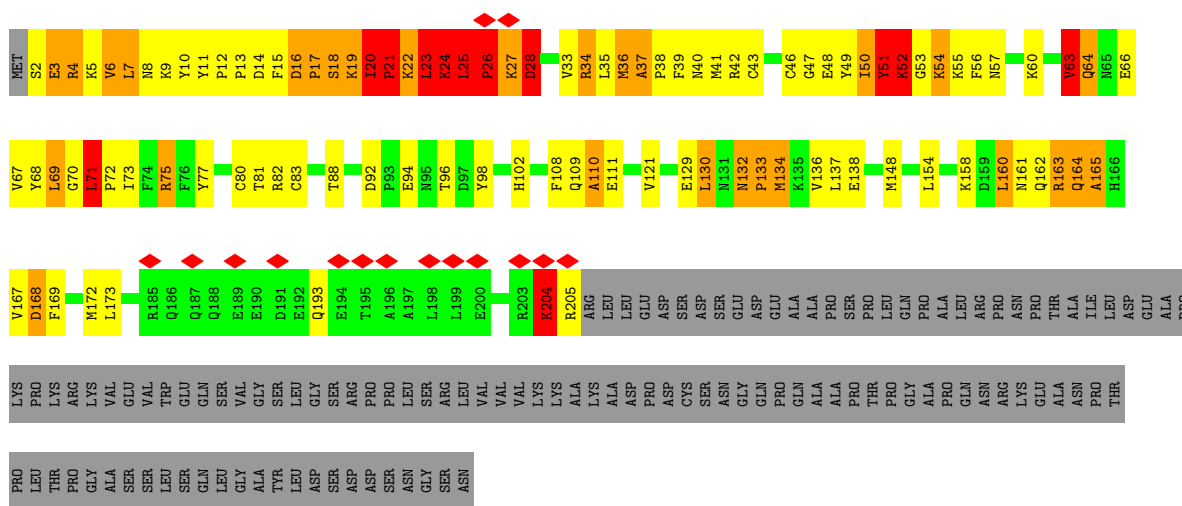
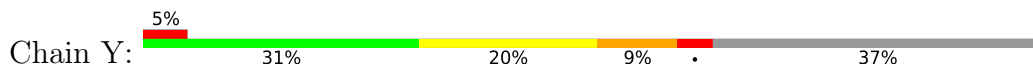


- Molecule 25: Pre-mRNA-splicing factor CWC25 homolog



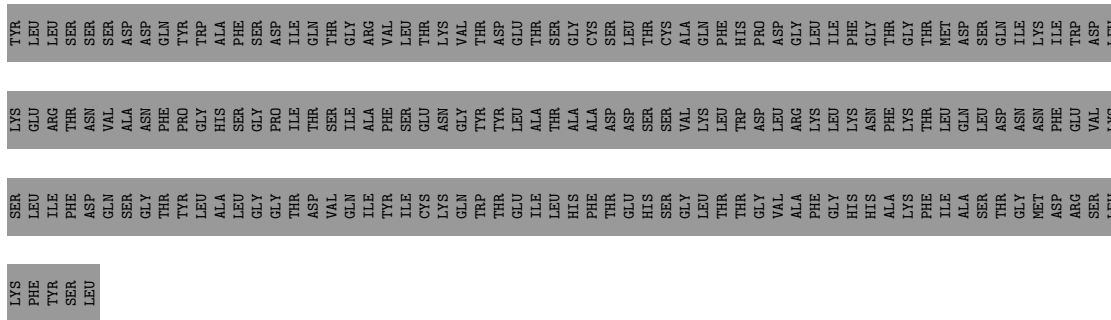
[illegible]

- Molecule 26: Coiled-coil domain-containing protein 94

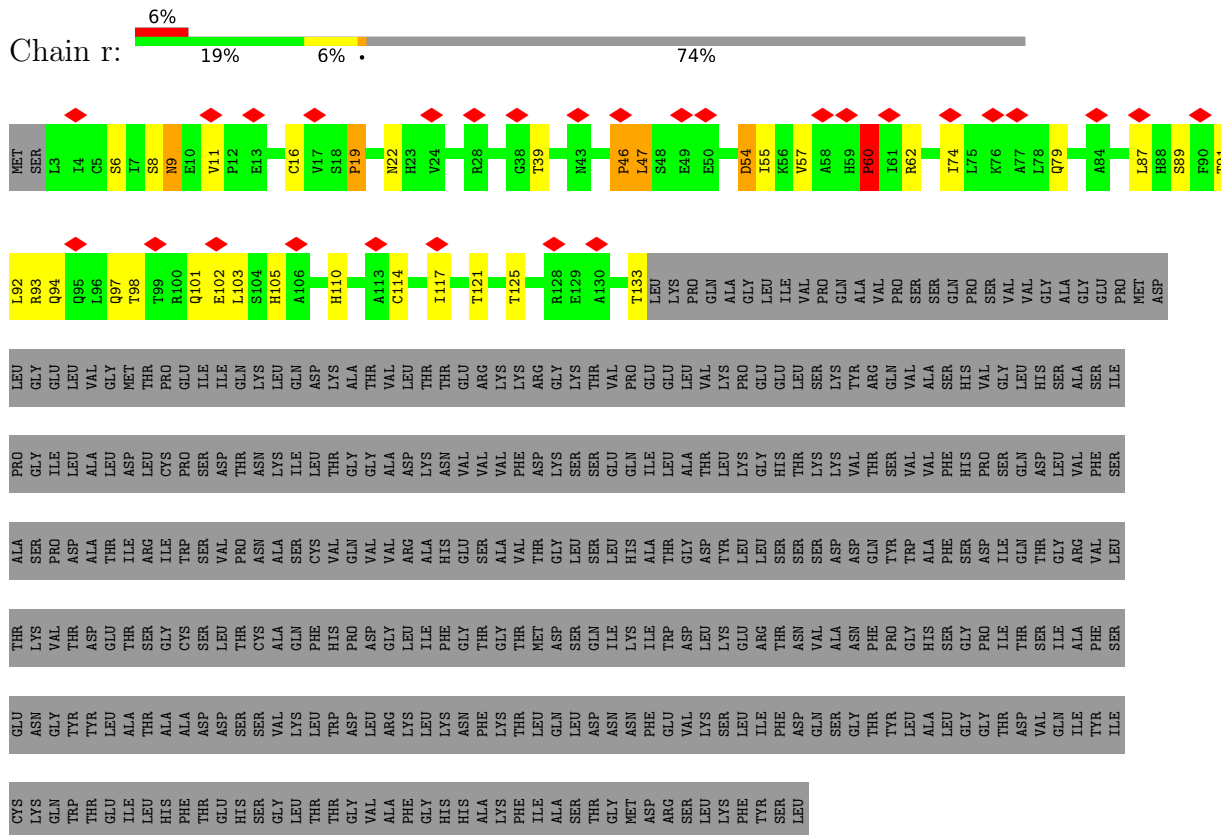


- Molecule 27: Pre-mRNA-splicing factor ATP-dependent RNA helicase PRP16

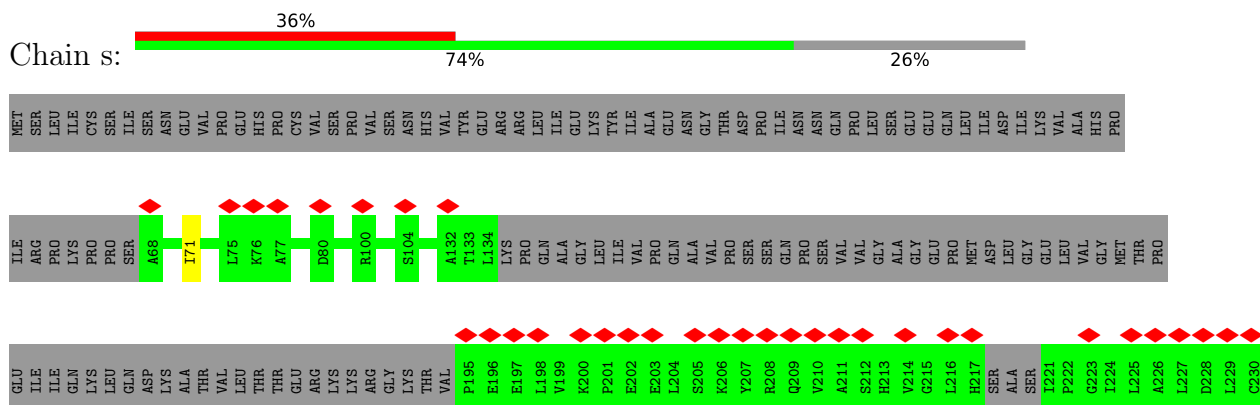
[illegible]

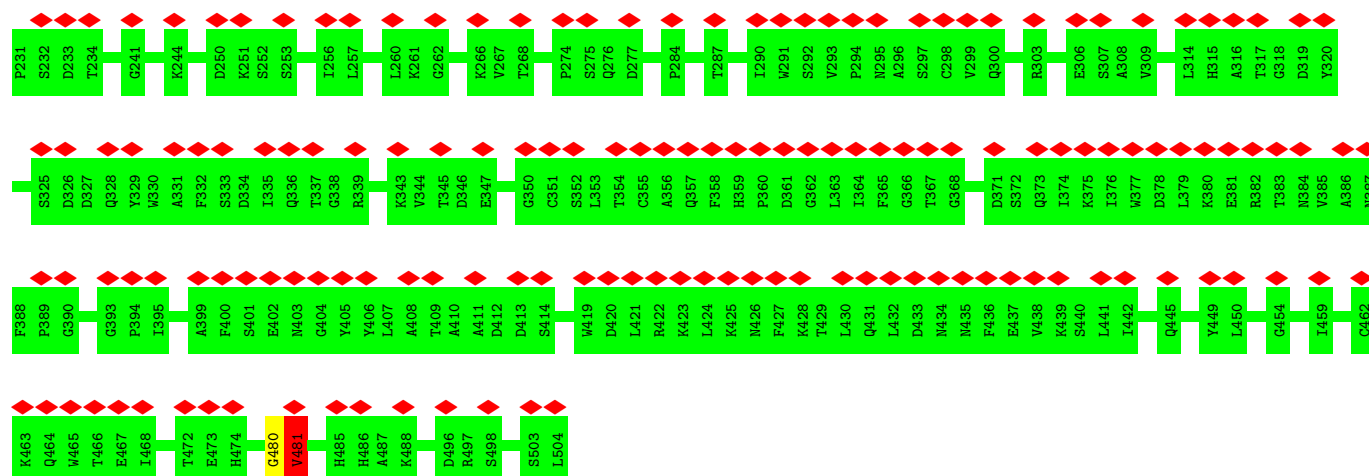


- Molecule 28: Pre-mRNA-processing factor 19

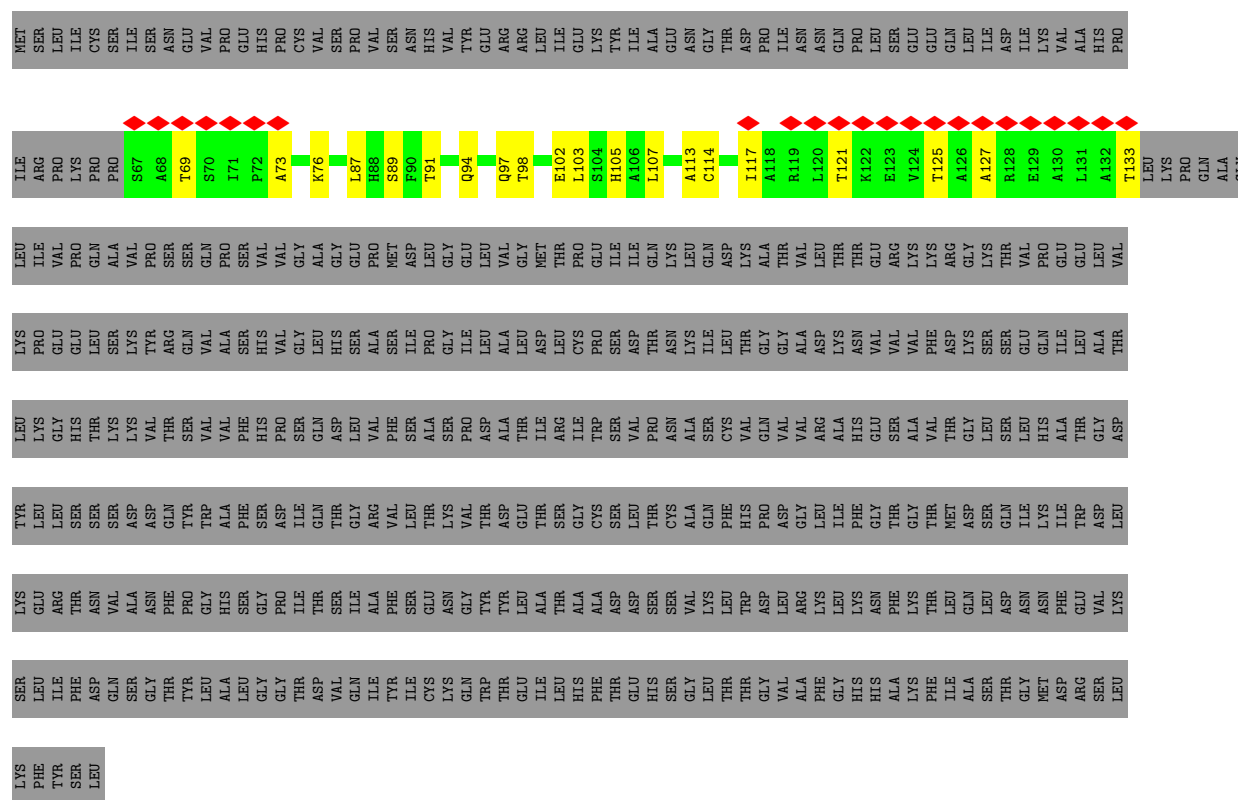


- Molecule 28: Pre-mRNA-processing factor 19

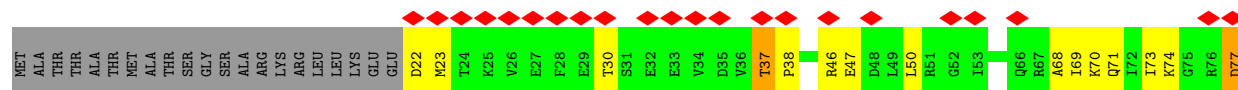
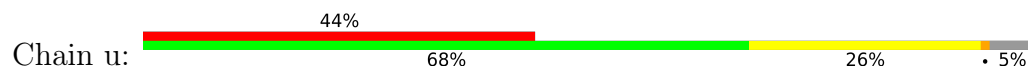


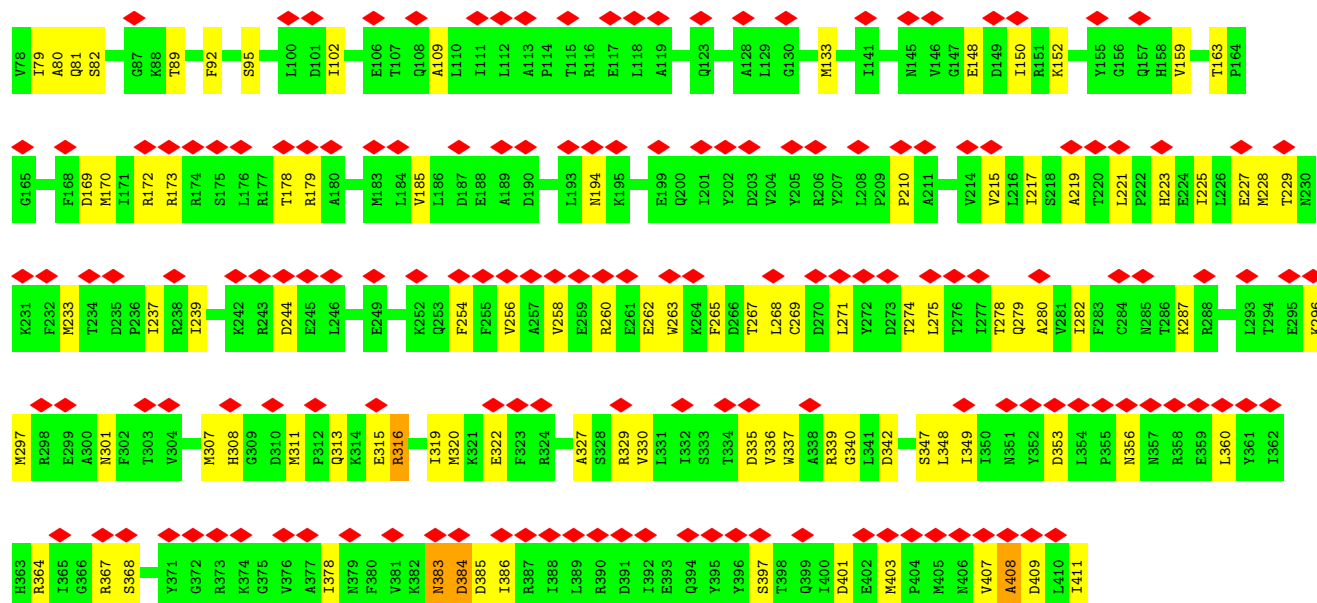


• Molecule 28: Pre-mRNA-processing factor 19

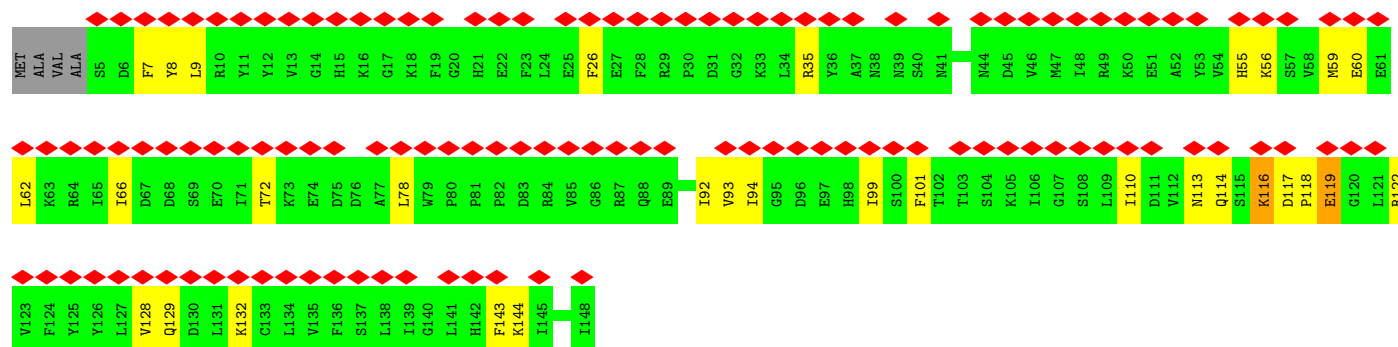
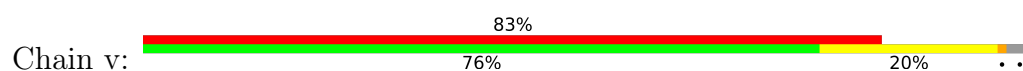


• Molecule 29: Eukaryotic initiation factor 4A-III

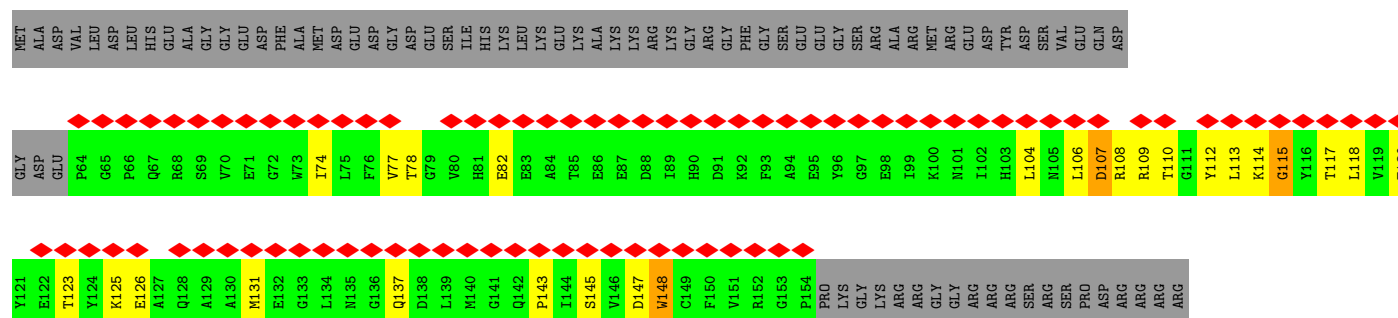
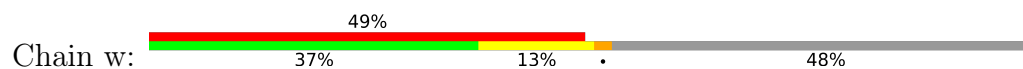




- Molecule 30: Protein mago nashi homolog 2

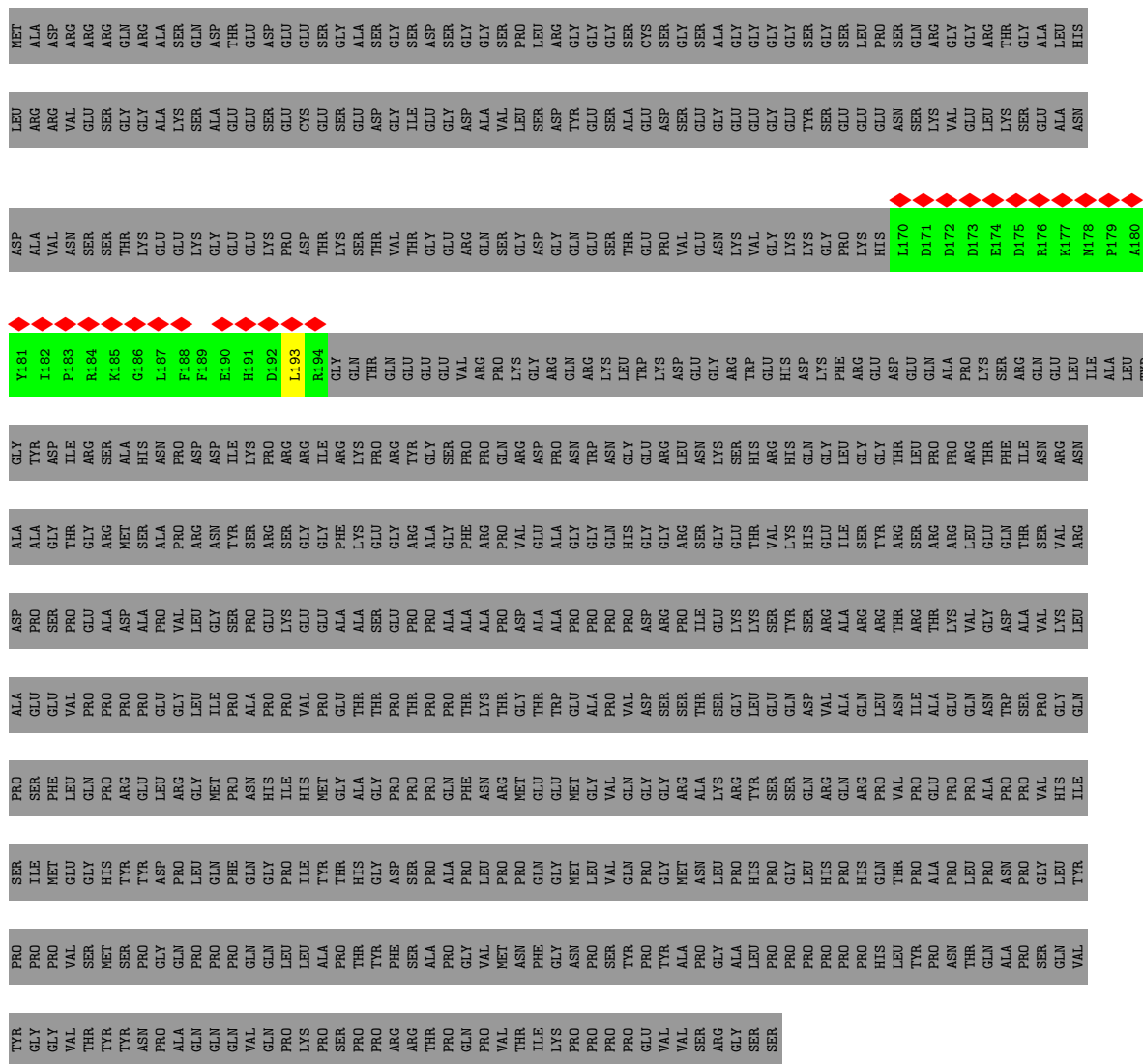


- Molecule 31: RNA-binding protein 8A

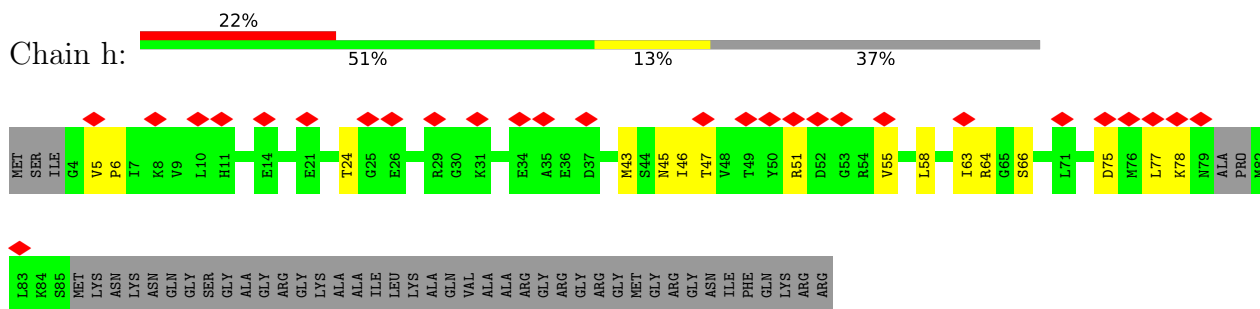


- Molecule 32: Protein CASC3

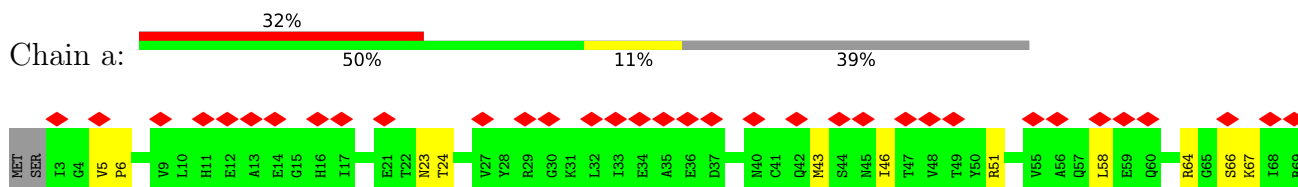




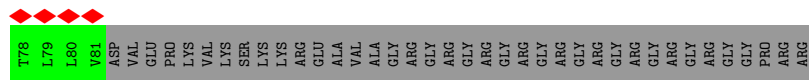
- Molecule 33: Small nuclear ribonucleoprotein Sm D3



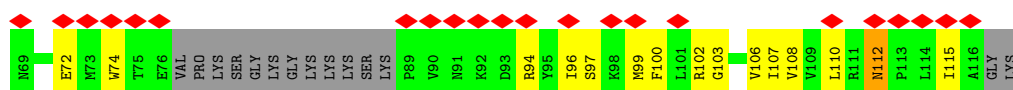
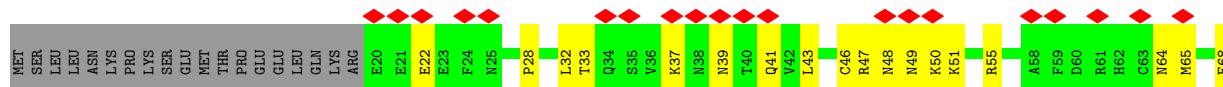
- Molecule 33: Small nuclear ribonucleoprotein Sm D3



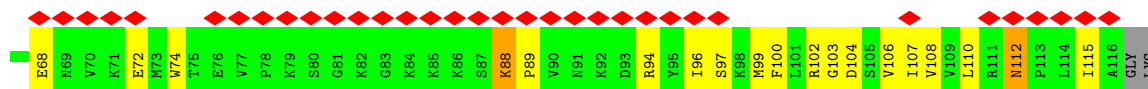
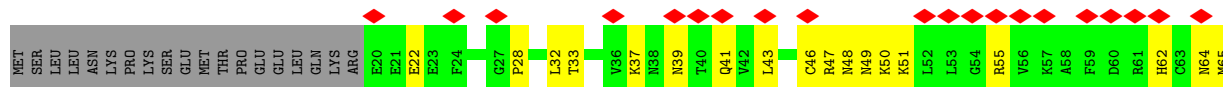




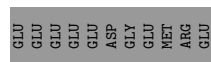
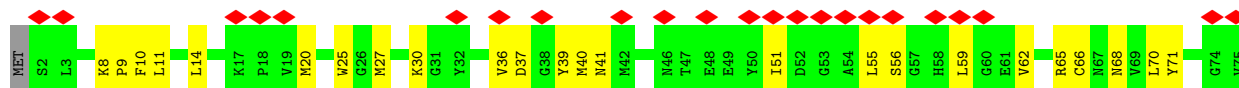
- Molecule 36: Small nuclear ribonucleoprotein Sm D2



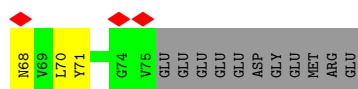
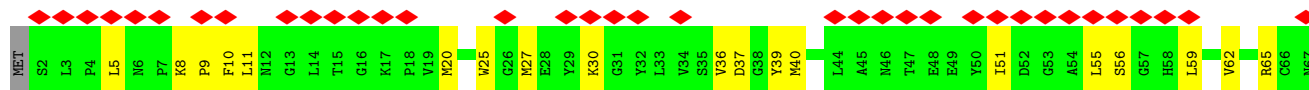
- Molecule 36: Small nuclear ribonucleoprotein Sm D2



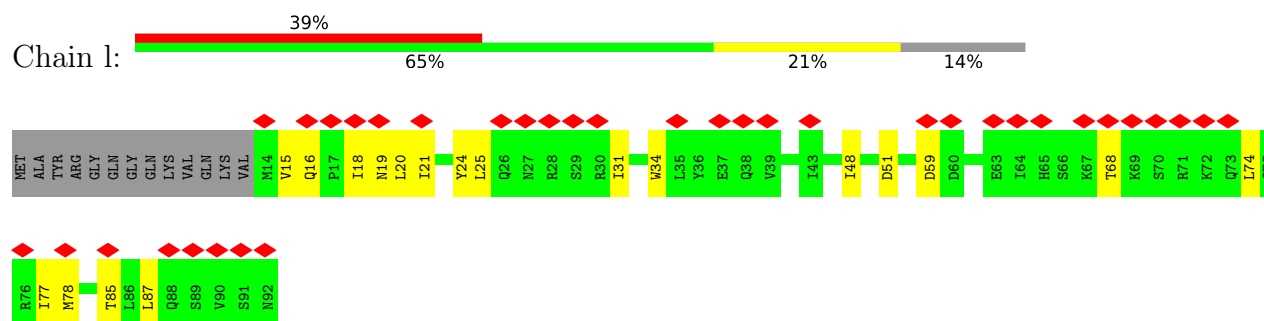
- Molecule 37: Small nuclear ribonucleoprotein F



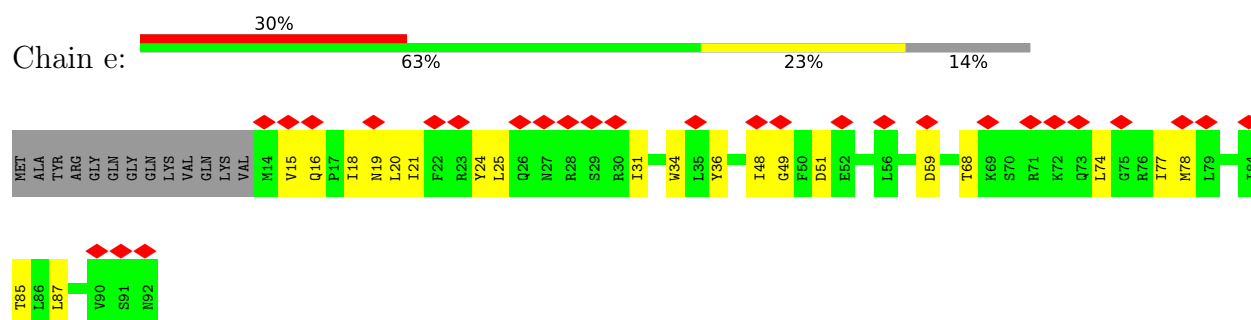
- Molecule 37: Small nuclear ribonucleoprotein F



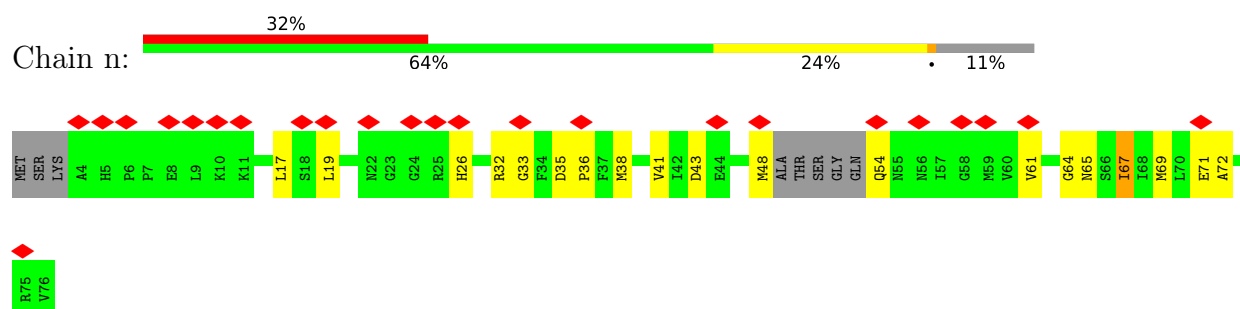
- Molecule 38: Small nuclear ribonucleoprotein E



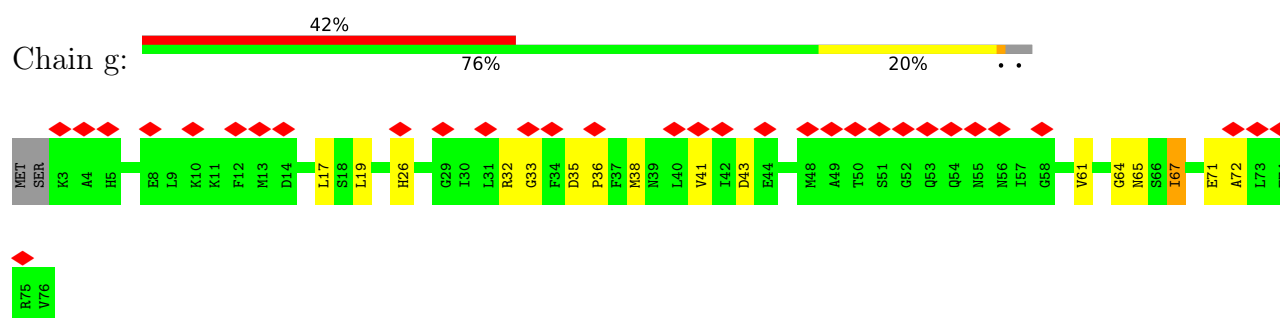
- Molecule 38: Small nuclear ribonucleoprotein E



- Molecule 39: Small nuclear ribonucleoprotein G

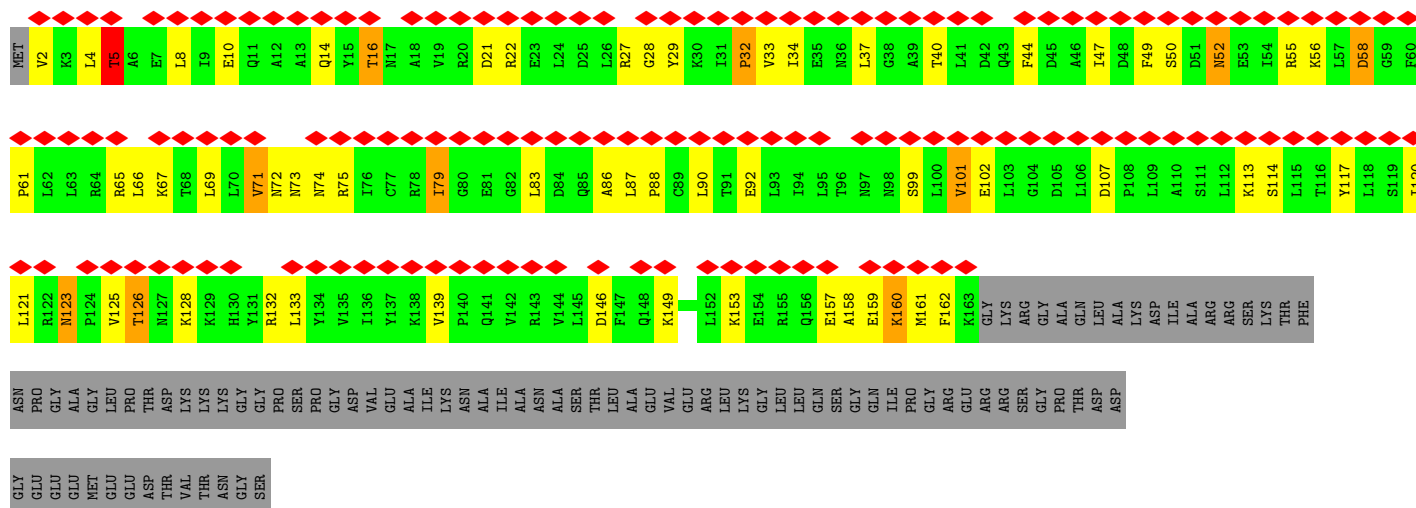


- Molecule 39: Small nuclear ribonucleoprotein G

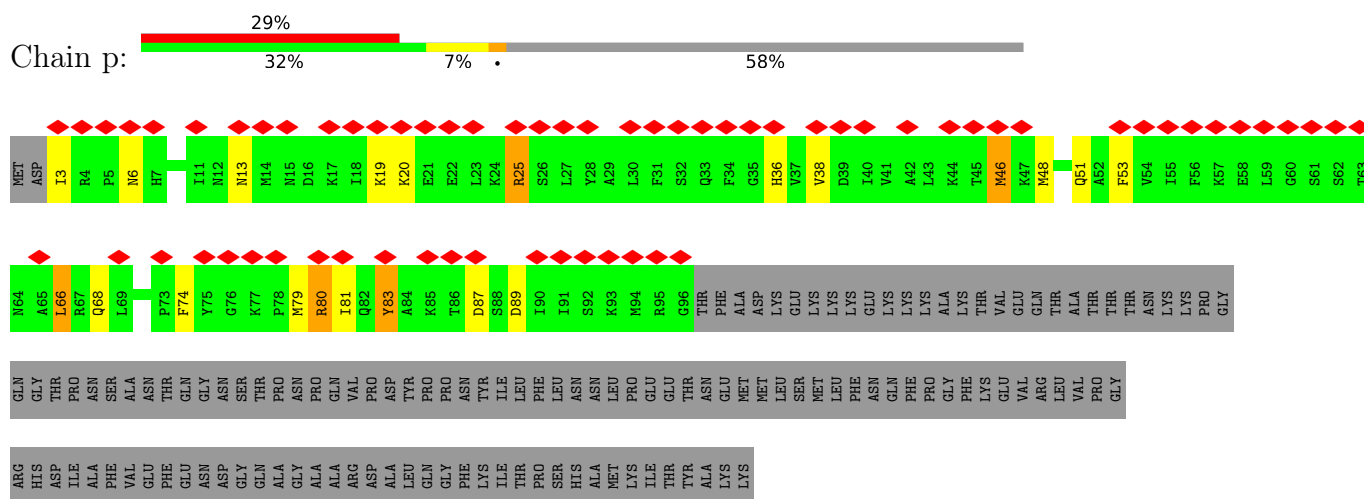


- Molecule 40: U2 small nuclear ribonucleoprotein A'

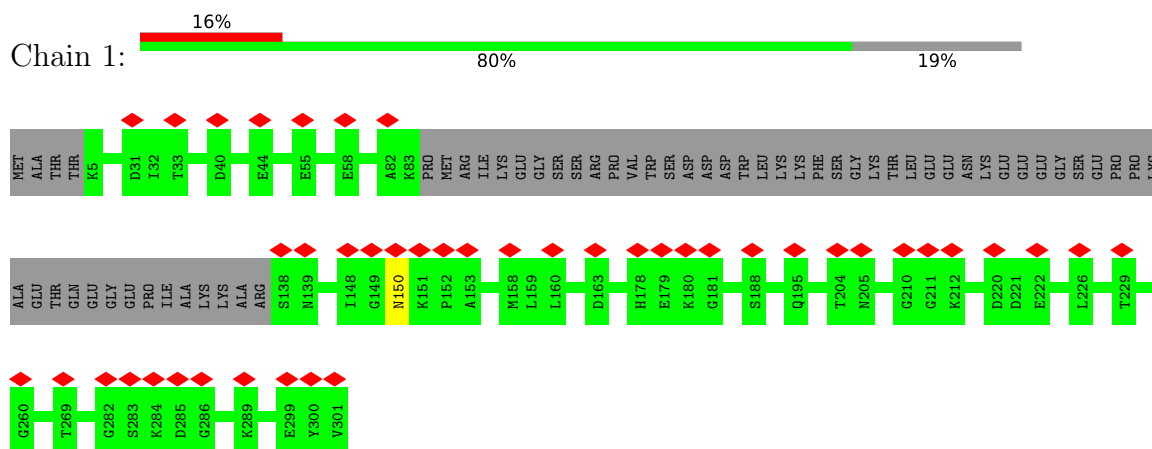




• Molecule 41: U2 small nuclear ribonucleoprotein B''



• Molecule 42: Peptidyl-prolyl cis-trans isomerase E

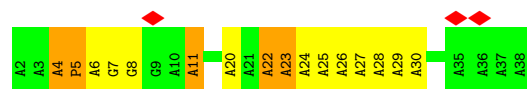


• Molecule 43: Peptidylprolyl isomerase domain and WD repeat-containing protein 1



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

- Molecule 45: UNKNOWN



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	53633	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.209	Depositor
Minimum map value	-0.105	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.029	Depositor
Map size ($\text{\AA}$)	535.2, 535.2, 535.2	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.338, 1.338, 1.338	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	A	1.29	90/17966 (0.5%)	1.34	108/24251 (0.4%)
2	B	0.69	1/1970 (0.1%)	0.96	6/3060 (0.2%)
3	C	1.09	11/6946 (0.2%)	1.28	41/9436 (0.4%)
4	D	0.55	0/7628	1.17	29/9528 (0.3%)
5	E	0.87	0/2392	1.00	6/3242 (0.2%)
6	F	0.58	0/2323	0.99	12/3619 (0.3%)
7	G	0.70	7/1820 (0.4%)	0.93	5/2819 (0.2%)
8	H	0.86	25/3283 (0.8%)	1.43	64/5096 (1.3%)
9	I	0.53	0/2724	0.91	18/3738 (0.5%)
10	J	0.81	2/3870 (0.1%)	1.14	6/5252 (0.1%)
11	K	1.08	12/981 (1.2%)	1.02	6/1317 (0.5%)
12	L	0.86	5/2914 (0.2%)	1.18	17/3929 (0.4%)
13	y	0.76	4/707 (0.6%)	1.12	5/953 (0.5%)
14	M	0.71	0/791	1.10	1/1058 (0.1%)
15	N	1.15	1/1210 (0.1%)	1.16	4/1622 (0.2%)
16	O	1.04	3/2324 (0.1%)	1.05	3/3135 (0.1%)
17	P	1.01	1/841 (0.1%)	1.29	3/1117 (0.3%)
18	R	1.03	8/1976 (0.4%)	1.34	11/2651 (0.4%)
19	S	0.81	0/1268	1.13	8/1714 (0.5%)
20	T	1.44	13/2526 (0.5%)	1.42	26/3443 (0.8%)
21	Q	0.38	0/5279	0.92	1/6583 (0.0%)
22	U	1.44	3/196 (1.5%)	1.53	4/265 (1.5%)
23	V	0.76	1/3453 (0.0%)	1.03	3/4640 (0.1%)
24	W	0.85	3/2336 (0.1%)	1.24	19/3027 (0.6%)
25	X	0.63	0/486	1.02	3/658 (0.5%)
26	Y	0.74	7/1450 (0.5%)	1.39	26/1975 (1.3%)
27	Z	0.87	2/2528 (0.1%)	1.75	38/3139 (1.2%)
28	q	0.98	9/929 (1.0%)	1.00	6/1260 (0.5%)
28	r	0.97	9/912 (1.0%)	1.02	6/1239 (0.5%)
28	s	3.23	4/1497 (0.3%)	1.30	4/1866 (0.2%)
28	t	0.91	6/480 (1.2%)	0.85	0/650
29	u	0.45	0/3175	1.00	14/4286 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
30	v	0.40	0/1225	0.84	3/1648 (0.2%)
31	w	0.40	0/748	0.98	4/1012 (0.4%)
32	x	0.46	0/221	0.92	0/296
33	a	0.63	0/616	0.85	0/830
33	h	0.65	0/627	0.86	0/842
34	b	0.71	0/685	1.01	3/913 (0.3%)
34	i	0.73	0/700	1.03	4/933 (0.4%)
35	c	0.74	0/649	0.98	0/877
35	j	0.74	0/657	0.98	0/888
36	d	0.94	0/778	1.10	2/1045 (0.2%)
36	k	0.95	0/696	1.07	1/935 (0.1%)
37	f	1.03	0/588	1.08	0/795
37	m	1.04	1/588 (0.2%)	1.08	0/795
38	e	0.85	0/660	1.06	1/886 (0.1%)
38	l	0.85	0/660	1.06	1/886 (0.1%)
39	g	0.71	0/576	0.95	1/771 (0.1%)
39	n	0.70	0/539	0.95	1/718 (0.1%)
40	o	0.81	0/1294	2.06	56/1754 (3.2%)
41	p	0.77	0/774	1.71	13/1035 (1.3%)
42	1	0.55	0/970	0.96	0/1209
43	2	0.85	0/1649	0.99	0/2035
44	3	0.97	1/682 (0.1%)	1.08	3/849 (0.4%)
45	4	0.65	0/184	1.38	3/255 (1.2%)
All	All	0.99	229/105947 (0.2%)	1.20	599/142775 (0.4%)

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
1	A	0	6
3	C	0	3
4	D	0	1
10	J	0	1
12	L	0	1
13	y	0	1
14	M	0	1
15	N	0	1
18	R	0	1
20	T	0	2
26	Y	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
27	Z	0	29
28	s	0	4
36	d	0	1
36	k	0	1
All	All	0	56

All (229) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	s	481[A]	VAL	N-CA	82.34	2.43	1.46
28	s	481[B]	VAL	N-CA	82.34	2.43	1.46
1	A	642	ARG	CD-NE	14.92	1.67	1.46
28	q	47	LEU	CB-CG	14.02	1.81	1.53
28	r	47	LEU	CB-CG	13.93	1.81	1.53
11	K	163	LEU	CB-CG	13.78	1.81	1.53
1	A	642	ARG	NE-CZ	13.26	1.47	1.33
28	s	481[A]	VAL	CA-C	11.93	1.67	1.52
28	s	481[B]	VAL	CA-C	11.93	1.67	1.52
11	K	106	CYS	CB-SG	-11.64	1.42	1.81
13	y	36	CYS	CB-SG	-9.12	1.51	1.81
3	C	387	ASP	CA-C	-8.89	1.48	1.52
11	K	132	CYS	CB-SG	-8.67	1.52	1.81
28	q	16	CYS	CB-SG	-8.64	1.52	1.81
28	r	16	CYS	CB-SG	-8.56	1.53	1.81
28	r	114	CYS	CB-SG	-8.41	1.53	1.81
28	t	114	CYS	CB-SG	-8.31	1.53	1.81
28	q	114	CYS	CB-SG	-8.21	1.54	1.81
1	A	316	PHE	C-N	-8.20	1.25	1.34
16	O	221	PRO	CA-C	-7.90	1.36	1.52
20	T	353	THR	CA-C	-7.73	1.43	1.52
1	A	483	GLN	CA-C	-7.66	1.43	1.52
8	H	142	C	C1'-N1	7.66	1.59	1.48
8	H	77	C	C1'-N1	7.60	1.59	1.48
24	W	278	LYS	CA-C	-7.54	1.44	1.53
11	K	186	VAL	CA-CB	-7.36	1.44	1.54
1	A	119	LEU	CA-C	-7.30	1.44	1.52
1	A	212	PRO	N-CA	-7.22	1.38	1.47
3	C	319	THR	CA-C	-7.20	1.44	1.52
8	H	55	U	C1'-N1	7.17	1.59	1.48
8	H	92	U	C1'-N1	7.16	1.59	1.48
7	G	-22	G	C1'-N9	-7.16	1.37	1.48
2	B	103	G	C1'-N9	-7.14	1.37	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	89	U	C1'-N1	7.12	1.59	1.48
8	H	54	U	C1'-N1	7.10	1.59	1.48
8	H	72	U	C1'-N1	7.10	1.59	1.48
8	H	74	U	C1'-N1	7.08	1.59	1.48
8	H	69	U	C1'-N1	7.06	1.59	1.48
1	A	1542	ILE	C-O	-7.05	1.16	1.24
8	H	182	U	C1'-N1	7.04	1.59	1.48
8	H	60	U	C1'-N1	7.00	1.58	1.48
8	H	150	U	C1'-N1	7.00	1.58	1.48
8	H	91	U	C1'-N1	6.99	1.58	1.48
16	O	54	VAL	CA-C	-6.97	1.44	1.52
8	H	58	U	C1'-N1	6.93	1.58	1.48
1	A	1416	ILE	CA-C	-6.88	1.45	1.52
7	G	-23	G	C1'-N9	-6.83	1.37	1.48
1	A	472	LEU	CA-C	-6.74	1.45	1.52
1	A	607	ASP	CA-C	-6.73	1.44	1.52
11	K	40	THR	CB-OG1	6.73	1.54	1.43
8	H	97	G	C1'-N9	-6.73	1.37	1.48
1	A	416	GLY	C-O	6.72	1.30	1.23
1	A	1329	SER	CA-C	-6.65	1.44	1.52
8	H	151	C	C1'-N1	6.61	1.58	1.48
1	A	1259	ILE	CA-C	-6.60	1.44	1.52
8	H	184	C	C1'-N1	6.55	1.58	1.48
8	H	73	C	C1'-N1	6.54	1.58	1.48
7	G	-19	A	C1'-N9	-6.53	1.38	1.48
8	H	141	C	C1'-N1	6.53	1.58	1.48
7	G	-20	A	C1'-N9	-6.52	1.38	1.48
8	H	148	C	C1'-N1	6.49	1.58	1.48
3	C	637	LEU	CA-C	-6.48	1.44	1.52
8	H	84	C	C1'-N1	6.47	1.58	1.48
8	H	71	C	C1'-N1	6.44	1.58	1.48
8	H	78	C	C1'-N1	6.44	1.58	1.48
8	H	70	C	C1'-N1	6.43	1.58	1.48
1	A	321	ASN	N-CA	-6.40	1.38	1.46
1	A	1563	HIS	CA-C	-6.39	1.45	1.52
3	C	876	PRO	N-CA	-6.38	1.39	1.47
18	R	221	GLY	C-N	6.38	1.40	1.33
15	N	101	CYS	CA-C	-6.35	1.45	1.52
3	C	317	CYS	CA-C	-6.32	1.45	1.52
27	Z	612	ALA	N-CA	6.28	1.53	1.46
1	A	593	ARG	CA-C	-6.28	1.44	1.52
1	A	798	GLY	C-N	6.28	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	533	LYS	N-CA	-6.28	1.38	1.46
1	A	1561	PHE	CA-C	-6.26	1.45	1.52
1	A	906	VAL	CA-CB	-6.26	1.49	1.54
1	A	581	ILE	CA-CB	-6.24	1.47	1.54
1	A	1541	THR	CA-C	-6.24	1.44	1.52
1	A	1325	LEU	N-CA	-6.22	1.37	1.46
1	A	141	ILE	CA-CB	-6.22	1.46	1.54
7	G	-21	A	C1'-N9	-6.18	1.38	1.48
1	A	125	ALA	C-O	-6.18	1.16	1.24
1	A	1549	VAL	N-CA	-6.15	1.38	1.46
1	A	1447	VAL	CA-C	-6.14	1.45	1.52
20	T	333	VAL	N-CA	-6.13	1.39	1.46
20	T	208	ARG	CA-C	-6.08	1.44	1.52
1	A	790	ARG	CA-C	-6.00	1.45	1.52
1	A	1019	TYR	CA-C	-5.98	1.46	1.53
1	A	941	LYS	CA-C	-5.98	1.45	1.52
1	A	1484	ILE	CA-CB	-5.96	1.47	1.54
1	A	894	VAL	CA-C	-5.95	1.45	1.52
1	A	1336	PRO	N-CA	-5.94	1.39	1.47
28	q	91	THR	CB-OG1	5.92	1.53	1.43
1	A	1541	THR	N-CA	-5.90	1.38	1.46
1	A	1314	VAL	C-O	-5.88	1.17	1.24
12	L	761	SER	CB-OG	5.88	1.53	1.42
13	y	50	ILE	CB-CG1	-5.87	1.41	1.53
1	A	1335	ILE	CA-C	-5.81	1.48	1.52
7	G	4	A	C1'-N9	-5.81	1.39	1.48
20	T	332	ALA	CA-C	-5.79	1.45	1.52
28	t	98	THR	CB-OG1	5.79	1.53	1.43
28	r	39	THR	CB-OG1	5.76	1.52	1.43
1	A	135	VAL	CA-C	-5.74	1.45	1.52
1	A	1757	GLU	C-N	5.71	1.41	1.33
28	t	133	THR	CB-OG1	5.71	1.52	1.43
1	A	221	ASN	CA-C	-5.70	1.45	1.52
1	A	1263	TRP	CA-C	-5.68	1.45	1.52
1	A	120	TYR	CA-C	-5.67	1.45	1.52
20	T	270	VAL	CA-C	-5.67	1.45	1.52
11	K	160	ILE	CB-CG1	-5.67	1.42	1.53
28	t	91	THR	CB-OG1	5.66	1.52	1.43
24	W	94	GLY	C-N	5.66	1.41	1.33
28	r	91	THR	CB-OG1	5.66	1.52	1.43
1	A	906	VAL	C-O	-5.65	1.18	1.23
1	A	272	ALA	CA-C	-5.65	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	q	39	THR	CB-OG1	5.63	1.52	1.43
20	T	376	ARG	CA-C	-5.62	1.45	1.52
1	A	1542	ILE	N-CA	-5.62	1.39	1.46
28	q	125	THR	CB-OG1	5.61	1.52	1.43
28	r	133	THR	CB-OG1	5.60	1.52	1.43
1	A	106	MET	C-N	-5.60	1.28	1.34
28	q	98	THR	CB-OG1	5.60	1.52	1.43
1	A	150	MET	CA-C	-5.58	1.45	1.52
28	r	125	THR	CB-OG1	5.58	1.52	1.43
8	H	110	A	C1'-N9	-5.56	1.39	1.48
28	r	98	THR	CB-OG1	5.54	1.52	1.43
26	Y	71	LEU	C-N	5.54	1.40	1.33
1	A	482	PHE	N-CA	-5.53	1.39	1.46
3	C	875	ILE	C-O	-5.53	1.17	1.24
1	A	1330	MET	N-CA	-5.52	1.38	1.45
1	A	221	ASN	N-CA	-5.51	1.39	1.46
28	q	133	THR	CB-OG1	5.51	1.52	1.43
1	A	799	PRO	N-CA	-5.50	1.40	1.47
22	U	3	ASN	CA-C	-5.50	1.47	1.53
11	K	128	SER	CB-OG	5.49	1.53	1.42
1	A	317	PRO	N-CA	-5.48	1.40	1.47
24	W	95	PRO	N-CD	5.48	1.55	1.47
28	t	125	THR	CB-OG1	5.48	1.52	1.43
1	A	1306	LYS	N-CA	-5.48	1.38	1.46
1	A	1328	LEU	CA-C	-5.47	1.45	1.52
26	Y	132	ASN	C-N	5.47	1.41	1.34
1	A	415	SER	C-O	-5.46	1.17	1.23
18	R	225	PRO	C-N	5.46	1.40	1.33
20	T	218	TRP	CA-C	-5.46	1.45	1.52
18	R	229	VAL	CA-C	-5.45	1.45	1.52
1	A	598	LEU	CA-C	-5.45	1.44	1.52
11	K	183	SER	CB-OG	5.44	1.53	1.42
1	A	1558	THR	CA-C	-5.42	1.45	1.52
12	L	705	THR	CB-OG1	5.42	1.52	1.43
28	t	89	SER	CB-OG	5.41	1.52	1.42
20	T	319	THR	CA-C	-5.40	1.45	1.52
13	y	37	THR	CB-OG1	5.39	1.52	1.43
1	A	750	TRP	CE2-CZ2	-5.39	1.28	1.39
28	r	89	SER	CB-OG	5.38	1.52	1.42
11	K	162	ASP	CA-CB	-5.38	1.44	1.53
10	J	203	LEU	N-CA	5.37	1.53	1.46
1	A	1629	ILE	N-CA	-5.36	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	136	U	C1'-N1	5.35	1.56	1.48
11	K	173	THR	CB-OG1	5.34	1.52	1.43
1	A	1230	LEU	CA-C	-5.33	1.46	1.52
1	A	904	HIS	N-CA	-5.33	1.39	1.46
3	C	369	PHE	C-O	-5.31	1.18	1.24
3	C	659	VAL	C-O	-5.31	1.18	1.23
16	O	20	PHE	C-O	-5.31	1.17	1.24
28	q	89	SER	CB-OG	5.30	1.52	1.42
1	A	1264	ASN	N-CA	-5.30	1.39	1.46
23	V	505	LYS	C-O	-5.29	1.17	1.24
1	A	505	ASN	CA-C	-5.29	1.46	1.52
1	A	1292	GLU	CA-C	-5.29	1.46	1.52
11	K	190	SER	CB-OG	5.28	1.52	1.42
1	A	489	TRP	CA-C	-5.27	1.45	1.52
1	A	335	PRO	N-CA	-5.27	1.40	1.47
11	K	187	SER	CB-OG	5.27	1.52	1.42
1	A	1475	ILE	CA-CB	-5.26	1.47	1.54
1	A	1380	ILE	CA-CB	-5.25	1.48	1.54
1	A	203	VAL	C-O	-5.25	1.17	1.24
1	A	610	HIS	CA-C	-5.24	1.46	1.52
26	Y	133	PRO	N-CD	5.24	1.55	1.47
1	A	1548	TYR	C-N	-5.24	1.28	1.33
1	A	983	LYS	CA-C	-5.24	1.46	1.52
1	A	107	PRO	N-CA	-5.24	1.40	1.47
1	A	597	LYS	CA-C	5.23	1.59	1.52
12	L	793	LEU	CA-CB	-5.23	1.45	1.53
3	C	899	SER	N-CA	-5.23	1.39	1.46
3	C	311	SER	CA-C	-5.23	1.47	1.53
1	A	716	ALA	CA-C	-5.21	1.46	1.52
12	L	726	SER	CB-OG	5.21	1.52	1.42
18	R	226	PRO	N-CD	5.20	1.55	1.47
12	L	46	CYS	CA-C	-5.20	1.46	1.52
1	A	120	TYR	C-O	5.20	1.30	1.23
26	Y	17	PRO	N-CD	5.19	1.55	1.47
1	A	134	TRP	CA-C	-5.18	1.46	1.52
18	R	223	PRO	N-CD	5.18	1.55	1.47
20	T	267	ASP	C-O	-5.18	1.18	1.24
3	C	258	ASN	N-CA	-5.17	1.39	1.45
1	A	170	ASP	CA-C	5.16	1.59	1.52
20	T	268	LYS	CA-C	-5.16	1.45	1.52
18	R	222	PRO	N-CD	5.15	1.54	1.47
1	A	531	THR	CA-C	-5.15	1.46	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	y	54	SER	CB-OG	5.15	1.52	1.42
27	Z	1092	ASN	CA-C	5.15	1.59	1.52
44	3	81	GLU	C-O	-5.13	1.17	1.24
1	A	828	PRO	CA-C	-5.13	1.47	1.52
20	T	216	ASN	CA-C	-5.13	1.46	1.53
1	A	749	TRP	CA-C	-5.13	1.46	1.52
18	R	225	PRO	N-CD	5.13	1.54	1.47
1	A	411	PHE	CA-C	-5.12	1.45	1.52
1	A	1758	PRO	N-CD	5.12	1.54	1.47
1	A	121	HIS	N-CA	-5.11	1.39	1.46
37	m	14	LEU	CA-C	5.10	1.59	1.52
10	J	340	GLN	C-O	-5.09	1.21	1.23
1	A	407	ALA	N-CA	-5.08	1.39	1.45
22	U	21	ARG	CA-C	-5.08	1.46	1.53
1	A	116	VAL	CA-C	-5.08	1.47	1.52
18	R	233	PRO	N-CD	5.06	1.54	1.47
26	Y	21	PRO	N-CD	5.06	1.54	1.47
1	A	1313	PRO	N-CA	-5.06	1.40	1.47
26	Y	16	ASP	C-N	5.05	1.40	1.34
26	Y	72	PRO	N-CD	5.04	1.54	1.47
1	A	747	ALA	CA-C	-5.04	1.46	1.52
1	A	455	VAL	CA-C	-5.03	1.46	1.52
20	T	465	ILE	N-CA	-5.02	1.40	1.46
1	A	1536	LEU	CA-CB	-5.01	1.45	1.53
20	T	280	VAL	N-CA	-5.01	1.40	1.46
17	P	31	SER	CA-C	-5.00	1.46	1.52
22	U	19	VAL	N-CA	-5.00	1.39	1.46
1	A	754	ALA	CA-C	-5.00	1.46	1.52

