



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 07:38 PM UTC

PDB ID : 7W59 / pdb_00007w59
EMDB ID : EMD-32317
Title : The cryo-EM structure of human pre-C*-I complex
Authors : Zhan, X.; Lu, Y.; Shi, Y.
Deposited on : 2021-11-29
Resolution : 3.60 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:

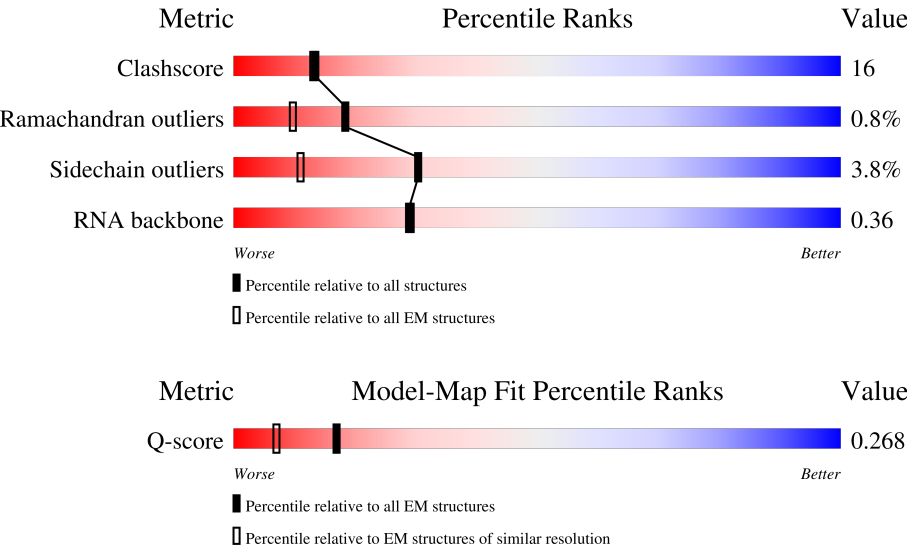
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.60 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.



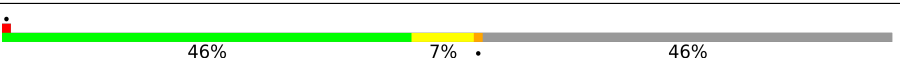
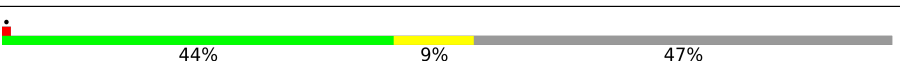
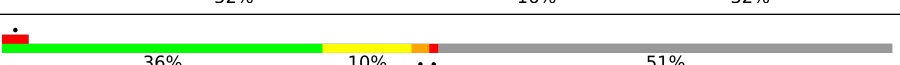
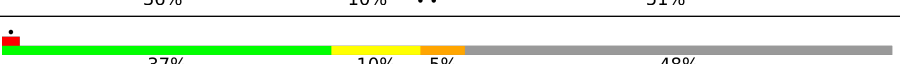
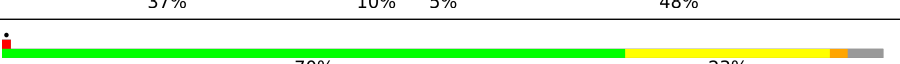
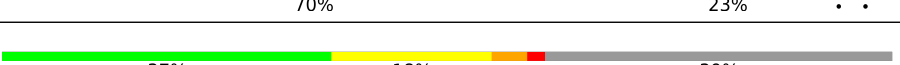
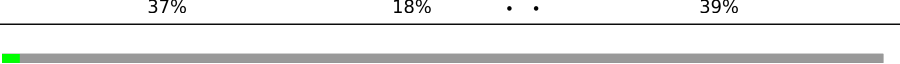
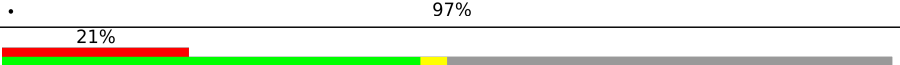
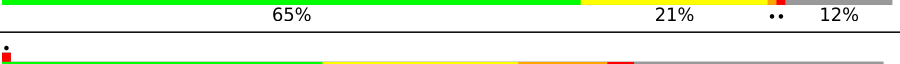
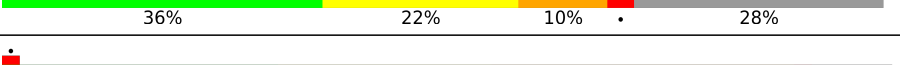
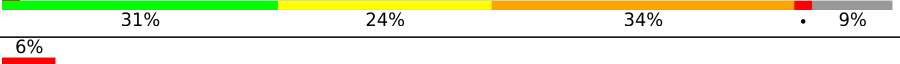
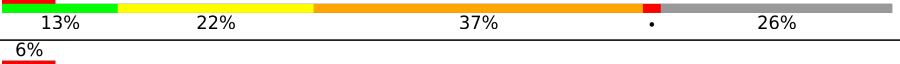
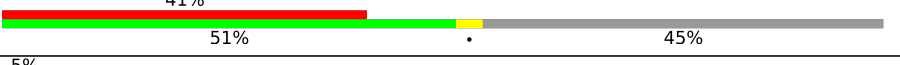
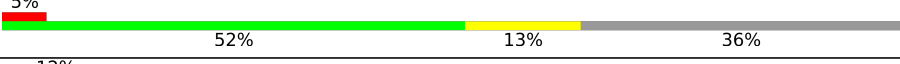
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	C	972	
3	E	357	

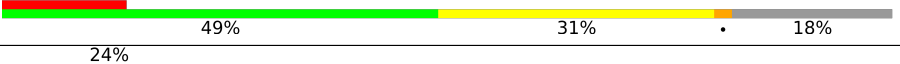
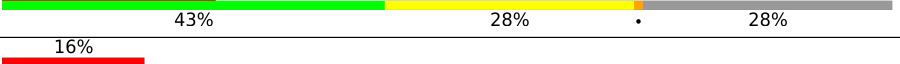
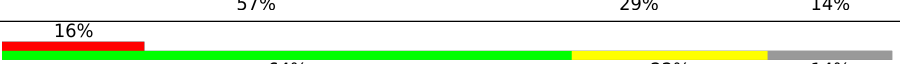
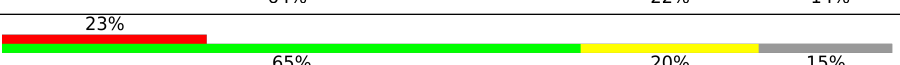
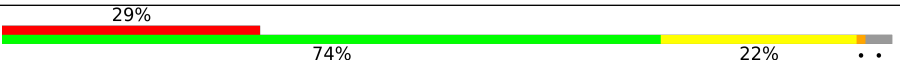
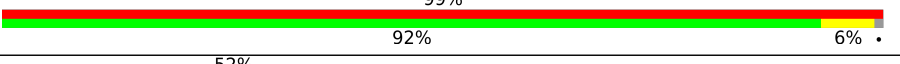
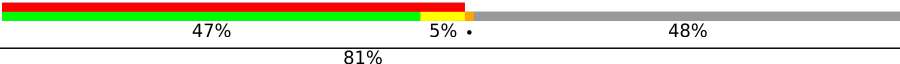
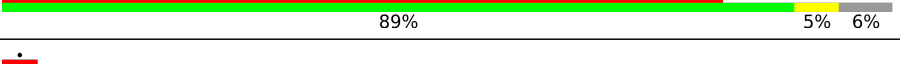
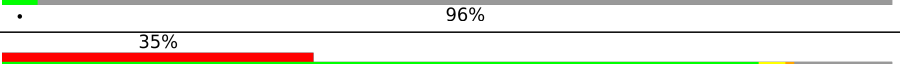
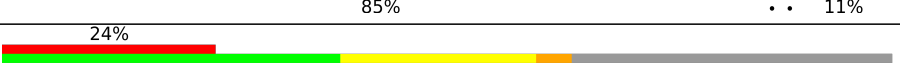
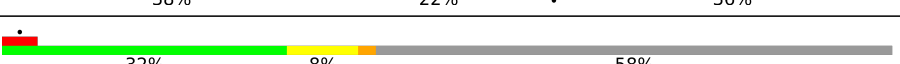
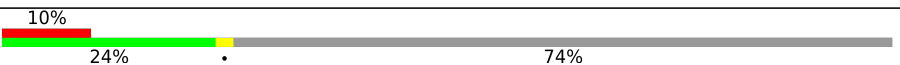
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Mol	Chain	Length	Quality of chain
4	4	46	
5	G	174	
6	J	848	
7	L	802	
8	M	243	
9	N	144	
10	O	420	
11	P	229	
12	R	536	
13	S	166	
14	T	514	
15	U	2752	
16	V	908	
17	W	579	
18	B	117	
19	F	107	
20	H	188	
21	b	240	
21	i	240	
22	X	254	
23	I	855	
24	y	301	
25	Y	1220	
26	a	126	
26	h	126	

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Mol	Chain	Length	Quality of chain
27	c	119	
27	j	119	
28	d	118	
28	k	118	
29	f	86	
29	m	86	
30	e	92	
30	l	92	
31	g	76	
31	n	76	
32	v	146	
33	w	174	
34	u	411	
35	x	703	
36	Q	1485	
37	o	255	
38	p	225	
39	q	504	
39	r	504	
39	s	504	
39	t	504	
40	K	225	

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
41	IHP	A	3000	-	-	X	-

2 Entry composition

There are 45 unique types of molecules in this entry. The entry contains 92315 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	1984	Total	C	N	O	S	0	0
			16449	10601	2879	2899	70		

- Molecule 2 is a protein called 116 kDa U5 small nuclear ribonucleoprotein component.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	862	Total	C	N	O	S	0	0
			6798	4347	1138	1281	32		

- Molecule 3 is a protein called U5 small nuclear ribonucleoprotein 40 kDa protein.

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

- Molecule 4 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	4	13	Total	C	N	O	P	0	0
			276	123	50	90	13		

- Molecule 5 is a RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	82	Total	C	N	O	P	0	0
			1510	666	210	552	82		

- Molecule 6 is a protein called Crooked neck-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	568	Total	C	N	O	S	0	0
			3814	2376	717	715	6		

- Molecule 7 is a protein called Cell division cycle 5-like protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	437	Total	C	N	O	S	0	0
			3015	1859	584	565	7		

- Molecule 8 is a protein called Pre-mRNA-splicing factor SYF2.

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

- Molecule 9 is a protein called Protein BUD31 homolog.

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

- Molecule 10 is a protein called Pre-mRNA-splicing factor RBM22.

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

- Molecule 11 is a protein called Spliceosome-associated protein CWC15 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	P	113	Total	C	N	O	S	0	0
			953	583	189	179	2		

- Molecule 12 is a protein called SNW domain-containing protein 1.

Mol	Chain	Residues	Atoms						AltConf	Trace
12	R	280	Total	C	N	O	P	S	0	0
			2243	1401	411	416	2	13		

- Molecule 13 is a protein called Peptidyl-prolyl cis-trans isomerase-like 1.

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

- Molecule 14 is a protein called Pleiotropic regulator 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	312	Total	C	N	O	S	0	0
			2454	1550	446	450	8		

- Molecule 15 is a protein called Serine/arginine repetitive matrix protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	U	72	Total	C	N	O	S	0	0
			422	257	82	82	1		

- Molecule 16 is a protein called Pre-mRNA-splicing factor CWC22 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	452	Total	C	N	O	S	0	0
			2632	1639	492	495	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	509	Total	C	N	O	S	0	0
			4129	2628	715	762	24		

- Molecule 18 is a RNA chain called U5 snRNA.

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

- Molecule 19 is a RNA chain called U6 snRNA.

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

- Molecule 20 is a RNA chain called U2 snRNA.

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

- Molecule 21 is a protein called Small nuclear ribonucleoprotein-associated proteins B and B'.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	b	102	Total	C	N	O	S	0	0
			786	492	148	139	7		
21	i	86	Total	C	N	O	S	0	0
			690	434	126	123	7		

- Molecule 22 is a protein called PSME3-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	X	69	Total	C	N	O	S	0	0
			616	380	111	124	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	I	617	Total	C	N	O	S	0	0
			3845	2380	721	733	11		

- Molecule 24 is a protein called Peptidyl-prolyl cis-trans isomerase E.

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

- Molecule 25 is a protein called ATP-dependent RNA helicase DHX8.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Y	667	Total	C	N	O	S	4	0
			3431	2057	680	693	1		

- Molecule 26 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	a	81	Total	C	N	O	S	0	0
			640	401	113	120	6		
26	h	81	Total	C	N	O	S	0	0
			633	397	112	118	6		

- Molecule 27 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	c	82	Total	C	N	O	S	0	0
			649	413	113	119	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
27	j	82	Total	C	N	O	S	0	0
			649	413	113	119	4		

- Molecule 28 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	d	97	Total	C	N	O	S	0	0
			776	488	143	140	5		
28	k	85	Total	C	N	O	S	0	0
			688	432	125	126	5		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	e	79	Total	C	N	O	S	0	0
			652	412	116	119	5		
30	l	78	Total	C	N	O	S	0	0
			644	407	115	118	4		

- Molecule 31 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	g	74	Total	C	N	O	S	0	0
			577	364	104	103	6		
31	n	69	Total	C	N	O	S	0	0
			538	342	96	94	6		

- Molecule 32 is a protein called Protein mago nashi homolog.

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

- Molecule 33 is a protein called RNA-binding protein 8A.

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

- Molecule 34 is a protein called Eukaryotic initiation factor 4A-III.

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

- Molecule 35 is a protein called Protein CASC3.

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

- Molecule 36 is a protein called RNA helicase aquarius.

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

- Molecule 37 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
37	o	162	Total	C	N	O	S	0	0
			1282	820	219	240	3		

- Molecule 38 is a protein called U2 small nuclear ribonucleoprotein B'.

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

- Molecule 39 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms				AltConf	Trace
39	q	132	Total	C	N	O	0	0
			659	395	132	132		
39	r	131	Total	C	N	O	0	0
			654	392	131	131		
39	s	132	Total	C	N	O	0	0
			659	395	132	132		

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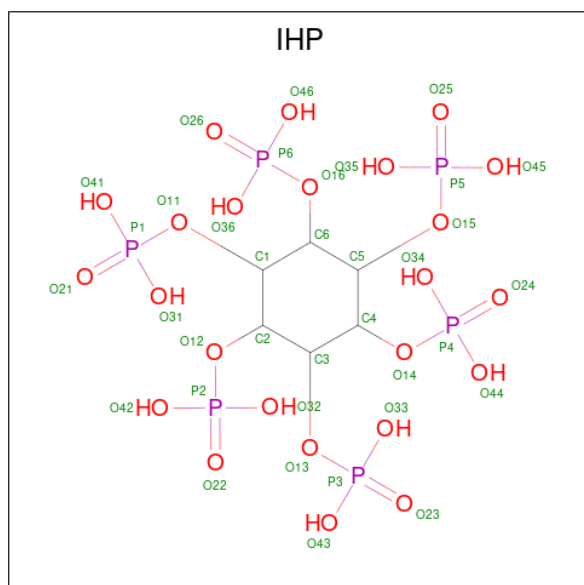
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Mol	Chain	Residues	Atoms				AltConf	Trace
39	t	131	Total	C	N	O	0	0
			654	392	131	131		

- Molecule 40 is a protein called Pre-mRNA-splicing factor SPF27.

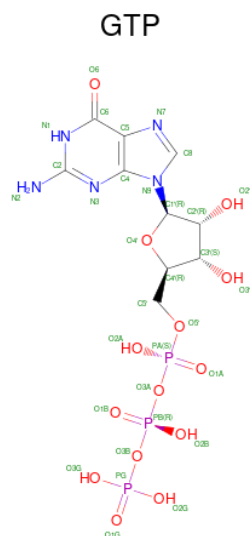
Mol	Chain	Residues	Atoms				AltConf	Trace
40	K	155	Total	C	N	O	0	0
			772	462	155	155		

- Molecule 41 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 42 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



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

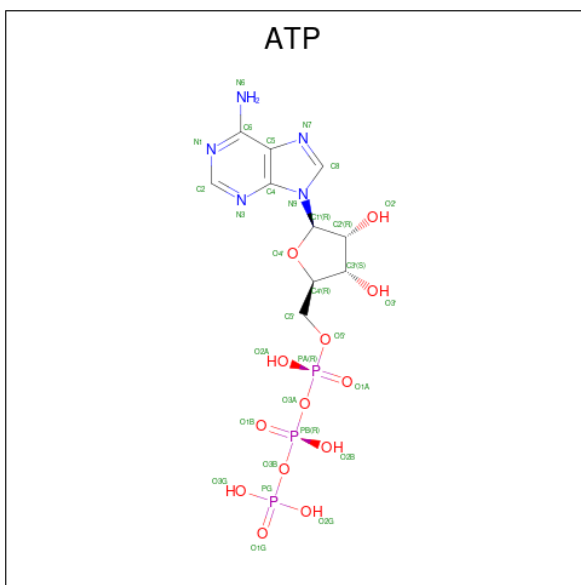
- Molecule 43 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

- Molecule 44 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
44	N	3	Total 3	Zn 3	0
44	O	3	Total 3	Zn 3	0

- Molecule 45 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $\text{C}_{10}\text{H}_{16}\text{N}_5\text{O}_{13}\text{P}_3$) (labeled as "Ligand of Interest" by depositor).

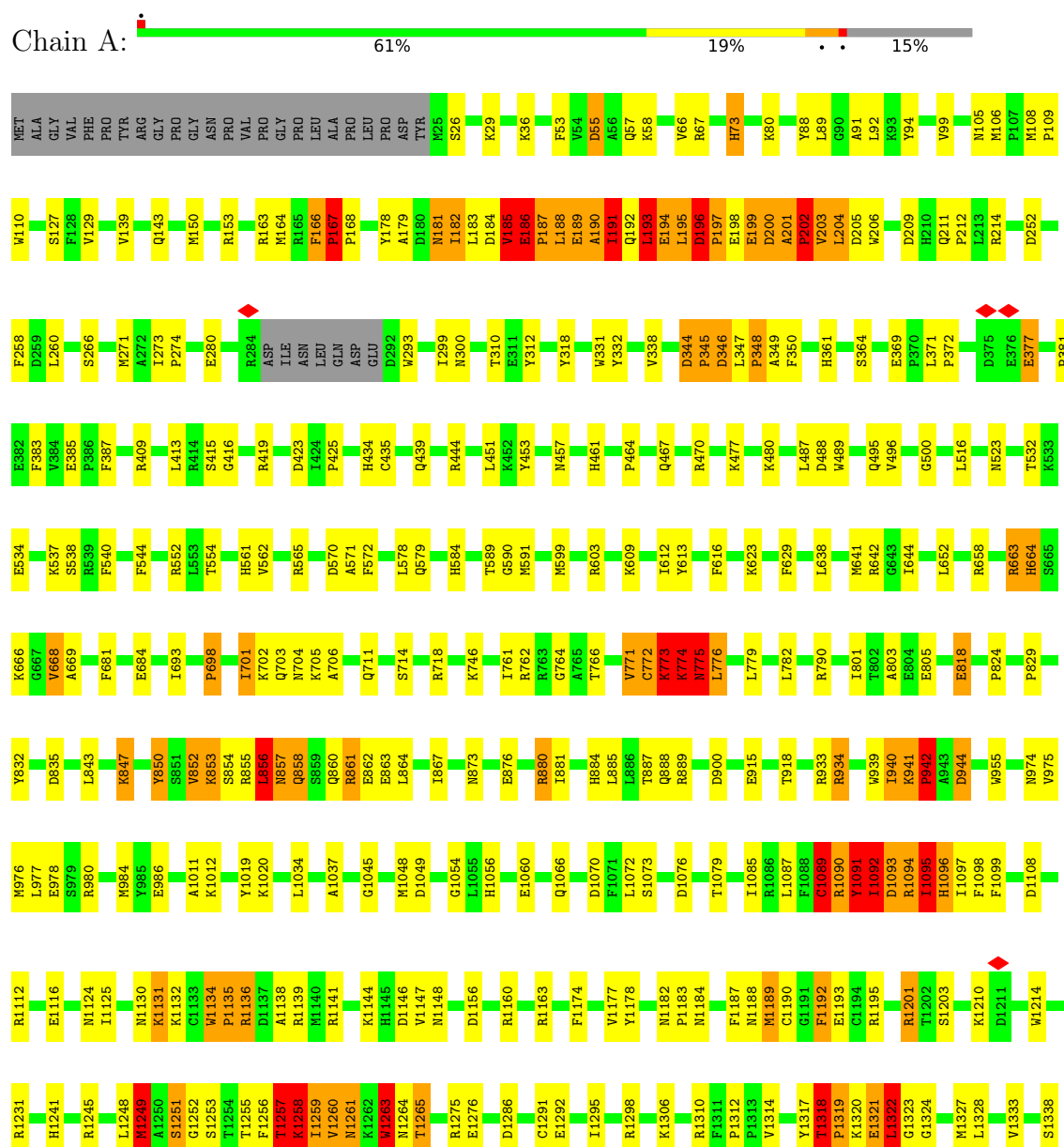


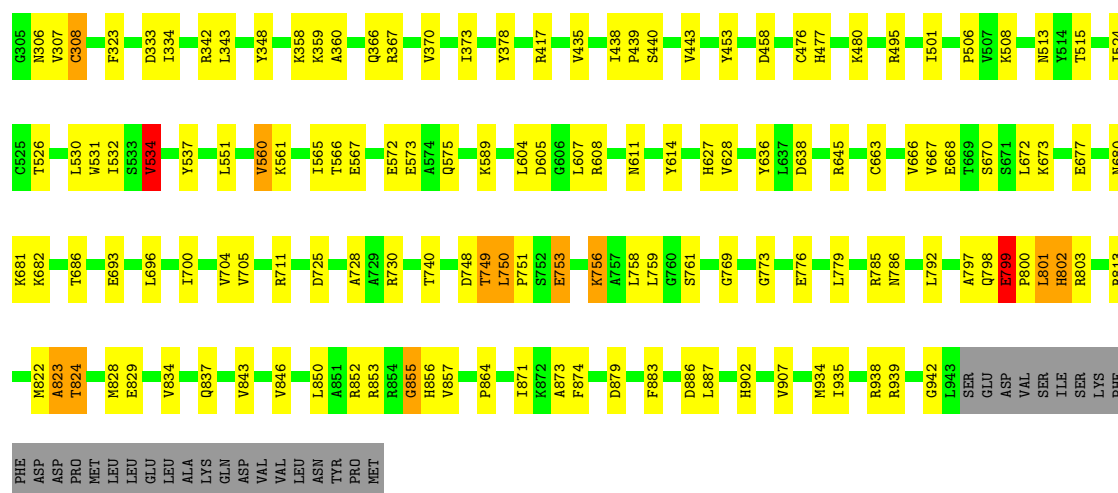
Mol	Chain	Residues	Atoms					AltConf
45	Q	1	Total 31	C 10	N 5	O 13	P 3	0

3 Residue-property plots

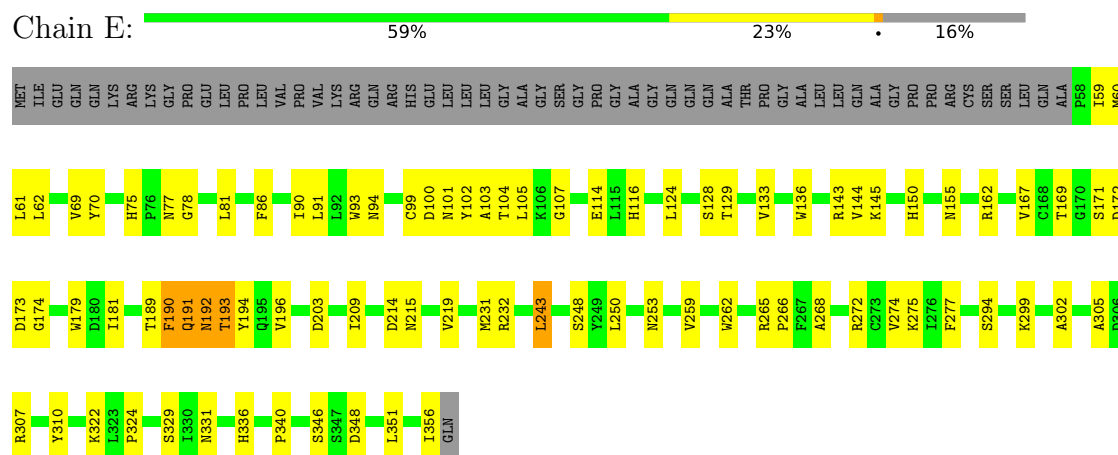
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

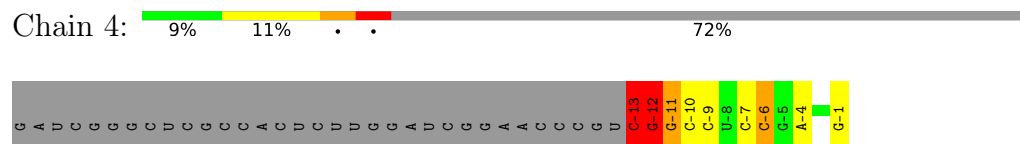




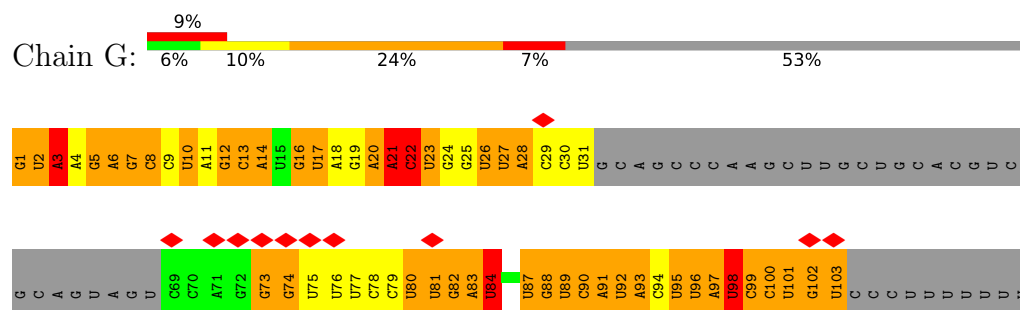
- Molecule 3: U5 small nuclear ribonucleoprotein 40 kDa protein



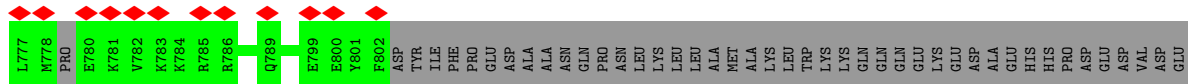
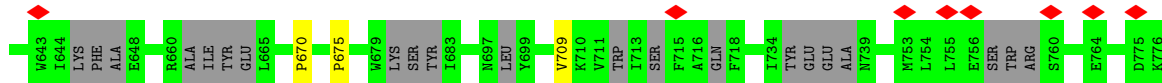
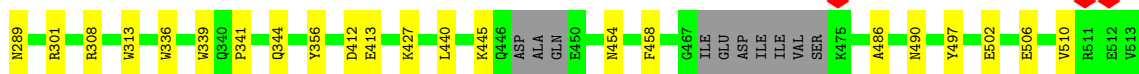
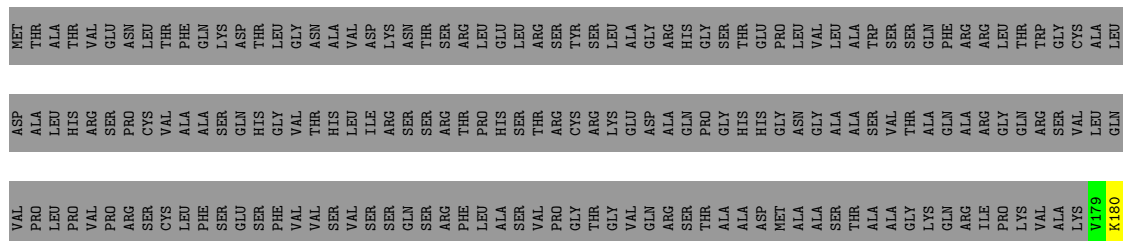
- Molecule 4: pre-mRNA



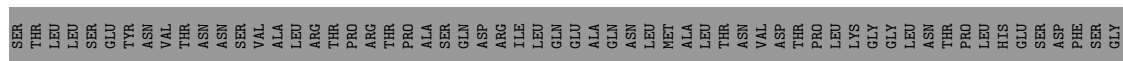
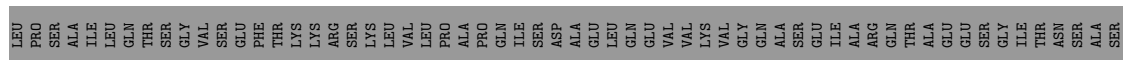
- Molecule 5: pre-mRNA

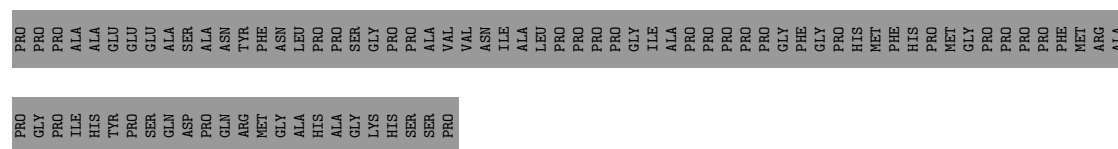


- Molecule 6: Crooked neck-like protein 1

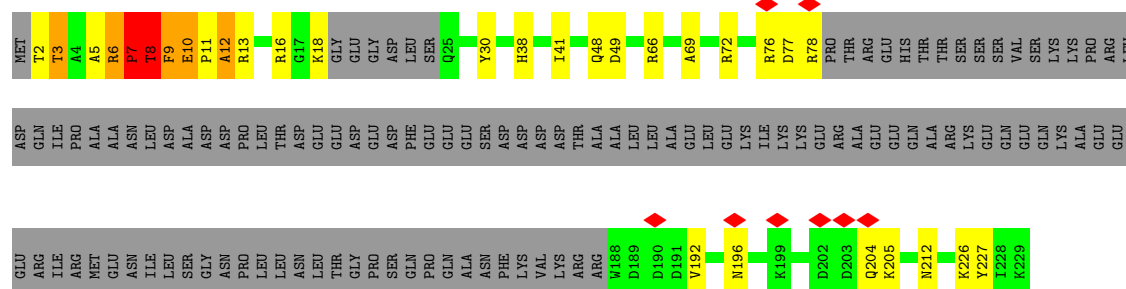


- Molecule 7: Cell division cycle 5-like protein

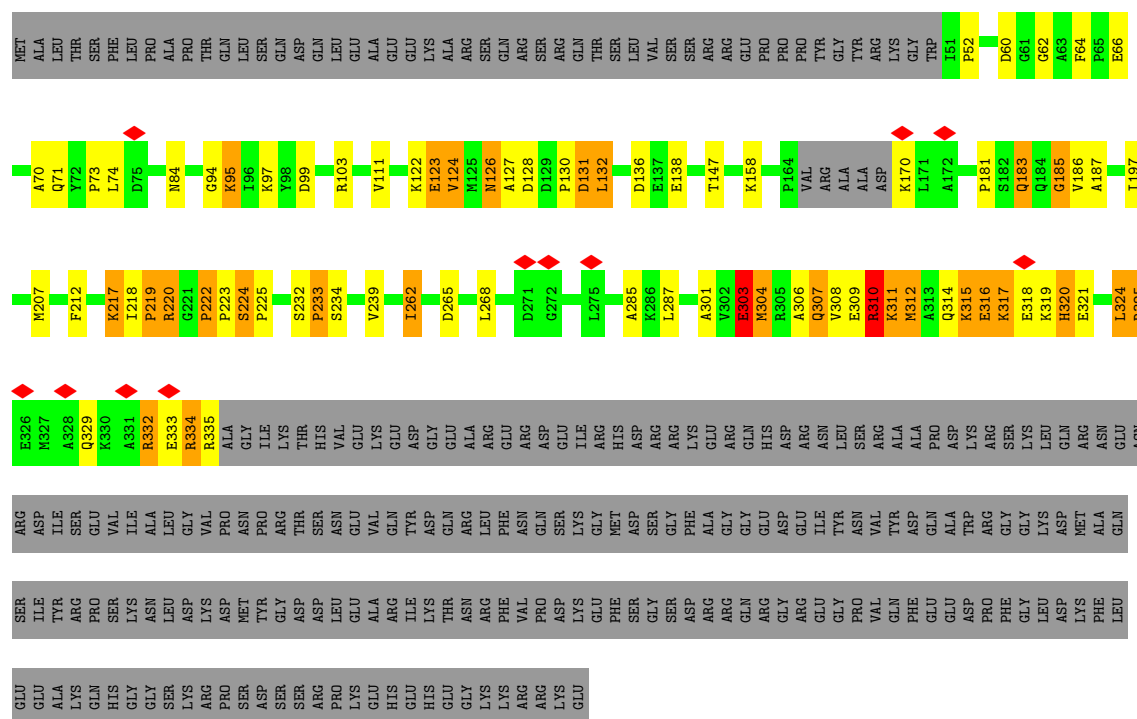




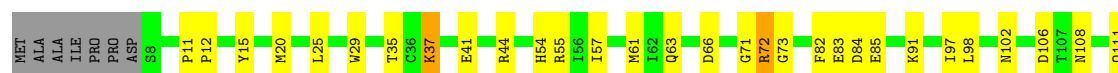
• Molecule 11: Spliceosome-associated protein CWC15 homolog



• Molecule 12: SNW domain-containing protein 1

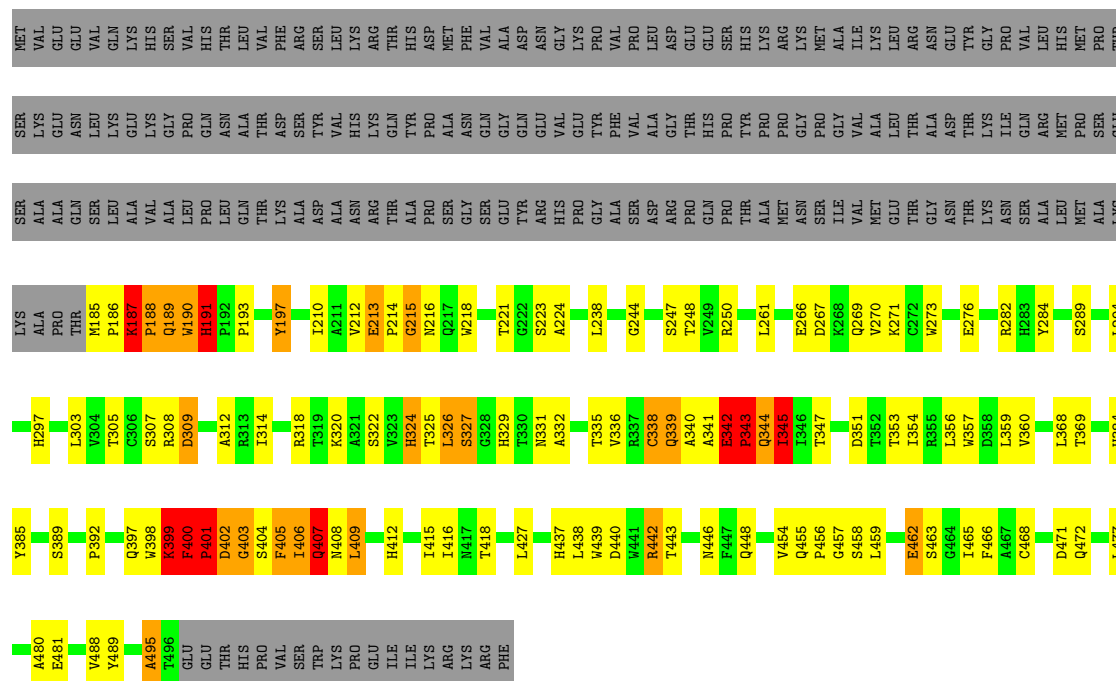
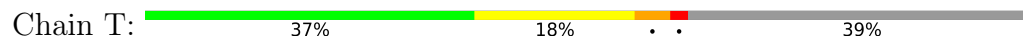