All (599) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	s	481[A]	VAL	N-CA-C	-26.68	68.71	108.46
28	s	481[B]	VAL	N-CA-C	-26.68	68.71	108.46
40	o	55	ARG	CD-NE-CZ	13.22	142.90	124.40
20	T	187	LYS	CA-C-N	13.12	132.88	119.76
20	T	187	LYS	C-N-CA	13.12	132.88	119.76
26	Y	13	PRO	N-CA-C	13.00	139.25	112.47
13	y	191	VAL	O-C-N	-12.43	109.72	121.91
26	Y	204	LYS	O-C-N	-12.02	109.69	122.07
40	o	49	PHE	CA-CB-CG	11.49	125.29	113.80
26	Y	14	ASP	N-CA-CB	-11.01	94.22	111.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	27	U	P-O3'-C3'	-10.62	104.26	120.20
29	u	37	THR	CA-C-N	10.61	130.38	119.56
29	u	37	THR	C-N-CA	10.61	130.38	119.56
31	w	114	LYS	N-CA-C	-10.48	93.65	110.20
44	3	86	GLY	CA-C-O	9.95	132.05	121.90
2	B	104	C	C2'-C3'-O3'	-9.93	94.61	109.50
27	Z	555	GLY	O-C-N	9.81	135.45	122.70
20	T	191	HIS	CA-C-N	9.31	126.36	119.66
20	T	191	HIS	C-N-CA	9.31	126.36	119.66
16	O	221	PRO	CA-C-O	9.19	146.55	119.00
24	W	382	ASN	CA-C-N	9.06	128.79	119.19
24	W	382	ASN	C-N-CA	9.06	128.79	119.19
40	o	58	ASP	CA-CB-CG	9.02	121.62	112.60
7	G	-3	A	C2'-C3'-O3'	-8.98	100.23	113.70
27	Z	555	GLY	CA-C-N	8.96	138.65	121.54
27	Z	555	GLY	C-N-CA	8.96	138.65	121.54
11	K	90	PRO	CA-CB-CG	8.81	121.24	104.50
1	A	332	TYR	N-CA-C	-8.71	95.83	109.07
4	D	124	LEU	N-CA-C	8.71	120.85	111.36
28	r	46	PRO	N-CA-CB	8.69	111.09	103.27
8	H	82	G	O3'-P-O5'	-8.65	91.03	104.00
3	C	144	CYS	N-CA-CB	8.64	123.53	110.22
8	H	84	C	O3'-P-O5'	-8.64	91.04	104.00
8	H	88	A	O3'-P-O5'	-8.63	91.05	104.00
15	N	101	CYS	CB-CA-C	-8.63	97.57	110.95
8	H	56	A	O3'-P-O5'	-8.63	91.06	104.00
8	H	91	U	O3'-P-O5'	-8.63	91.06	104.00
8	H	180	G	O3'-P-O5'	-8.62	91.07	104.00
8	H	73	C	O3'-P-O5'	-8.62	91.07	104.00
8	H	183	G	O3'-P-O5'	-8.62	91.08	104.00
8	H	181	G	O3'-P-O5'	-8.62	91.08	104.00
8	H	93	A	O3'-P-O5'	-8.61	91.08	104.00
8	H	72	U	O3'-P-O5'	-8.61	91.08	104.00
8	H	78	C	O3'-P-O5'	-8.61	91.09	104.00
8	H	182	U	O3'-P-O5'	-8.61	91.09	104.00
8	H	70	C	O3'-P-O5'	-8.60	91.10	104.00
8	H	150	U	O3'-P-O5'	-8.60	91.10	104.00
8	H	79	G	O3'-P-O5'	-8.59	91.11	104.00
8	H	141	C	O3'-P-O5'	-8.59	91.11	104.00
8	H	59	A	O3'-P-O5'	-8.59	91.12	104.00
8	H	81	G	O3'-P-O5'	-8.58	91.13	104.00
8	H	55	U	O3'-P-O5'	-8.58	91.13	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	80	A	O3'-P-O5'	-8.58	91.14	104.00
8	H	54	U	O3'-P-O5'	-8.57	91.14	104.00
8	H	92	U	O3'-P-O5'	-8.57	91.14	104.00
8	H	89	U	O3'-P-O5'	-8.57	91.14	104.00
8	H	149	A	O3'-P-O5'	-8.57	91.14	104.00
8	H	90	A	O3'-P-O5'	-8.57	91.15	104.00
8	H	83	A	O3'-P-O5'	-8.56	91.16	104.00
3	C	776	GLU	N-CA-C	8.56	124.93	113.97
8	H	68	G	O3'-P-O5'	-8.56	91.17	104.00
8	H	69	U	O3'-P-O5'	-8.55	91.17	104.00
8	H	113	G	O3'-P-O5'	-8.55	91.17	104.00
8	H	57	A	O3'-P-O5'	-8.55	91.17	104.00
8	H	71	C	O3'-P-O5'	-8.55	91.18	104.00
8	H	114	A	O3'-P-O5'	-8.54	91.18	104.00
8	H	148	C	O3'-P-O5'	-8.54	91.18	104.00
8	H	74	U	O3'-P-O5'	-8.54	91.20	104.00
1	A	211	GLN	CA-C-N	8.53	130.50	119.84
1	A	211	GLN	C-N-CA	8.53	130.50	119.84
8	H	77	C	O3'-P-O5'	-8.52	91.22	104.00
28	q	46	PRO	N-CA-CB	8.50	111.24	103.34
40	o	5	THR	N-CA-CB	-8.49	98.32	111.05
8	H	58	U	O3'-P-O5'	-8.48	91.29	104.00
44	3	6	GLN	CA-C-O	8.47	135.19	120.80
41	p	80	ARG	CD-NE-CZ	8.39	136.14	124.40
25	X	13	HIS	CA-C-N	8.35	128.00	119.56
25	X	13	HIS	C-N-CA	8.35	128.00	119.56
12	L	144	MET	N-CA-C	-8.29	96.56	109.25
24	W	279	LYS	N-CA-C	-8.24	93.25	110.80
1	A	1291	CYS	CB-CA-C	8.14	127.00	110.38
20	T	213	GLU	CA-C-N	8.10	129.96	119.84
20	T	213	GLU	C-N-CA	8.10	129.96	119.84
12	L	55	ASP	CA-C-N	8.09	127.75	119.82
12	L	55	ASP	C-N-CA	8.09	127.75	119.82
27	Z	611	TYR	CA-C-N	8.07	136.15	121.94
27	Z	611	TYR	C-N-CA	8.07	136.15	121.94
40	o	16	THR	CA-C-O	-8.05	111.75	120.36
22	U	19	VAL	CB-CA-C	-7.98	101.15	111.53
27	Z	624	LEU	N-CA-C	7.97	121.84	108.13
8	H	22	U	C1'-C2'-O2'	-7.95	96.48	108.40
18	R	101	ILE	CB-CA-C	-7.94	101.54	111.70
40	o	99	SER	N-CA-C	7.88	122.66	112.26
17	P	194	PHE	N-CA-C	7.86	121.72	109.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	677	VAL	CB-CA-C	-7.85	101.75	112.04
8	H	22	U	C2'-C3'-O3'	-7.82	101.97	113.70
16	O	23	LEU	N-CA-C	7.81	121.34	109.23
18	R	267	ARG	N-CA-C	7.77	122.58	113.18
1	A	799	PRO	N-CA-C	-7.76	98.61	111.26
2	B	12	U	C2'-C3'-O3'	-7.76	102.06	113.70
3	C	919	ARG	CA-C-N	7.74	127.45	119.56
3	C	919	ARG	C-N-CA	7.74	127.45	119.56
27	Z	1066	TRP	CA-C-N	7.73	130.85	120.65
27	Z	1066	TRP	C-N-CA	7.73	130.85	120.65
28	s	480	GLY	CA-C-N	7.71	133.66	122.94
28	s	480	GLY	C-N-CA	7.71	133.66	122.94
40	o	117	TYR	CA-C-O	7.67	128.45	120.40
21	Q	1379	TYR	N-CA-C	7.62	122.67	112.30
26	Y	14	ASP	N-CA-C	-7.61	101.14	111.87
8	H	168	A	P-O5'-C5'	-7.59	109.51	120.90
28	q	54	ASP	CA-CB-CG	-7.56	105.04	112.60
11	K	90	PRO	N-CA-CB	7.54	111.17	103.25
12	L	563	PRO	N-CA-CB	7.53	110.39	103.08
3	C	823	ALA	N-CA-C	7.48	120.75	110.06
1	A	873	ASN	CA-C-N	7.45	127.47	119.28
1	A	873	ASN	C-N-CA	7.45	127.47	119.28
28	q	60	PRO	N-CA-CB	7.41	111.03	103.25
1	A	81	PHE	N-CA-C	7.40	119.35	111.28
26	Y	51	TYR	N-CA-C	7.37	119.31	111.28
22	U	7	LEU	CA-C-N	7.36	127.71	119.32
22	U	7	LEU	C-N-CA	7.36	127.71	119.32
1	A	912	GLU	CA-C-N	7.31	127.65	119.32
1	A	912	GLU	C-N-CA	7.31	127.65	119.32
6	F	27	A	C1'-C2'-O2'	-7.31	97.44	108.40
1	A	276	GLY	CA-C-N	7.31	127.88	120.14
1	A	276	GLY	C-N-CA	7.31	127.88	120.14
11	K	78	PRO	N-CA-CB	7.28	110.89	103.25
9	I	588	PRO	N-CA-CB	7.28	110.14	103.08
1	A	167	PRO	CA-C-N	7.27	126.95	119.82
1	A	167	PRO	C-N-CA	7.27	126.95	119.82
4	D	1044	VAL	CA-C-N	7.27	126.77	118.85
4	D	1044	VAL	C-N-CA	7.27	126.77	118.85
8	H	167	U	O3'-P-O5'	-7.26	93.10	104.00
1	A	1415	GLY	CA-C-O	-7.23	117.52	122.22
29	u	408	ALA	N-CA-C	7.23	118.80	111.07
1	A	423	ASP	N-CA-C	-7.22	104.49	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	o	71	VAL	CA-C-N	7.21	131.63	120.75
40	o	71	VAL	C-N-CA	7.21	131.63	120.75
4	D	1666	THR	N-CA-C	7.19	121.50	112.87
6	F	51	U	C4'-C3'-O3'	-7.19	102.21	113.00
1	A	948	PRO	N-CA-C	7.19	119.47	110.70
18	R	225	PRO	CA-C-N	-7.15	112.61	119.76
18	R	225	PRO	C-N-CA	-7.15	112.61	119.76
40	o	21	ASP	CA-CB-CG	7.15	119.75	112.60
3	C	215	VAL	CB-CA-C	-7.13	102.52	112.14
7	G	2	U	C1'-C2'-O2'	-7.11	101.13	111.80
1	A	334	THR	CA-C-N	-7.11	112.67	119.85
1	A	334	THR	C-N-CA	-7.11	112.67	119.85
40	o	47	ILE	N-CA-CB	7.09	123.07	111.58
27	Z	798	VAL	N-CA-C	7.09	124.08	109.34
29	u	77	ASP	N-CA-C	-7.08	99.81	110.28
4	D	152	GLU	N-CA-C	-7.04	103.61	111.28
8	H	170	C	C3'-C2'-O2'	-7.02	104.08	114.60
13	y	40	PRO	N-CA-CB	7.01	110.18	103.52
20	T	220	VAL	CB-CA-C	-7.01	99.66	110.95
18	R	221	GLY	CA-C-N	-7.01	113.16	120.38
18	R	221	GLY	C-N-CA	-7.01	113.16	120.38
4	D	533	VAL	N-CA-C	6.99	118.86	112.29
8	H	23	A	C1'-C2'-O2'	-6.98	97.93	108.40
27	Z	604	ASN	N-CA-C	6.96	121.04	112.54
40	o	72	ASN	OD1-CG-ND2	6.96	129.56	122.60
1	A	1370	ARG	NE-CZ-NH2	6.96	125.46	119.20
9	I	475	PRO	N-CA-CB	6.95	110.89	103.52
40	o	107	ASP	CA-CB-CG	6.94	119.54	112.60
9	I	589	PRO	N-CA-CB	6.91	110.86	103.39
40	o	4	LEU	N-CA-C	-6.89	97.99	108.67
40	o	121	LEU	CA-C-O	6.89	128.88	121.44
14	M	160	PHE	N-CA-C	6.88	119.66	111.33
20	T	405	PHE	N-CA-C	6.88	119.80	111.82
26	Y	164	GLN	N-CA-C	6.88	118.86	111.36
9	I	160	PRO	N-CA-CB	6.87	110.46	103.25
6	F	53	A	C1'-C2'-O2'	6.86	118.68	108.40
40	o	75	ARG	NE-CZ-NH1	-6.85	114.65	121.50
1	A	1757	GLU	CA-C-N	-6.83	112.72	119.76
1	A	1757	GLU	C-N-CA	-6.83	112.72	119.76
1	A	642	ARG	NE-CZ-NH2	-6.82	113.06	119.20
26	Y	71	LEU	CA-C-N	-6.81	112.98	119.85
26	Y	71	LEU	C-N-CA	-6.81	112.98	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	798	GLY	O-C-N	6.79	128.56	121.77
9	I	551	PRO	N-CA-CB	6.78	110.71	103.52
9	I	162	PRO	N-CA-CB	6.78	110.70	103.52
41	p	53	PHE	CA-C-O	-6.77	112.87	120.32
1	A	937	PRO	CA-C-N	6.77	126.91	119.87
1	A	937	PRO	C-N-CA	6.77	126.91	119.87
9	I	342	PRO	N-CA-CB	6.75	110.34	103.25
28	r	54	ASP	CA-CB-CG	-6.74	105.86	112.60
40	o	58	ASP	N-CA-CB	-6.74	100.59	111.24
9	I	232	PRO	N-CA-CB	6.72	110.64	103.52
27	Z	794	ALA	CA-C-N	6.72	128.24	119.84
27	Z	794	ALA	C-N-CA	6.72	128.24	119.84
9	I	387	PRO	N-CA-CB	6.71	110.38	103.00
28	q	19	PRO	N-CA-CB	6.70	110.28	103.25
1	A	712	HIS	CB-CA-C	-6.68	99.70	110.79
28	r	19	PRO	N-CA-CB	6.67	110.23	102.76
26	Y	11	TYR	CA-C-N	6.66	127.24	120.38
26	Y	11	TYR	C-N-CA	6.66	127.24	120.38
1	A	455	VAL	CB-CA-C	-6.66	103.03	112.22
12	L	620	PRO	N-CA-CB	6.66	110.24	103.25
12	L	558	PRO	N-CA-CB	6.65	110.57	103.52
15	N	37	HIS	N-CA-CB	-6.65	102.11	111.62
1	A	1542	ILE	CA-C-N	-6.65	113.04	122.41
1	A	1542	ILE	C-N-CA	-6.65	113.04	122.41
2	B	48	A	C1'-C2'-O2'	6.63	118.34	108.40
8	H	164	C	C5'-C4'-O4'	-6.62	99.17	109.10
24	W	94	GLY	CA-C-N	-6.62	113.16	119.85
24	W	94	GLY	C-N-CA	-6.62	113.16	119.85
24	W	565	LYS	N-CA-C	6.61	118.90	108.79
12	L	594	PRO	N-CA-CB	6.60	110.18	103.25
3	C	799	GLU	CA-C-N	6.60	126.29	119.56
3	C	799	GLU	C-N-CA	6.60	126.29	119.56
3	C	148	CYS	CB-CA-C	6.58	122.04	110.85
9	I	722	GLU	N-CA-C	6.56	118.43	111.28
29	u	38	PRO	N-CA-C	6.55	122.36	113.84
9	I	816	PRO	N-CA-CB	6.55	110.46	103.52
13	y	165	PRO	N-CA-CB	6.50	109.39	103.08
13	y	164	PRO	N-CA-CB	6.48	109.37	103.08
1	A	617	ASN	CB-CA-C	-6.45	102.11	111.91
1	A	581	ILE	CB-CA-C	-6.44	103.73	111.97
1	A	642	ARG	NH1-CZ-NH2	6.43	127.65	119.30
26	Y	165	ALA	N-CA-C	6.42	118.86	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	L	564	PRO	N-CA-CB	6.41	110.31	103.52
11	K	40	THR	CA-CB-OG1	6.40	119.20	109.60
12	L	546	PRO	N-CA-CB	6.39	110.60	103.44
9	I	788	PRO	N-CA-CB	6.39	110.60	103.44
9	I	177	PRO	N-CA-CB	6.38	110.58	103.44
8	H	21	C	C2'-C3'-O3'	-6.38	104.14	113.70
9	I	463	PRO	N-CA-CB	6.38	109.94	103.25
24	W	460	SER	N-CA-C	6.37	118.23	111.28
24	W	106	ALA	CA-C-N	6.36	126.31	119.76
24	W	106	ALA	C-N-CA	6.36	126.31	119.76
8	H	32	U	C5'-C4'-C3'	-6.34	106.49	116.00
27	Z	988	LYS	CA-C-N	6.34	126.85	119.94
27	Z	988	LYS	C-N-CA	6.34	126.85	119.94
2	B	20	G	N9-C1'-C2'	6.34	123.50	114.00
40	o	55	ARG	NE-CZ-NH1	6.33	127.83	121.50
20	T	323	VAL	CB-CA-C	-6.33	103.87	111.97
1	A	1811	ASN	CA-C-N	6.33	126.81	119.47
1	A	1811	ASN	C-N-CA	6.33	126.81	119.47
45	4	7	GLY	N-CA-C	6.32	120.32	112.73
1	A	170	ASP	N-CA-C	6.31	118.93	110.35
9	I	518	PRO	N-CA-CB	6.31	110.21	103.52
9	I	394	PRO	N-CA-CB	6.31	110.50	103.44
8	H	168	A	C5'-C4'-C3'	-6.30	106.55	116.00
44	3	6	GLN	O-C-N	-6.30	112.91	123.00
29	u	68	ALA	N-CA-C	6.29	119.43	111.69
45	4	20	ALA	N-CA-C	6.29	118.13	111.28
40	o	40	THR	CA-C-N	6.27	131.50	122.40
40	o	40	THR	C-N-CA	6.27	131.50	122.40
28	r	60	PRO	N-CA-CB	6.26	109.83	103.25
40	o	87	LEU	CA-C-N	6.24	126.14	119.28
40	o	87	LEU	C-N-CA	6.24	126.14	119.28
1	A	1040	ILE	CB-CA-C	-6.24	103.72	112.14
8	H	169	C	P-O3'-C3'	6.22	129.53	120.20
10	J	188	GLN	N-CA-C	-6.21	97.58	110.80
20	T	192	PRO	O-C-N	6.20	124.06	121.15
12	L	151	MET	CB-CA-C	-6.20	101.15	110.88
20	T	354	ILE	CB-CA-C	-6.20	103.23	110.91
10	J	412	ASP	N-CA-C	6.19	117.63	108.60
3	C	89	LEU	N-CA-C	6.18	118.81	111.33
27	Z	913	ASP	CA-C-N	6.17	126.73	120.38
27	Z	913	ASP	C-N-CA	6.17	126.73	120.38
1	A	1571	ILE	CB-CA-C	-6.16	104.08	111.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	381	HIS	CA-C-N	6.16	127.54	119.84
20	T	381	HIS	C-N-CA	6.16	127.54	119.84
24	W	116	GLU	CA-C-N	6.15	126.50	119.92
24	W	116	GLU	C-N-CA	6.15	126.50	119.92
24	W	281	ILE	N-CA-C	6.14	117.51	111.67
30	v	144	LYS	N-CA-C	6.12	118.62	109.25
40	o	73	ASN	N-CA-C	6.12	119.81	111.17
1	A	204	LEU	N-CA-C	6.11	118.91	111.82
16	O	40	LYS	N-CA-C	6.11	117.63	110.97
1	A	132	ILE	CA-C-O	6.10	123.29	119.51
12	L	25	LYS	N-CA-C	6.10	119.19	111.69
3	C	843	VAL	CB-CA-C	-6.10	103.91	112.14
18	R	181	PRO	N-CA-C	6.09	125.02	112.47
29	u	339	ARG	N-CA-C	6.09	119.63	109.95
1	A	906	VAL	N-CA-C	6.06	114.83	107.61
12	L	548	PRO	N-CA-CB	6.05	110.22	103.44
1	A	1412	TRP	N-CA-C	6.04	118.36	111.11
41	p	89	ASP	CA-CB-CG	6.03	118.62	112.60
9	I	761	PRO	N-CA-CB	6.02	109.90	103.39
6	F	55	C	C3'-C2'-O2'	-6.02	101.67	110.70
20	T	327	SER	N-CA-C	-6.02	102.77	110.53
1	A	1567	PRO	CA-C-O	6.01	128.46	119.74
40	o	75	ARG	N-CA-CB	-6.01	102.62	111.51
3	C	264	ILE	CB-CA-C	-6.01	105.73	111.44
4	D	1006	LYS	CA-C-N	6.01	126.17	119.32
4	D	1006	LYS	C-N-CA	6.01	126.17	119.32
40	o	52	ASN	CA-CB-CG	6.01	118.61	112.60
1	A	1292	GLU	CB-CA-C	-6.00	100.84	110.79
6	F	66	C	C4'-C3'-O3'	-5.99	104.02	113.00
10	J	206	LEU	CA-C-N	-5.99	114.21	120.38
10	J	206	LEU	C-N-CA	-5.99	114.21	120.38
27	Z	1024	SER	N-CA-C	5.98	118.29	111.11
3	C	707	ILE	N-CA-C	5.97	118.56	111.09
19	S	128	ILE	CA-C-N	5.97	128.56	120.44
19	S	128	ILE	C-N-CA	5.97	128.56	120.44
6	F	65	G	P-O5'-C5'	-5.97	111.95	120.90
29	u	178	THR	N-CA-C	5.96	120.68	113.17
39	g	67	ILE	CB-CA-C	-5.96	104.80	111.23
40	o	79	ILE	CA-C-N	5.94	125.75	120.10
40	o	79	ILE	C-N-CA	5.94	125.75	120.10
41	p	46	MET	N-CA-C	-5.94	104.71	111.07
1	A	1568	THR	N-CA-C	-5.93	104.76	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	I	625	PRO	N-CA-CB	5.93	109.85	103.33
26	Y	132	ASN	CA-C-N	-5.93	112.47	119.05
26	Y	132	ASN	C-N-CA	-5.93	112.47	119.05
39	n	67	ILE	CB-CA-C	-5.92	104.84	111.23
40	o	123	ASN	OD1-CG-ND2	5.89	128.49	122.60
45	4	11	ALA	N-CA-C	5.89	117.38	111.07
40	o	27	ARG	CB-CA-C	-5.88	98.71	109.54
1	A	1330	MET	CA-CB-CG	-5.88	102.35	114.10
1	A	487	LEU	N-CA-C	5.87	119.12	109.85
1	A	387	PHE	N-CA-C	5.85	118.13	111.11
40	o	113	LYS	N-CA-C	5.85	118.41	111.33
40	o	50	SER	CA-C-O	5.85	127.75	121.55
3	C	922	GLU	CA-C-N	5.84	125.78	119.76
3	C	922	GLU	C-N-CA	5.84	125.78	119.76
8	H	163	G	O3'-P-O5'	-5.84	95.24	104.00
3	C	358	LYS	N-CA-C	-5.84	101.76	110.23
20	T	254	VAL	CB-CA-C	-5.84	102.44	110.96
27	Z	573	GLY	CA-C-N	5.84	132.69	121.54
27	Z	573	GLY	C-N-CA	5.84	132.69	121.54
1	A	1370	ARG	NE-CZ-NH1	-5.81	115.69	121.50
1	A	801	ILE	N-CA-C	5.81	118.31	111.05
1	A	167	PRO	N-CA-C	5.80	117.78	110.70
24	W	464	MET	CA-C-N	-5.80	113.05	119.19
24	W	464	MET	C-N-CA	-5.80	113.05	119.19
20	T	188	PRO	N-CA-C	5.78	120.27	111.19
11	K	107	VAL	CA-CB-CG1	5.78	120.23	110.40
1	A	1083	HIS	CA-C-N	5.78	125.90	119.32
1	A	1083	HIS	C-N-CA	5.78	125.90	119.32
1	A	1234	ASP	N-CA-C	5.76	117.64	111.36
20	T	187	LYS	CB-CA-C	5.75	115.28	111.20
29	u	336	VAL	N-CA-C	-5.75	103.99	112.04
13	y	166	PRO	N-CA-CB	5.74	109.37	103.23
3	C	536	ARG	N-CA-C	-5.73	100.95	109.83
5	E	309	VAL	CB-CA-C	-5.72	104.04	110.96
1	A	1278	VAL	N-CA-C	5.71	116.45	110.62
6	F	37	C	C4'-C3'-O3'	-5.71	104.44	113.00
27	Z	880	THR	CA-C-N	5.70	132.43	121.54
27	Z	880	THR	C-N-CA	5.70	132.43	121.54
40	o	149	LYS	CB-CA-C	-5.70	101.95	110.16
28	r	110	HIS	CA-CB-CG	5.70	119.50	113.80
3	C	544	VAL	CA-C-N	5.69	125.89	120.31
3	C	544	VAL	C-N-CA	5.69	125.89	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	164	C	P-O3'-C3'	5.69	128.73	120.20
1	A	243	ASN	N-CA-C	5.68	118.24	111.71
4	D	1135	LEU	CA-C-N	5.68	125.61	119.76
4	D	1135	LEU	C-N-CA	5.68	125.61	119.76
26	Y	21	PRO	CA-N-CD	-5.68	104.05	112.00
4	D	782	PHE	N-CA-C	5.67	118.02	109.41
40	o	27	ARG	CA-C-N	5.66	128.66	120.11
40	o	27	ARG	C-N-CA	5.66	128.66	120.11
29	u	210	PRO	N-CA-C	5.66	121.39	113.53
1	A	2153	THR	N-CA-C	-5.65	101.81	109.95
2	B	25	C	C1'-C2'-O2'	5.65	120.27	111.80
3	C	449	ILE	CB-CA-C	-5.64	104.52	112.14
27	Z	574	TYR	CA-C-N	5.64	131.85	121.70
27	Z	574	TYR	C-N-CA	5.64	131.85	121.70
3	C	747	ASP	N-CA-C	5.64	117.97	107.99
40	o	71	VAL	O-C-N	-5.63	115.53	122.57
4	D	1048	VAL	N-CA-C	-5.61	106.32	113.22
30	v	116	LYS	N-CA-C	-5.61	100.54	109.96
4	D	1291	LEU	CA-C-N	5.60	125.91	119.92
4	D	1291	LEU	C-N-CA	5.60	125.91	119.92
8	H	23	A	C3'-C2'-O2'	5.60	119.10	110.70
8	H	31	G	C4'-C3'-O3'	-5.60	104.60	113.00
27	Z	854	SER	CA-C-N	5.60	126.30	120.03
27	Z	854	SER	C-N-CA	5.60	126.30	120.03
26	Y	16	ASP	CA-C-N	-5.59	112.85	119.05
26	Y	16	ASP	C-N-CA	-5.59	112.85	119.05
1	A	118	VAL	CB-CA-C	-5.58	101.05	110.71
1	A	1615	HIS	N-CA-C	-5.58	101.44	109.48
19	S	66	ASP	CA-C-N	5.58	125.25	119.56
19	S	66	ASP	C-N-CA	5.58	125.25	119.56
1	A	1052	VAL	N-CA-C	5.57	115.70	110.30
34	i	52	LYS	CA-C-N	-5.56	114.20	119.76
34	i	52	LYS	C-N-CA	-5.56	114.20	119.76
6	F	50	A	C4'-C3'-C2'	-5.55	97.05	102.60
1	A	2225	LEU	N-CA-C	5.55	117.83	109.23
1	A	314	ILE	CA-CB-CG1	-5.55	100.97	110.40
1	A	1368	LEU	CB-CA-C	-5.54	101.26	110.68
18	R	96	ILE	N-CA-C	-5.54	102.37	109.30
1	A	1348	VAL	N-CA-C	5.54	119.80	112.04
18	R	251	ILE	CB-CA-C	-5.53	104.05	110.91
5	E	322	LYS	N-CA-C	-5.53	98.18	108.02
40	o	159	GLU	N-CA-C	-5.52	104.90	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	50	ALA	CA-C-N	5.52	125.35	119.28
17	P	50	ALA	C-N-CA	5.52	125.35	119.28
1	A	1318	THR	CA-C-N	5.52	125.46	119.78
1	A	1318	THR	C-N-CA	5.52	125.46	119.78
40	o	32	PRO	CA-C-N	5.51	130.66	122.99
40	o	32	PRO	C-N-CA	5.51	130.66	122.99
1	A	1311	PHE	CA-C-N	5.51	123.68	119.66
1	A	1311	PHE	C-N-CA	5.51	123.68	119.66
8	H	160	A	P-O5'-C5'	-5.51	112.63	120.90
1	A	2241	ASN	N-CA-C	5.50	118.30	110.10
8	H	165	A	N9-C1'-C2'	5.50	120.25	112.00
3	C	281	ILE	CB-CA-C	-5.50	104.93	111.97
20	T	307	SER	N-CA-C	5.50	117.55	109.24
1	A	664	HIS	N-CA-C	-5.49	100.85	109.25
1	A	2203	ASN	N-CA-C	5.49	120.80	109.11
40	o	16	THR	O-C-N	5.49	129.48	123.22
34	b	52	LYS	CA-C-N	-5.49	114.27	119.76
34	b	52	LYS	C-N-CA	-5.49	114.27	119.76
34	i	5	LYS	N-CA-C	5.49	118.18	111.82
31	w	115	GLY	N-CA-C	5.48	126.17	113.18
26	Y	92	ASP	CA-C-N	5.47	125.17	119.64
26	Y	92	ASP	C-N-CA	5.47	125.17	119.64
8	H	168	A	O4'-C1'-C2'	-5.47	102.13	107.60
8	H	157	G	P-O5'-C5'	-5.47	112.70	120.90
20	T	421	VAL	N-CA-C	5.47	116.15	108.17
40	o	34	ILE	CA-C-O	-5.46	114.29	120.74
40	o	132	ARG	CD-NE-CZ	5.46	132.05	124.40
5	E	284	PHE	N-CA-C	5.45	119.42	112.34
29	u	384	ASP	N-CA-C	5.45	117.64	111.11
24	W	151	LYS	N-CA-C	5.44	118.27	109.40
5	E	237	SER	N-CA-C	5.43	117.90	110.24
12	L	39	HIS	N-CA-C	-5.42	101.29	109.85
5	E	281	VAL	N-CA-C	5.41	116.10	108.36
1	A	487	LEU	N-CA-CB	-5.41	102.44	111.20
7	G	142	U	C4'-C3'-O3'	-5.41	104.89	113.00
3	C	744	ILE	CB-CA-C	-5.40	102.57	110.62
40	o	40	THR	N-CA-C	-5.40	106.19	112.89
3	C	469	ASP	CA-C-N	-5.40	113.72	119.98
3	C	469	ASP	C-N-CA	-5.40	113.72	119.98
10	J	356	TYR	N-CA-C	-5.40	102.21	110.14
41	p	25	ARG	CD-NE-CZ	5.38	131.94	124.40
24	W	470	SER	CA-C-N	5.38	125.05	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	W	470	SER	C-N-CA	5.38	125.05	119.56
3	C	907	VAL	CB-CA-C	-5.38	105.08	110.89
1	A	157	ASP	N-CA-C	5.38	119.94	112.90
5	E	156	SER	N-CA-C	5.38	116.70	108.42
1	A	427	VAL	CB-CA-C	-5.37	105.03	111.85
1	A	1566	ILE	CA-C-N	5.37	124.70	118.85
1	A	1566	ILE	C-N-CA	5.37	124.70	118.85
1	A	2100	THR	N-CA-C	-5.37	106.73	113.28
26	Y	12	PRO	CA-C-N	5.37	126.55	119.84
26	Y	12	PRO	C-N-CA	5.37	126.55	119.84
26	Y	41	MET	N-CA-C	5.37	116.57	108.46
1	A	1303	LEU	CA-C-N	-5.36	112.78	122.54
1	A	1303	LEU	C-N-CA	-5.36	112.78	122.54
7	G	-9	C	C1'-C2'-O2'	-5.36	103.76	111.80
1	A	1247	ILE	CB-CA-C	-5.36	104.91	112.14
3	C	567	GLU	CA-C-N	-5.35	113.15	119.84
3	C	567	GLU	C-N-CA	-5.35	113.15	119.84
3	C	815	VAL	CB-CA-C	-5.35	105.12	111.97
20	T	317	VAL	CB-CA-C	-5.35	105.03	112.04
3	C	420	CYS	CA-CB-SG	-5.35	102.09	114.40
27	Z	711	VAL	CA-C-N	5.35	131.32	121.85
27	Z	711	VAL	C-N-CA	5.35	131.32	121.85
40	o	125	VAL	CA-C-N	5.34	127.97	120.28
40	o	125	VAL	C-N-CA	5.34	127.97	120.28
18	R	229	VAL	CB-CA-C	-5.34	105.08	112.24
20	T	281	ILE	CB-CA-C	-5.34	106.36	111.06
6	F	50	A	C1'-C2'-O2'	5.34	116.41	108.40
1	A	1672	ASP	N-CA-C	5.33	116.90	111.14
6	F	50	A	C2'-C3'-O3'	5.33	121.69	113.70
34	i	65	ARG	CB-CG-CD	5.33	123.56	111.30
27	Z	703	HIS	CA-C-N	-5.33	118.14	123.04
27	Z	703	HIS	C-N-CA	-5.33	118.14	123.04
34	b	65	ARG	CB-CG-CD	5.33	123.55	111.30
27	Z	1092	ASN	CA-C-N	5.33	127.38	120.88
27	Z	1092	ASN	C-N-CA	5.33	127.38	120.88
4	D	2096	ALA	CA-C-N	5.32	125.53	120.31
4	D	2096	ALA	C-N-CA	5.32	125.53	120.31
4	D	153	ARG	N-CA-C	-5.32	105.48	111.28
26	Y	25	LEU	N-CA-C	5.30	121.53	109.81
41	p	6	ASN	N-CA-CB	-5.30	101.67	111.53
1	A	1117	HIS	CA-C-N	5.29	125.20	119.85
1	A	1117	HIS	C-N-CA	5.29	125.20	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	811	SER	N-CA-C	5.28	115.11	108.45
22	U	6	GLY	CA-C-O	5.28	126.57	122.29
27	Z	1051	ILE	CA-C-N	5.28	127.31	120.44
27	Z	1051	ILE	C-N-CA	5.28	127.31	120.44
40	o	146	ASP	CA-C-N	5.28	130.06	122.40
40	o	146	ASP	C-N-CA	5.28	130.06	122.40
40	o	33	VAL	N-CA-CB	-5.28	103.81	111.52
40	o	88	PRO	CB-CA-C	-5.28	103.98	112.21
26	Y	47	GLY	N-CA-C	-5.27	108.72	115.42
2	B	12	U	C4'-C3'-O3'	5.27	120.91	113.00
1	A	132	ILE	CA-C-N	5.27	126.43	119.84
1	A	132	ILE	C-N-CA	5.27	126.43	119.84
19	S	152	ARG	CA-C-N	5.26	125.18	119.76
19	S	152	ARG	C-N-CA	5.26	125.18	119.76
41	p	20	LYS	N-CA-C	5.26	117.42	111.11
28	r	74	ILE	CA-CB-CG1	5.26	119.34	110.40
12	L	143	ASP	N-CA-C	-5.26	99.21	108.20
4	D	749	GLY	N-CA-C	-5.26	108.43	114.69
4	D	1228	VAL	N-CA-C	5.25	116.61	110.62
4	D	1127	CYS	CA-C-N	5.25	125.56	119.47
4	D	1127	CYS	C-N-CA	5.25	125.56	119.47
1	A	1613	THR	N-CA-C	-5.25	101.88	109.59
1	A	429	ASN	N-CA-C	5.25	119.43	113.19
24	W	462	HIS	N-CA-C	5.24	117.07	111.36
18	R	143	ILE	CB-CA-C	-5.23	105.27	111.97
8	H	171	U	C2'-C3'-O3'	-5.23	105.86	113.70
4	D	1693	ARG	CA-C-N	5.22	125.03	119.28
4	D	1693	ARG	C-N-CA	5.22	125.03	119.28
27	Z	1091	VAL	N-CA-C	5.22	115.64	108.12
11	K	146	ILE	CA-CB-CG1	5.22	119.27	110.40
29	u	163	THR	N-CA-C	-5.22	103.61	110.39
41	p	48	MET	N-CA-C	5.21	119.63	113.28
3	C	552	ILE	CB-CA-C	-5.20	104.23	110.99
3	C	97	VAL	N-CA-C	5.20	116.09	110.21
4	D	488	LEU	N-CA-C	5.20	119.72	113.17
8	H	36	G	C4'-C3'-O3'	-5.20	105.20	113.00
12	L	83	ARG	NE-CZ-NH2	5.20	123.88	119.20
29	u	367	ARG	N-CA-C	-5.20	106.20	112.54
1	A	680	HIS	CB-CA-C	-5.20	102.72	110.88
26	Y	23	LEU	N-CA-C	5.19	117.84	111.82
20	T	414	ALA	N-CA-C	-5.19	100.25	108.14
1	A	166	PHE	N-CA-C	5.19	117.20	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	T	346	ILE	CB-CA-C	-5.19	103.39	110.96
15	N	100	LEU	N-CA-C	5.19	117.55	110.24
1	A	1657	THR	N-CA-C	5.18	115.38	108.38
1	A	1612	GLU	N-CA-C	-5.18	102.01	110.20
41	p	51	GLN	N-CA-C	5.18	117.55	109.52
41	p	36	HIS	CA-CB-CG	-5.17	108.63	113.80
1	A	1134	TRP	CA-C-N	5.17	125.16	119.89
1	A	1134	TRP	C-N-CA	5.17	125.16	119.89
26	Y	121	VAL	N-CA-C	5.16	115.89	110.62
41	p	68	GLN	OE1-CD-NE2	5.16	127.76	122.60
3	C	866	SER	CA-C-N	5.16	126.28	119.84
3	C	866	SER	C-N-CA	5.16	126.28	119.84
12	L	774	VAL	CA-CB-CG2	5.15	119.16	110.40
27	Z	1093	ILE	N-CA-C	5.14	115.42	110.74
36	k	99	MET	N-CA-C	5.14	116.88	108.76
4	D	572	ASP	N-CA-C	-5.14	103.36	110.35
19	S	32	ALA	CA-C-N	5.14	124.93	119.28
19	S	32	ALA	C-N-CA	5.14	124.93	119.28
1	A	1968	TRP	CA-C-N	5.14	126.26	119.84
1	A	1968	TRP	C-N-CA	5.14	126.26	119.84
1	A	1052	VAL	CB-CA-C	-5.14	105.39	111.81
4	D	1875	VAL	CA-C-N	5.14	124.58	119.24
4	D	1875	VAL	C-N-CA	5.14	124.58	119.24
3	C	809	ILE	O-C-N	5.13	123.70	120.42
12	L	137	ALA	N-CA-C	5.13	116.89	108.52
27	Z	977	MET	O-C-N	-5.13	115.76	122.59
8	H	160	A	C4'-C3'-C2'	-5.13	97.47	102.60
40	o	83	LEU	N-CA-C	5.13	117.54	111.33
8	H	170	C	O4'-C1'-C2'	-5.12	100.68	105.80
36	d	99	MET	N-CA-C	5.12	116.86	108.76
3	C	308	CYS	CB-CA-C	-5.12	100.75	109.51
40	o	90	LEU	CA-C-O	-5.12	113.19	120.51
3	C	307	VAL	N-CA-C	5.12	115.40	107.78
36	d	88	LYS	CG-CD-CE	-5.12	99.53	111.30
25	X	34	ARG	N-CA-C	5.11	116.85	111.28
28	q	60	PRO	CA-CB-CG	5.11	114.21	104.50
29	u	342	ASP	N-CA-C	5.11	117.04	107.99
10	J	275	ASN	N-CA-C	5.11	116.58	108.67
1	A	1774	ASN	N-CA-C	-5.10	105.72	111.28
41	p	83	TYR	CA-C-O	-5.10	115.23	121.05
28	q	110	HIS	CA-CB-CG	5.10	118.90	113.80
1	A	99	VAL	CB-CA-C	-5.10	105.26	112.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	36	A	C4'-C3'-O3'	-5.10	105.36	113.00
1	A	905	LEU	CA-C-N	-5.09	118.90	123.33
1	A	905	LEU	C-N-CA	-5.09	118.90	123.33
40	o	55	ARG	NE-CZ-NH2	-5.09	114.61	119.20
40	o	90	LEU	O-C-N	5.09	129.37	122.59
27	Z	740	PRO	CA-C-N	5.09	127.99	121.27
27	Z	740	PRO	C-N-CA	5.09	127.99	121.27
3	C	863	ILE	CA-C-O	5.09	122.15	119.15
7	G	-10	C	P-O5'-C5'	-5.09	113.27	120.90
20	T	401	PRO	N-CA-C	5.09	122.95	112.47
1	A	539	ARG	CB-CA-C	-5.09	101.28	109.72
8	H	160	A	N9-C1'-C2'	5.09	119.63	112.00
30	v	143	PHE	N-CA-C	5.09	120.14	113.88
1	A	1518	LEU	N-CA-C	5.08	121.63	110.80
8	H	156	U	C4'-C3'-C2'	5.08	107.68	102.60
6	F	62	C	C1'-C2'-O2'	5.08	116.02	108.40
24	W	399	LYS	N-CA-C	5.08	117.66	110.50
1	A	1190	CYS	CA-CB-SG	-5.08	102.72	114.40
23	V	459	ILE	CB-CA-C	-5.07	105.47	111.97
38	e	85	THR	N-CA-C	-5.07	105.94	112.68
8	H	155	C	P-O3'-C3'	5.07	127.80	120.20
31	w	148	TRP	N-CA-C	-5.06	103.36	110.50
31	w	107	ASP	N-CA-C	-5.06	102.15	109.59
26	Y	26	PRO	CA-N-CD	-5.05	104.92	112.00
15	N	102	CYS	CB-CA-C	-5.05	99.63	111.09
3	C	243	ILE	CB-CA-C	-5.04	105.52	111.97
23	V	483	GLU	N-CA-C	5.04	116.85	111.36
23	V	467	LEU	CB-CA-C	-5.04	100.40	110.42
20	T	479	THR	N-CA-C	5.03	117.60	109.40
40	o	28	GLY	N-CA-C	5.03	120.83	113.48
3	C	125	ASN	N-CA-C	5.03	116.45	111.07
38	l	85	THR	N-CA-C	-5.03	106.00	112.68
1	A	424	ILE	CA-C-N	5.02	126.12	119.84
1	A	424	ILE	C-N-CA	5.02	126.12	119.84
1	A	1963	GLU	CA-C-N	5.02	125.09	119.87
1	A	1963	GLU	C-N-CA	5.02	125.09	119.87
41	p	38	VAL	O-C-N	5.02	127.00	121.83
40	o	99	SER	N-CA-CB	-5.01	102.95	111.17
4	D	574	GLN	N-CA-C	5.01	117.85	111.69
3	C	310	SER	N-CA-C	5.01	116.60	109.14
20	T	253	ILE	CB-CA-C	-5.00	102.80	110.50
40	o	139	VAL	CA-C-N	5.00	124.66	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	o	139	VAL	C-N-CA	5.00	124.66	119.56

There are no chirality outliers.

All (56) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	166	PHE	Peptide
1	A	346	ASP	Peptide
1	A	408	PRO	Peptide
1	A	433	GLU	Peptide
1	A	642	ARG	Sidechain
1	A	941	LYS	Peptide
3	C	622	GLU	Peptide
3	C	736	GLY	Peptide
3	C	823	ALA	Peptide
4	D	430	LEU	Peptide
10	J	202	GLU	Peptide
12	L	202	ARG	Peptide
14	M	171	THR	Peptide
15	N	36	PRO	Peptide
18	R	94	GLY	Peptide
20	T	400	PHE	Mainchain,Peptide
26	Y	204	LYS	Mainchain
26	Y	34	ARG	Sidechain
26	Y	63	VAL	Peptide
27	Z	1023	TYR	Peptide
27	Z	1064	THR	Peptide
27	Z	1090	TYR	Peptide
27	Z	1113	THR	Peptide
27	Z	1119	TYR	Peptide
27	Z	475	LEU	Peptide
27	Z	479	MET	Peptide
27	Z	554	VAL	Peptide
27	Z	568	TYR	Peptide
27	Z	569	LEU	Peptide
27	Z	611	TYR	Peptide
27	Z	616	GLU	Peptide
27	Z	628	MET	Peptide
27	Z	711	VAL	Peptide
27	Z	721	GLU	Peptide
27	Z	740	PRO	Peptide
27	Z	747	MET	Peptide

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Mol	Chain	Res	Type	Group
27	Z	771	PRO	Peptide
27	Z	777	PRO	Peptide
27	Z	794	ALA	Peptide
27	Z	798	VAL	Mainchain,Peptide
27	Z	821	ILE	Peptide
27	Z	876	ASN	Peptide
27	Z	900	SER	Peptide
27	Z	904	GLN	Peptide
27	Z	905	ASP	Peptide
27	Z	962	SER	Peptide
27	Z	976	SER	Peptide
36	d	112	ASN	Peptide
36	k	112	ASN	Peptide
28	s	481[A]	VAL	Mainchain,Peptide
28	s	481[B]	VAL	Mainchain,Peptide
13	y	191	VAL	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	17519	0	16642	1178	0
2	B	1768	0	897	66	0
3	C	6795	0	6807	612	0
4	D	7632	0	1994	27	0
5	E	2338	0	2272	160	0
6	F	2075	0	1048	199	0
7	G	1641	0	835	255	0
8	H	2946	0	1494	261	0
9	I	2757	0	1234	24	0
10	J	3829	0	2907	133	0
11	K	979	0	741	23	0
12	L	2885	0	2427	278	0
13	y	704	0	525	46	0
14	M	775	0	767	102	0
15	N	1184	0	1190	72	0
16	O	2277	0	2260	176	0
17	P	829	0	814	74	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	R	1962	0	2011	286	0
19	S	1236	0	1210	183	0
20	T	2461	0	2420	156	0
21	Q	5288	0	1361	0	0
22	U	193	0	196	24	0
23	V	3410	0	3287	205	0
24	W	2310	0	1360	332	0
25	X	480	0	401	122	0
26	Y	1426	0	1210	274	0
27	Z	2540	0	677	12	0
28	q	918	0	801	16	0
28	r	901	0	777	14	0
28	s	1497	0	406	2	0
28	t	476	0	434	7	0
29	u	3126	0	3167	98	0
30	v	1196	0	1182	35	0
31	w	730	0	690	29	0
32	x	216	0	202	1	0
33	a	609	0	620	9	0
33	h	621	0	623	16	0
34	b	675	0	702	32	0
34	i	690	0	712	15	0
35	c	641	0	689	15	0
35	j	649	0	693	13	0
36	d	768	0	797	31	0
36	k	688	0	709	28	0
37	f	576	0	589	22	0
37	m	576	0	589	21	0
38	e	652	0	668	21	0
38	l	652	0	668	20	0
39	g	569	0	581	13	0
39	n	533	0	555	19	0
40	o	1277	0	1297	30	0
41	p	760	0	783	11	0
42	1	972	0	284	1	0
43	2	1664	0	449	11	0
44	3	684	0	198	0	0
45	4	184	0	180	34	0
46	A	36	0	6	10	0
47	C	32	0	12	7	0
48	C	1	0	0	0	0
48	F	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
48	u	1	0	0	0	0
49	D	54	0	24	1	0
50	N	3	0	0	2	0
50	O	3	0	0	0	0
50	Y	1	0	0	2	0
51	u	31	0	12	1	0
All	All	103906	0	79086	4873	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 27.

All (4873) 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)
19:S:57:ILE:HD13	24:W:97:ASN:CB	1.21	1.66
12:L:191:LEU:HD21	13:y:57:VAL:CB	1.24	1.64
1:A:1772:PHE:CD2	1:A:1813:ARG:HG2	1.21	1.63
28:r:47:LEU:CB	28:r:47:LEU:CG	1.81	1.59
1:A:853:LYS:HE2	7:G:148:U:C5	1.36	1.57
9:I:511:LEU:CB	9:I:547:LEU:CB	1.80	1.56
11:K:163:LEU:CB	11:K:163:LEU:CG	1.81	1.56
1:A:1320:LYS:HZ3	1:A:1526:LEU:CD2	0.93	1.56
1:A:1772:PHE:CZ	1:A:1813:ARG:HD2	1.38	1.54
1:A:1504:GLU:HA	1:A:1754:TYR:CE1	1.42	1.54
28:q:47:LEU:CB	28:q:47:LEU:CG	1.81	1.52
1:A:855:ARG:HG3	8:H:29:A:C2	1.43	1.50
1:A:1853:PRO:HG3	43:2:614:LYS:CA	1.38	1.50
19:S:57:ILE:CD1	24:W:97:ASN:CB	1.90	1.49
1:A:1772:PHE:CE2	1:A:1813:ARG:CD	1.93	1.48
1:A:1503:TRP:HZ3	1:A:1533:ARG:NE	1.09	1.46
1:A:1853:PRO:CG	43:2:614:LYS:CA	1.90	1.46
1:A:171:ASP:O	1:A:520:TYR:CD2	1.65	1.44
1:A:1772:PHE:CD2	1:A:1813:ARG:CG	1.99	1.44
26:Y:54:LYS:CG	26:Y:56:PHE:CZ	1.98	1.44
7:G:135:G:N2	8:H:41:U:H3	1.14	1.42
1:A:47:GLU:CB	1:A:50:LYS:NZ	1.82	1.42
19:S:57:ILE:CD1	24:W:97:ASN:HB3	1.43	1.41
1:A:855:ARG:HG3	8:H:29:A:N1	1.28	1.40
1:A:73:HIS:HD2	1:A:81:PHE:CE2	1.37	1.40
1:A:1853:PRO:CB	43:2:614:LYS:CA	1.98	1.40
1:A:80:LYS:NZ	15:N:37:HIS:CD2	1.89	1.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:853:LYS:CE	7:G:148:U:C5	2.05	1.39
12:L:191:LEU:O	12:L:196:ILE:CG1	1.70	1.39
5:E:260:ARG:NH1	5:E:273:CYS:SG	1.95	1.38
1:A:1527:ASN:HD22	7:G:149:G:N2	1.21	1.36
1:A:1853:PRO:HG3	43:2:614:LYS:C	1.48	1.36
3:C:387:ASP:O	3:C:388:VAL:HG12	1.20	1.36
1:A:47:GLU:HB2	1:A:50:LYS:NZ	1.04	1.36
3:C:680:ASN:OD1	3:C:682:LYS:CG	1.73	1.35
19:S:39:PHE:CB	19:S:129:PHE:CZ	2.10	1.34
19:S:149:SER:O	24:W:100:ARG:NH2	1.58	1.34
1:A:1853:PRO:HB3	43:2:614:LYS:CA	1.56	1.34
4:D:292:ILE:O	4:D:296:ALA:CA	1.75	1.33
5:E:267:PHE:CE2	11:K:194:GLU:HB3	1.63	1.33
5:E:267:PHE:CZ	11:K:194:GLU:O	1.82	1.33
3:C:445:ALA:O	3:C:449:ILE:N	1.59	1.32
4:D:152:GLU:O	4:D:156:GLU:N	1.59	1.31
4:D:292:ILE:O	4:D:296:ALA:N	1.60	1.31
26:Y:46:CYS:SG	26:Y:83:CYS:HB3	1.69	1.31
3:C:679:PRO:HB2	3:C:807:GLN:OE1	1.26	1.31
24:W:162:ASN:HD22	24:W:165:LEU:CD2	1.41	1.31
7:G:142:U:OP1	26:Y:33:VAL:HG13	1.27	1.30
4:D:151:LYS:O	4:D:155:LYS:N	1.62	1.30
1:A:155:LYS:NZ	1:A:624:GLY:O	1.63	1.29
1:A:855:ARG:CG	8:H:29:A:C2	2.13	1.29
3:C:670:SER:HA	3:C:823:ALA:CB	1.60	1.29
1:A:264:PHE:CZ	1:A:459:LEU:HD13	1.66	1.29
1:A:73:HIS:CD2	1:A:81:PHE:CE2	2.20	1.28
1:A:73:HIS:CD2	1:A:81:PHE:CZ	2.20	1.28
1:A:47:GLU:O	1:A:50:LYS:CG	1.80	1.28
12:L:101:GLU:OE1	26:Y:163:ARG:NH2	1.64	1.28
1:A:1320:LYS:NZ	1:A:1526:LEU:HD23	0.96	1.28
24:W:126:GLU:CG	24:W:130:ARG:NH1	1.96	1.28
26:Y:63:VAL:CG2	26:Y:73:ILE:O	1.81	1.28
19:S:39:PHE:HB2	19:S:129:PHE:CZ	1.66	1.27
1:A:1504:GLU:CA	1:A:1754:TYR:CE1	2.13	1.27
1:A:768:ASP:OD1	2:B:41:U:OP1	1.53	1.27
19:S:39:PHE:CG	19:S:129:PHE:HE2	1.53	1.26
1:A:80:LYS:NZ	15:N:37:HIS:NE2	1.78	1.26
1:A:1504:GLU:CA	1:A:1754:TYR:HE1	1.44	1.26
5:E:146:ARG:NH1	5:E:148:LYS:CE	1.98	1.26
12:L:191:LEU:HB3	12:L:196:ILE:CD1	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:39:PHE:CB	19:S:129:PHE:HZ	1.46	1.25
24:W:126:GLU:HG3	24:W:130:ARG:NH1	1.51	1.25
4:D:291:GLU:O	4:D:295:THR:N	1.66	1.25
3:C:680:ASN:OD1	3:C:682:LYS:HG2	1.23	1.25
8:H:32:U:O5'	25:X:17:LEU:HD12	1.09	1.25
3:C:114:TYR:OH	35:c:12:HIS:O	1.54	1.24
10:J:191:ALA:O	10:J:193:GLN:N	1.66	1.24
26:Y:54:LYS:HG3	26:Y:56:PHE:CE2	1.72	1.24
5:E:267:PHE:CE1	11:K:194:GLU:O	1.90	1.23
1:A:120:TYR:O	1:A:483:GLN:N	1.69	1.22
5:E:146:ARG:NH1	5:E:148:LYS:HE3	1.53	1.22
10:J:180:LYS:HG2	12:L:143:ASP:OD2	1.36	1.22
28:q:22:ASN:CB	28:r:55:ILE:HA	1.67	1.22
1:A:1772:PHE:CE2	1:A:1813:ARG:CG	2.20	1.22
19:S:57:ILE:HG23	24:W:99:PHE:CD2	1.74	1.22
24:W:204:ASP:OD1	24:W:205:VAL:HG23	1.36	1.22
1:A:227:ARG:HA	1:A:416:GLY:O	1.39	1.22
1:A:1772:PHE:CZ	1:A:1813:ARG:CD	2.10	1.22
12:L:191:LEU:CB	12:L:196:ILE:HD11	1.69	1.22
1:A:1772:PHE:CE2	1:A:1813:ARG:HG2	1.75	1.21
1:A:121:HIS:NE2	1:A:481:PHE:HB3	1.54	1.21
19:S:57:ILE:HD13	24:W:97:ASN:CG	1.66	1.21
19:S:131:ARG:HD3	19:S:132:VAL:O	1.09	1.20
6:F:48:A:H1'	12:L:33:ARG:NH1	1.57	1.20
3:C:497:LEU:HD13	3:C:577:PHE:CZ	1.75	1.20
12:L:192:ARG:HA	12:L:196:ILE:O	1.38	1.20
3:C:196:LYS:HE3	34:b:11:GLN:NE2	1.56	1.20
1:A:1320:LYS:CE	1:A:1526:LEU:HD23	1.71	1.19
26:Y:68:TYR:CE1	26:Y:69:LEU:HG	1.77	1.19
1:A:1771:LEU:CD2	1:A:1930:TYR:CB	2.20	1.19
1:A:1772:PHE:CE2	1:A:1813:ARG:HD2	1.67	1.19
19:S:39:PHE:CG	19:S:129:PHE:CE2	2.30	1.19
1:A:1771:LEU:CD2	1:A:1930:TYR:HB3	1.73	1.18
5:E:267:PHE:CE2	11:K:194:GLU:CB	2.25	1.18
12:L:191:LEU:CD2	13:y:57:VAL:CB	2.21	1.18
14:M:153:ARG:HA	14:M:160:PHE:CE2	1.76	1.18
1:A:1772:PHE:CE1	1:A:1813:ARG:HD2	1.79	1.18
24:W:210:GLU:HA	24:W:213:GLN:OE1	1.42	1.18
1:A:80:LYS:HZ1	15:N:37:HIS:CD2	1.55	1.18
25:X:37:ILE:HA	25:X:40:LEU:HD13	1.24	1.18
1:A:1772:PHE:CE2	1:A:1813:ARG:NE	2.12	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:449:ILE:CD1	3:C:466:SER:OG	1.90	1.17
7:G:2:U:HO2'	13:y:2:ALA:N	1.40	1.17
25:X:36:LYS:O	25:X:40:LEU:HD12	1.41	1.17
1:A:1503:TRP:CZ3	1:A:1533:ARG:NE	2.00	1.16
1:A:853:LYS:HG2	7:G:148:U:C4	1.81	1.16
3:C:230:ASP:OD2	3:C:259:LYS:CE	1.94	1.16
1:A:86:ARG:HH22	18:R:211:ARG:CG	1.57	1.16
1:A:1771:LEU:HD21	1:A:1930:TYR:CB	1.72	1.16
1:A:850:TYR:OH	1:A:863:GLU:HB3	1.43	1.16
24:W:140:ASP:HB3	24:W:153:ILE:CG2	1.74	1.16
24:W:162:ASN:ND2	24:W:165:LEU:HD21	1.61	1.16
5:E:74:PHE:CE1	5:E:81:LEU:HD21	1.82	1.15
19:S:57:ILE:CD1	24:W:97:ASN:CG	2.18	1.15
23:V:536:ILE:CG2	23:V:579:SER:CB	2.25	1.15
3:C:221:ILE:HD11	3:C:479:THR:OG1	1.46	1.14
18:R:101:ILE:O	18:R:104:GLN:HG3	1.48	1.14
26:Y:54:LYS:HG2	26:Y:56:PHE:CZ	1.67	1.14
1:A:1525:GLY:HA2	1:A:1528:GLN:HG2	1.29	1.13
3:C:705:VAL:HG23	3:C:717:PHE:CD2	1.83	1.13
7:G:21:A:N6	16:O:91:GLY:O	1.80	1.13
26:Y:54:LYS:CG	26:Y:56:PHE:CE2	2.30	1.13
3:C:216:THR:HG22	3:C:245:HIS:HE1	0.97	1.13
3:C:679:PRO:CB	3:C:807:GLN:OE1	1.95	1.13
6:F:28:A:O2'	15:N:39:GLY:HA2	1.48	1.13
3:C:465:MET:HE1	3:C:475:MET:HG3	1.14	1.13
3:C:507:VAL:HG11	3:C:565:ILE:HG23	1.30	1.13
12:L:191:LEU:O	12:L:196:ILE:HG12	1.32	1.13
1:A:1930:TYR:CE1	25:X:71:ASP:CB	2.32	1.13
3:C:196:LYS:HB2	34:b:7:SER:OG	1.49	1.13
7:G:-1:G:O3'	26:Y:4:ARG:HD2	1.49	1.12
19:S:57:ILE:CD1	24:W:97:ASN:OD1	1.97	1.12
19:S:131:ARG:CD	19:S:132:VAL:O	1.95	1.12
26:Y:19:LYS:O	26:Y:20:ILE:HG12	1.45	1.12
3:C:216:THR:HG22	3:C:245:HIS:CE1	1.85	1.12
6:F:27:A:OP1	15:N:41:ARG:NH2	1.83	1.12
16:O:21:PRO:O	24:W:110:MET:HE1	1.49	1.12
7:G:5:G:C2'	7:G:6:A:H2	1.61	1.11
15:N:125:LYS:HD2	24:W:167:VAL:O	1.44	1.11
19:S:39:PHE:HB3	19:S:129:PHE:CZ	1.85	1.11
1:A:439:GLN:NE2	1:A:614:TYR:CZ	2.18	1.11
7:G:6:A:H2'	7:G:7:G:O4'	1.47	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:168:A:H1'	39:n:48:MET:HE1	1.19	1.11
14:M:165:ASN:HB2	18:R:95:LYS:HA	1.22	1.11
14:M:153:ARG:HA	14:M:160:PHE:CZ	1.84	1.11
23:V:540:GLU:OE1	23:V:541:THR:HG23	1.48	1.11
1:A:1501:LEU:CD2	1:A:1753:LEU:HD13	1.79	1.11
1:A:172:GLU:OE2	26:Y:10:TYR:OH	1.66	1.11
19:S:57:ILE:HD13	24:W:97:ASN:HB2	1.16	1.11
19:S:57:ILE:HD12	24:W:97:ASN:HB3	1.25	1.11
23:V:520:GLU:O	23:V:523:GLU:CG	1.98	1.11
7:G:21:A:O2'	7:G:22:C:O5'	1.69	1.10
8:H:156:U:H6	8:H:156:U:H5''	1.10	1.10
30:v:72:THR:HG21	30:v:94:ILE:HD11	1.29	1.10
8:H:154:C:OP2	41:p:19:LYS:HG2	1.49	1.10
26:Y:28:ASP:OD2	26:Y:64:GLN:NE2	1.84	1.10
26:Y:54:LYS:HG3	26:Y:56:PHE:CZ	1.75	1.10
8:H:32:U:O5'	25:X:17:LEU:CD1	1.98	1.10
3:C:445:ALA:HB1	3:C:449:ILE:HG13	1.29	1.10
12:L:191:LEU:HD21	13:y:57:VAL:CG2	1.79	1.10
19:S:151:ASP:OD2	24:W:97:ASN:OD1	1.70	1.10
1:A:1771:LEU:HD21	1:A:1930:TYR:CA	1.80	1.10
17:P:193:VAL:HG23	17:P:194:PHE:CD2	1.86	1.10
26:Y:75:ARG:HD2	26:Y:77:TYR:CZ	1.87	1.10
1:A:73:HIS:NE2	1:A:81:PHE:CE1	2.20	1.09
10:J:214:ILE:HG22	10:J:219:GLU:HB3	1.14	1.09
19:S:150:GLN:HA	24:W:100:ARG:NH2	1.65	1.09
1:A:171:ASP:O	1:A:520:TYR:HD2	1.02	1.09
3:C:679:PRO:HD2	3:C:807:GLN:HB3	1.16	1.09
9:I:296:PHE:HA	9:I:305:SER:CB	1.80	1.09
26:Y:134:MET:HA	26:Y:134:MET:HE3	1.33	1.09
3:C:449:ILE:HD13	3:C:466:SER:OG	1.49	1.09
6:F:45:A:C5	26:Y:34:ARG:CZ	2.35	1.09
1:A:73:HIS:HD2	1:A:81:PHE:CD2	1.69	1.09
3:C:470:PRO:HB3	3:C:500:THR:HG23	1.34	1.09
19:S:57:ILE:CG2	24:W:99:PHE:HD2	1.65	1.09
1:A:276:GLY:O	1:A:448:GLN:NE2	1.83	1.09
1:A:1553:VAL:HG11	26:Y:7:LEU:HD12	1.18	1.09
14:M:194:ASP:O	14:M:196:TYR:N	1.84	1.08
3:C:196:LYS:HZ1	34:b:11:GLN:HG2	1.08	1.08
3:C:670:SER:HA	3:C:823:ALA:HB1	1.27	1.08
24:W:162:ASN:HB3	24:W:165:LEU:HD23	1.11	1.08
1:A:76:MET:CE	1:A:88:TYR:CD2	2.36	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:HIS:CE1	1:A:481:PHE:HB3	1.88	1.08
1:A:845:ARG:HH22	1:A:1439:ARG:HB3	1.12	1.08
23:V:496:CYS:O	23:V:500:GLN:HG3	1.50	1.08
25:X:6:LEU:HD22	26:Y:55:LYS:HE2	1.35	1.08
26:Y:68:TYR:HD1	26:Y:69:LEU:N	1.52	1.08
1:A:778:ARG:NH1	8:H:23:A:OP1	1.86	1.08
3:C:497:LEU:CD1	3:C:577:PHE:CZ	2.36	1.08
1:A:855:ARG:CB	8:H:29:A:H2	1.65	1.07
3:C:906:ILE:HD13	29:u:179:ARG:NH1	1.67	1.07
26:Y:34:ARG:HD3	26:Y:55:LYS:HD3	1.10	1.07
1:A:264:PHE:HE1	1:A:455:VAL:HG13	1.15	1.07
1:A:1494:TYR:CB	1:A:1744:ARG:HD3	1.84	1.07
3:C:230:ASP:OD2	3:C:259:LYS:HE2	1.49	1.07
3:C:465:MET:CE	3:C:475:MET:HG3	1.83	1.07
1:A:852:VAL:HG21	1:A:1449:LYS:HD2	1.36	1.07
1:A:264:PHE:CE1	1:A:455:VAL:HG13	1.90	1.07
5:E:266:PRO:HG2	12:L:785:GLN:HB2	1.37	1.07
8:H:105:G:H2'	8:H:106:G:H5''	1.37	1.07
24:W:162:ASN:HD22	24:W:165:LEU:HD21	0.93	1.06
25:X:37:ILE:HA	25:X:40:LEU:CD1	1.85	1.06
3:C:670:SER:CB	3:C:823:ALA:HB3	1.85	1.06
1:A:1771:LEU:HD21	1:A:1930:TYR:HB3	1.29	1.06
1:A:1853:PRO:HB3	43:2:614:LYS:N	1.67	1.06
3:C:449:ILE:HG21	3:C:457:VAL:HG11	1.36	1.06
8:H:40:C:H5'	26:Y:22:LYS:HB2	1.36	1.06
1:A:1463:LYS:NZ	7:G:152:C:OP2	1.88	1.06
1:A:1501:LEU:HD22	1:A:1753:LEU:HD13	1.14	1.06
26:Y:68:TYR:O	26:Y:70:GLY:N	1.89	1.06
1:A:47:GLU:O	1:A:50:LYS:HG3	0.88	1.05
12:L:161:ASN:ND2	12:L:163:GLN:O	1.88	1.05
12:L:191:LEU:HB3	12:L:196:ILE:HD11	1.08	1.05
20:T:399:LYS:CG	20:T:406:ILE:HD11	1.87	1.05
24:W:162:ASN:HB3	24:W:165:LEU:CD2	1.85	1.05
3:C:906:ILE:HD13	29:u:179:ARG:HH12	1.16	1.05
7:G:5:G:H2'	7:G:6:A:C2	1.91	1.05
1:A:168:PRO:CG	1:A:559:ASP:HB3	1.87	1.04
7:G:5:G:C4	7:G:6:A:N1	2.25	1.04
12:L:191:LEU:O	12:L:196:ILE:HG13	1.54	1.04
25:X:36:LYS:HZ3	25:X:36:LYS:HA	1.16	1.04
1:A:1527:ASN:ND2	7:G:149:G:N2	2.04	1.04
3:C:488:VAL:HG13	3:C:609:LYS:HE2	1.39	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:369:GLU:O	1:A:371:LEU:N	1.88	1.04
6:F:42:C:H2'	6:F:43:A:C8	1.91	1.04
12:L:161:ASN:CG	12:L:168:LYS:HE3	1.82	1.04
19:S:11:PRO:HB3	19:S:166:GLY:HA3	1.40	1.04
19:S:39:PHE:CB	19:S:129:PHE:CE2	2.40	1.04
1:A:86:ARG:HH22	18:R:211:ARG:HG2	1.16	1.04
26:Y:54:LYS:O	26:Y:56:PHE:CD2	2.09	1.04
3:C:196:LYS:CE	34:b:11:GLN:HE21	1.71	1.04
7:G:8:C:OP1	12:L:200:LYS:HE2	1.55	1.04
12:L:18:ILE:CG1	12:L:152:LEU:HD23	1.88	1.04
12:L:191:LEU:HD11	13:y:57:VAL:CG2	1.88	1.04
20:T:434:GLY:HA2	20:T:464:GLY:HA2	1.41	1.03
1:A:1494:TYR:HB3	1:A:1744:ARG:HD3	1.08	1.03
18:R:178:ARG:HD3	18:R:194:GLN:HE22	1.17	1.03
45:4:22:ALA:O	45:4:24:ALA:N	1.90	1.03
1:A:254:TYR:CZ	1:A:434:HIS:HB3	1.93	1.03
1:A:339:PHE:CE1	1:A:406:TRP:CE3	2.46	1.03
1:A:1533:ARG:NH1	1:A:1752:GLN:OE1	1.91	1.03
26:Y:63:VAL:HG22	26:Y:73:ILE:O	1.51	1.03
1:A:853:LYS:CG	7:G:148:U:C4	2.41	1.02
3:C:230:ASP:CG	3:C:259:LYS:HE2	1.84	1.02
3:C:387:ASP:O	3:C:388:VAL:CG1	2.07	1.02
3:C:511:GLY:O	3:C:576:ILE:CD1	2.07	1.02
4:D:291:GLU:O	4:D:295:THR:CA	2.05	1.02
14:M:153:ARG:CA	14:M:160:PHE:CE2	2.42	1.02
24:W:158:GLU:OE1	24:W:158:GLU:N	1.91	1.02
12:L:37:LEU:HD21	12:L:155:ALA:HB1	1.36	1.02
19:S:57:ILE:HD11	24:W:97:ASN:OD1	1.55	1.02
1:A:855:ARG:HB2	8:H:29:A:H2	1.25	1.02
8:H:32:U:P	25:X:17:LEU:HG	1.99	1.02
15:N:40:LYS:O	15:N:41:ARG:HG3	1.59	1.02
1:A:127:SER:OG	1:A:495:GLN:OE1	1.77	1.01
7:G:142:U:P	25:X:10:LYS:NZ	2.32	1.01
14:M:126:ASP:OD2	14:M:128:ALA:HB3	1.57	1.01
23:V:515:CYS:HA	23:V:521:TYR:HB2	1.42	1.01
25:X:5:ASP:OD1	25:X:7:ASN:N	1.91	1.01
25:X:12:TRP:HZ2	26:Y:35:LEU:CD2	1.72	1.01
1:A:254:TYR:CE2	1:A:434:HIS:HB2	1.94	1.01
7:G:135:G:N2	8:H:41:U:N3	1.92	1.01
12:L:198:ILE:C	12:L:199:GLN:HE21	1.67	1.01
3:C:703:GLU:OE2	3:C:740:THR:HG21	1.61	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:34:G:H2'	6:F:35:A:H5''	1.40	1.01
3:C:776:GLU:O	3:C:781:ASP:OD1	1.78	1.01
25:X:34:ARG:HA	25:X:37:ILE:CD1	1.90	1.01
1:A:80:LYS:HZ3	15:N:37:HIS:CD2	1.67	1.00
1:A:1791:HIS:CE1	1:A:1799:THR:HG23	1.94	1.00
3:C:448:LYS:O	3:C:452:THR:OG1	1.75	1.00
1:A:120:TYR:N	1:A:483:GLN:O	1.93	1.00
1:A:121:HIS:HA	1:A:482:PHE:HA	1.40	1.00
1:A:264:PHE:CE1	1:A:459:LEU:HD13	1.96	1.00
23:V:320:ARG:NH1	23:V:340:PHE:CE1	2.30	1.00
23:V:497:CYS:HB2	23:V:507:PHE:CG	1.96	1.00
26:Y:46:CYS:SG	26:Y:83:CYS:CB	2.49	1.00
1:A:168:PRO:HG3	1:A:559:ASP:HB3	1.39	1.00
12:L:162:THR:HG22	18:R:259:GLY:O	1.62	1.00
24:W:209:SER:HB2	24:W:212:GLU:HG3	1.44	1.00
24:W:420:ALA:O	24:W:438:ASP:N	1.93	1.00
23:V:455:PHE:HZ	23:V:489:LEU:HB2	1.25	1.00
5:E:267:PHE:HE2	11:K:194:GLU:CB	1.64	1.00
1:A:623:LYS:O	46:A:3000:IHP:P4	2.20	1.00
3:C:449:ILE:CG2	3:C:457:VAL:CG1	2.38	1.00
26:Y:68:TYR:HE1	26:Y:69:LEU:HG	1.12	1.00
26:Y:75:ARG:HD2	26:Y:77:TYR:OH	1.61	1.00
29:u:278:THR:HG23	29:u:279:GLN:H	1.26	0.99
19:S:11:PRO:HB3	19:S:165:SER:O	1.62	0.99
20:T:352:THR:HG22	20:T:373:LYS:C	1.86	0.99
5:E:267:PHE:CZ	11:K:194:GLU:HB3	1.95	0.99
6:F:45:A:C6	26:Y:34:ARG:CZ	2.44	0.99
12:L:178:GLU:CG	12:L:181:ARG:HD3	1.92	0.99
1:A:384:VAL:HG12	3:C:331:PHE:CD2	1.96	0.99
1:A:799:PRO:HD3	18:R:284:PHE:CE1	1.97	0.99
1:A:1320:LYS:HZ3	1:A:1526:LEU:CG	1.75	0.99
3:C:445:ALA:HB1	3:C:449:ILE:CG1	1.90	0.99
3:C:349:PHE:CD1	3:C:356:PHE:CE1	2.49	0.99
12:L:191:LEU:CA	12:L:196:ILE:HD11	1.92	0.99
12:L:52:GLU:OE2	12:L:134:THR:OG1	1.79	0.99
1:A:86:ARG:NH2	18:R:211:ARG:CG	2.24	0.99
1:A:1553:VAL:HG11	26:Y:7:LEU:CD1	1.92	0.99
7:G:21:A:H4'	7:G:22:C:OP1	1.62	0.99
1:A:1771:LEU:HD21	1:A:1930:TYR:HA	1.43	0.99
10:J:201:ARG:NE	10:J:201:ARG:O	1.94	0.99
8:H:32:U:OP1	25:X:17:LEU:N	1.94	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:166:LYS:HE3	12:L:170:LYS:NZ	1.78	0.99
1:A:380:LEU:HD23	3:C:349:PHE:CE1	1.98	0.98
45:4:4:ALA:CB	45:4:5:PRO:CD	2.40	0.98
23:V:548:ALA:CB	23:V:585:ILE:CB	2.41	0.98
3:C:680:ASN:OD1	3:C:682:LYS:CB	2.11	0.98
15:N:101:CYS:HB2	15:N:102:CYS:SG	2.04	0.98
1:A:76:MET:HE1	1:A:88:TYR:CD2	1.98	0.98
1:A:120:TYR:CE2	1:A:483:GLN:HB2	1.98	0.98
3:C:306:ASN:OD1	3:C:437:HIS:CE1	2.16	0.98
19:S:57:ILE:CG2	24:W:99:PHE:CD2	2.43	0.98
3:C:196:LYS:NZ	34:b:11:GLN:HG2	1.79	0.98
26:Y:63:VAL:HG23	26:Y:73:ILE:O	1.59	0.98
1:A:850:TYR:HE2	1:A:864:LEU:HB2	1.28	0.98
10:J:203:LEU:HD13	10:J:204:GLU:N	1.78	0.98
3:C:670:SER:CA	3:C:823:ALA:HB3	1.94	0.97
10:J:198:ALA:HB1	12:L:160:ALA:HA	1.46	0.97
24:W:162:ASN:ND2	24:W:165:LEU:CD2	2.20	0.97
3:C:711:ARG:HD3	3:C:730:ARG:HH11	1.29	0.97
10:J:180:LYS:CG	12:L:143:ASP:OD2	2.12	0.97
23:V:602:ARG:O	23:V:606:GLU:CG	2.13	0.97
26:Y:68:TYR:HE2	26:Y:94:GLU:HB2	1.29	0.97
8:H:168:A:H5''	8:H:168:A:C8	1.98	0.97
19:S:57:ILE:CG2	24:W:99:PHE:HB2	1.94	0.97
19:S:11:PRO:CB	19:S:165:SER:O	2.12	0.97
23:V:330:LYS:HZ3	29:u:50:LEU:HD23	1.27	0.97
1:A:805:GLU:OE2	17:P:194:PHE:HZ	1.43	0.97
3:C:670:SER:HA	3:C:823:ALA:HB3	1.43	0.97
6:F:35:A:OP1	12:L:203:LYS:HD2	1.65	0.97
18:R:65:PRO:HB2	19:S:90:LEU:HA	1.44	0.97
1:A:369:GLU:OE2	1:A:369:GLU:N	1.97	0.97
1:A:1772:PHE:CZ	1:A:1813:ARG:NE	2.31	0.97
7:G:5:G:C4	7:G:6:A:C2	2.52	0.96
19:S:100:MET:HG2	19:S:108:ASN:OD1	1.64	0.96
24:W:128:GLN:OE1	24:W:139:LEU:CD1	2.13	0.96
30:v:92:ILE:HG22	30:v:94:ILE:HG23	1.46	0.96
2:B:95:G:H5'	37:f:25:TRP:HH2	1.28	0.96
26:Y:7:LEU:O	26:Y:8:ASN:OD1	1.80	0.96
19:S:57:ILE:HG23	24:W:99:PHE:HD2	1.06	0.96
3:C:115:GLU:O	3:C:118:PHE:N	1.98	0.96
24:W:140:ASP:HB3	24:W:153:ILE:HG23	1.42	0.96
25:X:50:ARG:O	25:X:53:MET:N	1.99	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1504:GLU:HA	1:A:1754:TYR:CZ	1.99	0.96
5:E:146:ARG:HH11	5:E:148:LYS:HE2	1.28	0.96
1:A:1775:GLN:HG2	1:A:1859:LYS:CB	1.95	0.96
3:C:152:GLN:NE2	3:C:426:GLU:O	1.99	0.96
23:V:645:GLU:O	23:V:648:LYS:CG	2.14	0.96
26:Y:158:LYS:O	26:Y:163:ARG:CB	2.14	0.96
3:C:670:SER:CA	3:C:823:ALA:CB	2.44	0.95
1:A:850:TYR:HH	1:A:863:GLU:HB3	1.18	0.95
12:L:158:ARG:NE	26:Y:51:TYR:OH	1.99	0.95
45:4:4:ALA:HB1	45:4:5:PRO:CD	1.94	0.95
3:C:500:THR:HG22	3:C:545:PRO:HA	1.47	0.95
1:A:980:ARG:HG2	1:A:1094:ARG:HD2	1.45	0.95
1:A:1530:PRO:HG2	1:A:1533:ARG:HB3	1.48	0.95
7:G:5:G:H3'	7:G:6:A:C2	2.02	0.95
18:R:113:TYR:HB3	18:R:230:MET:HE1	1.46	0.95
20:T:352:THR:HG22	20:T:373:LYS:O	1.65	0.95
6:F:22:A:H5''	15:N:116:ASN:O	1.66	0.95
7:G:2:U:O2	7:G:142:U:O2'	1.83	0.95
7:G:27:U:O2'	7:G:28:A:O5'	1.85	0.95
7:G:5:G:C2'	7:G:6:A:C2	2.47	0.95
18:R:113:TYR:OH	20:T:402:ASP:OD1	1.85	0.95
8:H:156:U:H5''	8:H:156:U:C6	2.02	0.95
1:A:1021:ASP:OD1	8:H:24:A:N3	2.00	0.95
1:A:1493:THR:HG22	1:A:1747:ILE:HG22	1.49	0.95
1:A:1772:PHE:HD2	1:A:1813:ARG:HG2	1.13	0.95
3:C:349:PHE:HD1	3:C:356:PHE:CD1	1.85	0.94
3:C:855:GLY:O	3:C:856:HIS:HB3	1.63	0.94
7:G:5:G:C5	7:G:6:A:N1	2.35	0.94
24:W:130:ARG:HB3	24:W:167:VAL:HG11	1.49	0.94
7:G:8:C:OP1	12:L:200:LYS:CE	2.14	0.94
18:R:101:ILE:O	18:R:104:GLN:CG	2.16	0.94
26:Y:34:ARG:CD	26:Y:55:LYS:HD3	1.97	0.94
1:A:1580:HIS:CE1	26:Y:17:PRO:HG3	2.02	0.94
19:S:149:SER:O	24:W:100:ARG:CZ	2.16	0.94
1:A:151:MET:CE	1:A:628:GLY:O	2.16	0.94
3:C:711:ARG:NH2	3:C:730:ARG:O	2.00	0.94
24:W:140:ASP:HA	24:W:153:ILE:CD1	1.97	0.94
24:W:188:ASN:HD22	24:W:191:GLY:HA3	1.31	0.94
1:A:151:MET:HE3	1:A:628:GLY:O	1.68	0.94
1:A:264:PHE:CZ	1:A:459:LEU:CD1	2.50	0.94
24:W:140:ASP:HB2	24:W:153:ILE:HD13	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:114:TYR:CZ	35:c:12:HIS:O	2.20	0.94
6:F:86:U:O2'	6:F:87:C:O5'	1.83	0.94
7:G:17:U:O2	16:O:198:ILE:HD11	1.68	0.94
1:A:47:GLU:CB	1:A:50:LYS:HZ1	1.65	0.94
1:A:73:HIS:CD2	1:A:81:PHE:CE1	2.56	0.94
1:A:548:ARG:NH2	1:A:549:GLU:OE2	2.01	0.94
3:C:700:ILE:HG23	3:C:735:PHE:CD2	2.02	0.94
7:G:5:G:C3'	7:G:6:A:H2	1.81	0.94
12:L:178:GLU:HA	12:L:181:ARG:HG2	1.47	0.94
12:L:191:LEU:CD1	13:y:57:VAL:HG21	1.98	0.94
24:W:210:GLU:OE1	24:W:211:GLU:N	2.01	0.94
28:q:22:ASN:CB	28:r:55:ILE:CG1	2.46	0.94
1:A:853:LYS:CE	7:G:148:U:H5	1.57	0.94
26:Y:46:CYS:HG	50:Y:400:ZN:ZN	0.73	0.94
1:A:1525:GLY:CA	1:A:1528:GLN:HG2	1.98	0.94
5:E:267:PHE:HD1	12:L:788:TYR:CE2	1.84	0.94
6:F:8:C:H6	6:F:8:C:H5''	1.31	0.94
6:F:48:A:C1'	12:L:33:ARG:NH1	2.30	0.94
7:G:132:G:H1	8:H:44:U:H3	1.10	0.94
24:W:162:ASN:CB	24:W:165:LEU:HD23	1.96	0.94
26:Y:54:LYS:O	26:Y:56:PHE:CE2	2.19	0.94
18:R:171:LEU:HD12	18:R:201:GLU:OE1	1.67	0.93
18:R:303:GLU:OE2	18:R:307:GLN:NE2	1.99	0.93
23:V:536:ILE:HG21	23:V:579:SER:CB	1.97	0.93
9:I:640:ALA:HA	10:J:512:GLU:C	1.93	0.93
26:Y:34:ARG:HD3	26:Y:55:LYS:CD	1.96	0.93
3:C:670:SER:HB3	3:C:823:ALA:HB3	1.48	0.93
10:J:308:ARG:HG3	18:R:232:SEP:O	1.68	0.93
18:R:312:MET:HA	18:R:312:MET:HE3	1.49	0.93
5:E:119:THR:CG2	5:E:161:ARG:HB3	1.97	0.93
1:A:158:ARG:NH2	1:A:570:ASP:OD2	2.02	0.93
28:q:22:ASN:CB	28:r:55:ILE:CA	2.45	0.93
3:C:497:LEU:HD13	3:C:577:PHE:HZ	1.16	0.93
23:V:493:ILE:HD13	23:V:510:LEU:HD23	1.51	0.93
24:W:137:TYR:CD1	24:W:158:GLU:HB2	2.04	0.93
12:L:188:ARG:O	12:L:192:ARG:HG2	1.68	0.93
3:C:76:GLU:OE1	3:C:76:GLU:N	2.01	0.92
1:A:980:ARG:HG2	1:A:1094:ARG:CD	2.00	0.92
1:A:1881:ASN:OD1	45:4:11:ALA:HB2	1.69	0.92
3:C:449:ILE:HG21	3:C:457:VAL:CG1	1.97	0.92
5:E:146:ARG:NH1	5:E:148:LYS:HE2	1.82	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:680:ASN:CG	3:C:682:LYS:HG2	1.94	0.92
3:C:705:VAL:HG23	3:C:717:PHE:HD2	1.31	0.92
7:G:6:A:C2'	7:G:7:G:O4'	2.16	0.92
45:4:4:ALA:HB1	45:4:5:PRO:HD3	1.51	0.92
1:A:339:PHE:CE1	1:A:406:TRP:CZ3	2.58	0.92
1:A:1570:LYS:HE3	1:A:1574:ILE:HD11	1.48	0.92
15:N:128:VAL:HG13	15:N:130:ARG:H	1.35	0.92
26:Y:138:GLU:CA	27:Z:1096:GLY:O	2.18	0.92
3:C:452:THR:CG2	3:C:577:PHE:HD2	1.81	0.92
8:H:32:U:OP1	25:X:17:LEU:HG	1.69	0.92
9:I:236:GLN:CB	13:y:173:LEU:CB	2.47	0.92
1:A:1504:GLU:HB3	1:A:1752:GLN:HB3	1.49	0.92
3:C:244:LYS:HA	3:C:292:TYR:HD2	1.34	0.92
12:L:198:ILE:C	12:L:199:GLN:NE2	2.28	0.92
1:A:1501:LEU:O	45:4:28:ALA:HB2	1.69	0.92
1:A:235:MET:CE	1:A:411:PHE:HA	2.00	0.91
3:C:678:THR:HG21	3:C:683:ASN:HD22	1.34	0.91
26:Y:68:TYR:CD1	26:Y:69:LEU:N	2.37	0.91
1:A:86:ARG:NH2	18:R:211:ARG:HG3	1.84	0.91
19:S:150:GLN:CA	24:W:100:ARG:NH2	2.33	0.91
24:W:167:VAL:HG23	24:W:168:PHE:CD1	2.05	0.91
26:Y:54:LYS:HG2	26:Y:56:PHE:HZ	1.17	0.91
3:C:445:ALA:CB	3:C:449:ILE:HG13	2.01	0.91
10:J:220:LEU:HD11	10:J:224:LYS:HE3	1.53	0.91
18:R:262:ILE:HG21	18:R:267:ARG:NH1	1.85	0.91
25:X:12:TRP:HZ2	26:Y:35:LEU:HD21	1.33	0.91
16:O:234:LEU:O	16:O:271:PHE:HA	1.70	0.91
1:A:535:ARG:HD2	26:Y:3:GLU:O	1.70	0.91
3:C:674:CYS:SG	3:C:822:MET:SD	2.67	0.91
14:M:153:ARG:HG3	14:M:160:PHE:CE2	2.05	0.91
1:A:523:ASN:OD1	1:A:552:ARG:NH2	2.02	0.91
3:C:711:ARG:HD3	3:C:730:ARG:NH1	1.86	0.91
6:F:29:A:N6	7:G:16:G:O2'	2.04	0.91
12:L:154:GLU:HB3	26:Y:49:TYR:HE2	1.33	0.91
1:A:1525:GLY:HA2	1:A:1528:GLN:CG	2.01	0.91
3:C:476:CYS:HB3	3:C:565:ILE:HB	1.51	0.91
3:C:483:SER:HA	3:C:490:PHE:HB3	1.52	0.91
5:E:267:PHE:CZ	11:K:194:GLU:C	2.49	0.91
6:F:49:G:H1'	26:Y:51:TYR:CE2	2.05	0.91
7:G:147:C:C5'	7:G:148:U:OP2	2.19	0.91
10:J:192:GLU:HA	10:J:195:LEU:CD1	2.00	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:60:PHE:CE2	24:W:97:ASN:HA	2.04	0.91
6:F:45:A:C6	26:Y:34:ARG:NE	2.38	0.91
12:L:158:ARG:NH2	26:Y:51:TYR:OH	2.04	0.91
24:W:126:GLU:HG3	24:W:130:ARG:HH11	1.20	0.91
1:A:1771:LEU:HD23	1:A:1930:TYR:CB	2.01	0.90
12:L:191:LEU:HD11	13:y:57:VAL:HG23	1.52	0.90
23:V:536:ILE:O	23:V:578:SER:HB3	1.71	0.90
18:R:106:GLN:HG2	18:R:110:LYS:HE2	1.51	0.90
26:Y:54:LYS:CD	26:Y:56:PHE:CZ	2.55	0.90
1:A:232:LEU:HD22	1:A:404:LEU:HD13	1.53	0.90
1:A:254:TYR:CZ	1:A:434:HIS:CB	2.54	0.90
1:A:1760:GLU:OE2	1:A:1883:VAL:HG11	1.70	0.90
3:C:678:THR:OG1	3:C:680:ASN:O	1.89	0.90
6:F:45:A:N7	26:Y:34:ARG:NH1	2.18	0.90
9:I:641:GLU:H	10:J:512:GLU:CB	1.83	0.90
24:W:135:TYR:CE2	24:W:165:LEU:HD11	2.06	0.90
24:W:210:GLU:CA	24:W:213:GLN:OE1	2.18	0.90
1:A:67:ARG:HD3	1:A:179:ALA:HB2	1.51	0.90
7:G:134:U:O2	8:H:42:G:N2	2.05	0.90
8:H:168:A:C1'	39:n:48:MET:HE1	2.01	0.90
19:S:131:ARG:NH1	19:S:133:CYS:HA	1.85	0.90
6:F:42:C:C4	6:F:43:A:C6	2.59	0.90
12:L:104:LEU:HB3	26:Y:162:GLN:CB	2.00	0.90
19:S:58:LYS:H	24:W:99:PHE:HE2	1.17	0.90
1:A:305:ARG:HA	1:A:305:ARG:HH11	1.33	0.90
1:A:1501:LEU:HB2	45:4:28:ALA:CB	2.02	0.90
15:N:54:HIS:CD2	24:W:196:TRP:HZ3	1.89	0.90
15:N:124:SER:O	15:N:127:GLU:HG2	1.71	0.90
26:Y:25:LEU:H	26:Y:25:LEU:HD22	1.36	0.90
1:A:228:TRP:O	1:A:415:SER:HA	1.70	0.90
1:A:850:TYR:OH	1:A:863:GLU:CB	2.18	0.90
26:Y:138:GLU:HA	27:Z:1096:GLY:O	1.71	0.90
1:A:171:ASP:HB3	1:A:519:ASP:HB2	1.53	0.90
12:L:18:ILE:HG13	12:L:152:LEU:CD2	2.02	0.89
14:M:153:ARG:CB	14:M:160:PHE:CE2	2.54	0.89
14:M:162:PRO:HB3	14:M:167:LEU:HB2	1.54	0.89
16:O:89:GLU:OE1	24:W:103:GLN:HB2	1.72	0.89
26:Y:16:ASP:OD1	26:Y:18:SER:N	2.04	0.89
1:A:121:HIS:CG	1:A:481:PHE:O	2.25	0.89
3:C:221:ILE:CD1	3:C:479:THR:OG1	2.19	0.89
3:C:449:ILE:HD11	3:C:466:SER:OG	1.70	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:178:GLU:HG2	12:L:181:ARG:HD3	1.54	0.89
1:A:845:ARG:NH2	1:A:1439:ARG:HB3	1.86	0.89
29:u:278:THR:HG23	29:u:279:GLN:N	1.84	0.89
1:A:47:GLU:HB2	1:A:50:LYS:HZ3	1.08	0.89
1:A:171:ASP:C	1:A:520:TYR:HD2	1.81	0.89
1:A:338:VAL:HG23	3:C:867:PRO:HG3	1.53	0.89
2:B:95:G:H5''	36:d:47:ARG:HH22	1.38	0.89
6:F:47:A:H4'	6:F:48:A:OP1	1.70	0.89
18:R:82:MET:HE3	18:R:82:MET:C	1.97	0.89
19:S:34:LYS:HE3	19:S:78:TYR:CE2	2.07	0.89
13:y:54:SER:O	13:y:57:VAL:HG22	1.72	0.89
25:X:6:LEU:HB3	26:Y:36:MET:SD	2.11	0.89
14:M:165:ASN:HB2	18:R:95:LYS:CA	2.03	0.89
24:W:179:LYS:O	24:W:200:VAL:HG22	1.72	0.89
6:F:48:A:O2'	6:F:49:G:OP1	1.90	0.89
25:X:60:VAL:N	25:X:61:GLY:HA2	1.87	0.89
1:A:76:MET:HE1	1:A:88:TYR:CG	2.08	0.89
8:H:168:A:H1'	39:n:48:MET:CE	2.01	0.89
10:J:193:GLN:O	10:J:197:GLU:N	2.06	0.89
18:R:81:LYS:HA	18:R:81:LYS:NZ	1.88	0.89
6:F:42:C:H2'	6:F:43:A:H8	1.30	0.89
24:W:126:GLU:HG2	24:W:130:ARG:NH1	1.85	0.89
26:Y:19:LYS:O	26:Y:20:ILE:CG1	2.20	0.89
1:A:901:LEU:HD12	1:A:904:HIS:CE1	2.08	0.88
7:G:142:U:P	25:X:10:LYS:HZ1	1.93	0.88
45:4:4:ALA:CB	45:4:5:PRO:HD2	2.01	0.88
10:J:192:GLU:HA	10:J:195:LEU:HD13	1.54	0.88
12:L:191:LEU:C	12:L:196:ILE:CG1	2.45	0.88
1:A:675:GLN:OE1	6:F:70:A:OP1	1.89	0.88
9:I:600:ALA:HA	12:L:505:ARG:CB	2.04	0.88
23:V:642:GLU:O	23:V:645:GLU:CG	2.21	0.88
24:W:128:GLN:OE1	24:W:139:LEU:HD12	1.74	0.88
1:A:1341:ARG:NH2	1:A:1342:TRP:CZ2	2.42	0.88
1:A:73:HIS:CD2	1:A:81:PHE:CD2	2.57	0.88
8:H:40:C:H5''	26:Y:22:LYS:HG2	1.54	0.88
12:L:18:ILE:CD1	12:L:152:LEU:HD23	2.03	0.88
20:T:399:LYS:HG3	20:T:406:ILE:HD11	1.53	0.88
1:A:175:PRO:HG2	1:A:498:ARG:NH2	1.88	0.88
3:C:700:ILE:HG23	3:C:735:PHE:CE2	2.09	0.88
16:O:131:THR:HG22	24:W:108:ARG:HD3	1.56	0.88
3:C:77:VAL:HG12	20:T:197:TYR:C	1.98	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:81:LYS:HA	18:R:81:LYS:CE	2.02	0.88
1:A:70:ILE:HD13	1:A:495:GLN:HG3	1.55	0.88
12:L:39:HIS:HD2	12:L:151:MET:HE3	1.38	0.88
19:S:35:THR:C	19:S:129:PHE:HE1	1.80	0.88
1:A:850:TYR:CE2	1:A:864:LEU:HB2	2.08	0.88
3:C:678:THR:CG2	3:C:683:ASN:HB2	2.04	0.88
1:A:419:ARG:NH2	1:A:423:ASP:O	2.06	0.88
1:A:853:LYS:HG2	7:G:148:U:N3	1.88	0.88
1:A:1504:GLU:N	1:A:1754:TYR:HE1	1.69	0.88
3:C:523:GLN:OE1	3:C:524:ILE:N	2.07	0.88
20:T:399:LYS:HG2	20:T:406:ILE:HD11	1.53	0.88
23:V:537:HIS:HA	23:V:578:SER:HB2	1.54	0.88
3:C:488:VAL:HG13	3:C:609:LYS:CE	2.05	0.87
24:W:156:VAL:HG12	24:W:160:GLU:CD	1.99	0.87
1:A:86:ARG:NH2	18:R:211:ARG:HG2	1.85	0.87
1:A:623:LYS:HB3	46:A:3000:IHP:O34	1.72	0.87
3:C:465:MET:HE1	3:C:475:MET:CG	2.01	0.87
3:C:567:GLU:OE2	3:C:570:GLY:HA3	1.74	0.87
5:E:243:LEU:CD1	5:E:247:GLY:HA2	2.04	0.87
12:L:178:GLU:O	12:L:181:ARG:HG3	1.73	0.87
1:A:1758:PRO:HG3	45:4:8:GLY:O	1.73	0.87
3:C:679:PRO:CG	3:C:807:GLN:OE1	2.21	0.87
24:W:140:ASP:CB	24:W:153:ILE:CG2	2.53	0.87
25:X:34:ARG:HA	25:X:37:ILE:HD12	1.54	0.87
7:G:27:U:O4'	16:O:269:CYS:SG	2.31	0.87
10:J:191:ALA:N	12:L:17:GLU:OE1	2.07	0.87
10:J:192:GLU:CA	10:J:195:LEU:CD1	2.52	0.87
24:W:101:THR:CG2	24:W:104:MET:HG2	2.05	0.87
24:W:126:GLU:CG	24:W:130:ARG:HH12	1.86	0.87
1:A:80:LYS:HZ1	15:N:37:HIS:HD2	1.06	0.87
14:M:153:ARG:CA	14:M:160:PHE:HE2	1.82	0.87
24:W:135:TYR:CZ	24:W:165:LEU:HD11	2.10	0.87
25:X:36:LYS:HA	25:X:36:LYS:NZ	1.90	0.87
12:L:198:ILE:O	12:L:199:GLN:NE2	2.07	0.87
18:R:233:PRO:O	18:R:234:SER:OG	1.93	0.87
19:S:35:THR:O	19:S:129:PHE:HE1	1.57	0.87
25:X:36:LYS:O	25:X:40:LEU:CD1	2.23	0.87
1:A:227:ARG:CA	1:A:416:GLY:O	2.20	0.87
1:A:232:LEU:HD22	1:A:404:LEU:CD1	2.04	0.87
14:M:153:ARG:CB	14:M:160:PHE:HE2	1.87	0.87
6:F:43:A:H2'	6:F:44:G:H5'	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:48:A:H1'	12:L:33:ARG:CZ	2.05	0.87
14:M:153:ARG:HG3	14:M:160:PHE:HE2	1.40	0.87
30:v:110:ILE:O	30:v:114:GLN:HG2	1.74	0.86
6:F:34:G:C2'	6:F:35:A:H5''	2.04	0.86
7:G:27:U:C2'	7:G:28:A:O5'	2.22	0.86
18:R:178:ARG:HD3	18:R:194:GLN:NE2	1.90	0.86
26:Y:132:ASN:O	26:Y:136:VAL:HG23	1.74	0.86
34:b:46:ASP:OD2	34:b:64:LYS:HE3	1.75	0.86
1:A:433:GLU:OE1	1:A:436:PRO:HB3	1.74	0.86
1:A:855:ARG:CG	8:H:29:A:N1	2.24	0.86
1:A:1764:SER:HB3	1:A:1767:ASN:OD1	1.75	0.86
12:L:14:THR:HG23	12:L:152:LEU:HD11	1.56	0.86
12:L:18:ILE:HD11	12:L:152:LEU:HD23	1.56	0.86
24:W:155:SER:C	24:W:156:VAL:HG23	2.00	0.86
8:H:32:U:P	25:X:17:LEU:CG	2.64	0.86
16:O:131:THR:HG21	24:W:108:ARG:HG3	1.57	0.86
1:A:1494:TYR:HB3	1:A:1744:ARG:CD	2.01	0.86
1:A:1570:LYS:CE	1:A:1574:ILE:CD1	2.53	0.86
1:A:367:SER:O	1:A:369:GLU:N	2.08	0.86
1:A:1570:LYS:HE3	1:A:1574:ILE:CD1	2.05	0.86
18:R:81:LYS:HA	18:R:81:LYS:HZ2	1.38	0.86
24:W:137:TYR:CE1	24:W:158:GLU:HB3	2.10	0.86
34:i:46:ASP:OD2	34:i:64:LYS:HE3	1.75	0.86
10:J:325:ASN:HB2	14:M:172:HIS:HD2	1.39	0.86
12:L:191:LEU:HD11	13:y:57:VAL:HG21	1.56	0.86
19:S:9:TRP:O	19:S:11:PRO:HD3	1.76	0.86
1:A:1791:HIS:HE1	1:A:1799:THR:HG23	1.36	0.86
8:H:154:C:O2	8:H:176:G:N2	2.07	0.86
12:L:191:LEU:C	12:L:196:ILE:HG13	2.01	0.86
1:A:853:LYS:HE3	7:G:148:U:C5	2.11	0.85
18:R:220:ARG:NH1	18:R:220:ARG:HB2	1.91	0.85
19:S:150:GLN:HA	24:W:100:ARG:HH21	1.36	0.85
24:W:88:MET:HE1	24:W:89:PHE:HD2	1.41	0.85
26:Y:48:GLU:OE1	26:Y:80:CYS:SG	2.34	0.85
45:4:4:ALA:HB3	45:4:5:PRO:HD2	1.57	0.85
1:A:300:ASN:HB3	3:C:939:ARG:NH2	1.91	0.85
7:G:120:G:O2'	7:G:121:G:O4'	1.94	0.85
18:R:135:PRO:O	18:R:136:ASP:OD1	1.94	0.85
25:X:63:VAL:O	25:X:64:LYS:CB	2.24	0.85
26:Y:22:LYS:CE	26:Y:22:LYS:H	1.88	0.85
8:H:168:A:H5''	8:H:168:A:H8	1.36	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:140:ASP:CB	24:W:153:ILE:HD13	2.05	0.85
1:A:1768:TYR:CD2	1:A:2012:LEU:HD21	2.12	0.85
1:A:1771:LEU:CD2	1:A:1930:TYR:HA	2.05	0.85
3:C:449:ILE:HD11	3:C:466:SER:CB	2.06	0.85
3:C:701:GLU:HA	3:C:740:THR:OG1	1.75	0.85
24:W:210:GLU:HA	24:W:213:GLN:HB2	1.58	0.85
1:A:1771:LEU:HD23	1:A:1930:TYR:HB3	1.54	0.85
8:H:40:C:H5'	26:Y:22:LYS:CB	2.07	0.85
24:W:146:HIS:ND1	24:W:146:HIS:O	2.10	0.85
1:A:47:GLU:CA	1:A:50:LYS:NZ	2.39	0.85
1:A:1853:PRO:CG	43:2:614:LYS:C	2.33	0.85
3:C:705:VAL:HB	3:C:717:PHE:CE2	2.12	0.85
6:F:48:A:H1'	12:L:33:ARG:HH12	1.40	0.85
24:W:209:SER:CB	24:W:212:GLU:HG3	2.06	0.85
3:C:216:THR:CG2	3:C:245:HIS:HE1	1.84	0.85
8:H:98:G:N2	37:m:66:CYS:SG	2.50	0.85
12:L:166:LYS:HE3	12:L:170:LYS:HZ2	1.37	0.85
24:W:137:TYR:HA	24:W:154:GLY:HA3	1.59	0.85
24:W:182:LYS:O	24:W:182:LYS:HD3	1.76	0.85
6:F:48:A:C1'	12:L:33:ARG:HH12	1.87	0.85
14:M:194:ASP:C	14:M:196:TYR:H	1.84	0.85
16:O:20:PHE:CD1	18:R:177:ILE:HD11	2.11	0.85
19:S:35:THR:O	19:S:129:PHE:CE1	2.29	0.85
23:V:489:LEU:O	23:V:492:MET:HB2	1.77	0.85
3:C:365:SER:OG	3:C:371:GLU:OE2	1.94	0.84
3:C:711:ARG:HD3	3:C:730:ARG:HE	1.42	0.84
18:R:297:LYS:HE3	18:R:300:GLU:OE1	1.77	0.84
20:T:417:ASN:OD1	20:T:432:ASP:OD1	1.94	0.84
3:C:725:ASP:OD1	3:C:727:LEU:N	2.10	0.84
14:M:163:THR:OG1	14:M:166:SER:HB2	1.77	0.84
2:B:95:G:H4'	2:B:96:A:O4'	1.76	0.84
3:C:452:THR:HG22	3:C:577:PHE:HD2	1.42	0.84
6:F:27:A:N3	16:O:181:TYR:CE2	2.45	0.84
6:F:43:A:C2'	6:F:44:G:H5'	2.08	0.84
18:R:315:LYS:HE2	18:R:315:LYS:N	1.92	0.84
7:G:20:A:O2'	7:G:21:A:OP2	1.94	0.84
7:G:151:C:HO2'	7:G:152:C:P	2.01	0.84
22:U:23:LEU:H	23:V:474:HIS:HD2	1.25	0.84
23:V:493:ILE:CD1	23:V:510:LEU:HD23	2.06	0.84
24:W:109:ASN:HB2	24:W:114:TYR:CD1	2.12	0.84
1:A:152:ARG:HB3	1:A:152:ARG:HH11	1.39	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:263:PRO:HB2	18:R:266:LYS:HG2	1.56	0.84
7:G:-9:C:C4	22:U:18:TYR:CE1	2.65	0.84
3:C:196:LYS:NZ	34:b:11:GLN:CG	2.40	0.84
8:H:154:C:OP2	41:p:19:LYS:CG	2.25	0.84
5:E:162:ARG:NH2	5:E:203:ASP:O	2.10	0.84
12:L:178:GLU:HG3	12:L:181:ARG:HD3	1.57	0.84
12:L:191:LEU:CD2	13:y:57:VAL:HG21	2.08	0.84
18:R:78:ARG:H	18:R:78:ARG:NE	1.76	0.84
1:A:1853:PRO:HB3	43:2:613:THR:C	2.01	0.84
6:F:45:A:C5	26:Y:34:ARG:NH1	2.45	0.84
18:R:117:THR:O	18:R:120:VAL:HG12	1.78	0.84
3:C:488:VAL:CG1	3:C:609:LYS:HE2	2.08	0.83
14:M:153:ARG:CA	14:M:160:PHE:CZ	2.59	0.83
26:Y:158:LYS:HA	26:Y:163:ARG:CG	2.07	0.83
27:Z:833:PRO:CA	27:Z:919:ASN:CA	2.55	0.83
14:M:153:ARG:CG	14:M:160:PHE:HE2	1.90	0.83
14:M:160:PHE:HB3	14:M:161:PHE:CD1	2.14	0.83
1:A:1930:TYR:HE1	25:X:71:ASP:CB	1.87	0.83
3:C:482:TYR:HE2	3:C:493:PHE:CG	1.97	0.83
3:C:680:ASN:CG	3:C:682:LYS:CG	2.48	0.83
5:E:269:PRO:O	5:E:270:LYS:HB3	1.75	0.83
24:W:160:GLU:N	24:W:160:GLU:OE1	2.12	0.83
8:H:156:U:H6	8:H:156:U:C5'	1.89	0.83
19:S:57:ILE:HD11	24:W:97:ASN:CG	1.95	0.83
1:A:168:PRO:HG3	1:A:559:ASP:CB	2.07	0.83
8:H:152:G:N2	8:H:153:A:N7	2.26	0.83
10:J:406:PHE:CD2	10:J:411:MET:HE3	2.13	0.83
26:Y:68:TYR:CE2	26:Y:94:GLU:HB2	2.12	0.83
3:C:244:LYS:HA	3:C:292:TYR:CD2	2.13	0.83
3:C:348:TYR:CD1	3:C:359:LYS:HB3	2.14	0.83
12:L:37:LEU:HD21	12:L:155:ALA:CB	2.08	0.83
25:X:12:TRP:CZ2	26:Y:35:LEU:CD2	2.61	0.83
26:Y:158:LYS:O	26:Y:163:ARG:HB3	1.75	0.83
3:C:824:THR:HG23	3:C:824:THR:O	1.76	0.83
5:E:74:PHE:CE1	5:E:81:LEU:CD2	2.62	0.83
6:F:41:A:N1	7:G:6:A:N7	2.27	0.83
18:R:280:ILE:HD12	18:R:281:ASN:N	1.93	0.83
3:C:470:PRO:HB3	3:C:500:THR:CG2	2.08	0.83
22:U:23:LEU:H	23:V:474:HIS:CD2	1.97	0.83
24:W:188:ASN:ND2	24:W:191:GLY:HA3	1.93	0.83
26:Y:138:GLU:O	27:Z:1096:GLY:O	1.96	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:254:TYR:CE2	1:A:434:HIS:CB	2.61	0.83
3:C:196:LYS:HE3	34:b:11:GLN:HE21	0.76	0.83
14:M:153:ARG:CG	14:M:160:PHE:CE2	2.62	0.83
30:v:72:THR:CG2	30:v:94:ILE:HD11	2.08	0.83
7:G:-19:A:C2	29:u:172:ARG:NH2	2.47	0.83
19:S:39:PHE:CD1	19:S:129:PHE:HE2	1.97	0.83
1:A:615:ARG:O	1:A:618:THR:OG1	1.96	0.82
1:A:1502:PHE:CZ	1:A:1505:LYS:HD3	2.14	0.82
5:E:74:PHE:CE2	5:E:343:ILE:HG12	2.14	0.82
12:L:18:ILE:CG1	12:L:152:LEU:CD2	2.56	0.82
19:S:149:SER:C	24:W:100:ARG:NH2	2.37	0.82
1:A:1772:PHE:CD2	1:A:1813:ARG:CD	2.50	0.82
3:C:220:ARG:NH1	3:C:578:ARG:O	2.12	0.82
18:R:307:GLN:OE1	18:R:307:GLN:N	2.13	0.82
26:Y:54:LYS:HG2	26:Y:56:PHE:CE2	2.07	0.82
1:A:1775:GLN:HG2	1:A:1859:LYS:HB2	1.61	0.82
3:C:516:LEU:HD12	3:C:517:GLU:HG3	1.59	0.82
18:R:292:TYR:CE1	26:Y:167:VAL:HG21	2.14	0.82
3:C:230:ASP:OD2	3:C:259:LYS:NZ	2.12	0.82
5:E:146:ARG:HH11	5:E:148:LYS:CE	1.83	0.82
18:R:65:PRO:HG2	18:R:66:GLU:OE2	1.79	0.82
1:A:47:GLU:C	1:A:50:LYS:HG3	2.01	0.82
15:N:102:CYS:HG	50:N:202:ZN:ZN	0.89	0.82
19:S:60:PHE:CD2	24:W:98:PRO:HD2	2.15	0.82
1:A:47:GLU:CB	1:A:50:LYS:HZ2	1.66	0.82
9:I:600:ALA:O	12:L:505:ARG:CB	2.27	0.82
7:G:150:U:H2'	7:G:151:C:H5''	1.62	0.82
24:W:140:ASP:HA	24:W:153:ILE:HD11	1.61	0.82
26:Y:38:PRO:O	26:Y:52:LYS:HE3	1.77	0.82
6:F:42:C:C4	6:F:43:A:C5	2.68	0.82
18:R:134:ARG:O	18:R:136:ASP:N	2.12	0.82
24:W:140:ASP:CA	24:W:153:ILE:HG12	2.08	0.82
1:A:300:ASN:O	3:C:939:ARG:NH2	2.13	0.82
2:B:18:C:O2'	2:B:19:A:O5'	1.98	0.82
3:C:244:LYS:HB2	3:C:292:TYR:CE2	2.15	0.82
7:G:5:G:C3'	7:G:6:A:C2	2.62	0.82
1:A:855:ARG:HB2	8:H:29:A:C2	2.13	0.82
12:L:59:LYS:CD	12:L:91:ARG:NH1	2.43	0.81
1:A:852:VAL:HG23	7:G:148:U:O2	1.80	0.81
1:A:1530:PRO:HD2	1:A:1533:ARG:CZ	2.09	0.81
3:C:349:PHE:CD1	3:C:356:PHE:CD1	2.68	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:151:C:O2'	7:G:152:C:O5'	1.96	0.81
3:C:489:GLN:O	3:C:489:GLN:NE2	2.13	0.81
3:C:507:VAL:HG11	3:C:565:ILE:CG2	2.09	0.81
5:E:165:GLN:O	5:E:166:LEU:HD23	1.79	0.81
8:H:105:G:C2'	8:H:106:G:H5''	2.10	0.81
18:R:103:ARG:HB3	18:R:103:ARG:HH11	1.43	0.81
18:R:220:ARG:HB2	18:R:220:ARG:HH11	1.46	0.81
23:V:320:ARG:NH1	23:V:340:PHE:CZ	2.49	0.81
40:o:10:GLU:OE2	42:1:150:ASN:O	1.98	0.81
1:A:121:HIS:NE2	1:A:481:PHE:CB	2.42	0.81
1:A:235:MET:HE1	1:A:411:PHE:HA	1.61	0.81
1:A:247:THR:OG1	1:A:429:ASN:HB3	1.80	0.81
12:L:222:LEU:H	12:L:222:LEU:HD22	1.45	0.81
15:N:111:THR:HG21	15:N:115:THR:O	1.80	0.81
19:S:39:PHE:HB3	19:S:129:PHE:HZ	1.26	0.81
23:V:291:GLU:HG3	23:V:335:MET:SD	2.20	0.81
3:C:507:VAL:CG1	3:C:565:ILE:HG23	2.10	0.81
8:H:154:C:P	41:p:19:LYS:HD3	2.19	0.81
1:A:1501:LEU:C	45:4:28:ALA:HB2	2.06	0.81
9:I:236:GLN:N	13:y:170:ARG:HA	1.95	0.81
17:P:193:VAL:CG2	17:P:194:PHE:CD2	2.64	0.81
25:X:6:LEU:HD22	26:Y:55:LYS:CE	2.09	0.81
1:A:439:GLN:O	1:A:444:ARG:NH1	2.14	0.81
1:A:1504:GLU:N	1:A:1754:TYR:CE1	2.46	0.81
1:A:1775:GLN:HG2	1:A:1859:LYS:CG	2.11	0.81
3:C:196:LYS:HZ1	34:b:11:GLN:CG	1.93	0.81
19:S:39:PHE:HB2	19:S:129:PHE:CE2	2.09	0.81
19:S:39:PHE:CD2	19:S:129:PHE:CE2	2.68	0.81
1:A:338:VAL:O	3:C:266:GLU:HG2	1.81	0.81
1:A:623:LYS:O	46:A:3000:IHP:O44	1.99	0.81
1:A:1953:ILE:HD11	1:A:1986:LEU:HD11	1.63	0.81
3:C:449:ILE:HD11	3:C:466:SER:CA	2.11	0.81
13:y:14:ARG:HH22	26:Y:22:LYS:HB3	1.44	0.81
23:V:477:LEU:CD2	23:V:514:PHE:HE1	1.94	0.81
1:A:1257:THR:OG1	1:A:1527:ASN:OD1	1.97	0.81
1:A:1501:LEU:HB2	45:4:28:ALA:HB1	1.61	0.81
24:W:209:SER:O	24:W:213:GLN:N	2.13	0.81
14:M:160:PHE:HB3	14:M:161:PHE:HD1	1.46	0.80
16:O:171:GLY:HA2	24:W:208:PRO:CG	2.11	0.80
7:G:18:A:H5'	16:O:69:GLU:OE1	1.81	0.80
18:R:74:LEU:HD13	19:S:136:ILE:HG21	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:57:ILE:HG23	24:W:99:PHE:HB2	1.63	0.80
24:W:137:TYR:CE1	24:W:158:GLU:CB	2.65	0.80
1:A:264:PHE:HE1	1:A:455:VAL:CG1	1.94	0.80
3:C:196:LYS:HB2	34:b:7:SER:CB	2.10	0.80
3:C:711:ARG:HD3	3:C:730:ARG:NE	1.96	0.80
5:E:74:PHE:CZ	5:E:81:LEU:HD21	2.16	0.80
12:L:59:LYS:HG2	12:L:91:ARG:NH1	1.96	0.80
12:L:146:GLU:OE1	12:L:146:GLU:N	2.12	0.80
18:R:182:SER:HB2	24:W:112:SER:O	1.79	0.80
18:R:292:TYR:CZ	26:Y:167:VAL:HG11	2.15	0.80
25:X:6:LEU:HD12	25:X:6:LEU:O	1.82	0.80
25:X:35:LYS:HD2	25:X:35:LYS:N	1.96	0.80
26:Y:68:TYR:HE1	26:Y:69:LEU:CG	1.94	0.80
29:u:383:ASN:CG	29:u:384:ASP:H	1.89	0.80
30:v:129:GLN:HB3	31:w:108:ARG:HG3	1.64	0.80
1:A:245:LEU:HA	1:A:430:TRP:HZ2	1.46	0.80
20:T:213:GLU:HG3	20:T:218:TRP:CE2	2.16	0.80
1:A:805:GLU:OE2	17:P:194:PHE:CZ	2.33	0.80
16:O:131:THR:HG23	24:W:111:LEU:H	1.45	0.80
18:R:292:TYR:OH	26:Y:167:VAL:HG11	1.80	0.80
20:T:351:ASP:O	20:T:352:THR:OG1	1.99	0.80
26:Y:54:LYS:HD3	26:Y:56:PHE:CE1	2.17	0.80
5:E:248:SER:HB2	5:E:249:TYR:CD1	2.17	0.80
6:F:43:A:H2'	6:F:44:G:C5'	2.11	0.80
14:M:152:LEU:CD2	14:M:160:PHE:CZ	2.65	0.80
16:O:235:TYR:HD2	16:O:301:LYS:HB2	1.45	0.80
1:A:164:MET:HE1	1:A:560:SER:HA	1.63	0.80
1:A:364:SER:O	1:A:365:VAL:O	1.98	0.80
5:E:209:ILE:HG21	5:E:250:LEU:CD1	2.12	0.80
6:F:22:A:C5'	15:N:116:ASN:O	2.30	0.80
18:R:69:VAL:O	19:S:93:THR:HG21	1.81	0.80
19:S:57:ILE:HG21	24:W:99:PHE:HB2	1.63	0.80
29:u:79:ILE:HD11	29:u:229:THR:HG21	1.64	0.80
1:A:228:TRP:N	1:A:416:GLY:O	2.14	0.80
1:A:481:PHE:CE2	18:R:205:ASP:HA	2.17	0.80
3:C:131:ASN:ND2	3:C:495:ARG:HH12	1.79	0.80
7:G:142:U:P	25:X:10:LYS:HZ2	2.03	0.80
12:L:161:ASN:CG	12:L:168:LYS:CE	2.55	0.80
24:W:212:GLU:O	24:W:214:LYS:N	2.14	0.80
25:X:12:TRP:CZ2	26:Y:35:LEU:HD22	2.16	0.80
8:H:152:G:H5''	8:H:153:A:OP2	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:LYS:HE2	7:G:149:G:C6	2.17	0.80
9:I:641:GLU:N	10:J:512:GLU:CB	2.45	0.79
3:C:77:VAL:HG11	20:T:196:LEU:HG	1.63	0.79
3:C:306:ASN:OD1	3:C:437:HIS:ND1	2.14	0.79
24:W:154:GLY:O	24:W:156:VAL:HG23	1.82	0.79
1:A:293:TRP:CZ3	1:A:295:GLU:OE1	2.35	0.79
1:A:1775:GLN:HG2	1:A:1859:LYS:HG3	1.65	0.79
3:C:511:GLY:O	3:C:576:ILE:HD13	1.79	0.79
24:W:140:ASP:HB3	24:W:153:ILE:CG1	2.13	0.79
1:A:283:VAL:O	1:A:284:ARG:NE	2.15	0.79
26:Y:7:LEU:O	26:Y:7:LEU:HD13	1.83	0.79
1:A:810:TYR:OH	18:R:295:ASP:OD1	2.01	0.79
2:B:90:U:H5''	2:B:91:U:H5'	1.64	0.79
6:F:27:A:C4	16:O:181:TYR:CE2	2.70	0.79
16:O:20:PHE:CE1	18:R:177:ILE:HD11	2.17	0.79
19:S:101:ALA:HB1	24:W:95:PRO:HD3	1.65	0.79
23:V:473:ALA:O	23:V:477:LEU:HG	1.81	0.79
5:E:267:PHE:CE2	11:K:194:GLU:HB2	2.16	0.79
12:L:191:LEU:HB3	12:L:196:ILE:HD12	1.61	0.79
26:Y:19:LYS:C	26:Y:20:ILE:HG12	2.07	0.79
3:C:856:HIS:NE2	29:u:102:ILE:O	2.15	0.79
6:F:22:A:N7	24:W:130:ARG:NE	2.31	0.79
18:R:306:ALA:O	18:R:310:ARG:HG3	1.81	0.79
1:A:855:ARG:CB	8:H:29:A:C2	2.53	0.79
3:C:473:PRO:O	3:C:567:GLU:HB3	1.83	0.79
25:X:14:PRO:HD2	26:Y:98:TYR:OH	1.83	0.79
26:Y:68:TYR:O	26:Y:69:LEU:C	2.25	0.79
1:A:95:MET:HE2	1:A:503:MET:HE1	1.63	0.79
1:A:339:PHE:HE1	1:A:406:TRP:CZ3	2.01	0.79
16:O:253:TYR:CE1	19:S:93:THR:OG1	2.35	0.79
1:A:381:PRO:CD	3:C:334:ILE:HG22	2.13	0.79
3:C:244:LYS:HB2	3:C:292:TYR:HE2	1.47	0.79
5:E:265:ARG:H	5:E:272:ARG:NH2	1.80	0.79
12:L:172:ARG:NH1	26:Y:81:THR:O	2.16	0.79
19:S:11:PRO:CB	19:S:166:GLY:HA3	2.12	0.79
1:A:666:LYS:HB3	1:A:668:VAL:HG23	1.65	0.78
3:C:515:THR:O	3:C:517:GLU:N	2.16	0.78
3:C:738:ASP:HB2	3:C:740:THR:O	1.82	0.78
5:E:310:TYR:CE1	5:E:322:LYS:HD2	2.18	0.78
10:J:192:GLU:O	10:J:196:ARG:HB2	1.83	0.78
15:N:101:CYS:CB	15:N:102:CYS:SG	2.71	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:11:PRO:HB2	19:S:165:SER:O	1.83	0.78
23:V:471:GLU:OE2	23:V:475:LYS:HE3	1.81	0.78
26:Y:16:ASP:HB3	26:Y:19:LYS:HG2	1.65	0.78
1:A:168:PRO:HG2	1:A:559:ASP:HB3	1.64	0.78
1:A:664:HIS:NE2	1:A:666:LYS:HD3	1.98	0.78
6:F:50:A:OP1	12:L:165:LYS:CD	2.31	0.78
8:H:31:G:O3'	25:X:17:LEU:HG	1.82	0.78
38:l:20:LEU:HD22	38:l:24:TYR:CE2	2.18	0.78
12:L:18:ILE:HD11	12:L:152:LEU:CD2	2.14	0.78
19:S:149:SER:O	24:W:100:ARG:NH1	2.17	0.78
24:W:137:TYR:HE1	24:W:158:GLU:HB3	1.44	0.78
26:Y:23:LEU:O	26:Y:25:LEU:N	2.17	0.78
8:H:40:C:C5'	26:Y:22:LYS:CB	2.61	0.78
3:C:677:GLU:OE2	3:C:684:LYS:HG2	1.83	0.78
3:C:906:ILE:CD1	29:u:179:ARG:HH12	1.96	0.78
8:H:153:A:H2'	8:H:154:C:H5'	1.65	0.78
12:L:59:LYS:CG	12:L:91:ARG:NH1	2.47	0.78
20:T:306:CYS:SG	20:T:336:VAL:HB	2.22	0.78
3:C:471:ASP:H	3:C:499:GLY:HA2	1.47	0.78
7:G:-1:G:O3'	26:Y:4:ARG:CD	2.31	0.78
14:M:152:LEU:HD23	14:M:160:PHE:CZ	2.17	0.78
19:S:11:PRO:HB3	19:S:166:GLY:CA	2.14	0.78
19:S:60:PHE:HE2	24:W:97:ASN:HA	1.45	0.78
1:A:2286:VAL:CA	27:Z:696:PHE:O	2.32	0.78
5:E:266:PRO:CG	12:L:785:GLN:HB2	2.11	0.78
8:H:177:A:H5''	8:H:178:A:OP1	1.84	0.78
20:T:267:ASP:HB3	20:T:269:GLN:HG2	1.64	0.78
23:V:455:PHE:CZ	23:V:489:LEU:HB2	2.17	0.78
24:W:166:THR:OG1	24:W:169:GLU:HB3	1.84	0.78
8:H:101:U:H5''	8:H:102:U:H5'	1.64	0.78
10:J:361:ARG:HD3	14:M:161:PHE:CD2	2.18	0.78
26:Y:68:TYR:CD1	26:Y:69:LEU:HG	2.18	0.78
1:A:468:LYS:HD3	1:A:469:LYS:N	1.99	0.78
1:A:853:LYS:HG2	7:G:148:U:C5	2.19	0.78
3:C:750:LEU:O	3:C:754:VAL:HG23	1.84	0.78
20:T:292:TYR:CZ	20:T:308:ARG:HG3	2.18	0.78
26:Y:138:GLU:CB	27:Z:1097:MET:CA	2.62	0.78
1:A:758:ARG:HG2	17:P:227:TYR:CD2	2.19	0.77
23:V:537:HIS:O	23:V:578:SER:OG	2.00	0.77
24:W:101:THR:HG22	24:W:104:MET:HG2	1.66	0.77
38:e:20:LEU:HD22	38:e:24:TYR:CE2	2.18	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:805:GLU:CD	17:P:194:PHE:HZ	1.92	0.77
7:G:135:G:N2	7:G:136:U:N3	2.33	0.77
33:h:47:THR:CB	40:o:65:ARG:NH2	2.47	0.77
1:A:456:LEU:O	1:A:460:LYS:HG2	1.84	0.77
3:C:906:ILE:CD1	29:u:179:ARG:NH1	2.47	0.77
5:E:74:PHE:CD1	5:E:81:LEU:CD2	2.67	0.77
1:A:1494:TYR:CB	1:A:1744:ARG:CD	2.62	0.77
6:F:80:G:H5''	6:F:81:C:OP2	1.84	0.77
12:L:180:ARG:O	12:L:184:ALA:N	2.16	0.77
23:V:528:ILE:HA	23:V:531:GLU:CG	2.15	0.77
6:F:22:A:C6	24:W:130:ARG:HG2	2.20	0.77
20:T:352:THR:CG2	20:T:373:LYS:C	2.58	0.77
23:V:515:CYS:SG	23:V:522:MET:HA	2.24	0.77
37:m:70:LEU:HD22	37:m:71:TYR:HD2	1.50	0.77
1:A:362:ARG:O	1:A:362:ARG:NE	2.18	0.77
1:A:461:HIS:NE2	2:B:23:C:C6	2.53	0.77
6:F:35:A:P	12:L:203:LYS:HD2	2.25	0.77
8:H:32:U:P	25:X:17:LEU:CD1	2.72	0.77
12:L:154:GLU:CB	26:Y:49:TYR:HE2	1.96	0.77
20:T:434:GLY:HA2	20:T:464:GLY:CA	2.14	0.77
38:e:48:ILE:HD11	38:e:59:ASP:HB2	1.66	0.77
3:C:470:PRO:HA	3:C:499:GLY:HA2	1.67	0.77
25:X:12:TRP:HZ2	26:Y:35:LEU:HD22	1.48	0.77
25:X:41:GLN:N	25:X:41:GLN:HE21	1.82	0.77
1:A:1791:HIS:CE1	1:A:1799:THR:CG2	2.68	0.77
5:E:162:ARG:NH2	5:E:204:THR:HA	1.99	0.77
7:G:22:C:O2'	7:G:23:U:OP1	2.03	0.77
18:R:67:ILE:HG22	18:R:69:VAL:HG23	1.65	0.77
19:S:9:TRP:HE3	19:S:11:PRO:HD3	1.49	0.77
19:S:10:GLN:HA	19:S:29:TRP:CZ2	2.20	0.77
19:S:13:ASN:HA	19:S:25:LEU:O	1.85	0.77
26:Y:68:TYR:HE2	26:Y:94:GLU:CB	1.98	0.77
39:g:35:ASP:HB2	39:g:36:PRO:HD2	1.67	0.77
1:A:152:ARG:HH11	1:A:152:ARG:CB	1.96	0.76
1:A:299:ILE:HD13	1:A:1342:TRP:CZ3	2.21	0.76
12:L:18:ILE:HG23	12:L:37:LEU:CD2	2.15	0.76
16:O:177:GLU:OE1	16:O:177:GLU:N	2.18	0.76
18:R:181:PRO:O	18:R:182:SER:HB2	1.84	0.76
20:T:387:PHE:CE1	20:T:398:TRP:CD1	2.72	0.76
3:C:711:ARG:HD3	3:C:730:ARG:CZ	2.16	0.76
6:F:22:A:C8	24:W:130:ARG:CZ	2.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:71:GLY:O	24:W:93:PHE:HB2	1.86	0.76
1:A:230:PHE:N	1:A:414:ARG:O	2.18	0.76
3:C:471:ASP:OD1	3:C:472:GLY:N	2.19	0.76
12:L:161:ASN:OD1	12:L:168:LYS:HE3	1.86	0.76
18:R:181:PRO:O	24:W:112:SER:O	2.02	0.76
20:T:318:ARG:HG3	20:T:319:THR:HG23	1.67	0.76
23:V:497:CYS:CB	23:V:507:PHE:CG	2.68	0.76
24:W:179:LYS:O	24:W:200:VAL:CG2	2.33	0.76
38:l:48:ILE:HD11	38:l:59:ASP:HB2	1.66	0.76
1:A:1320:LYS:CE	1:A:1526:LEU:HA	2.14	0.76
16:O:21:PRO:O	24:W:110:MET:CE	2.29	0.76
23:V:548:ALA:HB1	23:V:586:PHE:N	2.00	0.76
1:A:1790:ILE:HG23	1:A:1800:THR:HG22	1.67	0.76
12:L:59:LYS:HE2	12:L:91:ARG:HH12	1.49	0.76
37:f:70:LEU:HD22	37:f:71:TYR:HD2	1.50	0.76
1:A:852:VAL:CG2	7:G:148:U:O2	2.33	0.76
3:C:125:ASN:O	3:C:126:SER:OG	2.04	0.76
3:C:705:VAL:HB	3:C:717:PHE:HE2	1.48	0.76
4:D:151:LYS:C	4:D:155:LYS:H	1.90	0.76
5:E:267:PHE:CD1	12:L:788:TYR:CE2	2.72	0.76
6:F:49:G:H1'	26:Y:51:TYR:HE2	1.49	0.76
7:G:2:U:C2	7:G:142:U:H1'	2.21	0.76
16:O:292:ILE:HG12	16:O:297:ARG:HA	1.66	0.76
19:S:34:LYS:HE3	19:S:78:TYR:HE2	1.47	0.76
23:V:457:ARG:HH21	23:V:457:ARG:HG3	1.51	0.76
12:L:161:ASN:OD1	12:L:168:LYS:CE	2.34	0.76
12:L:145:ASP:OD1	12:L:146:GLU:CD	2.29	0.76
28:q:8:SER:O	28:q:9:ASN:CB	2.34	0.76
1:A:623:LYS:CB	46:A:3000:IHP:O34	2.33	0.76
1:A:853:LYS:HE2	7:G:148:U:C6	2.13	0.76
3:C:445:ALA:HB3	3:C:466:SER:HA	1.66	0.76
5:E:267:PHE:HE2	11:K:194:GLU:HB3	1.13	0.76
12:L:191:LEU:C	12:L:196:ILE:HD11	2.10	0.76
19:S:101:ALA:HB1	24:W:95:PRO:CD	2.16	0.76
33:h:45:ASN:OD1	40:o:16:THR:CB	2.34	0.76
1:A:203:VAL:HG21	1:A:237:THR:CG2	2.14	0.76
1:A:1321:GLU:HG2	45:4:29:ALA:O	1.86	0.76
1:A:1504:GLU:CB	1:A:1752:GLN:HB3	2.16	0.76
7:G:19:G:H21	16:O:196:GLN:HG3	1.49	0.76
10:J:198:ALA:HB1	12:L:160:ALA:CA	2.14	0.76
10:J:203:LEU:HD13	10:J:204:GLU:H	1.49	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:152:LEU:CD2	14:M:160:PHE:CE1	2.70	0.76
18:R:66:GLU:OE2	18:R:66:GLU:N	2.19	0.76
24:W:178:ARG:CG	24:W:199:TYR:HE1	1.98	0.76
1:A:630:TRP:O	1:A:632:ALA:N	2.18	0.75
1:A:1889:LEU:HD11	1:A:2012:LEU:HG	1.68	0.75
5:E:231:MET:HB3	5:E:262:TRP:CZ3	2.21	0.75
9:I:720:ILE:O	9:I:721:LYS:CB	2.34	0.75
12:L:191:LEU:CD2	13:y:57:VAL:CG2	2.54	0.75
25:X:35:LYS:O	25:X:38:GLU:HG3	1.86	0.75
39:n:35:ASP:HB2	39:n:36:PRO:HD2	1.67	0.75
1:A:1503:TRP:HZ3	1:A:1533:ARG:CZ	1.98	0.75
3:C:711:ARG:CD	3:C:730:ARG:HE	1.99	0.75
5:E:258:THR:HG22	5:E:260:ARG:HG2	1.68	0.75
6:F:40:U:O2'	6:F:41:A:H5'	1.85	0.75
14:M:162:PRO:HB3	14:M:167:LEU:CB	2.16	0.75
19:S:20:MET:HE2	19:S:141:ARG:HB3	1.69	0.75
26:Y:158:LYS:HA	26:Y:163:ARG:HG3	1.68	0.75
36:d:50:LYS:HG2	36:d:74:TRP:HB3	1.68	0.75
1:A:47:GLU:HB2	1:A:50:LYS:HZ2	0.95	0.75
6:F:86:U:HO2'	6:F:87:C:P	2.08	0.75
7:G:5:G:C6	7:G:6:A:N6	2.55	0.75
7:G:134:U:H3	8:H:42:G:H1	1.31	0.75
1:A:229:GLN:HG2	1:A:415:SER:HB2	1.68	0.75
1:A:588:LEU:O	1:A:1551:PHE:CE1	2.40	0.75
1:A:1320:LYS:NZ	1:A:1526:LEU:CD2	1.78	0.75
3:C:482:TYR:HE2	3:C:493:PHE:CB	1.98	0.75
8:H:143:A:H3'	8:H:143:A:N3	2.00	0.75
23:V:449:GLU:HB3	23:V:452:LEU:CG	2.16	0.75
29:u:278:THR:HG21	29:u:347:SER:HB2	1.69	0.75
1:A:73:HIS:NE2	1:A:81:PHE:CZ	2.51	0.75
1:A:299:ILE:HD11	3:C:921:LEU:HD13	1.67	0.75
8:H:32:U:P	25:X:17:LEU:HD12	2.26	0.75
8:H:32:U:OP1	25:X:17:LEU:CG	2.34	0.75
12:L:156:ARG:O	12:L:160:ALA:N	2.18	0.75
16:O:253:TYR:HE1	19:S:93:THR:OG1	1.70	0.75
23:V:264:ILE:HG13	23:V:274:CYS:SG	2.26	0.75
25:X:37:ILE:CA	25:X:40:LEU:CD1	2.63	0.75
26:Y:16:ASP:OD1	26:Y:18:SER:OG	2.05	0.75
6:F:22:A:C8	24:W:130:ARG:NE	2.55	0.75
7:G:2:U:N3	7:G:142:U:O2	2.20	0.75
8:H:98:G:H1	37:m:41:ASN:HD21	1.34	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:70:ALA:O	18:R:71:GLN:O	2.05	0.75
1:A:1530:PRO:HG2	1:A:1533:ARG:CB	2.17	0.75
5:E:277:PHE:HE2	5:E:300:ILE:CD1	1.98	0.75
12:L:59:LYS:HG2	12:L:91:ARG:HH12	1.50	0.75
19:S:57:ILE:HG23	24:W:99:PHE:CG	2.21	0.75
24:W:126:GLU:CD	24:W:130:ARG:HH12	1.95	0.75
1:A:1570:LYS:HE2	1:A:1574:ILE:CD1	2.17	0.75
3:C:593:GLU:HG3	3:C:594:PRO:HD2	1.67	0.75
12:L:39:HIS:CD2	12:L:151:MET:HE3	2.20	0.75
19:S:9:TRP:HZ2	19:S:44:ARG:HD3	1.52	0.75
1:A:1504:GLU:HB2	1:A:1754:TYR:OH	1.86	0.75
3:C:69:ALA:HA	20:T:456:PRO:HG3	1.68	0.75
6:F:8:C:H5''	6:F:8:C:C6	2.19	0.75
24:W:140:ASP:N	24:W:153:ILE:HG12	2.02	0.75
1:A:168:PRO:CG	1:A:559:ASP:CB	2.64	0.74
1:A:666:LYS:CB	1:A:668:VAL:HG23	2.17	0.74
1:A:676:ARG:NH2	6:F:70:A:OP2	2.20	0.74
18:R:129:ASP:HB2	18:R:132:LEU:CD2	2.17	0.74
24:W:178:ARG:HD2	24:W:199:TYR:CD1	2.20	0.74
24:W:198:LYS:O	24:W:199:TYR:O	2.04	0.74
36:d:107:ILE:HG22	36:d:108:VAL:HG23	1.69	0.74
1:A:203:VAL:CG2	1:A:237:THR:CG2	2.65	0.74
3:C:508:LYS:O	3:C:566:THR:HG22	1.86	0.74
5:E:119:THR:HG21	5:E:161:ARG:CB	2.17	0.74
6:F:34:G:N2	7:G:13:C:C2	2.54	0.74
10:J:195:LEU:HD21	12:L:24:MET:HE3	1.69	0.74
16:O:20:PHE:CD1	18:R:177:ILE:CD1	2.70	0.74
6:F:1:G:O2'	15:N:99:ASN:ND2	2.20	0.74
8:H:153:A:C2'	8:H:154:C:H5'	2.17	0.74
19:S:9:TRP:CZ2	19:S:44:ARG:HD3	2.20	0.74
23:V:152:LEU:HA	23:V:387:MET:HE1	1.69	0.74
28:q:66:PRO:HD3	28:r:11:VAL:HG11	1.68	0.74
1:A:176:LEU:HD13	1:A:181:ASN:HD22	1.52	0.74
1:A:452:LYS:NZ	2:B:48:A:OP1	2.20	0.74
12:L:141:PRO:HG2	12:L:144:MET:HA	1.68	0.74
24:W:88:MET:CE	24:W:89:PHE:HD2	2.00	0.74
24:W:137:TYR:CB	24:W:159:ALA:HB2	2.18	0.74
24:W:140:ASP:CA	24:W:153:ILE:CD1	2.66	0.74
1:A:1320:LYS:NZ	1:A:1526:LEU:CG	2.42	0.74
3:C:449:ILE:CG2	3:C:457:VAL:HG11	2.04	0.74
3:C:510:LEU:HD22	3:C:514:TYR:CE2	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:406:PHE:CD2	10:J:411:MET:CE	2.70	0.74
19:S:131:ARG:NH1	19:S:132:VAL:O	2.20	0.74
36:k:107:ILE:HG22	36:k:108:VAL:HG23	1.69	0.74
1:A:1570:LYS:CE	1:A:1574:ILE:HD12	2.16	0.74
3:C:452:THR:O	3:C:577:PHE:HA	1.88	0.74
5:E:267:PHE:CE2	11:K:194:GLU:C	2.64	0.74
7:G:145:U:H3'	7:G:145:U:H6	1.53	0.74
19:S:119:THR:OG1	19:S:122:LEU:HD12	1.86	0.74
26:Y:138:GLU:C	27:Z:1096:GLY:O	2.31	0.74
1:A:76:MET:HE2	1:A:88:TYR:CD2	2.21	0.74
1:A:919:ASP:OD2	1:A:1012:LYS:HE3	1.88	0.74
5:E:287:ASN:O	5:E:289:LEU:HD23	1.88	0.74
1:A:1771:LEU:CD2	1:A:1930:TYR:HB2	2.15	0.74
3:C:348:TYR:CE1	3:C:359:LYS:HB3	2.22	0.74
5:E:243:LEU:HD11	5:E:247:GLY:HA2	1.68	0.74
7:G:20:A:H1'	16:O:193:LEU:HD21	1.70	0.74
7:G:151:C:OP1	7:G:151:C:H4'	1.85	0.74
1:A:366:LYS:O	1:A:368:GLN:N	2.21	0.74
1:A:760:ARG:NE	1:A:766:THR:OG1	2.19	0.74
15:N:40:LYS:C	15:N:41:ARG:HG3	2.13	0.74
16:O:247:ASP:OD2	16:O:294:ASN:ND2	2.21	0.74
24:W:135:TYR:CE2	24:W:165:LEU:CD1	2.70	0.74
26:Y:46:CYS:SG	50:Y:400:ZN:ZN	1.77	0.74
10:J:183:ALA:HB3	12:L:142:ILE:HG12	1.68	0.73
19:S:100:MET:CG	19:S:108:ASN:OD1	2.36	0.73
1:A:853:LYS:CE	7:G:148:U:C4	2.69	0.73
1:A:1570:LYS:HE2	1:A:1574:ILE:HD12	1.68	0.73
3:C:449:ILE:HG22	3:C:457:VAL:CG1	2.17	0.73
3:C:519:GLU:N	3:C:519:GLU:OE2	2.21	0.73
18:R:67:ILE:HG22	18:R:69:VAL:CG2	2.17	0.73
24:W:101:THR:HG23	24:W:104:MET:H	1.52	0.73
26:Y:75:ARG:CD	26:Y:77:TYR:OH	2.34	0.73
26:Y:165:ALA:HB3	26:Y:168:ASP:HB2	1.70	0.73
41:p:66:LEU:HD12	41:p:81:ILE:HG22	1.70	0.73
1:A:1502:PHE:CE2	1:A:1505:LYS:HB3	2.23	0.73
8:H:106:G:H4'	8:H:107:A:O4'	1.89	0.73
14:M:121:ASP:O	14:M:122:LEU:HD13	1.87	0.73
19:S:131:ARG:NH1	19:S:133:CYS:CA	2.51	0.73
23:V:515:CYS:HA	23:V:521:TYR:CB	2.17	0.73
36:k:50:LYS:HG2	36:k:74:TRP:HB3	1.68	0.73
1:A:1498:TRP:O	1:A:1501:LEU:HD12	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:131:THR:HG21	24:W:108:ARG:CG	2.17	0.73
19:S:131:ARG:HD3	19:S:132:VAL:C	2.09	0.73
20:T:385:TYR:O	20:T:400:PHE:HB2	1.88	0.73
31:w:109:ARG:HG3	31:w:110:THR:N	2.03	0.73
1:A:700:GLY:HA3	18:R:237:MET:HB2	1.69	0.73
1:A:758:ARG:HG2	17:P:227:TYR:CE2	2.23	0.73
3:C:516:LEU:CD1	3:C:517:GLU:HG3	2.18	0.73
6:F:43:A:C2'	6:F:44:G:C5'	2.66	0.73
7:G:6:A:H2'	7:G:7:G:C8	2.23	0.73
19:S:81:GLN:HA	19:S:108:ASN:O	1.88	0.73
26:Y:71:LEU:N	26:Y:71:LEU:HD12	2.03	0.73
26:Y:75:ARG:HD2	26:Y:77:TYR:CE1	2.23	0.73
1:A:47:GLU:CA	1:A:50:LYS:HZ1	1.97	0.73
3:C:680:ASN:OD1	3:C:682:LYS:HB2	1.86	0.73
25:X:41:GLN:HE21	25:X:41:GLN:CA	2.00	0.73
5:E:250:LEU:HD23	5:E:250:LEU:O	1.88	0.73
8:H:36:G:H1'	26:Y:4:ARG:NH2	2.02	0.73
8:H:153:A:H2'	8:H:154:C:C5'	2.19	0.73
24:W:154:GLY:O	24:W:156:VAL:CG2	2.35	0.73
1:A:853:LYS:HE2	7:G:148:U:H5	0.85	0.73
17:P:188:TRP:CE3	17:P:189:ASP:HB2	2.23	0.73
24:W:101:THR:O	24:W:102:GLN:C	2.30	0.73
25:X:5:ASP:HB3	25:X:8:LEU:HD12	1.69	0.73
26:Y:54:LYS:HD3	26:Y:56:PHE:CZ	2.23	0.73
26:Y:158:LYS:CA	26:Y:163:ARG:HG3	2.19	0.73
29:u:275:LEU:HG	29:u:348:LEU:HD23	1.71	0.73
24:W:212:GLU:C	24:W:214:LYS:H	1.97	0.73
26:Y:68:TYR:CE1	26:Y:69:LEU:CG	2.67	0.73
36:k:110:LEU:HD11	37:m:59:LEU:HB3	1.70	0.73
1:A:260:LEU:HD23	1:A:455:VAL:HG22	1.70	0.73
1:A:1495:PHE:CE1	1:A:1748:ARG:NE	2.56	0.73
3:C:711:ARG:CD	3:C:730:ARG:HH11	2.01	0.73
7:G:147:C:H5'	7:G:148:U:OP2	1.88	0.73
10:J:186:GLU:HA	10:J:186:GLU:OE2	1.88	0.73
23:V:603:LEU:HD12	23:V:639:LEU:HD13	1.71	0.73
25:X:6:LEU:CD2	26:Y:55:LYS:HE2	2.16	0.73
37:f:70:LEU:HD22	37:f:71:TYR:CD2	2.23	0.73
1:A:901:LEU:CD1	1:A:904:HIS:CE1	2.71	0.72
7:G:150:U:C2'	7:G:151:C:H5''	2.19	0.72
12:L:141:PRO:HG2	12:L:143:ASP:O	1.89	0.72
18:R:135:PRO:O	18:R:136:ASP:CG	2.32	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:58:GLU:O	25:X:61:GLY:HA3	1.89	0.72
33:h:47:THR:CB	40:o:65:ARG:HH22	2.02	0.72
1:A:381:PRO:HD2	3:C:334:ILE:CG2	2.19	0.72
1:A:799:PRO:HD3	18:R:284:PHE:CD1	2.23	0.72
5:E:74:PHE:HE2	5:E:343:ILE:HG12	1.54	0.72
5:E:146:ARG:HH12	5:E:148:LYS:HE3	1.50	0.72
6:F:5:U:H3'	6:F:7:G:H5''	1.71	0.72
24:W:162:ASN:HD22	24:W:165:LEU:HD22	1.49	0.72
30:v:99:ILE:HD12	30:v:101:PHE:CE1	2.24	0.72
6:F:22:A:C8	24:W:130:ARG:NH2	2.57	0.72
7:G:120:G:HO2'	7:G:121:G:C1'	2.00	0.72
1:A:1320:LYS:HZ3	1:A:1526:LEU:HD22	1.40	0.72
3:C:89:LEU:HD23	3:C:89:LEU:C	2.14	0.72
3:C:705:VAL:CG2	3:C:717:PHE:CD2	2.69	0.72
10:J:180:LYS:HB3	12:L:143:ASP:OD2	1.89	0.72
37:m:70:LEU:HD22	37:m:71:TYR:CD2	2.23	0.72
1:A:730:GLY:O	18:R:248:PRO:HG2	1.89	0.72
1:A:856:LEU:N	1:A:856:LEU:HD23	2.03	0.72
8:H:106:G:H21	8:H:107:A:N6	1.87	0.72
10:J:180:LYS:CB	12:L:143:ASP:OD2	2.36	0.72
12:L:158:ARG:CZ	26:Y:51:TYR:OH	2.37	0.72
16:O:235:TYR:HD1	16:O:271:PHE:HE1	1.37	0.72
23:V:449:GLU:HB3	23:V:452:LEU:HG	1.69	0.72
23:V:487:LYS:NZ	23:V:491:ASN:CG	2.47	0.72
24:W:140:ASP:CB	24:W:153:ILE:HG21	2.19	0.72
24:W:140:ASP:CB	24:W:153:ILE:CG1	2.68	0.72
36:d:110:LEU:HD11	37:f:59:LEU:HB3	1.69	0.72
1:A:300:ASN:C	3:C:939:ARG:HH21	1.97	0.72
1:A:462:ARG:HD2	1:A:462:ARG:N	2.05	0.72
16:O:131:THR:CG2	24:W:108:ARG:HD3	2.20	0.72
19:S:57:ILE:HG23	24:W:99:PHE:CB	2.19	0.72
24:W:140:ASP:CB	24:W:153:ILE:CD1	2.67	0.72
1:A:150:MET:SD	1:A:153:ARG:NH2	2.62	0.72
5:E:119:THR:HG21	5:E:161:ARG:HB3	1.72	0.72
16:O:137:LEU:HD11	24:W:104:MET:SD	2.30	0.72
16:O:240:GLY:HA3	16:O:296:ARG:HH12	1.55	0.72
1:A:1258:LYS:HG3	1:A:1527:ASN:HD21	1.55	0.72
1:A:1527:ASN:HD22	7:G:149:G:H22	1.32	0.72
3:C:671:SER:O	3:C:672:LEU:HD13	1.89	0.72
18:R:76:MET:HG2	19:S:95:ALA:CB	2.19	0.72
24:W:139:LEU:HD12	24:W:139:LEU:H	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:203:VAL:HG23	1:A:237:THR:HG21	1.72	0.72
1:A:684:GLU:OE1	20:T:266:GLU:OE1	2.08	0.72
12:L:154:GLU:CB	26:Y:49:TYR:CE2	2.73	0.72
23:V:548:ALA:HB3	23:V:585:ILE:CB	2.19	0.72
24:W:137:TYR:HD1	24:W:158:GLU:HB2	1.51	0.72
24:W:155:SER:O	24:W:156:VAL:HG23	1.90	0.72
25:X:34:ARG:HA	25:X:37:ILE:HD11	1.70	0.72
1:A:193:LEU:HD12	1:A:194:GLU:H	1.55	0.72
1:A:434:HIS:ND1	1:A:435:CYS:SG	2.62	0.72
8:H:179:C:H2'	8:H:180:G:H8	1.53	0.72
24:W:101:THR:O	24:W:104:MET:N	2.22	0.72
26:Y:20:ILE:HD13	26:Y:20:ILE:N	2.04	0.72
3:C:250:ARG:HE	3:C:451:HIS:CD2	2.07	0.71
1:A:155:LYS:CE	1:A:624:GLY:O	2.38	0.71
1:A:855:ARG:C	1:A:856:LEU:HD23	2.14	0.71
7:G:4:A:H2'	7:G:5:G:O4'	1.89	0.71
8:H:10:C:C5	14:M:198:ARG:CZ	2.73	0.71
18:R:74:LEU:HD13	19:S:136:ILE:CG2	2.20	0.71
23:V:584:LYS:HG3	23:V:634:ILE:HG12	1.71	0.71
24:W:491:GLN:O	24:W:493:ARG:N	2.23	0.71
26:Y:67:VAL:HB	26:Y:71:LEU:O	1.90	0.71
26:Y:109:GLN:O	26:Y:111:GLU:N	2.21	0.71
1:A:1527:ASN:ND2	7:G:149:G:C2	2.55	0.71
12:L:38:LEU:HA	12:L:151:MET:HE1	1.73	0.71
12:L:176:LEU:HD13	12:L:176:LEU:C	2.15	0.71
23:V:540:GLU:OE1	23:V:541:THR:N	2.24	0.71
24:W:162:ASN:CB	24:W:165:LEU:CD2	2.63	0.71
30:v:72:THR:HG21	30:v:94:ILE:CD1	2.16	0.71
3:C:726:LEU:HD12	3:C:726:LEU:O	1.89	0.71
6:F:68:C:C5	20:T:285:HIS:CD2	2.78	0.71
20:T:434:GLY:CA	20:T:464:GLY:HA2	2.19	0.71
23:V:468:ASP:O	23:V:506:PHE:CE2	2.43	0.71
1:A:121:HIS:HE2	1:A:481:PHE:HB3	1.52	0.71
1:A:549:GLU:OE1	1:A:552:ARG:NH1	2.23	0.71
1:A:1953:ILE:HD11	1:A:1986:LEU:CD1	2.19	0.71
5:E:264:VAL:HA	5:E:272:ARG:HH21	1.55	0.71
29:u:275:LEU:O	29:u:275:LEU:HD23	1.90	0.71
7:G:2:U:O2'	13:y:2:ALA:N	2.21	0.71
12:L:18:ILE:CD1	12:L:152:LEU:CD2	2.68	0.71
19:S:11:PRO:HB3	19:S:165:SER:C	2.15	0.71
19:S:88:PRO:O	19:S:91:LYS:HE3	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:549:LYS:O	23:V:552:ALA:HB3	1.91	0.71
26:Y:19:LYS:C	26:Y:20:ILE:CG1	2.57	0.71
1:A:76:MET:CE	1:A:506:LEU:HD11	2.21	0.71
1:A:107:PRO:O	1:A:111:GLU:OE1	2.08	0.71
6:F:59:G:O2'	6:F:60:C:OP1	2.09	0.71
1:A:1321:GLU:OE1	45:4:25:ALA:O	2.08	0.71
23:V:536:ILE:HG22	23:V:579:SER:CB	2.21	0.71
1:A:73:HIS:NE2	1:A:81:PHE:CD1	2.59	0.71
1:A:264:PHE:CE2	1:A:459:LEU:CD1	2.73	0.71
1:A:1370:ARG:NH1	23:V:506:PHE:CG	2.59	0.71
1:A:1949:ARG:HD2	1:A:1986:LEU:HD21	1.72	0.71
18:R:312:MET:HA	18:R:312:MET:CE	2.21	0.71
1:A:181:ASN:O	1:A:185:VAL:HG22	1.90	0.71
1:A:673:THR:O	1:A:677:VAL:HG23	1.91	0.71
3:C:700:ILE:HA	3:C:705:VAL:CG1	2.21	0.71
23:V:536:ILE:O	23:V:578:SER:CB	2.39	0.71
1:A:229:GLN:CG	1:A:415:SER:HB2	2.21	0.70
3:C:706:GLN:HE21	3:C:708:THR:H	1.38	0.70
19:S:102:ASN:C	24:W:94:GLY:HA2	2.16	0.70
1:A:81:PHE:O	1:A:83:HIS:N	2.24	0.70
3:C:508:LYS:HB3	3:C:566:THR:HG23	1.72	0.70
8:H:154:C:H2'	8:H:155:C:C6	2.26	0.70
10:J:353:GLU:OE1	10:J:358:GLU:HB3	1.91	0.70
1:A:76:MET:CE	1:A:88:TYR:CG	2.70	0.70
1:A:155:LYS:CE	1:A:624:GLY:C	2.64	0.70
3:C:474:LEU:HD23	3:C:474:LEU:C	2.16	0.70
9:I:296:PHE:CA	9:I:305:SER:CB	2.66	0.70
23:V:514:PHE:O	23:V:521:TYR:CG	2.44	0.70
24:W:140:ASP:HB3	24:W:153:ILE:CB	2.21	0.70
29:u:69:ILE:O	29:u:73:ILE:HG12	1.91	0.70
1:A:1084:PRO:HG2	17:P:188:TRP:CE3	2.27	0.70
3:C:93:ILE:HD11	20:T:240:LEU:HD23	1.70	0.70
3:C:490:PHE:CZ	3:C:612:LYS:HD2	2.26	0.70
3:C:678:THR:HG21	3:C:683:ASN:ND2	2.06	0.70
7:G:141:C:C2'	7:G:142:U:H5'	2.21	0.70
19:S:10:GLN:HB3	19:S:29:TRP:CE3	2.27	0.70
1:A:748:ASP:OD1	17:P:214:THR:CG2	2.40	0.70
3:C:457:VAL:CB	3:C:462:GLY:HA3	2.22	0.70
3:C:679:PRO:HG2	3:C:807:GLN:OE1	1.91	0.70
5:E:267:PHE:HE2	11:K:194:GLU:HB2	1.51	0.70
18:R:189:ASN:HD21	18:R:195:ARG:NH2	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:449:GLU:CG	23:V:452:LEU:HD12	2.21	0.70
26:Y:25:LEU:HD22	26:Y:25:LEU:N	2.05	0.70
1:A:126:ILE:HG21	18:R:207:MET:HE2	1.74	0.70
1:A:481:PHE:CD2	18:R:205:ASP:HA	2.27	0.70
6:F:41:A:H61	7:G:6:A:H62	1.37	0.70
6:F:87:C:OP2	14:M:193:ARG:HA	1.92	0.70
7:G:135:G:C2	7:G:136:U:C4	2.79	0.70
20:T:267:ASP:O	20:T:268:LYS:HG3	1.91	0.70
25:X:12:TRP:CZ2	26:Y:35:LEU:HD21	2.24	0.70
1:A:1775:GLN:CG	1:A:1859:LYS:HG3	2.22	0.70
3:C:196:LYS:CB	34:b:7:SER:OG	2.35	0.70
5:E:74:PHE:CE2	5:E:343:ILE:CG1	2.73	0.70
7:G:-2:C:H3'	7:G:-1:G:H5''	1.74	0.70
12:L:14:THR:HG23	12:L:152:LEU:CD1	2.21	0.70
19:S:60:PHE:CE2	24:W:98:PRO:HD3	2.25	0.70
1:A:671:THR:OG1	6:F:69:A:OP1	2.08	0.70
8:H:106:G:C5'	36:k:47:ARG:HH22	2.05	0.70
16:O:137:LEU:HD21	24:W:104:MET:HE1	1.74	0.70
1:A:228:TRP:O	1:A:415:SER:CA	2.39	0.70
6:F:22:A:H8	24:W:130:ARG:NH2	1.90	0.70
7:G:1:G:N2	7:G:1:G:OP2	2.23	0.70
10:J:181:ASN:HD22	10:J:181:ASN:H	1.40	0.70
13:y:31:PHE:CG	13:y:32:LEU:N	2.60	0.70
23:V:637:GLY:O	23:V:644:ARG:NH2	2.25	0.70
1:A:1504:GLU:CB	1:A:1754:TYR:HE1	2.05	0.70
7:G:150:U:C3'	7:G:151:C:H5''	2.22	0.70
17:P:66:ARG:HB2	17:P:66:ARG:HH11	1.55	0.70
20:T:366:VAL:HG21	20:T:402:ASP:HA	1.72	0.70
22:U:1:MET:SD	22:U:1:MET:N	2.54	0.70
26:Y:134:MET:HE3	26:Y:134:MET:CA	2.14	0.70
1:A:76:MET:SD	1:A:88:TYR:CG	2.85	0.69
1:A:645:THR:HB	1:A:646:PRO:HD3	1.74	0.69
1:A:1498:TRP:HA	1:A:1501:LEU:CD1	2.21	0.69
6:F:40:U:C2'	6:F:41:A:H5'	2.21	0.69
7:G:6:A:H2'	7:G:7:G:C1'	2.22	0.69
10:J:191:ALA:O	10:J:192:GLU:C	2.34	0.69
14:M:152:LEU:O	14:M:156:HIS:CD2	2.45	0.69
16:O:144:SER:HA	16:O:148:LEU:HD13	1.73	0.69
19:S:58:LYS:N	24:W:99:PHE:HE2	1.89	0.69
3:C:736:GLY:CA	3:C:770:PHE:CE2	2.75	0.69
7:G:146:C:H1'	8:H:33:G:N2	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:191:LEU:C	12:L:196:ILE:CD1	2.66	0.69
1:A:1553:VAL:CG1	26:Y:7:LEU:CD1	2.69	0.69
3:C:449:ILE:HD11	3:C:466:SER:HA	1.74	0.69
18:R:232:SEP:HA	18:R:232:SEP:O1P	1.92	0.69
23:V:468:ASP:O	23:V:506:PHE:HE2	1.74	0.69
1:A:71:ARG:HD2	1:A:177:ASP:OD2	1.92	0.69
1:A:794:TYR:OH	1:A:989:ASP:OD2	2.07	0.69
1:A:850:TYR:OH	1:A:863:GLU:CG	2.41	0.69
1:A:1868:MET:HE2	1:A:1872:LEU:HD11	1.73	0.69
13:y:54:SER:C	13:y:57:VAL:HG22	2.17	0.69
30:v:119:GLU:OE1	30:v:119:GLU:HA	1.91	0.69
1:A:1503:TRP:O	1:A:1504:GLU:HG3	1.91	0.69
6:F:33:G:H5''	6:F:33:G:H8	1.57	0.69
5:E:267:PHE:HD1	12:L:788:TYR:CD2	2.11	0.69
23:V:477:LEU:HD21	23:V:514:PHE:HE1	1.54	0.69
24:W:123:PHE:CZ	24:W:168:PHE:CD2	2.80	0.69
1:A:121:HIS:ND1	1:A:481:PHE:O	2.25	0.69
1:A:293:TRP:HZ3	1:A:295:GLU:OE1	1.76	0.69
1:A:1870:ASP:HB2	1:A:1871:PRO:HD3	1.75	0.69
8:H:150:U:H3	8:H:181:G:H1	1.41	0.69
9:I:600:ALA:CA	12:L:505:ARG:CB	2.71	0.69
12:L:172:ARG:NH1	26:Y:82:ARG:HA	2.08	0.69
16:O:197:ASN:OD1	16:O:198:ILE:N	2.24	0.69
17:P:72:ARG:NH1	17:P:72:ARG:HB2	2.08	0.69
19:S:39:PHE:HB2	19:S:129:PHE:HZ	1.10	0.69
24:W:201:ASP:OD1	24:W:201:ASP:N	2.23	0.69
1:A:76:MET:HE3	1:A:506:LEU:HD11	1.74	0.69
1:A:377:GLU:O	1:A:378:PHE:HB3	1.91	0.69
1:A:384:VAL:HG12	3:C:331:PHE:CG	2.28	0.69
1:A:853:LYS:CD	7:G:148:U:C5	2.74	0.69
1:A:880:ARG:HG3	1:A:881:ILE:N	2.06	0.69
1:A:1083:HIS:NE2	17:P:189:ASP:OD1	2.22	0.69
3:C:725:ASP:OD1	3:C:728:ALA:N	2.25	0.69
6:F:88:G:H4'	14:M:121:ASP:HB2	1.75	0.69
8:H:153:A:N6	8:H:177:A:C2	2.60	0.69
10:J:353:GLU:OE1	10:J:358:GLU:CB	2.41	0.69
18:R:103:ARG:HH11	18:R:103:ARG:CB	2.04	0.69
19:S:102:ASN:ND2	19:S:104:GLY:O	2.26	0.69
1:A:76:MET:HE1	1:A:88:TYR:CB	2.22	0.69
3:C:482:TYR:CE2	3:C:493:PHE:HB2	2.28	0.69
3:C:709:TRP:HB3	3:C:713:LYS:HD2	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:152:G:O3'	8:H:153:A:O4'	2.11	0.69
25:X:5:ASP:HB3	25:X:8:LEU:CD1	2.21	0.69
1:A:338:VAL:CG2	3:C:867:PRO:HG3	2.23	0.69
1:A:721:LYS:O	1:A:1022:MET:HE3	1.93	0.69
1:A:1364:LEU:HD12	23:V:461:LEU:HB3	1.75	0.69
3:C:87:GLN:OE1	3:C:91:GLU:HG2	1.92	0.69
5:E:266:PRO:HG2	12:L:785:GLN:CB	2.20	0.69
7:G:20:A:H1'	16:O:193:LEU:CD2	2.22	0.69
18:R:76:MET:HE3	19:S:140:ASN:OD1	1.93	0.69
1:A:1493:THR:HG22	1:A:1747:ILE:CG2	2.21	0.68
3:C:705:VAL:HG23	3:C:717:PHE:CE2	2.27	0.68
5:E:74:PHE:CD1	5:E:81:LEU:HD23	2.28	0.68
5:E:146:ARG:HH12	5:E:148:LYS:CE	1.99	0.68
12:L:135:LYS:HZ3	12:L:136:PRO:HD2	1.58	0.68
16:O:26:THR:OG1	16:O:159:ARG:NH2	2.25	0.68
20:T:314:ILE:HD12	20:T:324:HIS:HB2	1.75	0.68
20:T:455:GLN:HG3	20:T:485:THR:HG21	1.76	0.68
5:E:178:LEU:CD1	5:E:222:LEU:CD2	2.70	0.68
5:E:264:VAL:HA	5:E:272:ARG:NH2	2.07	0.68
7:G:16:G:O2'	7:G:17:U:OP2	2.10	0.68
16:O:262:THR:HB	16:O:271:PHE:HB2	1.73	0.68
18:R:81:LYS:HZ2	18:R:81:LYS:CA	2.04	0.68
18:R:106:GLN:CG	18:R:110:LYS:HE2	2.22	0.68
24:W:140:ASP:HB3	24:W:153:ILE:HG12	1.74	0.68
1:A:1501:LEU:O	45:4:28:ALA:CB	2.41	0.68
1:A:1953:ILE:CD1	1:A:1986:LEU:CD1	2.71	0.68
2:B:21:A:O3'	2:B:22:U:H4'	1.94	0.68
3:C:256:CYS:SG	3:C:308:CYS:HB2	2.33	0.68
3:C:737:PRO:HG3	3:C:774:THR:OG1	1.93	0.68
24:W:88:MET:SD	24:W:89:PHE:HB2	2.33	0.68
26:Y:22:LYS:H	26:Y:22:LYS:HE3	1.57	0.68
3:C:452:THR:HB	3:C:577:PHE:CD2	2.27	0.68
10:J:360:ASP:O	10:J:363:ARG:HG3	1.93	0.68
12:L:158:ARG:HB3	12:L:158:ARG:HH11	1.58	0.68
26:Y:134:MET:HE3	26:Y:137:LEU:HD12	1.75	0.68
29:u:73:ILE:HD11	29:u:95:SER:HA	1.75	0.68
36:k:33:THR:HG22	36:k:37:LYS:HE2	1.76	0.68
1:A:1495:PHE:CE1	1:A:1748:ARG:HD3	2.29	0.68
1:A:1768:TYR:CD2	1:A:2012:LEU:CD2	2.77	0.68
3:C:452:THR:CG2	3:C:577:PHE:CD2	2.72	0.68
6:F:22:A:C5	24:W:130:ARG:HG2	2.29	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:18:ILE:HG13	12:L:152:LEU:HD21	1.74	0.68
12:L:59:LYS:CE	12:L:91:ARG:HH12	2.07	0.68
23:V:547:VAL:O	23:V:550:MET:N	2.27	0.68
24:W:178:ARG:CG	24:W:199:TYR:CE1	2.76	0.68
1:A:277:PRO:HA	1:A:448:GLN:CG	2.24	0.68
1:A:700:GLY:C	1:A:701:ILE:HD13	2.19	0.68
1:A:1881:ASN:OD1	45:4:11:ALA:CB	2.40	0.68
2:B:90:U:O4'	33:a:66:SER:HB3	1.92	0.68
6:F:42:C:H2'	6:F:43:A:O4'	1.93	0.68
10:J:214:ILE:H	10:J:214:ILE:HD12	1.59	0.68
14:M:145:ASP:HB2	14:M:148:THR:OG1	1.93	0.68
17:P:188:TRP:CZ3	17:P:189:ASP:HB2	2.28	0.68
23:V:536:ILE:HG23	23:V:579:SER:CB	2.21	0.68
30:v:92:ILE:CG2	30:v:94:ILE:HG23	2.21	0.68
34:b:18:ARG:NH1	34:b:52:LYS:HB2	2.09	0.68
1:A:439:GLN:NE2	1:A:614:TYR:OH	2.27	0.68
10:J:353:GLU:OE2	10:J:361:ARG:NH2	2.27	0.68
18:R:262:ILE:HG13	18:R:263:PRO:HD2	1.76	0.68
25:X:48:ARG:O	25:X:51:GLU:CB	2.41	0.68
1:A:255:PHE:HE1	1:A:432:ARG:O	1.75	0.68
3:C:360:ALA:H	3:C:361:PRO:HD3	1.59	0.68
3:C:705:VAL:CB	3:C:717:PHE:CE2	2.76	0.68
5:E:108:HIS:CE1	5:E:128:SER:CB	2.77	0.68
6:F:40:U:H2'	6:F:41:A:H5'	1.75	0.68
8:H:101:U:O4'	33:h:66:SER:HB3	1.92	0.68
12:L:59:LYS:CD	12:L:91:ARG:HH12	2.05	0.68
12:L:59:LYS:CG	12:L:91:ARG:HH12	2.06	0.68
26:Y:158:LYS:HA	26:Y:163:ARG:HG2	1.74	0.68
1:A:1813:ARG:HB3	1:A:1813:ARG:CZ	2.24	0.68
3:C:736:GLY:CA	3:C:770:PHE:HE2	2.07	0.68
4:D:166:ASP:O	4:D:169:TYR:N	2.26	0.68
6:F:41:A:C6	6:F:42:C:N4	2.61	0.68
12:L:154:GLU:HG3	12:L:155:ALA:N	2.06	0.68
1:A:44:ARG:HD2	1:A:45:TYR:CE2	2.28	0.68
1:A:91:ALA:O	1:A:93:LYS:N	2.27	0.68
1:A:203:VAL:CG2	1:A:237:THR:HG21	2.23	0.68
1:A:298:ASP:O	1:A:302:ILE:HG12	1.94	0.68
1:A:1771:LEU:HD23	1:A:1930:TYR:HB2	1.75	0.68
3:C:350:ASN:CG	3:C:353:THR:HG23	2.19	0.68
6:F:31:U:C2'	6:F:32:U:H5'	2.24	0.68
6:F:35:A:OP1	12:L:203:LYS:CD	2.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:135:G:N2	7:G:136:U:H3	1.92	0.68
17:P:63:LEU:O	17:P:63:LEU:HD23	1.94	0.68
18:R:88:ILE:CG2	18:R:96:ILE:CG2	2.71	0.68
19:S:58:LYS:N	24:W:99:PHE:CE2	2.61	0.68
1:A:1772:PHE:CD2	1:A:1813:ARG:HD2	2.22	0.67
3:C:482:TYR:CE2	3:C:493:PHE:CB	2.77	0.67
8:H:143:A:H2'	8:H:144:C:H6	1.59	0.67
26:Y:22:LYS:H	26:Y:22:LYS:CD	2.05	0.67
1:A:171:ASP:OD2	1:A:519:ASP:OD2	2.12	0.67
1:A:1738:PRO:HG3	1:A:1839:TRP:CE2	2.29	0.67
3:C:453:TYR:CZ	3:C:575:GLN:HB2	2.28	0.67
3:C:705:VAL:CG2	3:C:717:PHE:CE2	2.77	0.67
15:N:102:CYS:SG	50:N:202:ZN:ZN	1.81	0.67
19:S:34:LYS:CE	19:S:78:TYR:CE2	2.77	0.67
20:T:185:MET:CB	20:T:186:PRO:HD3	2.24	0.67
20:T:272:CYS:HB3	20:T:282:ARG:HG3	1.77	0.67
23:V:330:LYS:O	23:V:333:GLN:HG3	1.94	0.67
23:V:548:ALA:HB1	23:V:585:ILE:CB	2.25	0.67
1:A:663:ARG:NH1	6:F:64:U:OP2	2.27	0.67
1:A:1528:GLN:OE1	1:A:1528:GLN:HA	1.94	0.67
1:A:1580:HIS:CE1	26:Y:17:PRO:CG	2.77	0.67
3:C:534:VAL:HG12	3:C:535:ALA:H	1.59	0.67
5:E:243:LEU:HD12	5:E:247:GLY:HA2	1.76	0.67
5:E:246:GLU:HB2	5:E:248:SER:OG	1.94	0.67
6:F:40:U:H2'	6:F:41:A:C5'	2.25	0.67
7:G:27:U:H2'	7:G:28:A:O5'	1.94	0.67
7:G:151:C:H1'	7:G:152:C:H5'	1.77	0.67
8:H:168:A:C8	8:H:168:A:C5'	2.75	0.67
24:W:140:ASP:CB	24:W:153:ILE:HG12	2.24	0.67
34:i:18:ARG:NH1	34:i:52:LYS:HB2	2.09	0.67
1:A:134:TRP:HB3	1:A:418:THR:CG2	2.25	0.67
1:A:162:LYS:HZ2	1:A:1690:ASP:HB2	1.60	0.67
5:E:66:GLU:HB2	5:E:87:ASP:OD2	1.94	0.67
1:A:122:ILE:CD1	1:A:483:GLN:HG3	2.24	0.67
1:A:228:TRP:O	1:A:416:GLY:N	2.26	0.67
1:A:852:VAL:CG2	1:A:1449:LYS:HD2	2.21	0.67
1:A:1352:HIS:CD2	22:U:5:ILE:HD13	2.30	0.67
1:A:1504:GLU:OE2	1:A:1752:GLN:CD	2.37	0.67
6:F:50:A:OP1	12:L:165:LYS:HD3	1.95	0.67
7:G:-1:G:H4'	7:G:1:G:O2'	1.94	0.67
23:V:225:LYS:HG2	23:V:405:ILE:HG12	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:48:GLU:CD	26:Y:80:CYS:SG	2.77	0.67
1:A:464:PRO:HG2	2:B:20:G:H2'	1.77	0.67
1:A:1772:PHE:HE2	1:A:1813:ARG:NE	1.86	0.67
7:G:-12:G:H4'	7:G:-11:G:OP1	1.94	0.67
8:H:156:U:C6	8:H:156:U:C5'	2.72	0.67
12:L:166:LYS:HE3	12:L:170:LYS:HZ1	1.56	0.67
19:S:10:GLN:HB3	19:S:29:TRP:CD2	2.30	0.67
6:F:27:A:O2'	6:F:28:A:C8	2.48	0.67
7:G:2:U:O2	7:G:142:U:H1'	1.95	0.67
7:G:138:A:OP2	7:G:138:A:O4'	2.12	0.67
8:H:151:C:H2'	8:H:152:G:H8	1.60	0.67
10:J:191:ALA:C	10:J:193:GLN:N	2.52	0.67
13:y:14:ARG:HB3	26:Y:20:ILE:HG21	1.77	0.67
24:W:139:LEU:HD12	24:W:139:LEU:N	2.08	0.67
25:X:5:ASP:HB3	25:X:8:LEU:CG	2.24	0.67
29:u:335:ASP:OD1	29:u:364:ARG:HD2	1.95	0.67
1:A:344:ASP:N	1:A:344:ASP:OD1	2.28	0.67
1:A:980:ARG:CG	1:A:1094:ARG:HD2	2.24	0.67
1:A:1341:ARG:NH2	1:A:1342:TRP:CH2	2.63	0.67
1:A:1495:PHE:CE1	1:A:1748:ARG:CD	2.78	0.67
3:C:510:LEU:HD22	3:C:514:TYR:CD2	2.30	0.67
25:X:28:GLN:HA	25:X:28:GLN:OE1	1.93	0.67
31:w:106:LEU:HD23	31:w:113:LEU:HD23	1.77	0.67
1:A:339:PHE:CE1	1:A:406:TRP:HE3	2.12	0.67
1:A:1761:PRO:O	1:A:1762:TYR:O	2.12	0.67
8:H:75:A:H61	8:H:77:C:H42	1.43	0.67
8:H:153:A:C3'	8:H:154:C:H5'	2.25	0.67
12:L:178:GLU:O	12:L:181:ARG:CG	2.43	0.67
24:W:123:PHE:CE1	24:W:168:PHE:CE2	2.83	0.67
26:Y:108:PHE:HD1	26:Y:109:GLN:H	1.43	0.67
38:l:20:LEU:HD12	39:n:41:VAL:HG13	1.77	0.67
1:A:254:TYR:OH	1:A:434:HIS:HB3	1.95	0.67
3:C:568:PRO:O	3:C:569:ARG:HB3	1.94	0.67
16:O:137:LEU:HD12	16:O:140:ALA:HB3	1.76	0.67
19:S:150:GLN:CA	24:W:100:ARG:HH21	1.99	0.67
24:W:101:THR:HG22	24:W:104:MET:CG	2.24	0.67
24:W:156:VAL:HG12	24:W:160:GLU:OE1	1.94	0.67
1:A:89:LEU:HD22	1:A:656:LEU:HD22	1.76	0.66
1:A:229:GLN:HA	1:A:414:ARG:O	1.94	0.66
3:C:221:ILE:CG1	3:C:479:THR:OG1	2.43	0.66
3:C:244:LYS:CB	3:C:292:TYR:CE2	2.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:445:ALA:C	3:C:449:ILE:HG13	2.20	0.66
3:C:508:LYS:HE3	3:C:566:THR:HG21	1.77	0.66
15:N:125:LYS:CD	24:W:167:VAL:O	2.34	0.66
18:R:78:ARG:H	18:R:78:ARG:CD	2.05	0.66
26:Y:70:GLY:C	26:Y:71:LEU:HD12	2.20	0.66
36:d:33:THR:HG22	36:d:37:LYS:HE2	1.76	0.66
1:A:83:HIS:CE1	7:G:16:G:O6	2.47	0.66
1:A:1504:GLU:CB	1:A:1754:TYR:CE1	2.78	0.66
25:X:50:ARG:O	25:X:52:GLU:N	2.28	0.66
34:i:18:ARG:NH1	34:i:52:LYS:CB	2.58	0.66
1:A:171:ASP:O	1:A:520:TYR:CG	2.44	0.66
1:A:1993:LYS:HD2	1:A:1993:LYS:O	1.95	0.66
2:B:19:A:H2'	2:B:20:G:H5''	1.78	0.66
7:G:5:G:C6	7:G:6:A:C6	2.84	0.66
8:H:151:C:C2	8:H:152:G:C8	2.83	0.66
8:H:151:C:O2	8:H:152:G:C8	2.48	0.66
12:L:200:LYS:O	12:L:201:LYS:HB2	1.95	0.66
1:A:155:LYS:HD2	1:A:626:GLY:O	1.96	0.66
3:C:114:TYR:CE1	35:c:12:HIS:HB3	2.30	0.66
7:G:7:G:O2'	7:G:8:C:H5'	1.95	0.66
7:G:150:U:H2'	7:G:151:C:O4'	1.95	0.66
14:M:194:ASP:C	14:M:196:TYR:N	2.45	0.66
18:R:113:TYR:OH	20:T:402:ASP:O	2.13	0.66
19:S:77:ILE:HG13	19:S:78:TYR:HD1	1.59	0.66
38:e:20:LEU:HD12	39:g:41:VAL:HG13	1.77	0.66
1:A:76:MET:SD	1:A:88:TYR:CD1	2.88	0.66
3:C:572:GLU:HG3	3:C:573:GLU:H	1.60	0.66
6:F:31:U:O2'	6:F:32:U:H5'	1.95	0.66
16:O:243:ILE:HG12	16:O:294:ASN:HD22	1.60	0.66
7:G:141:C:H2'	7:G:142:U:H5'	1.76	0.66
18:R:88:ILE:H	18:R:88:ILE:HD12	1.61	0.66
18:R:124:VAL:HG13	18:R:125:MET:H	1.60	0.66
18:R:132:LEU:HD23	18:R:132:LEU:H	1.60	0.66
34:b:18:ARG:NH1	34:b:52:LYS:CB	2.58	0.66
6:F:85:U:H3'	6:F:86:U:H5'	1.77	0.66
7:G:146:C:C2	8:H:33:G:C2	2.83	0.66
16:O:28:LEU:HD23	18:R:195:ARG:HE	1.61	0.66
18:R:74:LEU:CB	19:S:136:ILE:HG21	2.26	0.66
20:T:355:ARG:C	20:T:356:LEU:HD12	2.20	0.66
23:V:279:THR:O	23:V:283:GLU:HG3	1.95	0.66
26:Y:70:GLY:O	26:Y:71:LEU:HG	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:116:HIS:O	5:E:124:LEU:HD12	1.95	0.66
7:G:13:C:H2'	7:G:14:A:C8	2.31	0.66
18:R:69:VAL:O	19:S:93:THR:CG2	2.43	0.66
1:A:245:LEU:HA	1:A:430:TRP:CZ2	2.28	0.66
1:A:630:TRP:O	1:A:631:ALA:C	2.37	0.66
1:A:1488:THR:HB	1:A:1537:TRP:O	1.96	0.66
1:A:1495:PHE:CE1	1:A:1748:ARG:CZ	2.79	0.66
1:A:1758:PRO:CG	45:4:8:GLY:O	2.44	0.66
3:C:389:ASP:OD1	3:C:389:ASP:N	2.26	0.66
7:G:147:C:O5'	7:G:148:U:OP2	2.14	0.66
20:T:342:GLU:HB3	20:T:343:PRO:CD	2.26	0.66
26:Y:134:MET:CE	26:Y:137:LEU:HD12	2.26	0.66
40:o:5:THR:HG22	40:o:8:LEU:H	1.60	0.66
1:A:75:ASP:OD1	1:A:75:ASP:N	2.26	0.66
1:A:232:LEU:HD21	3:C:412:ILE:HD11	1.77	0.66
3:C:363:SER:O	3:C:364:SER:OG	2.11	0.66
3:C:750:LEU:C	3:C:750:LEU:HD12	2.21	0.66
8:H:11:G:N7	14:M:198:ARG:NH1	2.43	0.66
13:y:14:ARG:NH2	26:Y:22:LYS:HB3	2.10	0.66
1:A:339:PHE:CD1	1:A:406:TRP:CE3	2.84	0.65
14:M:152:LEU:O	14:M:156:HIS:HD2	1.79	0.65
24:W:137:TYR:CD1	24:W:158:GLU:CB	2.79	0.65
1:A:282:LEU:C	1:A:282:LEU:HD23	2.20	0.65
3:C:457:VAL:HB	3:C:462:GLY:HA3	1.78	0.65
3:C:463:GLU:OE1	3:C:463:GLU:N	2.30	0.65
5:E:108:HIS:CE1	5:E:128:SER:HB3	2.31	0.65
7:G:6:A:O2'	7:G:7:G:O4'	2.15	0.65
12:L:178:GLU:HG3	12:L:181:ARG:CD	2.26	0.65
17:P:30:TYR:OH	18:R:164:PRO:HD3	1.96	0.65
17:P:66:ARG:HH11	17:P:66:ARG:CB	2.09	0.65
24:W:128:GLN:OE1	24:W:139:LEU:HD11	1.94	0.65
1:A:95:MET:HE2	1:A:503:MET:CE	2.26	0.65
1:A:151:MET:SD	1:A:628:GLY:C	2.80	0.65
1:A:845:ARG:HH22	1:A:1439:ARG:CB	1.99	0.65
12:L:30:GLN:OE1	12:L:33:ARG:NE	2.28	0.65
23:V:320:ARG:HH12	23:V:340:PHE:HE1	1.33	0.65
24:W:123:PHE:CZ	24:W:168:PHE:CE2	2.84	0.65
30:v:122:ARG:HG2	30:v:122:ARG:HH11	1.61	0.65
8:H:32:U:OP1	25:X:17:LEU:CB	2.44	0.65
8:H:114:A:H61	8:H:142:C:H42	1.44	0.65
10:J:204:GLU:HG3	10:J:204:GLU:O	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:459:LEU:HD12	20:T:460:ASP:H	1.61	0.65
23:V:330:LYS:NZ	29:u:47:GLU:HG3	2.12	0.65
1:A:300:ASN:HB3	3:C:939:ARG:HH21	1.62	0.65
1:A:380:LEU:O	3:C:354:ARG:HG3	1.97	0.65
1:A:853:LYS:CG	7:G:148:U:C5	2.77	0.65
5:E:178:LEU:HD11	5:E:222:LEU:CD2	2.26	0.65
12:L:59:LYS:HD3	12:L:91:ARG:NH1	2.10	0.65
16:O:147:LEU:O	16:O:151:ALA:N	2.29	0.65
24:W:178:ARG:HD2	24:W:199:TYR:HD1	1.62	0.65
1:A:225:TYR:O	1:A:418:THR:OG1	2.11	0.65
1:A:377:GLU:O	1:A:378:PHE:CB	2.44	0.65
3:C:482:TYR:HE2	3:C:493:PHE:CD2	2.14	0.65
3:C:700:ILE:HG21	3:C:741:GLY:O	1.97	0.65
5:E:153:PHE:O	5:E:171:SER:HB2	1.97	0.65
19:S:61:MET:HE1	24:W:95:PRO:HG3	1.78	0.65
12:L:141:PRO:CG	12:L:143:ASP:O	2.44	0.65
12:L:172:ARG:HH12	26:Y:81:THR:C	2.05	0.65
20:T:327:SER:O	20:T:357:TRP:HH2	1.80	0.65
1:A:853:LYS:HG3	7:G:148:U:C4	2.32	0.65
1:A:1210:LYS:O	1:A:1212:GLY:N	2.29	0.65
1:A:1578:ARG:O	1:A:1579:ALA:HB3	1.97	0.65
3:C:824:THR:O	3:C:824:THR:CG2	2.45	0.65
7:G:21:A:N6	16:O:92:LEU:HD23	2.12	0.65
1:A:175:PRO:HG2	1:A:498:ARG:CZ	2.27	0.65
1:A:853:LYS:HE3	7:G:148:U:C4	2.30	0.65
1:A:1758:PRO:HG2	45:4:8:GLY:C	2.22	0.65
3:C:66:TYR:CD2	20:T:457:GLY:HA2	2.32	0.65
4:D:152:GLU:O	4:D:156:GLU:CA	2.45	0.65
7:G:-23:G:N2	29:u:356:ASN:HD22	1.94	0.65
12:L:181:ARG:NH2	12:L:185:LEU:CD2	2.60	0.65
18:R:171:LEU:CD1	18:R:201:GLU:CD	2.70	0.65
19:S:9:TRP:HE3	19:S:11:PRO:CD	2.10	0.65
20:T:439:TRP:CZ3	20:T:446:ASN:HB2	2.31	0.65
36:k:32:LEU:HD22	36:k:65:MET:HE3	1.79	0.65
1:A:97:HIS:HD2	1:A:473:PHE:CZ	2.15	0.64
1:A:378:PHE:CD1	1:A:379:GLU:N	2.65	0.64
1:A:380:LEU:HD23	3:C:349:PHE:HE1	1.55	0.64
1:A:748:ASP:OD1	17:P:214:THR:HG23	1.96	0.64
3:C:476:CYS:CB	3:C:565:ILE:HB	2.27	0.64
3:C:680:ASN:HD21	3:C:682:LYS:HG3	1.62	0.64
6:F:43:A:O2'	6:F:44:G:H5'	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:68:THR:HA	16:O:83:THR:HG22	1.77	0.64
18:R:76:MET:HE1	19:S:136:ILE:CD1	2.26	0.64
1:A:1320:LYS:CE	1:A:1526:LEU:CD2	2.53	0.64
1:A:1764:SER:OG	1:A:1765:SER:N	2.28	0.64
16:O:196:GLN:HE21	16:O:208:PRO:HG2	1.61	0.64
26:Y:158:LYS:O	26:Y:163:ARG:HB2	1.97	0.64
1:A:379:GLU:CB	3:C:354:ARG:O	2.45	0.64
1:A:1772:PHE:HE2	1:A:1813:ARG:HE	1.41	0.64
5:E:277:PHE:HE2	5:E:300:ILE:HD13	1.61	0.64
7:G:8:C:OP1	12:L:200:LYS:HE3	1.97	0.64
8:H:36:G:C1'	26:Y:4:ARG:NH2	2.60	0.64
8:H:153:A:H3'	8:H:154:C:H5'	1.79	0.64
12:L:59:LYS:HD3	12:L:91:ARG:HH11	1.62	0.64
19:S:13:ASN:HD22	19:S:24:VAL:HG11	1.62	0.64
1:A:387:PHE:CD1	3:C:327:TYR:CE1	2.85	0.64
3:C:96:PRO:HB3	20:T:276:GLU:OE2	1.98	0.64
3:C:482:TYR:CE2	3:C:493:PHE:CD2	2.86	0.64
18:R:232:SEP:O1P	18:R:233:PRO:HD3	1.97	0.64
18:R:303:GLU:O	18:R:307:GLN:CD	2.40	0.64
20:T:458:SER:OG	20:T:459:LEU:N	2.30	0.64
22:U:20:GLN:HE22	23:V:478:LYS:HD2	1.62	0.64
23:V:452:LEU:N	23:V:452:LEU:HD23	2.13	0.64
25:X:5:ASP:HB3	25:X:8:LEU:HG	1.79	0.64
1:A:435:CYS:HB3	7:G:-11:G:H22	1.62	0.64
1:A:661:GLU:CD	18:R:214:ILE:HD11	2.22	0.64
1:A:792:HIS:CE1	18:R:279:HIS:HE1	2.14	0.64
1:A:1868:MET:CE	1:A:1872:LEU:HD11	2.27	0.64
2:B:12:U:O2'	2:B:13:C:O5'	2.15	0.64
3:C:86:THR:O	20:T:239:LYS:O	2.15	0.64
3:C:680:ASN:ND2	3:C:682:LYS:HG3	2.12	0.64
12:L:38:LEU:HA	12:L:151:MET:CE	2.28	0.64
16:O:22:ILE:HG23	24:W:112:SER:HB3	1.79	0.64
16:O:253:TYR:OH	19:S:91:LYS:HB3	1.97	0.64
19:S:10:GLN:OE1	19:S:10:GLN:N	2.31	0.64
24:W:137:TYR:HB2	24:W:159:ALA:HB2	1.79	0.64
1:A:155:LYS:HZ1	1:A:624:GLY:C	1.88	0.64
1:A:271:MET:HE1	1:A:313:LYS:HD2	1.78	0.64
1:A:1524:SER:O	1:A:1528:GLN:N	2.31	0.64
3:C:256:CYS:SG	3:C:308:CYS:CB	2.86	0.64
3:C:452:THR:HG22	3:C:577:PHE:CD2	2.29	0.64
3:C:678:THR:HG21	3:C:683:ASN:HB2	1.76	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:126:C:H4'	7:G:127:U:OP2	1.97	0.64
10:J:183:ALA:O	12:L:141:PRO:HA	1.98	0.64
23:V:455:PHE:HZ	23:V:489:LEU:CB	2.06	0.64
26:Y:160:LEU:HD23	26:Y:161:ASN:H	1.62	0.64
1:A:134:TRP:HB3	1:A:418:THR:HG21	1.79	0.64
3:C:473:PRO:O	3:C:474:LEU:HB3	1.96	0.64
3:C:488:VAL:HG13	3:C:609:LYS:NZ	2.12	0.64
7:G:153:C:H3'	7:G:153:C:H6	1.61	0.64
24:W:140:ASP:CA	24:W:153:ILE:CG1	2.74	0.64
26:Y:42:ARG:HG3	26:Y:49:TYR:CE1	2.33	0.64
3:C:62:ASP:OD1	3:C:62:ASP:N	2.28	0.64
6:F:45:A:C5	26:Y:34:ARG:NH2	2.66	0.64
8:H:147:G:H2'	8:H:148:C:H6	1.62	0.64
10:J:203:LEU:CD1	10:J:204:GLU:N	2.58	0.64
10:J:203:LEU:CD1	10:J:204:GLU:H	2.11	0.64
12:L:168:LYS:O	12:L:172:ARG:HG3	1.98	0.64
16:O:276:THR:HG23	16:O:279:ALA:H	1.62	0.64
18:R:119:LEU:C	18:R:119:LEU:HD13	2.23	0.64
19:S:60:PHE:CE2	24:W:98:PRO:CD	2.81	0.64
26:Y:2:SER:O	26:Y:3:GLU:HG3	1.98	0.64
1:A:176:LEU:HD13	1:A:181:ASN:ND2	2.12	0.64
1:A:338:VAL:O	3:C:266:GLU:CG	2.46	0.64
1:A:1211:ASP:O	1:A:1213:VAL:N	2.30	0.64
1:A:1930:TYR:CD1	25:X:71:ASP:CB	2.80	0.64
3:C:481:MET:SD	3:C:492:ALA:HB2	2.37	0.64
3:C:572:GLU:HG3	3:C:573:GLU:N	2.12	0.64
5:E:178:LEU:HD21	5:E:208:ILE:CD1	2.28	0.64
6:F:42:C:C2'	6:F:43:A:C8	2.75	0.64
8:H:32:U:C5'	25:X:17:LEU:HD12	2.24	0.64
16:O:115:GLU:HB3	18:R:218:ILE:HG21	1.80	0.64
18:R:110:LYS:HD2	18:R:110:LYS:C	2.23	0.64
23:V:493:ILE:HD13	23:V:510:LEU:CD2	2.26	0.64
26:Y:130:LEU:O	26:Y:134:MET:HG2	1.98	0.64
1:A:299:ILE:CD1	3:C:921:LEU:HD13	2.27	0.64
1:A:468:LYS:HD3	1:A:469:LYS:H	1.61	0.64
1:A:1758:PRO:CG	45:4:8:GLY:C	2.71	0.64
2:B:95:G:H5'	37:f:25:TRP:CH2	2.21	0.64
6:F:85:U:H3'	6:F:86:U:C5'	2.28	0.64
7:G:130:A:O5'	7:G:130:A:H8	1.81	0.64
8:H:164:C:H6	8:H:164:C:H5'	1.63	0.64
9:I:600:ALA:C	12:L:505:ARG:CB	2.71	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:M:160:PHE:C	14:M:162:PRO:HD3	2.22	0.64
24:W:210:GLU:OE1	24:W:210:GLU:N	2.31	0.64
25:X:60:VAL:H	25:X:61:GLY:HA2	1.63	0.64
3:C:350:ASN:ND2	3:C:353:THR:HG23	2.13	0.63
7:G:150:U:H3'	7:G:151:C:H5''	1.80	0.63
1:A:481:PHE:CE2	18:R:205:ASP:CA	2.81	0.63
1:A:1527:ASN:CB	7:G:149:G:H22	2.11	0.63
3:C:456:GLY:O	3:C:457:VAL:HG22	1.99	0.63
6:F:22:A:N6	24:W:130:ARG:HG2	2.14	0.63
10:J:192:GLU:C	10:J:195:LEU:HD12	2.23	0.63
10:J:406:PHE:CG	10:J:411:MET:HE2	2.33	0.63
16:O:224:ASP:O	16:O:302:TRP:NE1	2.31	0.63
5:E:146:ARG:CZ	5:E:148:LYS:HE3	2.27	0.63
5:E:251:LEU:HG	5:E:291:CYS:SG	2.39	0.63
10:J:192:GLU:C	10:J:195:LEU:CD1	2.70	0.63
18:R:67:ILE:HD13	18:R:67:ILE:N	2.13	0.63
24:W:97:ASN:C	24:W:99:PHE:H	2.06	0.63
3:C:65:TYR:HD2	17:P:216:ARG:HD3	1.63	0.63
12:L:61:THR:CG2	12:L:91:ARG:HH22	2.11	0.63
12:L:191:LEU:O	12:L:196:ILE:CD1	2.44	0.63
18:R:179:TYR:HD1	24:W:115:ALA:HB2	1.61	0.63
18:R:262:ILE:CG2	18:R:267:ARG:NH1	2.61	0.63
36:d:32:LEU:HD22	36:d:65:MET:HE3	1.79	0.63
1:A:663:ARG:NH2	6:F:65:G:N7	2.47	0.63
1:A:1416:ILE:HB	1:A:1417:PRO:HD3	1.78	0.63
1:A:1848:LEU:HD22	1:A:1914:MET:HE3	1.80	0.63
3:C:452:THR:CB	3:C:577:PHE:HD2	2.12	0.63
18:R:76:MET:CE	19:S:136:ILE:HD11	2.28	0.63
26:Y:19:LYS:O	26:Y:20:ILE:CB	2.47	0.63
31:w:125:LYS:HG3	31:w:126:GLU:N	2.12	0.63
1:A:165:ARG:NH2	1:A:1690:ASP:OD2	2.31	0.63
7:G:4:A:C6	7:G:5:G:C5	2.86	0.63
7:G:148:U:O2'	7:G:149:G:OP2	2.17	0.63
12:L:13:ASN:ND2	12:L:139:PRO:HA	2.13	0.63
31:w:123:THR:HG1	31:w:126:GLU:HG3	1.62	0.63
1:A:109:PRO:HD3	1:A:630:TRP:CZ2	2.33	0.63
1:A:1502:PHE:HE2	1:A:1505:LYS:HB3	1.63	0.63
15:N:54:HIS:CD2	24:W:196:TRP:CZ3	2.81	0.63
16:O:78:LYS:O	16:O:97:ARG:NH2	2.32	0.63
18:R:262:ILE:HG13	18:R:263:PRO:CD	2.28	0.63
1:A:1094:ARG:HH11	1:A:1094:ARG:HB2	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:856:HIS:CE1	29:u:102:ILE:HG22	2.33	0.63
6:F:35:A:C5'	6:F:35:A:H8	2.12	0.63
12:L:61:THR:HG23	12:L:91:ARG:HH22	1.62	0.63
14:M:152:LEU:HD23	14:M:160:PHE:HZ	1.64	0.63
23:V:477:LEU:HD21	23:V:514:PHE:CE1	2.34	0.63
24:W:140:ASP:CB	24:W:153:ILE:HG23	2.23	0.63
2:B:32:C:OP1	17:P:33:ARG:CZ	2.47	0.63
3:C:497:LEU:HD11	3:C:577:PHE:CZ	2.32	0.63
6:F:6:C:OP2	6:F:6:C:H4'	1.99	0.63
7:G:2:U:H1'	13:y:2:ALA:N	2.14	0.63
10:J:204:GLU:OE1	12:L:168:LYS:HA	1.98	0.63
15:N:116:ASN:OD1	15:N:116:ASN:N	2.32	0.63
20:T:185:MET:SD	20:T:442:ARG:NH1	2.71	0.63
1:A:44:ARG:HD2	1:A:45:TYR:CZ	2.34	0.62
3:C:93:ILE:HD11	20:T:240:LEU:CD2	2.29	0.62
3:C:360:ALA:N	3:C:361:PRO:HD3	2.14	0.62
10:J:297:ASN:OD1	12:L:223:GLY:O	2.16	0.62
18:R:66:GLU:OE2	19:S:89:ASP:O	2.16	0.62
23:V:329:ASP:O	23:V:333:GLN:HG2	1.99	0.62
3:C:250:ARG:NE	3:C:451:HIS:NE2	2.47	0.62
3:C:495:ARG:HD2	3:C:497:LEU:HD23	1.81	0.62
4:D:508:GLY:HA3	49:D:2201:ADP:H8	1.64	0.62
6:F:27:A:N3	16:O:181:TYR:HE2	1.97	0.62
7:G:5:G:N3	7:G:6:A:C2	2.66	0.62
23:V:600:ASN:HA	23:V:639:LEU:HD21	1.80	0.62
30:v:9:LEU:CD1	30:v:92:ILE:HG12	2.29	0.62
1:A:203:VAL:HG21	1:A:237:THR:HG22	1.81	0.62
1:A:203:VAL:CG2	1:A:237:THR:HB	2.30	0.62
8:H:152:G:C2	8:H:153:A:C5	2.87	0.62
10:J:323:LEU:HD21	14:M:182:MET:HE2	1.82	0.62
18:R:263:PRO:CB	18:R:266:LYS:HG2	2.29	0.62
1:A:671:THR:HG1	6:F:69:A:P	2.22	0.62
3:C:675:PHE:HD1	3:C:675:PHE:H	1.47	0.62
3:C:679:PRO:HD3	3:C:811:THR:OG1	2.00	0.62
6:F:46:G:H2'	6:F:47:A:C8	2.33	0.62
7:G:150:U:H3'	7:G:150:U:H6	1.65	0.62
14:M:152:LEU:HD21	14:M:160:PHE:CE1	2.34	0.62
16:O:171:GLY:HA2	24:W:208:PRO:CD	2.29	0.62
16:O:196:GLN:NE2	16:O:209:VAL:HG23	2.14	0.62
29:u:278:THR:HG21	29:u:347:SER:CB	2.29	0.62
38:l:74:LEU:HB3	38:l:77:ILE:HD11	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:587:GLN:HA	1:A:1550:GLY:O	2.00	0.62
7:G:5:G:C5	7:G:6:A:C6	2.87	0.62
10:J:406:PHE:CE2	10:J:411:MET:CE	2.83	0.62
16:O:19:ASP:OD1	16:O:20:PHE:N	2.33	0.62
23:V:250:LYS:HD3	23:V:288:ASP:CG	2.24	0.62
25:X:58:GLU:C	25:X:61:GLY:HA3	2.25	0.62
1:A:97:HIS:CD2	1:A:473:PHE:CZ	2.87	0.62
1:A:264:PHE:CE1	1:A:455:VAL:CG1	2.75	0.62
1:A:658:ARG:HD2	1:A:663:ARG:NH2	2.14	0.62
1:A:1352:HIS:CD2	22:U:5:ILE:CD1	2.82	0.62
1:A:1553:VAL:CG1	26:Y:7:LEU:HD12	2.11	0.62
1:A:1738:PRO:HG3	1:A:1839:TRP:CD2	2.33	0.62
1:A:1873:GLU:OE1	45:4:6:ALA:C	2.41	0.62
3:C:295:ASP:OD1	3:C:297:ASN:N	2.32	0.62
3:C:701:GLU:HA	3:C:740:THR:HG1	1.64	0.62
3:C:749:THR:O	3:C:753:GLU:N	2.27	0.62
8:H:154:C:H2'	8:H:155:C:H6	1.62	0.62
10:J:203:LEU:HD13	10:J:204:GLU:CB	2.29	0.62
12:L:135:LYS:NZ	12:L:136:PRO:HD2	2.13	0.62
16:O:137:LEU:HD21	24:W:104:MET:CE	2.29	0.62
20:T:185:MET:HB3	20:T:186:PRO:HD3	1.81	0.62
23:V:549:LYS:O	23:V:552:ALA:N	2.32	0.62
38:e:74:LEU:HB3	38:e:77:ILE:HD11	1.81	0.62
1:A:731:LEU:HD12	1:A:732:PRO:HD2	1.81	0.62
1:A:1307:MET:SD	1:A:1547:VAL:HB	2.40	0.62
5:E:267:PHE:HD1	12:L:788:TYR:HE2	1.42	0.62
6:F:36:A:C2'	6:F:37:C:O5'	2.48	0.62
8:H:153:A:N6	8:H:177:A:H2	1.98	0.62
12:L:18:ILE:CG2	12:L:37:LEU:CD2	2.77	0.62
18:R:74:LEU:CD1	19:S:136:ILE:HG21	2.29	0.62
40:o:123:ASN:O	40:o:126:THR:HB	1.99	0.62
1:A:1502:PHE:HZ	1:A:1505:LYS:HD3	1.64	0.62
5:E:108:HIS:CE1	5:E:128:SER:HB2	2.35	0.62
8:H:143:A:H2'	8:H:144:C:C6	2.35	0.62
13:y:54:SER:O	13:y:57:VAL:CG2	2.47	0.62
16:O:31:ASN:OD1	16:O:33:TYR:N	2.27	0.62
20:T:349:SER:OG	20:T:351:ASP:OD1	2.18	0.62
26:Y:134:MET:N	26:Y:134:MET:SD	2.73	0.62
26:Y:165:ALA:CB	26:Y:168:ASP:HB2	2.28	0.62
1:A:919:ASP:OD2	1:A:1012:LYS:CE	2.47	0.62
1:A:1341:ARG:HH21	1:A:1342:TRP:HZ2	1.47	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1504:GLU:OE2	1:A:1752:GLN:OE1	2.17	0.62
3:C:456:GLY:C	3:C:457:VAL:HG13	2.25	0.62
5:E:277:PHE:HE2	5:E:300:ILE:HD12	1.63	0.62
6:F:45:A:H2	26:Y:57:ASN:HD21	1.44	0.62
7:G:2:U:H3	7:G:144:A:H61	1.48	0.62
7:G:145:U:H3'	7:G:145:U:C6	2.35	0.62
12:L:181:ARG:NH2	12:L:185:LEU:HD22	2.14	0.62
14:M:162:PRO:CB	14:M:167:LEU:HB2	2.27	0.62
15:N:38:GLU:C	15:N:40:LYS:H	2.08	0.62
18:R:119:LEU:HD13	18:R:119:LEU:O	1.98	0.62
18:R:281:ASN:OD1	18:R:282:GLU:N	2.33	0.62
20:T:267:ASP:O	20:T:268:LYS:CB	2.47	0.62
31:w:78:THR:HG22	31:w:145:SER:HB2	1.80	0.62
1:A:384:VAL:HA	3:C:331:PHE:CE2	2.35	0.62
1:A:697:MET:HE2	18:R:245:TRP:CZ3	2.35	0.62
5:E:119:THR:HG23	5:E:161:ARG:HB3	1.80	0.62
7:G:-3:A:O2'	7:G:-2:C:H5'	2.00	0.62
7:G:-1:G:HO3'	26:Y:4:ARG:HD2	1.65	0.62
14:M:198:ARG:HG3	14:M:198:ARG:O	2.00	0.62
18:R:77:GLY:HA2	18:R:78:ARG:NH2	2.14	0.62
23:V:575:THR:O	23:V:580:ARG:NH1	2.33	0.62
26:Y:75:ARG:CD	26:Y:77:TYR:CZ	2.77	0.62
1:A:338:VAL:HG21	3:C:867:PRO:CD	2.30	0.61
3:C:465:MET:CE	3:C:475:MET:CG	2.70	0.61
6:F:49:G:N7	12:L:33:ARG:HG3	2.15	0.61
18:R:220:ARG:HH11	18:R:220:ARG:CB	2.11	0.61
28:q:22:ASN:CB	28:r:55:ILE:CB	2.78	0.61
29:u:223:HIS:O	29:u:227:GLU:HG3	1.99	0.61
1:A:260:LEU:CD2	1:A:455:VAL:HG22	2.30	0.61
1:A:1498:TRP:HA	1:A:1501:LEU:HD11	1.82	0.61
9:I:802:ALA:HB2	26:Y:193:GLN:CB	2.31	0.61
12:L:199:GLN:HE21	12:L:199:GLN:N	1.97	0.61
13:y:47:ARG:HA	13:y:50:ILE:CG1	2.30	0.61
18:R:123:GLU:OE1	18:R:124:VAL:N	2.30	0.61
25:X:36:LYS:HZ3	25:X:36:LYS:CA	2.03	0.61
29:u:275:LEU:CD2	29:u:330:VAL:HG22	2.30	0.61
31:w:78:THR:CG2	31:w:145:SER:HB2	2.29	0.61
1:A:141:ILE:HG12	1:A:426:LEU:CD2	2.30	0.61
1:A:1495:PHE:CZ	1:A:1748:ARG:HD3	2.36	0.61
3:C:65:TYR:CD2	17:P:216:ARG:HD3	2.34	0.61
3:C:470:PRO:HA	3:C:499:GLY:CA	2.29	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:705:VAL:HG22	3:C:705:VAL:O	2.00	0.61
3:C:809:ILE:HB	3:C:810:PRO:HD3	1.82	0.61
12:L:191:LEU:CD1	13:y:57:VAL:CG2	2.60	0.61
19:S:9:TRP:CE3	19:S:11:PRO:CG	2.83	0.61
28:r:8:SER:O	28:r:9:ASN:CB	2.47	0.61
1:A:1332:HIS:ND1	1:A:1359:HIS:CE1	2.68	0.61
2:B:19:A:O2'	2:B:20:G:OP1	2.12	0.61
9:I:640:ALA:HA	10:J:512:GLU:CB	2.31	0.61
14:M:152:LEU:HD23	14:M:152:LEU:C	2.24	0.61
18:R:185:GLY:O	18:R:186:VAL:HG22	2.00	0.61
19:S:57:ILE:HG21	24:W:97:ASN:HB2	1.82	0.61
23:V:483:GLU:O	23:V:486:THR:N	2.33	0.61
24:W:210:GLU:CA	24:W:213:GLN:HB2	2.28	0.61
1:A:1772:PHE:CG	1:A:1813:ARG:CG	2.77	0.61
3:C:596:ASN:HD22	3:C:596:ASN:N	1.97	0.61
4:D:151:LYS:O	4:D:154:ARG:C	2.41	0.61
18:R:55:LEU:O	18:R:73:PRO:O	2.19	0.61
20:T:339:GLN:NE2	20:T:342:GLU:O	2.34	0.61
30:v:119:GLU:OE1	30:v:119:GLU:CA	2.49	0.61
1:A:155:LYS:HE3	1:A:624:GLY:C	2.24	0.61
6:F:51:U:OP1	26:Y:54:LYS:HA	1.99	0.61
7:G:20:A:O2'	7:G:21:A:P	2.58	0.61
24:W:290:GLY:CA	24:W:571:TRP:O	2.49	0.61
1:A:1889:LEU:HD21	1:A:1891:LEU:HD21	1.82	0.61
3:C:446:LYS:HB3	3:C:447:PRO:HD3	1.83	0.61
3:C:449:ILE:CG2	3:C:457:VAL:HG12	2.26	0.61
6:F:34:G:C5'	6:F:34:G:H8	2.14	0.61
7:G:152:C:O2'	7:G:153:C:O2	2.13	0.61
10:J:408:ASP:OD1	10:J:442:ARG:HG2	2.00	0.61
12:L:101:GLU:CD	26:Y:163:ARG:HH21	2.09	0.61
14:M:126:ASP:OD2	14:M:128:ALA:CB	2.42	0.61
24:W:126:GLU:HG2	24:W:130:ARG:CZ	2.30	0.61
26:Y:7:LEU:O	26:Y:8:ASN:CG	2.44	0.61
1:A:73:HIS:CD2	1:A:81:PHE:CD1	2.88	0.61
3:C:115:GLU:O	3:C:116:MET:C	2.43	0.61
6:F:7:G:H5'	6:F:7:G:H8	1.66	0.61
18:R:292:TYR:CD1	26:Y:167:VAL:HG21	2.35	0.61
3:C:91:GLU:OE1	3:C:91:GLU:HA	2.01	0.61
3:C:301:SER:O	3:C:304:LEU:N	2.30	0.61
12:L:146:GLU:HG2	12:L:147:ASP:OD1	2.01	0.61
20:T:292:TYR:CE2	20:T:308:ARG:HG3	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:264:ILE:HD13	23:V:269:ALA:HB3	1.81	0.61
23:V:330:LYS:NZ	29:u:50:LEU:HD23	2.11	0.61
25:X:5:ASP:CB	25:X:8:LEU:HD12	2.31	0.61
1:A:48:LYS:O	1:A:53:PHE:CG	2.54	0.61
1:A:283:VAL:HG13	1:A:284:ARG:H	1.64	0.61
1:A:1338:SER:OG	1:A:1351:THR:N	2.28	0.61
1:A:1530:PRO:HD2	1:A:1533:ARG:NH2	2.15	0.61
5:E:178:LEU:HD21	5:E:208:ILE:HD13	1.82	0.61
8:H:40:C:C5'	26:Y:22:LYS:HB2	2.18	0.61
8:H:112:G:H2'	8:H:113:G:H8	1.65	0.61
8:H:142:C:C2'	8:H:143:A:H5'	2.30	0.61
18:R:76:MET:HE1	19:S:136:ILE:HD11	1.81	0.61
18:R:171:LEU:HD12	18:R:201:GLU:CD	2.25	0.61
18:R:171:LEU:CD1	18:R:201:GLU:OE1	2.44	0.61
24:W:88:MET:HE1	24:W:89:PHE:CD2	2.30	0.61
24:W:135:TYR:HB3	24:W:137:TYR:CE1	2.35	0.61
24:W:180:LYS:HB3	24:W:199:TYR:HA	1.83	0.61
29:u:229:THR:HG23	29:u:233:MET:SD	2.41	0.61
1:A:299:ILE:HD13	1:A:1342:TRP:CE3	2.36	0.60
1:A:305:ARG:HA	1:A:305:ARG:NH1	2.09	0.60
1:A:623:LYS:CD	46:A:3000:IHP:O43	2.49	0.60
1:A:1589:ILE:HD13	1:A:1705:ILE:HD12	1.83	0.60
3:C:619:THR:C	3:C:620:LYS:HG3	2.25	0.60
8:H:10:C:C4	14:M:198:ARG:NH1	2.69	0.60
10:J:195:LEU:HD12	10:J:195:LEU:H	1.66	0.60
16:O:283:ALA:O	16:O:287:SER:OG	2.18	0.60
18:R:314:GLN:HA	18:R:314:GLN:NE2	2.16	0.60
25:X:50:ARG:C	25:X:52:GLU:N	2.57	0.60
29:u:278:THR:O	29:u:329:ARG:HD2	2.01	0.60
1:A:82:ARG:HB3	1:A:83:HIS:ND1	2.17	0.60
1:A:378:PHE:C	1:A:379:GLU:HG2	2.25	0.60
1:A:850:TYR:HE2	1:A:864:LEU:CB	2.09	0.60
3:C:478:THR:OG1	3:C:563:ALA:O	2.14	0.60
3:C:516:LEU:HD13	3:C:516:LEU:C	2.26	0.60
8:H:157:G:H5''	8:H:157:G:H8	1.65	0.60
25:X:36:LYS:C	25:X:40:LEU:HD12	2.25	0.60
26:Y:54:LYS:CG	26:Y:56:PHE:HZ	1.78	0.60
1:A:402:ILE:HG21	3:C:268:LYS:HE3	1.82	0.60
6:F:85:U:O2'	6:F:86:U:H5''	2.00	0.60
18:R:237:MET:HE2	18:R:237:MET:HA	1.82	0.60
24:W:109:ASN:HB2	24:W:114:TYR:HD1	1.63	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:GLU:CA	1:A:50:LYS:HZ2	2.06	0.60
1:A:122:ILE:N	1:A:481:PHE:O	2.34	0.60
1:A:344:ASP:OD1	1:A:347:LEU:CD1	2.49	0.60
1:A:569:VAL:O	1:A:570:ASP:CB	2.50	0.60
1:A:750:TRP:CZ2	1:A:778:ARG:HG2	2.36	0.60
1:A:758:ARG:NH2	1:A:775:ASN:ND2	2.50	0.60
10:J:192:GLU:OE2	10:J:196:ARG:NH1	2.34	0.60
17:P:72:ARG:HB2	17:P:72:ARG:HH11	1.66	0.60
20:T:339:GLN:HG2	20:T:340:ALA:N	2.16	0.60
23:V:483:GLU:O	23:V:486:THR:OG1	2.20	0.60
24:W:128:GLN:CD	24:W:139:LEU:CD1	2.74	0.60
1:A:158:ARG:HH12	1:A:573:GLN:HE21	1.48	0.60
1:A:344:ASP:OD1	1:A:347:LEU:HD12	2.00	0.60
1:A:758:ARG:NH1	1:A:900:ASP:OD2	2.30	0.60
1:A:1501:LEU:HD22	1:A:1753:LEU:CD1	2.09	0.60
1:A:1930:TYR:OH	25:X:71:ASP:O	2.14	0.60
6:F:35:A:H5''	6:F:35:A:H8	1.66	0.60
6:F:42:C:N4	6:F:43:A:C6	2.68	0.60
24:W:178:ARG:HD3	24:W:201:ASP:OD2	2.02	0.60
29:u:148:GLU:OE1	29:u:148:GLU:HA	2.01	0.60
1:A:382:GLU:HA	3:C:354:ARG:NH1	2.16	0.60
3:C:444:GLY:O	3:C:447:PRO:HD2	2.02	0.60
18:R:88:ILE:O	19:S:20:MET:SD	2.60	0.60
20:T:327:SER:O	20:T:357:TRP:CH2	2.53	0.60
20:T:356:LEU:HD12	20:T:356:LEU:N	2.14	0.60
20:T:455:GLN:HG2	20:T:456:PRO:CD	2.32	0.60
1:A:368:GLN:OE1	1:A:368:GLN:HA	2.00	0.60
1:A:439:GLN:NE2	1:A:614:TYR:CE2	2.49	0.60
1:A:1332:HIS:HE1	1:A:1358:SER:O	1.85	0.60
1:A:1772:PHE:CD1	1:A:1813:ARG:HD2	2.31	0.60
7:G:5:G:N9	7:G:6:A:C2	2.69	0.60
19:S:150:GLN:C	24:W:100:ARG:HH21	2.10	0.60
26:Y:163:ARG:CG	26:Y:163:ARG:HH11	2.15	0.60
1:A:71:ARG:NH1	1:A:177:ASP:OD2	2.32	0.60
3:C:471:ASP:N	3:C:499:GLY:HA2	2.16	0.60
10:J:296:ARG:HD2	12:L:225:TYR:CZ	2.36	0.60
10:J:493:ALA:HB1	10:J:499:ARG:CB	2.32	0.60
12:L:233:GLN:OE1	12:L:233:GLN:HA	2.01	0.60
18:R:104:GLN:NE2	18:R:105:GLY:N	2.50	0.60
29:u:383:ASN:CG	29:u:384:ASP:N	2.58	0.60
1:A:623:LYS:HD3	46:A:3000:IHP:O43	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:830:LEU:HD21	26:Y:148:MET:CB	2.31	0.60
3:C:87:GLN:OE1	3:C:91:GLU:CG	2.49	0.60
7:G:22:C:HO2'	7:G:23:U:P	2.24	0.60
1:A:44:ARG:HG3	1:A:45:TYR:CD2	2.37	0.60
5:E:114:GLU:CD	5:E:116:HIS:HE2	2.09	0.60
5:E:233:GLY:O	5:E:260:ARG:NH2	2.35	0.60
8:H:106:G:N2	8:H:107:A:C6	2.67	0.60
18:R:90:VAL:CG1	18:R:94:GLY:O	2.50	0.60
20:T:455:GLN:HG2	20:T:456:PRO:HD3	1.83	0.60
23:V:483:GLU:O	23:V:486:THR:CB	2.49	0.60
25:X:36:LYS:HE2	25:X:36:LYS:N	2.17	0.60
26:Y:161:ASN:O	26:Y:165:ALA:N	2.31	0.60
3:C:359:LYS:HE3	3:C:359:LYS:O	2.02	0.59
3:C:710:ASN:O	3:C:713:LYS:N	2.31	0.59
3:C:779:LEU:HB3	3:C:934:MET:HE1	1.83	0.59
6:F:27:A:O2'	6:F:28:A:N7	2.36	0.59
12:L:102:PHE:CE1	12:L:106:LYS:HG2	2.37	0.59
17:P:193:VAL:HG23	17:P:194:PHE:CE2	2.34	0.59
19:S:57:ILE:HG22	24:W:99:PHE:CD2	2.35	0.59
24:W:146:HIS:HB3	24:W:148:VAL:O	2.01	0.59
24:W:198:LYS:O	24:W:199:TYR:C	2.45	0.59
40:o:133:LEU:HD12	40:o:158:ALA:HB2	1.84	0.59
1:A:529:THR:OG1	8:H:38:A:OP1	2.18	0.59
1:A:1768:TYR:CE2	1:A:2012:LEU:HD22	2.38	0.59
1:A:1953:ILE:CD1	1:A:1986:LEU:HD11	2.31	0.59
5:E:263:ASP:HB3	5:E:274:VAL:HG21	1.84	0.59
16:O:132:ARG:HG3	16:O:137:LEU:HD23	1.83	0.59
26:Y:64:GLN:HE21	26:Y:64:GLN:H	1.50	0.59
1:A:678:GLU:OE2	1:A:774:LYS:NZ	2.33	0.59
1:A:1134:TRP:O	1:A:1139:ARG:NH1	2.34	0.59
1:A:1495:PHE:CZ	1:A:1748:ARG:HG2	2.36	0.59
1:A:1501:LEU:CB	45:4:28:ALA:CB	2.79	0.59
1:A:1853:PRO:CB	43:2:614:LYS:N	2.48	0.59
3:C:186:VAL:HG22	3:C:535:ALA:HA	1.85	0.59
8:H:106:G:H5'	36:k:47:ARG:HH22	1.66	0.59
12:L:15:GLU:OE1	12:L:41:LYS:NZ	2.36	0.59
18:R:74:LEU:HD23	18:R:74:LEU:C	2.27	0.59
23:V:449:GLU:HB3	23:V:452:LEU:HD12	1.84	0.59
24:W:128:GLN:CD	24:W:139:LEU:HD11	2.28	0.59
26:Y:70:GLY:H	26:Y:71:LEU:HD12	1.67	0.59
3:C:474:LEU:HD11	3:C:501:ILE:HG12	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:18:ILE:CG2	12:L:37:LEU:HD23	2.31	0.59
12:L:77:LEU:CD2	18:R:285:ALA:HA	2.32	0.59
16:O:133:PRO:HD2	16:O:137:LEU:HD22	1.84	0.59
16:O:155:PRO:HD3	18:R:188:PHE:CD1	2.38	0.59
20:T:342:GLU:HB3	20:T:343:PRO:HD3	1.83	0.59
23:V:603:LEU:HA	23:V:606:GLU:CG	2.33	0.59
30:v:8:TYR:HB3	30:v:93:VAL:HB	1.83	0.59
1:A:120:TYR:O	1:A:483:GLN:O	2.20	0.59
1:A:1580:HIS:NE2	26:Y:17:PRO:CG	2.65	0.59
3:C:298:LEU:HD13	3:C:298:LEU:N	2.18	0.59
3:C:736:GLY:HA2	3:C:770:PHE:CE2	2.38	0.59
5:E:265:ARG:H	5:E:272:ARG:HH21	1.47	0.59
18:R:66:GLU:OE1	19:S:31:HIS:NE2	2.35	0.59
18:R:124:VAL:HG22	18:R:125:MET:N	2.16	0.59
23:V:330:LYS:HZ2	29:u:47:GLU:HG3	1.68	0.59
23:V:487:LYS:HZ1	23:V:491:ASN:CG	2.10	0.59
26:Y:134:MET:HA	26:Y:134:MET:CE	2.21	0.59
1:A:73:HIS:CD2	1:A:81:PHE:CG	2.89	0.59
1:A:530:LEU:O	13:y:7:LYS:HD3	2.02	0.59
1:A:1017:ILE:HD12	1:A:1024:HIS:NE2	2.17	0.59
1:A:1382:SER:HA	1:A:1415:GLY:HA2	1.84	0.59
1:A:1953:ILE:CD1	1:A:1986:LEU:HD13	2.32	0.59
3:C:674:CYS:HG	3:C:822:MET:CE	2.16	0.59
5:E:267:PHE:CD1	12:L:788:TYR:HE2	2.18	0.59
8:H:15:U:C2'	8:H:16:U:OP2	2.50	0.59
23:V:514:PHE:O	23:V:521:TYR:CB	2.51	0.59
23:V:609:GLN:O	23:V:612:PHE:N	2.36	0.59
1:A:120:TYR:CZ	1:A:483:GLN:HB2	2.38	0.59
1:A:120:TYR:CD1	1:A:483:GLN:O	2.56	0.59
1:A:152:ARG:HH11	1:A:152:ARG:CG	2.15	0.59
1:A:280:GLU:OE2	1:A:281:PRO:HD2	2.03	0.59
8:H:154:C:OP1	41:p:19:LYS:HD3	2.03	0.59
19:S:20:MET:HE2	19:S:141:ARG:CB	2.31	0.59
30:v:99:ILE:HD12	30:v:101:PHE:CZ	2.38	0.59
1:A:1567:PRO:HB2	8:H:36:G:OP1	2.01	0.59
14:M:118:LYS:HA	14:M:118:LYS:HZ3	1.67	0.59
1:A:44:ARG:CG	1:A:45:TYR:CD2	2.85	0.59
1:A:91:ALA:O	1:A:92:LEU:C	2.45	0.59
1:A:1870:ASP:HB2	1:A:1871:PRO:CD	2.32	0.59
10:J:195:LEU:HD21	12:L:24:MET:CE	2.32	0.59
17:P:193:VAL:CG2	17:P:194:PHE:CE2	2.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:622:ARG:HA	23:V:625:ARG:HH11	1.68	0.59
24:W:167:VAL:CG2	24:W:168:PHE:CD1	2.85	0.59
1:A:384:VAL:HG12	3:C:331:PHE:HD2	1.61	0.59
1:A:1501:LEU:CB	45:4:28:ALA:HB2	2.33	0.59
7:G:150:U:C3'	7:G:151:C:C5'	2.80	0.59
19:S:60:PHE:CD2	24:W:98:PRO:CD	2.86	0.59
19:S:61:MET:HE1	24:W:95:PRO:CG	2.32	0.59
1:A:151:MET:CE	1:A:628:GLY:C	2.75	0.58
1:A:384:VAL:HG12	3:C:331:PHE:CB	2.33	0.58
1:A:1502:PHE:CE2	1:A:1505:LYS:HD3	2.37	0.58
2:B:95:G:C5'	36:d:47:ARG:HH22	2.12	0.58
3:C:680:ASN:CG	3:C:682:LYS:HG3	2.26	0.58
3:C:706:GLN:NE2	3:C:708:THR:OG1	2.35	0.58
17:P:73:GLU:O	17:P:76:ARG:HG2	2.03	0.58
19:S:10:GLN:HA	19:S:29:TRP:CH2	2.38	0.58
24:W:130:ARG:O	24:W:134:THR:OG1	2.21	0.58
29:u:46:ARG:HD3	29:u:133:MET:HE3	1.85	0.58
37:m:70:LEU:CD2	37:m:71:TYR:HD2	2.16	0.58
37:f:70:LEU:CD2	37:f:71:TYR:HD2	2.16	0.58
1:A:76:MET:SD	1:A:88:TYR:CD2	2.95	0.58
1:A:181:ASN:N	1:A:181:ASN:OD1	2.35	0.58
3:C:259:LYS:HG3	47:C:1500:GTP:C6	2.38	0.58
4:D:127:GLN:O	4:D:128:PRO:O	2.21	0.58
16:O:57:TRP:CD1	16:O:57:TRP:C	2.81	0.58
16:O:245:GLU:O	16:O:248:LEU:N	2.36	0.58
24:W:109:ASN:HB2	24:W:114:TYR:CE1	2.38	0.58
25:X:31:GLU:OE1	25:X:31:GLU:HA	2.02	0.58
25:X:33:GLU:O	25:X:37:ILE:HG13	2.03	0.58
1:A:47:GLU:HA	1:A:50:LYS:HZ1	1.66	0.58
1:A:1768:TYR:CE2	1:A:2012:LEU:CD2	2.86	0.58
3:C:221:ILE:HD11	3:C:479:THR:HG1	1.65	0.58
5:E:310:TYR:CE1	5:E:322:LYS:CD	2.86	0.58
7:G:125:C:OP1	7:G:125:C:H3'	2.03	0.58
14:M:163:THR:N	14:M:166:SER:HB3	2.18	0.58
20:T:345:ILE:HB	20:T:357:TRP:HB2	1.85	0.58
24:W:144:ASP:N	24:W:144:ASP:OD1	2.36	0.58
26:Y:54:LYS:HG3	26:Y:54:LYS:O	2.03	0.58
1:A:537:LYS:HD2	6:F:37:C:N4	2.18	0.58
1:A:1508:GLY:C	25:X:24:TRP:NE1	2.61	0.58
3:C:259:LYS:CG	47:C:1500:GTP:C6	2.86	0.58
3:C:449:ILE:CD1	3:C:466:SER:CB	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:C:H5''	26:Y:22:LYS:CG	2.29	0.58
13:y:67:GLU:HA	13:y:70:ILE:HG12	1.85	0.58
16:O:235:TYR:CD2	16:O:301:LYS:HB2	2.33	0.58
18:R:76:MET:N	18:R:76:MET:SD	2.76	0.58
29:u:278:THR:CG2	29:u:279:GLN:N	2.57	0.58
1:A:1074:PHE:CD1	1:A:1080:GLU:HG2	2.38	0.58
1:A:1317:TYR:CE1	1:A:1329:SER:HB2	2.38	0.58
3:C:220:ARG:O	3:C:448:LYS:CE	2.52	0.58
5:E:87:ASP:O	5:E:88:ARG:CB	2.51	0.58
17:P:63:LEU:HD23	17:P:63:LEU:C	2.28	0.58
18:R:124:VAL:HG22	18:R:126:ASN:H	1.68	0.58
1:A:60:ASP:OD1	1:A:60:ASP:N	2.36	0.58
1:A:284:ARG:NH1	2:B:35:U:O2'	2.36	0.58
1:A:379:GLU:CA	3:C:354:ARG:O	2.51	0.58
3:C:509:VAL:O	3:C:510:LEU:HD23	2.04	0.58
3:C:669:THR:CG2	3:C:690:GLU:OE1	2.52	0.58
3:C:750:LEU:O	3:C:750:LEU:HD12	2.03	0.58
4:D:290:LEU:O	4:D:294:LYS:N	2.28	0.58
10:J:188:GLN:HG3	12:L:140:ASP:OD1	2.03	0.58
10:J:300:ASP:OD2	18:R:101:ILE:HD11	2.02	0.58
16:O:123:ARG:O	16:O:126:SER:OG	2.16	0.58
18:R:171:LEU:HD23	18:R:171:LEU:O	2.03	0.58
18:R:189:ASN:HD21	18:R:195:ARG:HH22	1.50	0.58
23:V:631:PHE:HB2	23:V:640:THR:HG21	1.84	0.58
24:W:156:VAL:HG12	24:W:160:GLU:OE2	2.03	0.58
26:Y:40:ASN:HB2	26:Y:50:ILE:O	2.03	0.58
1:A:86:ARG:HG3	1:A:87:VAL:N	2.17	0.58
1:A:663:ARG:HH11	6:F:63:C:H3'	1.68	0.58
10:J:192:GLU:N	10:J:195:LEU:HD11	2.18	0.58
10:J:311:GLN:OE1	10:J:311:GLN:N	2.33	0.58
18:R:303:GLU:O	18:R:307:GLN:HG2	2.04	0.58
23:V:606:GLU:HB3	23:V:608:LEU:HG	1.86	0.58
31:w:109:ARG:HG3	31:w:110:THR:HG23	1.86	0.58
1:A:825:ILE:HB	1:A:1001:VAL:HG12	1.86	0.58
3:C:669:THR:HG22	3:C:690:GLU:HB3	1.84	0.58
6:F:22:A:C6	24:W:130:ARG:CG	2.86	0.58
12:L:52:GLU:OE2	12:L:134:THR:N	2.36	0.58
16:O:240:GLY:HA3	16:O:296:ARG:HH22	1.68	0.58
26:Y:16:ASP:CG	26:Y:18:SER:HG	2.11	0.58
33:h:45:ASN:HB3	40:o:22:ARG:NH1	2.18	0.58
40:o:101:VAL:HG23	40:o:102:GLU:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1320:LYS:NZ	1:A:1526:LEU:CB	2.52	0.58
5:E:165:GLN:HG3	5:E:181:ILE:HD11	1.85	0.58
8:H:154:C:O2'	8:H:155:C:H5'	2.04	0.58
12:L:145:ASP:O	12:L:146:GLU:C	2.46	0.58
14:M:124:PHE:O	14:M:125:SER:OG	2.15	0.58
16:O:233:THR:HA	16:O:272:ILE:O	2.03	0.58
20:T:399:LYS:HG2	20:T:406:ILE:CD1	2.31	0.58
24:W:178:ARG:NH1	24:W:202:GLU:HG2	2.18	0.58
1:A:122:ILE:HD13	1:A:483:GLN:CG	2.32	0.58
1:A:853:LYS:HG2	7:G:148:U:C2	2.39	0.58
3:C:87:GLN:HG2	3:C:91:GLU:HG2	1.86	0.58
3:C:700:ILE:CG2	3:C:735:PHE:CD2	2.83	0.58
5:E:277:PHE:CE2	5:E:300:ILE:CD1	2.85	0.58
8:H:31:G:O3'	25:X:17:LEU:CD1	2.52	0.58
16:O:102:SER:OG	16:O:139:LYS:NZ	2.25	0.58
18:R:76:MET:HG2	19:S:95:ALA:HB1	1.85	0.58
18:R:148:ARG:HG3	18:R:148:ARG:HH11	1.68	0.58
18:R:231:HIS:H	18:R:231:HIS:CD2	2.22	0.58
19:S:131:ARG:HH11	19:S:132:VAL:C	2.12	0.58
23:V:497:CYS:CB	23:V:507:PHE:CB	2.81	0.58
1:A:300:ASN:CB	3:C:939:ARG:NH2	2.66	0.57
17:P:31:SER:N	17:P:34:ASP:OD2	2.37	0.57
17:P:35:LEU:HB3	17:P:36:PRO:HD2	1.86	0.57
19:S:131:ARG:HH11	19:S:133:CYS:CA	2.17	0.57
1:A:48:LYS:O	1:A:53:PHE:CD2	2.57	0.57
1:A:120:TYR:CE1	1:A:484:SER:C	2.82	0.57
1:A:682:ASP:OD2	8:H:21:C:H4'	2.03	0.57
10:J:214:ILE:HD12	10:J:214:ILE:N	2.18	0.57
14:M:153:ARG:CB	14:M:160:PHE:CZ	2.87	0.57
16:O:84:CYS:O	16:O:85:LEU:HB2	2.03	0.57
24:W:99:PHE:O	24:W:99:PHE:HD1	1.86	0.57
25:X:14:PRO:CD	26:Y:98:TYR:OH	2.51	0.57
1:A:282:LEU:HD23	1:A:282:LEU:O	2.05	0.57
1:A:587:GLN:O	1:A:587:GLN:HG2	2.04	0.57
3:C:678:THR:CG2	3:C:683:ASN:CB	2.80	0.57
5:E:87:ASP:O	5:E:88:ARG:HG3	2.04	0.57
6:F:48:A:N3	12:L:33:ARG:NH2	2.52	0.57
8:H:31:G:O3'	25:X:17:LEU:CG	2.50	0.57
12:L:37:LEU:CD2	12:L:155:ALA:CB	2.81	0.57
14:M:151:ARG:HH11	14:M:151:ARG:HG2	1.69	0.57
25:X:37:ILE:O	25:X:40:LEU:HB2	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:LYS:O	46:A:3000:IHP:O24	2.22	0.57
3:C:573:GLU:N	3:C:573:GLU:OE1	2.37	0.57
3:C:906:ILE:HG21	29:u:179:ARG:HH12	1.69	0.57
10:J:224:LYS:HE2	10:J:255:LEU:HD13	1.85	0.57
15:N:128:VAL:HG13	15:N:130:ARG:N	2.14	0.57
16:O:226:PRO:HB2	16:O:277:ARG:HH21	1.68	0.57
18:R:106:GLN:HG2	18:R:110:LYS:CE	2.28	0.57
23:V:449:GLU:HB3	23:V:452:LEU:CD1	2.33	0.57
28:q:58:ALA:HB1	28:r:6:SER:HA	1.87	0.57
31:w:77:VAL:HB	31:w:117:THR:CG2	2.33	0.57
39:n:19:LEU:O	39:n:26:HIS:HD2	1.88	0.57
1:A:339:PHE:CD1	1:A:406:TRP:CZ3	2.93	0.57
1:A:758:ARG:HH12	1:A:900:ASP:CG	2.13	0.57
1:A:1021:ASP:OD1	8:H:24:A:C2	2.56	0.57
1:A:1754:TYR:N	1:A:1754:TYR:CD1	2.73	0.57
4:D:291:GLU:C	4:D:295:THR:H	2.03	0.57
5:E:250:LEU:CD2	5:E:262:TRP:HB2	2.35	0.57
12:L:161:ASN:OD1	12:L:168:LYS:HE2	2.02	0.57
13:y:57:VAL:HG23	13:y:58:ALA:N	2.19	0.57
1:A:593:ARG:NH1	1:A:1565:LYS:HE3	2.20	0.57
1:A:1215:ASN:HB3	1:A:1224:ARG:CD	2.35	0.57
3:C:196:LYS:HD2	34:b:7:SER:HB2	1.86	0.57
3:C:706:GLN:NE2	3:C:708:THR:H	2.02	0.57
7:G:150:U:H3'	7:G:151:C:C5'	2.34	0.57
39:g:19:LEU:O	39:g:26:HIS:HD2	1.88	0.57
1:A:249:LEU:HD22	1:A:254:TYR:HB2	1.86	0.57
1:A:381:PRO:HD2	3:C:334:ILE:HG22	1.78	0.57
1:A:675:GLN:OE1	6:F:70:A:P	2.63	0.57
1:A:1356:GLY:O	22:U:15:THR:HG22	2.04	0.57
7:G:-2:C:N4	7:G:-1:G:C2	2.73	0.57
8:H:152:G:N2	8:H:153:A:C5	2.73	0.57
10:J:225:LEU:CD2	12:L:211:ASN:HB2	2.35	0.57
10:J:325:ASN:CB	14:M:172:HIS:HD2	2.16	0.57
17:P:76:ARG:HG3	17:P:77:ASP:N	2.19	0.57
23:V:497:CYS:HB2	23:V:507:PHE:CB	2.34	0.57
24:W:182:LYS:HD3	24:W:182:LYS:C	2.28	0.57
25:X:6:LEU:HD12	25:X:6:LEU:C	2.30	0.57
1:A:464:PRO:O	1:A:465:LYS:HB3	2.05	0.57
1:A:805:GLU:CD	17:P:194:PHE:CZ	2.81	0.57
3:C:93:ILE:O	3:C:94:ILE:HB	2.04	0.57
3:C:671:SER:C	3:C:672:LEU:HD22	2.30	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:45:A:N6	26:Y:34:ARG:NE	2.53	0.57
12:L:49:ARG:HD3	12:L:49:ARG:O	2.04	0.57
12:L:144:MET:CB	12:L:149:LEU:HD21	2.35	0.57
14:M:154:GLU:HG3	14:M:155:LYS:N	2.19	0.57
14:M:176:THR:O	14:M:179:ILE:N	2.38	0.57
15:N:54:HIS:HD2	24:W:196:TRP:HZ3	1.48	0.57
15:N:127:GLU:HG3	24:W:135:TYR:OH	2.05	0.57
20:T:351:ASP:C	20:T:352:THR:OG1	2.48	0.57
23:V:330:LYS:HA	23:V:333:GLN:CG	2.34	0.57
24:W:135:TYR:CZ	24:W:165:LEU:CD1	2.85	0.57
1:A:232:LEU:HD22	1:A:404:LEU:HD12	1.86	0.57
1:A:384:VAL:HG12	3:C:331:PHE:HB3	1.87	0.57
1:A:1758:PRO:HG2	45:4:8:GLY:CA	2.35	0.57
3:C:445:ALA:CB	3:C:466:SER:HA	2.35	0.57
7:G:142:U:OP2	25:X:10:LYS:NZ	2.29	0.57
18:R:282:GLU:O	18:R:284:PHE:N	2.37	0.57
19:S:10:GLN:CB	19:S:29:TRP:CD2	2.88	0.57
19:S:151:ASP:CG	24:W:97:ASN:OD1	2.47	0.57
20:T:347:THR:CG2	20:T:357:TRP:HE1	2.18	0.57
20:T:351:ASP:C	20:T:352:THR:HG1	2.09	0.57
24:W:97:ASN:ND2	24:W:97:ASN:H	2.02	0.57
26:Y:26:PRO:O	26:Y:27:LYS:CB	2.52	0.57
26:Y:64:GLN:HE21	26:Y:64:GLN:N	2.03	0.57
29:u:268:LEU:HD11	29:u:282:ILE:HD13	1.87	0.57
3:C:487:GLY:HA3	3:C:489:GLN:OE1	2.05	0.57
3:C:508:LYS:HB3	3:C:566:THR:CG2	2.35	0.57
3:C:749:THR:OG1	3:C:752:SER:HB2	2.04	0.57
7:G:145:U:C6	7:G:145:U:C3'	2.87	0.57
12:L:166:LYS:O	12:L:169:ARG:HB3	2.05	0.57
14:M:118:LYS:HA	14:M:118:LYS:NZ	2.20	0.57
14:M:179:ILE:HG13	14:M:180:ASP:N	2.19	0.57
18:R:70:ALA:O	18:R:71:GLN:C	2.48	0.57
23:V:478:LYS:HA	23:V:478:LYS:HE3	1.87	0.57
24:W:101:THR:O	24:W:103:GLN:N	2.38	0.57
29:u:315:GLU:O	29:u:319:ILE:HG12	2.05	0.57
40:o:2:VAL:HG11	40:o:29:TYR:O	2.05	0.57
1:A:120:TYR:HE1	1:A:484:SER:C	2.13	0.56
1:A:229:GLN:HA	1:A:415:SER:HA	1.85	0.56
1:A:332:TYR:HB3	3:C:177:ARG:O	2.05	0.56
2:B:23:C:O2'	2:B:24:G:O5'	2.21	0.56
5:E:277:PHE:CE2	5:E:300:ILE:HD13	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:152:G:N2	8:H:153:A:C8	2.73	0.56
12:L:144:MET:O	12:L:149:LEU:CD1	2.53	0.56
18:R:74:LEU:HB3	19:S:136:ILE:HG12	1.87	0.56
18:R:82:MET:HE3	18:R:82:MET:O	2.04	0.56
20:T:306:CYS:SG	20:T:336:VAL:CG1	2.93	0.56
1:A:232:LEU:HD13	1:A:401:GLY:HA2	1.85	0.56
1:A:642:ARG:NE	2:B:55:C:O2	2.37	0.56
1:A:748:ASP:OD1	17:P:214:THR:HG21	2.05	0.56
3:C:572:GLU:O	3:C:573:GLU:HB2	2.04	0.56
3:C:680:ASN:ND2	3:C:682:LYS:CG	2.68	0.56
6:F:36:A:H2'	6:F:37:C:O5'	2.05	0.56
6:F:85:U:O2'	6:F:86:U:OP1	2.22	0.56
7:G:12:G:H2'	7:G:13:C:C5	2.40	0.56
8:H:57:A:H2'	8:H:58:U:H6	1.70	0.56
12:L:176:LEU:O	12:L:176:LEU:HD22	2.05	0.56
19:S:131:ARG:NH1	19:S:133:CYS:CB	2.68	0.56
26:Y:68:TYR:O	26:Y:71:LEU:HD12	2.06	0.56
1:A:517:HIS:CD2	26:Y:10:TYR:CD1	2.93	0.56
1:A:1494:TYR:CD2	1:A:1494:TYR:O	2.58	0.56
1:A:1860:GLN:HG2	1:A:1883:VAL:HB	1.86	0.56
3:C:223:ASP:OD1	3:C:495:ARG:NH2	2.39	0.56
3:C:426:GLU:O	3:C:427:PHE:HB2	2.05	0.56
6:F:43:A:H2'	6:F:44:G:O5'	2.04	0.56
6:F:88:G:C4'	14:M:121:ASP:HB2	2.35	0.56
7:G:21:A:C2	16:O:152:ARG:HB2	2.41	0.56
8:H:68:G:H2'	8:H:69:U:H6	1.70	0.56
8:H:181:G:H2'	8:H:182:U:H6	1.71	0.56
14:M:118:LYS:HG3	14:M:119:ASN:N	2.20	0.56
17:P:188:TRP:CG	17:P:189:ASP:H	2.23	0.56
19:S:77:ILE:HG13	19:S:78:TYR:CD1	2.38	0.56
1:A:264:PHE:CE1	1:A:459:LEU:CD1	2.81	0.56
1:A:1307:MET:HE2	1:A:1548:TYR:HB3	1.87	0.56
3:C:152:GLN:CD	3:C:426:GLU:O	2.49	0.56
8:H:91:U:H2'	8:H:92:U:H6	1.71	0.56
8:H:179:C:H2'	8:H:180:G:C8	2.38	0.56
16:O:177:GLU:HG3	24:W:202:GLU:OE1	2.05	0.56
18:R:176:TYR:HB2	24:W:118:ALA:O	2.06	0.56
19:S:13:ASN:HD22	19:S:24:VAL:CG1	2.19	0.56
24:W:162:ASN:CG	24:W:165:LEU:CD2	2.78	0.56
25:X:5:ASP:OD1	25:X:6:LEU:N	2.38	0.56
29:u:77:ASP:HB3	29:u:233:MET:HE2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
37:m:11:LEU:CD1	37:m:40:MET:HE2	2.35	0.56
1:A:178:TYR:CD2	1:A:491:GLU:HB2	2.40	0.56
1:A:253:ASN:HB3	3:C:893:GLY:O	2.05	0.56
1:A:570:ASP:OD1	1:A:571:ALA:N	2.38	0.56
1:A:1370:ARG:HH12	23:V:506:PHE:HB3	1.70	0.56
3:C:674:CYS:SG	3:C:822:MET:HE1	2.45	0.56
3:C:677:GLU:HA	3:C:683:ASN:O	2.05	0.56
14:M:190:ILE:HG12	14:M:193:ARG:NH2	2.20	0.56
18:R:55:LEU:CB	18:R:73:PRO:O	2.53	0.56
26:Y:163:ARG:HG2	26:Y:163:ARG:NH1	2.21	0.56
1:A:364:SER:O	1:A:365:VAL:C	2.48	0.56
1:A:434:HIS:CE1	1:A:435:CYS:SG	2.98	0.56
1:A:1853:PRO:CA	43:2:614:LYS:CA	2.82	0.56
3:C:449:ILE:HG22	3:C:457:VAL:HG13	1.88	0.56
8:H:70:C:H2'	8:H:71:C:H6	1.71	0.56
8:H:83:A:H2'	8:H:84:C:H6	1.71	0.56
8:H:88:A:H2'	8:H:89:U:H6	1.71	0.56
8:H:141:C:C2	8:H:142:C:C5	2.94	0.56
20:T:342:GLU:CB	20:T:343:PRO:CD	2.83	0.56
24:W:140:ASP:HA	24:W:153:ILE:CG1	2.35	0.56
24:W:178:ARG:CD	24:W:199:TYR:CD1	2.88	0.56
25:X:60:VAL:N	25:X:61:GLY:CA	2.62	0.56
37:m:70:LEU:HD23	37:m:70:LEU:C	2.31	0.56
1:A:107:PRO:O	1:A:111:GLU:CD	2.48	0.56
1:A:232:LEU:HD11	3:C:385:VAL:O	2.05	0.56
8:H:54:U:H2'	8:H:55:U:H6	1.71	0.56
8:H:69:U:C2	8:H:70:C:C5	2.94	0.56
12:L:102:PHE:CE1	12:L:106:LYS:CG	2.88	0.56
15:N:117:CYS:SG	15:N:119:CYS:HB3	2.42	0.56
30:v:117:ASP:N	30:v:118:PRO:HD3	2.21	0.56
1:A:89:LEU:HD13	1:A:660:PHE:HZ	1.71	0.56
1:A:227:ARG:C	1:A:416:GLY:O	2.48	0.56
1:A:1504:GLU:CB	1:A:1754:TYR:OH	2.53	0.56
1:A:1881:ASN:OD1	45:4:11:ALA:CA	2.54	0.56
1:A:1949:ARG:CD	1:A:1986:LEU:HD21	2.34	0.56
3:C:617:LEU:HD11	3:C:629:ILE:HG23	1.87	0.56
8:H:150:U:C2	8:H:151:C:C5	2.94	0.56
8:H:183:G:H2'	8:H:184:C:H6	1.71	0.56
9:I:508:ASP:O	9:I:547:LEU:CB	2.54	0.56
1:A:276:GLY:C	1:A:448:GLN:HE21	2.05	0.56
1:A:1527:ASN:ND2	7:G:149:G:H22	1.93	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:673:LYS:HG3	3:C:686:THR:CG2	2.36	0.56
5:E:119:THR:HG21	5:E:161:ARG:HB2	1.87	0.56
6:F:42:C:C2'	6:F:43:A:O4'	2.54	0.56
7:G:148:U:OP1	7:G:148:U:H4'	2.05	0.56
10:J:290:ARG:NH2	14:M:179:ILE:HD11	2.21	0.56
12:L:154:GLU:HB3	26:Y:49:TYR:CE2	2.24	0.56
23:V:497:CYS:O	23:V:500:GLN:HB2	2.05	0.56
1:A:283:VAL:HG22	1:A:284:ARG:HG2	1.88	0.56
1:A:799:PRO:CD	18:R:284:PHE:CD1	2.89	0.56
1:A:1208:THR:HG21	23:V:553:HIS:CD2	2.41	0.56
2:B:47:A:O2'	2:B:48:A:H5''	2.06	0.56
3:C:91:GLU:O	20:T:278:ASN:ND2	2.38	0.56
8:H:73:C:C2	8:H:74:U:C5	2.94	0.56
8:H:77:C:C2	8:H:78:C:C5	2.93	0.56
8:H:90:A:H2'	8:H:91:U:H6	1.70	0.56
8:H:91:U:C2	8:H:92:U:C5	2.94	0.56
12:L:154:GLU:O	12:L:158:ARG:HG2	2.06	0.56
18:R:74:LEU:HD23	18:R:75:ASP:OD1	2.06	0.56
18:R:280:ILE:HD12	18:R:280:ILE:C	2.30	0.56
23:V:316:PHE:CE2	23:V:343:ARG:HD3	2.41	0.56
38:l:20:LEU:HD22	38:l:24:TYR:CZ	2.40	0.56
34:b:56:SER:HB2	34:b:59:ALA:O	2.06	0.56
38:e:20:LEU:HD22	38:e:24:TYR:CZ	2.40	0.56
1:A:89:LEU:HD13	1:A:660:PHE:CZ	2.41	0.55
1:A:569:VAL:O	1:A:570:ASP:HB2	2.04	0.55
3:C:439:PRO:HB2	3:C:443:VAL:HB	1.88	0.55
6:F:28:A:H1'	15:N:39:GLY:O	2.05	0.55
6:F:41:A:C2	7:G:6:A:N7	2.74	0.55
8:H:70:C:C2	8:H:71:C:C5	2.94	0.55