• Molecule 13: Peptidyl-prolyl cis-trans isomerase-like 1

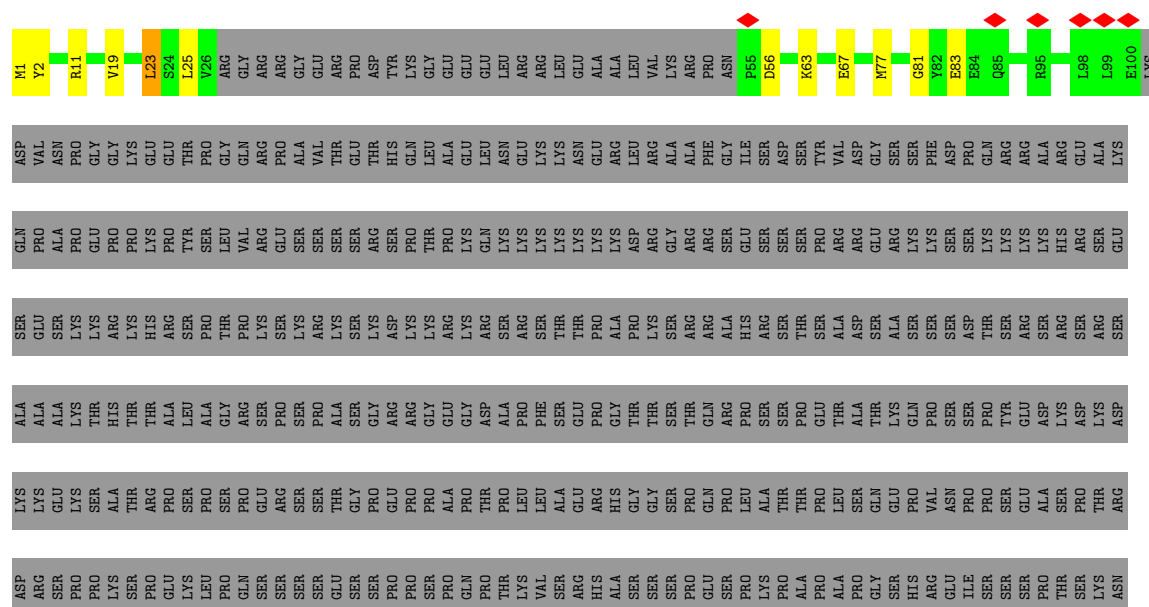




• Molecule 14: Pleiotropic regulator 1

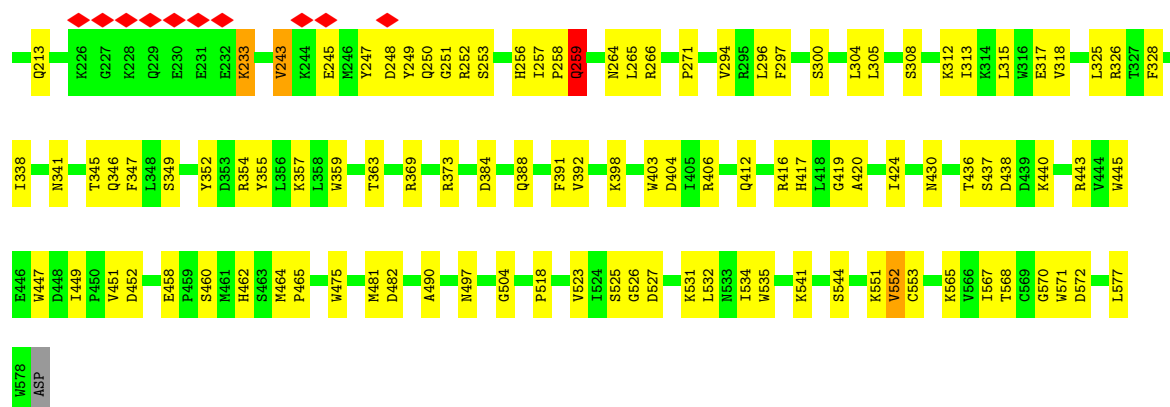


• Molecule 15: Serine/arginine repetitive matrix protein 2

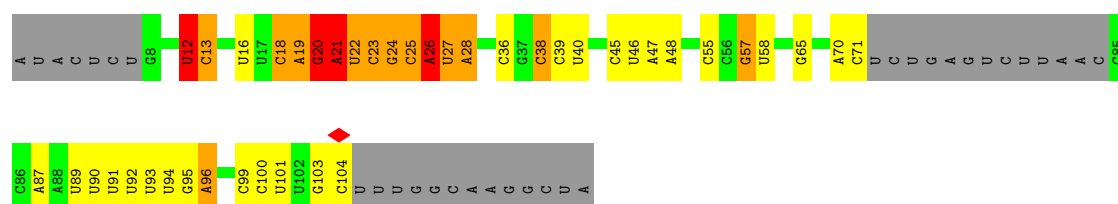




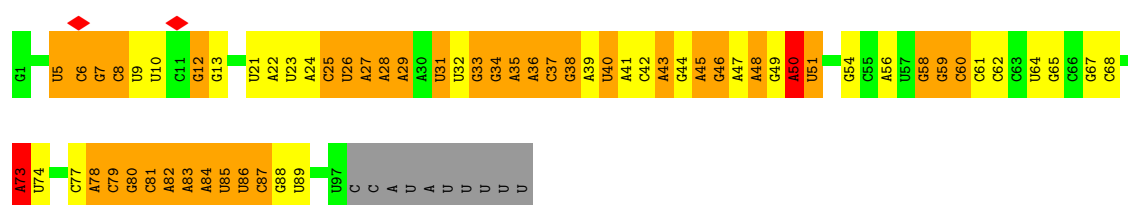
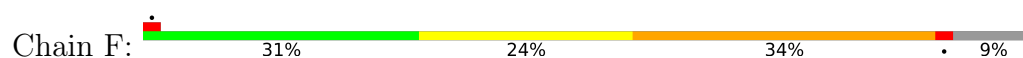




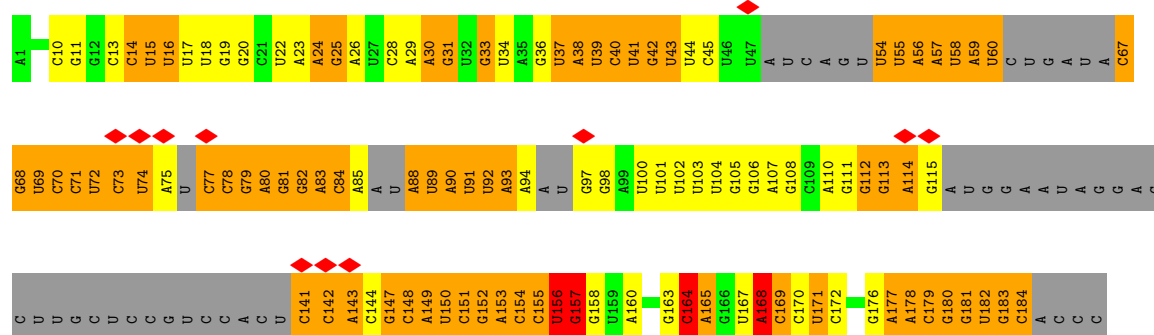
• Molecule 18: U5 snRNA



• Molecule 19: U6 snRNA

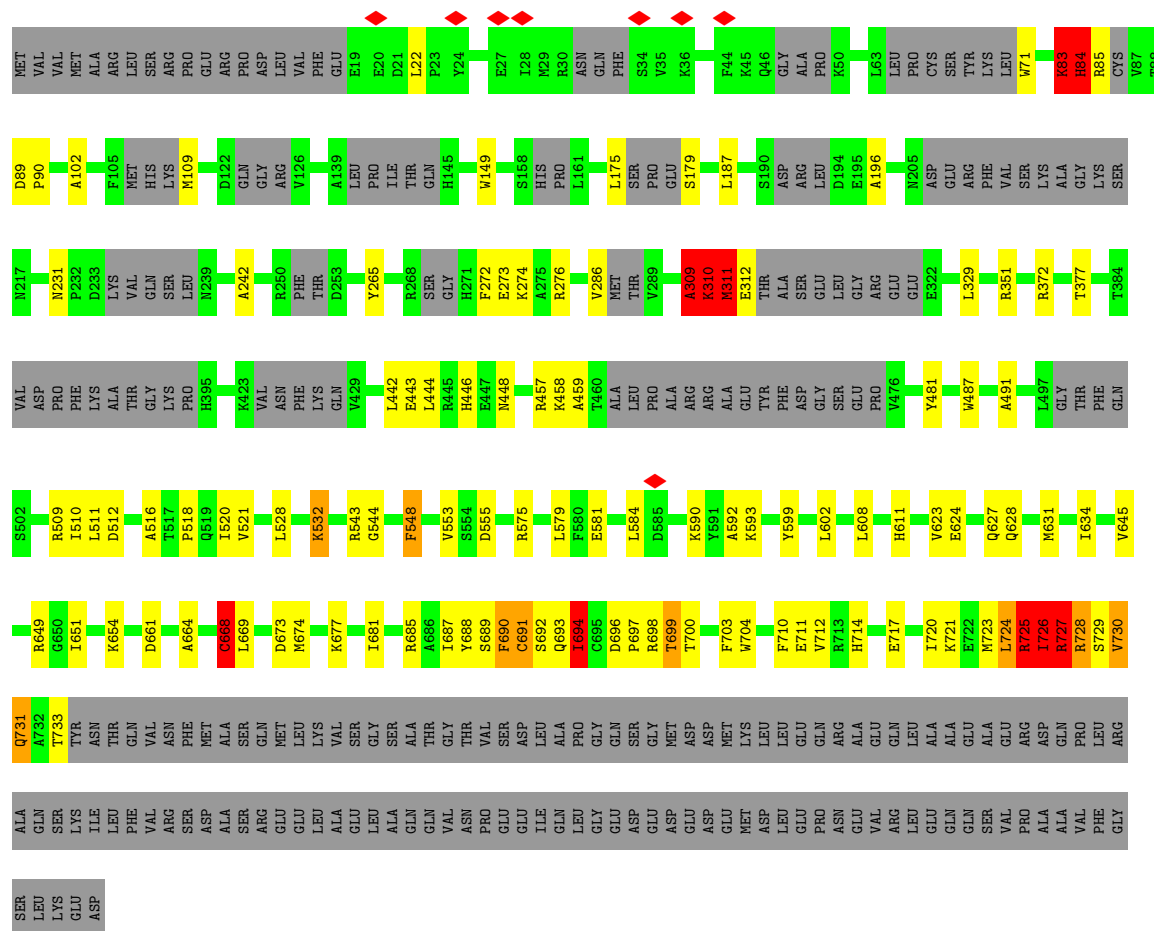


• Molecule 20: U2 snRNA

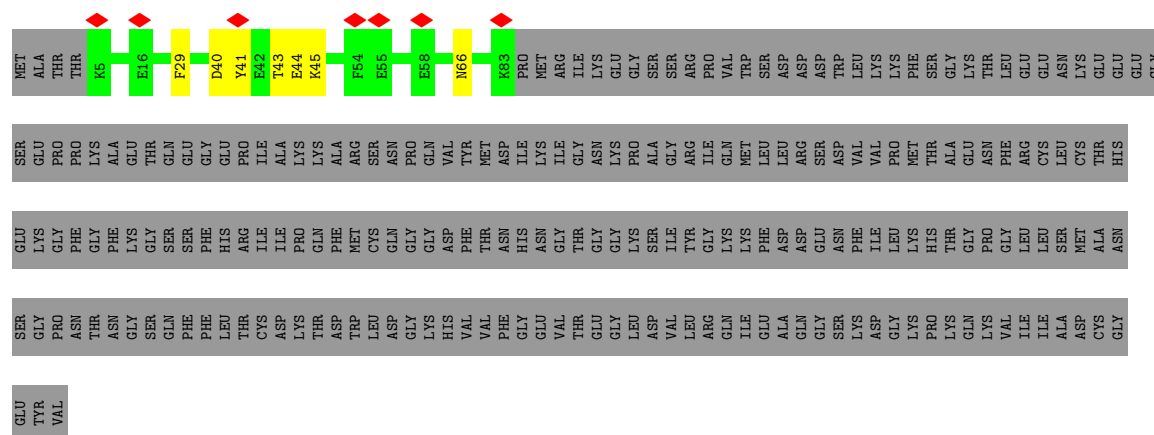


• Molecule 21: Small nuclear ribonucleoprotein-associated proteins B and B'

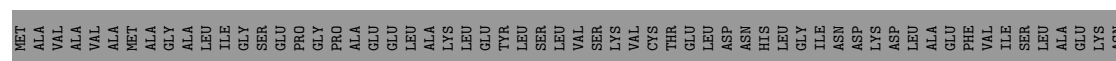
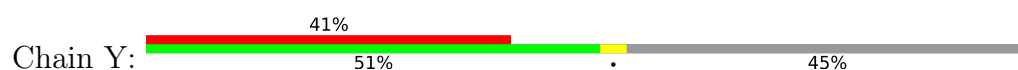




● Molecule 24: Peptidyl-prolyl cis-trans isomerase E

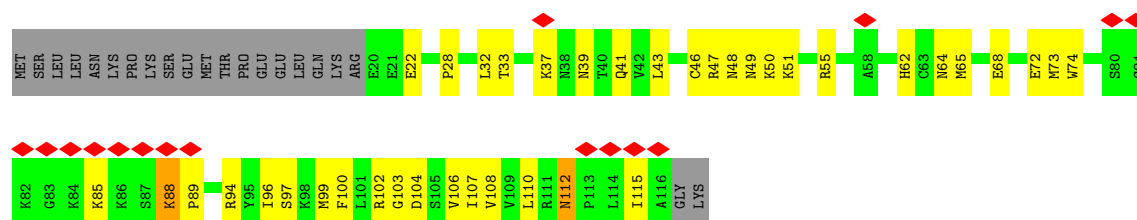


● Molecule 25: ATP-dependent RNA helicase DHX8

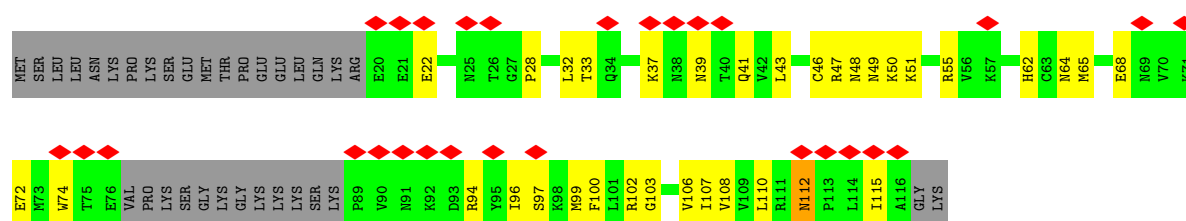




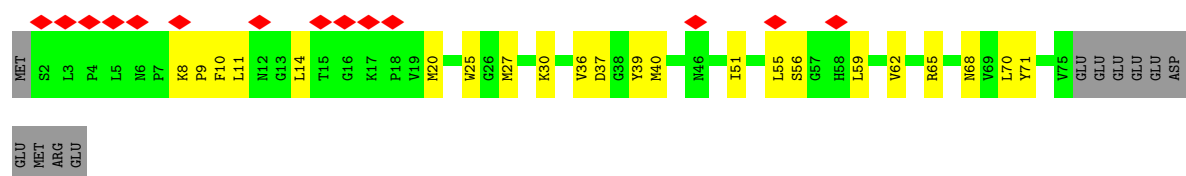
- Molecule 28: Small nuclear ribonucleoprotein Sm D2



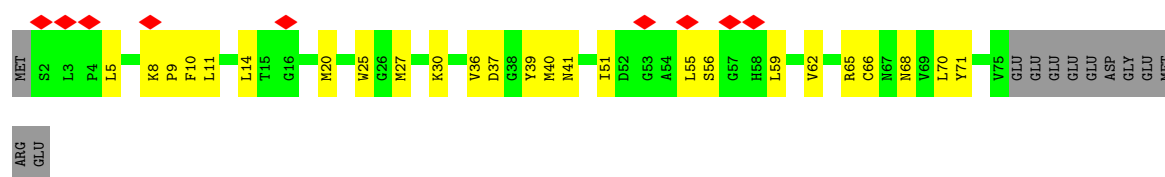
- Molecule 28: Small nuclear ribonucleoprotein Sm D2



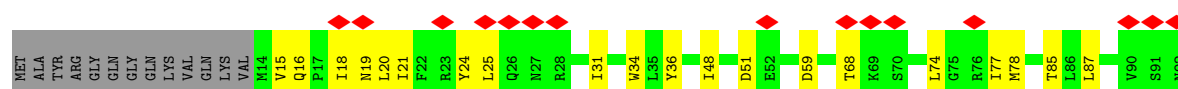
- Molecule 29: Small nuclear ribonucleoprotein F



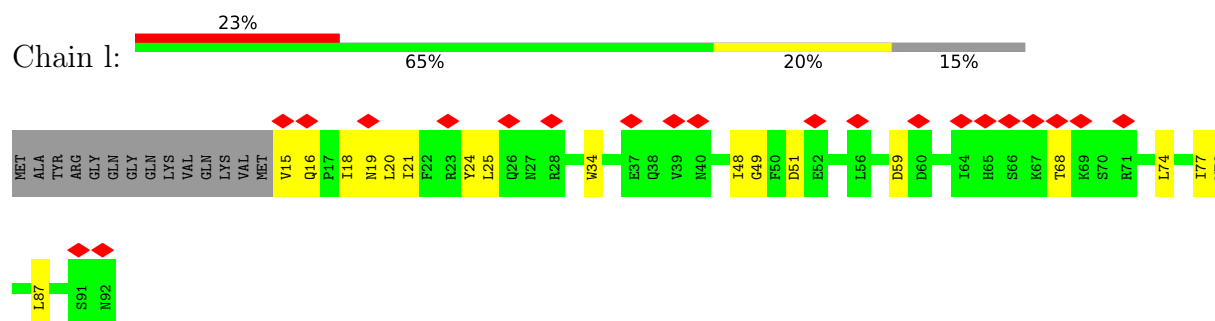
- Molecule 29: Small nuclear ribonucleoprotein F



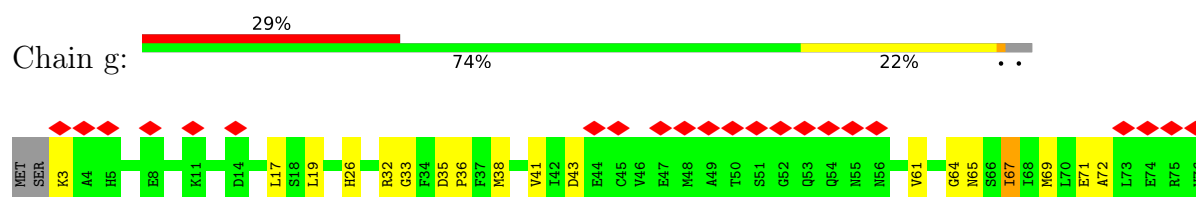
- Molecule 30: Small nuclear ribonucleoprotein E



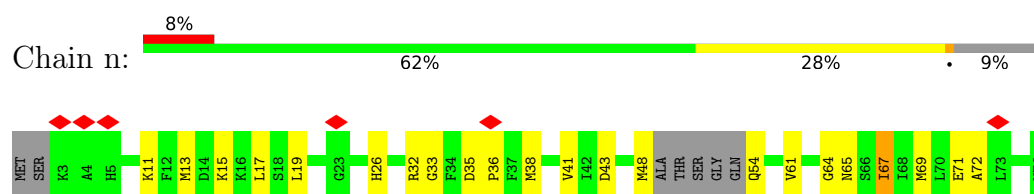
- Molecule 30: Small nuclear ribonucleoprotein E