8:H:149:A:H2'	8:H:150:U:H6	1.71	0.55
8:H:150:U:H2'	8:H:151:C:H6	1.71	0.55
10:J:220:LEU:HD13	10:J:220:LEU:C	2.31	0.55
10:J:355:ARG:NH2	14:M:139:THR:HG23	2.22	0.55
10:J:433:ARG:HH12	10:J:461:LYS:CB	2.19	0.55
17:P:33:ARG:HG3	17:P:33:ARG:HH11	1.71	0.55
19:S:58:LYS:HB3	24:W:99:PHE:CE2	2.41	0.55
24:W:185:ASP:O	24:W:186:ALA:HB3	2.06	0.55
26:Y:22:LYS:HD2	26:Y:22:LYS:O	2.05	0.55
29:u:275:LEU:HD23	29:u:275:LEU:C	2.31	0.55
37:f:11:LEU:CD1	37:f:40:MET:HE2	2.35	0.55
1:A:44:ARG:NH2	5:E:285:GLU:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:675:GLN:OE1	6:F:70:A:H5''	2.06	0.55
1:A:792:HIS:HE1	18:R:279:HIS:HE1	1.52	0.55
3:C:185:PRO:HG3	3:C:482:TYR:CZ	2.41	0.55
3:C:559:ILE:C	3:C:559:ILE:HD12	2.31	0.55
3:C:679:PRO:HD2	3:C:807:GLN:CB	2.10	0.55
7:G:22:C:O2	7:G:22:C:H2'	2.05	0.55
7:G:138:A:H2'	7:G:139:U:O5'	2.07	0.55
8:H:71:C:H2'	8:H:72:U:H6	1.70	0.55
8:H:183:G:C4	8:H:184:C:C5	2.94	0.55
10:J:191:ALA:O	10:J:193:GLN:CA	2.54	0.55
10:J:406:PHE:CE2	10:J:411:MET:HE3	2.41	0.55
12:L:154:GLU:HB2	26:Y:49:TYR:CE2	2.42	0.55
20:T:185:MET:SD	20:T:442:ARG:NH2	2.75	0.55
37:m:8:LYS:HB3	37:m:9:PRO:HD3	1.88	0.55
1:A:151:MET:SD	1:A:628:GLY:O	2.65	0.55
1:A:356:ILE:HG22	1:A:357:ASN:N	2.20	0.55
1:A:1502:PHE:CE2	1:A:1505:LYS:CB	2.88	0.55
3:C:631:GLY:HA3	3:C:637:LEU:HD21	1.88	0.55
7:G:-12:G:O2'	7:G:-11:G:P	2.64	0.55
8:H:73:C:H2'	8:H:74:U:H6	1.70	0.55
8:H:147:G:C4	8:H:148:C:C5	2.94	0.55
16:O:106:ASP:CG	16:O:107:MET:H	2.15	0.55
16:O:236:VAL:O	16:O:269:CYS:HA	2.06	0.55
24:W:207:LYS:HG3	24:W:208:PRO:O	2.06	0.55
26:Y:43:CYS:SG	26:Y:46:CYS:HB2	2.47	0.55
1:A:387:PHE:CE1	3:C:327:TYR:CD1	2.95	0.55
1:A:701:ILE:HD13	1:A:701:ILE:N	2.22	0.55
1:A:1498:TRP:CA	1:A:1501:LEU:HD12	2.36	0.55
5:E:310:TYR:CZ	5:E:322:LYS:HD2	2.42	0.55
7:G:153:C:C3'	7:G:153:C:C6	2.90	0.55
8:H:72:U:C2	8:H:73:C:C5	2.94	0.55
8:H:181:G:C4	8:H:182:U:C5	2.95	0.55
10:J:406:PHE:CD1	10:J:411:MET:HE2	2.41	0.55
25:X:6:LEU:HD23	26:Y:55:LYS:CG	2.35	0.55
26:Y:38:PRO:O	26:Y:52:LYS:CE	2.51	0.55
1:A:517:HIS:NE2	26:Y:10:TYR:CE1	2.75	0.55
1:A:1425:LYS:HB3	7:G:154:U:O2	2.05	0.55
1:A:1495:PHE:CD1	1:A:1748:ARG:CZ	2.90	0.55
1:A:1797:ASN:OD1	8:H:45:C:O2'	2.11	0.55
3:C:196:LYS:NZ	34:b:11:GLN:HG3	2.21	0.55
5:E:162:ARG:CZ	5:E:203:ASP:O	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:260:ARG:NH1	5:E:276:ILE:HD11	2.22	0.55
16:O:196:GLN:HE22	16:O:209:VAL:HG23	1.71	0.55
19:S:101:ALA:CB	24:W:95:PRO:HD3	2.36	0.55
24:W:178:ARG:HG3	24:W:199:TYR:HE1	1.69	0.55
29:u:89:THR:HB	51:u:702:ATP:O1A	2.06	0.55
36:d:88:LYS:HG3	36:d:89:PRO:HD2	1.89	0.55
1:A:203:VAL:HG23	1:A:237:THR:CG2	2.34	0.55
1:A:229:GLN:HG2	1:A:415:SER:CB	2.36	0.55
1:A:339:PHE:C	1:A:340:ILE:HD13	2.31	0.55
1:A:982:GLU:CD	1:A:1169:GLN:HG3	2.31	0.55
1:A:1495:PHE:CZ	1:A:1748:ARG:CD	2.89	0.55
1:A:1531:ASN:ND2	8:H:35:A:OP1	2.39	0.55
1:A:1771:LEU:CD2	1:A:1930:TYR:CA	2.56	0.55
3:C:385:VAL:HG23	3:C:386:GLY:N	2.20	0.55
3:C:452:THR:CB	3:C:577:PHE:CD2	2.89	0.55
7:G:148:U:O2'	7:G:149:G:P	2.65	0.55
8:H:77:C:H2'	8:H:78:C:H6	1.70	0.55
18:R:86:LEU:O	18:R:86:LEU:HD12	2.06	0.55
23:V:484:SER:C	23:V:486:THR:H	2.15	0.55
23:V:571:SER:HB2	23:V:573:GLU:HB3	1.89	0.55
23:V:625:ARG:O	23:V:629:ASN:HB3	2.07	0.55
24:W:167:VAL:HG23	24:W:168:PHE:HD1	1.69	0.55
24:W:188:ASN:ND2	24:W:191:GLY:CA	2.68	0.55
26:Y:3:GLU:HB3	26:Y:5:LYS:O	2.06	0.55
28:q:94:GLN:O	28:q:97:GLN:CG	2.55	0.55
37:f:70:LEU:HD23	37:f:70:LEU:C	2.31	0.55
1:A:226:GLN:HA	1:A:418:THR:OG1	2.06	0.55
2:B:94:U:H2'	2:B:95:G:H5''	1.89	0.55
3:C:482:TYR:CD2	3:C:493:PHE:HB2	2.42	0.55
3:C:510:LEU:HB3	3:C:576:ILE:HD11	1.89	0.55
5:E:250:LEU:HD22	5:E:262:TRP:HB2	1.88	0.55
5:E:284:PHE:HZ	24:W:120:ILE:HD13	1.70	0.55
8:H:83:A:C4	8:H:84:C:C5	2.95	0.55
10:J:192:GLU:CA	10:J:195:LEU:HD11	2.34	0.55
15:N:139:CYS:SG	15:N:140:ARG:N	2.80	0.55
16:O:228:ASP:O	16:O:277:ARG:NH2	2.40	0.55
18:R:129:ASP:HB2	18:R:132:LEU:HD21	1.88	0.55
24:W:135:TYR:CB	24:W:137:TYR:CE1	2.89	0.55
26:Y:49:TYR:C	26:Y:50:ILE:HD13	2.32	0.55
34:i:52:LYS:HE3	35:j:53:VAL:HG21	1.88	0.55
1:A:1567:PRO:HG2	1:A:1568:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1771:LEU:HG	1:A:1772:PHE:N	2.22	0.55
3:C:313:GLN:HB2	47:C:1500:GTP:C6	2.41	0.55
4:D:292:ILE:C	4:D:296:ALA:N	2.57	0.55
10:J:408:ASP:OD1	10:J:443:ILE:HG22	2.07	0.55
11:K:163:LEU:CG	11:K:163:LEU:CA	2.80	0.55
16:O:232:THR:HG22	16:O:277:ARG:HA	1.89	0.55
18:R:135:PRO:HD3	20:T:385:TYR:CE1	2.42	0.55
18:R:171:LEU:HD11	18:R:201:GLU:CD	2.32	0.55
20:T:233:LEU:HD23	20:T:233:LEU:C	2.32	0.55
20:T:356:LEU:N	20:T:356:LEU:CD1	2.70	0.55
36:k:94:ARG:HE	36:k:96:ILE:HD11	1.72	0.55
45:4:29:ALA:O	45:4:30:ALA:HB3	2.06	0.55
1:A:226:GLN:OE1	1:A:417:ARG:NE	2.31	0.55
1:A:623:LYS:HG2	46:A:3000:IHP:O34	2.07	0.55
4:D:146:GLU:O	4:D:149:ARG:N	2.40	0.55
7:G:142:U:OP1	26:Y:33:VAL:CG1	2.23	0.55
8:H:10:C:C5	14:M:198:ARG:NH1	2.75	0.55
8:H:59:A:H2'	8:H:60:U:H6	1.71	0.55
8:H:59:A:C4	8:H:60:U:C5	2.95	0.55
8:H:71:C:C2	8:H:72:U:C5	2.94	0.55
8:H:88:A:C4	8:H:89:U:C5	2.95	0.55
8:H:105:G:C6	35:j:20:LYS:HD3	2.42	0.55
10:J:323:LEU:HD21	14:M:182:MET:CE	2.37	0.55
18:R:315:LYS:HE2	18:R:315:LYS:CA	2.37	0.55
23:V:641:ASP:O	23:V:644:ARG:N	2.39	0.55
24:W:137:TYR:CG	24:W:159:ALA:HB2	2.42	0.55
1:A:89:LEU:O	1:A:89:LEU:HD23	2.05	0.55
5:E:108:HIS:ND1	5:E:128:SER:CB	2.70	0.55
5:E:153:PHE:HD1	5:E:153:PHE:H	1.54	0.55
6:F:26:U:O2'	6:F:27:A:P	2.65	0.55
6:F:68:C:C6	20:T:285:HIS:CD2	2.95	0.55
8:H:54:U:C2	8:H:55:U:C5	2.94	0.55
8:H:68:G:C4	8:H:69:U:C5	2.95	0.55
12:L:721:LEU:HA	12:L:724:TYR:CG	2.41	0.55
13:y:54:SER:HA	13:y:57:VAL:CG2	2.37	0.55
37:f:8:LYS:HB3	37:f:9:PRO:HD3	1.88	0.55
1:A:283:VAL:HG13	1:A:284:ARG:N	2.22	0.54
1:A:1791:HIS:HE1	1:A:1799:THR:CG2	2.13	0.54
3:C:220:ARG:HG2	3:C:479:THR:HG21	1.89	0.54
3:C:457:VAL:HA	3:C:462:GLY:HA3	1.88	0.54
3:C:511:GLY:O	3:C:576:ILE:HD12	2.02	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:161:ARG:NH1	5:E:203:ASP:OD1	2.40	0.54
8:H:27:U:O2'	8:H:28:C:H5'	2.06	0.54
11:K:135:TRP:O	11:K:138:TYR:CG	2.60	0.54
12:L:144:MET:O	12:L:149:LEU:HD11	2.07	0.54
14:M:151:ARG:NE	14:M:151:ARG:HA	2.22	0.54
28:t:102:GLU:O	28:t:105:HIS:CG	2.60	0.54
1:A:348:PRO:HB3	1:A:394:TYR:CE2	2.43	0.54
1:A:406:TRP:CZ3	3:C:265:LEU:O	2.60	0.54
1:A:579:GLN:NE2	1:A:613:TYR:CE1	2.74	0.54
1:A:596:TYR:O	1:A:597:LYS:C	2.50	0.54
1:A:855:ARG:NH2	8:H:29:A:H61	2.05	0.54
1:A:1370:ARG:NH1	23:V:506:PHE:CB	2.70	0.54
3:C:452:THR:O	3:C:577:PHE:CA	2.55	0.54
4:D:1048:VAL:O	4:D:1050:GLU:N	2.40	0.54
5:E:87:ASP:O	5:E:88:ARG:HB2	2.08	0.54
7:G:5:G:H2'	7:G:6:A:N3	2.20	0.54
19:S:131:ARG:HH12	19:S:133:CYS:HA	1.68	0.54
23:V:536:ILE:HG23	23:V:579:SER:CA	2.36	0.54
31:w:123:THR:OG1	31:w:126:GLU:HG3	2.07	0.54
1:A:356:ILE:HG22	1:A:357:ASN:H	1.72	0.54
1:A:436:PRO:O	1:A:437:ALA:HB3	2.07	0.54
1:A:460:LYS:NZ	2:B:49:A:OP2	2.41	0.54
3:C:196:LYS:HD2	34:b:7:SER:CB	2.37	0.54
8:H:15:U:H2'	8:H:16:U:OP2	2.06	0.54
8:H:69:U:H2'	8:H:70:C:H6	1.70	0.54
23:V:533:TYR:HA	23:V:536:ILE:HG13	1.89	0.54
26:Y:15:PHE:C	26:Y:15:PHE:CD1	2.85	0.54
1:A:1243:ARG:HD2	1:A:1450:GLN:OE1	2.06	0.54
3:C:69:ALA:HA	20:T:456:PRO:CG	2.37	0.54
8:H:90:A:C4	8:H:91:U:C5	2.95	0.54
12:L:11:TRP:CE2	12:L:41:LYS:HE2	2.41	0.54
20:T:455:GLN:NE2	20:T:456:PRO:HD2	2.22	0.54
23:V:287:ASP:HB3	23:V:331:ARG:CZ	2.37	0.54
25:X:6:LEU:HD23	26:Y:55:LYS:HG3	1.89	0.54
25:X:36:LYS:CA	25:X:36:LYS:CE	2.85	0.54
29:u:287:LYS:HG2	29:u:308:HIS:HB2	1.89	0.54
34:b:52:LYS:HE3	35:c:53:VAL:HG21	1.88	0.54
36:d:94:ARG:HE	36:d:96:ILE:HD11	1.72	0.54
1:A:162:LYS:NZ	1:A:1690:ASP:HB2	2.22	0.54
1:A:1109:LEU:HD11	17:P:188:TRP:HZ2	1.73	0.54
6:F:34:G:H8	6:F:34:G:O5'	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:40:U:C2'	6:F:41:A:C5'	2.85	0.54
8:H:149:A:C4	8:H:150:U:C5	2.95	0.54
8:H:153:A:C3'	8:H:154:C:C5'	2.85	0.54
15:N:38:GLU:O	15:N:40:LYS:N	2.38	0.54
16:O:243:ILE:HG22	16:O:244:THR:O	2.08	0.54
20:T:267:ASP:O	20:T:268:LYS:CG	2.56	0.54
22:U:23:LEU:O	22:U:23:LEU:HD13	2.08	0.54
25:X:5:ASP:CB	25:X:8:LEU:CD1	2.86	0.54
26:Y:50:ILE:HD13	26:Y:50:ILE:N	2.22	0.54
26:Y:138:GLU:CB	27:Z:1096:GLY:C	2.81	0.54
29:u:30:THR:HG23	29:u:239:ILE:HA	1.89	0.54
1:A:120:TYR:HE1	1:A:485:THR:HB	1.72	0.54
1:A:623:LYS:CG	46:A:3000:IHP:O34	2.55	0.54
1:A:705:LYS:O	1:A:708:THR:N	2.40	0.54
8:H:72:U:H2'	8:H:73:C:H6	1.71	0.54
8:H:141:C:H2'	8:H:142:C:H6	1.71	0.54
10:J:218:GLU:HG3	10:J:219:GLU:OE2	2.07	0.54
18:R:237:MET:SD	18:R:241:GLU:CD	2.91	0.54
23:V:330:LYS:HA	23:V:333:GLN:CD	2.32	0.54
36:d:50:LYS:HG2	36:d:74:TRP:CB	2.36	0.54
1:A:758:ARG:CG	17:P:227:TYR:CE2	2.91	0.54
1:A:1790:ILE:CG2	1:A:1798:LEU:HB3	2.37	0.54
3:C:490:PHE:HZ	3:C:612:LYS:HD2	1.69	0.54
16:O:50:ARG:NH1	16:O:122:GLU:OE1	2.41	0.54
16:O:166:SER:HA	16:O:169:VAL:HG12	1.89	0.54
18:R:70:ALA:HA	19:S:93:THR:CG2	2.38	0.54
18:R:89:GLN:OE1	19:S:155:ASP:OD2	2.26	0.54
18:R:231:HIS:H	18:R:231:HIS:HD2	1.56	0.54
23:V:457:ARG:HG3	23:V:457:ARG:NH2	2.18	0.54
23:V:489:LEU:O	23:V:492:MET:CB	2.53	0.54
23:V:493:ILE:CD1	23:V:510:LEU:CD2	2.82	0.54
26:Y:64:GLN:NE2	26:Y:64:GLN:HA	2.23	0.54
1:A:148:TRP:CH2	1:A:616:PHE:HB2	2.42	0.54
1:A:155:LYS:NZ	1:A:624:GLY:C	2.56	0.54
1:A:1494:TYR:CG	1:A:1744:ARG:NE	2.75	0.54
1:A:1504:GLU:HB3	1:A:1752:GLN:CB	2.30	0.54
7:G:140:A:C2	8:H:38:A:C2	2.96	0.54
8:H:40:C:H4'	26:Y:24:LYS:NZ	2.23	0.54
10:J:192:GLU:O	10:J:196:ARG:CB	2.56	0.54
18:R:297:LYS:CE	18:R:300:GLU:OE1	2.50	0.54
24:W:135:TYR:HB3	24:W:137:TYR:HE1	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:14:GLN:HG2	40:o:22:ARG:NH2	2.21	0.54
1:A:299:ILE:HD13	1:A:1342:TRP:CH2	2.43	0.54
1:A:331:TRP:C	1:A:331:TRP:HE3	2.14	0.54
1:A:387:PHE:HE1	3:C:327:TYR:CD1	2.26	0.54
1:A:465:LYS:HG3	1:A:465:LYS:O	2.08	0.54
1:A:799:PRO:CD	18:R:284:PHE:CE1	2.83	0.54
1:A:1505:LYS:HE3	45:4:23:ALA:HB2	1.90	0.54
3:C:481:MET:SD	3:C:559:ILE:HD11	2.48	0.54
6:F:45:A:C4	26:Y:34:ARG:NH2	2.75	0.54
7:G:134:U:C2'	7:G:135:G:H5'	2.38	0.54
10:J:218:GLU:HG3	10:J:219:GLU:N	2.23	0.54
12:L:184:ALA:O	12:L:188:ARG:HB2	2.08	0.54
17:P:41:ILE:HD11	20:T:318:ARG:HB2	1.90	0.54
20:T:287:HIS:CE1	20:T:313:ARG:HG3	2.43	0.54
20:T:384:HIS:O	20:T:385:TYR:CB	2.55	0.54
23:V:549:LYS:HG2	23:V:589:GLU:HB2	1.89	0.54
12:L:186:GLN:OE1	12:L:186:GLN:HA	2.08	0.54
15:N:27:GLN:NE2	15:N:31:GLU:OE2	2.41	0.54
16:O:80:VAL:HG11	16:O:94:ILE:HD11	1.90	0.54
18:R:309:GLU:OE1	18:R:309:GLU:HA	2.08	0.54
25:X:37:ILE:CA	25:X:40:LEU:HD12	2.37	0.54
36:k:50:LYS:HG2	36:k:74:TRP:CB	2.36	0.54
1:A:278:LYS:NZ	7:G:-9:C:OP1	2.37	0.53
1:A:1527:ASN:HB2	7:G:149:G:H22	1.71	0.53
1:A:1863:VAL:HG11	1:A:1868:MET:HB2	1.89	0.53
2:B:18:C:C2'	2:B:19:A:O5'	2.56	0.53
3:C:742:PRO:HB2	3:C:786:ASN:H	1.72	0.53
5:E:178:LEU:CD1	5:E:222:LEU:HD22	2.37	0.53
5:E:232:ARG:O	5:E:262:TRP:HH2	1.92	0.53
7:G:2:U:O4	26:Y:4:ARG:NH2	2.41	0.53
12:L:178:GLU:CA	12:L:181:ARG:HG2	2.30	0.53
15:N:40:LYS:O	15:N:41:ARG:CG	2.47	0.53
15:N:40:LYS:C	15:N:41:ARG:CG	2.81	0.53
18:R:52:PRO:O	18:R:53:ARG:HB2	2.09	0.53
23:V:152:LEU:HA	23:V:387:MET:CE	2.36	0.53
24:W:135:TYR:O	24:W:158:GLU:HG2	2.08	0.53
29:u:307:MET:HE1	29:u:320:MET:HG2	1.90	0.53
34:i:56:SER:HB2	34:i:59:ALA:O	2.07	0.53
35:c:68:PHE:HB2	36:d:100:PHE:HB3	1.91	0.53
1:A:1160:ARG:NH1	17:P:189:ASP:OD2	2.41	0.53
1:A:1761:PRO:O	1:A:1762:TYR:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:702:ASN:O	3:C:703:GLU:HB2	2.07	0.53
7:G:26:U:H3'	16:O:235:TYR:OH	2.09	0.53
12:L:18:ILE:HG12	12:L:152:LEU:HD23	1.85	0.53
12:L:59:LYS:HE2	12:L:91:ARG:NH1	2.20	0.53
14:M:193:ARG:O	14:M:196:TYR:HB2	2.08	0.53
18:R:103:ARG:HH11	18:R:103:ARG:CG	2.21	0.53
23:V:477:LEU:HD23	23:V:514:PHE:HE1	1.72	0.53
23:V:532:GLN:CG	23:V:536:ILE:HG12	2.38	0.53
1:A:40:LEU:HD11	24:W:124:MET:SD	2.48	0.53
1:A:1527:ASN:HB2	7:G:149:G:N2	2.23	0.53
3:C:129:ILE:HG22	3:C:199:LEU:HB3	1.90	0.53
3:C:360:ALA:N	3:C:361:PRO:CD	2.71	0.53
6:F:42:C:C6	6:F:43:A:N7	2.77	0.53
7:G:5:G:O5'	7:G:5:G:H8	1.90	0.53
7:G:153:C:H3'	7:G:153:C:C6	2.42	0.53
8:H:57:A:C4	8:H:58:U:C5	2.95	0.53
12:L:162:THR:CG2	18:R:259:GLY:O	2.46	0.53
31:w:104:LEU:HD22	31:w:113:LEU:HD13	1.91	0.53
1:A:148:TRP:CZ2	1:A:616:PHE:HA	2.44	0.53
1:A:338:VAL:CG2	3:C:867:PRO:CG	2.86	0.53
5:E:320:LEU:O	24:W:84:THR:HG22	2.09	0.53
8:H:154:C:OP2	41:p:19:LYS:CD	2.56	0.53
18:R:312:MET:HE3	18:R:312:MET:CA	2.31	0.53
23:V:537:HIS:HA	23:V:578:SER:CB	2.31	0.53
26:Y:43:CYS:SG	26:Y:46:CYS:CB	2.97	0.53
28:q:53:ILE:CG1	28:r:22:ASN:CB	2.86	0.53
29:u:313:GLN:HA	29:u:316:ARG:HG3	1.90	0.53
39:g:17:LEU:HD23	39:g:72:ALA:HA	1.91	0.53
1:A:151:MET:HE1	1:A:629:PHE:HA	1.91	0.53
1:A:628:GLY:O	1:A:629:PHE:HB2	2.08	0.53
1:A:946:GLU:OE2	1:A:954:LYS:HE3	2.07	0.53
3:C:906:ILE:HB	29:u:179:ARG:HH22	1.73	0.53
6:F:41:A:H61	7:G:6:A:N6	2.06	0.53
12:L:733:LYS:O	12:L:736:ASN:CG	2.52	0.53
15:N:128:VAL:CG1	15:N:130:ARG:HB3	2.38	0.53
16:O:24:CYS:HB2	16:O:27:CYS:SG	2.49	0.53
20:T:318:ARG:HH11	20:T:318:ARG:CG	2.22	0.53
23:V:525:PHE:O	23:V:528:ILE:CG1	2.57	0.53
26:Y:75:ARG:HG3	26:Y:75:ARG:O	2.07	0.53
29:u:383:ASN:OD1	29:u:384:ASP:N	2.38	0.53
30:v:55:HIS:CE1	30:v:56:LYS:HG2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:v:99:ILE:HD12	30:v:101:PHE:HE1	1.70	0.53
1:A:309:ARG:HH21	22:U:1:MET:HE2	1.74	0.53
1:A:755:HIS:CE1	17:P:220:HIS:ND1	2.77	0.53
1:A:758:ARG:HD2	1:A:779:LEU:HD11	1.90	0.53
1:A:1490:PHE:HB2	1:A:1537:TRP:CH2	2.43	0.53
2:B:27:U:O2'	2:B:28:A:O5'	2.23	0.53
3:C:96:PRO:CB	20:T:276:GLU:OE2	2.56	0.53
6:F:33:G:H5''	6:F:33:G:C8	2.42	0.53
10:J:359:VAL:O	10:J:363:ARG:HG2	2.09	0.53
12:L:18:ILE:HG23	12:L:37:LEU:HD22	1.88	0.53
23:V:374:ASP:HB2	23:V:376:TYR:CZ	2.42	0.53
24:W:100:ARG:NH1	24:W:100:ARG:HG2	2.22	0.53
24:W:481:MET:O	24:W:483:ASN:N	2.41	0.53
26:Y:204:LYS:O	26:Y:205:ARG:C	2.51	0.53
30:v:129:GLN:CB	31:w:108:ARG:HG3	2.36	0.53
1:A:1384:ARG:NH2	1:A:1414:ARG:NH1	2.57	0.53
1:A:1534:PHE:CD1	1:A:1534:PHE:C	2.86	0.53
10:J:187:VAL:O	10:J:188:GLN:HB2	2.08	0.53
12:L:198:ILE:HD13	13:y:54:SER:OG	2.09	0.53
18:R:230:MET:HG2	18:R:230:MET:O	2.08	0.53
24:W:192:PHE:CD1	24:W:192:PHE:C	2.86	0.53
28:q:22:ASN:CB	28:r:54:ASP:O	2.56	0.53
1:A:980:ARG:HG2	1:A:1094:ARG:HD3	1.84	0.53
1:A:1204:TYR:HE1	3:C:917:VAL:HG11	1.74	0.53
5:E:108:HIS:ND1	5:E:128:SER:HB2	2.24	0.53
7:G:-9:C:C5	22:U:18:TYR:CE1	2.97	0.53
10:J:205:LEU:O	10:J:206:LEU:HG	2.09	0.53
23:V:515:CYS:SG	23:V:522:MET:CA	2.94	0.53
24:W:178:ARG:HG3	24:W:199:TYR:CE1	2.43	0.53
1:A:980:ARG:O	1:A:1168:VAL:HG13	2.09	0.53
1:A:1455:TRP:H	1:A:1455:TRP:CD1	2.25	0.53
3:C:700:ILE:HA	3:C:705:VAL:HG12	1.89	0.53
3:C:710:ASN:O	3:C:712:LYS:N	2.42	0.53
6:F:38:G:H2'	6:F:39:A:C8	2.43	0.53
10:J:191:ALA:C	10:J:193:GLN:H	2.13	0.53
10:J:325:ASN:HB2	14:M:172:HIS:CD2	2.31	0.53
10:J:360:ASP:HA	10:J:363:ARG:HD2	1.91	0.53
16:O:235:TYR:CD1	16:O:271:PHE:HE1	2.24	0.53
24:W:178:ARG:CD	24:W:199:TYR:CE1	2.92	0.53
24:W:181:PHE:N	24:W:181:PHE:CD1	2.76	0.53
29:u:46:ARG:NH1	29:u:133:MET:HE3	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:275:LEU:HD21	29:u:330:VAL:HG22	1.90	0.53
36:d:107:ILE:HG22	36:d:108:VAL:CG2	2.39	0.53
1:A:191:ILE:HG23	1:A:572:PHE:CZ	2.44	0.53
1:A:758:ARG:NH1	1:A:900:ASP:CG	2.67	0.53
3:C:943:LEU:HD23	3:C:943:LEU:N	2.24	0.53
10:J:203:LEU:CD1	10:J:204:GLU:HG2	2.39	0.53
14:M:153:ARG:CA	14:M:160:PHE:HZ	2.19	0.53
14:M:153:ARG:HB2	14:M:160:PHE:CZ	2.44	0.53
16:O:116:TYR:OH	18:R:222:PRO:HD3	2.08	0.53
17:P:32:SER:O	17:P:35:LEU:HD12	2.09	0.53
20:T:387:PHE:CD1	20:T:387:PHE:C	2.87	0.53
20:T:392:PRO:HA	20:T:414:ALA:O	2.10	0.53
29:u:80:ALA:HB3	29:u:217:ILE:HD13	1.91	0.53
31:w:125:LYS:CG	31:w:126:GLU:N	2.71	0.53
1:A:121:HIS:CD2	1:A:481:PHE:O	2.61	0.52
1:A:227:ARG:H	1:A:417:ARG:HA	1.75	0.52
1:A:1801:LYS:HD3	1:A:1802:PRO:HD2	1.91	0.52
5:E:178:LEU:CD2	5:E:208:ILE:CD1	2.87	0.52
6:F:58:G:O2'	6:F:59:G:P	2.67	0.52
12:L:101:GLU:O	12:L:105:ASP:HB2	2.08	0.52
18:R:303:GLU:O	18:R:307:GLN:OE1	2.27	0.52
19:S:34:LYS:CE	19:S:78:TYR:CD2	2.91	0.52
23:V:515:CYS:SG	23:V:521:TYR:C	2.92	0.52
24:W:176:GLU:HG3	24:W:176:GLU:O	2.09	0.52
24:W:536:ASP:O	24:W:540:THR:N	2.41	0.52
26:Y:2:SER:O	26:Y:3:GLU:CG	2.57	0.52
39:n:17:LEU:HD23	39:n:72:ALA:HA	1.91	0.52
1:A:67:ARG:HD3	1:A:179:ALA:CB	2.34	0.52
1:A:122:ILE:HD13	1:A:483:GLN:HG3	1.90	0.52
1:A:1320:LYS:CD	1:A:1526:LEU:HD23	2.35	0.52
1:A:1332:HIS:CE1	1:A:1358:SER:O	2.61	0.52
3:C:680:ASN:OD1	3:C:682:LYS:HG3	1.92	0.52
7:G:7:G:OP2	7:G:7:G:H8	1.93	0.52
8:H:147:G:H2'	8:H:148:C:C6	2.43	0.52
9:I:729:SER:O	9:I:732:ALA:HB3	2.09	0.52
16:O:106:ASP:OD1	16:O:107:MET:N	2.41	0.52
17:P:30:TYR:OH	18:R:164:PRO:CG	2.57	0.52
23:V:525:PHE:O	23:V:528:ILE:N	2.41	0.52
23:V:530:LYS:O	23:V:532:GLN:N	2.42	0.52
25:X:37:ILE:CA	25:X:40:LEU:HD13	2.15	0.52
28:r:117:ILE:O	28:r:121:THR:HG23	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:307:MET:HA	29:u:311:MET:SD	2.49	0.52
1:A:254:TYR:O	1:A:434:HIS:HD2	1.91	0.52
1:A:1786:TYR:CE1	1:A:1833:LEU:HB3	2.45	0.52
3:C:196:LYS:HZ2	34:b:11:GLN:HG3	1.74	0.52
3:C:711:ARG:CZ	3:C:730:ARG:O	2.57	0.52
6:F:40:U:H2'	6:F:41:A:O5'	2.09	0.52
6:F:58:G:O2'	6:F:59:G:OP1	2.23	0.52
17:P:228:ILE:HD12	17:P:228:ILE:N	2.23	0.52
18:R:262:ILE:HG21	18:R:267:ARG:HH11	1.71	0.52
23:V:573:GLU:OE1	23:V:574:THR:N	2.42	0.52
24:W:178:ARG:HG2	24:W:199:TYR:HE1	1.74	0.52
29:u:383:ASN:O	29:u:386:ILE:HG22	2.09	0.52
1:A:94:TYR:HB2	18:R:207:MET:HE1	1.91	0.52
1:A:168:PRO:HG2	1:A:559:ASP:CB	2.36	0.52
1:A:171:ASP:CG	1:A:519:ASP:OD2	2.53	0.52
1:A:1580:HIS:NE2	26:Y:17:PRO:HG3	2.22	0.52
1:A:1723:LYS:CB	1:A:1724:PRO:HD3	2.39	0.52
2:B:32:C:OP1	17:P:33:ARG:NH2	2.42	0.52
3:C:516:LEU:HB2	3:C:575:GLN:HE22	1.73	0.52
12:L:158:ARG:HB3	12:L:158:ARG:NH1	2.25	0.52
23:V:218:LEU:HD23	23:V:218:LEU:C	2.35	0.52
23:V:234:LEU:HD21	23:V:263:LEU:HD13	1.92	0.52
30:v:94:ILE:HG13	30:v:94:ILE:O	2.09	0.52
35:j:68:PHE:HB2	36:k:100:PHE:HB3	1.90	0.52
1:A:121:HIS:CE1	1:A:481:PHE:O	2.63	0.52
1:A:750:TRP:CE2	1:A:778:ARG:HG2	2.44	0.52
1:A:781:ARG:NH2	8:H:24:A:H5'	2.25	0.52
3:C:445:ALA:CA	3:C:449:ILE:HG13	2.38	0.52
5:E:162:ARG:HH22	5:E:204:THR:HA	1.74	0.52
12:L:20:LYS:HE3	12:L:54:LEU:HD11	1.91	0.52
13:y:191:VAL:O	13:y:192:ILE:C	2.51	0.52
15:N:101:CYS:HB2	15:N:102:CYS:HG	1.74	0.52
16:O:97:ARG:NH1	16:O:136:MET:HE2	2.25	0.52
18:R:113:TYR:CB	18:R:230:MET:HE1	2.30	0.52
19:S:101:ALA:HB1	24:W:95:PRO:HD2	1.90	0.52
20:T:267:ASP:O	20:T:268:LYS:HB2	2.10	0.52
20:T:318:ARG:HH11	20:T:319:THR:HG23	1.74	0.52
20:T:454:VAL:CG2	20:T:463:SER:OG	2.58	0.52
1:A:61:MET:HB2	1:A:120:TYR:OH	2.10	0.52
1:A:433:GLU:OE1	1:A:436:PRO:CB	2.54	0.52
3:C:66:TYR:HB3	20:T:456:PRO:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:150:ILE:HD11	3:C:535:ALA:HB2	1.92	0.52
7:G:142:U:O5'	25:X:10:LYS:NZ	2.42	0.52
8:H:164:C:H5'	8:H:164:C:C6	2.44	0.52
10:J:192:GLU:CA	10:J:195:LEU:HD13	2.27	0.52
16:O:171:GLY:HA2	24:W:208:PRO:HG2	1.90	0.52
18:R:262:ILE:CG1	18:R:263:PRO:HD2	2.39	0.52
20:T:454:VAL:HG12	20:T:455:GLN:N	2.24	0.52
20:T:459:LEU:HD12	20:T:460:ASP:N	2.25	0.52
23:V:565:LEU:HD22	23:V:608:LEU:HD13	1.90	0.52
26:Y:80:CYS:HB2	26:Y:83:CYS:SG	2.49	0.52
1:A:245:LEU:HD22	1:A:430:TRP:CH2	2.44	0.52
1:A:339:PHE:HE1	1:A:406:TRP:HZ3	1.54	0.52
1:A:372:PRO:HG3	3:C:341:LYS:O	2.10	0.52
1:A:1530:PRO:CD	1:A:1533:ARG:NH1	2.73	0.52
3:C:82:GLN:HG3	20:T:238:LEU:H	1.74	0.52
3:C:93:ILE:HD13	20:T:230:ILE:HD13	1.92	0.52
3:C:902:HIS:ND1	3:C:903:HIS:HB2	2.25	0.52
6:F:25:C:H4'	6:F:26:U:O5'	2.09	0.52
7:G:21:A:O2'	7:G:22:C:C5'	2.58	0.52
7:G:146:C:H2'	7:G:147:C:O4'	2.10	0.52
16:O:165:CYS:HB2	16:O:181:TYR:HB2	1.90	0.52
18:R:95:LYS:HD3	18:R:95:LYS:N	2.25	0.52
19:S:60:PHE:CZ	24:W:98:PRO:HD3	2.45	0.52
20:T:347:THR:O	20:T:354:ILE:HG23	2.10	0.52
24:W:531:LYS:CA	24:W:546:PHE:O	2.58	0.52
25:X:58:GLU:C	25:X:61:GLY:CA	2.83	0.52
1:A:204:LEU:HD23	1:A:205:ASP:OD1	2.09	0.52
1:A:1258:LYS:CG	1:A:1527:ASN:HD21	2.22	0.52
3:C:300:LEU:HD13	3:C:300:LEU:N	2.25	0.52
6:F:45:A:C6	26:Y:34:ARG:NH1	2.73	0.52
8:H:40:C:C5'	26:Y:22:LYS:HG2	2.34	0.52
14:M:124:PHE:HE2	14:M:127:TYR:CE1	2.28	0.52
18:R:65:PRO:CB	19:S:90:LEU:HA	2.28	0.52
18:R:185:GLY:C	18:R:186:VAL:HG13	2.35	0.52
23:V:556:TYR:CG	23:V:557:THR:N	2.78	0.52
24:W:97:ASN:C	24:W:99:PHE:N	2.66	0.52
26:Y:25:LEU:N	26:Y:25:LEU:CD2	2.73	0.52
29:u:71:GLN:HG3	29:u:237:ILE:HG21	1.92	0.52
1:A:206:TRP:CD1	1:A:213:LEU:HD21	2.45	0.52
1:A:699:GLU:H	1:A:699:GLU:CD	2.18	0.52
1:A:1248:LEU:HD21	1:A:1295:ILE:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1530:PRO:CG	1:A:1533:ARG:NH1	2.73	0.52
3:C:143:THR:HB	47:C:1500:GTP:O1A	2.09	0.52
7:G:8:C:H2'	7:G:9:C:C6	2.45	0.52
24:W:155:SER:C	24:W:156:VAL:CG2	2.72	0.52
40:o:5:THR:CG2	40:o:8:LEU:H	2.23	0.52
1:A:651:TRP:CD1	6:F:66:C:H1'	2.44	0.52
1:A:682:ASP:CG	8:H:21:C:H4'	2.35	0.52
1:A:733:THR:N	1:A:734:PRO:CD	2.72	0.52
1:A:1880:PRO:O	45:4:8:GLY:HA2	2.10	0.52
3:C:388:VAL:O	3:C:388:VAL:HG22	2.10	0.52
6:F:68:C:C4	20:T:285:HIS:CG	2.98	0.52
14:M:160:PHE:HB3	14:M:161:PHE:CE1	2.44	0.52
16:O:149:LYS:HD2	16:O:290:LYS:NZ	2.25	0.52
19:S:36:CYS:HA	19:S:129:PHE:CE1	2.45	0.52
24:W:166:THR:OG1	24:W:169:GLU:CB	2.56	0.52
24:W:210:GLU:CD	24:W:211:GLU:H	2.11	0.52
25:X:50:ARG:O	25:X:51:GLU:C	2.52	0.52
26:Y:68:TYR:CD1	26:Y:68:TYR:C	2.88	0.52
3:C:333:ASP:OD1	3:C:333:ASP:N	2.42	0.51
5:E:229:TYR:CE2	5:E:272:ARG:NH1	2.77	0.51
14:M:163:THR:N	14:M:166:SER:CB	2.73	0.51
19:S:110:SER:O	19:S:111:GLN:C	2.50	0.51
24:W:109:ASN:CB	24:W:114:TYR:HD1	2.23	0.51
24:W:137:TYR:CE1	24:W:158:GLU:HB2	2.33	0.51
25:X:36:LYS:N	25:X:36:LYS:CE	2.73	0.51
1:A:672:VAL:HG21	20:T:267:ASP:OD1	2.10	0.51
3:C:89:LEU:O	3:C:91:GLU:N	2.43	0.51
3:C:600:LEU:N	3:C:601:PRO:HD2	2.25	0.51
3:C:678:THR:HG23	3:C:683:ASN:H	1.75	0.51
6:F:68:C:C4	20:T:285:HIS:CD2	2.99	0.51
6:F:85:U:C3'	6:F:86:U:C5'	2.89	0.51
7:G:6:A:N3	7:G:6:A:C5'	2.73	0.51
10:J:189:ILE:HG23	10:J:189:ILE:O	2.10	0.51
12:L:104:LEU:HD13	26:Y:162:GLN:O	2.10	0.51
16:O:88:LEU:HD11	24:W:111:LEU:HG	1.93	0.51
24:W:97:ASN:HD22	24:W:97:ASN:N	2.08	0.51
24:W:132:PHE:CD1	24:W:132:PHE:C	2.88	0.51
24:W:481:MET:C	24:W:483:ASN:H	2.18	0.51
26:Y:64:GLN:NE2	26:Y:64:GLN:CA	2.73	0.51
38:e:87:LEU:HB2	39:g:61:VAL:HB	1.92	0.51
1:A:364:SER:C	1:A:365:VAL:O	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ARG:NH1	1:A:900:ASP:OD1	2.44	0.51
3:C:710:ASN:O	3:C:711:ARG:C	2.53	0.51
6:F:22:A:C5	24:W:130:ARG:CG	2.92	0.51
6:F:45:A:C5'	6:F:45:A:N3	2.73	0.51
8:H:100:U:O2'	33:h:64:ARG:NH2	2.43	0.51
14:M:156:HIS:CD2	14:M:156:HIS:N	2.77	0.51
16:O:113:ASN:O	16:O:116:TYR:N	2.43	0.51
19:S:9:TRP:CE3	19:S:11:PRO:HG2	2.45	0.51
19:S:35:THR:O	19:S:129:PHE:CZ	2.63	0.51
20:T:306:CYS:SG	20:T:336:VAL:CB	2.97	0.51
1:A:468:LYS:HD3	1:A:468:LYS:C	2.35	0.51
1:A:794:TYR:HD1	1:A:800:TYR:CE2	2.29	0.51
1:A:1508:GLY:C	25:X:24:TRP:HE1	2.18	0.51
3:C:700:ILE:CG2	3:C:741:GLY:O	2.57	0.51
5:E:153:PHE:N	5:E:153:PHE:CD1	2.78	0.51
11:K:196:GLU:O	11:K:199:ILE:CG1	2.59	0.51
15:N:43:VAL:O	15:N:47:TRP:NE1	2.44	0.51
16:O:88:LEU:CD1	24:W:111:LEU:HG	2.41	0.51
16:O:283:ALA:O	16:O:287:SER:CB	2.58	0.51
20:T:297:HIS:HD2	20:T:338:CYS:SG	2.34	0.51
22:U:9:THR:HG23	22:U:9:THR:O	2.09	0.51
22:U:20:GLN:HE21	23:V:474:HIS:CE1	2.29	0.51
23:V:449:GLU:CB	23:V:452:LEU:HD12	2.39	0.51
1:A:128:PHE:CD1	1:A:473:PHE:CZ	2.98	0.51
1:A:312:TYR:N	1:A:312:TYR:CD1	2.78	0.51
3:C:499:GLY:C	3:C:500:THR:HG23	2.36	0.51
4:D:114:GLU:O	4:D:117:LEU:N	2.44	0.51
5:E:74:PHE:CD1	5:E:81:LEU:HD21	2.29	0.51
5:E:231:MET:SD	5:E:262:TRP:CE3	3.04	0.51
16:O:75:SER:O	16:O:79:ASN:N	2.43	0.51
26:Y:46:CYS:O	26:Y:82:ARG:NH1	2.43	0.51
29:u:256:VAL:CG2	29:u:403:MET:HE2	2.41	0.51
1:A:115:ASP:HB3	1:A:486:LYS:HE2	1.91	0.51
1:A:308:ILE:HG22	1:A:308:ILE:O	2.09	0.51
1:A:588:LEU:O	1:A:1551:PHE:HE1	1.90	0.51
1:A:1494:TYR:CG	1:A:1744:ARG:CD	2.93	0.51
7:G:151:C:H1'	7:G:152:C:C5'	2.41	0.51
8:H:154:C:OP2	41:p:19:LYS:HD3	2.09	0.51
10:J:195:LEU:CD2	12:L:24:MET:HE3	2.39	0.51
19:S:11:PRO:CA	19:S:166:GLY:HA3	2.41	0.51
24:W:189:ILE:O	24:W:189:ILE:HG13	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:41:GLN:CA	25:X:41:GLN:NE2	2.73	0.51
1:A:1306:LYS:NZ	2:B:38:C:O2'	2.44	0.51
1:A:1509:PHE:CB	25:X:21:GLU:CB	2.89	0.51
3:C:715:GLY:HA2	3:C:729:ALA:HB1	1.93	0.51
8:H:107:A:C6	8:H:108:G:C5	2.98	0.51
12:L:154:GLU:HB2	26:Y:49:TYR:CD2	2.46	0.51
14:M:176:THR:O	14:M:177:GLU:C	2.53	0.51
18:R:74:LEU:HB3	19:S:136:ILE:HG21	1.92	0.51
18:R:125:MET:O	18:R:126:ASN:HB3	2.11	0.51
28:r:47:LEU:CG	28:r:47:LEU:CA	2.82	0.51
33:h:55:VAL:HG21	40:o:67:LYS:NZ	2.25	0.51
1:A:1580:HIS:NE2	26:Y:17:PRO:HB3	2.26	0.51
3:C:753:GLU:C	3:C:755:ASP:H	2.19	0.51
6:F:50:A:OP1	12:L:165:LYS:HD2	2.10	0.51
7:G:21:A:H61	16:O:91:GLY:C	2.17	0.51
10:J:294:HIS:HE1	12:L:230:GLU:HB2	1.75	0.51
12:L:146:GLU:O	12:L:149:LEU:N	2.44	0.51
15:N:126:LEU:O	24:W:134:THR:CG2	2.58	0.51
16:O:36:MET:HE2	16:O:57:TRP:CE3	2.46	0.51
16:O:88:LEU:HD13	24:W:112:SER:HA	1.93	0.51
17:P:30:TYR:OH	18:R:164:PRO:CD	2.59	0.51
23:V:260:VAL:O	23:V:264:ILE:HG12	2.11	0.51
24:W:88:MET:SD	24:W:89:PHE:CB	2.98	0.51
26:Y:19:LYS:C	26:Y:20:ILE:HD13	2.35	0.51
3:C:457:VAL:HG12	3:C:462:GLY:CA	2.41	0.51
3:C:674:CYS:SG	3:C:822:MET:CE	2.99	0.51
3:C:749:THR:HG1	3:C:752:SER:HB2	1.74	0.51
4:D:441:GLY:O	4:D:693:THR:N	2.36	0.51
6:F:58:G:H2'	6:F:59:G:C8	2.46	0.51
6:F:88:G:H1'	14:M:121:ASP:HB3	1.93	0.51
13:y:10:THR:O	13:y:13:ALA:HB3	2.10	0.51
23:V:484:SER:C	23:V:486:THR:N	2.67	0.51
26:Y:130:LEU:N	26:Y:130:LEU:CD1	2.73	0.51
29:u:225:ILE:HD13	29:u:228:MET:HE3	1.93	0.51
29:u:307:MET:HE1	29:u:320:MET:SD	2.51	0.51
31:w:82:GLU:CG	31:w:112:TYR:HB3	2.40	0.51
1:A:203:VAL:CG2	1:A:237:THR:CB	2.88	0.51
1:A:434:HIS:C	1:A:434:HIS:HD1	2.19	0.51
1:A:748:ASP:HA	17:P:214:THR:HG21	1.92	0.51
1:A:762:ARG:HH12	17:P:226:LYS:NZ	2.09	0.51
3:C:65:TYR:C	3:C:66:TYR:CG	2.85	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:215:VAL:HG11	3:C:242:LEU:HD22	1.93	0.51
3:C:240:GLU:OE2	3:C:292:TYR:OH	2.18	0.51
15:N:1:MET:HB3	15:N:2:PRO:HD3	1.93	0.51
16:O:44:GLU:HA	16:O:50:ARG:O	2.10	0.51
16:O:75:SER:OG	16:O:76:LYS:N	2.44	0.51
20:T:385:TYR:CE2	20:T:400:PHE:HB3	2.46	0.51
1:A:122:ILE:CD1	1:A:483:GLN:CG	2.89	0.50
1:A:409:ARG:N	1:A:410:PRO:HD2	2.26	0.50
1:A:1498:TRP:HA	1:A:1501:LEU:HD12	1.89	0.50
3:C:456:GLY:O	3:C:457:VAL:HG13	2.11	0.50
5:E:276:ILE:C	5:E:277:PHE:HD1	2.19	0.50
6:F:43:A:O2'	6:F:44:G:C5'	2.58	0.50
6:F:48:A:HO2'	6:F:49:G:P	2.23	0.50
10:J:201:ARG:NE	10:J:203:LEU:HA	2.25	0.50
12:L:177:GLU:OE1	12:L:177:GLU:HA	2.11	0.50
23:V:291:GLU:OE1	23:V:331:ARG:NH2	2.43	0.50
24:W:162:ASN:CG	24:W:165:LEU:HD21	2.31	0.50
28:q:127:ALA:HB1	28:t:127:ALA:HB1	1.92	0.50
36:k:41:GLN:H	36:k:115:ILE:HB	1.76	0.50
40:o:102:GLU:HG2	40:o:128:LYS:HZ1	1.75	0.50
1:A:527:VAL:O	13:y:12:LEU:HD22	2.10	0.50
1:A:589:THR:OG1	1:A:590:GLY:N	2.44	0.50
3:C:301:SER:O	3:C:303:LEU:N	2.44	0.50
5:E:178:LEU:N	5:E:178:LEU:HD23	2.25	0.50
5:E:276:ILE:C	5:E:277:PHE:CD1	2.89	0.50
7:G:141:C:OP1	26:Y:60:LYS:NZ	2.42	0.50
10:J:201:ARG:O	10:J:203:LEU:N	2.44	0.50
18:R:134:ARG:O	18:R:135:PRO:C	2.54	0.50
23:V:536:ILE:CG2	23:V:579:SER:CA	2.89	0.50
34:i:50:LYS:HG2	34:i:51:ILE:HG13	1.93	0.50
37:f:20:MET:HE2	37:f:30:LYS:HB2	1.94	0.50
1:A:435:CYS:HB3	7:G:-11:G:N2	2.25	0.50
1:A:1436:TRP:CH2	1:A:1437:ARG:NH2	2.80	0.50
3:C:705:VAL:HG21	3:C:718:PHE:CZ	2.47	0.50
8:H:153:A:C2'	8:H:154:C:C5'	2.86	0.50
10:J:315:LYS:NZ	14:M:189:GLN:HE22	2.09	0.50
12:L:103:LEU:O	12:L:107:ALA:HB2	2.11	0.50
16:O:20:PHE:CE1	18:R:197:ILE:HD13	2.46	0.50
16:O:256:GLY:HA2	18:R:70:ALA:CB	2.42	0.50
26:Y:163:ARG:CG	26:Y:163:ARG:NH1	2.73	0.50
1:A:331:TRP:C	1:A:331:TRP:CE3	2.90	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:TRP:CD1	1:A:630:TRP:H	2.30	0.50
2:B:100:C:H2'	2:B:101:U:C6	2.47	0.50
3:C:569:ARG:HE	3:C:569:ARG:C	2.20	0.50
5:E:74:PHE:HE1	5:E:95:VAL:HG22	1.77	0.50
18:R:229:VAL:HG23	18:R:230:MET:N	2.27	0.50
19:S:10:GLN:HA	19:S:29:TRP:CE2	2.46	0.50
30:v:7:PHE:CE1	30:v:94:ILE:HG22	2.46	0.50
30:v:128:VAL:HG12	30:v:132:LYS:HE2	1.93	0.50
36:d:41:GLN:H	36:d:115:ILE:HB	1.76	0.50
1:A:95:MET:N	1:A:96:PRO:HD2	2.26	0.50
2:B:94:U:H5	36:d:104:ASP:O	1.94	0.50
3:C:846:VAL:HG22	3:C:887:LEU:HD11	1.94	0.50
8:H:40:C:OP1	13:y:14:ARG:NH2	2.45	0.50
8:H:111:G:O3'	8:H:112:G:O4'	2.29	0.50
10:J:203:LEU:HD13	10:J:204:GLU:CA	2.40	0.50
10:J:232:GLU:HG3	12:L:210:TYR:CE1	2.46	0.50
10:J:252:GLU:OE1	10:J:260:ARG:HB3	2.12	0.50
16:O:235:TYR:HD1	16:O:271:PHE:CE1	2.24	0.50
17:P:66:ARG:HH11	17:P:66:ARG:CG	2.24	0.50
18:R:135:PRO:O	18:R:136:ASP:CB	2.58	0.50
23:V:294:ILE:HG22	23:V:298:LYS:HE3	1.94	0.50
24:W:153:ILE:O	24:W:153:ILE:HG13	2.11	0.50
24:W:181:PHE:H	24:W:200:VAL:HG13	1.76	0.50
30:v:9:LEU:HD22	30:v:66:ILE:HD11	1.93	0.50
1:A:712:HIS:CG	18:R:250:CYS:HB2	2.47	0.50
1:A:760:ARG:NH2	1:A:766:THR:OG1	2.44	0.50
1:A:1904:ASP:O	1:A:1908:LYS:HG2	2.11	0.50
3:C:493:PHE:HD2	3:C:551:LEU:HD21	1.76	0.50
5:E:243:LEU:HD11	5:E:247:GLY:CA	2.41	0.50
6:F:22:A:H8	24:W:130:ARG:HH21	1.60	0.50
12:L:72:LEU:HD21	12:L:103:LEU:HD12	1.93	0.50
24:W:123:PHE:CZ	24:W:168:PHE:HD2	2.28	0.50
25:X:36:LYS:HA	25:X:36:LYS:CE	2.41	0.50
1:A:97:HIS:HD2	1:A:473:PHE:HZ	1.59	0.50
1:A:519:ASP:C	1:A:519:ASP:OD1	2.54	0.50
3:C:709:TRP:N	3:C:709:TRP:CD1	2.79	0.50
4:D:127:GLN:O	4:D:128:PRO:C	2.54	0.50
5:E:119:THR:CG2	5:E:161:ARG:CB	2.73	0.50
7:G:20:A:Cl'	16:O:193:LEU:HD21	2.40	0.50
13:y:10:THR:O	13:y:13:ALA:N	2.45	0.50
14:M:163:THR:CB	14:M:166:SER:HB2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:72:GLN:O	16:O:75:SER:OG	2.19	0.50
17:P:191:ASP:N	17:P:191:ASP:OD1	2.45	0.50
19:S:57:ILE:CG2	24:W:99:PHE:CB	2.75	0.50
20:T:300:ILE:O	20:T:301:ASP:HB2	2.11	0.50
31:w:74:ILE:HD13	31:w:120:GLU:HG3	1.93	0.50
1:A:386:PRO:HD3	3:C:372:PHE:CE1	2.46	0.50
1:A:1503:TRP:CZ3	1:A:1533:ARG:CD	2.90	0.50
3:C:259:LYS:HG2	47:C:1500:GTP:C6	2.46	0.50
3:C:336:TYR:CD1	3:C:336:TYR:C	2.89	0.50
5:E:267:PHE:CZ	11:K:194:GLU:CB	2.73	0.50
7:G:7:G:H2'	7:G:8:C:C6	2.47	0.50
14:M:168:LEU:HD23	14:M:168:LEU:H	1.76	0.50
23:V:166:ILE:O	23:V:170:ILE:HG12	2.12	0.50
29:u:322:GLU:HG3	29:u:327:ALA:HB3	1.93	0.50
38:l:87:LEU:HB2	39:n:61:VAL:HB	1.92	0.50
1:A:347:LEU:HD13	1:A:351:TYR:OH	2.12	0.50
1:A:381:PRO:HD2	3:C:334:ILE:HG21	1.91	0.50
2:B:87:A:H2'	37:f:39:TYR:CE2	2.47	0.50
3:C:221:ILE:O	3:C:448:LYS:NZ	2.45	0.50
3:C:619:THR:O	3:C:620:LYS:HG3	2.12	0.50
6:F:27:A:C2	16:O:181:TYR:CE2	3.00	0.50
7:G:21:A:C6	16:O:92:LEU:HD23	2.46	0.50
7:G:150:U:H2'	7:G:151:C:C5'	2.37	0.50
8:H:153:A:H3'	8:H:154:C:C5'	2.38	0.50
12:L:172:ARG:HH12	26:Y:82:ARG:HA	1.75	0.50
26:Y:39:PHE:CD1	26:Y:39:PHE:C	2.89	0.50
37:f:51:ILE:HG22	37:f:56:SER:HB2	1.93	0.50
38:e:15:VAL:O	39:g:33:GLY:HA3	2.12	0.50
1:A:273:ILE:CG2	1:A:274:PRO:HD2	2.42	0.49
1:A:525:LYS:HD2	26:Y:10:TYR:HB2	1.94	0.49
1:A:592:TYR:CD1	1:A:592:TYR:C	2.90	0.49
1:A:790:ARG:CZ	1:A:986:GLU:OE2	2.60	0.49
1:A:1365:ILE:O	23:V:465:SER:HB2	2.12	0.49
1:A:1489:LEU:HD12	1:A:1536:LEU:O	2.12	0.49
1:A:1949:ARG:HD2	1:A:1986:LEU:CD2	2.39	0.49
2:B:23:C:HO2'	2:B:24:G:P	2.34	0.49
3:C:335:ASN:OD1	3:C:336:TYR:N	2.45	0.49
3:C:499:GLY:O	3:C:500:THR:CG2	2.60	0.49
3:C:854:ARG:NH1	3:C:879:ASP:OD2	2.44	0.49
5:E:74:PHE:HE1	5:E:95:VAL:CG2	2.25	0.49
5:E:228:THR:HG22	5:E:229:TYR:HD1	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:188:LEU:C	11:K:188:LEU:HD13	2.36	0.49
18:R:79:LYS:NZ	18:R:80:LYS:NZ	2.60	0.49
18:R:282:GLU:C	18:R:284:PHE:N	2.66	0.49
20:T:318:ARG:HG3	20:T:318:ARG:HH11	1.76	0.49
20:T:329:HIS:CE1	20:T:355:ARG:HG3	2.46	0.49
26:Y:109:GLN:CD	26:Y:110:ALA:N	2.69	0.49
1:A:348:PRO:O	1:A:350:PHE:N	2.45	0.49
1:A:1210:LYS:O	1:A:1211:ASP:C	2.54	0.49
1:A:1487:HIS:O	1:A:1541:THR:OG1	2.26	0.49
1:A:1503:TRP:CZ3	1:A:1533:ARG:CZ	2.84	0.49
3:C:350:ASN:HB3	3:C:353:THR:HG23	1.94	0.49
3:C:659:VAL:HG12	3:C:660:VAL:N	2.26	0.49
5:E:263:ASP:O	5:E:272:ARG:NE	2.32	0.49
6:F:27:A:C2	16:O:181:TYR:CD2	3.00	0.49
8:H:36:G:HI1'	26:Y:4:ARG:HH22	1.75	0.49
16:O:161:ARG:NH2	16:O:182:ARG:HD2	2.28	0.49
18:R:103:ARG:CG	18:R:103:ARG:NH1	2.75	0.49
23:V:536:ILE:HG23	23:V:579:SER:HA	1.94	0.49
38:l:20:LEU:HD13	39:n:61:VAL:CG2	2.42	0.49
33:a:75:ASP:O	33:a:78:LYS:HG2	2.12	0.49
1:A:120:TYR:CE1	1:A:485:THR:HB	2.47	0.49
1:A:726:TRP:CE3	1:A:726:TRP:O	2.65	0.49
1:A:1384:ARG:NH2	1:A:1414:ARG:HH11	2.10	0.49
3:C:381:LEU:CD2	3:C:416:LEU:HD22	2.42	0.49
3:C:387:ASP:O	3:C:389:ASP:OD1	2.30	0.49
8:H:107:A:C2	8:H:108:G:C4	3.01	0.49
10:J:406:PHE:CD2	10:J:411:MET:HE2	2.45	0.49
16:O:155:PRO:HG3	18:R:188:PHE:HA	1.94	0.49
16:O:253:TYR:CD1	19:S:93:THR:OG1	2.63	0.49
18:R:77:GLY:HA2	18:R:78:ARG:CZ	2.43	0.49
20:T:281:ILE:HD12	20:T:282:ARG:HG2	1.93	0.49
24:W:88:MET:SD	24:W:88:MET:C	2.95	0.49
24:W:207:LYS:HB2	24:W:207:LYS:NZ	2.27	0.49
26:Y:33:VAL:HG12	26:Y:34:ARG:O	2.12	0.49
37:m:20:MET:HE2	37:m:30:LYS:HB2	1.94	0.49
37:m:51:ILE:HG22	37:m:56:SER:HB2	1.94	0.49
1:A:152:ARG:CG	1:A:152:ARG:NH1	2.73	0.49
1:A:467:GLN:HE21	2:B:19:A:N6	2.10	0.49
1:A:1328:LEU:HD22	1:A:1368:LEU:HD21	1.95	0.49
3:C:363:SER:O	3:C:364:SER:CB	2.60	0.49
5:E:265:ARG:N	5:E:272:ARG:HH21	2.10	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:81:C:H4'	6:F:82:A:OP2	2.12	0.49
7:G:5:G:C5'	7:G:5:G:C8	2.96	0.49
8:H:106:G:H5'	37:m:25:TRP:HH2	1.76	0.49
17:P:41:ILE:HD11	20:T:318:ARG:HA	1.93	0.49
23:V:234:LEU:CD2	23:V:263:LEU:HD13	2.42	0.49
23:V:466:SER:HB2	23:V:471:GLU:CD	2.37	0.49
26:Y:70:GLY:N	26:Y:71:LEU:HD12	2.26	0.49
1:A:117:PRO:HG2	1:A:131:GLU:HB2	1.94	0.49
1:A:121:HIS:HD2	1:A:482:PHE:CE1	2.30	0.49
1:A:461:HIS:NE2	2:B:23:C:C5	2.80	0.49
1:A:1489:LEU:HD11	1:A:1536:LEU:HD22	1.94	0.49
3:C:753:GLU:O	3:C:755:ASP:N	2.45	0.49
8:H:27:U:C2'	8:H:28:C:H5'	2.42	0.49
12:L:144:MET:CB	12:L:149:LEU:HD11	2.43	0.49
18:R:128:ASP:OD1	20:T:384:HIS:CD2	2.66	0.49
20:T:442:ARG:HB3	20:T:443:THR:HG23	1.95	0.49
23:V:549:LYS:O	23:V:552:ALA:CB	2.60	0.49
24:W:178:ARG:HH12	24:W:202:GLU:HG2	1.77	0.49
33:h:75:ASP:O	33:h:78:LYS:HG2	2.12	0.49
38:l:15:VAL:O	39:n:33:GLY:HA3	2.12	0.49
1:A:76:MET:SD	1:A:88:TYR:CE1	3.05	0.49
1:A:115:ASP:CB	1:A:486:LYS:HE2	2.43	0.49
1:A:823:SER:OG	1:A:933:ARG:NH1	2.46	0.49
1:A:1525:GLY:C	1:A:1528:GLN:HG2	2.37	0.49
1:A:1530:PRO:CD	1:A:1533:ARG:CZ	2.86	0.49
1:A:1868:MET:HE3	1:A:1872:LEU:HG	1.94	0.49
2:B:93:U:O2'	37:f:65:ARG:NH2	2.46	0.49
3:C:911:PRO:HB2	3:C:934:MET:HE3	1.95	0.49
6:F:35:A:OP1	12:L:203:LYS:HG3	2.13	0.49
7:G:150:U:C3'	7:G:150:U:C6	2.96	0.49
8:H:104:U:O2'	37:m:65:ARG:NH2	2.45	0.49
16:O:240:GLY:HA3	16:O:296:ARG:NH1	2.24	0.49
18:R:303:GLU:O	18:R:307:GLN:CG	2.61	0.49
19:S:34:LYS:HE3	19:S:78:TYR:CD2	2.47	0.49
23:V:151:SER:O	23:V:155:GLN:HG3	2.13	0.49
29:u:70:LYS:O	29:u:74:LYS:HG3	2.13	0.49
29:u:185:VAL:HG22	29:u:215:VAL:HB	1.94	0.49
38:e:20:LEU:HD13	39:g:61:VAL:CG2	2.43	0.49
1:A:850:TYR:HD2	1:A:864:LEU:HD13	1.78	0.49
1:A:1012:LYS:O	1:A:1015:VAL:HG13	2.13	0.49
1:A:1275:ARG:HD2	1:A:1375:TRP:CD2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1949:ARG:HD3	1:A:1986:LEU:HD11	1.93	0.49
2:B:89:U:O2'	33:a:64:ARG:NH2	2.43	0.49
5:E:162:ARG:HH21	5:E:204:THR:HA	1.78	0.49
5:E:263:ASP:OD1	5:E:272:ARG:HB3	2.13	0.49
7:G:-2:C:C3'	7:G:-1:G:H5''	2.43	0.49
7:G:150:U:H3'	7:G:150:U:C6	2.47	0.49
23:V:497:CYS:HA	23:V:500:GLN:OE1	2.12	0.49
24:W:210:GLU:CB	24:W:213:GLN:OE1	2.61	0.49
24:W:290:GLY:HA2	24:W:573:GLY:HA2	1.94	0.49
25:X:35:LYS:C	25:X:36:LYS:HE2	2.38	0.49
26:Y:169:PHE:O	26:Y:173:LEU:CB	2.61	0.49
34:b:50:LYS:HG2	34:b:51:ILE:HG13	1.93	0.49
1:A:89:LEU:CD2	1:A:656:LEU:HD22	2.42	0.49
1:A:259:ASP:C	1:A:259:ASP:OD1	2.55	0.49
1:A:1930:TYR:HE1	25:X:71:ASP:N	2.09	0.49
1:A:2003:THR:CB	25:X:47:GLU:CB	2.91	0.49
3:C:334:ILE:HD12	3:C:334:ILE:O	2.13	0.49
5:E:67:GLY:H	5:E:87:ASP:CG	2.20	0.49
12:L:158:ARG:HH21	26:Y:51:TYR:HH	1.54	0.49
14:M:153:ARG:HB2	14:M:160:PHE:CE2	2.47	0.49
23:V:455:PHE:O	23:V:459:ILE:HG12	2.12	0.49
26:Y:138:GLU:CB	27:Z:1096:GLY:O	2.60	0.49
1:A:120:TYR:CZ	1:A:483:GLN:CB	2.96	0.49
1:A:299:ILE:CD1	1:A:1342:TRP:CZ3	2.95	0.49
3:C:510:LEU:HD22	3:C:514:TYR:HE2	1.75	0.49
3:C:736:GLY:N	3:C:770:PHE:HE2	2.10	0.49
6:F:34:G:C5'	6:F:34:G:C8	2.95	0.49
7:G:135:G:N2	8:H:41:U:C2	2.77	0.49
14:M:160:PHE:CB	14:M:161:PHE:HD1	2.20	0.49
16:O:35:ARG:HD3	24:W:129:ARG:NH1	2.27	0.49
18:R:81:LYS:HA	18:R:81:LYS:HE3	1.87	0.49
18:R:189:ASN:HD21	18:R:195:ARG:CZ	2.26	0.49
24:W:100:ARG:HB3	24:W:104:MET:HB3	1.95	0.49
26:Y:70:GLY:H	26:Y:71:LEU:CD1	2.26	0.49
31:w:77:VAL:HB	31:w:117:THR:HG22	1.95	0.49
1:A:122:ILE:HD12	1:A:483:GLN:HG3	1.94	0.49
1:A:304:ILE:HD12	3:C:921:LEU:HD12	1.94	0.49
1:A:494:LEU:HD21	1:A:562:VAL:HG21	1.95	0.49
1:A:1211:ASP:C	1:A:1213:VAL:N	2.71	0.49
1:A:1330:MET:HG3	1:A:1367:ASN:HD21	1.76	0.49
1:A:1488:THR:O	1:A:1540:PRO:HG2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:301:SER:C	3:C:303:LEU:N	2.68	0.49
7:G:147:C:C4'	7:G:148:U:OP2	2.60	0.49
9:I:640:ALA:HA	10:J:512:GLU:O	2.11	0.49
18:R:215:ASN:HD22	18:R:216:LYS:N	2.11	0.49
23:V:506:PHE:CD1	23:V:506:PHE:C	2.90	0.49
24:W:88:MET:CE	24:W:89:PHE:CD2	2.90	0.49
24:W:140:ASP:HB2	24:W:153:ILE:HG21	1.93	0.49
26:Y:70:GLY:C	26:Y:71:LEU:HG	2.37	0.49
28:r:94:GLN:O	28:r:97:GLN:CG	2.60	0.49
1:A:44:ARG:CG	1:A:45:TYR:CE2	2.96	0.48
1:A:760:ARG:CZ	1:A:766:THR:OG1	2.61	0.48
1:A:1307:MET:HE1	1:A:1549:VAL:O	2.13	0.48
1:A:1370:ARG:NH1	23:V:506:PHE:CD2	2.78	0.48
1:A:1868:MET:CE	1:A:1872:LEU:CD1	2.91	0.48
2:B:20:G:H1'	2:B:21:A:OP1	2.12	0.48
5:E:164:PRO:O	5:E:166:LEU:HG	2.13	0.48
6:F:39:A:C2'	6:F:40:U:H5'	2.43	0.48
8:H:98:G:H2'	37:m:39:TYR:CE2	2.47	0.48
12:L:59:LYS:CE	12:L:91:ARG:NH1	2.71	0.48
13:y:54:SER:CA	13:y:57:VAL:HG22	2.43	0.48
18:R:55:LEU:CA	18:R:73:PRO:O	2.61	0.48
18:R:184:GLN:O	18:R:188:PHE:HB2	2.13	0.48
19:S:34:LYS:HE2	19:S:78:TYR:CD2	2.48	0.48
19:S:131:ARG:HH12	19:S:133:CYS:CB	2.26	0.48
23:V:608:LEU:O	23:V:612:PHE:HB2	2.12	0.48
26:Y:19:LYS:C	26:Y:20:ILE:CD1	2.86	0.48
26:Y:109:GLN:CD	26:Y:110:ALA:H	2.21	0.48
26:Y:158:LYS:O	26:Y:163:ARG:CG	2.60	0.48
3:C:297:ASN:HD22	3:C:298:LEU:CD1	2.26	0.48
3:C:499:GLY:O	3:C:500:THR:HG23	2.13	0.48
3:C:709:TRP:CD1	3:C:709:TRP:H	2.30	0.48
10:J:260:ARG:HH12	12:L:215:PRO:HD3	1.78	0.48
20:T:342:GLU:O	20:T:343:PRO:C	2.56	0.48
20:T:384:HIS:O	20:T:385:TYR:HB3	2.13	0.48
20:T:399:LYS:HG3	20:T:406:ILE:CD1	2.37	0.48
24:W:189:ILE:O	24:W:190:ASP:HB2	2.13	0.48
26:Y:70:GLY:C	26:Y:71:LEU:CG	2.85	0.48
26:Y:138:GLU:CB	27:Z:1097:MET:N	2.76	0.48
1:A:134:TRP:HB3	1:A:418:THR:HG22	1.95	0.48
1:A:732:PRO:HG2	18:R:247:ILE:CD1	2.43	0.48
1:A:1275:ARG:HD2	1:A:1375:TRP:CE2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:116:MET:O	3:C:119:LEU:HB3	2.13	0.48
3:C:291:MET:CG	3:C:292:TYR:CE1	2.96	0.48
3:C:438:ILE:CD1	3:C:438:ILE:N	2.76	0.48
5:E:269:PRO:O	5:E:270:LYS:CB	2.54	0.48
16:O:147:LEU:HA	16:O:150:LEU:HG	1.94	0.48
24:W:127:GLN:HG3	24:W:168:PHE:CE2	2.48	0.48
29:u:349:ILE:HG12	29:u:368:SER:HB3	1.95	0.48
1:A:300:ASN:C	3:C:939:ARG:NH2	2.66	0.48
5:E:161:ARG:HH11	5:E:161:ARG:CG	2.26	0.48
6:F:77:C:C2'	6:F:78:A:H5'	2.44	0.48
13:y:54:SER:HA	13:y:57:VAL:HG22	1.95	0.48
15:N:65:TYR:OH	15:N:93:LYS:HE2	2.14	0.48
18:R:55:LEU:C	18:R:73:PRO:O	2.56	0.48
18:R:73:PRO:HG2	18:R:74:LEU:H	1.79	0.48
20:T:302:VAL:HG23	20:T:315:TRP:O	2.14	0.48
23:V:625:ARG:O	23:V:629:ASN:CB	2.62	0.48
24:W:88:MET:SD	24:W:89:PHE:N	2.86	0.48
26:Y:42:ARG:HG3	26:Y:49:TYR:HE1	1.76	0.48
26:Y:70:GLY:C	26:Y:71:LEU:CD1	2.85	0.48
29:u:89:THR:HA	29:u:92:PHE:CE2	2.48	0.48
40:o:66:LEU:HD21	40:o:69:LEU:HG	1.95	0.48
37:f:10:PHE:CE2	38:e:78:MET:HB2	2.49	0.48
1:A:279:PHE:CE1	1:A:452:LYS:HE3	2.48	0.48
1:A:323:LEU:N	1:A:324:PRO:CD	2.77	0.48
1:A:412:ASN:OD1	1:A:413:LEU:HD23	2.13	0.48
3:C:557:GLN:N	3:C:558:PRO:HD2	2.29	0.48
5:E:266:PRO:CD	12:L:785:GLN:HB2	2.43	0.48
6:F:28:A:C6	16:O:167:PHE:CG	3.01	0.48
6:F:36:A:HO2'	6:F:37:C:P	2.36	0.48
7:G:6:A:O2'	7:G:7:G:H5'	2.13	0.48
25:X:36:LYS:N	25:X:36:LYS:CD	2.76	0.48
30:v:9:LEU:HD12	30:v:92:ILE:HG12	1.95	0.48
1:A:258:PHE:HZ	1:A:275:GLY:O	1.96	0.48
1:A:758:ARG:NH2	1:A:775:ASN:HD22	2.11	0.48
3:C:244:LYS:CA	3:C:292:TYR:CD2	2.92	0.48
3:C:349:PHE:HB2	3:C:356:PHE:CE1	2.48	0.48
3:C:507:VAL:HG12	3:C:508:LYS:N	2.29	0.48
3:C:749:THR:O	3:C:753:GLU:HB2	2.14	0.48
23:V:622:ARG:HA	23:V:625:ARG:NH1	2.29	0.48
25:X:41:GLN:HE21	25:X:41:GLN:HA	1.77	0.48
26:Y:129:GLU:C	26:Y:130:LEU:HD12	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:k:107:ILE:HG22	36:k:108:VAL:CG2	2.39	0.48
2:B:92:U:O4	34:b:38:MET:HG3	2.14	0.48
3:C:297:ASN:HB3	3:C:298:LEU:HD13	1.95	0.48
3:C:690:GLU:HB2	3:C:691:PRO:HD2	1.95	0.48
8:H:103:U:O4	34:i:38:MET:HG3	2.14	0.48
9:I:712:VAL:O	9:I:713:ARG:C	2.57	0.48
10:J:197:GLU:HG2	12:L:156:ARG:HD3	1.95	0.48
16:O:55:PHE:CE1	18:R:199:MET:HE1	2.48	0.48
18:R:51:ILE:N	18:R:52:PRO:CD	2.77	0.48
19:S:20:MET:CE	19:S:141:ARG:HD2	2.44	0.48
23:V:493:ILE:HD11	23:V:510:LEU:HD23	1.94	0.48
24:W:101:THR:HG23	24:W:104:MET:N	2.25	0.48
26:Y:68:TYR:HB3	26:Y:71:LEU:HD13	1.95	0.48
1:A:232:LEU:CD1	3:C:385:VAL:O	2.61	0.48
3:C:349:PHE:CD1	3:C:356:PHE:HE1	2.22	0.48
3:C:401:ILE:HD11	3:C:423:PHE:HB2	1.95	0.48
6:F:43:A:C2	7:G:5:G:N1	2.82	0.48
10:J:192:GLU:HA	10:J:195:LEU:HD11	1.87	0.48
12:L:14:THR:HG21	12:L:148:GLU:HB3	1.96	0.48
14:M:163:THR:H	14:M:166:SER:CB	2.27	0.48
18:R:74:LEU:CG	19:S:136:ILE:HG21	2.44	0.48
23:V:467:LEU:O	23:V:468:ASP:CB	2.62	0.48
23:V:502:THR:HG22	23:V:503:TYR:N	2.29	0.48
23:V:532:GLN:O	23:V:536:ILE:HG13	2.14	0.48
24:W:97:ASN:ND2	24:W:97:ASN:O	2.47	0.48
26:Y:39:PHE:O	26:Y:39:PHE:HD1	1.97	0.48
1:A:203:VAL:HG12	1:A:207:PHE:CD1	2.49	0.48
1:A:406:TRP:HZ3	3:C:265:LEU:O	1.96	0.48
1:A:1295:ILE:HG13	1:A:1296:GLN:N	2.28	0.48
6:F:35:A:C5'	6:F:35:A:C8	2.93	0.48
6:F:50:A:HO2'	6:F:51:U:P	2.36	0.48
7:G:4:A:N6	7:G:5:G:C6	2.82	0.48
7:G:13:C:H2'	7:G:14:A:H8	1.75	0.48
7:G:136:U:H2'	7:G:137:C:C6	2.48	0.48
7:G:149:G:O2'	7:G:150:U:O5'	2.24	0.48
12:L:104:LEU:HD13	26:Y:162:GLN:C	2.39	0.48
23:V:152:LEU:HA	23:V:387:MET:SD	2.54	0.48
23:V:497:CYS:CB	23:V:507:PHE:HB3	2.44	0.48
26:Y:6:VAL:HG12	26:Y:8:ASN:O	2.13	0.48
1:A:549:GLU:CD	1:A:552:ARG:NH1	2.72	0.48
1:A:666:LYS:HB2	1:A:668:VAL:HG23	1.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:HIS:ND1	18:R:250:CYS:HB2	2.29	0.48
1:A:984:MET:HG3	1:A:1048:MET:HE1	1.95	0.48
3:C:196:LYS:HZ2	34:b:11:GLN:CG	2.26	0.48
3:C:250:ARG:NE	3:C:451:HIS:CD2	2.76	0.48
3:C:457:VAL:HG12	3:C:462:GLY:HA3	1.96	0.48
3:C:855:GLY:O	3:C:856:HIS:CB	2.44	0.48
8:H:32:U:H2'	8:H:33:G:O4'	2.14	0.48
8:H:69:U:H2'	8:H:70:C:C6	2.49	0.48
8:H:143:A:N3	8:H:143:A:C3'	2.73	0.48
12:L:52:GLU:CD	12:L:134:THR:HG1	2.04	0.48
16:O:171:GLY:HA2	24:W:208:PRO:HD3	1.95	0.48
20:T:213:GLU:HG3	20:T:218:TRP:NE1	2.29	0.48
23:V:525:PHE:O	23:V:526:GLU:C	2.55	0.48
24:W:100:ARG:HG2	24:W:100:ARG:HH11	1.78	0.48
24:W:110:MET:HG3	24:W:110:MET:O	2.12	0.48
29:u:244:ASP:HB2	29:u:397:SER:HB2	1.95	0.48
30:v:113:ASN:HA	30:v:118:PRO:HB3	1.95	0.48
33:h:24:THR:O	33:h:51:ARG:NH1	2.46	0.48
33:h:45:ASN:HB3	40:o:22:ARG:HH11	1.79	0.48
1:A:277:PRO:HA	1:A:448:GLN:HG3	1.95	0.47
1:A:379:GLU:HA	3:C:354:ARG:O	2.13	0.47
1:A:1084:PRO:HG2	17:P:188:TRP:CD2	2.49	0.47
3:C:514:TYR:CD1	3:C:515:THR:N	2.82	0.47
3:C:673:LYS:HB3	3:C:688:ILE:HG22	1.96	0.47
7:G:21:A:N6	16:O:92:LEU:HA	2.28	0.47
8:H:40:C:C5'	26:Y:22:LYS:CG	2.91	0.47
8:H:90:A:H5'	24:W:499:LYS:CA	2.43	0.47
16:O:27:CYS:O	16:O:28:LEU:C	2.56	0.47
16:O:146:MET:O	16:O:149:LYS:N	2.40	0.47
18:R:265:ASP:OD2	18:R:266:LYS:HD3	2.13	0.47
31:w:77:VAL:HB	31:w:117:THR:HG23	1.95	0.47
1:A:1889:LEU:CD1	1:A:2012:LEU:HG	2.42	0.47
5:E:219:VAL:HB	5:E:229:TYR:HB2	1.95	0.47
5:E:267:PHE:CZ	11:K:194:GLU:CA	2.97	0.47
7:G:2:U:H3	7:G:144:A:N6	2.11	0.47
7:G:149:G:HO2'	7:G:150:U:P	2.36	0.47
18:R:103:ARG:NH2	18:R:110:LYS:O	2.40	0.47
20:T:246:ILE:HB	20:T:267:ASP:OD1	2.15	0.47
20:T:416:ILE:O	20:T:416:ILE:HD13	2.14	0.47
37:m:10:PHE:CE2	38:l:78:MET:HB2	2.49	0.47
1:A:385:GLU:OE1	1:A:386:PRO:HD2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1531:ASN:C	1:A:1531:ASN:OD1	2.57	0.47
1:A:1813:ARG:HB3	1:A:1813:ARG:NH1	2.30	0.47
3:C:93:ILE:O	3:C:94:ILE:CB	2.62	0.47
3:C:150:ILE:CD1	3:C:535:ALA:HB2	2.44	0.47
7:G:2:U:O2	7:G:144:A:N1	2.47	0.47
10:J:216:ASP:O	10:J:219:GLU:N	2.47	0.47
10:J:219:GLU:OE1	12:L:189:ARG:NE	2.46	0.47
20:T:185:MET:CB	20:T:186:PRO:CD	2.90	0.47
20:T:213:GLU:HB2	20:T:218:TRP:O	2.13	0.47
23:V:523:GLU:CG	23:V:524:SER:N	2.76	0.47
23:V:540:GLU:OE1	23:V:541:THR:CG2	2.41	0.47
24:W:210:GLU:HA	24:W:213:GLN:CD	2.27	0.47
29:u:307:MET:HE2	29:u:319:ILE:CG2	2.44	0.47
36:k:108:VAL:CG1	37:m:62:VAL:HG13	2.45	0.47
1:A:210:HIS:CD2	1:A:210:HIS:C	2.92	0.47
1:A:238:LEU:HB3	1:A:411:PHE:HE1	1.79	0.47
1:A:409:ARG:HD2	1:A:409:ARG:O	2.14	0.47
2:B:20:G:OP1	2:B:20:G:H4'	2.12	0.47
3:C:221:ILE:HG23	3:C:495:ARG:HB3	1.96	0.47
5:E:209:ILE:HG21	5:E:250:LEU:HD11	1.93	0.47
6:F:12:G:H2'	6:F:13:G:O4'	2.15	0.47
8:H:151:C:C2	8:H:152:G:N7	2.82	0.47
10:J:360:ASP:HA	10:J:363:ARG:CG	2.44	0.47
17:P:30:TYR:HH	18:R:164:PRO:HD3	1.78	0.47
22:U:23:LEU:N	23:V:474:HIS:HD2	2.03	0.47
23:V:470:GLU:OE2	23:V:513:ARG:NH1	2.44	0.47
23:V:576:THR:O	23:V:579:SER:N	2.47	0.47
24:W:126:GLU:CD	24:W:130:ARG:NH1	2.57	0.47
24:W:127:GLN:CG	24:W:168:PHE:CE2	2.97	0.47
24:W:491:GLN:O	24:W:492:ASN:C	2.57	0.47
25:X:7:ASN:OD1	26:Y:36:MET:O	2.31	0.47
25:X:36:LYS:H	25:X:36:LYS:HD2	1.80	0.47
1:A:47:GLU:OE1	1:A:47:GLU:N	2.35	0.47
1:A:155:LYS:HD2	1:A:626:GLY:C	2.39	0.47
1:A:299:ILE:CD1	1:A:1342:TRP:CH2	2.98	0.47
3:C:114:TYR:HE1	35:c:12:HIS:HB3	1.73	0.47
3:C:678:THR:HG23	3:C:683:ASN:CA	2.43	0.47
6:F:28:A:O4'	15:N:41:ARG:HA	2.15	0.47
6:F:49:G:O2'	26:Y:51:TYR:CD2	2.48	0.47
7:G:22:C:O2'	7:G:23:U:P	2.71	0.47
10:J:436:TYR:OH	10:J:458:PHE:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:O:292:ILE:HG23	16:O:296:ARG:C	2.40	0.47
18:R:120:VAL:CG2	18:R:121:PRO:HD2	2.44	0.47
18:R:176:TYR:OH	24:W:122:ASP:OD1	2.28	0.47
28:q:47:LEU:CG	28:q:47:LEU:CA	2.81	0.47
1:A:91:ALA:O	1:A:94:TYR:N	2.43	0.47
1:A:232:LEU:HD13	1:A:404:LEU:HD12	1.95	0.47
1:A:378:PHE:CD1	1:A:378:PHE:C	2.93	0.47
1:A:464:PRO:HG3	2:B:20:G:N3	2.30	0.47
1:A:1614:ILE:HG22	1:A:1615:HIS:O	2.14	0.47
1:A:1758:PRO:HG3	45:4:8:GLY:C	2.37	0.47
2:B:12:U:H3	2:B:65:G:H1	1.62	0.47
7:G:134:U:H2'	7:G:135:G:H5'	1.96	0.47
12:L:158:ARG:NE	26:Y:51:TYR:CZ	2.77	0.47
13:y:30:PRO:HD2	13:y:87:TRP:HH2	1.79	0.47
20:T:257:ARG:HD3	20:T:301:ASP:OD1	2.14	0.47
25:X:30:HIS:CG	26:Y:69:LEU:CD2	2.98	0.47
30:v:99:ILE:CD1	30:v:101:PHE:HE1	2.27	0.47
35:j:20:LYS:HE2	35:j:63:ASN:O	2.15	0.47
1:A:121:HIS:HD2	1:A:482:PHE:CZ	2.31	0.47
1:A:195:LEU:H	1:A:195:LEU:HD12	1.80	0.47
1:A:229:GLN:CB	1:A:415:SER:HB2	2.45	0.47
1:A:232:LEU:HD21	3:C:412:ILE:CD1	2.44	0.47
1:A:330:THR:O	1:A:331:TRP:CB	2.62	0.47
1:A:340:ILE:HD13	1:A:340:ILE:N	2.29	0.47
1:A:606:LYS:NZ	1:A:1548:TYR:O	2.26	0.47
1:A:623:LYS:HG2	46:A:3000:IHP:O43	2.13	0.47
1:A:948:PRO:N	1:A:949:PRO:HD2	2.29	0.47
1:A:1094:ARG:HH11	1:A:1094:ARG:CB	2.27	0.47
1:A:1539:SER:N	1:A:1540:PRO:CD	2.78	0.47
1:A:1835:GLN:OE1	1:A:1835:GLN:HA	2.14	0.47
1:A:1853:PRO:HB3	43:2:613:THR:O	2.12	0.47
3:C:477:HIS:HD1	3:C:478:THR:N	2.12	0.47
3:C:559:ILE:HD12	3:C:559:ILE:O	2.15	0.47
5:E:178:LEU:CD2	5:E:208:ILE:HD13	2.44	0.47
5:E:255:MET:C	5:E:257:ASN:H	2.21	0.47
6:F:85:U:C2'	6:F:86:U:H5''	2.45	0.47
8:H:153:A:C8	8:H:154:C:H5'	2.50	0.47
12:L:49:ARG:HD3	12:L:49:ARG:C	2.38	0.47
16:O:226:PRO:HG3	16:O:302:TRP:CH2	2.50	0.47
16:O:236:VAL:HB	16:O:270:ALA:O	2.15	0.47
17:P:64:GLU:OE2	17:P:68:ARG:NE	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:88:ILE:HD12	18:R:88:ILE:N	2.29	0.47
18:R:282:GLU:O	18:R:285:ALA:N	2.36	0.47
19:S:125:LYS:HE3	19:S:125:LYS:N	2.30	0.47
24:W:137:TYR:OH	24:W:165:LEU:HG	2.14	0.47
25:X:35:LYS:N	25:X:35:LYS:CD	2.73	0.47
30:v:7:PHE:HE1	30:v:94:ILE:HG22	1.80	0.47
31:w:125:LYS:HZ3	31:w:126:GLU:CG	2.27	0.47
33:a:43:MET:HB3	33:a:46:ILE:HD11	1.97	0.47
35:c:6:PHE:CD1	35:c:6:PHE:C	2.93	0.47
36:d:108:VAL:CG1	37:f:62:VAL:HG13	2.44	0.47
1:A:120:TYR:CG	1:A:483:GLN:O	2.68	0.47
1:A:127:SER:CB	1:A:495:GLN:OE1	2.61	0.47
1:A:279:PHE:CZ	1:A:452:LYS:HG3	2.49	0.47
1:A:380:LEU:HD23	3:C:349:PHE:CZ	2.48	0.47
3:C:366:GLN:O	3:C:367:ARG:C	2.58	0.47
5:E:243:LEU:CD1	5:E:247:GLY:CA	2.84	0.47
6:F:44:G:O5'	6:F:44:G:H8	1.98	0.47
7:G:12:G:H2'	7:G:13:C:C6	2.50	0.47
16:O:193:LEU:HD23	16:O:193:LEU:O	2.15	0.47
1:A:1494:TYR:CB	1:A:1744:ARG:NE	2.78	0.47
1:A:1788:VAL:HG22	1:A:1800:THR:HB	1.97	0.47
3:C:457:VAL:CA	3:C:462:GLY:HA3	2.44	0.47
7:G:136:U:H2'	7:G:137:C:O4'	2.14	0.47
8:H:40:C:H4'	26:Y:24:LYS:HZ2	1.80	0.47
10:J:406:PHE:HB3	10:J:411:MET:HG2	1.96	0.47
15:N:27:GLN:HE21	15:N:31:GLU:HG2	1.79	0.47
30:v:26:PHE:HA	30:v:35:ARG:O	2.14	0.47
37:m:36:VAL:HG12	37:m:37:ASP:N	2.29	0.47
1:A:332:TYR:C	1:A:332:TYR:CD1	2.92	0.47
1:A:712:HIS:CE1	18:R:250:CYS:HB2	2.50	0.47
1:A:1210:LYS:HE2	1:A:1211:ASP:H	1.79	0.47
1:A:1215:ASN:CG	1:A:1224:ARG:HD3	2.41	0.47
1:A:1498:TRP:C	1:A:1501:LEU:HD12	2.39	0.47
1:A:1763:LEU:HG	1:A:1862:ILE:HD13	1.97	0.47
3:C:115:GLU:O	3:C:118:PHE:CA	2.61	0.47
3:C:244:LYS:HG3	3:C:292:TYR:CD2	2.50	0.47
3:C:490:PHE:CE1	3:C:612:LYS:HD2	2.49	0.47
3:C:567:GLU:O	3:C:567:GLU:HG3	2.15	0.47
5:E:277:PHE:CE2	5:E:300:ILE:HD12	2.46	0.47
6:F:86:U:C2	14:M:196:TYR:CE2	3.03	0.47
8:H:83:A:H2'	8:H:84:C:C6	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:203:LEU:HD13	10:J:204:GLU:HB3	1.96	0.47
14:M:156:HIS:CD2	14:M:156:HIS:H	2.33	0.47
16:O:68:THR:HA	16:O:83:THR:CG2	2.45	0.47
23:V:515:CYS:SG	23:V:522:MET:N	2.88	0.47
23:V:527:GLY:O	23:V:530:LYS:N	2.47	0.47
25:X:38:GLU:OE2	25:X:39:GLU:HA	2.15	0.47
40:o:2:VAL:O	40:o:2:VAL:HG13	2.13	0.47
33:a:24:THR:O	33:a:51:ARG:NH1	2.46	0.47
37:f:36:VAL:HG12	37:f:37:ASP:N	2.29	0.47
1:A:1790:ILE:HG22	1:A:1798:LEU:HB3	1.96	0.46
3:C:470:PRO:CA	3:C:499:GLY:HA2	2.42	0.46
3:C:569:ARG:C	3:C:569:ARG:NE	2.73	0.46
7:G:2:U:O2	7:G:142:U:C2'	2.62	0.46
7:G:132:G:N2	8:H:44:U:O2	2.38	0.46
8:H:90:A:H2'	8:H:91:U:C6	2.50	0.46
12:L:178:GLU:O	12:L:179:ALA:C	2.58	0.46
12:L:181:ARG:HG3	12:L:182:LEU:H	1.80	0.46
17:P:227:TYR:N	17:P:227:TYR:CD1	2.82	0.46
19:S:57:ILE:CG1	24:W:97:ASN:OD1	2.59	0.46
24:W:97:ASN:ND2	24:W:97:ASN:N	2.60	0.46
26:Y:75:ARG:HH11	26:Y:75:ARG:HB2	1.80	0.46
31:w:125:LYS:NZ	31:w:126:GLU:HG3	2.29	0.46
40:o:14:GLN:HG3	40:o:44:PHE:HE1	1.80	0.46
40:o:153:LYS:O	40:o:157:GLU:HG3	2.15	0.46
1:A:299:ILE:HD11	3:C:921:LEU:CD1	2.39	0.46
1:A:401:GLY:HA3	3:C:386:GLY:HA2	1.98	0.46
1:A:425:PRO:HG3	2:B:26:A:H5'	1.97	0.46
1:A:1089:CYS:SG	1:A:1096:HIS:CD2	3.08	0.46
1:A:1378:GLU:HB3	1:A:1416:ILE:HD11	1.97	0.46
1:A:1657:THR:OG1	1:A:1658:GLN:N	2.48	0.46
3:C:350:ASN:CB	3:C:353:THR:HG23	2.45	0.46
6:F:41:A:N6	6:F:42:C:H42	2.13	0.46
8:H:54:U:H2'	8:H:55:U:C6	2.50	0.46
10:J:191:ALA:O	10:J:194:LEU:N	2.47	0.46
10:J:239:ARG:C	10:J:239:ARG:HD3	2.41	0.46
11:K:134:ALA:C	11:K:137:VAL:HG22	2.40	0.46
12:L:39:HIS:O	12:L:40:ARG:HB2	2.14	0.46
12:L:102:PHE:CD1	12:L:102:PHE:C	2.93	0.46
16:O:230:THR:H	16:O:277:ARG:CZ	2.27	0.46
24:W:159:ALA:HB3	24:W:160:GLU:OE1	2.14	0.46
27:Z:1114:PRO:C	27:Z:1116:TYR:H	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:269:CYS:SG	29:u:297:MET:HE1	2.56	0.46
31:w:82:GLU:HG3	31:w:112:TYR:HB3	1.96	0.46
36:k:46:CYS:HB3	36:k:48:ASN:OD1	2.15	0.46
40:o:56:LYS:HG2	40:o:58:ASP:HB2	1.97	0.46
40:o:92:GLU:OE1	41:p:25:ARG:NE	2.39	0.46
1:A:338:VAL:HG21	3:C:267:LEU:CD2	2.46	0.46
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	1.96	0.46
1:A:1211:ASP:O	1:A:1212:GLY:C	2.58	0.46
1:A:1215:ASN:HB3	1:A:1224:ARG:NE	2.31	0.46
1:A:1530:PRO:HG3	1:A:1533:ARG:NH1	2.30	0.46
2:B:29:A:O2'	2:B:30:A:H5'	2.15	0.46
3:C:185:PRO:HD3	3:C:482:TYR:CE1	2.50	0.46
6:F:22:A:H3'	15:N:115:THR:HG21	1.96	0.46
6:F:43:A:N6	6:F:44:G:O6	2.48	0.46
7:G:-8:U:C6	22:U:16:ASN:HA	2.50	0.46
8:H:149:A:H2'	8:H:150:U:C6	2.50	0.46
13:y:63:ALA:O	13:y:65:LEU:N	2.47	0.46
17:P:54:VAL:HG13	17:P:59:PHE:HZ	1.80	0.46
18:R:77:GLY:HA2	18:R:78:ARG:HH21	1.78	0.46
19:S:13:ASN:ND2	19:S:24:VAL:CG1	2.79	0.46
23:V:547:VAL:O	23:V:548:ALA:C	2.58	0.46
24:W:167:VAL:CG2	24:W:168:PHE:CE1	2.98	0.46
30:v:56:LYS:O	30:v:60:GLU:HG2	2.15	0.46
39:n:64:GLY:HA2	39:n:67:ILE:HD12	1.97	0.46
40:o:61:PRO:O	40:o:86:ALA:HB1	2.16	0.46
38:e:68:THR:O	38:e:68:THR:HG22	2.15	0.46
1:A:595:LYS:HG3	2:B:45:C:OP1	2.15	0.46
1:A:648:LEU:HD23	1:A:648:LEU:HA	1.79	0.46
3:C:725:ASP:OD1	3:C:727:LEU:CA	2.64	0.46
3:C:853:ARG:O	3:C:854:ARG:CB	2.62	0.46
4:D:151:LYS:O	4:D:154:ARG:CA	2.63	0.46
5:E:177:LYS:C	5:E:178:LEU:HD23	2.41	0.46
7:G:21:A:O2'	7:G:22:C:P	2.71	0.46
8:H:81:G:H2'	8:H:82:G:H8	1.81	0.46
8:H:91:U:H2'	8:H:92:U:C6	2.50	0.46
16:O:110:SER:OG	16:O:113:ASN:ND2	2.48	0.46
16:O:113:ASN:O	16:O:114:LYS:C	2.58	0.46
17:P:48:GLN:O	17:P:49:ASP:CB	2.64	0.46
20:T:318:ARG:HH11	20:T:319:THR:CG2	2.28	0.46
23:V:352:ILE:HG22	23:V:353:ILE:HG13	1.98	0.46
26:Y:3:GLU:CB	26:Y:5:LYS:O	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:225:ILE:HA	29:u:228:MET:HE3	1.96	0.46
1:A:55:ASP:OD1	1:A:55:ASP:N	2.45	0.46
1:A:232:LEU:O	1:A:404:LEU:HD11	2.16	0.46
1:A:790:ARG:NH2	1:A:986:GLU:HG2	2.30	0.46
1:A:986:GLU:O	1:A:1029:GLY:HA2	2.15	0.46
1:A:1494:TYR:CG	1:A:1744:ARG:HD3	2.45	0.46
7:G:-2:C:H2'	7:G:-1:G:OP1	2.15	0.46
7:G:129:G:H4'	7:G:130:A:OP1	2.16	0.46
8:H:77:C:H2'	8:H:78:C:C6	2.49	0.46
8:H:183:G:H2'	8:H:184:C:C6	2.50	0.46
18:R:280:ILE:HD12	18:R:281:ASN:H	1.75	0.46
19:S:81:GLN:HB3	19:S:108:ASN:N	2.31	0.46
31:w:107:ASP:OD1	31:w:109:ARG:HG2	2.14	0.46
36:d:46:CYS:HB3	36:d:48:ASN:OD1	2.15	0.46
1:A:338:VAL:HG21	3:C:867:PRO:HD2	1.98	0.46
1:A:362:ARG:C	1:A:362:ARG:CD	2.88	0.46
1:A:852:VAL:HG23	7:G:148:U:C2	2.49	0.46
1:A:904:HIS:HA	17:P:227:TYR:O	2.15	0.46
1:A:1253:SER:CB	8:H:34:U:O2'	2.63	0.46
1:A:1416:ILE:CB	1:A:1417:PRO:HD3	2.45	0.46
1:A:1489:LEU:HG	1:A:1539:SER:OG	2.15	0.46
3:C:193:THR:HG22	3:C:428:THR:HG21	1.97	0.46
7:G:6:A:H2'	7:G:7:G:N9	2.31	0.46
8:H:107:A:C6	8:H:108:G:C6	3.04	0.46
8:H:142:C:H2'	8:H:143:A:H5'	1.98	0.46
12:L:161:ASN:ND2	12:L:161:ASN:C	2.73	0.46
16:O:234:LEU:HB2	16:O:272:ILE:HB	1.98	0.46
17:P:228:ILE:N	17:P:228:ILE:CD1	2.78	0.46
18:R:195:ARG:HB3	18:R:195:ARG:HH11	1.80	0.46
22:U:1:MET:O	22:U:3:ASN:N	2.48	0.46
23:V:478:LYS:HE3	23:V:478:LYS:CA	2.45	0.46
1:A:434:HIS:ND1	1:A:434:HIS:C	2.73	0.46
1:A:1171:GLU:OE1	1:A:1171:GLU:N	2.46	0.46
1:A:1341:ARG:CZ	1:A:1342:TRP:CZ2	2.98	0.46
1:A:1592:ASP:O	1:A:1596:VAL:HG23	2.16	0.46
3:C:349:PHE:CG	3:C:356:PHE:CE1	3.03	0.46
3:C:385:VAL:CG2	3:C:386:GLY:N	2.78	0.46
6:F:80:G:H5''	6:F:81:C:P	2.56	0.46
12:L:191:LEU:CG	13:y:57:VAL:HG21	2.43	0.46
14:M:154:GLU:HG3	14:M:155:LYS:HG3	1.97	0.46
17:P:227:TYR:N	17:P:227:TYR:HD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:66:GLU:OE2	19:S:90:LEU:HD23	2.16	0.46
19:S:131:ARG:HH12	19:S:133:CYS:CA	2.27	0.46
20:T:297:HIS:CD2	20:T:338:CYS:SG	3.09	0.46
23:V:294:ILE:HD13	23:V:335:MET:O	2.16	0.46
23:V:585:ILE:O	23:V:586:PHE:C	2.58	0.46
25:X:58:GLU:O	25:X:61:GLY:CA	2.62	0.46
29:u:265:PHE:CZ	29:u:296:LYS:HG2	2.51	0.46
29:u:275:LEU:CD2	29:u:330:VAL:CG2	2.94	0.46
35:c:20:LYS:HE2	35:c:63:ASN:O	2.15	0.46
38:e:16:GLN:HB3	38:e:19:ASN:OD1	2.16	0.46
1:A:67:ARG:HE	1:A:67:ARG:HB2	1.58	0.46
1:A:201:ALA:HA	1:A:204:LEU:HB3	1.98	0.46
1:A:387:PHE:CE1	3:C:327:TYR:CE1	3.03	0.46
1:A:388:LEU:HB3	1:A:391:THR:OG1	2.16	0.46
1:A:801:ILE:O	1:A:802:THR:HB	2.15	0.46
1:A:948:PRO:HB2	1:A:949:PRO:HD3	1.97	0.46
1:A:1487:HIS:HB3	1:A:1541:THR:OG1	2.16	0.46
1:A:1504:GLU:OE2	1:A:1752:GLN:NE2	2.49	0.46
1:A:1527:ASN:CB	7:G:149:G:N2	2.79	0.46
1:A:1578:ARG:O	1:A:1579:ALA:CB	2.64	0.46
2:B:93:U:O4	36:d:64:ASN:ND2	2.42	0.46
3:C:678:THR:HG23	3:C:683:ASN:N	2.31	0.46
4:D:1349:GLY:HA2	4:D:1491:SER:O	2.16	0.46
5:E:232:ARG:O	5:E:262:TRP:CH2	2.69	0.46
5:E:260:ARG:CZ	5:E:276:ILE:HD11	2.46	0.46
5:E:274:VAL:C	5:E:275:LYS:HG3	2.40	0.46
6:F:42:C:C5	6:F:43:A:C5	3.03	0.46
7:G:143:U:C5	25:X:9:LYS:HG2	2.51	0.46
7:G:146:C:C6	7:G:146:C:H5"	2.51	0.46
8:H:24:A:H3'	8:H:25:G:H5"	1.96	0.46
8:H:114:A:H2'	8:H:115:G:H8	1.81	0.46
12:L:18:ILE:HG21	12:L:37:LEU:HD23	1.97	0.46
12:L:141:PRO:HG2	12:L:144:MET:CA	2.40	0.46
14:M:124:PHE:CD1	14:M:125:SER:N	2.84	0.46
16:O:22:ILE:HD13	24:W:111:LEU:HD23	1.97	0.46
18:R:106:GLN:OE1	18:R:225:PRO:HD2	2.15	0.46
19:S:9:TRP:C	19:S:11:PRO:HD3	2.39	0.46
20:T:409:LEU:HD12	20:T:409:LEU:N	2.31	0.46
23:V:530:LYS:C	23:V:532:GLN:N	2.74	0.46
45:4:24:ALA:O	45:4:27:ALA:HB3	2.15	0.46
1:A:120:TYR:CD2	1:A:483:GLN:HB2	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASN:HD21	22:U:8:PRO:HA	1.81	0.46
1:A:317:PRO:HB2	1:A:327:VAL:HG11	1.98	0.46
1:A:437:ALA:O	1:A:439:GLN:HG2	2.15	0.46
1:A:658:ARG:N	17:P:29:GLN:OE1	2.49	0.46
1:A:1848:LEU:HD22	1:A:1914:MET:CE	2.44	0.46
3:C:259:LYS:HG2	47:C:1500:GTP:N1	2.31	0.46
3:C:671:SER:OG	3:C:672:LEU:HD22	2.15	0.46
3:C:678:THR:HG21	3:C:683:ASN:CB	2.43	0.46
5:E:87:ASP:O	5:E:88:ARG:CG	2.63	0.46
8:H:59:A:H2'	8:H:60:U:C6	2.50	0.46
8:H:181:G:H2'	8:H:182:U:C6	2.50	0.46
12:L:83:ARG:HH11	12:L:93:ALA:HB3	1.81	0.46
12:L:789:ALA:O	12:L:792:LEU:CG	2.64	0.46
16:O:255:PHE:C	18:R:70:ALA:HB2	2.40	0.46
24:W:137:TYR:CD2	24:W:137:TYR:O	2.69	0.46
33:h:43:MET:HB3	33:h:46:ILE:HD11	1.97	0.46
35:j:61:ARG:HB3	35:j:64:ASN:HD22	1.80	0.46
1:A:371:LEU:CD1	3:C:347:ILE:HD11	2.46	0.46
3:C:680:ASN:HD21	3:C:682:LYS:CG	2.27	0.46
5:E:178:LEU:CD1	5:E:222:LEU:HD21	2.46	0.46
6:F:22:A:P	15:N:115:THR:OG1	2.74	0.46
8:H:71:C:H2'	8:H:72:U:C6	2.50	0.46
8:H:72:U:H2'	8:H:73:C:C6	2.50	0.46
10:J:323:LEU:O	14:M:178:GLU:HG2	2.15	0.46
10:J:344:GLN:HG2	14:M:132:LEU:HD21	1.98	0.46
15:N:5:LYS:HD2	15:N:77:TYR:OH	2.16	0.46
16:O:78:LYS:HG3	16:O:202:TYR:CZ	2.50	0.46
16:O:84:CYS:HB3	16:O:86:LEU:HG	1.98	0.46
18:R:101:ILE:O	18:R:104:GLN:HG2	2.08	0.46
23:V:548:ALA:HB1	23:V:585:ILE:C	2.41	0.46
25:X:5:ASP:OD1	25:X:7:ASN:HB2	2.16	0.46
25:X:46:GLU:O	25:X:49:ALA:HB3	2.16	0.46
36:k:33:THR:CG2	36:k:37:LYS:HE2	2.46	0.46
1:A:34:ALA:HA	5:E:213:ILE:CD1	2.46	0.45
1:A:61:MET:HB3	1:A:62:PRO:HD2	1.98	0.45
1:A:359:ILE:O	1:A:360:SER:HB3	2.16	0.45
1:A:461:HIS:CE1	2:B:23:C:C6	3.03	0.45
1:A:781:ARG:O	1:A:785:LYS:HG3	2.15	0.45
1:A:901:LEU:HD13	1:A:904:HIS:HE1	1.80	0.45
2:B:22:U:O2	2:B:22:U:H2'	2.15	0.45
8:H:13:C:N3	14:M:197:SER:OG	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:73:C:H2'	8:H:74:U:C6	2.50	0.45
8:H:80:A:H2'	8:H:81:G:H8	1.81	0.45
8:H:88:A:H2'	8:H:89:U:C6	2.50	0.45
8:H:157:G:H5''	8:H:157:G:C8	2.50	0.45
12:L:19:LEU:CD1	12:L:34:ILE:HG21	2.46	0.45
14:M:161:PHE:HD1	14:M:161:PHE:N	2.14	0.45
15:N:128:VAL:HG11	15:N:130:ARG:HB3	1.96	0.45
18:R:88:ILE:HG22	18:R:96:ILE:HG23	1.98	0.45
25:X:39:GLU:OE1	25:X:40:LEU:N	2.50	0.45
38:l:68:THR:HG22	38:l:68:THR:O	2.15	0.45
36:d:72:GLU:HG2	36:d:74:TRP:CE3	2.51	0.45
39:g:64:GLY:HA2	39:g:67:ILE:HD12	1.97	0.45
1:A:374:ASP:O	1:A:375:ASP:HB3	2.16	0.45
1:A:588:LEU:C	1:A:1551:PHE:CD1	2.94	0.45
1:A:1321:GLU:CG	45:4:29:ALA:O	2.61	0.45
1:A:1675:ASP:C	1:A:1675:ASP:OD1	2.59	0.45
2:B:57:G:H2'	2:B:58:U:H5'	1.99	0.45
3:C:457:VAL:CG1	3:C:462:GLY:HA3	2.46	0.45
3:C:495:ARG:HG3	3:C:495:ARG:O	2.16	0.45
5:E:157:CYS:HA	5:E:168:CYS:O	2.16	0.45
6:F:45:A:N3	6:F:45:A:H5''	2.30	0.45
8:H:68:G:H2'	8:H:69:U:C6	2.50	0.45
15:N:51:ARG:HG3	24:W:196:TRP:CD2	2.51	0.45
16:O:63:MET:SD	16:O:160:ASN:HB2	2.56	0.45
16:O:97:ARG:HH12	16:O:136:MET:HE2	1.81	0.45
18:R:88:ILE:HG21	18:R:96:ILE:CG2	2.46	0.45
24:W:101:THR:N	24:W:104:MET:HB2	2.31	0.45
24:W:203:LYS:HA	24:W:203:LYS:HD2	1.58	0.45
24:W:210:GLU:HB3	24:W:213:GLN:OE1	2.15	0.45
38:l:16:GLN:HB3	38:l:19:ASN:OD1	2.16	0.45
1:A:1416:ILE:HD13	1:A:1416:ILE:HA	1.82	0.45
6:F:42:C:O2'	6:F:43:A:H5'	2.16	0.45
7:G:7:G:H2'	7:G:8:C:H6	1.81	0.45
9:I:712:VAL:O	9:I:715:GLY:N	2.49	0.45
12:L:199:GLN:NE2	12:L:199:GLN:N	2.60	0.45
13:y:3:ARG:H	13:y:3:ARG:HG2	1.50	0.45
16:O:90:TYR:HB3	16:O:92:LEU:HD12	1.98	0.45
18:R:178:ARG:CD	18:R:194:GLN:NE2	2.72	0.45
18:R:265:ASP:OD1	18:R:265:ASP:N	2.49	0.45
19:S:34:LYS:HG3	19:S:78:TYR:CE2	2.52	0.45
26:Y:129:GLU:C	26:Y:130:LEU:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:w:131:MET:HE1	31:w:148:TRP:CD1	2.51	0.45
39:g:35:ASP:HB2	39:g:36:PRO:CD	2.42	0.45
1:A:44:ARG:CD	1:A:45:TYR:CE2	2.99	0.45
1:A:118:VAL:HG12	1:A:119:LEU:N	2.31	0.45
1:A:380:LEU:O	3:C:354:ARG:CG	2.64	0.45
1:A:615:ARG:HE	1:A:615:ARG:HB2	1.59	0.45
1:A:1320:LYS:HE2	1:A:1526:LEU:HG	1.99	0.45
1:A:1508:GLY:O	25:X:24:TRP:NE1	2.49	0.45
1:A:1758:PRO:O	45:4:5:PRO:HG2	2.17	0.45
2:B:23:C:O2'	2:B:24:G:H2'	2.16	0.45
3:C:65:TYR:O	3:C:66:TYR:CB	2.65	0.45
3:C:66:TYR:N	3:C:66:TYR:CD1	2.81	0.45
3:C:196:LYS:HB2	34:b:7:SER:HB3	1.96	0.45
3:C:502:HIS:ND1	3:C:543:ARG:HB3	2.32	0.45
3:C:926:ALA:HA	3:C:929:LEU:HG	1.98	0.45
5:E:146:ARG:NH1	5:E:148:LYS:NZ	2.62	0.45
8:H:56:A:H2'	8:H:57:A:H8	1.82	0.45
8:H:58:U:H2'	8:H:59:A:H8	1.82	0.45
8:H:180:G:H2'	8:H:181:G:H8	1.81	0.45
10:J:360:ASP:HA	10:J:363:ARG:CD	2.46	0.45
10:J:406:PHE:CB	10:J:411:MET:HG2	2.47	0.45
14:M:202:TYR:C	14:M:202:TYR:CD1	2.93	0.45
15:N:101:CYS:HB3	15:N:102:CYS:SG	2.54	0.45
19:S:66:ASP:C	19:S:66:ASP:OD1	2.60	0.45
20:T:387:PHE:CZ	20:T:398:TRP:CD1	3.04	0.45
20:T:459:LEU:HB3	20:T:462:GLU:HG3	1.98	0.45
26:Y:75:ARG:NE	26:Y:77:TYR:OH	2.50	0.45
26:Y:109:GLN:CG	26:Y:110:ALA:H	2.28	0.45
35:j:6:PHE:CD1	35:j:6:PHE:C	2.93	0.45
35:c:61:ARG:HB3	35:c:64:ASN:HD22	1.80	0.45
1:A:298:ASP:OD1	1:A:300:ASN:N	2.48	0.45
1:A:1094:ARG:HH11	1:A:1094:ARG:CG	2.30	0.45
3:C:183:SER:OG	3:C:480:LYS:NZ	2.50	0.45
3:C:445:ALA:CB	3:C:449:ILE:CG1	2.73	0.45
3:C:524:ILE:O	3:C:525:CYS:SG	2.74	0.45
5:E:260:ARG:CD	5:E:276:ILE:HG12	2.47	0.45
8:H:150:U:H2'	8:H:151:C:C6	2.50	0.45
10:J:375:ASP:O	10:J:376:VAL:C	2.58	0.45
12:L:18:ILE:HD11	12:L:152:LEU:HG	1.98	0.45
18:R:196:VAL:HG11	24:W:120:ILE:HD12	1.98	0.45
20:T:455:GLN:CG	20:T:456:PRO:CD	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:330:LYS:HZ3	29:u:50:LEU:CD2	2.14	0.45
23:V:576:THR:O	23:V:580:ARG:N	2.36	0.45
24:W:167:VAL:HG23	24:W:168:PHE:N	2.32	0.45
31:w:125:LYS:HZ3	31:w:126:GLU:HG3	1.81	0.45
39:n:38:MET:HE2	39:n:67:ILE:HG21	1.98	0.45
1:A:280:GLU:OE1	22:U:9:THR:HG21	2.17	0.45
1:A:1930:TYR:HE1	25:X:71:ASP:CA	2.29	0.45
3:C:497:LEU:CD1	3:C:577:PHE:CE1	2.94	0.45
8:H:82:G:H2'	8:H:83:A:H8	1.82	0.45
8:H:92:U:H2'	8:H:93:A:H8	1.82	0.45
8:H:148:C:H2'	8:H:149:A:H8	1.82	0.45
14:M:142:ILE:O	14:M:142:ILE:HG13	2.15	0.45
14:M:161:PHE:CD1	14:M:161:PHE:N	2.84	0.45
16:O:56:ARG:HG2	16:O:67:LYS:HB3	1.98	0.45
18:R:248:PRO:HA	18:R:249:PRO:HD3	1.80	0.45
26:Y:168:ASP:O	26:Y:172:MET:CB	2.65	0.45
29:u:307:MET:HA	29:u:311:MET:CE	2.47	0.45
34:b:18:ARG:NH1	34:b:52:LYS:HB3	2.31	0.45
1:A:121:HIS:HA	1:A:481:PHE:O	2.17	0.45
1:A:805:GLU:OE1	17:P:194:PHE:CZ	2.69	0.45
1:A:974:ASN:HB2	1:A:1178:TYR:HB3	1.97	0.45
1:A:1070:ASP:C	1:A:1070:ASP:OD1	2.60	0.45
4:D:419:GLY:C	4:D:421:HIS:H	2.25	0.45
7:G:-9:C:C4	22:U:18:TYR:CZ	3.03	0.45
7:G:120:G:O2'	7:G:121:G:O5'	2.34	0.45
7:G:135:G:C2	7:G:136:U:N3	2.85	0.45
8:H:93:A:H2'	8:H:94:A:H8	1.82	0.45
8:H:141:C:H2'	8:H:142:C:C6	2.50	0.45
8:H:182:U:H2'	8:H:183:G:H8	1.81	0.45
12:L:178:GLU:HA	12:L:181:ARG:CG	2.33	0.45
16:O:131:THR:O	16:O:132:ARG:HB2	2.17	0.45
19:S:39:PHE:CD1	19:S:129:PHE:CE2	2.88	0.45
20:T:342:GLU:CB	20:T:343:PRO:HD2	2.47	0.45
20:T:454:VAL:HG22	20:T:463:SER:OG	2.16	0.45
23:V:537:HIS:C	23:V:578:SER:HG	2.18	0.45
36:k:48:ASN:O	36:k:49:ASN:HB2	2.17	0.45
33:a:77:LEU:HD12	33:a:77:LEU:N	2.32	0.45
38:e:18:ILE:HA	38:e:21:ILE:HD12	1.97	0.45
1:A:75:ASP:HB2	1:A:77:THR:OG1	2.16	0.45
1:A:89:LEU:CD2	1:A:656:LEU:CD2	2.95	0.45
1:A:293:TRP:CE3	1:A:293:TRP:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:758:ARG:CG	17:P:227:TYR:HE2	2.30	0.45
1:A:857:ASN:OD1	1:A:857:ASN:C	2.59	0.45
1:A:1488:THR:C	1:A:1540:PRO:HG2	2.41	0.45
1:A:1752:GLN:O	1:A:1754:TYR:CE1	2.70	0.45
1:A:1791:HIS:ND1	1:A:1799:THR:CG2	2.79	0.45
5:E:267:PHE:CE2	11:K:194:GLU:CA	2.96	0.45
6:F:42:C:C2'	6:F:43:A:H8	2.14	0.45
6:F:44:G:O5'	6:F:44:G:C8	2.70	0.45
7:G:2:U:O2	7:G:142:U:C1'	2.62	0.45
8:H:84:C:H2'	8:H:85:A:H8	1.82	0.45
10:J:190:THR:HA	12:L:17:GLU:CD	2.42	0.45
12:L:86:ALA:HB3	12:L:87:PRO:CD	2.46	0.45
16:O:197:ASN:O	16:O:201:ARG:HG3	2.17	0.45
19:S:82:PHE:H	19:S:108:ASN:H	1.64	0.45
20:T:316:ASP:C	20:T:316:ASP:OD1	2.58	0.45
29:u:148:GLU:OE1	29:u:148:GLU:CA	2.65	0.45
36:k:22:GLU:OE1	36:k:22:GLU:HA	2.17	0.45
36:d:43:LEU:HD11	36:d:51:LYS:HB3	1.99	0.45
39:g:32:ARG:HG3	39:g:43:ASP:HB2	1.99	0.45
39:g:38:MET:HE2	39:g:67:ILE:HG21	1.98	0.45
1:A:148:TRP:HE3	1:A:629:PHE:CD1	2.35	0.45
1:A:277:PRO:HA	1:A:448:GLN:HG2	1.98	0.45
1:A:318:TYR:O	3:C:645:ARG:NH1	2.49	0.45
1:A:370:PRO:O	1:A:371:LEU:C	2.60	0.45
1:A:388:LEU:HD21	3:C:395:THR:HG23	1.99	0.45
1:A:464:PRO:HG3	2:B:20:G:C2	2.51	0.45
8:H:70:C:H2'	8:H:71:C:C6	2.49	0.45
8:H:152:G:O2'	8:H:153:A:H1'	2.16	0.45
13:y:36:CYS:SG	13:y:37:THR:N	2.88	0.45
14:M:152:LEU:CD2	14:M:160:PHE:HZ	2.19	0.45
16:O:20:PHE:CG	16:O:21:PRO:HD2	2.51	0.45
1:A:345:PRO:O	1:A:346:ASP:O	2.35	0.45
1:A:587:GLN:HA	1:A:1550:GLY:C	2.42	0.45
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.70	0.45
1:A:684:GLU:OE2	20:T:290:ALA:HB2	2.16	0.45
1:A:1690:ASP:OD1	1:A:1691:ASN:N	2.49	0.45
3:C:144:CYS:SG	3:C:148:CYS:SG	3.15	0.45
3:C:926:ALA:N	3:C:927:PRO:HD2	2.32	0.45
5:E:246:GLU:HB2	5:E:248:SER:HG	1.81	0.45
6:F:42:C:O2'	6:F:43:A:O4'	2.35	0.45
7:G:4:A:C2	7:G:5:G:C4	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:129:G:O3'	7:G:130:A:C8	2.70	0.45
12:L:52:GLU:CD	12:L:133:GLU:HB2	2.41	0.45
16:O:58:CYS:HB2	16:O:65:PHE:CE1	2.52	0.45
16:O:259:ARG:HD2	16:O:273:GLN:HG2	1.99	0.45
18:R:176:TYR:HH	24:W:122:ASP:CG	2.24	0.45
19:S:103:ALA:N	24:W:94:GLY:HA2	2.32	0.45
29:u:82:SER:O	29:u:219:ALA:HA	2.17	0.45
29:u:274:THR:HG21	29:u:409:ASP:OD1	2.17	0.45
34:i:17:MET:HE1	34:i:82:VAL:HG22	1.99	0.45
38:l:18:ILE:HA	38:l:21:ILE:HD12	1.97	0.45
38:e:25:LEU:C	38:e:25:LEU:HD23	2.42	0.45
1:A:365:VAL:HG12	1:A:366:LYS:N	2.32	0.44
1:A:671:THR:OG1	6:F:69:A:P	2.75	0.44
1:A:1436:TRP:CH2	1:A:1437:ARG:CZ	3.00	0.44
1:A:1768:TYR:O	1:A:1768:TYR:CD1	2.70	0.44
2:B:42:U:H2'	2:B:43:U:O4'	2.17	0.44
3:C:191:PRO:HG2	3:C:426:GLU:OE1	2.17	0.44
3:C:671:SER:CB	3:C:672:LEU:HD22	2.46	0.44
5:E:132:THR:HG21	5:E:146:ARG:HG2	1.99	0.44
5:E:178:LEU:HG	5:E:188:GLN:HB2	1.98	0.44
5:E:266:PRO:O	12:L:788:TYR:CD1	2.70	0.44
6:F:9:U:H2'	6:F:10:U:C6	2.52	0.44
7:G:5:G:C1'	7:G:6:A:H2	2.27	0.44
10:J:192:GLU:O	10:J:196:ARG:N	2.45	0.44
10:J:201:ARG:HE	10:J:203:LEU:HA	1.81	0.44
12:L:106:LYS:CE	12:L:106:LYS:HA	2.47	0.44
16:O:35:ARG:NH1	24:W:129:ARG:HH12	2.15	0.44
16:O:205:ILE:O	16:O:207:ASP:N	2.50	0.44
18:R:181:PRO:O	18:R:182:SER:CB	2.58	0.44
18:R:281:ASN:OD1	18:R:283:ASN:N	2.48	0.44
18:R:282:GLU:O	18:R:283:ASN:C	2.56	0.44
24:W:97:ASN:H	24:W:97:ASN:HD22	1.65	0.44
26:Y:27:LYS:C	26:Y:28:ASP:CG	2.86	0.44
29:u:81:GLN:HB2	29:u:221:LEU:HD12	1.99	0.44
39:n:32:ARG:HG3	39:n:43:ASP:HB2	1.99	0.44
36:d:22:GLU:OE1	36:d:22:GLU:HA	2.17	0.44
1:A:853:LYS:HE3	7:G:148:U:O4	2.16	0.44
1:A:1723:LYS:HB2	1:A:1724:PRO:HD3	1.99	0.44
1:A:1772:PHE:CG	1:A:1813:ARG:HD2	2.51	0.44
3:C:388:VAL:HA	3:C:392:LEU:HB2	1.99	0.44
7:G:120:G:HO2'	7:G:121:G:C4'	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:20:LYS:CE	12:L:54:LEU:HD11	2.47	0.44
13:y:57:VAL:CG2	13:y:58:ALA:N	2.80	0.44
15:N:117:CYS:C	15:N:119:CYS:N	2.73	0.44
16:O:294:ASN:O	16:O:296:ARG:HG3	2.17	0.44
18:R:67:ILE:HG22	18:R:69:VAL:HG21	1.97	0.44
18:R:126:ASN:HD22	18:R:128:ASP:H	1.66	0.44
20:T:347:THR:HG21	20:T:357:TRP:HE1	1.81	0.44
20:T:358:ASP:HB2	20:T:365:ARG:HD2	2.00	0.44
31:w:109:ARG:CG	31:w:110:THR:N	2.77	0.44
38:l:25:LEU:HD23	38:l:25:LEU:C	2.42	0.44
1:A:70:ILE:HD13	1:A:495:GLN:CG	2.38	0.44
1:A:331:TRP:HE3	1:A:332:TYR:CA	2.31	0.44
1:A:1862:ILE:CG2	1:A:1887:SER:OG	2.66	0.44
3:C:89:LEU:C	3:C:89:LEU:CD2	2.82	0.44
3:C:334:ILE:HD12	3:C:334:ILE:C	2.42	0.44
3:C:779:LEU:HD11	3:C:825:PRO:HB2	1.99	0.44
8:H:74:U:H2'	8:H:75:A:H8	1.82	0.44
8:H:78:C:H2'	8:H:79:G:H8	1.81	0.44
8:H:143:A:OP2	8:H:143:A:C2	2.71	0.44
15:N:60:ILE:HD13	15:N:78:CYS:HB3	1.99	0.44
18:R:52:PRO:HB3	18:R:57:ASP:OD2	2.17	0.44
18:R:123:GLU:C	18:R:124:VAL:HG12	2.41	0.44
19:S:38:ASN:HD22	19:S:100:MET:CE	2.30	0.44
19:S:81:GLN:HB3	19:S:108:ASN:H	1.82	0.44
20:T:393:ASP:O	20:T:413:ASN:ND2	2.49	0.44
23:V:369:MET:O	23:V:369:MET:HE3	2.17	0.44
25:X:5:ASP:OD2	25:X:7:ASN:HB2	2.18	0.44
25:X:39:GLU:C	25:X:39:GLU:CD	2.85	0.44
29:u:148:GLU:OE2	29:u:152:LYS:HE2	2.17	0.44
36:k:72:GLU:HG2	36:k:74:TRP:CE3	2.52	0.44
34:b:37:HIS:O	34:b:38:MET:HB2	2.18	0.44
36:d:48:ASN:O	36:d:49:ASN:HB2	2.17	0.44
38:e:20:LEU:CD2	38:e:24:TYR:CZ	3.00	0.44
1:A:193:LEU:HB3	1:A:208:TYR:OH	2.17	0.44
1:A:684:GLU:OE1	20:T:266:GLU:HB3	2.18	0.44
1:A:767:VAL:CG2	2:B:39:C:O2'	2.65	0.44
1:A:800:TYR:CG	3:C:59:LEU:HD13	2.52	0.44
1:A:979:SER:HB2	1:A:1168:VAL:CG1	2.47	0.44
1:A:1330:MET:HG2	1:A:1330:MET:O	2.18	0.44
1:A:1759:THR:O	1:A:1760:GLU:HG2	2.17	0.44
3:C:242:LEU:HD23	3:C:242:LEU:HA	1.84	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:446:LYS:HA	3:C:449:ILE:HD12	1.98	0.44
3:C:534:VAL:HG12	3:C:535:ALA:N	2.31	0.44
5:E:276:ILE:O	5:E:277:PHE:HD1	2.00	0.44
6:F:27:A:P	15:N:41:ARG:HH21	2.40	0.44
7:G:134:U:O2'	7:G:135:G:H5'	2.17	0.44
12:L:77:LEU:HD21	18:R:285:ALA:HB2	2.00	0.44
13:y:8:ALA:O	13:y:13:ALA:HB1	2.17	0.44
16:O:258:ILE:HG22	16:O:260:THR:N	2.32	0.44
23:V:497:CYS:HA	23:V:500:GLN:CD	2.43	0.44
28:t:73:ALA:O	28:t:76:LYS:CG	2.65	0.44
33:h:5:VAL:HB	33:h:6:PRO:HD3	2.00	0.44
34:b:18:ARG:HB2	34:b:83:GLU:HG2	2.00	0.44
1:A:47:GLU:C	1:A:50:LYS:CG	2.77	0.44
1:A:76:MET:SD	1:A:88:TYR:CE2	3.10	0.44
1:A:80:LYS:NZ	15:N:37:HIS:HD2	1.69	0.44
1:A:328:HIS:C	1:A:329:LEU:HD23	2.43	0.44
1:A:382:GLU:C	1:A:382:GLU:CD	2.85	0.44
1:A:697:MET:HE2	18:R:245:TRP:HZ3	1.80	0.44
5:E:267:PHE:CD1	12:L:788:TYR:CD2	2.99	0.44
6:F:5:U:H5'	6:F:6:C:OP2	2.17	0.44
6:F:42:C:N1	6:F:43:A:C8	2.85	0.44
8:H:79:G:H2'	8:H:80:A:H8	1.82	0.44
10:J:192:GLU:N	10:J:195:LEU:CD1	2.80	0.44
11:K:134:ALA:O	11:K:137:VAL:HG22	2.17	0.44
12:L:176:LEU:C	12:L:176:LEU:CD1	2.86	0.44
15:N:17:LEU:HD12	15:N:18:ILE:HG23	1.98	0.44
20:T:306:CYS:SG	20:T:336:VAL:HG12	2.57	0.44
23:V:182:ILE:O	23:V:186:LEU:HG	2.17	0.44
23:V:231:GLU:O	23:V:235:LYS:HG3	2.18	0.44
24:W:205:VAL:HG12	24:W:206:ALA:N	2.33	0.44
26:Y:75:ARG:HD3	26:Y:88:THR:CG2	2.48	0.44
34:b:17:MET:HE1	34:b:82:VAL:HG22	1.99	0.44
1:A:794:TYR:CE1	1:A:799:PRO:HA	2.53	0.44
1:A:1495:PHE:CZ	1:A:1748:ARG:CG	3.01	0.44
3:C:60:HIS:ND1	3:C:60:HIS:O	2.50	0.44
3:C:674:CYS:HB2	3:C:818:SER:HB3	2.00	0.44
8:H:89:U:H2'	8:H:90:A:H8	1.82	0.44
9:I:433:ALA:O	9:I:437:CYS:N	2.50	0.44
12:L:102:PHE:CE1	12:L:106:LYS:HG3	2.52	0.44
12:L:141:PRO:CG	12:L:144:MET:HA	2.43	0.44
12:L:200:LYS:O	12:L:201:LYS:CB	2.64	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:167:VAL:HG23	24:W:168:PHE:CE1	2.52	0.44
24:W:176:GLU:O	24:W:177:LYS:C	2.60	0.44
28:t:117:ILE:O	28:t:121:THR:HG23	2.18	0.44
29:u:267:THR:O	29:u:271:LEU:HD13	2.17	0.44
1:A:73:HIS:HA	1:A:81:PHE:CE2	2.53	0.44
1:A:705:LYS:H	1:A:705:LYS:HG2	1.53	0.44
1:A:1314:VAL:HG13	1:A:1315:VAL:N	2.31	0.44
1:A:1336:PRO:HB3	1:A:1353:PHE:CE1	2.53	0.44
1:A:1531:ASN:OD1	1:A:1531:ASN:O	2.36	0.44
3:C:297:ASN:HD22	3:C:298:LEU:HD12	1.83	0.44
3:C:439:PRO:O	3:C:440:SER:CB	2.66	0.44
3:C:673:LYS:HG3	3:C:686:THR:HG23	2.00	0.44
3:C:890:HIS:CE1	7:G:-12:G:C6	3.05	0.44
5:E:248:SER:HB2	5:E:249:TYR:CE1	2.53	0.44
5:E:274:VAL:C	5:E:275:LYS:CG	2.91	0.44
7:G:8:C:P	12:L:200:LYS:HE3	2.57	0.44
12:L:18:ILE:HD11	12:L:152:LEU:CG	2.47	0.44
14:M:121:ASP:OD1	14:M:122:LEU:N	2.51	0.44
18:R:79:LYS:HZ3	18:R:80:LYS:NZ	2.16	0.44
18:R:109:ASP:OD1	18:R:110:LYS:N	2.51	0.44
18:R:148:ARG:HG3	18:R:148:ARG:NH1	2.31	0.44
18:R:179:TYR:CE2	18:R:181:PRO:HG3	2.52	0.44
20:T:459:LEU:HG	20:T:461:SER:OG	2.18	0.44
23:V:512:GLY:O	23:V:513:ARG:C	2.60	0.44
25:X:5:ASP:N	25:X:8:LEU:HD12	2.32	0.44
25:X:38:GLU:C	25:X:38:GLU:CD	2.86	0.44
33:h:77:LEU:N	33:h:77:LEU:HD12	2.32	0.44
34:i:52:LYS:HG3	34:i:52:LYS:O	2.18	0.44
36:k:43:LEU:HD11	36:k:51:LYS:HB3	1.99	0.44
38:l:20:LEU:CD2	38:l:24:TYR:CZ	3.00	0.44
40:o:120:ILE:HG22	40:o:120:ILE:O	2.16	0.44
1:A:351:TYR:HA	3:C:270:PRO:HG3	1.98	0.44
3:C:67:PRO:O	3:C:68:THR:C	2.61	0.44
3:C:392:LEU:HD12	3:C:392:LEU:O	2.18	0.44
3:C:514:TYR:CD1	3:C:514:TYR:C	2.94	0.44
3:C:637:LEU:HD23	3:C:637:LEU:HA	1.88	0.44
3:C:669:THR:HG22	3:C:690:GLU:CB	2.48	0.44
3:C:726:LEU:HD12	3:C:726:LEU:C	2.42	0.44
7:G:121:G:H2'	7:G:122:U:OP2	2.18	0.44
8:H:55:U:H2'	8:H:56:A:H8	1.82	0.44
15:N:15:TRP:HE3	15:N:74:LEU:HD11	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:N:47:TRP:HB2	15:N:48:PRO:HD3	1.99	0.44
18:R:88:ILE:CG2	18:R:96:ILE:HG23	2.48	0.44
19:S:150:GLN:C	24:W:100:ARG:NH2	2.73	0.44
20:T:185:MET:HB2	20:T:186:PRO:HD3	1.98	0.44
23:V:234:LEU:HB3	23:V:370:LEU:HD12	2.00	0.44
24:W:126:GLU:O	24:W:130:ARG:HD3	2.18	0.44
30:v:7:PHE:HE2	30:v:62:LEU:HD23	1.82	0.44
1:A:30:LEU:HB3	5:E:194:TYR:CZ	2.53	0.44
1:A:47:GLU:C	1:A:50:LYS:HZ2	2.25	0.44
1:A:79:ARG:HD2	1:A:79:ARG:O	2.18	0.44
1:A:81:PHE:O	1:A:82:ARG:C	2.59	0.44
1:A:373:ASP:OD1	1:A:374:ASP:N	2.51	0.44
1:A:387:PHE:HD1	3:C:327:TYR:CE1	2.33	0.44
1:A:587:GLN:HG3	1:A:1550:GLY:O	2.17	0.44
1:A:705:LYS:O	1:A:706:ALA:C	2.61	0.44
1:A:1136:ARG:HB2	1:A:1345:GLN:HA	1.99	0.44
1:A:1179:SER:C	1:A:1181:ASP:N	2.75	0.44
1:A:1498:TRP:CA	1:A:1501:LEU:CD1	2.94	0.44
1:A:1862:ILE:HG22	1:A:1887:SER:OG	2.18	0.44
1:A:1993:LYS:HD2	1:A:1993:LYS:C	2.43	0.44
3:C:481:MET:HE2	3:C:559:ILE:HD11	2.00	0.44
6:F:43:A:C6	6:F:44:G:C6	3.06	0.44
16:O:185:LYS:HG2	16:O:186:PRO:HD2	2.00	0.44
20:T:225:ASP:O	20:T:226:ARG:HB2	2.18	0.44
24:W:100:ARG:HB3	24:W:104:MET:CB	2.47	0.44
33:a:5:VAL:HB	33:a:6:PRO:HD3	2.00	0.44
1:A:379:GLU:HB2	3:C:354:ARG:O	2.17	0.43
1:A:661:GLU:HA	18:R:213:LYS:HA	2.00	0.43
1:A:906:VAL:HA	1:A:907:PRO:HD3	1.81	0.43
1:A:1334:LEU:HD23	1:A:1334:LEU:HA	1.77	0.43
7:G:-12:G:HO2'	7:G:-11:G:P	2.41	0.43
7:G:145:U:H6	7:G:145:U:C3'	2.21	0.43
7:G:152:C:C6	7:G:152:C:OP1	2.71	0.43
24:W:181:PHE:N	24:W:181:PHE:HD1	2.15	0.43
25:X:5:ASP:CG	25:X:7:ASN:HB2	2.43	0.43
25:X:41:GLN:N	25:X:41:GLN:NE2	2.60	0.43
26:Y:68:TYR:O	26:Y:70:GLY:CA	2.64	0.43
31:w:123:THR:OG1	31:w:126:GLU:CG	2.66	0.43
1:A:109:PRO:HD3	1:A:630:TRP:HZ2	1.83	0.43
1:A:593:ARG:HH12	1:A:1565:LYS:HE3	1.82	0.43
1:A:1761:PRO:C	1:A:1762:TYR:O	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:413:ARG:HB2	3:C:414:PRO:HD3	1.99	0.43
3:C:474:LEU:C	3:C:474:LEU:CD2	2.87	0.43
3:C:505:GLN:HG2	3:C:506:PRO:HD2	2.00	0.43
8:H:168:A:C2'	39:n:48:MET:HE1	2.46	0.43
10:J:258:ILE:HG12	12:L:232:TYR:CD1	2.53	0.43
16:O:229:LYS:HA	16:O:277:ARG:NH1	2.33	0.43
20:T:471:ASP:C	20:T:471:ASP:OD1	2.61	0.43
23:V:620:ASN:HB3	23:V:623:ASN:HB2	1.99	0.43
25:X:36:LYS:N	25:X:36:LYS:HD2	2.32	0.43
33:h:55:VAL:HG21	40:o:67:LYS:HZ1	1.82	0.43
37:m:65:ARG:HG3	37:m:65:ARG:HH11	1.83	0.43
34:b:52:LYS:HG3	34:b:52:LYS:O	2.18	0.43
2:B:12:U:O2'	2:B:13:C:P	2.77	0.43
2:B:95:G:C6	38:e:36:TYR:O	2.71	0.43
3:C:96:PRO:CD	20:T:276:GLU:OE2	2.66	0.43
3:C:381:LEU:HD23	3:C:416:LEU:HD22	1.99	0.43
3:C:445:ALA:HB1	3:C:449:ILE:CD1	2.46	0.43
12:L:61:THR:O	12:L:91:ARG:NH2	2.50	0.43
12:L:63:TRP:CD1	12:L:67:GLU:HG2	2.53	0.43
16:O:45:CYS:SG	16:O:48:CYS:N	2.92	0.43
20:T:439:TRP:CE3	20:T:446:ASN:HB2	2.52	0.43
1:A:385:GLU:HB3	1:A:386:PRO:HD2	2.00	0.43
1:A:407:ALA:HA	1:A:408:PRO:HD3	1.87	0.43
1:A:802:THR:HG22	1:A:803:ALA:N	2.34	0.43
1:A:802:THR:HG22	1:A:804:GLU:HG2	2.01	0.43
1:A:995:ARG:HA	1:A:995:ARG:HD2	1.80	0.43
1:A:1166:THR:OG1	1:A:1167:THR:N	2.48	0.43
3:C:134:LEU:HD22	3:C:228:PHE:HE1	1.83	0.43
5:E:251:LEU:CG	5:E:291:CYS:SG	3.05	0.43
5:E:277:PHE:CD1	5:E:277:PHE:N	2.83	0.43
6:F:50:A:O2'	6:F:51:U:H5'	2.19	0.43
7:G:146:C:C2	8:H:33:G:N2	2.86	0.43
8:H:113:G:H2'	8:H:114:A:H8	1.82	0.43
10:J:323:LEU:HD22	14:M:174:PRO:HG3	1.99	0.43
14:M:166:SER:O	14:M:167:LEU:HD13	2.18	0.43
16:O:28:LEU:CD2	18:R:195:ARG:HE	2.29	0.43
23:V:520:GLU:C	23:V:523:GLU:CG	2.85	0.43
24:W:89:PHE:CD1	24:W:89:PHE:O	2.71	0.43
24:W:458:GLU:O	24:W:459:PRO:C	2.59	0.43
26:Y:19:LYS:N	26:Y:19:LYS:CD	2.81	0.43
26:Y:42:ARG:HG3	26:Y:49:TYR:CD1	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:u:307:MET:HE1	29:u:320:MET:CG	2.49	0.43
1:A:61:MET:CE	15:N:104:ARG:HD2	2.49	0.43
1:A:330:THR:O	1:A:331:TRP:HB2	2.17	0.43
3:C:295:ASP:OD1	3:C:297:ASN:HB2	2.19	0.43
3:C:349:PHE:CG	3:C:356:PHE:HE1	2.36	0.43
5:E:277:PHE:CE1	5:E:317:ARG:HG2	2.53	0.43
6:F:34:G:C3'	6:F:35:A:H5''	2.46	0.43
7:G:153:C:H5'	7:G:154:U:O4	2.18	0.43
8:H:57:A:H2'	8:H:58:U:C6	2.50	0.43
14:M:165:ASN:HB2	18:R:95:LYS:CB	2.48	0.43
16:O:253:TYR:HH	19:S:91:LYS:HB3	1.82	0.43
18:R:69:VAL:C	19:S:93:THR:HG21	2.44	0.43
18:R:88:ILE:HG22	18:R:96:ILE:CG2	2.49	0.43
18:R:183:GLN:HB3	18:R:188:PHE:CD2	2.54	0.43
18:R:262:ILE:CG1	18:R:263:PRO:CD	2.96	0.43
26:Y:26:PRO:O	26:Y:27:LYS:HB2	2.18	0.43
26:Y:37:ALA:N	26:Y:53:GLY:HA2	2.33	0.43
29:u:23:MET:O	29:u:227:GLU:HG2	2.19	0.43
29:u:265:PHE:CE1	29:u:297:MET:HE3	2.53	0.43
29:u:278:THR:CG2	29:u:279:GLN:H	2.05	0.43
34:i:18:ARG:NH1	34:i:52:LYS:HB3	2.31	0.43
38:e:51:ASP:C	38:e:51:ASP:OD1	2.61	0.43
1:A:106:MET:HG2	1:A:489:TRP:CZ2	2.53	0.43
1:A:371:LEU:HD12	1:A:372:PRO:HD2	2.01	0.43
1:A:380:LEU:CD2	3:C:349:PHE:CE1	2.86	0.43
1:A:412:ASN:OD1	1:A:412:ASN:C	2.62	0.43
1:A:643:GLY:O	1:A:646:PRO:HD2	2.19	0.43
1:A:1091:TYR:O	1:A:1092:ILE:HB	2.19	0.43
1:A:1539:SER:OG	1:A:1540:PRO:HD3	2.19	0.43
3:C:90:THR:O	3:C:92:PRO:HD3	2.19	0.43
3:C:350:ASN:HB3	3:C:353:THR:CG2	2.49	0.43
6:F:43:A:C2'	6:F:44:G:O5'	2.67	0.43
8:H:178:A:N3	8:H:178:A:H2'	2.34	0.43
16:O:259:ARG:HG3	16:O:274:PHE:C	2.44	0.43
17:P:226:LYS:HD3	17:P:227:TYR:HE1	1.83	0.43
18:R:208:GLU:OE2	18:R:211:ARG:NH1	2.51	0.43
19:S:56:ILE:HD12	19:S:153:PRO:HG3	2.00	0.43
34:i:18:ARG:HB2	34:i:83:GLU:HG2	1.99	0.43
34:i:37:HIS:O	34:i:38:MET:HB2	2.17	0.43
38:l:34:TRP:CD1	38:l:34:TRP:N	2.86	0.43
1:A:44:ARG:HG2	1:A:45:TYR:CD2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:ARG:HE	1:A:86:ARG:HB2	1.65	0.43
1:A:394:TYR:N	1:A:394:TYR:CD1	2.86	0.43
1:A:675:GLN:OE1	6:F:70:A:C5'	2.66	0.43
1:A:901:LEU:CD1	1:A:904:HIS:HE1	2.26	0.43
3:C:89:LEU:C	3:C:91:GLU:N	2.76	0.43
3:C:712:LYS:O	3:C:716:GLU:HG3	2.18	0.43
7:G:146:C:O2	8:H:33:G:C2	2.72	0.43
14:M:122:LEU:N	14:M:122:LEU:HD22	2.34	0.43
18:R:82:MET:HE3	18:R:82:MET:CA	2.48	0.43
18:R:113:TYR:HB3	18:R:230:MET:CE	2.32	0.43
18:R:113:TYR:CG	18:R:118:ASP:OD2	2.72	0.43
18:R:124:VAL:HG22	18:R:125:MET:H	1.83	0.43
18:R:316:GLU:HG3	18:R:316:GLU:O	2.19	0.43
19:S:131:ARG:HH12	19:S:133:CYS:HB2	1.83	0.43
23:V:330:LYS:C	23:V:333:GLN:HG3	2.44	0.43
23:V:577:SER:HA	23:V:580:ARG:HD2	2.01	0.43
24:W:517:SER:O	24:W:518:PRO:C	2.60	0.43
31:w:131:MET:HE2	31:w:147:ASP:C	2.44	0.43
37:f:65:ARG:HH11	37:f:65:ARG:HG3	1.83	0.43
38:e:20:LEU:HD13	39:g:61:VAL:HG22	2.00	0.43
1:A:235:MET:CE	1:A:411:PHE:CA	2.84	0.43
1:A:790:ARG:HA	3:C:60:HIS:CD2	2.52	0.43
1:A:1320:LYS:HE2	1:A:1526:LEU:HA	1.99	0.43
1:A:1758:PRO:HG2	45:4:8:GLY:N	2.34	0.43
1:A:1763:LEU:O	1:A:1767:ASN:HB2	2.19	0.43
6:F:8:C:C6	6:F:8:C:C5'	2.98	0.43
8:H:154:C:O2'	8:H:155:C:C5'	2.66	0.43
12:L:703:MET:O	12:L:707:ALA:HB3	2.18	0.43
12:L:717:MET:O	12:L:721:LEU:N	2.48	0.43
14:M:160:PHE:C	14:M:161:PHE:HD1	2.27	0.43
15:N:59:TYR:CZ	15:N:63:LEU:HD11	2.53	0.43
15:N:125:LYS:HD3	15:N:125:LYS:HA	1.74	0.43
18:R:116:TYR:CD1	18:R:116:TYR:C	2.97	0.43
19:S:125:LYS:HB3	19:S:126:HIS:CE1	2.54	0.43
23:V:631:PHE:CD1	23:V:634:ILE:HD12	2.54	0.43
26:Y:52:LYS:CD	26:Y:52:LYS:C	2.91	0.43
1:A:86:ARG:HH21	18:R:211:ARG:HG3	1.74	0.43
1:A:380:LEU:O	3:C:354:ARG:NH1	2.51	0.43
1:A:380:LEU:H	1:A:380:LEU:HD22	1.84	0.43
1:A:517:HIS:CD2	26:Y:10:TYR:CG	3.06	0.43
1:A:1433:ASP:OD1	1:A:1439:ARG:NH2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:C:H2'	2:B:100:C:C6	2.53	0.43
3:C:61:GLU:OE1	3:C:62:ASP:N	2.51	0.43
3:C:115:GLU:C	3:C:117:ASP:N	2.76	0.43
3:C:196:LYS:CE	34:b:11:GLN:CG	2.97	0.43
3:C:829:GLU:HG3	3:C:830:PRO:HD2	2.01	0.43
5:E:321:TYR:OH	5:E:356:ILE:HG23	2.19	0.43
7:G:23:U:C6	7:G:23:U:H5''	2.54	0.43
8:H:142:C:O2'	8:H:143:A:H5'	2.18	0.43
12:L:86:ALA:HB1	12:L:91:ARG:O	2.18	0.43
12:L:104:LEU:HA	12:L:107:ALA:HB3	2.00	0.43
12:L:178:GLU:O	12:L:181:ARG:N	2.52	0.43
16:O:230:THR:H	16:O:277:ARG:NH1	2.17	0.43
16:O:278:GLN:O	16:O:282:VAL:HG23	2.19	0.43
18:R:238:THR:HG22	18:R:240:LYS:H	1.84	0.43
19:S:155:ASP:OD1	19:S:155:ASP:C	2.62	0.43
20:T:284:TYR:N	20:T:284:TYR:CD1	2.86	0.43
23:V:294:ILE:HD13	23:V:335:MET:C	2.43	0.43
24:W:381:PHE:O	24:W:382:ASN:C	2.60	0.43
35:j:67:TYR:HB2	36:k:100:PHE:O	2.19	0.43
39:n:35:ASP:HB2	39:n:36:PRO:CD	2.42	0.43
1:A:151:MET:SD	1:A:628:GLY:HA3	2.59	0.43
1:A:1162:PRO:HG3	17:P:194:PHE:CZ	2.54	0.43
1:A:1253:SER:OG	8:H:34:U:O2'	1.90	0.43
1:A:1298:ARG:HA	1:A:1298:ARG:HD2	1.66	0.43
1:A:1424:GLN:O	1:A:1427:ARG:HD3	2.18	0.43
3:C:289:ILE:CD1	3:C:300:LEU:HD21	2.49	0.43
8:H:112:G:H2'	8:H:113:G:C8	2.50	0.43
8:H:153:A:H2'	8:H:154:C:H5''	1.99	0.43
12:L:147:ASP:O	12:L:151:MET:HG3	2.19	0.43
14:M:168:LEU:HD23	14:M:168:LEU:N	2.34	0.43
18:R:120:VAL:HG23	18:R:121:PRO:HD2	2.01	0.43
18:R:178:ARG:CD	18:R:194:GLN:HE22	2.07	0.43
23:V:577:SER:N	23:V:580:ARG:HH11	2.16	0.43
24:W:155:SER:O	24:W:156:VAL:CG2	2.61	0.43
36:k:68:GLU:HA	36:k:97:SER:O	2.19	0.43
35:c:67:TYR:HB2	36:d:100:PHE:O	2.19	0.43
45:4:23:ALA:O	45:4:26:ALA:HB3	2.19	0.43
1:A:381:PRO:CG	3:C:334:ILE:HG22	2.49	0.42
1:A:464:PRO:HD2	2:B:20:G:O2'	2.19	0.42
1:A:758:ARG:HH21	1:A:775:ASN:ND2	2.17	0.42
1:A:1363:GLN:O	1:A:1364:LEU:HG	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1685:LEU:HD23	1:A:1685:LEU:HA	1.84	0.42
1:A:1930:TYR:CE1	25:X:71:ASP:CA	3.01	0.42
2:B:24:G:O2'	2:B:26:A:C5	2.71	0.42
2:B:94:U:O2'	2:B:95:G:H3'	2.18	0.42
3:C:77:VAL:HG12	20:T:197:TYR:CA	2.49	0.42
3:C:259:LYS:HG2	47:C:1500:GTP:C2	2.53	0.42
3:C:291:MET:HG2	3:C:292:TYR:CE1	2.54	0.42
3:C:481:MET:SD	3:C:492:ALA:CB	3.06	0.42
5:E:114:GLU:CD	5:E:116:HIS:NE2	2.76	0.42
8:H:36:G:H1'	26:Y:4:ARG:HH21	1.83	0.42
10:J:376:VAL:HB	10:J:411:MET:HE1	2.01	0.42
14:M:159:GLU:OE2	14:M:167:LEU:HB3	2.19	0.42
16:O:79:ASN:OD1	24:W:111:LEU:HD11	2.18	0.42
18:R:70:ALA:HA	19:S:93:THR:HG21	2.01	0.42
18:R:79:LYS:NZ	18:R:80:LYS:HZ1	2.17	0.42
18:R:125:MET:HG3	18:R:129:ASP:OD2	2.19	0.42
18:R:314:GLN:NE2	18:R:314:GLN:CA	2.80	0.42
19:S:38:ASN:HD22	19:S:100:MET:HE1	1.82	0.42
24:W:210:GLU:C	24:W:213:GLN:HB2	2.44	0.42
26:Y:75:ARG:HD3	26:Y:88:THR:HG23	2.01	0.42
29:u:271:LEU:HD11	29:u:408:ALA:HB1	2.00	0.42
29:u:403:MET:HG3	29:u:411:ILE:HD12	2.00	0.42
38:l:51:ASP:C	38:l:51:ASP:OD1	2.61	0.42
1:A:148:TRP:CZ2	1:A:616:PHE:CA	3.02	0.42
1:A:1759:THR:C	1:A:1760:GLU:HG2	2.43	0.42
3:C:70:GLU:C	3:C:70:GLU:CD	2.87	0.42
5:E:348:ASP:C	5:E:348:ASP:OD1	2.62	0.42
8:H:101:U:H4'	34:i:73:ARG:NH2	2.34	0.42
8:H:157:G:H2'	8:H:158:G:O4'	2.19	0.42
10:J:216:ASP:O	10:J:218:GLU:N	2.52	0.42
12:L:196:ILE:O	12:L:196:ILE:HG13	2.18	0.42
15:N:126:LEU:O	24:W:134:THR:HG22	2.18	0.42
18:R:266:LYS:CD	18:R:266:LYS:N	2.82	0.42
24:W:185:ASP:OD1	24:W:185:ASP:N	2.52	0.42
35:j:63:ASN:HA	36:k:102:ARG:CZ	2.50	0.42
34:b:50:LYS:C	34:b:51:ILE:HG13	2.44	0.42
35:c:66:ARG:CZ	36:d:48:ASN:HB3	2.49	0.42
38:e:34:TRP:N	38:e:34:TRP:CD1	2.86	0.42
1:A:369:GLU:HB2	1:A:370:PRO:HD2	2.00	0.42
1:A:1868:MET:HE3	1:A:1872:LEU:CD1	2.49	0.42
1:A:1946:ASN:ND2	1:A:1949:ARG:HE	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:A:H5'	2:B:93:U:OP2	2.19	0.42
3:C:856:HIS:CE1	29:u:102:ILE:CG2	3.00	0.42
10:J:185:ALA:HA	12:L:142:ILE:HD13	2.00	0.42
19:S:10:GLN:CA	19:S:29:TRP:CE2	3.01	0.42
20:T:309:ASP:C	20:T:309:ASP:OD1	2.59	0.42
20:T:406:ILE:HG22	20:T:407:GLN:N	2.33	0.42
24:W:168:PHE:CD1	24:W:168:PHE:N	2.87	0.42
29:u:73:ILE:CD1	29:u:95:SER:HA	2.46	0.42
29:u:260:ARG:HG2	29:u:262:GLU:H	1.83	0.42
1:A:785:LYS:HE2	1:A:785:LYS:HB3	1.80	0.42
1:A:1132:LYS:HA	1:A:1139:ARG:NH1	2.34	0.42
6:F:35:A:OP1	12:L:203:LYS:CG	2.67	0.42
12:L:146:GLU:CG	12:L:147:ASP:OD1	2.68	0.42
12:L:192:ARG:HA	12:L:196:ILE:HG13	2.01	0.42
15:N:30:ARG:HA	15:N:30:ARG:HD2	1.86	0.42
16:O:157:TYR:C	16:O:159:ARG:H	2.27	0.42
18:R:314:GLN:C	18:R:315:LYS:HE2	2.43	0.42
19:S:102:ASN:OD1	19:S:107:THR:O	2.37	0.42
20:T:495:ALA:O	20:T:496:THR:C	2.62	0.42
23:V:644:ARG:O	23:V:647:LEU:HB2	2.19	0.42
25:X:37:ILE:HG13	25:X:37:ILE:H	1.56	0.42
26:Y:28:ASP:OD2	26:Y:64:GLN:CD	2.59	0.42
29:u:307:MET:HE2	29:u:319:ILE:HG22	2.01	0.42
30:v:72:THR:CG2	30:v:94:ILE:CD1	2.89	0.42
1:A:298:ASP:OD1	1:A:298:ASP:C	2.62	0.42
1:A:593:ARG:NH1	1:A:1565:LYS:CE	2.82	0.42
1:A:684:GLU:CD	20:T:290:ALA:HB2	2.45	0.42
1:A:762:ARG:HH12	17:P:226:LYS:CE	2.33	0.42
3:C:275:TYR:OH	3:C:345:GLY:HA2	2.19	0.42
3:C:323:PHE:CE2	3:C:424:PHE:HE1	2.37	0.42
3:C:669:THR:HG22	3:C:690:GLU:OE1	2.19	0.42
6:F:48:A:N3	12:L:33:ARG:NH1	2.68	0.42
7:G:-19:A:N3	29:u:169:ASP:OD2	2.52	0.42
7:G:135:G:N2	7:G:136:U:C4	2.87	0.42
11:K:157:ARG:O	11:K:160:ILE:CG1	2.68	0.42
13:y:69:ARG:O	13:y:73:LEU:HG	2.20	0.42
24:W:135:TYR:CE2	24:W:165:LEU:HD12	2.54	0.42
24:W:571:TRP:C	24:W:573:GLY:N	2.78	0.42
29:u:254:PHE:HA	29:u:401:ASP:O	2.18	0.42
1:A:258:PHE:CD2	1:A:434:HIS:HA	2.55	0.42
1:A:304:ILE:CD1	3:C:921:LEU:HD12	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:539:ARG:NH2	6:F:64:U:H1'	2.35	0.42
1:A:835:ASP:OD1	1:A:836:THR:N	2.53	0.42
1:A:976:MET:HE2	1:A:976:MET:HB2	1.89	0.42
1:A:1495:PHE:CE2	1:A:1748:ARG:HG2	2.55	0.42
3:C:301:SER:C	3:C:303:LEU:H	2.25	0.42
3:C:589:LYS:HB3	3:C:659:VAL:O	2.20	0.42
8:H:155:C:H2'	8:H:156:U:H5''	2.02	0.42
12:L:39:HIS:HD2	12:L:151:MET:CE	2.18	0.42
17:P:58:ASP:OD2	17:P:61:ARG:HB2	2.19	0.42
18:R:67:ILE:CG1	18:R:71:GLN:OE1	2.68	0.42
18:R:314:GLN:CA	18:R:314:GLN:HE21	2.32	0.42
20:T:455:GLN:HG3	20:T:485:THR:CG2	2.48	0.42
24:W:571:TRP:O	24:W:573:GLY:N	2.52	0.42
28:r:102:GLU:HA	28:r:105:HIS:CG	2.54	0.42
29:u:265:PHE:CE1	29:u:297:MET:CE	3.03	0.42
30:v:7:PHE:HD2	30:v:59:MET:HE3	1.84	0.42
1:A:193:LEU:HD12	1:A:194:GLU:N	2.29	0.42
1:A:470:ARG:CZ	1:A:470:ARG:HB2	2.49	0.42
1:A:733:THR:OG1	1:A:734:PRO:HD3	2.20	0.42
1:A:843:LEU:HD23	1:A:843:LEU:HA	1.91	0.42
1:A:1838:LYS:HE3	1:A:1867:GLY:C	2.44	0.42
3:C:220:ARG:HD3	3:C:477:HIS:NE2	2.34	0.42
7:G:138:A:C2'	7:G:139:U:O5'	2.68	0.42
8:H:98:G:H5'	8:H:104:U:OP2	2.19	0.42
10:J:240:THR:O	10:J:241:VAL:HB	2.19	0.42
14:M:153:ARG:HG3	14:M:160:PHE:CD2	2.49	0.42
14:M:200:ARG:H	14:M:200:ARG:HD2	1.84	0.42
15:N:70:ILE:HG23	15:N:74:LEU:HD23	2.01	0.42
16:O:62:ARG:C	16:O:63:MET:HE2	2.45	0.42
16:O:104:LYS:HG3	16:O:139:LYS:HZ1	1.84	0.42
16:O:226:PRO:HD3	16:O:281:GLU:HG2	2.02	0.42
19:S:11:PRO:HB3	19:S:166:GLY:N	2.34	0.42
20:T:225:ASP:O	20:T:226:ARG:CB	2.67	0.42
20:T:454:VAL:CG1	20:T:455:GLN:N	2.81	0.42
24:W:172:GLN:HG3	24:W:173:LYS:N	2.33	0.42
25:X:34:ARG:CA	25:X:37:ILE:HD12	2.37	0.42
29:u:22:ASP:C	29:u:22:ASP:OD1	2.61	0.42
31:w:137:GLN:O	31:w:143:PRO:HA	2.19	0.42
1:A:232:LEU:N	1:A:233:PRO:CD	2.83	0.42
1:A:300:ASN:CB	3:C:939:ARG:HH21	2.30	0.42
1:A:384:VAL:HA	3:C:331:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:801:ILE:O	1:A:802:THR:CB	2.67	0.42
1:A:1201:ARG:O	1:A:1203:SER:N	2.50	0.42
1:A:2332:ASP:C	1:A:2334:TYR:H	2.28	0.42
3:C:461:LEU:HD23	3:C:461:LEU:HA	1.78	0.42
3:C:474:LEU:HD12	3:C:500:THR:O	2.20	0.42
3:C:941:LYS:HG2	3:C:942:GLY:N	2.34	0.42
6:F:95:G:C6	8:H:4:G:C6	3.08	0.42
7:G:146:C:H3'	7:G:147:C:H5''	2.02	0.42
8:H:41:U:O5'	8:H:41:U:H6	2.03	0.42
12:L:52:GLU:OE2	12:L:134:THR:CB	2.67	0.42
12:L:161:ASN:ND2	12:L:161:ASN:O	2.50	0.42
15:N:24:GLU:HG2	24:W:189:ILE:HD13	2.01	0.42
16:O:24:CYS:HB3	16:O:26:THR:H	1.85	0.42
16:O:45:CYS:O	16:O:49:ALA:HA	2.18	0.42
16:O:133:PRO:HG2	16:O:137:LEU:HB2	2.01	0.42
16:O:147:LEU:HD12	16:O:148:LEU:N	2.34	0.42
26:Y:46:CYS:C	26:Y:48:GLU:H	2.26	0.42
28:t:94:GLN:O	28:t:97:GLN:CG	2.68	0.42
30:v:78:LEU:HB3	30:v:116:LYS:HB2	2.02	0.42
1:A:89:LEU:CD2	1:A:89:LEU:C	2.93	0.42
1:A:141:ILE:HG12	1:A:426:LEU:HD23	1.99	0.42
1:A:629:PHE:CD2	1:A:629:PHE:O	2.73	0.42
1:A:697:MET:SD	1:A:705:LYS:HD2	2.60	0.42
1:A:703:GLN:NE2	1:A:703:GLN:HA	2.33	0.42
1:A:1366:PRO:HD2	1:A:1474:MET:CE	2.50	0.42
2:B:23:C:O2'	2:B:24:G:H3'	2.19	0.42
2:B:90:U:H4'	34:b:73:ARG:NH2	2.34	0.42
3:C:71:GLU:C	3:C:71:GLU:CD	2.88	0.42
3:C:512:GLU:HG3	3:C:562:THR:O	2.19	0.42
7:G:-5:G:O2'	7:G:-4:A:H5''	2.19	0.42
12:L:135:LYS:HG3	12:L:136:PRO:N	2.34	0.42
15:N:128:VAL:HG13	15:N:130:ARG:CB	2.48	0.42
16:O:35:ARG:CZ	24:W:129:ARG:NH1	2.83	0.42
16:O:241:ASP:CG	16:O:268:GLN:HE21	2.28	0.42
17:P:228:ILE:O	17:P:229:LYS:C	2.63	0.42
18:R:103:ARG:O	18:R:106:GLN:N	2.48	0.42
18:R:189:ASN:HD22	18:R:189:ASN:HA	1.42	0.42
18:R:307:GLN:N	18:R:307:GLN:CD	2.78	0.42
20:T:233:LEU:HD23	20:T:233:LEU:O	2.20	0.42
24:W:128:GLN:NE2	24:W:139:LEU:HD11	2.35	0.42
38:l:20:LEU:HD13	39:n:61:VAL:HG22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:o:56:LYS:HE2	40:o:58:ASP:CG	2.44	0.42
40:o:161:MET:O	40:o:162:PHE:HB2	2.19	0.42
37:f:65:ARG:HG3	37:f:65:ARG:NH1	2.35	0.42
1:A:76:MET:HE2	1:A:88:TYR:CE2	2.55	0.42
1:A:120:TYR:CA	1:A:483:GLN:O	2.64	0.42
1:A:344:ASP:OD1	1:A:347:LEU:HD11	2.19	0.42
1:A:381:PRO:O	1:A:383:PHE:N	2.52	0.42
1:A:384:VAL:O	1:A:385:GLU:HG2	2.20	0.42
1:A:428:LYS:HE3	1:A:454:TYR:CE1	2.55	0.42
1:A:700:GLY:HA3	18:R:237:MET:CB	2.42	0.42
1:A:1768:TYR:CD1	1:A:1768:TYR:C	2.98	0.42
2:B:92:U:C3'	2:B:93:U:H5'	2.50	0.42
3:C:114:TYR:CE1	35:c:12:HIS:O	2.70	0.42
3:C:465:MET:HE1	3:C:475:MET:CE	2.50	0.42
7:G:152:C:H4'	7:G:153:C:OP1	2.19	0.42
10:J:214:ILE:C	10:J:216:ASP:N	2.78	0.42
10:J:368:ARG:O	10:J:372:VAL:HG23	2.20	0.42
12:L:144:MET:O	12:L:149:LEU:HD12	2.20	0.42
18:R:179:TYR:CD1	24:W:115:ALA:HB2	2.49	0.42
34:i:50:LYS:C	34:i:51:ILE:HG13	2.44	0.42
1:A:54:VAL:HG23	1:A:54:VAL:O	2.20	0.41
1:A:507:LEU:HA	1:A:507:LEU:HD12	1.79	0.41
3:C:700:ILE:HD11	3:C:744:ILE:HD11	2.02	0.41
3:C:703:GLU:OE2	3:C:740:THR:CG2	2.50	0.41
8:H:104:U:O4	36:k:64:ASN:ND2	2.42	0.41
10:J:340:GLN:N	10:J:341:PRO:HD3	2.35	0.41
15:N:12:PRO:HG2	15:N:74:LEU:HA	2.01	0.41
18:R:90:VAL:HG11	18:R:94:GLY:O	2.20	0.41
18:R:124:VAL:HG22	18:R:126:ASN:N	2.34	0.41
20:T:223:SER:OG	20:T:224:ALA:N	2.53	0.41
20:T:399:LYS:CG	20:T:406:ILE:CD1	2.78	0.41
23:V:467:LEU:O	23:V:468:ASP:HB2	2.19	0.41
23:V:484:SER:O	23:V:486:THR:N	2.53	0.41
23:V:497:CYS:HA	23:V:500:GLN:CG	2.50	0.41
23:V:520:GLU:HA	23:V:523:GLU:CG	2.50	0.41
24:W:155:SER:O	24:W:156:VAL:CB	2.67	0.41
25:X:12:TRP:CH2	26:Y:35:LEU:HD22	2.54	0.41
26:Y:22:LYS:CD	26:Y:22:LYS:N	2.73	0.41
29:u:173:ARG:HH21	29:u:173:ARG:CB	2.33	0.41
35:j:66:ARG:CZ	36:k:48:ASN:HB3	2.49	0.41
36:k:103:GLY:O	36:k:106:VAL:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
38:l:18:ILE:H	38:l:18:ILE:HG13	1.70	0.41
40:o:37:LEU:HB2	40:o:61:PRO:HD3	2.00	0.41
34:b:9:MET:HE2	35:c:39:HIS:HE1	1.84	0.41
36:d:68:GLU:HA	36:d:97:SER:O	2.19	0.41
1:A:137:GLU:N	1:A:138:PRO:HD2	2.35	0.41
1:A:206:TRP:CE3	1:A:212:PRO:HB3	2.55	0.41
1:A:676:ARG:NH2	6:F:70:A:P	2.93	0.41
1:A:1149:LEU:O	1:A:1153:VAL:HG23	2.20	0.41
1:A:1330:MET:O	1:A:1330:MET:CG	2.68	0.41
1:A:1370:ARG:HH12	23:V:506:PHE:CB	2.33	0.41
6:F:8:C:H6	6:F:8:C:C5'	2.15	0.41
6:F:27:A:C4	16:O:181:TYR:HE2	2.27	0.41
8:H:107:A:N1	8:H:108:G:C5	2.88	0.41
17:P:73:GLU:C	17:P:73:GLU:CD	2.88	0.41
24:W:182:LYS:N	24:W:182:LYS:CD	2.82	0.41
29:u:353:ASP:O	29:u:364:ARG:NH2	2.53	0.41
34:i:9:MET:HE2	35:j:39:HIS:HE1	1.84	0.41
36:k:28:PRO:HD2	37:m:37:ASP:HB3	2.02	0.41
37:m:65:ARG:HB3	37:m:68:ASN:HD22	1.85	0.41
40:o:52:ASN:HB2	40:o:74:ASN:OD1	2.20	0.41
35:c:63:ASN:HA	36:d:102:ARG:CZ	2.50	0.41
1:A:121:HIS:HE2	1:A:481:PHE:CB	2.22	0.41
1:A:184:ASP:OD1	15:N:1:MET:N	2.35	0.41
1:A:795:LEU:HD23	1:A:795:LEU:HA	1.91	0.41
1:A:912:GLU:HG3	1:A:913:PRO:HD2	2.01	0.41
1:A:947:PRO:HA	1:A:948:PRO:HD3	1.74	0.41
1:A:1210:LYS:C	1:A:1212:GLY:N	2.76	0.41
1:A:1268:ILE:HG21	1:A:1268:ILE:HD13	1.72	0.41
1:A:1427:ARG:H	1:A:1427:ARG:HG2	1.66	0.41
3:C:70:GLU:CD	3:C:71:GLU:N	2.79	0.41
3:C:445:ALA:O	3:C:449:ILE:CA	2.59	0.41
3:C:445:ALA:CB	3:C:449:ILE:CD1	2.98	0.41
3:C:452:THR:HB	3:C:577:PHE:CE2	2.54	0.41
3:C:675:PHE:CD1	3:C:675:PHE:N	2.88	0.41
4:D:1583:ASP:C	4:D:1585:GLN:H	2.26	0.41
6:F:45:A:OP1	6:F:45:A:H4'	2.20	0.41
6:F:79:C:N4	12:L:166:LYS:HE2	2.35	0.41
7:G:-11:G:H5'	7:G:-10:C:C5	2.55	0.41
12:L:222:LEU:HD22	12:L:222:LEU:N	2.22	0.41
14:M:160:PHE:CB	14:M:161:PHE:CD1	2.94	0.41
18:R:247:ILE:HA	18:R:248:PRO:HD3	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:50:ARG:C	25:X:52:GLU:H	2.27	0.41
29:u:378:ILE:HD13	29:u:403:MET:HE1	2.02	0.41
30:v:122:ARG:HG2	30:v:122:ARG:NH1	2.30	0.41
36:k:39:ASN:OD1	36:k:55:ARG:HD3	2.21	0.41
1:A:48:LYS:HG2	1:A:49:ARG:N	2.35	0.41
1:A:75:ASP:C	1:A:77:THR:H	2.27	0.41
1:A:143:GLN:O	1:A:146:SER:HB3	2.20	0.41
1:A:300:ASN:CA	3:C:939:ARG:NH2	2.84	0.41
1:A:417:ARG:NH2	2:B:58:U:O3'	2.48	0.41
1:A:596:TYR:O	1:A:598:LEU:N	2.54	0.41
1:A:758:ARG:HD2	1:A:779:LEU:CD1	2.50	0.41
1:A:1109:LEU:HD11	17:P:188:TRP:CZ2	2.53	0.41
1:A:1318:THR:HA	1:A:1319:PRO:HD3	1.76	0.41
3:C:97:VAL:CG1	17:P:47:THR:OG1	2.69	0.41
3:C:220:ARG:O	3:C:448:LYS:HE3	2.21	0.41
5:E:67:GLY:N	5:E:87:ASP:OD1	2.41	0.41
6:F:45:A:O2'	6:F:46:G:P	2.79	0.41
7:G:150:U:C6	7:G:151:C:H5''	2.55	0.41
12:L:25:LYS:O	18:R:256:ASN:ND2	2.49	0.41
12:L:99:HIS:O	12:L:102:PHE:HB3	2.19	0.41
12:L:179:ALA:O	12:L:183:ALA:CB	2.69	0.41
15:N:113:PHE:HD1	18:R:200:VAL:HG21	1.86	0.41
16:O:248:LEU:O	16:O:252:PHE:HD2	2.03	0.41
19:S:98:LEU:HD21	19:S:129:PHE:HD2	1.84	0.41
20:T:188:PRO:HG3	20:T:443:THR:HG21	2.01	0.41
20:T:292:TYR:CE2	20:T:308:ARG:CG	3.03	0.41
23:V:225:LYS:HE3	23:V:405:ILE:CG1	2.50	0.41
23:V:512:GLY:O	23:V:515:CYS:HB2	2.20	0.41
24:W:123:PHE:HZ	24:W:168:PHE:HD2	1.68	0.41
26:Y:67:VAL:O	26:Y:67:VAL:HG23	2.19	0.41
28:q:81:GLU:O	28:q:85:VAL:HG23	2.20	0.41
29:u:109:ALA:HB3	29:u:159:VAL:HG22	2.02	0.41
29:u:258:VAL:HB	29:u:263:TRP:HB2	2.02	0.41
33:a:58:LEU:HD22	39:g:71:GLU:CD	2.45	0.41
36:d:39:ASN:OD1	36:d:55:ARG:HD3	2.21	0.41
38:e:24:TYR:CD1	38:e:31:ILE:HD11	2.56	0.41
1:A:86:ARG:HH22	18:R:211:ARG:HA	1.85	0.41
1:A:283:VAL:O	1:A:284:ARG:CZ	2.67	0.41
1:A:331:TRP:HE3	1:A:332:TYR:N	2.18	0.41
1:A:464:PRO:HG2	2:B:20:G:C2'	2.47	0.41
1:A:1352:HIS:ND1	22:U:21:ARG:HA	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1494:TYR:HB2	1:A:1710:ASN:ND2	2.35	0.41
5:E:255:MET:O	5:E:257:ASN:N	2.54	0.41
6:F:77:C:H2'	6:F:78:A:H5'	2.02	0.41
7:G:6:A:N3	7:G:6:A:H5'	2.35	0.41
16:O:157:TYR:C	16:O:159:ARG:N	2.77	0.41
20:T:455:GLN:CG	20:T:456:PRO:HD2	2.51	0.41
26:Y:158:LYS:CB	26:Y:163:ARG:HG3	2.49	0.41
29:u:79:ILE:HD11	29:u:229:THR:CG2	2.44	0.41
29:u:268:LEU:HD11	29:u:282:ILE:CD1	2.51	0.41
1:A:151:MET:SD	1:A:628:GLY:CA	3.08	0.41
1:A:292:ASP:O	1:A:294:ASN:ND2	2.54	0.41
1:A:302:ILE:O	3:C:936:LYS:NZ	2.49	0.41
1:A:338:VAL:HG22	3:C:267:LEU:HD23	2.02	0.41
1:A:380:LEU:CD2	3:C:349:PHE:HE1	2.26	0.41
1:A:440:PRO:O	1:A:441:VAL:C	2.64	0.41
1:A:1249:MET:HE3	1:A:1249:MET:HB2	2.00	0.41
1:A:1288:LEU:HD23	1:A:1288:LEU:HA	1.77	0.41
1:A:1370:ARG:HA	1:A:1370:ARG:HD2	1.84	0.41
3:C:65:TYR:O	3:C:66:TYR:CG	2.73	0.41
4:D:577:LYS:O	4:D:581:SER:N	2.54	0.41
7:G:26:U:H2'	7:G:27:U:C5'	2.51	0.41
8:H:102:U:O2'	35:j:61:ARG:NH1	2.51	0.41
8:H:152:G:H2'	8:H:153:A:C1'	2.51	0.41
9:I:296:PHE:CB	9:I:305:SER:O	2.68	0.41
15:N:2:PRO:HG2	15:N:4:VAL:H	1.84	0.41
15:N:75:TYR:CZ	15:N:79:ILE:HD11	2.55	0.41
16:O:155:PRO:HD3	18:R:188:PHE:CE1	2.56	0.41
18:R:103:ARG:O	18:R:104:GLN:C	2.64	0.41
19:S:131:ARG:CD	19:S:131:ARG:C	2.93	0.41
38:l:24:TYR:CD1	38:l:31:ILE:HD11	2.56	0.41
1:A:107:PRO:O	1:A:108:MET:HB2	2.21	0.41
1:A:293:TRP:CH2	1:A:295:GLU:OE1	2.73	0.41
1:A:1161:LEU:HA	1:A:1162:PRO:HD3	1.89	0.41
1:A:1755:SER:OG	1:A:1757:GLU:OE1	2.39	0.41
1:A:1889:LEU:HD12	1:A:2013:GLY:HA3	2.02	0.41
3:C:73:TYR:HB3	3:C:77:VAL:HG21	2.02	0.41
3:C:221:ILE:HG13	3:C:479:THR:OG1	2.20	0.41
3:C:736:GLY:HA3	3:C:770:PHE:CE2	2.53	0.41
3:C:738:ASP:OD1	3:C:738:ASP:N	2.54	0.41
3:C:863:ILE:HD12	3:C:868:LEU:HB2	2.03	0.41
5:E:152:SER:OG	5:E:153:PHE:HD1	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:31:U:H2'	6:F:32:U:H5'	2.02	0.41
6:F:41:A:N6	6:F:42:C:N4	2.68	0.41
6:F:42:C:C5	6:F:43:A:N7	2.88	0.41
7:G:18:A:N1	16:O:196:GLN:O	2.53	0.41
8:H:103:U:C3'	8:H:104:U:H5'	2.50	0.41
12:L:172:ARG:O	12:L:176:LEU:N	2.43	0.41
17:P:63:LEU:C	17:P:63:LEU:CD2	2.93	0.41
18:R:71:GLN:HE21	18:R:71:GLN:HB2	1.61	0.41
18:R:106:GLN:N	18:R:106:GLN:CD	2.79	0.41
18:R:134:ARG:NH2	20:T:339:GLN:OE1	2.54	0.41
23:V:515:CYS:SG	23:V:521:TYR:O	2.78	0.41
23:V:548:ALA:HB2	23:V:585:ILE:CB	2.42	0.41
25:X:5:ASP:CB	25:X:8:LEU:HG	2.47	0.41
26:Y:39:PHE:CD1	26:Y:39:PHE:O	2.74	0.41
26:Y:63:VAL:HA	26:Y:64:GLN:HG2	2.01	0.41
29:u:169:ASP:OD1	29:u:170:MET:HE2	2.20	0.41
37:m:65:ARG:HG3	37:m:65:ARG:NH1	2.35	0.41
41:p:74:PHE:CG	41:p:79:MET:HE3	2.55	0.41
1:A:211:GLN:HA	1:A:212:PRO:HD3	1.82	0.41
1:A:1868:MET:HE3	1:A:1868:MET:HB3	1.91	0.41
3:C:152:GLN:OE1	3:C:426:GLU:O	2.39	0.41
3:C:220:ARG:O	3:C:448:LYS:HE2	2.21	0.41
3:C:297:ASN:ND2	3:C:297:ASN:C	2.79	0.41
3:C:392:LEU:N	3:C:393:PRO:CD	2.84	0.41
3:C:441:PRO:O	3:C:444:GLY:HA3	2.20	0.41
3:C:457:VAL:O	3:C:458:ASP:CB	2.67	0.41
3:C:853:ARG:O	3:C:854:ARG:HB3	2.20	0.41
6:F:43:A:C6	6:F:44:G:O6	2.73	0.41
7:G:135:G:C2	7:G:136:U:O4	2.73	0.41
7:G:150:U:H6	7:G:151:C:H5''	1.86	0.41
8:H:171:U:H2'	8:H:172:C:O4'	2.21	0.41
10:J:412:ASP:O	10:J:413:GLU:C	2.63	0.41
10:J:423:GLU:OE1	10:J:423:GLU:HA	2.20	0.41
12:L:145:ASP:OD1	12:L:146:GLU:OE1	2.38	0.41
20:T:294:LEU:HD23	20:T:294:LEU:N	2.36	0.41
22:U:1:MET:O	22:U:2:TYR:C	2.64	0.41
23:V:452:LEU:N	23:V:452:LEU:CD2	2.81	0.41
23:V:466:SER:HB2	23:V:471:GLU:HB3	2.02	0.41
23:V:606:GLU:CB	23:V:608:LEU:HG	2.50	0.41
24:W:97:ASN:O	24:W:99:PHE:N	2.53	0.41
24:W:127:GLN:HG2	24:W:168:PHE:CE2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:163:ARG:HG2	26:Y:163:ARG:HH11	1.81	0.41
35:j:3:LEU:O	35:j:6:PHE:HB3	2.21	0.41
38:e:21:ILE:HA	38:e:24:TYR:HD2	1.86	0.41
1:A:148:TRP:CZ3	1:A:612:ILE:HG23	2.56	0.41
1:A:203:VAL:HG21	1:A:237:THR:CB	2.51	0.41
1:A:225:TYR:O	1:A:418:THR:CB	2.68	0.41
1:A:282:LEU:C	1:A:282:LEU:CD2	2.93	0.41
1:A:309:ARG:NH2	22:U:1:MET:HE2	2.34	0.41
1:A:456:LEU:HD23	1:A:456:LEU:HA	1.87	0.41
1:A:1237:MET:HE1	1:A:1283:GLU:CD	2.46	0.41
1:A:1364:LEU:HD13	23:V:462:ALA:HA	2.03	0.41
1:A:1573:LEU:HD23	1:A:1573:LEU:HA	1.92	0.41
1:A:1641:ARG:HG3	1:A:1641:ARG:NH1	2.35	0.41
3:C:354:ARG:CG	3:C:354:ARG:HH11	2.34	0.41
3:C:457:VAL:C	3:C:458:ASP:CG	2.88	0.41
3:C:489:GLN:N	3:C:489:GLN:CD	2.78	0.41
3:C:513:ASN:O	3:C:513:ASN:ND2	2.54	0.41
3:C:707:ILE:HD11	3:C:735:PHE:HB2	2.01	0.41
3:C:710:ASN:C	3:C:712:LYS:N	2.77	0.41
5:E:209:ILE:HG21	5:E:250:LEU:HD12	1.99	0.41
6:F:25:C:C4'	6:F:26:U:OP2	2.69	0.41
6:F:42:C:N3	6:F:43:A:C5	2.89	0.41
6:F:86:U:C2'	6:F:87:C:O5'	2.67	0.41
7:G:6:A:C2'	7:G:7:G:C8	2.99	0.41
7:G:7:G:C8	7:G:7:G:OP2	2.72	0.41
7:G:27:U:HO2'	7:G:28:A:C5'	2.21	0.41
7:G:146:C:C6	7:G:146:C:C5'	3.03	0.41
7:G:149:G:O2'	7:G:150:U:P	2.79	0.41
8:H:168:A:C2	39:n:54:GLN:CB	3.04	0.41
11:K:92:PRO:O	11:K:93:SER:C	2.64	0.41
12:L:151:MET:O	12:L:154:GLU:HG3	2.21	0.41
12:L:161:ASN:ND2	12:L:168:LYS:HE3	2.29	0.41
12:L:191:LEU:CG	13:y:57:VAL:CG2	2.98	0.41
12:L:214:ILE:O	12:L:215:PRO:C	2.63	0.41
15:N:56:LYS:HE2	15:N:83:TYR:O	2.20	0.41
19:S:25:LEU:HD12	19:S:25:LEU:N	2.36	0.41
19:S:35:THR:C	19:S:129:PHE:CE1	2.73	0.41
20:T:297:HIS:CE1	20:T:300:ILE:HD12	2.56	0.41
20:T:339:GLN:CG	20:T:340:ALA:N	2.84	0.41
23:V:177:ASN:O	23:V:180:ILE:HG22	2.21	0.41
23:V:503:TYR:HB2	23:V:546:ASN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:V:530:LYS:O	23:V:531:GLU:C	2.64	0.41
23:V:571:SER:CB	23:V:573:GLU:HB3	2.50	0.41
24:W:100:ARG:HH11	24:W:100:ARG:CG	2.33	0.41
26:Y:43:CYS:HB3	26:Y:46:CYS:HB2	2.03	0.41
28:q:117:ILE:HG13	28:t:117:ILE:HG22	2.01	0.41
29:u:271:LEU:O	29:u:275:LEU:HB2	2.21	0.41
29:u:275:LEU:HD21	29:u:280:ALA:HB3	2.03	0.41
30:v:129:GLN:HB3	31:w:108:ARG:CG	2.45	0.41
31:w:131:MET:HE1	31:w:148:TRP:CG	2.56	0.41
32:x:193:LEU:HD23	32:x:193:LEU:HA	1.68	0.41
38:l:21:ILE:HA	38:l:24:TYR:HD2	1.86	0.41
36:d:103:GLY:O	36:d:106:VAL:HG23	2.20	0.41
1:A:47:GLU:CB	1:A:50:LYS:HZ3	1.93	0.41
1:A:61:MET:HB3	1:A:62:PRO:CD	2.51	0.41
1:A:300:ASN:O	3:C:936:LYS:HG2	2.21	0.41
1:A:346:ASP:O	1:A:347:LEU:C	2.64	0.41
1:A:758:ARG:O	1:A:758:ARG:HG3	2.20	0.41
1:A:937:PRO:CB	1:A:938:PRO:HD2	2.51	0.41
1:A:1508:GLY:O	25:X:24:TRP:CE2	2.74	0.41
3:C:230:ASP:OD2	3:C:259:LYS:HE3	2.09	0.41
3:C:235:VAL:HG13	3:C:239:THR:OG1	2.22	0.41
3:C:518:ASP:N	3:C:519:GLU:OE2	2.54	0.41
3:C:641:MET:HE2	3:C:655:VAL:HG21	2.01	0.41
3:C:705:VAL:HG21	3:C:718:PHE:CE2	2.56	0.41
4:D:1481:ILE:C	4:D:1483:ARG:H	2.28	0.41
6:F:9:U:O2'	6:F:10:U:O4'	2.39	0.41
6:F:33:G:C2'	6:F:34:G:O5'	2.69	0.41
6:F:51:U:H2'	6:F:52:U:O4'	2.21	0.41
9:I:616:TYR:O	9:I:618:ARG:N	2.54	0.41
13:y:54:SER:HA	13:y:57:VAL:HG21	2.02	0.41
16:O:134:VAL:HG12	16:O:135:GLY:N	2.37	0.41
16:O:235:TYR:HA	16:O:271:PHE:HD1	1.86	0.41
19:S:12:PRO:CD	19:S:166:GLY:HA2	2.51	0.41
29:u:46:ARG:HD3	29:u:133:MET:CE	2.51	0.41
33:h:58:LEU:HD22	39:n:71:GLU:CD	2.45	0.41
40:o:37:LEU:HB2	40:o:61:PRO:CD	2.51	0.41
41:p:3:ILE:HG22	41:p:83:TYR:HB2	2.02	0.41
45:4:4:ALA:HB3	45:4:5:PRO:CD	2.27	0.41
1:A:406:TRP:CH2	3:C:265:LEU:O	2.75	0.40
2:B:20:G:C1'	2:B:21:A:OP1	2.69	0.40
3:C:300:LEU:N	3:C:300:LEU:CD1	2.84	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:490:PHE:CD1	3:C:490:PHE:N	2.90	0.40
3:C:704:VAL:O	3:C:709:TRP:CZ2	2.74	0.40
3:C:934:MET:HE2	3:C:934:MET:HB2	1.93	0.40
4:D:642:THR:C	4:D:644:GLU:H	2.29	0.40
6:F:42:C:O2'	6:F:43:A:C5'	2.69	0.40
6:F:55:C:H2'	6:F:56:A:O4'	2.21	0.40
8:H:106:G:H5'	36:k:47:ARG:NH2	2.34	0.40
10:J:206:LEU:HD21	12:L:171:ALA:HB1	2.02	0.40
16:O:144:SER:O	16:O:145:ASP:C	2.64	0.40
16:O:240:GLY:HA3	16:O:296:ARG:NH2	2.34	0.40
17:P:44:ARG:HG3	20:T:258:SER:CA	2.51	0.40
18:R:69:VAL:HG12	18:R:70:ALA:N	2.36	0.40
18:R:155:VAL:O	18:R:159:VAL:HG23	2.20	0.40
20:T:187:LYS:N	20:T:188:PRO:HD3	2.37	0.40
20:T:209:CYS:O	20:T:221:THR:HA	2.21	0.40
20:T:318:ARG:CG	20:T:318:ARG:NH1	2.82	0.40
24:W:98:PRO:O	24:W:99:PHE:C	2.63	0.40
26:Y:52:LYS:C	26:Y:52:LYS:HD2	2.46	0.40
26:Y:109:GLN:O	26:Y:110:ALA:C	2.63	0.40
26:Y:109:GLN:C	26:Y:111:GLU:N	2.79	0.40
29:u:46:ARG:HH11	29:u:133:MET:HE3	1.85	0.40
40:o:160:LYS:O	40:o:161:MET:C	2.63	0.40
36:d:28:PRO:HD2	37:f:37:ASP:HB3	2.02	0.40
36:d:33:THR:CG2	36:d:37:LYS:HE2	2.46	0.40
36:d:110:LEU:CD1	37:f:59:LEU:HB3	2.46	0.40
1:A:347:LEU:O	1:A:348:PRO:C	2.63	0.40
1:A:1255:THR:HG23	8:H:33:G:O2'	2.21	0.40
1:A:1772:PHE:CD1	1:A:1772:PHE:C	2.99	0.40
2:B:27:U:HO2'	2:B:28:A:P	2.44	0.40
3:C:64:LYS:HE2	3:C:64:LYS:HA	2.02	0.40
6:F:48:A:C4	12:L:33:ARG:NH1	2.70	0.40
7:G:-1:G:O3'	26:Y:4:ARG:CG	2.70	0.40
7:G:21:A:H61	16:O:92:LEU:HA	1.87	0.40
7:G:22:C:O2	7:G:22:C:C2'	2.70	0.40
7:G:145:U:O4	25:X:9:LYS:NZ	2.54	0.40
8:H:149:A:C6	8:H:150:U:C4	3.09	0.40
8:H:183:G:C6	8:H:184:C:N4	2.89	0.40
10:J:216:ASP:O	10:J:217:GLU:C	2.64	0.40
10:J:296:ARG:HD2	12:L:225:TYR:CE1	2.56	0.40
10:J:360:ASP:C	10:J:363:ARG:HG3	2.45	0.40
12:L:40:ARG:HG3	26:Y:109:GLN:NE2	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:66:GLU:CD	12:L:66:GLU:H	2.30	0.40
12:L:86:ALA:HB3	12:L:87:PRO:HD3	2.03	0.40
12:L:181:ARG:O	12:L:185:LEU:N	2.42	0.40
16:O:256:GLY:HA2	18:R:70:ALA:HB3	2.04	0.40
17:P:26:LEU:HD12	17:P:26:LEU:HA	1.92	0.40
17:P:193:VAL:HG21	17:P:194:PHE:CE2	2.56	0.40
18:R:249:PRO:O	18:R:250:CYS:C	2.64	0.40
19:S:9:TRP:CE3	19:S:11:PRO:CD	2.95	0.40
22:U:25:LEU:C	22:U:25:LEU:HD12	2.46	0.40
23:V:489:LEU:O	23:V:492:MET:N	2.55	0.40
24:W:101:THR:C	24:W:103:GLN:N	2.79	0.40
33:h:63:ILE:HG12	39:n:69:MET:HG3	2.03	0.40
41:p:13:ASN:HB2	41:p:80:ARG:HH21	1.86	0.40
36:d:62:HIS:O	36:d:103:GLY:HA3	2.21	0.40
1:A:158:ARG:HH12	1:A:573:GLN:NE2	2.16	0.40
1:A:280:GLU:CD	1:A:281:PRO:HD2	2.46	0.40
1:A:587:GLN:CA	1:A:1550:GLY:O	2.67	0.40
1:A:1629:ILE:HB	1:A:1662:ILE:HB	2.03	0.40
3:C:445:ALA:O	3:C:448:LYS:N	2.54	0.40
3:C:614:TYR:HA	3:C:615:PRO:HD3	1.86	0.40
5:E:115:LEU:O	5:E:116:HIS:CD2	2.74	0.40
7:G:27:U:CI'	16:O:269:CYS:SG	3.09	0.40
8:H:18:U:O2	18:R:257:ALA:HB3	2.22	0.40
8:H:31:G:O3'	25:X:17:LEU:HD11	2.22	0.40
8:H:112:G:O5'	8:H:112:G:H8	2.04	0.40
9:I:520:ILE:O	9:I:524:TYR:N	2.54	0.40
10:J:194:LEU:HD11	12:L:152:LEU:HD22	2.03	0.40
10:J:220:LEU:O	10:J:223:TYR:HB3	2.21	0.40
12:L:181:ARG:HG3	12:L:182:LEU:N	2.37	0.40
15:N:37:HIS:CD2	15:N:37:HIS:O	2.74	0.40
15:N:40:LYS:O	15:N:44:GLU:HB3	2.21	0.40
18:R:106:GLN:NE2	18:R:106:GLN:CA	2.84	0.40
20:T:210:ILE:HG12	20:T:221:THR:HG22	2.02	0.40
20:T:318:ARG:NH1	20:T:319:THR:CG2	2.85	0.40
23:V:612:PHE:CZ	23:V:631:PHE:HE2	2.39	0.40
26:Y:20:ILE:HG22	26:Y:21:PRO:CD	2.51	0.40
27:Z:975:VAL:C	27:Z:977:MET:O	2.64	0.40
28:t:113:ALA:O	28:t:117:ILE:HG23	2.21	0.40
30:v:92:ILE:CG2	30:v:94:ILE:CG2	2.95	0.40
37:f:5:LEU:O	38:e:49:GLY:HA3	2.22	0.40
37:f:65:ARG:HB3	37:f:68:ASN:HD22	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:312:TYR:CE2	3:C:882:GLY:HA3	2.56	0.40
1:A:598:LEU:N	1:A:598:LEU:HD12	2.35	0.40
1:A:2332:ASP:O	1:A:2334:TYR:N	2.54	0.40
3:C:97:VAL:HG13	17:P:47:THR:OG1	2.21	0.40
3:C:576:ILE:HG22	3:C:577:PHE:O	2.22	0.40
3:C:592:VAL:HG12	3:C:603:MET:SD	2.62	0.40
6:F:90:G:C2	8:H:9:U:C2	3.09	0.40
7:G:10:U:H2'	7:G:11:A:O4'	2.22	0.40
8:H:160:A:H2'	8:H:161:U:O4'	2.22	0.40
12:L:77:LEU:HD21	18:R:285:ALA:CB	2.52	0.40
16:O:239:LEU:HG	16:O:240:GLY:O	2.22	0.40
17:P:72:ARG:NH1	17:P:72:ARG:CB	2.83	0.40
22:U:25:LEU:C	22:U:25:LEU:CD1	2.94	0.40
23:V:585:ILE:O	23:V:588:GLN:N	2.54	0.40
24:W:157:GLU:HB3	24:W:158:GLU:OE1	2.21	0.40
24:W:210:GLU:O	24:W:213:GLN:HB2	2.20	0.40
26:Y:130:LEU:N	26:Y:130:LEU:HD13	2.36	0.40
26:Y:133:PRO:O	26:Y:137:LEU:HG	2.22	0.40
35:c:3:LEU:O	35:c:6:PHE:HB3	2.20	0.40
1:A:152:ARG:HB3	1:A:152:ARG:NH1	2.21	0.40
1:A:338:VAL:CG2	3:C:267:LEU:HD23	2.51	0.40
1:A:370:PRO:HG3	3:C:304:LEU:CD2	2.52	0.40
1:A:678:GLU:CD	1:A:774:LYS:NZ	2.80	0.40
1:A:1630:LEU:HD21	1:A:1696:PRO:HG3	2.03	0.40
2:B:19:A:H2'	2:B:20:G:C5'	2.49	0.40
3:C:87:GLN:OE1	3:C:91:GLU:HG3	2.22	0.40
3:C:114:TYR:HD1	3:C:115:GLU:HG3	1.86	0.40
3:C:673:LYS:CG	3:C:686:THR:HG23	2.52	0.40
3:C:706:GLN:HE21	3:C:708:THR:N	2.13	0.40
6:F:42:C:C2	6:F:43:A:C4	3.10	0.40
7:G:1:G:C6	7:G:145:U:O4'	2.74	0.40
7:G:9:C:H2'	7:G:10:U:C6	2.57	0.40
12:L:741:GLN:O	12:L:744:GLN:CG	2.69	0.40
13:y:64:GLY:O	13:y:65:LEU:HB2	2.21	0.40
14:M:167:LEU:O	18:R:96:ILE:HD11	2.22	0.40
19:S:15:TYR:HB2	19:S:163:TYR:HB2	2.02	0.40
19:S:65:GLY:O	19:S:110:SER:OG	2.40	0.40
20:T:281:ILE:CD1	20:T:282:ARG:HG2	2.50	0.40
23:V:472:CYS:CB	23:V:510:LEU:HD11	2.52	0.40
23:V:549:LYS:HA	23:V:589:GLU:HG2	2.04	0.40
23:V:600:ASN:HA	23:V:639:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:Y:7:LEU:HD22	26:Y:7:LEU:HA	1.87	0.40
26:Y:109:GLN:OE1	26:Y:110:ALA:N	2.54	0.40
28:q:106:ALA:O	28:q:109:GLN:CG	2.69	0.40
29:u:150:ILE:HD11	29:u:173:ARG:HH22	1.86	0.40
35:j:20:LYS:O	35:j:66:ARG:NH2	2.55	0.40
33:a:23:ASN:ND2	33:a:67:LYS:HA	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2247/2335 (96%)	2100 (94%)	107 (5%)	40 (2%)	6	35
3	C	856/972 (88%)	779 (91%)	57 (7%)	20 (2%)	5	31
4	D	1900/2136 (89%)	1799 (95%)	96 (5%)	5 (0%)	36	70
5	E	297/357 (83%)	272 (92%)	16 (5%)	9 (3%)	3	25
9	I	493/855 (58%)	475 (96%)	10 (2%)	8 (2%)	7	37
10	J	530/848 (62%)	483 (91%)	30 (6%)	17 (3%)	3	24
11	K	144/225 (64%)	134 (93%)	6 (4%)	4 (3%)	4	27
12	L	401/802 (50%)	375 (94%)	19 (5%)	7 (2%)	7	36
13	y	106/307 (34%)	98 (92%)	8 (8%)	0	100	100
14	M	89/243 (37%)	80 (90%)	3 (3%)	6 (7%)	1	14
15	N	141/144 (98%)	126 (89%)	12 (8%)	3 (2%)	5	32
16	O	279/420 (66%)	247 (88%)	26 (9%)	6 (2%)	5	31
17	P	92/229 (40%)	82 (89%)	9 (10%)	1 (1%)	11	44
18	R	235/536 (44%)	207 (88%)	14 (6%)	14 (6%)	1	15
19	S	157/166 (95%)	144 (92%)	10 (6%)	3 (2%)	6	34