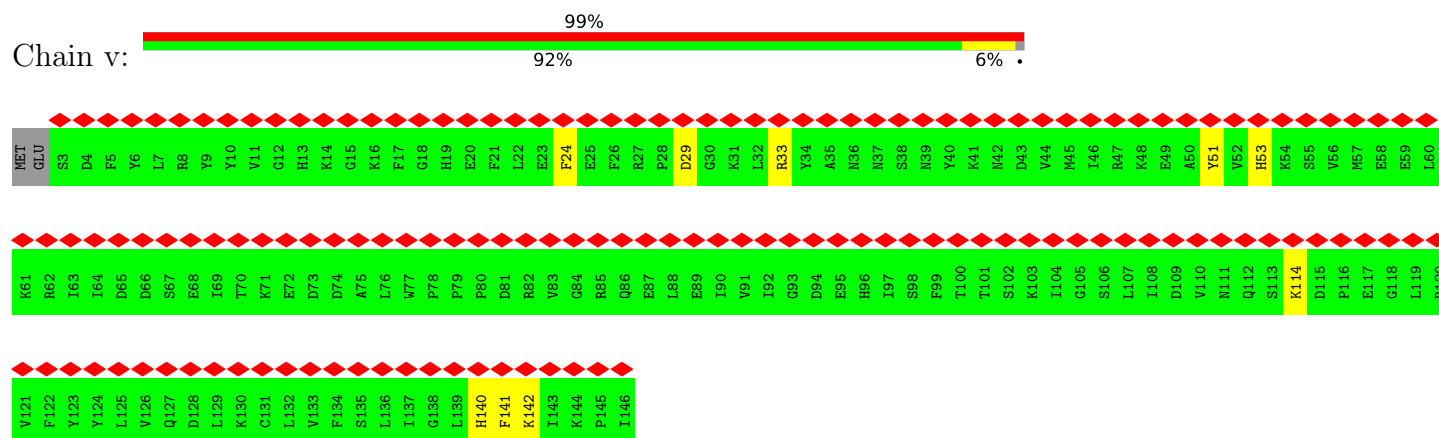
- Molecule 31: Small nuclear ribonucleoprotein G



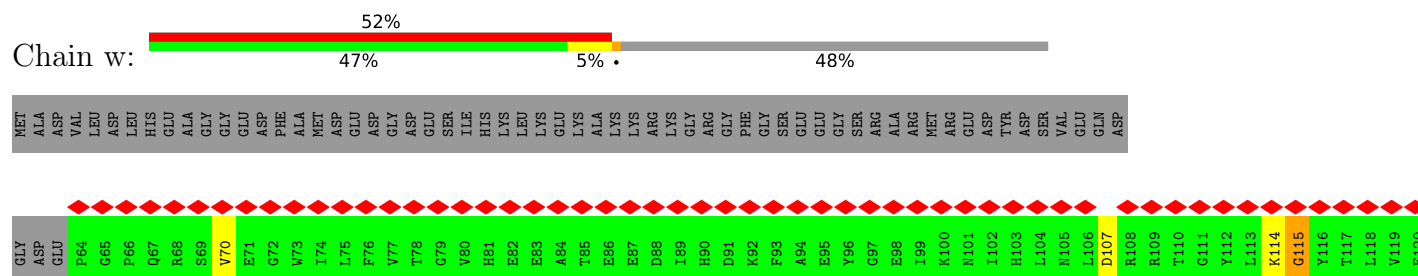
- Molecule 31: Small nuclear ribonucleoprotein G



- Molecule 32: Protein mago nashi homolog



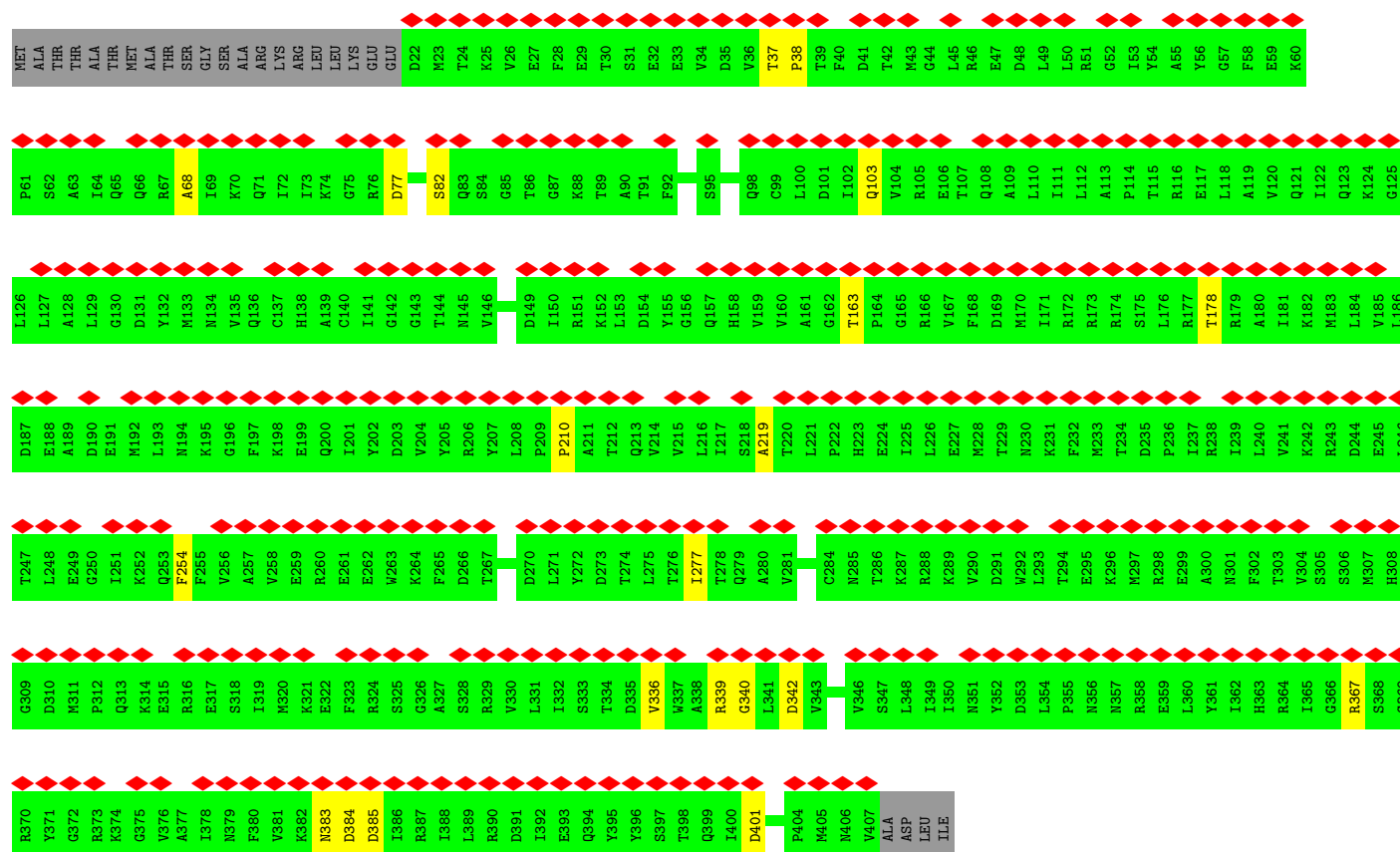
- Molecule 33: RNA-binding protein 8A





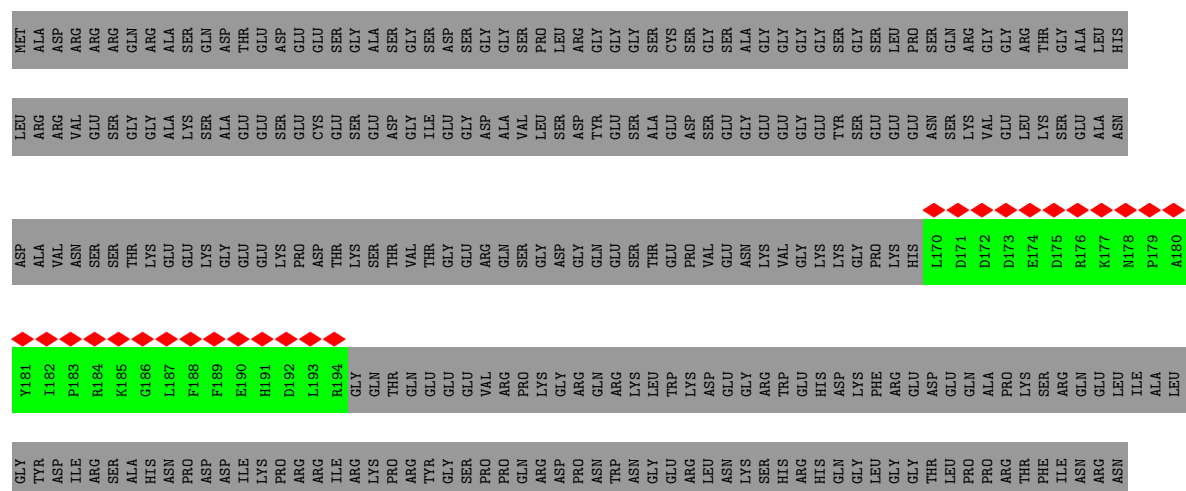
• Molecule 34: Eukaryotic initiation factor 4A-III

Chain u:

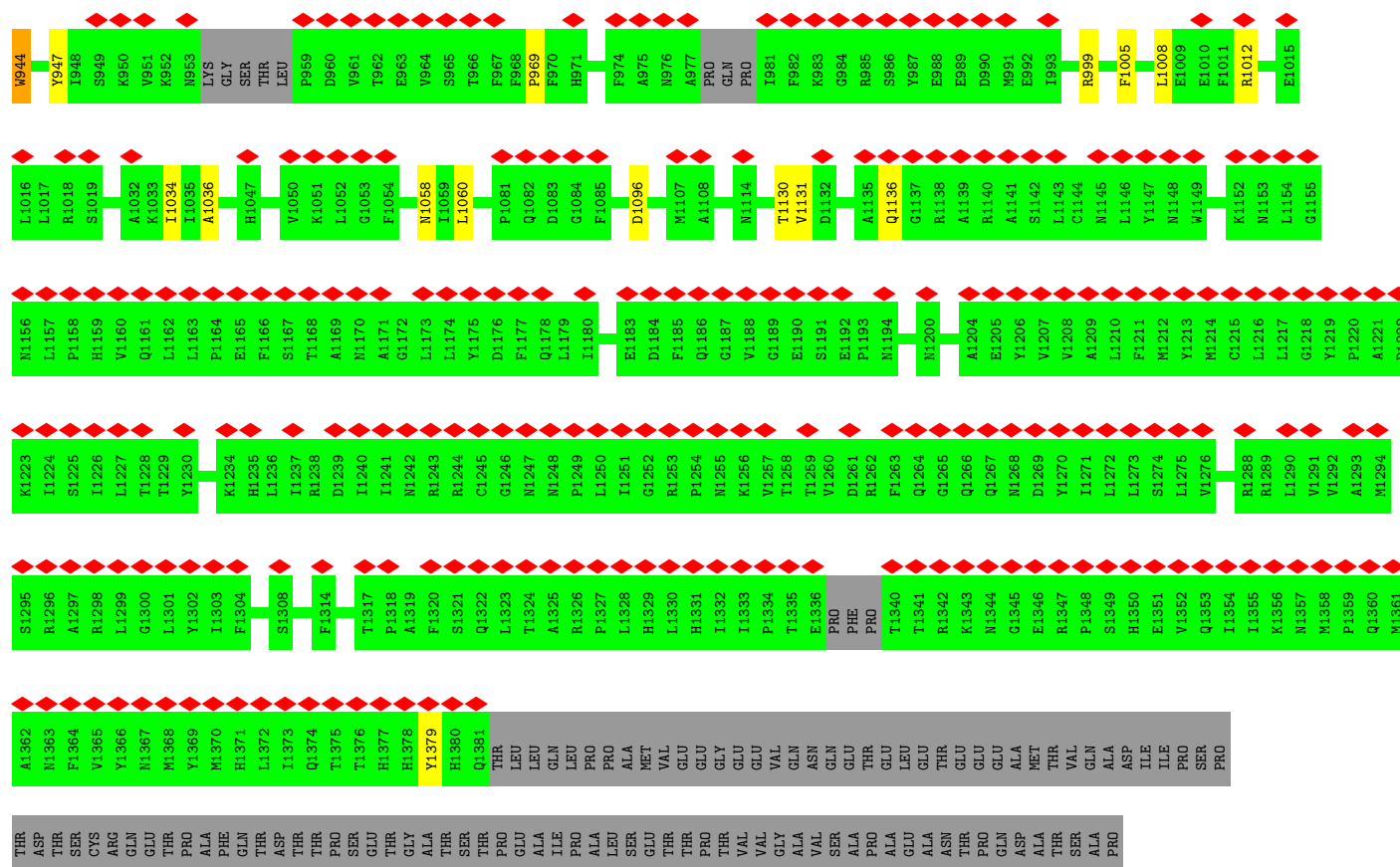


• Molecule 35: Protein CASC3

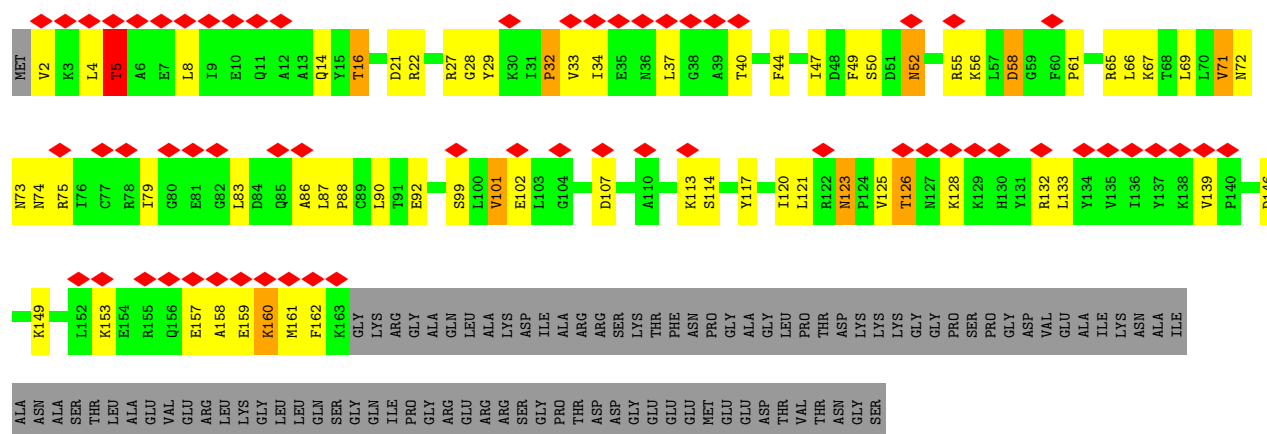
Chain x:





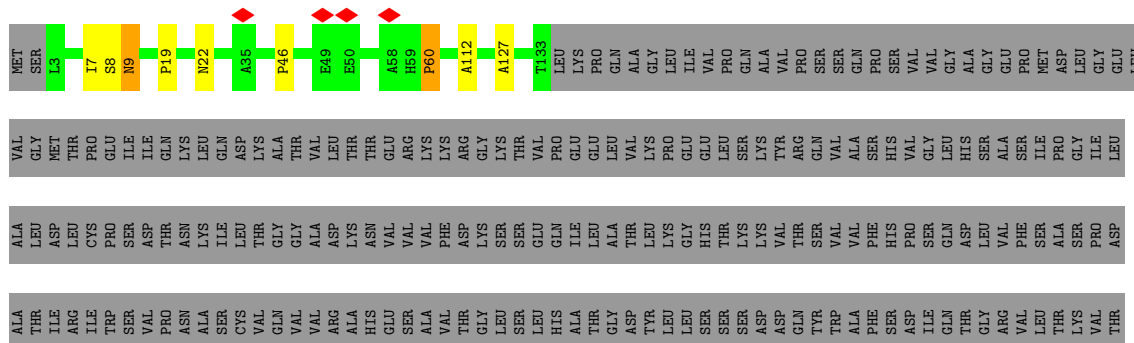


• Molecule 37: U2 small nuclear ribonucleoprotein A'

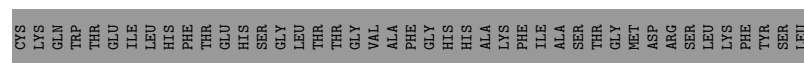


• Molecule 38: U2 small nuclear ribonucleoprotein B'

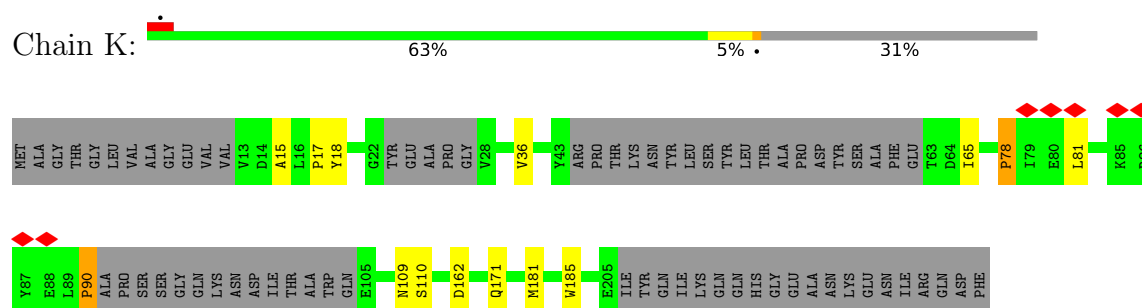








- Molecule 40: Pre-mRNA-splicing factor SPF27



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	192274	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)	1200	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	3.470	Depositor
Minimum map value	-1.736	Depositor
Average map value	0.012	Depositor
Map value standard deviation	0.092	Depositor
Recommended contour level	0.38	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: GTP, IHP, MG, ATP, ZN, 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	0.92	74/16897 (0.4%)	1.12	132/22917 (0.6%)
2	C	0.64	6/6950 (0.1%)	0.95	28/9443 (0.3%)
3	E	0.54	0/2392	0.83	7/3242 (0.2%)
4	4	0.72	0/307	1.00	3/476 (0.6%)
5	G	0.62	2/1674 (0.1%)	1.43	39/2594 (1.5%)
6	J	0.64	7/3856 (0.2%)	0.92	21/5234 (0.4%)
7	L	0.50	0/3046	0.81	10/4115 (0.2%)
8	M	0.47	0/1119	0.78	2/1497 (0.1%)
9	N	0.78	0/1210	1.00	9/1622 (0.6%)
10	O	0.53	0/2344	0.80	2/3163 (0.1%)
11	P	0.72	1/967 (0.1%)	1.19	8/1285 (0.6%)
12	R	0.83	5/2262 (0.2%)	1.21	19/3031 (0.6%)
13	S	0.52	1/1268 (0.1%)	0.82	2/1714 (0.1%)
14	T	1.15	20/2519 (0.8%)	1.36	35/3433 (1.0%)
15	U	0.50	0/424	0.85	2/582 (0.3%)
16	V	0.42	0/2642	0.82	0/3602
17	W	0.47	0/4237	0.92	11/5723 (0.2%)
18	B	0.60	2/1970 (0.1%)	0.82	6/3060 (0.2%)
19	F	0.48	0/2323	0.82	3/3619 (0.1%)
20	H	0.85	26/3305 (0.8%)	1.41	60/5130 (1.2%)
21	b	0.77	0/797	1.05	4/1062 (0.4%)
21	i	0.73	0/700	1.03	4/933 (0.4%)
22	X	1.12	1/621 (0.2%)	2.08	17/822 (2.1%)
23	I	0.62	0/3871	1.45	30/5283 (0.6%)
24	y	0.49	0/389	1.05	0/540
25	Y	1.00	1/3436 (0.0%)	1.52	26/4774 (0.5%)
26	a	0.66	0/646	0.85	0/867
26	h	0.65	0/639	0.86	0/857
27	c	0.74	0/657	0.98	0/888
27	j	0.74	0/657	0.98	0/888
28	d	0.94	1/786 (0.1%)	1.10	2/1053 (0.2%)
28	k	0.95	0/696	1.07	1/935 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
29	f	1.04	1/588 (0.2%)	1.08	0/795
29	m	1.04	1/588 (0.2%)	1.08	0/795
30	e	0.84	0/660	1.06	1/886 (0.1%)
30	l	0.85	0/652	1.06	0/876
31	g	0.71	0/584	0.95	1/779 (0.1%)
31	n	0.70	0/544	0.96	1/725 (0.1%)
32	v	0.47	0/710	1.03	3/987 (0.3%)
33	w	0.47	0/444	1.21	4/614 (0.7%)
34	u	0.51	0/1906	1.20	13/2653 (0.5%)
35	x	0.53	0/123	1.12	0/170
36	Q	0.53	8/6565 (0.1%)	1.07	34/9143 (0.4%)
37	o	0.81	0/1299	2.05	54/1761 (3.1%)
38	p	0.77	0/774	1.71	12/1035 (1.2%)
39	q	0.62	0/658	1.04	3/919 (0.3%)
39	r	0.57	0/653	0.99	3/912 (0.3%)
39	s	0.60	0/658	1.11	4/919 (0.4%)
39	t	0.62	0/653	0.94	3/912 (0.3%)
40	K	0.56	1/768 (0.1%)	0.95	2/1067 (0.2%)
All	All	0.73	158/94434 (0.2%)	1.12	621/130332 (0.5%)