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
20	T	311/514 (60%)	282 (91%)	17 (6%)	12 (4%)	2	21
21	Q	1304/1485 (88%)	1279 (98%)	25 (2%)	0	100	100
22	U	24/2752 (1%)	20 (83%)	3 (12%)	1 (4%)	2	20
23	V	444/908 (49%)	413 (93%)	26 (6%)	5 (1%)	11	44
24	W	436/579 (75%)	385 (88%)	32 (7%)	19 (4%)	2	20
25	X	69/425 (16%)	65 (94%)	2 (3%)	2 (3%)	3	26
26	Y	202/323 (62%)	182 (90%)	6 (3%)	14 (7%)	1	13
27	Z	611/1227 (50%)	517 (85%)	61 (10%)	33 (5%)	1	17
28	q	130/504 (26%)	119 (92%)	7 (5%)	4 (3%)	3	25
28	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	7	37
28	s	369/504 (73%)	352 (95%)	16 (4%)	1 (0%)	36	70
28	t	65/504 (13%)	64 (98%)	0	1 (2%)	8	39
29	u	388/411 (94%)	376 (97%)	9 (2%)	3 (1%)	16	52
30	v	142/148 (96%)	138 (97%)	4 (3%)	0	100	100
31	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	11	44
32	x	23/703 (3%)	22 (96%)	1 (4%)	0	100	100
33	a	75/126 (60%)	74 (99%)	1 (1%)	0	100	100
33	h	76/126 (60%)	75 (99%)	1 (1%)	0	100	100
34	b	81/229 (35%)	79 (98%)	2 (2%)	0	100	100
34	i	84/229 (37%)	82 (98%)	2 (2%)	0	100	100
35	c	79/119 (66%)	76 (96%)	3 (4%)	0	100	100
35	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
36	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
36	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
37	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
37	m	72/86 (84%)	68 (94%)	4 (6%)	0	100	100
38	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
38	l	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
39	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
39	n	64/76 (84%)	62 (97%)	2 (3%)	0	100	100
40	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
41	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
42	1	239/301 (79%)	232 (97%)	7 (3%)	0	100	100
43	2	386/646 (60%)	358 (93%)	20 (5%)	8 (2%)	5	32
44	3	167/754 (22%)	165 (99%)	2 (1%)	0	100	100
45	4	35/37 (95%)	29 (83%)	2 (6%)	4 (11%)	0	5
All	All	14867/26150 (57%)	13893 (93%)	719 (5%)	255 (2%)	9	36