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	15
2	C	0	5
6	J	0	3
9	N	0	3
10	O	0	1
11	P	0	3
12	R	0	6
17	W	0	1
23	I	0	5
28	d	0	1
28	k	0	1
36	Q	0	1
All	All	0	45

All (158) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	92	PRO	N-CA	16.17	1.67	1.47
36	Q	525	PRO	N-CA	15.81	1.67	1.47
1	A	345	PRO	N-CA	15.55	1.68	1.47
14	T	191	HIS	C-N	13.26	1.49	1.33
1	A	942	PRO	C-O	-13.00	1.07	1.24
1	A	1319	PRO	C-O	-12.81	1.08	1.23
1	A	1472	THR	C-O	-10.60	1.11	1.24
12	R	219	PRO	C-O	-10.46	1.11	1.23
25	Y	426	LEU	C-N	9.88	1.50	1.34
12	R	222	PRO	C-O	-9.55	1.13	1.24
1	A	771	VAL	C-O	-9.54	1.13	1.24
1	A	1470	TYR	C-O	-9.16	1.11	1.24
14	T	343	PRO	C-O	-9.13	1.12	1.24
1	A	776	LEU	C-O	-9.11	1.12	1.24
14	T	405	PHE	C-O	-8.95	1.15	1.23
1	A	773	LYS	C-O	-8.83	1.13	1.24
1	A	191	ILE	C-O	-8.77	1.15	1.23
1	A	1089	CYS	C-O	-8.77	1.13	1.24
1	A	1318	THR	C-O	-8.71	1.12	1.24
14	T	212	VAL	C-O	-8.68	1.14	1.24
1	A	1096	HIS	C-O	-8.63	1.12	1.24
6	J	239	ARG	C-O	-8.49	1.13	1.24
1	A	1090	ARG	C-O	-8.47	1.13	1.24
2	C	91	GLU	C-N	8.47	1.43	1.33
1	A	940	ILE	C-O	-8.42	1.15	1.24
1	A	1093	ASP	C-O	-8.41	1.12	1.24
14	T	214	PRO	C-O	-8.23	1.13	1.24
36	Q	934	TYR	C-O	8.17	1.34	1.24
1	A	344	ASP	C-N	7.99	1.44	1.33
1	A	1092	ILE	C-O	-7.84	1.14	1.24
1	A	1471	ARG	C-O	-7.76	1.14	1.24
1	A	1319	PRO	N-CD	-7.76	1.36	1.47
1	A	1263	TRP	C-O	-7.75	1.15	1.24
2	C	92	PRO	C-O	-7.68	1.15	1.23
20	H	77	C	C1'-N1	7.63	1.59	1.48
1	A	1264	ASN	C-O	-7.63	1.15	1.24
1	A	1265	THR	C-O	-7.63	1.14	1.24
1	A	1553	VAL	C-O	-7.63	1.15	1.24
20	H	142	C	C1'-N1	7.62	1.59	1.48
1	A	1563	HIS	C-O	-7.57	1.14	1.23
1	A	663	ARG	C-O	-7.50	1.14	1.23
14	T	399	LYS	C-O	-7.50	1.14	1.23
1	A	775	ASN	C-O	-7.47	1.14	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1163	ARG	C-O	-7.47	1.15	1.24
12	R	132	LEU	C-O	-7.43	1.15	1.23
1	A	1257	THR	C-O	-7.41	1.15	1.24
1	A	1322	LEU	C-O	-7.41	1.14	1.24
6	J	207	PRO	C-O	-7.33	1.18	1.25
14	T	345	ILE	C-O	-7.33	1.15	1.24
1	A	1260	VAL	C-O	-7.32	1.15	1.24
18	B	103	G	C1'-N9	-7.30	1.37	1.48
1	A	1508	GLY	C-O	7.24	1.33	1.23
20	H	55	U	C1'-N1	7.19	1.59	1.48
20	H	92	U	C1'-N1	7.16	1.59	1.48
20	H	54	U	C1'-N1	7.15	1.59	1.48
2	C	67	PRO	C-O	-7.13	1.15	1.23
6	J	208	PRO	C-O	-7.12	1.19	1.25
20	H	72	U	C1'-N1	7.12	1.59	1.48
20	H	89	U	C1'-N1	7.11	1.59	1.48
20	H	74	U	C1'-N1	7.10	1.59	1.48
20	H	69	U	C1'-N1	7.10	1.59	1.48
1	A	1465	TRP	C-O	-7.06	1.15	1.23
20	H	60	U	C1'-N1	7.05	1.59	1.48
20	H	91	U	C1'-N1	7.02	1.58	1.48
20	H	58	U	C1'-N1	7.02	1.58	1.48
1	A	934	ARG	C-O	-7.02	1.12	1.23
20	H	150	U	C1'-N1	7.01	1.58	1.48
20	H	182	U	C1'-N1	6.95	1.58	1.48
36	Q	531	TRP	C-N	6.94	1.50	1.33
1	A	1473	ASP	C-O	-6.92	1.15	1.24
1	A	1469	ASN	C-O	-6.85	1.14	1.24
5	G	21	A	O3'-P	-6.75	1.51	1.61
20	H	97	G	C1'-N9	-6.70	1.38	1.48
36	Q	935	PHE	C-O	-6.69	1.15	1.24
1	A	772	CYS	C-O	-6.69	1.16	1.24
20	H	151	C	C1'-N1	6.66	1.58	1.48
20	H	141	C	C1'-N1	6.62	1.58	1.48
1	A	167	PRO	C-O	-6.62	1.17	1.24
1	A	182	ILE	C-O	-6.61	1.16	1.24
20	H	73	C	C1'-N1	6.60	1.58	1.48
1	A	941	LYS	C-O	-6.58	1.16	1.24
20	H	184	C	C1'-N1	6.57	1.58	1.48
20	H	71	C	C1'-N1	6.54	1.58	1.48
1	A	348	PRO	C-O	-6.54	1.16	1.23
20	H	148	C	C1'-N1	6.50	1.58	1.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	H	67	C	C1'-N1	6.49	1.58	1.48
20	H	78	C	C1'-N1	6.48	1.58	1.48
1	A	1094	ARG	C-O	-6.47	1.15	1.23
20	H	70	C	C1'-N1	6.47	1.58	1.48
20	H	84	C	C1'-N1	6.45	1.58	1.48
14	T	406	ILE	C-O	-6.44	1.16	1.24
1	A	1496	PRO	C-O	-6.42	1.16	1.24
1	A	1459	ARG	C-O	-6.38	1.15	1.24
1	A	942	PRO	N-CD	-6.29	1.39	1.47
6	J	209	PRO	C-O	-6.29	1.19	1.25
1	A	1091	TYR	C-O	-6.19	1.16	1.24
14	T	403	GLY	C-O	-6.18	1.17	1.23
14	T	213	GLU	C-O	-6.17	1.16	1.24
1	A	1560	ILE	C-O	-6.17	1.16	1.24
1	A	1561	PHE	C-O	-6.10	1.16	1.23
1	A	1256	PHE	C-O	-6.09	1.17	1.24
1	A	187	PRO	C-O	-6.09	1.16	1.24
1	A	168	PRO	C-O	-5.96	1.16	1.24
1	A	190	ALA	C-O	-5.92	1.15	1.23
14	T	327	SER	CA-CB	-5.90	1.44	1.53
36	Q	930	GLU	N-CA	5.83	1.53	1.46
1	A	1095	ILE	C-O	-5.82	1.17	1.24
1	A	201	ALA	C-O	-5.80	1.16	1.24
36	Q	937	LEU	C-O	5.79	1.30	1.24
1	A	202	PRO	C-O	-5.79	1.16	1.24
5	G	98	U	O3'-P	-5.78	1.52	1.61
14	T	409	LEU	C-O	-5.76	1.17	1.24
1	A	187	PRO	N-CD	-5.75	1.39	1.47
6	J	240	THR	C-O	-5.74	1.16	1.24
22	X	76	LYS	C-O	-5.72	1.17	1.24
1	A	197	PRO	C-O	-5.70	1.17	1.24
1	A	669	ALA	C-O	-5.69	1.16	1.24
1	A	1562	MET	C-O	-5.69	1.17	1.24
6	J	244	ASN	C-O	-5.63	1.16	1.24
6	J	243	SER	CA-CB	-5.59	1.44	1.53
14	T	404	SER	CA-CB	-5.53	1.44	1.53
20	H	110	A	C1'-N9	-5.53	1.39	1.48
1	A	1528	GLN	C-O	-5.49	1.17	1.24
1	A	193	LEU	C-O	-5.48	1.17	1.23
1	A	349	ALA	C-O	-5.45	1.17	1.24
1	A	1554	GLN	C-O	-5.43	1.17	1.23
11	P	11	PRO	C-O	-5.41	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	Q	933	GLY	C-O	5.41	1.30	1.23
1	A	668	VAL	C-O	-5.40	1.17	1.24
2	C	94	ILE	C-O	-5.39	1.17	1.24
40	K	162	ASP	CA-CB	-5.38	1.44	1.53
1	A	1753	LEU	C-O	-5.35	1.17	1.24
1	A	1494	TYR	C-O	-5.34	1.17	1.24
14	T	215	GLY	C-O	-5.34	1.16	1.23
13	S	72	ARG	C-N	-5.33	1.30	1.33
36	Q	941	MET	C-O	5.32	1.30	1.24
14	T	191	HIS	C-O	-5.29	1.17	1.23
1	A	1468	ASN	C-O	-5.29	1.17	1.24
14	T	344	GLN	C-O	-5.27	1.17	1.24
1	A	167	PRO	N-CD	-5.27	1.40	1.47
14	T	326	LEU	C-O	-5.25	1.17	1.24
14	T	463	SER	C-O	-5.24	1.17	1.23
12	R	306	ALA	C-O	-5.22	1.18	1.24
1	A	1461	ASP	C-O	-5.22	1.17	1.24
1	A	1749	LYS	C-O	-5.22	1.17	1.24
12	R	220	ARG	C-O	-5.21	1.17	1.23
14	T	400	PHE	C-O	-5.19	1.17	1.24
1	A	192	GLN	C-O	-5.17	1.18	1.24
1	A	774	LYS	C-O	-5.16	1.18	1.24
1	A	1557	LEU	C-O	-5.15	1.17	1.24
2	C	81	VAL	C-O	-5.13	1.18	1.24
29	f	14	LEU	CA-C	5.09	1.59	1.52
1	A	186	GLU	C-O	-5.08	1.17	1.23
1	A	185	VAL	C-O	-5.07	1.18	1.24
29	m	14	LEU	CA-C	5.05	1.59	1.52
18	B	96	A	C1'-N9	-5.02	1.40	1.48
28	d	73	MET	CA-C	-5.01	1.46	1.52
14	T	338	CYS	C-O	-5.00	1.18	1.23