All (255) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	92	LEU
1	A	167	PRO
1	A	188	LEU
1	A	331	TRP
1	A	346	ASP
1	A	365	VAL
1	A	367	SER
1	A	368	GLN
1	A	570	ASP
1	A	629	PHE
1	A	706	ALA
1	A	942	PRO
1	A	1518	LEU
1	A	1762	TYR
1	A	1828	ALA
3	C	156	GLU
3	C	388	VAL
3	C	427	PHE
3	C	444	GLY
3	C	457	VAL
3	C	458	ASP
3	C	516	LEU
3	C	824	THR
4	D	128	PRO
4	D	957	VAL
4	D	1584	ILE
5	E	193	THR
9	I	463	PRO
9	I	721	LYS

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Mol	Chain	Res	Type
9	I	797	PHE
10	J	188	GLN
10	J	191	ALA
10	J	192	GLU
10	J	202	GLU
10	J	203	LEU
10	J	205	LEU
10	J	216	ASP
10	J	413	GLU
11	K	78	PRO
11	K	90	PRO
12	L	138	ARG
12	L	146	GLU
12	L	201	LYS
12	L	203	LYS
14	M	157	GLY
14	M	195	LYS
15	N	36	PRO
16	O	20	PHE
16	O	107	MET
17	P	49	ASP
18	R	71	GLN
18	R	135	PRO
18	R	136	ASP
18	R	186	VAL
18	R	223	PRO
19	S	164	PRO
20	T	186	PRO
20	T	268	LYS
20	T	341	ALA
20	T	343	PRO
20	T	495	ALA
23	V	596	LEU
23	V	597	PRO
24	W	156	VAL
24	W	199	TYR
24	W	205	VAL
24	W	213	GLN
24	W	279	LYS
24	W	299	LEU
24	W	325	LEU
24	W	372	ASN