All (621) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	344	ASP	CA-C-N	20.68	142.03	119.28
1	A	344	ASP	C-N-CA	20.68	142.03	119.28
1	A	856	LEU	CA-C-N	17.52	155.00	121.54
1	A	856	LEU	C-N-CA	17.52	155.00	121.54
36	Q	531	TRP	CA-C-N	17.41	141.60	119.84
36	Q	531	TRP	C-N-CA	17.41	141.60	119.84
36	Q	524	LYS	CA-C-N	17.29	141.46	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	Q	524	LYS	C-N-CA	17.29	141.46	119.84
14	T	191	HIS	CA-C-N	17.02	137.91	120.38
14	T	191	HIS	C-N-CA	17.02	137.91	120.38
1	A	1515	TRP	N-CA-CB	16.70	138.72	110.49
5	G	1	G	C1'-C2'-O2'	-16.53	87.01	111.80
2	C	91	GLU	CA-C-N	14.74	136.79	120.13
2	C	91	GLU	C-N-CA	14.74	136.79	120.13
11	P	7	PRO	N-CA-CB	-14.61	87.91	103.25
1	A	775	ASN	CA-CB-CG	-14.43	98.17	112.60
1	A	1470	TYR	CB-CA-C	-13.69	85.28	109.24
2	C	85	ASP	CB-CA-C	-13.69	86.77	110.45
1	A	1261	ASN	CB-CA-C	-13.66	88.12	110.79
1	A	1318	THR	CA-CB-OG1	-13.64	89.14	109.60
37	o	55	ARG	CD-NE-CZ	13.11	142.76	124.40
1	A	1261	ASN	CA-CB-CG	-13.04	99.56	112.60
14	T	343	PRO	CB-CA-C	12.91	132.87	111.56
5	G	130	G	C4'-C3'-O3'	12.62	131.93	113.00
1	A	940	ILE	CA-C-N	-12.39	109.22	122.85
1	A	940	ILE	C-N-CA	-12.39	109.22	122.85
13	S	72	ARG	CB-CA-C	-12.37	84.80	109.67
1	A	187	PRO	N-CD-CG	-12.34	84.69	103.20
1	A	1264	ASN	CB-CA-C	-12.26	90.43	110.79
5	G	84	U	C2'-C3'-O3'	-12.13	95.51	113.70
23	I	83	LYS	O-C-N	-12.07	109.64	122.07
23	I	84	HIS	O-C-N	-12.02	109.69	122.07
23	I	310	LYS	O-C-N	-12.00	109.71	122.07
23	I	311	MET	O-C-N	-11.97	109.74	122.07
1	A	1472	THR	CB-CA-C	-11.95	90.95	110.79
23	I	309	ALA	O-C-N	-11.90	109.81	122.07
22	X	107	GLU	CB-CA-C	-11.60	92.67	110.88
37	o	49	PHE	CA-CB-CG	11.46	125.27	113.80
22	X	115	TYR	CB-CA-C	11.43	130.29	110.85
14	T	401	PRO	CA-N-CD	-11.41	96.03	112.00
2	C	91	GLU	O-C-N	-11.37	110.97	121.20
22	X	96	GLN	CB-CA-C	-11.32	92.00	110.79
1	A	772	CYS	CA-CB-SG	-11.00	89.10	114.40
1	A	187	PRO	N-CA-CB	-10.93	91.78	103.25
1	A	942	PRO	N-CA-C	-10.79	90.24	112.47
2	C	67	PRO	CB-CA-C	-10.70	95.84	110.60
34	u	37	THR	CA-C-N	10.66	130.44	119.56
34	u	37	THR	C-N-CA	10.66	130.44	119.56
14	T	343	PRO	CA-N-CD	-10.63	97.12	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1496	PRO	CB-CA-C	-10.63	95.08	112.62
33	w	114	LYS	N-CA-C	-10.47	93.65	110.20
12	R	310	ARG	CB-CA-C	-10.45	94.48	110.88
1	A	186	GLU	CB-CA-C	-10.37	88.95	110.31
1	A	1507	SER	O-C-N	-10.11	109.04	122.38
5	G	98	U	C3'-C2'-O2'	10.01	125.71	110.70
3	E	193	THR	CA-CB-OG1	-9.97	94.65	109.60
18	B	104	C	C2'-C3'-O3'	-9.94	94.59	109.50
1	A	1265	THR	CA-CB-OG1	-9.86	94.81	109.60
23	I	458	LYS	O-C-N	9.74	132.10	122.07
23	I	459	ALA	O-C-N	9.68	132.04	122.07
1	A	167	PRO	N-CA-C	-9.66	98.91	110.70
14	T	401	PRO	CB-CA-C	9.61	127.42	111.56
1	A	1090	ARG	CB-CG-CD	-9.61	89.21	111.30
1	A	167	PRO	CA-N-CD	-9.58	98.58	112.00
23	I	457	ARG	O-C-N	9.57	131.93	122.07
22	X	86	GLU	CB-CG-CD	9.56	128.85	112.60
5	G	124	G	C2'-C3'-O3'	9.52	123.78	109.50
36	Q	934	TYR	CA-C-N	-9.46	107.51	122.65
36	Q	934	TYR	C-N-CA	-9.46	107.51	122.65
39	s	46	PRO	N-CA-CB	9.43	111.19	103.36
23	I	694	ILE	CA-C-N	9.34	134.85	120.75
23	I	694	ILE	C-N-CA	9.34	134.85	120.75
2	C	68	THR	CB-CA-C	-9.34	90.48	111.30
36	Q	935	PHE	CB-CA-C	9.31	126.30	110.56
5	G	98	U	C2'-C3'-O3'	-9.30	99.74	113.70
1	A	167	PRO	CB-CA-C	9.29	122.25	110.92
5	G	127	G	C4'-C3'-O3'	9.28	126.92	113.00
5	G	121	C	C4'-C3'-O3'	9.26	126.89	113.00
1	A	1459	ARG	CB-CG-CD	-9.20	90.15	111.30
1	A	166	PHE	CA-CB-CG	-9.17	104.63	113.80
37	o	58	ASP	CA-CB-CG	9.08	121.68	112.60
1	A	934	ARG	CG-CD-NE	-9.05	92.08	112.00
36	Q	944	TRP	CA-C-N	-9.03	108.00	120.38
36	Q	944	TRP	C-N-CA	-9.03	108.00	120.38
1	A	383	PHE	N-CA-C	-8.99	102.89	114.04
7	L	124	LYS	N-CA-C	8.90	124.27	112.35
5	G	125	C	C4'-C3'-O3'	8.88	122.72	109.40
1	A	1754	TYR	CB-CA-C	-8.87	93.64	111.91
18	B	12	U	C4'-C3'-O3'	8.80	122.60	109.40
2	C	855	GLY	N-CA-C	8.78	123.27	112.73
25	Y	687	ALA	CA-C-N	8.74	133.93	120.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	687	ALA	C-N-CA	8.74	133.93	120.82
23	I	458	LYS	CA-C-O	-8.74	111.65	120.82
1	A	1091	TYR	CA-C-O	-8.72	111.13	120.46
1	A	1319	PRO	CB-CA-C	-8.72	99.53	110.95
39	r	46	PRO	N-CA-CB	8.69	111.09	103.27
6	J	240	THR	CA-CB-OG1	-8.68	96.58	109.60
20	H	183	G	O3'-P-O5'	-8.66	91.01	104.00
23	I	459	ALA	CA-C-O	-8.65	111.74	120.82
20	H	82	G	O3'-P-O5'	-8.64	91.03	104.00
20	H	77	C	O3'-P-O5'	-8.63	91.05	104.00
20	H	59	A	O3'-P-O5'	-8.63	91.06	104.00
20	H	113	G	O3'-P-O5'	-8.63	91.06	104.00
2	C	114	TYR	CB-CA-C	-8.62	92.78	110.38
20	H	91	U	O3'-P-O5'	-8.62	91.07	104.00
20	H	78	C	O3'-P-O5'	-8.62	91.07	104.00
20	H	141	C	O3'-P-O5'	-8.61	91.08	104.00
20	H	150	U	O3'-P-O5'	-8.61	91.09	104.00
20	H	180	G	O3'-P-O5'	-8.61	91.09	104.00
20	H	74	U	O3'-P-O5'	-8.61	91.09	104.00
20	H	56	A	O3'-P-O5'	-8.60	91.10	104.00
20	H	73	C	O3'-P-O5'	-8.60	91.09	104.00
20	H	148	C	O3'-P-O5'	-8.60	91.10	104.00
20	H	68	G	O3'-P-O5'	-8.60	91.11	104.00
5	G	130	G	N9-C1'-C2'	-8.59	99.11	112.00
20	H	182	U	O3'-P-O5'	-8.59	91.11	104.00
36	Q	936	PHE	N-CA-C	-8.59	101.88	111.07
20	H	54	U	O3'-P-O5'	-8.59	91.12	104.00
20	H	57	A	O3'-P-O5'	-8.59	91.12	104.00
20	H	89	U	O3'-P-O5'	-8.59	91.12	104.00
20	H	93	A	O3'-P-O5'	-8.59	91.12	104.00
20	H	181	G	O3'-P-O5'	-8.58	91.12	104.00
20	H	79	G	O3'-P-O5'	-8.58	91.13	104.00
20	H	55	U	O3'-P-O5'	-8.58	91.14	104.00
20	H	80	A	O3'-P-O5'	-8.58	91.14	104.00
20	H	72	U	O3'-P-O5'	-8.57	91.14	104.00
20	H	90	A	O3'-P-O5'	-8.57	91.14	104.00
20	H	149	A	O3'-P-O5'	-8.57	91.15	104.00
20	H	58	U	O3'-P-O5'	-8.56	91.15	104.00
20	H	88	A	O3'-P-O5'	-8.56	91.16	104.00
20	H	83	A	O3'-P-O5'	-8.56	91.16	104.00
20	H	92	U	O3'-P-O5'	-8.56	91.16	104.00
20	H	69	U	O3'-P-O5'	-8.55	91.17	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	H	81	G	O3'-P-O5'	-8.55	91.18	104.00
20	H	84	C	O3'-P-O5'	-8.55	91.18	104.00
14	T	339	GLN	CB-CA-C	-8.55	93.08	109.66
23	I	457	ARG	CA-C-O	-8.55	111.84	120.82
20	H	71	C	O3'-P-O5'	-8.54	91.19	104.00
20	H	114	A	O3'-P-O5'	-8.54	91.20	104.00
7	L	9	GLY	CA-C-N	8.52	137.31	121.97
7	L	9	GLY	C-N-CA	8.52	137.31	121.97
20	H	70	C	O3'-P-O5'	-8.52	91.22	104.00
20	H	67	C	O3'-P-O5'	-8.51	91.23	104.00
37	o	5	THR	N-CA-CB	-8.51	98.29	111.05
5	G	124	G	C3'-C2'-O2'	8.49	127.33	114.60
1	A	200	ASP	CA-CB-CG	-8.48	104.11	112.60
1	A	345	PRO	CA-N-CD	-8.45	100.17	112.00
39	q	46	PRO	N-CA-CB	8.44	111.19	103.34
23	I	725	ARG	N-CA-C	-8.34	102.19	111.28
38	p	80	ARG	CD-NE-CZ	8.29	136.00	124.40
5	G	1	G	C4'-C3'-O3'	8.26	121.79	109.40
22	X	108	GLU	CB-CA-C	-8.25	97.92	110.88
4	4	-12	G	N9-C1'-C2'	-8.23	99.65	112.00
39	s	60	PRO	N-CA-CB	8.18	111.83	103.25
1	A	166	PHE	CA-C-N	8.17	128.79	120.38
1	A	166	PHE	C-N-CA	8.17	128.79	120.38
6	J	208	PRO	CB-CA-C	-8.16	103.72	111.39
25	Y	1040	GLY	N-CA-C	8.15	122.82	111.25
6	J	238	ASN	CA-CB-CG	-8.12	104.48	112.60
5	G	1	G	N9-C1'-C2'	-8.11	101.84	114.00
1	A	1459	ARG	CA-C-O	-8.06	110.27	119.79
37	o	16	THR	CA-C-O	-8.03	111.76	120.36
22	X	103	GLN	CB-CA-C	-7.91	98.47	110.88
14	T	187	LYS	CA-C-N	7.90	129.72	119.84
14	T	187	LYS	C-N-CA	7.90	129.72	119.84
37	o	99	SER	N-CA-C	7.90	122.69	112.26
11	P	8	THR	CB-CA-C	7.90	126.14	110.42
2	C	92	PRO	CA-N-CD	-7.89	100.95	112.00
37	o	47	ILE	N-CA-CB	7.88	123.03	111.52
1	A	1096	HIS	CA-C-O	-7.85	112.22	120.70
7	L	54	LEU	N-CA-C	7.85	119.84	111.28
5	G	21	A	O3'-P-O5'	7.78	115.67	104.00
22	X	64	ARG	CB-CA-C	-7.70	98.01	110.79
1	A	1090	ARG	CG-CD-NE	-7.69	95.07	112.00
36	Q	1379	TYR	N-CA-C	7.69	122.76	112.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	130	G	C1'-C2'-O2'	-7.68	96.87	108.40
37	o	117	TYR	CA-C-O	7.68	128.46	120.40
14	T	344	GLN	N-CA-CB	7.67	123.46	110.49
36	Q	929	CYS	O-C-N	-7.59	112.53	122.39
20	H	168	A	P-O5'-C5'	-7.57	109.54	120.90
1	A	1563	HIS	CA-CB-CG	-7.54	106.26	113.80
4	4	-12	G	C4'-C3'-O3'	7.50	124.24	113.00
1	A	186	GLU	CB-CG-CD	-7.47	99.89	112.60
39	q	60	PRO	N-CA-CB	7.42	111.04	103.25
1	A	664	HIS	CA-CB-CG	-7.42	106.38	113.80
1	A	1461	ASP	CB-CA-C	-7.39	96.61	109.02
18	B	20	G	N9-C1'-C2'	7.37	125.05	114.00
2	C	823	ALA	N-CA-C	7.36	120.48	108.26
1	A	1497	THR	CA-CB-OG1	-7.32	98.62	109.60
1	A	1560	ILE	CA-C-O	-7.32	112.44	120.71
40	K	90	PRO	N-CA-CB	7.32	111.05	103.00
5	G	124	G	C1'-C2'-O2'	7.30	122.75	111.80
20	H	22	U	C2'-C3'-O3'	-7.29	102.77	113.70
20	H	167	U	O3'-P-O5'	-7.28	93.09	104.00
14	T	400	PHE	CA-CB-CG	-7.26	106.54	113.80
5	G	119	A	C2'-C3'-O3'	-7.25	98.63	109.50
14	T	407	GLN	CB-CG-CD	-7.24	100.29	112.60
40	K	78	PRO	N-CA-CB	7.23	110.84	103.25
2	C	92	PRO	CB-CA-C	-7.22	102.66	111.11
36	Q	96	CYS	N-CA-C	-7.21	103.42	111.28
1	A	940	ILE	CA-C-O	-7.21	112.23	120.95
37	o	71	VAL	CA-C-N	7.20	131.63	120.75
37	o	71	VAL	C-N-CA	7.20	131.63	120.75
20	H	31	G	N9-C1'-C2'	-7.20	101.20	112.00
1	A	1523	ARG	N-CA-CB	-7.19	99.59	110.01
5	G	129	U	C3'-C2'-O2'	7.17	121.45	110.70
39	t	60	PRO	N-CA-CB	7.17	111.33	103.30
1	A	663	ARG	CG-CD-NE	-7.15	96.27	112.00
1	A	1556	ASP	CB-CA-C	-7.14	99.67	110.88
37	o	21	ASP	CA-CB-CG	7.13	119.73	112.60
34	u	77	ASP	N-CA-C	-7.08	99.81	110.28
5	G	120	G	C2'-C3'-O3'	7.06	120.09	109.50
1	A	350	PHE	CA-C-O	-7.05	112.57	120.54
1	A	1560	ILE	N-CA-CB	-7.04	103.05	110.72
23	I	726	ILE	N-CA-CB	7.01	121.10	110.58
20	H	170	C	C3'-C2'-O2'	-7.01	104.08	114.60
37	o	72	ASN	OD1-CG-ND2	7.00	129.60	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	T	400	PHE	CA-C-N	7.00	128.58	119.84
14	T	400	PHE	C-N-CA	7.00	128.58	119.84
1	A	187	PRO	N-CA-C	6.99	126.86	112.47
5	G	120	G	O4'-C1'-N9	-6.95	97.78	108.20
1	A	940	ILE	N-CA-C	-6.93	99.69	108.84
3	E	192	ASN	CA-C-N	6.92	134.76	121.54
3	E	192	ASN	C-N-CA	6.92	134.76	121.54
1	A	345	PRO	N-CA-C	-6.92	104.31	113.65
12	R	223	PRO	CB-CA-C	-6.92	96.96	110.10
25	Y	685	ASP	CA-C-N	6.92	134.75	121.54
25	Y	685	ASP	C-N-CA	6.92	134.75	121.54
37	o	107	ASP	CA-CB-CG	6.91	119.51	112.60
1	A	941	LYS	N-CA-C	6.90	120.48	108.75
37	o	4	LEU	N-CA-C	-6.90	97.98	108.67
14	T	214	PRO	CB-CA-C	-6.88	102.08	111.85
5	G	130	G	C2'-C3'-O3'	-6.87	103.40	113.70
37	o	121	LEU	CA-C-O	6.87	128.85	121.44
1	A	1096	HIS	CA-C-N	6.86	132.59	122.71
1	A	1096	HIS	C-N-CA	6.86	132.59	122.71
37	o	75	ARG	NE-CZ-NH1	-6.85	114.65	121.50
1	A	1257	THR	CA-CB-OG1	-6.84	99.33	109.60
1	A	1259	ILE	CB-CA-C	-6.83	102.92	112.14
2	C	85	ASP	CA-C-N	6.83	134.14	122.12
2	C	85	ASP	C-N-CA	6.83	134.14	122.12
39	t	46	PRO	N-CA-CB	6.83	110.42	103.25
14	T	309	ASP	O-C-N	6.80	131.17	122.39
38	p	53	PHE	CA-C-O	-6.79	112.86	120.32
1	A	1509	PHE	CA-C-O	-6.78	113.70	120.82
6	J	675	PRO	N-CA-CB	6.77	110.36	103.25
25	Y	686	GLU	CA-C-N	6.77	134.47	121.54
25	Y	686	GLU	C-N-CA	6.77	134.47	121.54
1	A	1459	ARG	CA-C-N	-6.76	112.06	122.60
1	A	1459	ARG	C-N-CA	-6.76	112.06	122.60
14	T	399	LYS	CB-CA-C	-6.76	96.92	111.78
12	R	310	ARG	CB-CG-CD	-6.74	95.79	111.30
37	o	58	ASP	N-CA-CB	-6.74	100.59	111.24
5	G	122	U	C5'-C4'-C3'	-6.73	105.91	116.00
6	J	604	PRO	N-CA-CB	6.73	110.32	103.25
1	A	1753	LEU	N-CA-CB	-6.71	99.88	110.69
12	R	303	GLU	CB-CG-CD	6.71	124.00	112.60
1	A	1761	PRO	N-CA-C	-6.70	100.67	111.19
39	q	19	PRO	N-CA-CB	6.68	110.26	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	799	GLU	CB-CA-C	6.67	116.81	111.00
5	G	127	G	C1'-C2'-O2'	-6.66	98.42	108.40
20	H	164	C	C5'-C4'-O4'	-6.66	99.12	109.10
25	Y	689	GLU	N-CA-C	-6.62	97.27	108.26
9	N	40	LYS	CA-C-N	6.61	134.17	121.54
9	N	40	LYS	C-N-CA	6.61	134.17	121.54
39	r	19	PRO	N-CA-CB	6.61	110.16	102.76
34	u	38	PRO	N-CA-C	6.60	122.42	113.84
1	A	1094	ARG	CA-C-O	-6.58	114.24	121.87
5	G	80	U	C2'-C3'-O3'	-6.57	103.84	113.70
23	I	728	ARG	CB-CA-C	-6.56	100.49	110.92
1	A	856	LEU	N-CA-C	6.55	120.48	111.71
22	X	89	PHE	CA-C-O	-6.54	113.62	120.55
2	C	92	PRO	CA-C-O	-6.53	113.33	120.97
1	A	663	ARG	CB-CA-C	-6.53	98.48	109.65
36	Q	99	ASN	CB-CA-C	-6.53	100.63	110.88
39	t	19	PRO	N-CA-CB	6.51	110.08	103.25
14	T	343	PRO	CA-C-O	-6.49	108.80	120.60
1	A	167	PRO	N-CD-CG	-6.48	93.48	103.20
11	P	6	ARG	CB-CA-C	-6.48	98.84	109.27
1	A	1556	ASP	N-CA-C	6.47	117.99	111.07
37	o	87	LEU	CA-C-N	6.46	126.22	119.05
37	o	87	LEU	C-N-CA	6.46	126.22	119.05
17	W	318	VAL	N-CA-C	6.46	117.14	110.36
1	A	850	TYR	CB-CA-C	-6.46	101.11	111.18
1	A	1522	GLN	CA-C-N	6.46	128.83	120.44
1	A	1522	GLN	C-N-CA	6.46	128.83	120.44
5	G	22	C	C4'-C3'-O3'	-6.46	103.32	113.00
6	J	637	PRO	N-CA-CB	6.44	110.35	103.52
18	B	12	U	C2'-C3'-O3'	-6.44	99.84	109.50
17	W	77	LYS	CA-C-N	-6.43	113.93	122.99
17	W	77	LYS	C-N-CA	-6.43	113.93	122.99
5	G	119	A	C3'-C2'-O2'	6.41	124.22	114.60
1	A	1091	TYR	N-CA-CB	-6.41	99.83	110.47
37	o	55	ARG	NE-CZ-NH1	6.39	127.89	121.50
1	A	775	ASN	CB-CA-C	-6.39	96.96	110.31
1	A	776	LEU	N-CA-C	-6.38	104.98	112.89
6	J	187	VAL	CA-C-N	6.37	133.70	121.54
6	J	187	VAL	C-N-CA	6.37	133.70	121.54
1	A	1095	ILE	CA-C-O	-6.36	113.71	120.39
11	P	8	THR	CA-CB-OG1	-6.35	100.07	109.60
39	s	19	PRO	N-CA-CB	6.34	109.91	103.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1321	GLU	CA-C-O	-6.34	113.70	120.42
36	Q	933	GLY	O-C-N	6.33	128.27	122.19
12	R	222	PRO	CB-CA-C	-6.32	103.21	110.92
34	u	68	ALA	N-CA-C	6.31	119.45	111.69
1	A	774	LYS	CB-CA-C	-6.31	100.94	110.90
37	o	40	THR	CA-C-N	6.29	131.53	122.40
37	o	40	THR	C-N-CA	6.29	131.53	122.40
5	G	97	A	C2'-C3'-O3'	6.29	118.93	109.50