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Mol	Chain	Res	Type
24	W	492	ASN
25	X	51	GLU
25	X	64	LYS
26	Y	24	LYS
26	Y	25	LEU
26	Y	27	LYS
26	Y	37	ALA
26	Y	69	LEU
26	Y	110	ALA
27	Z	556	GLU
27	Z	574	TYR
27	Z	614	ARG
27	Z	711	VAL
27	Z	748	PRO
27	Z	771	PRO
27	Z	795	PRO
27	Z	821	ILE
27	Z	881	THR
27	Z	978	LEU
27	Z	1087	ILE
27	Z	1099	CYS
27	Z	1114	PRO
28	q	59	HIS
28	q	60	PRO
28	s	71	ILE
28	t	69	THR
29	u	383	ASN
43	2	114	LYS
43	2	186	PRO
43	2	233	PRO
43	2	239	VAL
43	2	282	TYR
43	2	382	ASN
45	4	4	ALA
45	4	22	ALA
45	4	23	ALA
1	A	308	ILE
1	A	349	ALA
1	A	370	PRO
1	A	374	ASP
1	A	382	GLU
1	A	383	PHE

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Mol	Chain	Res	Type
1	A	631	ALA
1	A	1212	GLY
3	C	90	THR
3	C	364	SER
3	C	711	ARG
4	D	151	LYS
9	I	618	ARG
9	I	634	ILE
10	J	217	GLU
10	J	341	PRO
10	J	376	VAL
10	J	709	VAL
14	M	120	PRO
15	N	39	GLY
16	O	132	ARG
16	O	206	ASN
18	R	191	GLY
19	S	12	PRO
20	T	301	ASP
22	U	2	TYR
23	V	485	GLN
24	W	177	LYS
24	W	191	GLY
24	W	318	VAL
24	W	482	ASP
26	Y	96	THR
27	Z	570	HIS
27	Z	608	GLU
27	Z	778	ILE
27	Z	796	ASP
27	Z	798	VAL
27	Z	1085	LYS
27	Z	1098	PRO
28	q	9	ASN
29	u	340	GLY
29	u	385	ASP
31	w	115	GLY
40	o	160	LYS
1	A	51	PHE
1	A	212	PRO
1	A	378	PHE
1	A	1092	ILE

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Mol	Chain	Res	Type
1	A	1831	LYS
1	A	1947	ASN
3	C	63	LYS
5	E	60	MET
5	E	88	ARG
5	E	256	ASP
9	I	601	GLN
9	I	752	ALA
10	J	190	THR
18	R	104	GLN
18	R	173	PRO
18	R	250	CYS
20	T	406	ILE
23	V	578	SER
24	W	102	GLN
26	Y	21	PRO
26	Y	52	LYS
26	Y	102	HIS
27	Z	615	PHE
27	Z	641	ALA
27	Z	822	ASP
27	Z	982	ALA
28	q	19	PRO
28	r	9	ASN
43	2	336	PRO
1	A	363	HIS
1	A	480	LYS
1	A	1363	GLN
3	C	754	VAL
3	C	856	HIS
5	E	162	ARG
9	I	617	GLU
10	J	189	ILE
10	J	206	LEU
10	J	604	PRO
11	K	65	ILE
12	L	132	PRO
12	L	585	TYR
16	O	134	VAL
18	R	124	VAL
18	R	234	SER
18	R	283	ASN

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Mol	Chain	Res	Type
19	S	10	GLN
20	T	401	PRO
24	W	554	ILE
26	Y	28	ASP
26	Y	66	GLU
27	Z	509	MET
27	Z	605	LEU
27	Z	777	PRO
27	Z	904	GLN
27	Z	1110	MET
27	Z	1112	TYR
27	Z	1151	VAL
40	o	32	PRO
1	A	359	ILE
1	A	1339	ASP
1	A	1517	LYS
3	C	361	PRO
3	C	615	PRO
5	E	159	PRO
16	O	239	LEU
18	R	126	ASN
20	T	185	MET
20	T	189	GLN
20	T	226	ARG
24	W	301	GLY
24	W	330	GLY
26	Y	20	ILE
43	2	283	PRO
1	A	903	SER
1	A	1275	ARG
1	A	2013	GLY
3	C	94	ILE
3	C	360	ALA
3	C	623	GLU
5	E	270	LYS
14	M	161	PHE
18	R	249	PRO
23	V	609	GLN
24	W	376	PRO
24	W	549	HIS
27	Z	1103	PRO
3	C	66	TYR

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Mol	Chain	Res	Type
5	E	149	GLY
12	L	215	PRO
11	K	17	PRO
1	A	186	GLU
10	J	241	VAL
14	M	174	PRO
20	T	411	GLY
26	Y	26	PRO
27	Z	1109	GLY
4	D	585	ILE
5	E	324	PRO
14	M	144	PRO
15	N	4	VAL
28	r	60	PRO
45	4	5	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1778/2108 (84%)	1628 (92%)	150 (8%)	10	32
3	C	760/866 (88%)	694 (91%)	66 (9%)	9	31
5	E	256/300 (85%)	243 (95%)	13 (5%)	21	45
10	J	241/751 (32%)	216 (90%)	25 (10%)	7	24
11	K	54/196 (28%)	46 (85%)	8 (15%)	3	15
12	L	193/709 (27%)	155 (80%)	38 (20%)	1	9
13	y	33/256 (13%)	30 (91%)	3 (9%)	9	29
14	M	85/209 (41%)	61 (72%)	24 (28%)	0	3
15	N	130/130 (100%)	124 (95%)	6 (5%)	24	47
16	O	253/361 (70%)	248 (98%)	5 (2%)	48	66
17	P	90/203 (44%)	80 (89%)	10 (11%)	6	22
18	R	210/457 (46%)	153 (73%)	57 (27%)	0	3

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
19	S	129/134 (96%)	120 (93%)	9 (7%)	14	38
20	T	269/441 (61%)	252 (94%)	17 (6%)	16	40
22	U	21/2432 (1%)	16 (76%)	5 (24%)	1	5
23	V	324/838 (39%)	305 (94%)	19 (6%)	18	42
24	W	115/502 (23%)	73 (64%)	42 (36%)	0	1
25	X	33/381 (9%)	20 (61%)	13 (39%)	0	1
26	Y	114/289 (39%)	85 (75%)	29 (25%)	0	4
28	q	78/435 (18%)	71 (91%)	7 (9%)	9	30
28	r	76/435 (18%)	65 (86%)	11 (14%)	3	16
28	t	40/435 (9%)	37 (92%)	3 (8%)	12	35
29	u	344/361 (95%)	337 (98%)	7 (2%)	48	66
30	v	132/134 (98%)	131 (99%)	1 (1%)	73	77
31	w	76/143 (53%)	75 (99%)	1 (1%)	61	72
32	x	23/581 (4%)	23 (100%)	0	100	100
33	a	68/101 (67%)	68 (100%)	0	100	100
33	h	68/101 (67%)	68 (100%)	0	100	100
34	b	76/167 (46%)	73 (96%)	3 (4%)	28	51
34	i	77/167 (46%)	74 (96%)	3 (4%)	28	51
35	c	76/101 (75%)	74 (97%)	2 (3%)	40	61
35	j	77/101 (76%)	75 (97%)	2 (3%)	40	61
36	d	88/110 (80%)	87 (99%)	1 (1%)	65	74
36	k	80/110 (73%)	79 (99%)	1 (1%)	61	72
37	f	63/74 (85%)	61 (97%)	2 (3%)	34	56
37	m	63/74 (85%)	61 (97%)	2 (3%)	34	56
38	e	74/84 (88%)	74 (100%)	0	100	100
38	l	74/84 (88%)	74 (100%)	0	100	100
39	g	62/66 (94%)	61 (98%)	1 (2%)	55	69
39	n	59/66 (89%)	58 (98%)	1 (2%)	53	68
40	o	138/218 (63%)	132 (96%)	6 (4%)	26	49
41	p	82/195 (42%)	79 (96%)	3 (4%)	30	52
45	4	1/1 (100%)	1 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	7083/15907 (44%)	6487 (92%)	596 (8%)	12	32

All (596) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	44	ARG
1	A	48	LYS
1	A	49	ARG
1	A	55	ASP
1	A	58	LYS
1	A	59	GLU
1	A	60	ASP
1	A	75	ASP
1	A	77	THR
1	A	78	ASN
1	A	82	ARG
1	A	86	ARG
1	A	88	TYR
1	A	89	LEU
1	A	152	ARG
1	A	165	ARG
1	A	180	ASP
1	A	181	ASN
1	A	185	VAL
1	A	200	ASP
1	A	204	LEU
1	A	212	PRO
1	A	232	LEU
1	A	233	PRO
1	A	250	VAL
1	A	258	PHE
1	A	284	ARG
1	A	294	ASN
1	A	295	GLU
1	A	304	ILE
1	A	310	THR
1	A	325	HIS
1	A	329	LEU
1	A	330	THR
1	A	331	TRP
1	A	336	ASN
1	A	338	VAL

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Mol	Chain	Res	Type
1	A	344	ASP
1	A	359	ILE
1	A	361	HIS
1	A	362	ARG
1	A	363	HIS
1	A	364	SER
1	A	371	LEU
1	A	377	GLU
1	A	379	GLU
1	A	380	LEU
1	A	383	PHE
1	A	388	LEU
1	A	389	LYS
1	A	391	THR
1	A	394	TYR
1	A	409	ARG
1	A	413	LEU
1	A	433	GLU
1	A	439	GLN
1	A	459	LEU
1	A	462	ARG
1	A	467	GLN
1	A	468	LYS
1	A	533	LYS
1	A	546	LEU
1	A	548	ARG
1	A	579	GLN
1	A	601	GLN
1	A	621	VAL
1	A	630	TRP
1	A	670	LYS
1	A	671	THR
1	A	673	THR
1	A	674	LYS
1	A	675	GLN
1	A	690	MET
1	A	697	MET
1	A	701	ILE
1	A	705	LYS
1	A	726	TRP
1	A	744	LYS
1	A	762	ARG

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Mol	Chain	Res	Type
1	A	767	VAL
1	A	804	GLU
1	A	847	LYS
1	A	851	SER
1	A	855	ARG
1	A	856	LEU
1	A	861	ARG
1	A	880	ARG
1	A	883	ARG
1	A	904	HIS
1	A	948	PRO
1	A	1032	ARG
1	A	1089	CYS
1	A	1094	ARG
1	A	1141	ARG
1	A	1168	VAL
1	A	1179	SER
1	A	1210	LYS
1	A	1211	ASP
1	A	1224	ARG
1	A	1246	GLN
1	A	1249	MET
1	A	1279	VAL
1	A	1315	VAL
1	A	1321	GLU
1	A	1337	GLN
1	A	1361	GLU
1	A	1363	GLN
1	A	1370	ARG
1	A	1393	ARG
1	A	1414	ARG
1	A	1417	PRO
1	A	1427	ARG
1	A	1449	LYS
1	A	1504	GLU
1	A	1526	LEU
1	A	1532	ARG
1	A	1534	PHE
1	A	1570	LYS
1	A	1615	HIS
1	A	1626	CYS
1	A	1641	ARG

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Mol	Chain	Res	Type
1	A	1678	ARG
1	A	1681	ARG
1	A	1732	LYS
1	A	1738	PRO
1	A	1754	TYR
1	A	1756	SER
1	A	1757	GLU
1	A	1763	LEU
1	A	1766	GLN
1	A	1768	TYR
1	A	1770	GLU
1	A	1771	LEU
1	A	1774	ASN
1	A	1790	ILE
1	A	1794	PHE
1	A	1813	ARG
1	A	1831	LYS
1	A	1833	LEU
1	A	1865	ARG
1	A	1868	MET
1	A	1885	LYS
1	A	1887	SER
1	A	1888	GLU
1	A	1889	LEU
1	A	1898	LYS
1	A	1949	ARG
1	A	1958	LYS
1	A	1968	TRP
1	A	1986	LEU
3	C	61	GLU
3	C	62	ASP
3	C	63	LYS
3	C	64	LYS
3	C	68	THR
3	C	71	GLU
3	C	87	GLN
3	C	92	PRO
3	C	97	VAL
3	C	295	ASP
3	C	297	ASN
3	C	298	LEU
3	C	300	LEU

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Mol	Chain	Res	Type
3	C	333	ASP
3	C	336	TYR
3	C	354	ARG
3	C	357	THR
3	C	359	LYS
3	C	362	THR
3	C	366	GLN
3	C	389	ASP
3	C	427	PHE
3	C	428	THR
3	C	438	ILE
3	C	448	LYS
3	C	450	GLU
3	C	452	THR
3	C	454	THR
3	C	457	VAL
3	C	458	ASP
3	C	463	GLU
3	C	468	CYS
3	C	474	LEU
3	C	475	MET
3	C	489	GLN
3	C	490	PHE
3	C	495	ARG
3	C	512	GLU
3	C	517	GLU
3	C	519	GLU
3	C	540	GLU
3	C	569	ARG
3	C	572	GLU
3	C	573	GLU
3	C	596	ASN
3	C	673	LYS
3	C	675	PHE
3	C	677	GLU
3	C	680	ASN
3	C	704	VAL
3	C	706	GLN
3	C	709	TRP
3	C	724	TRP
3	C	725	ASP
3	C	726	LEU

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Mol	Chain	Res	Type
3	C	730	ARG
3	C	738	ASP
3	C	749	THR
3	C	750	LEU
3	C	813	ARG
3	C	826	ARG
3	C	856	HIS
3	C	885	THR
3	C	939	ARG
3	C	941	LYS
3	C	943	LEU
5	E	74	PHE
5	E	153	PHE
5	E	161	ARG
5	E	178	LEU
5	E	215	ASN
5	E	229	TYR
5	E	243	LEU
5	E	248	SER
5	E	250	LEU
5	E	265	ARG
5	E	270	LYS
5	E	271	GLU
5	E	289	LEU
10	J	181	ASN
10	J	186	GLU
10	J	188	GLN
10	J	189	ILE
10	J	195	LEU
10	J	196	ARG
10	J	200	GLU
10	J	201	ARG
10	J	203	LEU
10	J	212	GLN
10	J	214	ILE
10	J	215	THR
10	J	217	GLU
10	J	218	GLU
10	J	219	GLU
10	J	220	LEU
10	J	221	ASN
10	J	229	LYS

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Mol	Chain	Res	Type
10	J	237	LYS
10	J	239	ARG
10	J	281	LYS
10	J	308	ARG
10	J	363	ARG
10	J	410	HIS
10	J	411	MET
11	K	38	GLU
11	K	90	PRO
11	K	117	GLN
11	K	126	LEU
11	K	147	GLU
11	K	168	LYS
11	K	171	GLN
11	K	173	THR
12	L	33	ARG
12	L	37	LEU
12	L	67	GLU
12	L	83	ARG
12	L	91	ARG
12	L	101	GLU
12	L	106	LYS
12	L	131	ASN
12	L	135	LYS
12	L	140	ASP
12	L	143	ASP
12	L	146	GLU
12	L	147	ASP
12	L	154	GLU
12	L	158	ARG
12	L	159	LEU
12	L	161	ASN
12	L	163	GLN
12	L	165	LYS
12	L	175	GLN
12	L	176	LEU
12	L	178	GLU
12	L	180	ARG
12	L	185	LEU
12	L	186	GLN
12	L	188	ARG
12	L	199	GLN

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Mol	Chain	Res	Type
12	L	203	LYS
12	L	204	ARG
12	L	206	ARG
12	L	219	LYS
12	L	222	LEU
12	L	227	THR
12	L	228	SER
12	L	235	LEU
12	L	731	LEU
12	L	761	SER
12	L	781	GLU
13	y	3	ARG
13	y	12	LEU
13	y	40	PRO
14	M	118	LYS
14	M	122	LEU
14	M	124	PHE
14	M	142	ILE
14	M	145	ASP
14	M	146	MET
14	M	147	GLU
14	M	148	THR
14	M	150	GLU
14	M	151	ARG
14	M	152	LEU
14	M	154	GLU
14	M	155	LYS
14	M	156	HIS
14	M	159	GLU
14	M	167	LEU
14	M	168	LEU
14	M	177	GLU
14	M	178	GLU
14	M	179	ILE
14	M	195	LYS
14	M	197	SER
14	M	198	ARG
14	M	200	ARG
15	N	24	GLU
15	N	41	ARG
15	N	42	LYS
15	N	102	CYS

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Mol	Chain	Res	Type
15	N	116	ASN
15	N	125	LYS
16	O	45	CYS
16	O	69	GLU
16	O	74	CYS
16	O	115	GLU
16	O	150	LEU
17	P	29	GLN
17	P	33	ARG
17	P	66	ARG
17	P	67	GLU
17	P	74	LYS
17	P	76	ARG
17	P	78	ARG
17	P	212	ASN
17	P	224	MET
17	P	229	LYS
18	R	56	GLU
18	R	66	GLU
18	R	67	ILE
18	R	71	GLN
18	R	72	TYR
18	R	75	ASP
18	R	78	ARG
18	R	79	LYS
18	R	80	LYS
18	R	81	LYS
18	R	82	MET
18	R	86	LEU
18	R	89	GLN
18	R	92	SER
18	R	95	LYS
18	R	96	ILE
18	R	103	ARG
18	R	104	GLN
18	R	106	GLN
18	R	110	LYS
18	R	111	VAL
18	R	115	LYS
18	R	122	LYS
18	R	125	MET
18	R	128	ASP