39	r	60	PRO	N-CA-CB	6.28	109.84	103.25
5	G	1	G	C2'-C3'-O3'	6.27	118.90	109.50
22	X	106	GLU	CA-C-N	-6.27	112.29	120.44
22	X	106	GLU	C-N-CA	-6.27	112.29	120.44
6	J	210	PRO	CB-CA-C	-6.26	103.21	111.23
20	H	168	A	C5'-C4'-C3'	-6.26	106.61	116.00
6	J	670	PRO	N-CA-CB	6.23	110.42	103.44
20	H	169	C	P-O3'-C3'	6.23	129.55	120.20
1	A	1469	ASN	CB-CA-C	-6.22	100.04	110.56
12	R	320	HIS	CB-CA-C	6.22	122.61	110.67
18	B	26	A	P-O5'-C5'	-6.22	111.58	120.90
3	E	189	THR	CA-C-N	-6.21	114.36	123.05
3	E	189	THR	C-N-CA	-6.21	114.36	123.05
1	A	1749	LYS	N-CA-C	-6.20	104.97	112.54
1	A	1318	THR	N-CA-CB	-6.18	100.28	109.98
20	H	31	G	C4'-C3'-O3'	6.18	122.27	113.00
14	T	400	PHE	CB-CA-C	6.15	122.29	110.17
23	I	690	PHE	N-CA-C	-6.14	103.52	111.02
23	I	726	ILE	O-C-N	6.14	128.16	121.83
6	J	412	ASP	CA-C-N	6.14	128.83	120.54
6	J	412	ASP	C-N-CA	6.14	128.83	120.54
1	A	1249	MET	N-CA-C	-6.13	103.75	111.11
32	v	142	LYS	N-CA-C	6.13	118.64	109.25
2	C	93	ILE	CB-CA-C	-6.13	104.84	111.59
14	T	343	PRO	N-CA-C	-6.13	99.84	112.47
37	o	73	ASN	N-CA-C	6.12	119.80	111.17
1	A	1263	TRP	CA-C-O	-6.12	114.07	120.55
12	R	303	GLU	N-CA-C	-6.10	104.75	111.82
34	u	339	ARG	N-CA-C	6.10	119.64	109.95
5	G	3	A	N9-C1'-C2'	-6.09	102.86	112.00
1	A	1192	PHE	N-CA-C	6.06	119.05	110.50
1	A	1514	LYS	CA-C-N	-6.06	109.97	121.54
1	A	1514	LYS	C-N-CA	-6.06	109.97	121.54
37	o	52	ASN	CA-CB-CG	6.04	118.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	191	GLN	CB-CA-C	-6.03	101.21	110.26
1	A	1265	THR	CA-C-N	6.03	133.34	121.58
1	A	1265	THR	C-N-CA	6.03	133.34	121.58
23	I	377	THR	CB-CA-C	-6.03	101.42	110.88
6	J	566	PRO	N-CA-CB	6.01	110.17	103.44
1	A	1514	LYS	CA-C-O	-6.01	111.92	120.51
36	Q	944	TRP	CA-C-O	-6.00	111.92	120.51
1	A	771	VAL	CA-C-O	-6.00	114.71	120.95
7	L	214	ILE	N-CA-C	-5.99	102.43	108.96
14	T	342	GLU	CB-CA-C	5.99	121.97	110.17
36	Q	933	GLY	CA-C-O	-5.99	114.58	120.75
34	u	178	THR	N-CA-C	5.99	120.71	113.17
38	p	89	ASP	CA-CB-CG	5.98	118.58	112.60
37	o	75	ARG	N-CA-CB	-5.98	102.66	111.51
14	T	213	GLU	N-CA-CB	-5.98	100.59	109.98
31	g	67	ILE	CB-CA-C	-5.96	104.80	111.23
36	Q	942	SER	CA-C-N	-5.95	111.43	121.18
36	Q	942	SER	C-N-CA	-5.95	111.43	121.18
7	L	134	THR	N-CA-C	5.94	117.84	111.36
31	n	67	ILE	CB-CA-C	-5.94	104.81	111.23
23	I	481	TYR	N-CA-C	5.94	118.71	111.82
12	R	320	HIS	CA-CB-CG	-5.94	107.86	113.80
1	A	202	PRO	CB-CA-C	-5.92	102.34	112.64
12	R	217	LYS	CB-CA-C	-5.92	98.98	109.70
22	X	98	GLU	CB-CA-C	-5.92	100.97	110.79
15	U	83	GLU	CA-C-N	5.91	132.83	121.54
15	U	83	GLU	C-N-CA	5.91	132.83	121.54
38	p	46	MET	N-CA-C	-5.90	104.76	111.07
37	o	27	ARG	CB-CA-C	-5.89	98.69	109.54
20	H	163	G	O3'-P-O5'	-5.89	95.17	104.00
23	I	726	ILE	CA-C-O	-5.89	114.61	120.85
1	A	1556	ASP	CA-C-O	-5.88	114.65	120.82
22	X	106	GLU	CA-C-O	-5.87	113.72	120.24
37	o	123	ASN	OD1-CG-ND2	5.87	128.47	122.60
5	G	125	C	P-O3'-C3'	5.87	129.00	120.20
1	A	1094	ARG	CB-CA-C	-5.86	97.66	109.68
1	A	1255	THR	CA-CB-OG1	-5.85	100.82	109.60
36	Q	943	ARG	CA-C-N	-5.85	110.37	121.54
36	Q	943	ARG	C-N-CA	-5.85	110.37	121.54
5	G	122	U	C1'-C2'-O2'	5.85	117.17	108.40
14	T	409	LEU	CA-C-O	-5.84	114.46	120.54
6	J	413	GLU	N-CA-C	5.84	118.12	111.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	419	PHE	CA-CB-CG	5.83	119.64	113.80
6	J	244	ASN	CA-CB-CG	-5.82	106.78	112.60
1	A	203	VAL	CA-C-O	-5.80	113.53	120.78
37	o	50	SER	CA-C-O	5.80	127.70	121.55
1	A	1509	PHE	N-CA-C	5.78	117.25	111.07
36	Q	930	GLU	CA-C-N	5.77	129.83	120.60
36	Q	930	GLU	C-N-CA	5.77	129.83	120.60
1	A	773	LYS	CA-C-O	-5.77	114.44	120.55
19	F	73	A	C2'-C3'-O3'	-5.75	100.87	109.50
1	A	1920	TYR	CA-C-N	5.74	130.32	121.19
1	A	1920	TYR	C-N-CA	5.74	130.32	121.19
34	u	336	VAL	N-CA-C	-5.74	104.00	112.04
23	I	457	ARG	N-CA-C	5.72	117.20	111.07
5	G	122	U	C2'-C3'-O3'	5.71	122.27	113.70
1	A	1093	ASP	CA-C-O	-5.71	112.96	119.41
5	G	121	C	C3'-C2'-O2'	5.71	119.26	110.70
17	W	317	GLU	CA-C-N	5.71	127.96	120.60
17	W	317	GLU	C-N-CA	5.71	127.96	120.60
19	F	50	A	C1'-C2'-O2'	5.70	116.94	108.40
20	H	164	C	P-O3'-C3'	5.67	128.70	120.20
37	o	27	ARG	CA-C-N	5.67	128.67	120.11
37	o	27	ARG	C-N-CA	5.67	128.67	120.11
2	C	801	LEU	CA-C-N	5.66	127.87	120.28
2	C	801	LEU	C-N-CA	5.66	127.87	120.28
32	v	114	LYS	N-CA-C	-5.66	100.45	109.96
1	A	1553	VAL	CA-C-O	-5.66	114.50	120.39
37	o	71	VAL	O-C-N	-5.66	115.50	122.57
1	A	1256	PHE	CA-CB-CG	-5.64	108.16	113.80
21	i	52	LYS	CA-C-N	-5.64	114.12	119.76
21	i	52	LYS	C-N-CA	-5.64	114.12	119.76
12	R	219	PRO	CA-C-O	-5.63	114.92	121.34
37	o	149	LYS	CB-CA-C	-5.63	102.05	110.16
14	T	407	GLN	CA-C-N	-5.62	112.69	122.37
14	T	407	GLN	C-N-CA	-5.62	112.69	122.37
5	G	120	G	P-O3'-C3'	5.62	128.63	120.20
5	G	127	G	C2'-C3'-O3'	-5.62	105.27	113.70
25	Y	418	ASP	CA-C-N	-5.61	115.14	123.11
25	Y	418	ASP	C-N-CA	-5.61	115.14	123.11
1	A	1054	GLY	N-CA-C	-5.61	106.01	112.29
11	P	9	PHE	CA-C-N	-5.61	116.27	123.16
11	P	9	PHE	C-N-CA	-5.61	116.27	123.16
9	N	33	GLU	CB-CA-C	-5.60	100.41	110.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	350	PHE	CA-CB-CG	-5.59	108.21	113.80
36	Q	525	PRO	N-CA-C	-5.58	100.96	112.47
9	N	42	LYS	CA-C-N	5.58	132.02	121.97
9	N	42	LYS	C-N-CA	5.58	132.02	121.97
19	F	73	A	C3'-C2'-O2'	5.58	122.97	114.60
7	L	7	LYS	CA-C-N	5.57	130.41	121.17
7	L	7	LYS	C-N-CA	5.57	130.41	121.17
20	H	157	G	P-O5'-C5'	-5.56	112.56	120.90
14	T	325	THR	CA-CB-OG1	-5.55	101.27	109.60
34	u	384	ASP	N-CA-C	5.55	117.77	111.11
37	o	159	GLU	N-CA-C	-5.54	104.88	111.69
7	L	9	GLY	O-C-N	5.54	129.32	122.78
37	o	16	THR	O-C-N	5.54	129.53	123.22
17	W	74	PRO	N-CA-CB	-5.53	97.44	103.25
2	C	560	VAL	CA-C-N	5.53	129.98	121.19
2	C	560	VAL	C-N-CA	5.53	129.98	121.19
20	H	165	A	N9-C1'-C2'	5.53	120.29	112.00
1	A	1472	THR	CA-CB-OG1	-5.52	101.31	109.60
11	P	12	ALA	CA-C-O	-5.52	115.70	121.55
37	o	34	ILE	CA-C-O	-5.52	114.22	120.74
36	Q	93	SER	N-CA-CB	5.52	118.84	110.28
20	H	168	A	O4'-C1'-C2'	-5.51	102.09	107.60
37	o	32	PRO	CA-C-N	5.51	130.65	122.99
37	o	32	PRO	C-N-CA	5.51	130.65	122.99
21	i	5	LYS	N-CA-C	5.50	118.20	111.82
25	Y	680	ALA	N-CA-C	-5.50	104.81	112.45
21	b	5	LYS	N-CA-C	5.50	118.19	111.82
20	H	160	A	P-O5'-C5'	-5.49	112.66	120.90
25	Y	688	HIS	CA-C-N	5.49	130.51	122.39
25	Y	688	HIS	C-N-CA	5.49	130.51	122.39
1	A	1552	GLN	CA-C-N	-5.48	115.81	123.10
1	A	1552	GLN	C-N-CA	-5.48	115.81	123.10
14	T	407	GLN	CB-CA-C	-5.48	99.52	110.42
36	Q	940	VAL	CA-C-O	-5.48	115.36	121.17
1	A	1465	TRP	CA-C-N	-5.47	115.34	123.11
1	A	1465	TRP	C-N-CA	-5.47	115.34	123.11
36	Q	935	PHE	CA-C-N	-5.47	113.33	120.44
36	Q	935	PHE	C-N-CA	-5.47	113.33	120.44
14	T	406	ILE	CA-C-O	-5.47	115.05	120.85
1	A	663	ARG	CA-C-O	-5.46	115.04	121.16
37	o	40	THR	N-CA-C	-5.46	106.12	112.89
21	b	52	LYS	CA-C-N	-5.46	114.30	119.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	b	52	LYS	C-N-CA	-5.46	114.30	119.76
37	o	132	ARG	CD-NE-CZ	5.46	132.04	124.40
2	C	753	GLU	N-CA-CB	5.45	118.78	110.44
25	Y	1183	VAL	N-CA-C	5.45	114.21	106.53
25	Y	419	PHE	CB-CA-C	5.45	119.67	110.79
12	R	130	PRO	CA-C-N	5.44	127.57	120.28
12	R	130	PRO	C-N-CA	5.44	127.57	120.28
33	w	115	GLY	N-CA-C	5.44	126.07	113.18
1	A	1503	TRP	CA-C-N	-5.42	115.46	123.05
1	A	1503	TRP	C-N-CA	-5.42	115.46	123.05
2	C	534	VAL	N-CA-C	-5.42	101.91	109.45
12	R	303	GLU	CB-CA-C	5.42	121.07	110.67
1	A	196	ASP	CA-C-O	-5.42	115.22	119.66
17	W	204	ASP	CA-C-N	5.41	130.23	121.95
17	W	204	ASP	C-N-CA	5.41	130.23	121.95
12	R	304	MET	CB-CG-SD	-5.39	96.53	112.70
14	T	389	SER	CA-C-N	-5.37	118.48	122.18
14	T	389	SER	C-N-CA	-5.37	118.48	122.18
3	E	192	ASN	O-C-N	5.37	128.27	122.15
36	Q	999	ARG	CA-C-N	5.37	127.47	120.28
36	Q	999	ARG	C-N-CA	5.37	127.47	120.28
17	W	266	ARG	CA-C-N	5.36	128.46	120.90
17	W	266	ARG	C-N-CA	5.36	128.46	120.90
25	Y	975	ARG	CA-C-N	5.36	127.40	120.44
25	Y	975	ARG	C-N-CA	5.36	127.40	120.44
1	A	1496	PRO	N-CA-CB	-5.35	97.44	103.33
6	J	356	TYR	CA-C-N	-5.34	111.33	121.54
6	J	356	TYR	C-N-CA	-5.34	111.33	121.54
38	p	25	ARG	CD-NE-CZ	5.34	131.88	124.40
1	A	1556	ASP	CA-C-N	-5.33	114.16	122.37
1	A	1556	ASP	C-N-CA	-5.33	114.16	122.37
21	b	65	ARG	CB-CG-CD	5.33	123.57	111.30
4	4	-13	C	C4'-C3'-O3'	5.33	117.40	109.40
25	Y	841	ILE	N-CA-CB	5.33	117.79	110.54
10	O	30	GLU	CA-C-N	-5.33	114.20	121.61
10	O	30	GLU	C-N-CA	-5.33	114.20	121.61
21	i	65	ARG	CB-CG-CD	5.33	123.55	111.30
2	C	515	THR	CA-C-N	5.32	127.73	120.54
2	C	515	THR	C-N-CA	5.32	127.73	120.54
22	X	76	LYS	CB-CA-C	-5.32	101.81	110.85
25	Y	1169	ASP	N-CA-C	-5.32	100.95	109.04
37	o	146	ASP	CA-C-N	5.32	130.11	122.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	o	146	ASP	C-N-CA	5.32	130.11	122.40
39	s	54	ASP	N-CA-CB	-5.32	102.22	110.46
1	A	192	GLN	CB-CA-C	-5.31	102.19	110.74
2	C	824	THR	N-CA-C	5.31	123.40	112.40
9	N	34	THR	CA-CB-OG1	-5.30	101.64	109.60
37	o	33	VAL	N-CA-CB	-5.30	103.77	111.52
37	o	125	VAL	CA-C-N	5.30	127.92	120.28
37	o	125	VAL	C-N-CA	5.30	127.92	120.28
1	A	941	LYS	CA-C-O	-5.30	115.45	121.28
38	p	6	ASN	N-CA-CB	-5.30	101.67	111.53
36	Q	934	TYR	N-CA-CB	5.28	119.42	110.49
13	S	130	GLY	N-CA-C	5.28	118.83	110.96
9	N	42	LYS	O-C-N	5.27	129.35	122.87
14	T	189	GLN	CB-CA-C	5.27	121.01	111.06
1	A	1319	PRO	CA-C-O	-5.26	115.35	122.08
22	X	68	GLU	CA-C-N	-5.24	113.31	120.44
22	X	68	GLU	C-N-CA	-5.24	113.31	120.44
37	o	113	LYS	N-CA-C	5.24	118.46	111.75
14	T	403	GLY	CA-C-O	-5.24	116.80	121.41
20	H	171	U	C2'-C3'-O3'	-5.24	105.84	113.70
38	p	20	LYS	N-CA-C	5.23	117.39	111.11
23	I	668	CYS	N-CA-C	-5.22	105.27	111.69
37	o	88	PRO	CB-CA-C	-5.22	104.01	112.62
7	L	52	GLU	N-CA-C	5.21	117.04	111.36
34	u	163	THR	N-CA-C	-5.21	103.62	110.39
14	T	324	HIS	CB-CA-C	-5.21	99.26	110.45
23	I	727	ARG	O-C-N	5.21	127.64	122.12
20	H	156	U	C4'-C3'-C2'	5.20	107.80	102.60
2	C	359	LYS	CA-CB-CG	5.19	124.48	114.10
1	A	1095	ILE	N-CA-CB	-5.19	104.25	111.41
23	I	231	ASN	O-C-N	5.18	125.09	120.48
25	Y	1052	TRP	CA-C-N	5.18	127.17	120.44
25	Y	1052	TRP	C-N-CA	5.18	127.17	120.44
38	p	68	GLN	OE1-CD-NE2	5.18	127.78	122.60
33	w	148	TRP	N-CA-C	-5.18	103.20	110.50
22	X	96	GLN	CB-CG-CD	-5.17	103.80	112.60
38	p	51	GLN	N-CA-C	5.17	117.54	109.52
37	o	55	ARG	NE-CZ-NH2	-5.17	114.55	119.20
34	u	367	ARG	N-CA-C	-5.17	106.24	112.54
1	A	1462	GLY	CA-C-N	-5.16	115.88	123.00
1	A	1462	GLY	C-N-CA	-5.16	115.88	123.00
1	A	1513	MET	CA-C-N	-5.16	111.68	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1513	MET	C-N-CA	-5.16	111.68	121.54
37	o	83	LEU	N-CA-C	5.16	117.57	111.33
11	P	7	PRO	N-CA-C	5.16	123.09	112.47
9	N	43	VAL	N-CA-CB	5.15	119.72	111.23
25	Y	619	ARG	CA-C-N	5.15	127.49	120.54
25	Y	619	ARG	C-N-CA	5.15	127.49	120.54
37	o	90	LEU	CA-C-O	-5.15	113.15	120.51
38	p	48	MET	N-CA-C	5.14	119.56	113.28
23	I	22	LEU	O-C-N	5.13	125.04	120.48
34	u	342	ASP	N-CA-C	5.13	117.07	107.99
12	R	126	ASN	CB-CA-C	-5.12	110.69	116.63
28	d	88	LYS	CG-CD-CE	-5.12	99.52	111.30
18	B	21	A	C2'-C3'-O3'	-5.12	106.02	113.70
1	A	1264	ASN	CA-CB-CG	-5.12	107.48	112.60
5	G	121	C	C4'-C3'-C2'	5.11	107.71	102.60
20	H	22	U	C1'-C2'-O2'	-5.11	100.73	108.40
38	p	36	HIS	CA-CB-CG	-5.11	108.69	113.80
28	k	99	MET	N-CA-C	5.11	116.84	108.76
6	J	239	ARG	CG-CD-NE	-5.11	100.76	112.00
33	w	107	ASP	N-CA-C	-5.10	102.09	109.59
17	W	79	VAL	N-CA-C	5.10	114.12	106.42
34	u	210	PRO	N-CA-C	5.10	121.35	113.75
20	H	160	A	C4'-C3'-C2'	-5.10	97.50	102.60
23	I	487	TRP	N-CA-C	5.10	116.92	111.36
22	X	57	ARG	N-CA-C	-5.10	105.62	111.07
14	T	495	ALA	N-CA-C	5.09	117.61	111.40
23	I	149	TRP	O-C-N	5.09	125.01	120.48
5	G	125	C	C3'-C2'-O2'	5.08	122.23	114.60
1	A	197	PRO	CB-CA-C	-5.08	104.23	112.62
38	p	83	TYR	CA-C-O	-5.08	115.26	121.05
25	Y	417	PRO	CA-C-N	-5.08	115.60	123.17
25	Y	417	PRO	C-N-CA	-5.08	115.60	123.17
37	o	90	LEU	O-C-N	5.07	129.34	122.59
28	d	99	MET	N-CA-C	5.06	116.76	108.76
36	Q	100	GLU	CA-C-N	-5.06	111.92	120.58
36	Q	100	GLU	C-N-CA	-5.06	111.92	120.58
5	G	1	G	C3'-C2'-O2'	5.06	122.19	114.60
30	e	85	THR	N-CA-C	-5.06	105.95	112.68
12	R	181	PRO	N-CA-C	5.06	120.42	113.84
8	M	124	PHE	CA-C-N	5.06	129.23	121.19
8	M	124	PHE	C-N-CA	5.06	129.23	121.19
20	H	155	C	P-O3'-C3'	5.06	127.78	120.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	38	GLU	CB-CA-C	5.05	118.76	109.46
2	C	753	GLU	CA-C-N	5.05	128.45	120.47
2	C	753	GLU	C-N-CA	5.05	128.45	120.47
1	A	847	LYS	CB-CA-C	-5.05	102.27	110.85
12	R	304	MET	CB-CA-C	-5.05	102.93	110.90
37	o	139	VAL	CA-C-N	5.05	124.71	119.56
37	o	139	VAL	C-N-CA	5.05	124.71	119.56
20	H	160	A	N9-C1'-C2'	5.04	119.57	112.00
23	I	444	LEU	O-C-N	5.04	127.26	122.07
37	o	28	GLY	N-CA-C	5.03	120.83	113.48
5	G	122	U	N1-C1'-C2'	-5.03	104.45	112.00
23	I	89	ASP	O-C-N	5.03	124.96	120.48
32	v	141	PHE	N-CA-C	5.03	120.06	113.88
1	A	1258	LYS	CA-C-O	-5.02	115.23	120.55
20	H	170	C	O4'-C1'-C2'	-5.02	100.78	105.80
36	Q	935	PHE	N-CA-C	-5.02	106.75	112.92
1	A	1460	HIS	N-CA-CB	5.02	118.51	110.73
12	R	70	ALA	CA-C-N	5.02	128.79	121.31
12	R	70	ALA	C-N-CA	5.02	128.79	121.31
6	J	242	ILE	CA-C-O	-5.01	113.97	120.03
6	J	201	ARG	CA-C-N	5.01	129.47	122.36
6	J	201	ARG	C-N-CA	5.01	129.47	122.36
1	A	1831	LYS	N-CA-C	5.01	121.46	110.80
37	o	99	SER	N-CA-CB	-5.01	102.96	111.17
14	T	190	TRP	CA-C-O	-5.00	115.94	122.14
1	A	1505	LYS	CB-CA-C	5.00	117.70	109.90