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Mol	Chain	Res	Type
18	R	133	GLN
18	R	137	GLU
18	R	158	LYS
18	R	170	LYS
18	R	171	LEU
18	R	181	PRO
18	R	183	GLN
18	R	186	VAL
18	R	189	ASN
18	R	195	ARG
18	R	211	ARG
18	R	212	PHE
18	R	213	LYS
18	R	214	ILE
18	R	215	ASN
18	R	216	LYS
18	R	220	ARG
18	R	231	HIS
18	R	241	GLU
18	R	250	CYS
18	R	264	LEU
18	R	265	ASP
18	R	266	LYS
18	R	267	ARG
18	R	268	LEU
18	R	279	HIS
18	R	280	ILE
18	R	297	LYS
18	R	307	GLN
18	R	312	MET
18	R	314	GLN
18	R	315	LYS
19	S	10	GLN
19	S	15	TYR
19	S	20	MET
19	S	91	LYS
19	S	102	ASN
19	S	108	ASN
19	S	125	LYS
19	S	129	PHE
19	S	131	ARG
20	T	257	ARG

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Mol	Chain	Res	Type
20	T	282	ARG
20	T	308	ARG
20	T	318	ARG
20	T	387	PHE
20	T	399	LYS
20	T	400	PHE
20	T	401	PRO
20	T	402	ASP
20	T	412	HIS
20	T	416	ILE
20	T	418	THR
20	T	455	GLN
20	T	460	ASP
20	T	461	SER
20	T	463	SER
20	T	478	LEU
22	U	1	MET
22	U	11	ARG
22	U	20	GLN
22	U	23	LEU
22	U	25	LEU
23	V	333	GLN
23	V	344	LYS
23	V	387	MET
23	V	452	LEU
23	V	457	ARG
23	V	461	LEU
23	V	465	SER
23	V	467	LEU
23	V	471	GLU
23	V	478	LYS
23	V	490	CYS
23	V	510	LEU
23	V	513	ARG
23	V	514	PHE
23	V	533	TYR
23	V	535	THR
23	V	540	GLU
23	V	577	SER
23	V	597	PRO
24	W	84	THR
24	W	88	MET

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Mol	Chain	Res	Type
24	W	92	GLU
24	W	93	PHE
24	W	96	GLU
24	W	97	ASN
24	W	100	ARG
24	W	108	ARG
24	W	126	GLU
24	W	127	GLN
24	W	129	ARG
24	W	130	ARG
24	W	134	THR
24	W	139	LEU
24	W	144	ASP
24	W	146	HIS
24	W	148	VAL
24	W	152	TYR
24	W	156	VAL
24	W	157	GLU
24	W	158	GLU
24	W	160	GLU
24	W	165	LEU
24	W	169	GLU
24	W	170	THR
24	W	172	GLN
24	W	177	LYS
24	W	178	ARG
24	W	180	LYS
24	W	181	PHE
24	W	182	LYS
24	W	187	SER
24	W	198	LYS
24	W	200	VAL
24	W	201	ASP
24	W	203	LYS
24	W	204	ASP
24	W	207	LYS
24	W	209	SER
24	W	210	GLU
24	W	212	GLU
24	W	213	GLN
25	X	6	LEU
25	X	7	ASN

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Mol	Chain	Res	Type
25	X	9	LYS
25	X	15	GLN
25	X	24	TRP
25	X	25	LYS
25	X	29	LYS
25	X	31	GLU
25	X	35	LYS
25	X	36	LYS
25	X	37	ILE
25	X	38	GLU
25	X	41	GLN
26	Y	3	GLU
26	Y	4	ARG
26	Y	6	VAL
26	Y	7	LEU
26	Y	9	LYS
26	Y	18	SER
26	Y	19	LYS
26	Y	20	ILE
26	Y	22	LYS
26	Y	23	LEU
26	Y	24	LYS
26	Y	25	LEU
26	Y	28	ASP
26	Y	36	MET
26	Y	50	ILE
26	Y	51	TYR
26	Y	52	LYS
26	Y	54	LYS
26	Y	63	VAL
26	Y	64	GLN
26	Y	71	LEU
26	Y	75	ARG
26	Y	130	LEU
26	Y	134	MET
26	Y	154	LEU
26	Y	160	LEU
26	Y	163	ARG
26	Y	164	GLN
26	Y	168	ASP
28	q	19	PRO
28	q	28	ARG

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Mol	Chain	Res	Type
28	q	46	PRO
28	q	56	LYS
28	q	103	LEU
28	q	107	LEU
28	q	114	CYS
28	r	19	PRO
28	r	46	PRO
28	r	57	VAL
28	r	60	PRO
28	r	62	ARG
28	r	79	GLN
28	r	87	LEU
28	r	92	LEU
28	r	93	ARG
28	r	101	GLN
28	r	103	LEU
28	t	87	LEU
28	t	103	LEU
28	t	107	LEU
29	u	37	THR
29	u	194	ASN
29	u	301	ASN
29	u	316	ARG
29	u	337	TRP
29	u	360	LEU
29	u	407	VAL
30	v	119	GLU
31	w	118	LEU
34	i	13	ILE
34	i	57	LYS
34	i	58	GLN
35	j	4	VAL
35	j	40	LEU
36	k	112	ASN
37	m	27	MET
37	m	55	LEU
39	n	65	ASN
40	o	5	THR
40	o	71	VAL
40	o	79	ILE
40	o	101	VAL
40	o	114	SER

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Mol	Chain	Res	Type
40	o	126	THR
41	p	46	MET
41	p	66	LEU
41	p	87	ASP
34	b	13	ILE
34	b	57	LYS
34	b	58	GLN
35	c	4	VAL
35	c	40	LEU
36	d	112	ASN
37	f	27	MET
37	f	55	LEU
39	g	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (128) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	73	HIS
1	A	78	ASN
1	A	97	HIS
1	A	210	HIS
1	A	270	ASN
1	A	294	ASN
1	A	297	ASN
1	A	325	HIS
1	A	333	HIS
1	A	573	GLN
1	A	584	HIS
1	A	587	GLN
1	A	601	GLN
1	A	659	GLN
1	A	775	ASN
1	A	792	HIS
1	A	904	HIS
1	A	924	GLN
1	A	1035	GLN
1	A	1075	GLN
1	A	1096	HIS
1	A	1215	ASN
1	A	1227	GLN
1	A	1359	HIS

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Mol	Chain	Res	Type
1	A	1527	ASN
1	A	1531	ASN
1	A	1717	ASN
1	A	1946	ASN
3	C	245	HIS
3	C	297	ASN
3	C	437	HIS
3	C	513	ASN
3	C	548	ASN
3	C	575	GLN
3	C	596	ASN
3	C	706	GLN
3	C	890	HIS
3	C	892	GLN
5	E	101	ASN
5	E	108	HIS
5	E	165	GLN
5	E	188	GLN
5	E	225	ASN
5	E	253	ASN
10	J	181	ASN
10	J	212	GLN
10	J	221	ASN
11	K	171	GLN
12	L	13	ASN
12	L	39	HIS
12	L	73	HIS
12	L	99	HIS
12	L	175	GLN
12	L	199	GLN
12	L	211	ASN
13	y	48	GLN
14	M	134	GLN
14	M	156	HIS
14	M	172	HIS
14	M	189	GLN
15	N	27	GLN
15	N	54	HIS
15	N	99	ASN
15	N	107	GLN
15	N	136	HIS
16	O	113	ASN

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Mol	Chain	Res	Type
16	O	163	HIS
16	O	196	GLN
16	O	254	GLN
16	O	268	GLN
16	O	294	ASN
18	R	89	GLN
18	R	104	GLN
18	R	126	ASN
18	R	189	ASN
18	R	194	GLN
18	R	215	ASN
18	R	231	HIS
18	R	242	GLN
18	R	314	GLN
19	S	13	ASN
19	S	54	HIS
19	S	63	GLN
19	S	150	GLN
20	T	217	GLN
20	T	285	HIS
20	T	297	HIS
20	T	384	HIS
20	T	413	ASN
20	T	417	ASN
20	T	446	ASN
20	T	451	HIS
20	T	455	GLN
22	U	20	GLN
23	V	474	HIS
23	V	553	HIS
24	W	162	ASN
24	W	172	GLN
25	X	41	GLN
26	Y	8	ASN
26	Y	57	ASN
26	Y	64	GLN
26	Y	107	ASN
26	Y	164	GLN
29	u	157	GLN
29	u	301	ASN
29	u	356	ASN
29	u	394	GLN

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Mol	Chain	Res	Type
33	h	60	GLN
34	i	22	GLN
34	i	76	ASN
35	j	64	ASN
36	k	34	GLN
37	m	58	HIS
38	l	65	HIS
39	n	65	ASN
40	o	156	GLN
41	p	7	HIS
33	a	60	GLN
34	b	11	GLN
34	b	22	GLN
34	b	76	ASN
35	c	64	ASN
36	d	34	GLN
37	f	58	HIS
38	e	65	HIS
39	g	65	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	82/117 (70%)	17 (20%)	6 (7%)
6	F	96/107 (89%)	45 (46%)	17 (17%)
7	G	85/275 (30%)	50 (58%)	8 (9%)
8	H	132/188 (70%)	26 (19%)	4 (3%)
All	All	395/687 (57%)	138 (34%)	35 (8%)

All (138) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	13	C
2	B	19	A
2	B	20	G
2	B	21	A
2	B	22	U
2	B	23	C
2	B	24	G
2	B	25	C

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Mol	Chain	Res	Type
2	B	26	A
2	B	28	A
2	B	36	C
2	B	38	C
2	B	45	C
2	B	57	G
2	B	70	A
2	B	71	C
6	F	5	U
6	F	6	C
6	F	7	G
6	F	8	C
6	F	10	U
6	F	12	G
6	F	25	C
6	F	26	U
6	F	27	A
6	F	28	A
6	F	29	A
6	F	31	U
6	F	33	G
6	F	34	G
6	F	35	A
6	F	36	A
6	F	37	C
6	F	38	G
6	F	45	A
6	F	46	G
6	F	47	A
6	F	48	A
6	F	49	G
6	F	50	A
6	F	51	U
6	F	54	G
6	F	55	C
6	F	56	A
6	F	59	G
6	F	60	C
6	F	61	C
6	F	62	C
6	F	67	G
6	F	68	C

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Mol	Chain	Res	Type
6	F	74	U
6	F	78	A
6	F	79	C
6	F	80	G
6	F	81	C
6	F	82	A
6	F	83	A
6	F	84	A
6	F	85	U
6	F	86	U
6	F	87	C
7	G	-11	G
7	G	-6	C
7	G	-1	G
7	G	2	U
7	G	3	A
7	G	5	G
7	G	6	A
7	G	7	G
7	G	8	C
7	G	10	U
7	G	11	A
7	G	12	G
7	G	13	C
7	G	14	A
7	G	17	U
7	G	21	A
7	G	22	C
7	G	23	U
7	G	24	G
7	G	25	G
7	G	26	U
7	G	27	U
7	G	28	A
7	G	29	C
7	G	30	C
7	G	31	U
7	G	120	G
7	G	121	G
7	G	122	U
7	G	123	U
7	G	124	U

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Mol	Chain	Res	Type
7	G	125	C
7	G	126	C
7	G	127	U
7	G	128	U
7	G	129	G
7	G	130	A
7	G	138	A
7	G	142	U
7	G	143	U
7	G	145	U
7	G	146	C
7	G	147	C
7	G	148	U
7	G	149	G
7	G	150	U
7	G	151	C
7	G	152	C
7	G	153	C
7	G	154	U
8	H	13	C
8	H	15	U
8	H	16	U
8	H	17	U
8	H	19	G
8	H	22	U
8	H	24	A
8	H	25	G
8	H	29	A
8	H	30	A
8	H	31	G
8	H	112	G
8	H	143	A
8	H	147	G
8	H	152	G
8	H	153	A
8	H	154	C
8	H	156	U
8	H	157	G
8	H	164	C
8	H	165	A
8	H	168	A
8	H	169	C

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Mol	Chain	Res	Type
8	H	177	A
8	H	178	A
8	H	179	C

All (35) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	12	U
2	B	18	C
2	B	19	A
2	B	20	G
2	B	25	C
2	B	27	U
6	F	5	U
6	F	7	G
6	F	25	C
6	F	26	U
6	F	33	G
6	F	34	G
6	F	35	A
6	F	36	A
6	F	45	A
6	F	47	A
6	F	48	A
6	F	50	A
6	F	58	G
6	F	59	G
6	F	81	C
6	F	84	A
6	F	86	U
7	G	-12	G
7	G	16	G
7	G	20	A
7	G	21	A
7	G	22	C
7	G	23	U
7	G	146	C
7	G	152	C
8	H	15	U
8	H	156	U
8	H	164	C
8	H	168	A

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

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
18	SEP	R	224	18	8,9,10	0.84	0	7,12,14	1.19	0
18	SEP	R	232	18	8,9,10	0.75	0	7,12,14	1.46	1 (14%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
18	SEP	R	224	18	-	3/6/8/10	-
18	SEP	R	232	18	-	3/6/8/10	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
18	R	232	SEP	OG-CB-CA	-2.55	105.67	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
18	R	224	SEP	CB-OG-P-O1P
18	R	224	SEP	CB-OG-P-O2P
18	R	224	SEP	CB-OG-P-O3P
18	R	232	SEP	N-CA-CB-OG
18	R	232	SEP	CA-CB-OG-P
18	R	232	SEP	C-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
18	R	232	SEP	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 14 are monoatomic - leaving 5 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	$\# Z > 2$
49	ADP	D	2202	-	28,29,29	1.36	4 (14%)	43,45,45	1.86	9 (20%)
51	ATP	u	702	48	32,33,33	1.22	3 (9%)	48,52,52	1.84	8 (16%)
46	IHP	A	3000	-	36,36,36	1.03	2 (5%)	60,60,60	1.74	15 (25%)
49	ADP	D	2201	-	28,29,29	1.44	5 (17%)	43,45,45	1.79	7 (16%)
47	GTP	C	1500	48	33,34,34	1.45	5 (15%)	50,54,54	2.05	10 (20%)

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
49	ADP	D	2202	-	-	2/16/32/32	0/3/3/3
51	ATP	u	702	48	-	0/22/38/38	0/3/3/3
46	IHP	A	3000	-	-	6/30/54/54	0/1/1/1
49	ADP	D	2201	-	-	8/16/32/32	0/3/3/3
47	GTP	C	1500	48	-	8/22/38/38	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	D	2201	ADP	C5-C4	4.77	1.47	1.39
49	D	2202	ADP	C5-C4	4.46	1.47	1.39
47	C	1500	GTP	C5-N7	-3.75	1.31	1.39
47	C	1500	GTP	C6-N1	-3.29	1.32	1.38
51	u	702	ATP	C4-N9	-3.19	1.31	1.37
47	C	1500	GTP	PA-O3A	3.16	1.62	1.59
46	A	3000	IHP	P5-O45	-2.93	1.43	1.54
51	u	702	ATP	PB-O3B	2.77	1.62	1.59
46	A	3000	IHP	P2-O12	2.73	1.64	1.59
49	D	2202	ADP	C5-C6	2.64	1.48	1.41
47	C	1500	GTP	C8-N9	-2.61	1.31	1.37
47	C	1500	GTP	C4-N9	-2.58	1.31	1.38
49	D	2201	ADP	C5-C6	2.56	1.48	1.41
49	D	2202	ADP	C5-N7	-2.43	1.34	1.39
49	D	2201	ADP	C5-N7	-2.36	1.34	1.39
49	D	2201	ADP	C8-N7	2.36	1.36	1.31
49	D	2202	ADP	C8-N7	2.29	1.36	1.31
49	D	2201	ADP	PA-O3A	2.28	1.62	1.59
51	u	702	ATP	C5-N7	-2.13	1.35	1.39

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	C	1500	GTP	C5-C4-N3	-7.08	117.12	128.39
51	u	702	ATP	C5-C4-N3	-6.36	117.96	126.72
49	D	2202	ADP	C5-C4-N3	-6.35	117.97	126.72
47	C	1500	GTP	C2-N3-C4	5.99	122.62	112.30
49	D	2201	ADP	C5-C4-N3	-5.86	118.65	126.72
47	C	1500	GTP	N9-C4-N3	5.76	137.47	125.95
49	D	2202	ADP	N3-C4-N9	4.84	135.40	127.17
49	D	2201	ADP	N3-C4-N9	4.62	135.03	127.17
46	A	3000	IHP	O35-P5-O15	-4.53	88.20	105.85
51	u	702	ATP	N3-C2-N1	-4.15	122.30	128.58
46	A	3000	IHP	O45-P5-O35	4.12	123.25	107.80
51	u	702	ATP	N3-C4-N9	4.06	134.08	127.17
51	u	702	ATP	C4-C5-N7	-4.05	105.95	110.58
49	D	2202	ADP	C2-N3-C4	3.88	121.30	111.83
49	D	2201	ADP	C2-N3-C4	3.69	120.83	111.83
46	A	3000	IHP	P3-O13-C3	-3.68	113.60	123.43
49	D	2202	ADP	C4-C5-N7	-3.65	106.41	110.58
46	A	3000	IHP	O16-C6-C1	3.64	116.50	108.76
51	u	702	ATP	C2-N3-C4	3.63	120.70	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
47	C	1500	GTP	O6-C6-C5	-3.56	117.12	126.53
46	A	3000	IHP	C6-C1-C2	-3.22	103.36	110.43
49	D	2201	ADP	N3-C2-N1	-3.22	123.71	128.58
49	D	2201	ADP	C4-C5-N7	-3.17	106.95	110.58
51	u	702	ATP	N9-C8-N7	-3.17	109.44	113.94
51	u	702	ATP	C5-N7-C8	3.12	108.35	103.45
47	C	1500	GTP	C2-N1-C6	-3.06	119.56	125.11
49	D	2202	ADP	N3-C2-N1	-3.00	124.04	128.58
47	C	1500	GTP	O2G-PG-O3B	2.91	114.38	104.64
47	C	1500	GTP	C5-C6-N1	2.90	120.62	113.25
47	C	1500	GTP	O2A-PA-O3A	2.81	114.88	107.27
46	A	3000	IHP	O44-P4-O34	2.74	118.08	107.80
46	A	3000	IHP	C5-C6-C1	-2.66	104.58	110.43
49	D	2202	ADP	C5-N7-C8	2.58	107.51	103.45
51	u	702	ATP	C4-N9-C8	2.44	108.30	105.74
46	A	3000	IHP	O15-C5-C4	-2.39	103.68	108.76
46	A	3000	IHP	P6-O16-C6	-2.37	117.10	123.43
46	A	3000	IHP	O31-P1-O11	-2.37	96.62	105.85
46	A	3000	IHP	O12-C2-C3	2.33	113.72	108.76
49	D	2202	ADP	C4-N9-C8	2.30	108.15	105.74
47	C	1500	GTP	O4'-C4'-C3'	2.28	109.67	105.15
49	D	2201	ADP	C4-N9-C8	2.27	108.12	105.74
49	D	2201	ADP	C5-N7-C8	2.26	107.01	103.45
46	A	3000	IHP	O45-P5-O15	-2.26	97.03	105.85
46	A	3000	IHP	O35-P5-O25	2.24	119.57	110.83
49	D	2202	ADP	C3'-C2'-C1'	2.22	105.66	101.46
47	C	1500	GTP	C6-C5-N7	2.12	134.15	130.29
46	A	3000	IHP	C4-C3-C2	2.07	114.98	110.43
46	A	3000	IHP	O42-P2-O22	2.06	118.84	110.83
49	D	2202	ADP	C6-C5-N7	2.02	135.99	132.09

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
46	A	3000	IHP	C4-C5-O15-P5
46	A	3000	IHP	C6-C5-O15-P5
47	C	1500	GTP	PB-O3B-PG-O3G
47	C	1500	GTP	C5'-O5'-PA-O1A
47	C	1500	GTP	C5'-O5'-PA-O2A
49	D	2201	ADP	PA-O3A-PB-O2B
49	D	2201	ADP	C5'-O5'-PA-O1A

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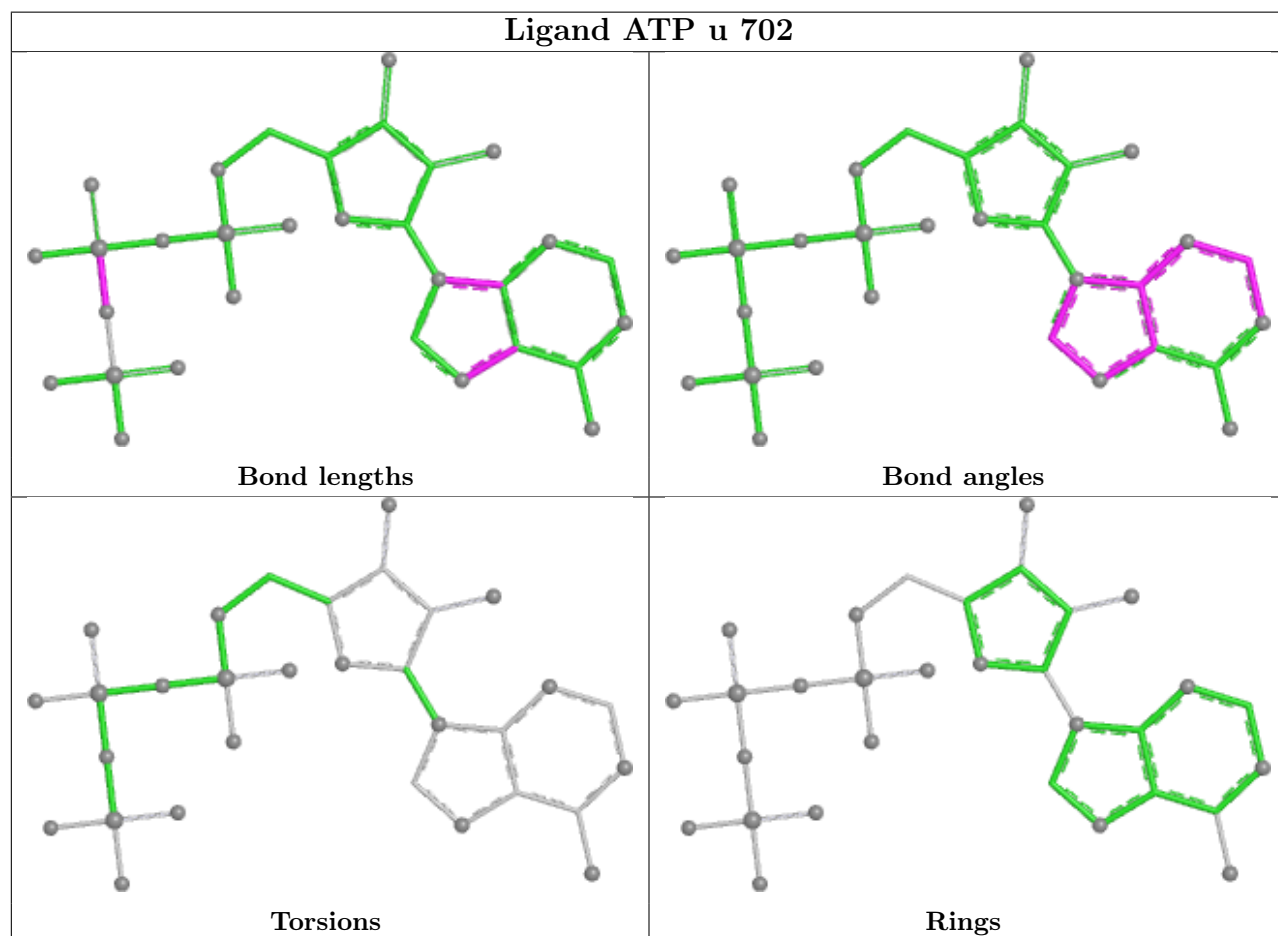
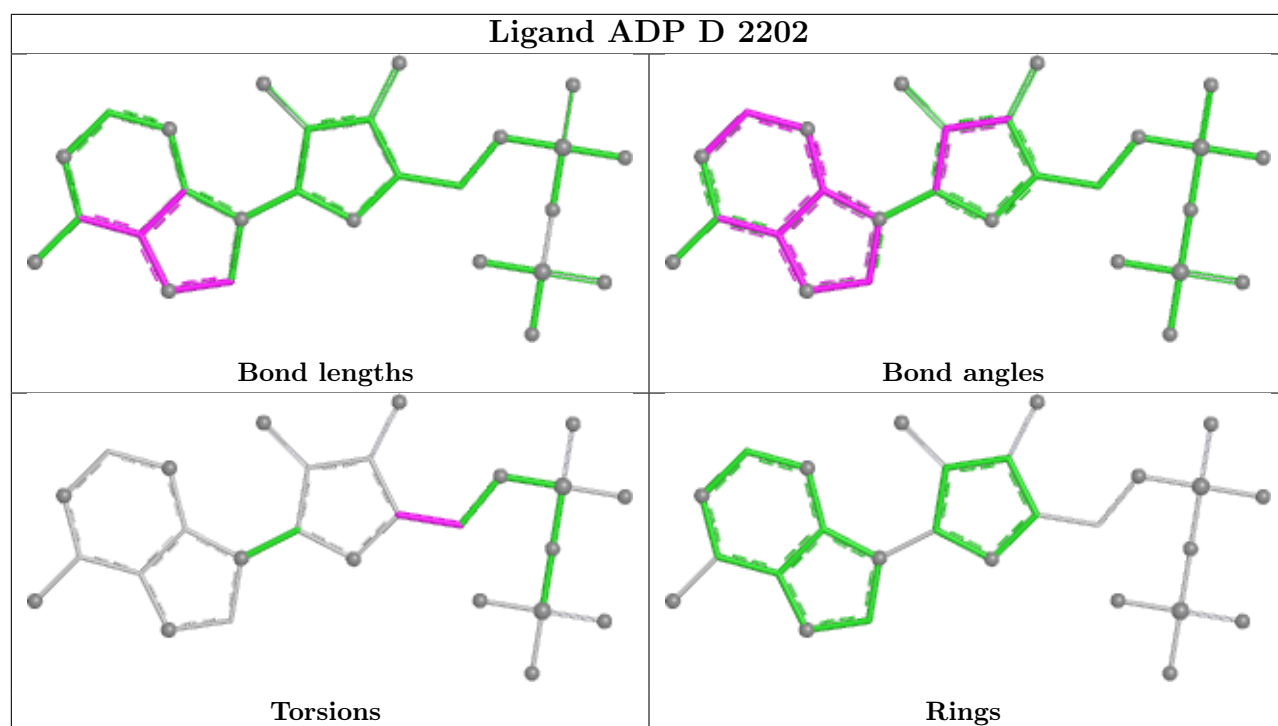
Mol	Chain	Res	Type	Atoms
49	D	2201	ADP	C5'-O5'-PA-O2A
49	D	2201	ADP	C5'-O5'-PA-O3A
47	C	1500	GTP	O4'-C4'-C5'-O5'
47	C	1500	GTP	C3'-C4'-C5'-O5'
49	D	2201	ADP	C3'-C4'-C5'-O5'
49	D	2201	ADP	O4'-C4'-C5'-O5'
49	D	2202	ADP	C3'-C4'-C5'-O5'
49	D	2202	ADP	O4'-C4'-C5'-O5'
47	C	1500	GTP	C5'-O5'-PA-O3A
46	A	3000	IHP	C1-O11-P1-O21
46	A	3000	IHP	C2-O12-P2-O22
46	A	3000	IHP	C5-O15-P5-O25
49	D	2201	ADP	PA-O3A-PB-O1B
49	D	2201	ADP	PA-O3A-PB-O3B
47	C	1500	GTP	PG-O3B-PB-O2B
46	A	3000	IHP	C1-O11-P1-O31
47	C	1500	GTP	PG-O3B-PB-O1B

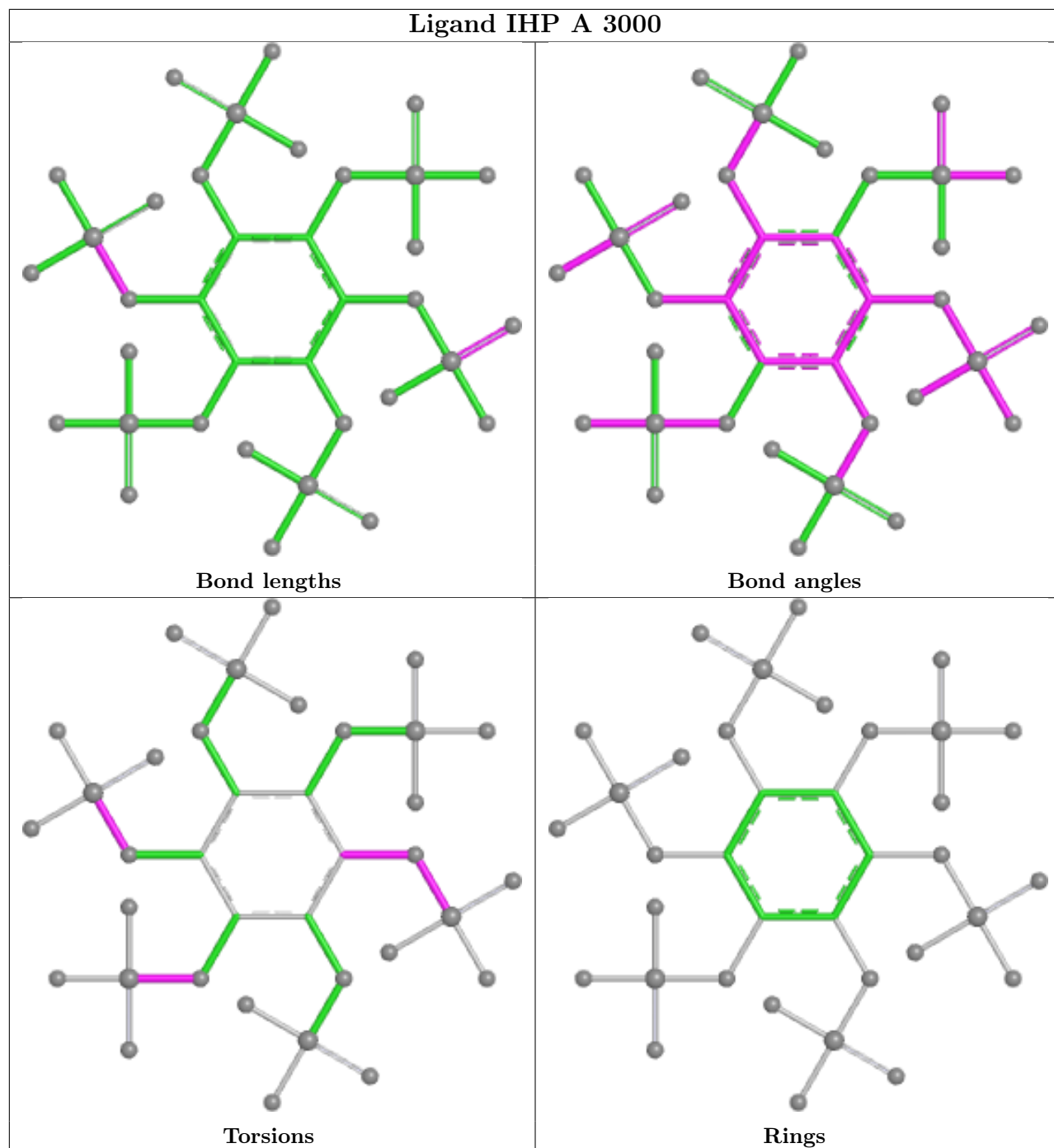
There are no ring outliers.

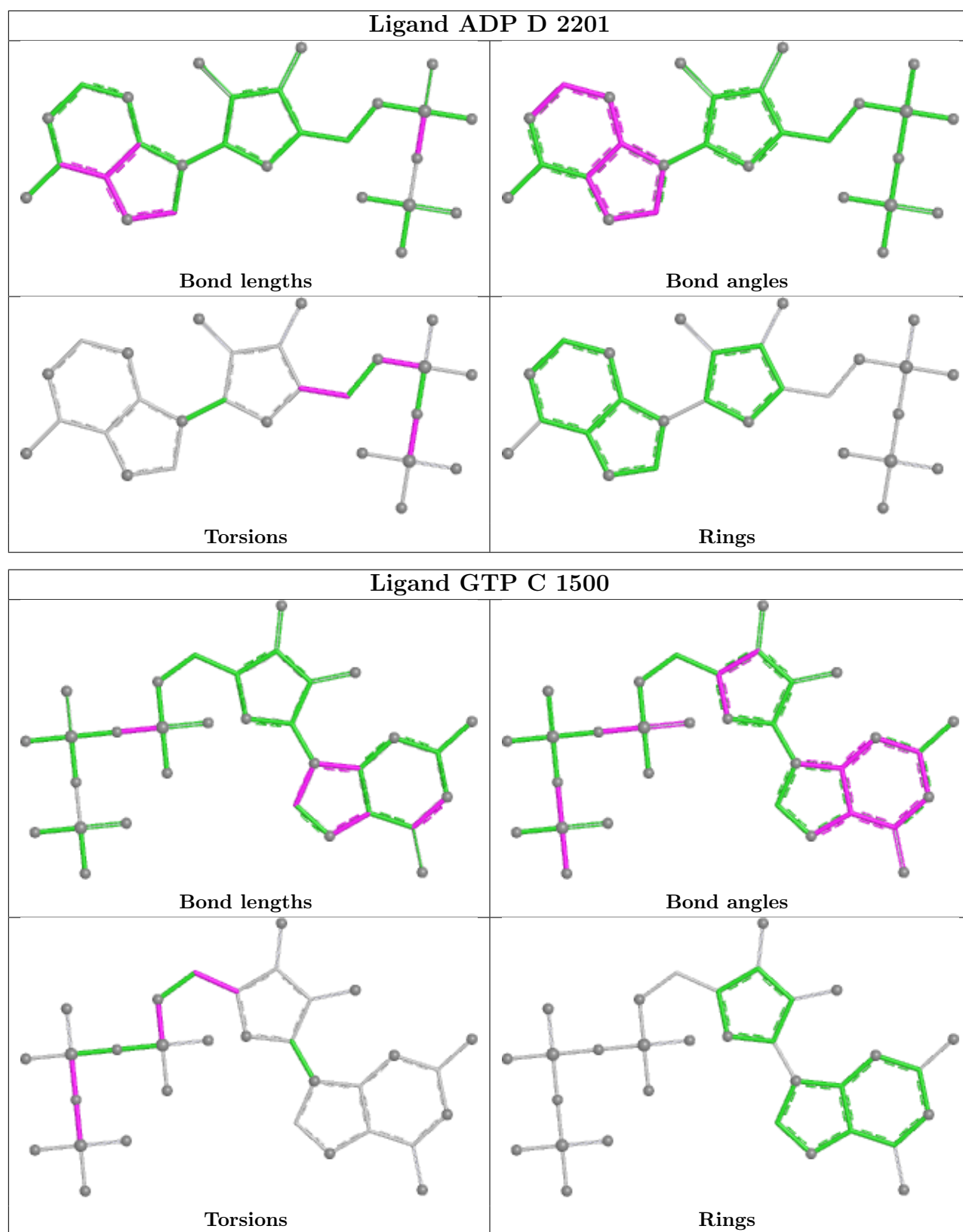
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
51	u	702	ATP	1	0
46	A	3000	IHP	10	0
49	D	2201	ADP	1	0
47	C	1500	GTP	7	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

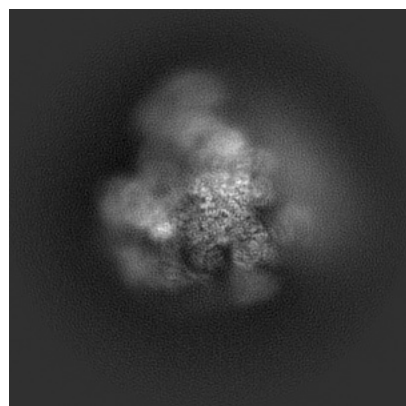
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6864. These allow visual inspection of the internal detail of the map and identification of artifacts.

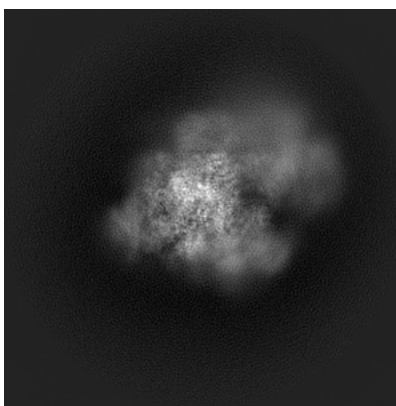
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

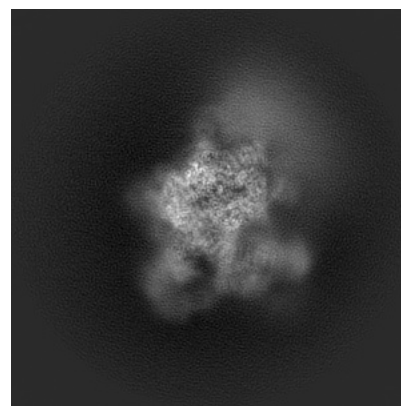
6.1.1 Primary map



X

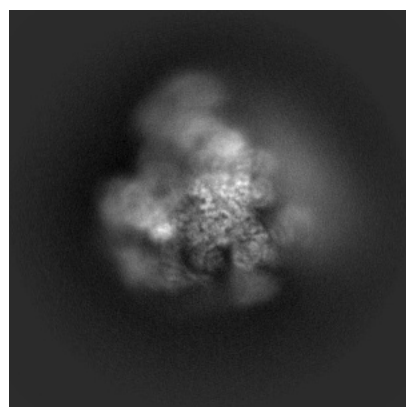


Y

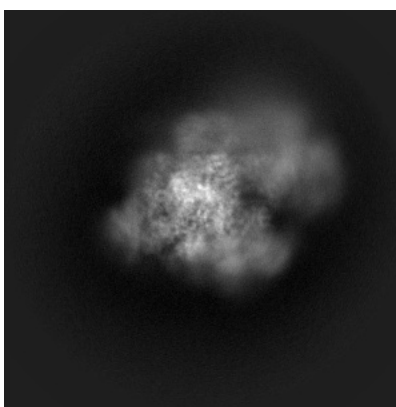


Z

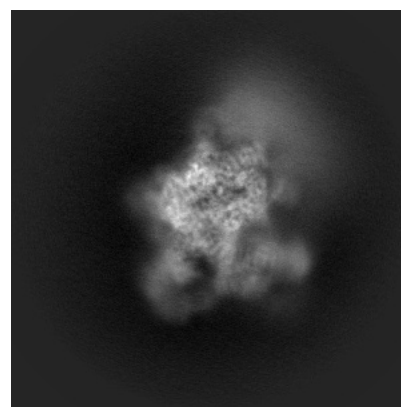
6.1.2 Raw map



X



Y

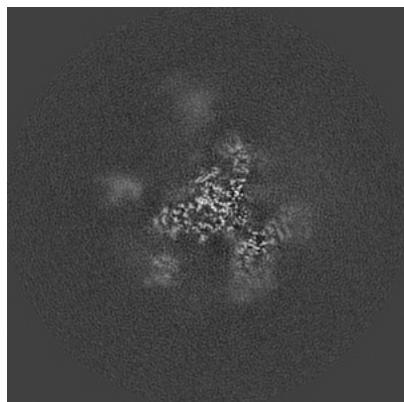


Z

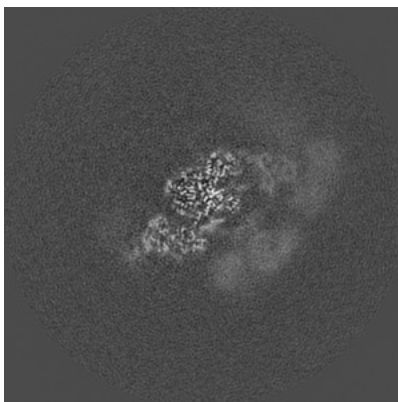
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

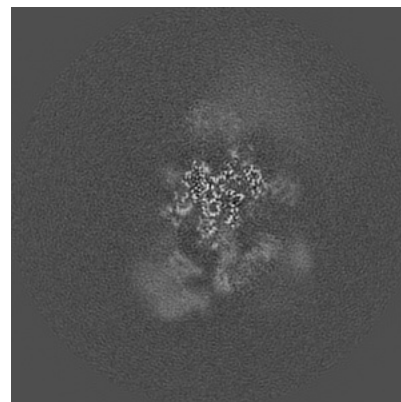
6.2.1 Primary map



X Index: 200

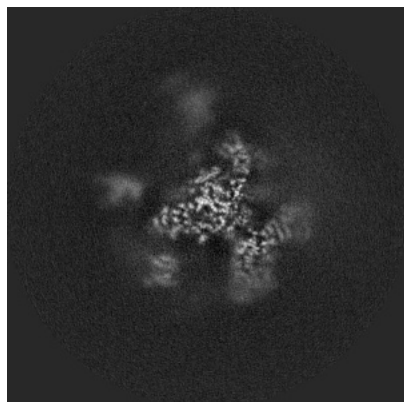


Y Index: 200

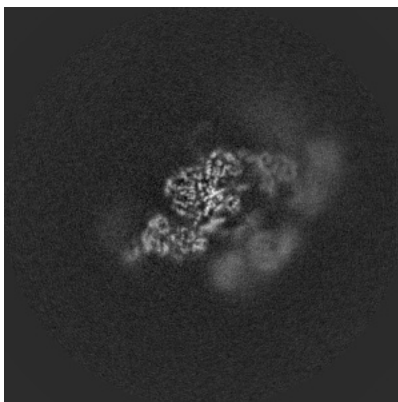


Z Index: 200

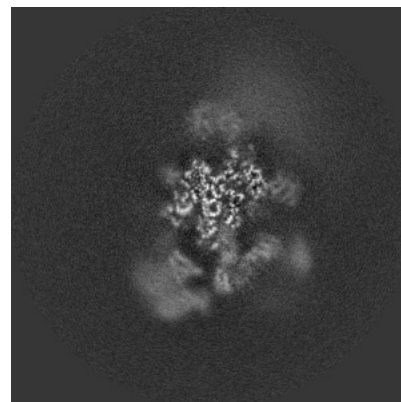
6.2.2 Raw map



X Index: 200



Y Index: 200

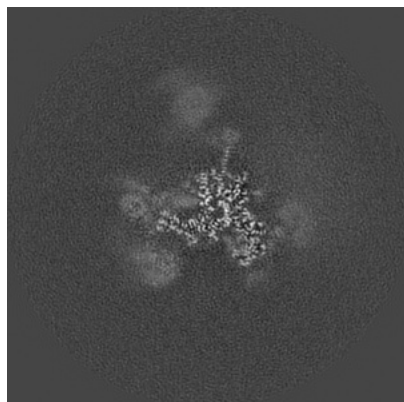


Z Index: 200

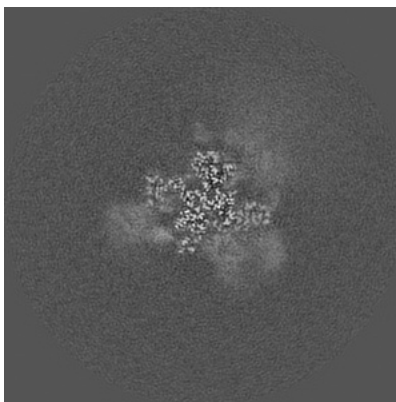
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

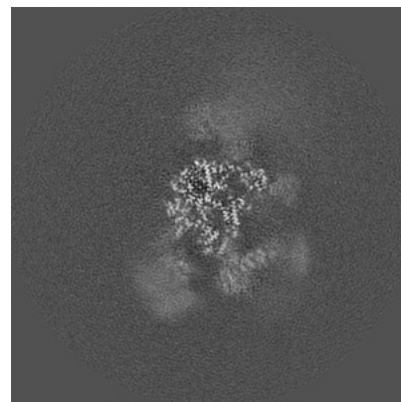
6.3.1 Primary map



X Index: 210

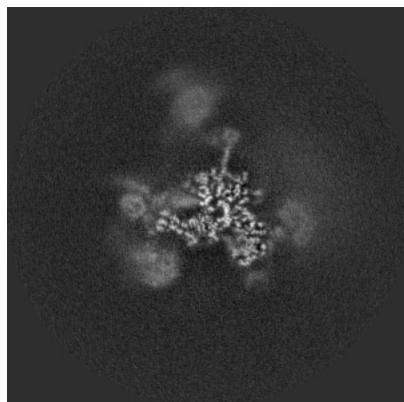


Y Index: 229

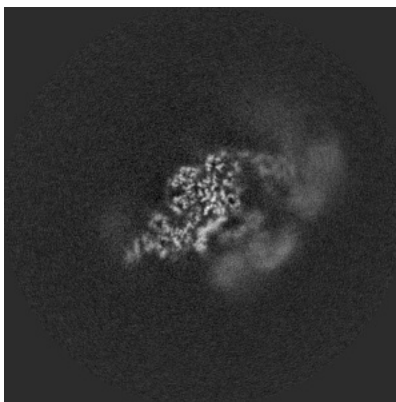


Z Index: 194

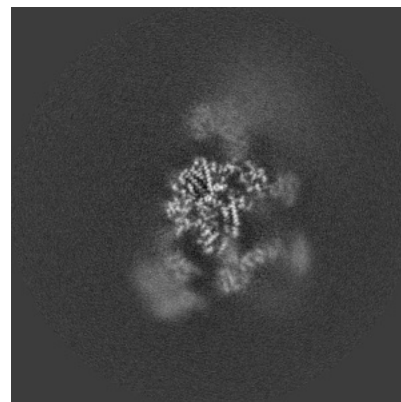
6.3.2 Raw map



X Index: 210



Y Index: 197

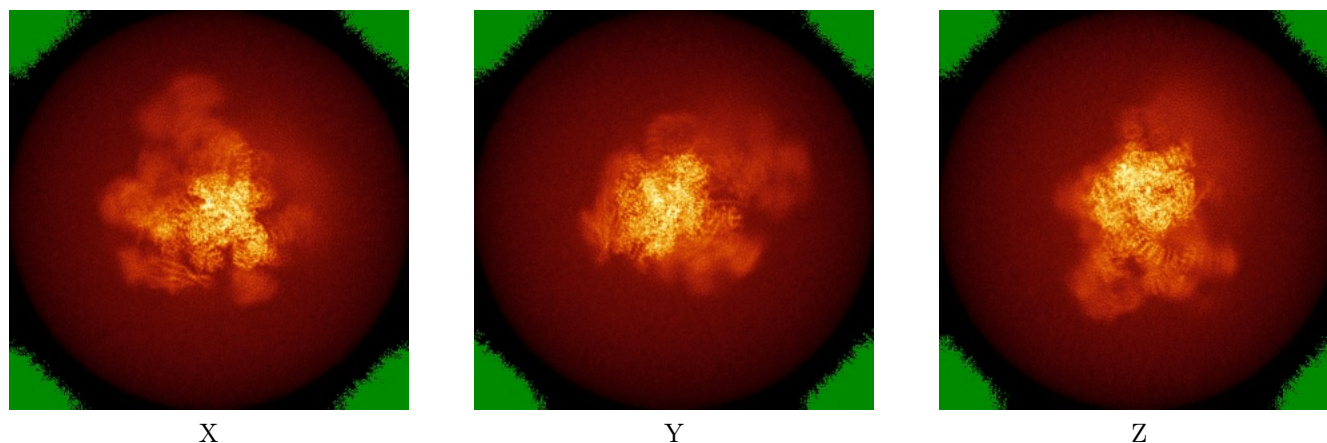


Z Index: 195

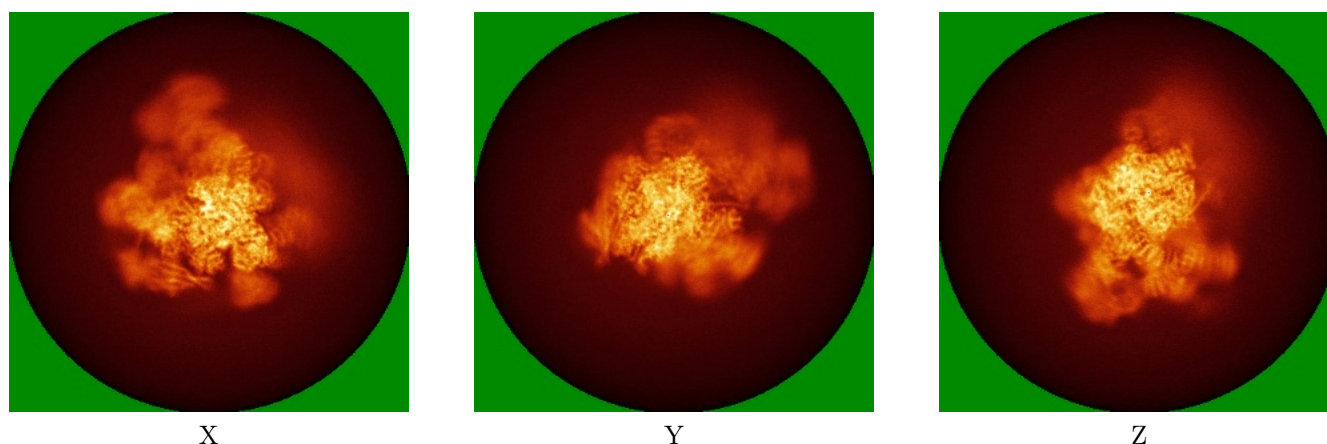
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



6.4.2 Raw map



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](#)

This section was not generated.

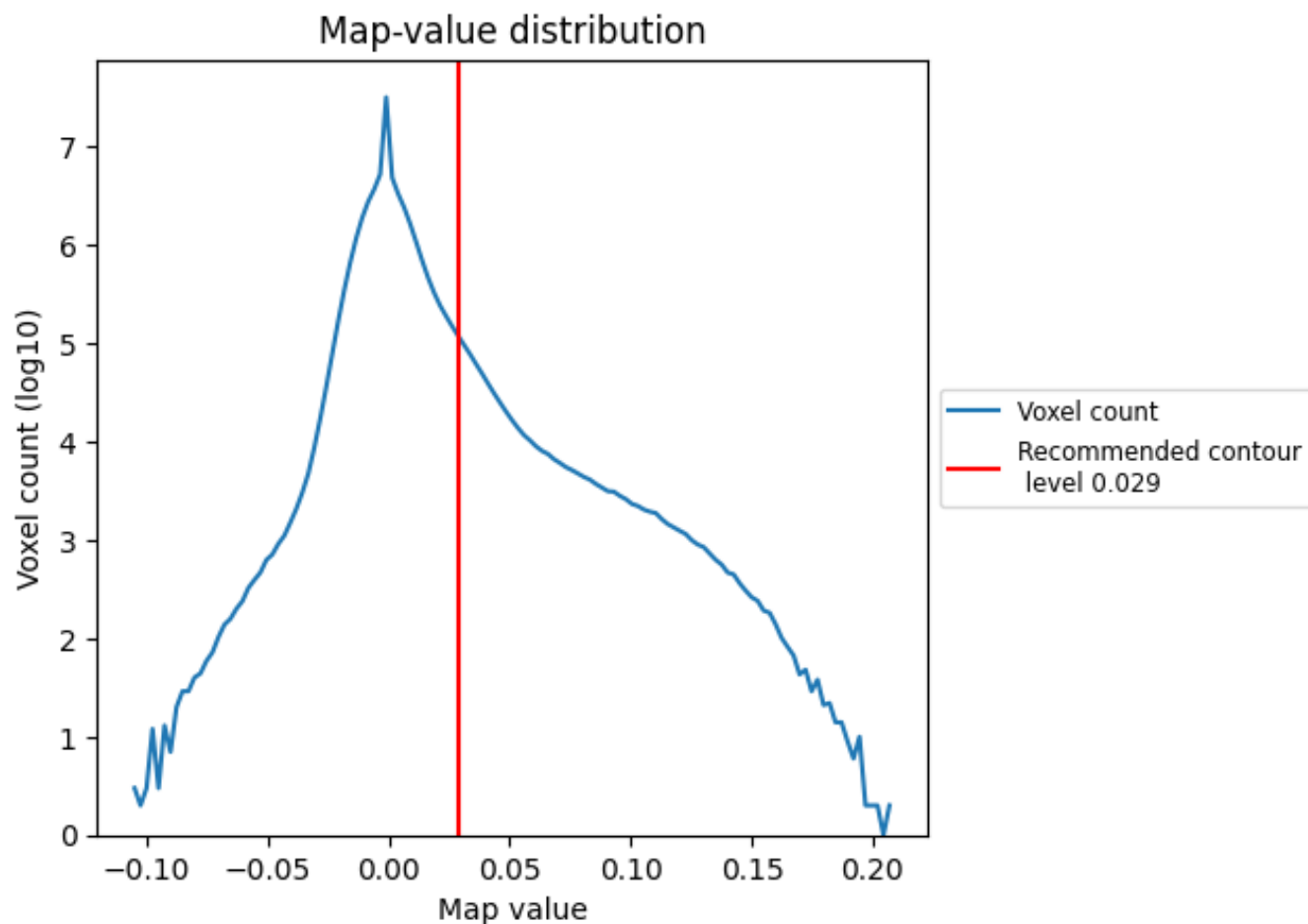
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

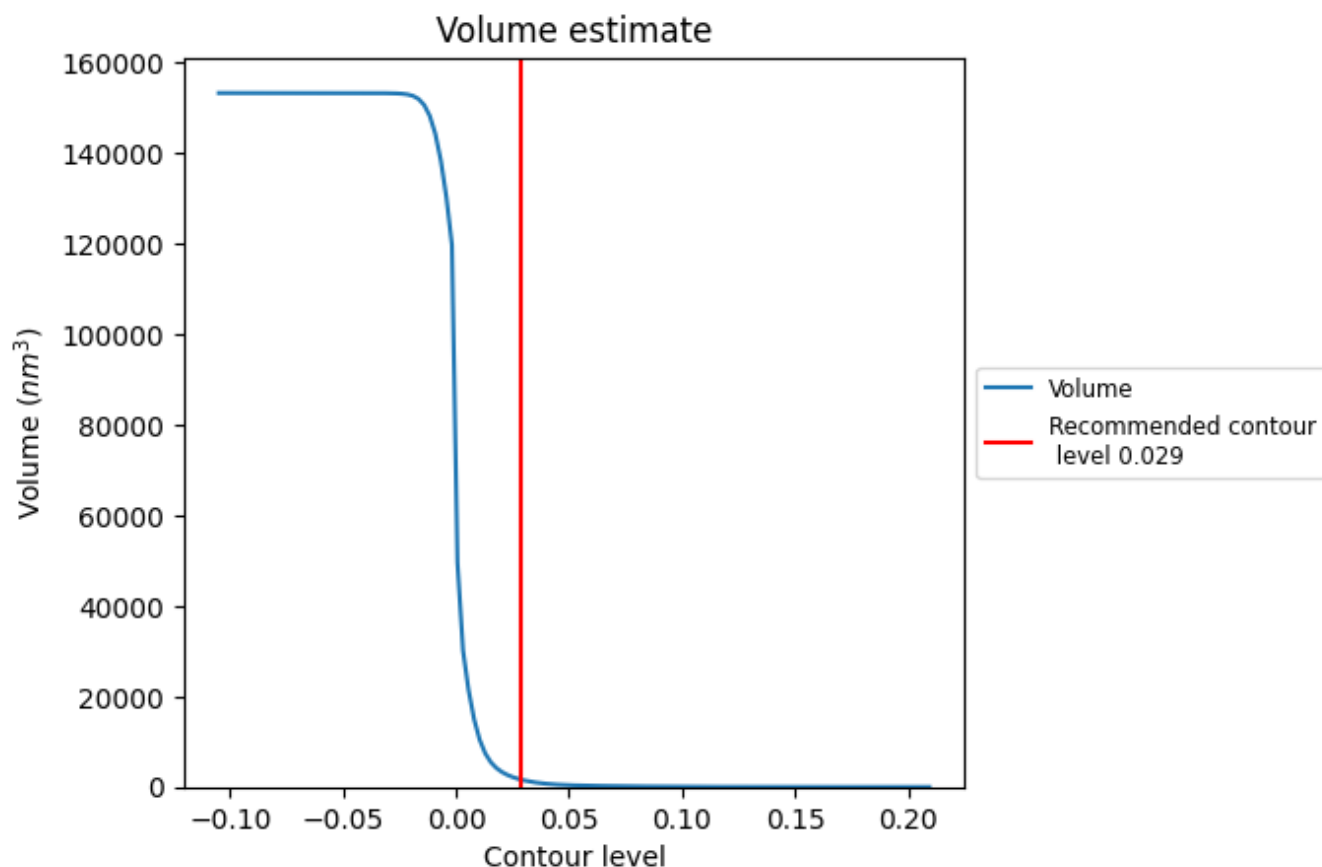
This section contains the results of statistical analysis of the map.

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.

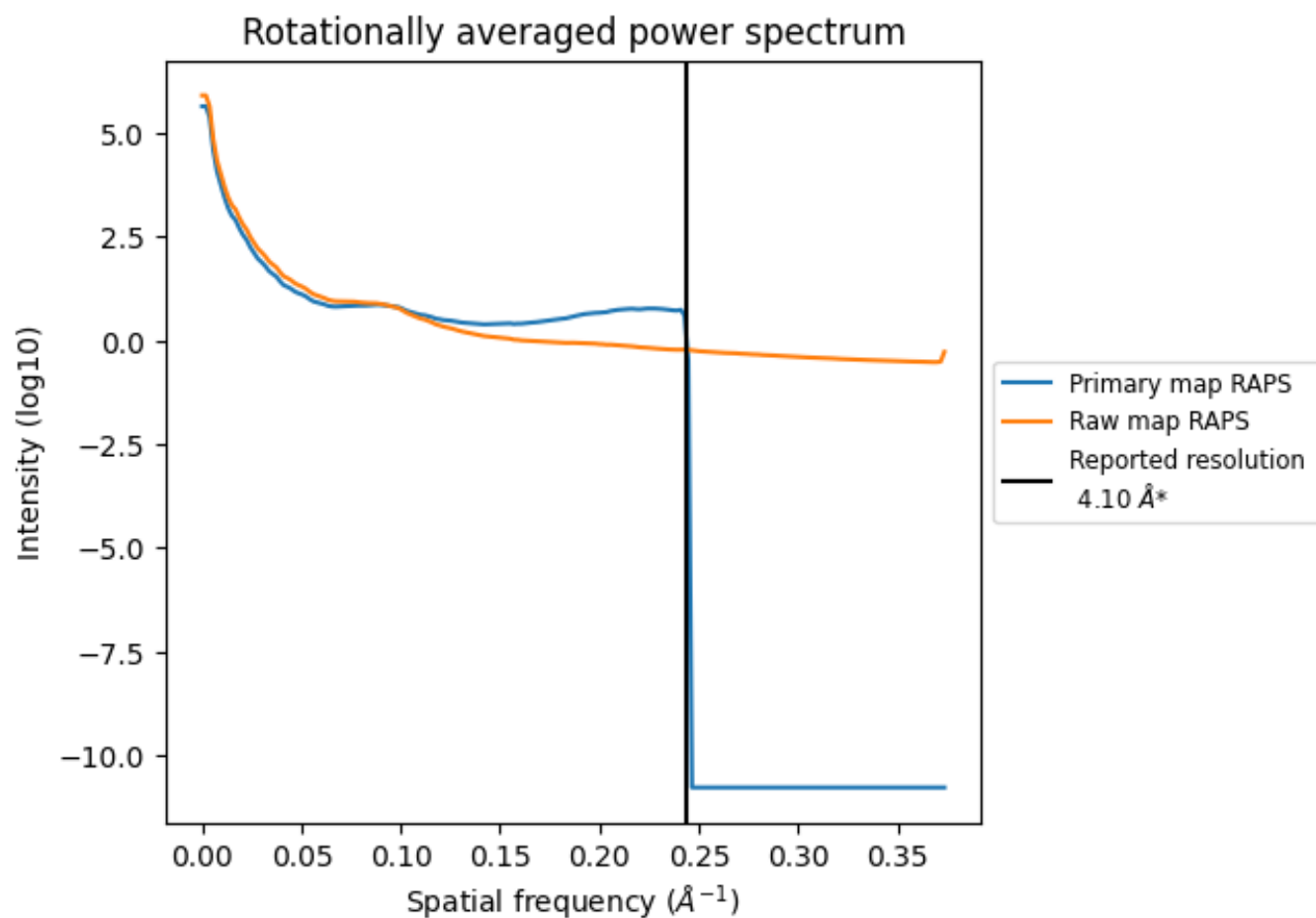
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1595 nm³; this corresponds to an approximate mass of 1441 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 ⓘ

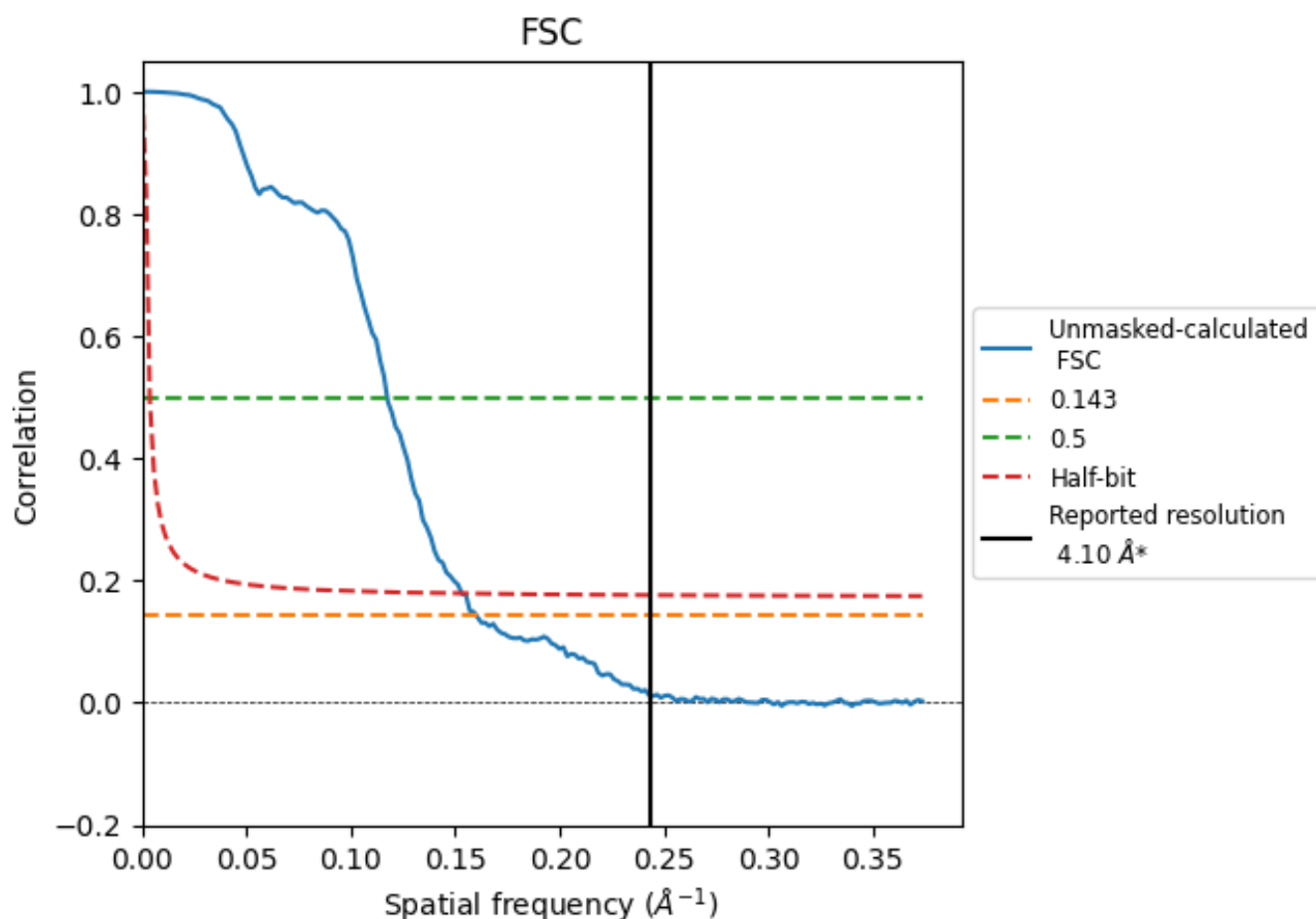


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 $0.244 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

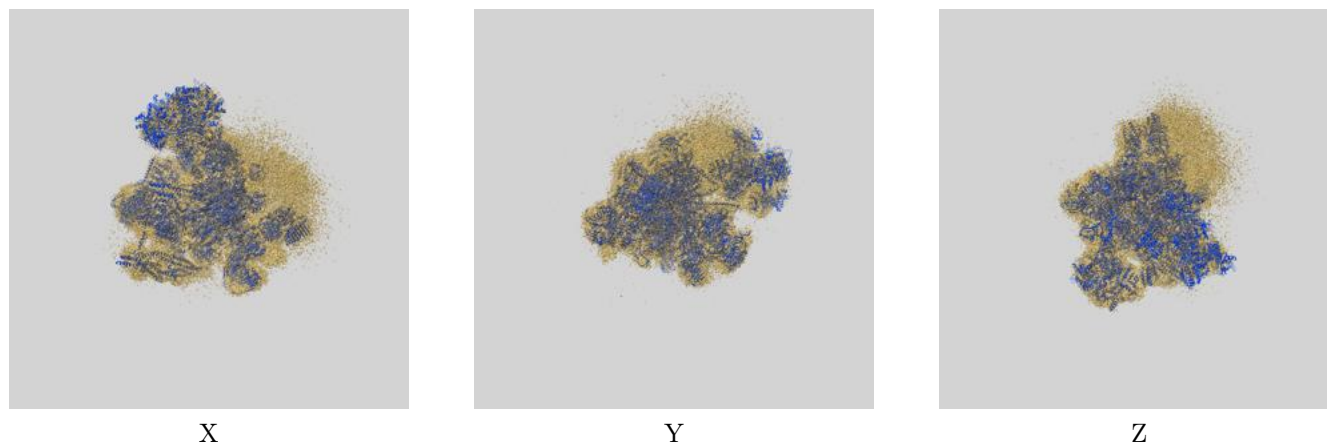
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	6.25	8.52	6.53

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.25 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

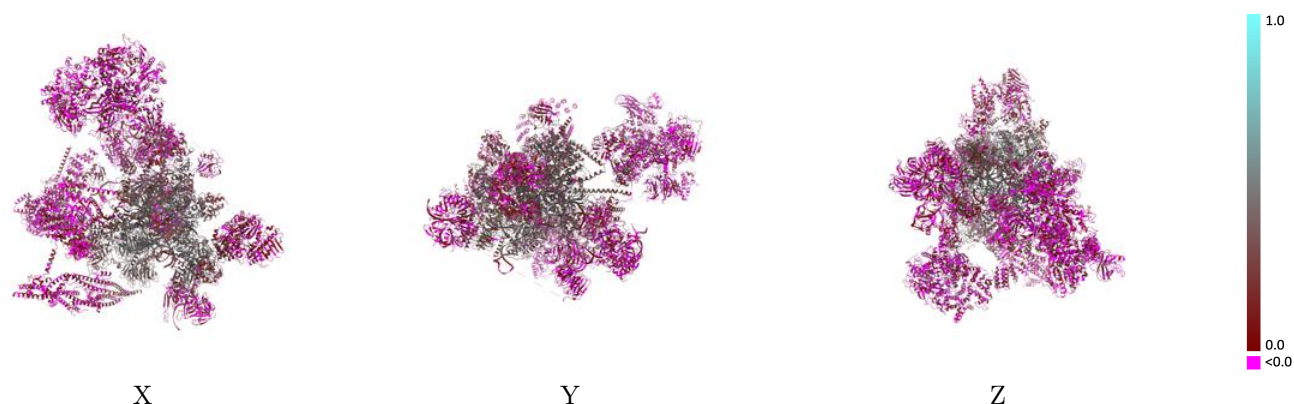
This section contains information regarding the fit between EMDB map EMD-6864 and PDB model 5YZG. Per-residue inclusion information can be found in section 3 on page 16.

9.1 Map-model overlay [i](#)



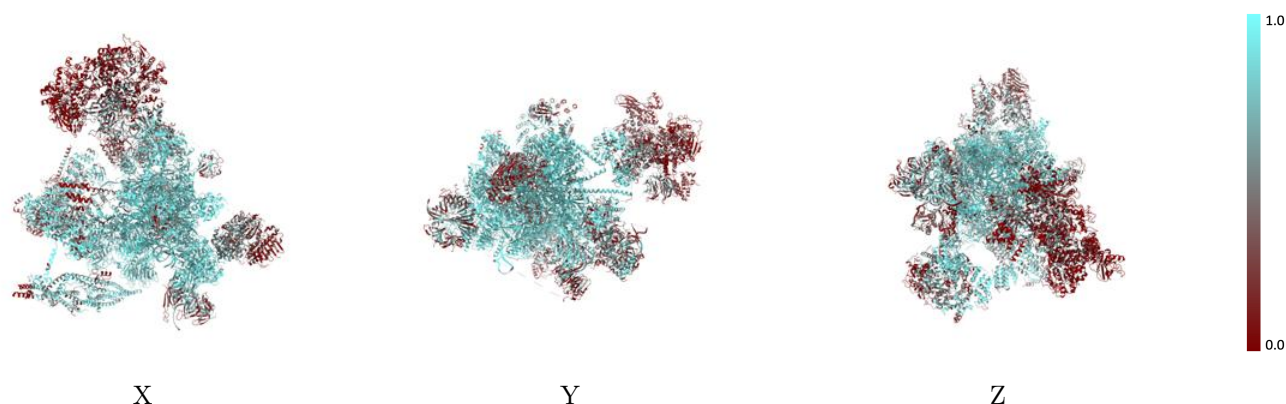
The images above show the 3D surface view of the map at the recommended contour level 0.029 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



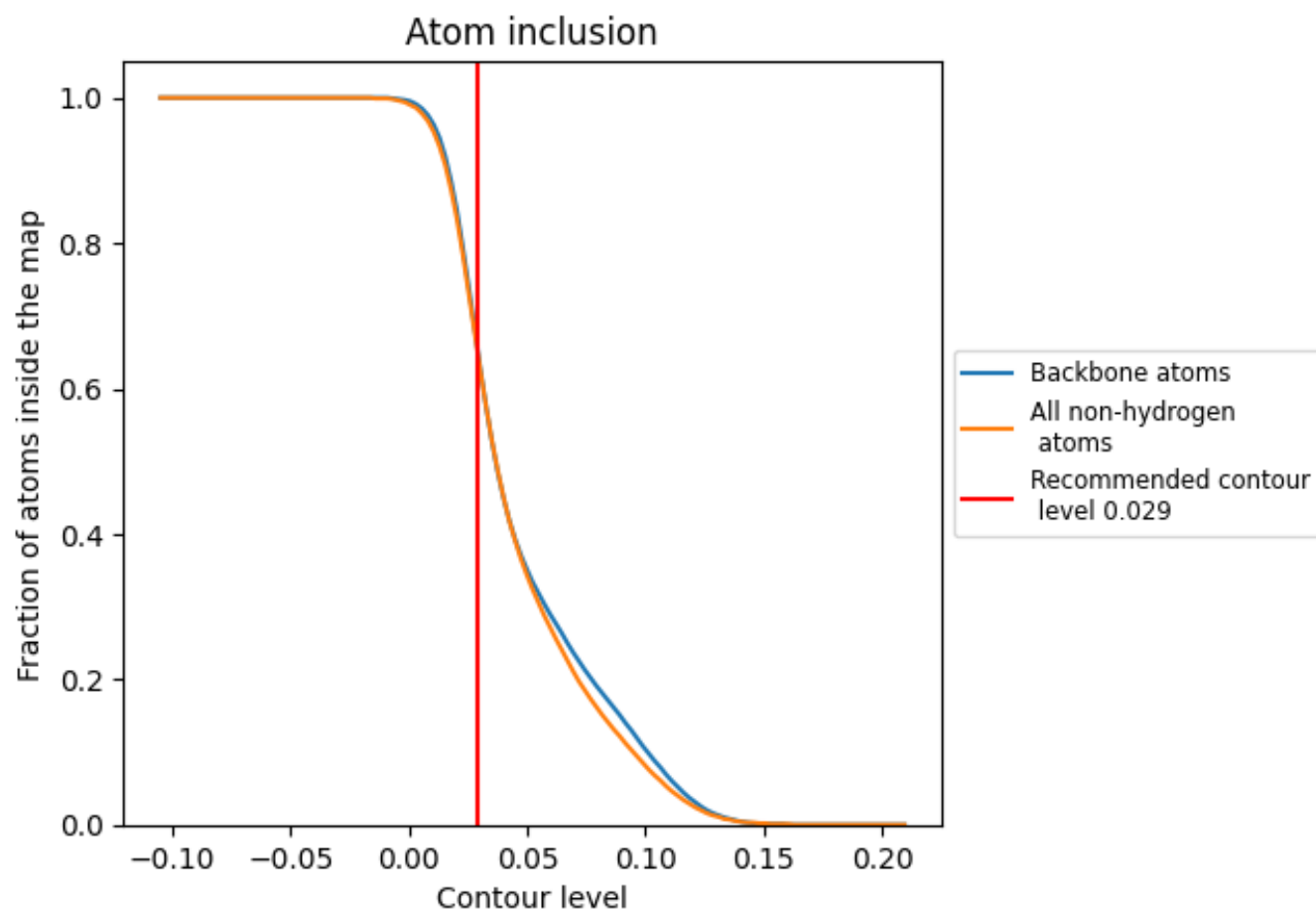
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.029).

9.4 Atom inclusion [i](#)



At the recommended contour level, 65% of all backbone atoms, 65% 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 (0.029) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6510	 0.2050
1	 0.7200	 0.1430
2	 0.4000	 0.0390
3	 0.4680	 0.1560
4	 0.8700	 0.3750
A	 0.8370	 0.3780
B	 0.8520	 0.2730
C	 0.8680	 0.3820
D	 0.1460	 0.0280
E	 0.8900	 0.3500
F	 0.8650	 0.2960
G	 0.8510	 0.2700
H	 0.6310	 0.0890
I	 0.7740	 0.0680
J	 0.7230	 0.2200
K	 0.7130	 0.0690
L	 0.7540	 0.2330
M	 0.6960	 0.2110
N	 0.8730	 0.4120
O	 0.8470	 0.3230
P	 0.8100	 0.3700
Q	 0.4890	 0.0330
R	 0.8270	 0.3610
S	 0.8430	 0.3040
T	 0.9240	 0.4440
U	 0.9360	 0.4430
V	 0.6770	 0.2120
W	 0.7040	 0.1780
X	 0.8270	 0.3130
Y	 0.8360	 0.3570
Z	 0.6210	 0.1250
a	 0.3930	 0.0090
b	 0.3740	 0.0240
c	 0.4240	 0.0370
d	 0.4010	 0.0410



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Chain	Atom inclusion	Q-score
e	 0.5360	 0.0140
f	 0.4080	 0.0310
g	 0.4810	 0.0080
h	 0.5260	 0.0240
i	 0.4030	 -0.0170
j	 0.4980	 0.0360
k	 0.4200	 0.0330
l	 0.4910	 -0.0020
m	 0.5670	 0.0230
n	 0.5660	 0.0530
o	 0.1710	 0.0460
p	 0.3100	 -0.0180
q	 0.4200	 0.0250
r	 0.6580	 0.0370
s	 0.4310	 0.0090
t	 0.5920	 0.0430
u	 0.4450	 0.0850
v	 0.1650	 0.0720
w	 0.1540	 0.0230
x	 0.0860	 0.0040
y	 0.7300	 0.1960