There are no chirality outliers.

All (45) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1019	TYR	Peptide
1	A	1201	ARG	Peptide
1	A	1210	LYS	Peptide
1	A	1338	SER	Peptide
1	A	1507	SER	Mainchain
1	A	1686	ASP	Peptide
1	A	186	GLU	Mainchain
1	A	1879	PHE	Peptide
1	A	196	ASP	Mainchain
1	A	377	GLU	Peptide
1	A	385	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	A	55	ASP	Peptide
1	A	698	PRO	Peptide
1	A	73	HIS	Peptide
1	A	775	ASN	Sidechain
2	C	308	CYS	Peptide
2	C	358	LYS	Peptide
2	C	360	ALA	Peptide
2	C	534	VAL	Peptide
2	C	902	HIS	Peptide
23	I	309	ALA	Mainchain
23	I	310	LYS	Mainchain
23	I	311	MET	Mainchain
23	I	83	LYS	Mainchain
23	I	84	HIS	Mainchain
6	J	215	THR	Peptide
6	J	216	ASP	Peptide
6	J	237	LYS	Mainchain
9	N	136	HIS	Peptide
9	N	3	LYS	Peptide
9	N	4	VAL	Peptide
10	O	63	MET	Peptide
11	P	204	GLN	Peptide
11	P	30	TYR	Peptide
11	P	48	GLN	Peptide
36	Q	90	TYR	Mainchain
12	R	183	GLN	Peptide
12	R	185	GLY	Peptide
12	R	212	PHE	Peptide
12	R	303	GLU	Mainchain
12	R	66	GLU	Peptide
12	R	94	GLY	Peptide
17	W	518	PRO	Peptide
28	d	112	ASN	Peptide
28	k	112	ASN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16449	0	16375	659	0
2	C	6798	0	6815	184	0
3	E	2338	0	2275	81	0
4	4	276	0	142	16	0
5	G	1510	0	760	206	0
6	J	3814	0	2902	58	0
7	L	3015	0	2570	92	0
8	M	1098	0	1082	32	0
9	N	1184	0	1190	31	0
10	O	2296	0	2284	75	0
11	P	953	0	939	46	0
12	R	2243	0	2298	86	0
13	S	1236	0	1210	42	0
14	T	2454	0	2413	149	0
15	U	422	0	291	13	0
16	V	2632	0	1734	21	0
17	W	4129	0	4040	133	0
18	B	1768	0	897	66	0
19	F	2075	0	1048	182	0
20	H	2966	0	1505	279	0
21	b	786	0	811	48	0
21	i	690	0	712	15	0
22	X	616	0	605	140	0
23	I	3845	0	2729	192	0
24	y	390	0	190	12	0
25	Y	3431	0	1662	47	0
26	a	640	0	657	15	0
26	h	633	0	645	15	0
27	c	649	0	693	10	0
27	j	649	0	693	13	0
28	d	776	0	819	32	0
28	k	688	0	709	29	0
29	f	576	0	589	21	0
29	m	576	0	589	22	0
30	e	652	0	668	20	0
30	l	644	0	659	23	0
31	g	577	0	603	15	0
31	n	538	0	557	25	0
32	v	711	0	299	6	0
33	w	445	0	203	6	0
34	u	1907	0	845	5	0
35	x	124	0	51	0	0
36	Q	6562	0	2836	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
37	o	1282	0	1305	28	0
38	p	760	0	783	12	0
39	q	659	0	296	19	0
39	r	654	0	294	8	0
39	s	659	0	296	20	0
39	t	654	0	294	10	0
40	K	772	0	342	11	0
41	A	36	0	6	9	0
42	C	32	0	12	2	0
43	C	1	0	0	0	0
43	F	6	0	0	0	0
43	Q	2	0	0	0	0
44	N	3	0	0	0	0
44	O	3	0	0	0	0
45	Q	31	0	12	5	0
All	All	92315	0	75234	2699	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 16.

All (2699) 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)
23:I:265:TYR:CB	23:I:274:LYS:CB	1.84	1.53
36:Q:943:ARG:CB	36:Q:969:PRO:CB	1.82	1.53
36:Q:525:PRO:N	36:Q:525:PRO:CA	1.67	1.52
1:A:345:PRO:N	1:A:345:PRO:CA	1.68	1.46
14:T:297:HIS:CE1	14:T:340:ALA:HB2	1.51	1.45
1:A:1045:GLY:HA3	1:A:1090:ARG:NH2	1.35	1.38
5:G:82:G:H4'	17:W:541:LYS:NZ	1.40	1.32
1:A:856:LEU:O	1:A:860:GLN:HB2	1.25	1.31
14:T:188:PRO:HB3	14:T:440:ASP:OD2	1.13	1.31
23:I:273:GLU:HA	36:Q:357:ALA:CB	1.63	1.28
1:A:857:ASN:O	1:A:861:ARG:CD	1.81	1.26
1:A:1515:TRP:CB	20:H:30:A:C4	2.18	1.26
5:G:73:G:O2'	5:G:74:G:O4'	1.54	1.25
1:A:857:ASN:C	1:A:861:ARG:HD3	1.61	1.25
1:A:1501:LEU:HD12	1:A:1753:LEU:CD1	1.66	1.25
23:I:704:TRP:CZ3	23:I:727:ARG:HG3	1.71	1.25
1:A:858:GLN:CA	1:A:861:ARG:HD3	1.66	1.25
36:Q:801:GLN:O	45:Q:1501:ATP:N6	1.66	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:I:696:ASP:OD1	23:I:697:PRO:HD2	1.26	1.25
20:H:79:G:C5'	24:y:40:ASP:CB	2.15	1.24
22:X:100:ILE:O	22:X:103:GLN:HB2	1.24	1.24
17:W:83:PRO:HB3	17:W:87:THR:OG1	1.34	1.23
2:C:852:ARG:NH2	4:4:-13:C:H2'	1.50	1.22
1:A:534:GLU:OE2	19:F:38:G:OP1	1.58	1.22
3:E:266:PRO:HG2	7:L:785:GLN:CB	1.71	1.21
14:T:185:MET:HG3	14:T:186:PRO:CD	1.69	1.21
1:A:858:GLN:O	1:A:861:ARG:HG2	1.39	1.21
1:A:584:HIS:HE1	41:A:3000:IHP:O26	1.21	1.20
14:T:185:MET:CG	14:T:186:PRO:HD3	1.72	1.20
1:A:537:LYS:HD2	19:F:37:C:N4	1.54	1.20
1:A:857:ASN:O	1:A:861:ARG:HD2	1.34	1.20
17:W:73:ASP:OD2	17:W:74:PRO:HD2	1.38	1.19
25:Y:413:LYS:O	25:Y:419:PHE:HD1	1.24	1.18
6:J:237:LYS:NZ	19:F:79:C:OP2	1.76	1.17
1:A:2001:SER:OG	22:X:54:LEU:HD21	1.44	1.17
7:L:174:LYS:NZ	19:F:80:G:OP1	1.77	1.16
2:C:68:THR:OG1	2:C:71:GLU:HB2	1.45	1.16
14:T:213:GLU:HG3	14:T:218:TRP:CE2	1.80	1.16
36:Q:801:GLN:C	45:Q:1501:ATP:HN62	1.53	1.16
5:G:21:A:O2'	5:G:22:C:O5'	1.64	1.15
1:A:1515:TRP:CB	20:H:30:A:C5	2.28	1.15
23:I:273:GLU:CA	36:Q:357:ALA:HB2	1.77	1.15
1:A:1135:PRO:HD2	1:A:1138:ALA:HB3	1.24	1.14
7:L:4:ILE:HD11	22:X:78:MET:HE3	1.26	1.14
23:I:286:VAL:O	23:I:351:ARG:CB	1.95	1.14
5:G:21:A:CI'	10:O:152:ARG:NH2	2.11	1.14
17:W:259:GLN:OE1	31:n:13:MET:HG3	1.46	1.13
20:H:154:C:OP2	38:p:19:LYS:HG2	1.49	1.13
1:A:1565:LYS:O	1:A:1567:PRO:HD3	1.49	1.13
14:T:188:PRO:CB	14:T:440:ASP:OD2	1.97	1.12
23:I:71:TRP:CB	24:y:29:PHE:O	1.98	1.12
14:T:188:PRO:HG3	14:T:443:THR:OG1	1.47	1.11
20:H:79:G:H5'	24:y:40:ASP:CB	1.78	1.11
23:I:273:GLU:HA	36:Q:357:ALA:HB2	1.11	1.11
20:H:36:G:H2'	20:H:37:U:H5'	1.31	1.11
1:A:861:ARG:HB3	1:A:861:ARG:HH11	1.16	1.11
1:A:584:HIS:CE1	41:A:3000:IHP:O26	2.02	1.10
7:L:129:ASP:OD2	7:L:130:PRO:HD2	1.51	1.10
7:L:65:ARG:NH2	23:I:721:LYS:NZ	2.00	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:LYS:HE2	5:G:126:G:O2'	1.47	1.10
3:E:93:TRP:HZ3	21:b:105:GLY:O	1.33	1.10
20:H:79:G:H5''	24:y:40:ASP:CB	1.80	1.10
1:A:1554:GLN:HA	1:A:1561:PHE:HB3	1.16	1.09
14:T:455:GLN:HG2	14:T:456:PRO:HD2	1.14	1.09
36:Q:801:GLN:C	45:Q:1501:ATP:N6	2.08	1.09
5:G:2:U:O2	19:F:45:A:N6	1.85	1.09
11:P:212:ASN:HB3	14:T:458:SER:N	1.67	1.09
20:H:36:G:C2'	20:H:37:U:H5'	1.83	1.09
23:I:84:HIS:CB	23:I:90:PRO:HA	1.82	1.09
23:I:681:ILE:HG23	23:I:710:PHE:CZ	1.88	1.08
20:H:168:A:H1'	31:n:48:MET:HE1	1.19	1.08
1:A:858:GLN:HA	1:A:861:ARG:HD3	1.33	1.08
5:G:21:A:H1'	10:O:152:ARG:HH21	1.05	1.08
1:A:1501:LEU:HD12	1:A:1753:LEU:HD11	1.14	1.08
19:F:34:G:H2'	19:F:35:A:H5''	1.30	1.08
19:F:39:A:C2'	19:F:40:U:H5'	1.82	1.08
20:H:156:U:H6	20:H:156:U:H5''	1.10	1.08
1:A:858:GLN:N	1:A:861:ARG:HD3	1.69	1.07
1:A:1793:THR:HG21	19:F:43:A:H5''	1.36	1.07
23:I:175:LEU:CB	23:I:179:SER:CB	2.33	1.07
1:A:361:HIS:HE1	16:V:324:HIS:HA	1.20	1.07
5:G:21:A:OP2	10:O:193:LEU:HD21	1.51	1.07
1:A:857:ASN:C	1:A:861:ARG:CD	2.26	1.06
20:H:105:G:H2'	20:H:106:G:H5''	1.37	1.06
1:A:166:PHE:HB3	1:A:167:PRO:HD2	1.11	1.06
1:A:1468:ASN:OD1	5:G:130:G:C5'	2.04	1.06
1:A:191:ILE:HG22	1:A:572:PHE:CZ	1.90	1.06
3:E:59:ILE:HD11	17:W:82:ASN:HD21	1.10	1.05
17:W:79:VAL:HG21	21:b:114:ILE:HD11	1.05	1.04
39:q:60:PRO:CB	39:s:93:ARG:C	2.30	1.04
1:A:195:LEU:H	1:A:195:LEU:HD12	1.23	1.03
14:T:297:HIS:HE1	14:T:340:ALA:HB2	1.23	1.03
39:s:71:ILE:CB	39:t:81:GLU:CB	2.36	1.03
20:H:40:C:H4'	20:H:41:U:OP1	1.56	1.03
5:G:100:C:H2'	5:G:101:U:C6	1.93	1.02
1:A:1501:LEU:CD1	1:A:1753:LEU:CD1	2.38	1.02
20:H:30:A:H1'	22:X:73:PHE:CE1	1.94	1.02
23:I:187:LEU:HA	23:I:196:ALA:HB1	1.38	1.02
20:H:39:U:H6	20:H:39:U:H5''	1.23	1.01
1:A:1468:ASN:OD1	5:G:130:G:H5'	1.61	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:30:A:H1'	22:X:73:PHE:HE1	1.23	1.01
19:F:86:U:O2'	19:F:87:C:O5'	1.78	1.01
7:L:124:LYS:CE	7:L:129:ASP:OD2	2.08	1.01
1:A:1495:PHE:HE2	1:A:1748:ARG:NE	1.59	1.01
11:P:3:THR:CG2	19:F:79:C:C2	2.44	1.01
12:R:317:LYS:HA	12:R:317:LYS:NZ	1.76	1.01
39:s:112:ALA:O	40:K:15:ALA:HB1	1.60	1.01
3:E:192:ASN:HD22	3:E:196:VAL:HG22	1.24	1.00
2:C:68:THR:OG1	2:C:71:GLU:CB	2.10	1.00
25:Y:413:LYS:O	25:Y:419:PHE:CD1	2.14	1.00
1:A:1468:ASN:CG	5:G:130:G:H5'	1.87	1.00
5:G:91:A:C2	20:H:39:U:O2	2.14	1.00
14:T:455:GLN:HG2	14:T:456:PRO:CD	1.91	1.00
14:T:297:HIS:CE1	14:T:340:ALA:CB	2.43	1.00
19:F:8:C:H6	19:F:8:C:H5''	1.23	1.00
1:A:106:MET:HE3	1:A:561:HIS:NE2	1.76	1.00
1:A:887:THR:HB	7:L:122:LYS:HE2	1.43	1.00
1:A:856:LEU:O	1:A:860:GLN:CB	2.10	0.99
1:A:1997:VAL:HG13	22:X:54:LEU:CD2	1.90	0.99
12:R:332:ARG:HG2	12:R:332:ARG:HH11	1.19	0.99
17:W:79:VAL:CG2	21:b:114:ILE:HD11	1.92	0.99
1:A:1997:VAL:CG1	22:X:54:LEU:CD2	2.41	0.99
23:I:704:TRP:CE3	23:I:727:ARG:HG3	1.97	0.99
1:A:2001:SER:OG	22:X:54:LEU:CD2	2.10	0.99
23:I:691:CYS:SG	23:I:694:ILE:CG2	2.50	0.99
1:A:1386:TRP:HB3	25:Y:410:VAL:CG2	1.92	0.99
17:W:79:VAL:HG21	21:b:114:ILE:CD1	1.93	0.98
1:A:1045:GLY:CA	1:A:1090:ARG:NH2	2.26	0.98
20:H:168:A:H5''	20:H:168:A:C8	1.98	0.98
5:G:20:A:HO2'	10:O:193:LEU:HD21	1.22	0.98
5:G:6:A:N1	19:F:41:A:N1	2.11	0.98
32:v:29:ASP:CB	33:w:154:PRO:CB	2.42	0.98
1:A:858:GLN:HA	1:A:861:ARG:CD	1.93	0.98
5:G:21:A:H1'	10:O:152:ARG:NH2	1.73	0.98
5:G:21:A:H4'	5:G:22:C:OP1	1.60	0.98
17:W:72:LEU:HD23	17:W:83:PRO:HG3	1.42	0.98
19:F:34:G:C2'	19:F:35:A:H5''	1.94	0.97
1:A:361:HIS:CE1	16:V:324:HIS:HA	1.98	0.97
1:A:1418:ARG:HH12	1:A:1464:LEU:HA	1.27	0.97
20:H:40:C:O2'	20:H:41:U:H5''	1.64	0.97
17:W:83:PRO:HB3	17:W:87:THR:HG1	1.19	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:21:A:N9	10:O:152:ARG:NH2	2.11	0.97
1:A:1318:THR:CG2	1:A:1324:GLY:HA3	1.94	0.96
2:C:673:LYS:NZ	15:U:56:ASP:CB	2.28	0.96
2:C:852:ARG:NH2	4:4:-13:C:C6	2.32	0.96
1:A:1456:THR:OG1	1:A:1461:ASP:OD2	1.81	0.96
5:G:95:U:O2'	5:G:96:U:H5'	1.64	0.96
14:T:213:GLU:HG3	14:T:218:TRP:CZ2	2.01	0.96
1:A:1554:GLN:HA	1:A:1561:PHE:CB	1.95	0.95
5:G:82:G:H4'	17:W:541:LYS:HZ3	0.96	0.95
19:F:39:A:H2'	19:F:40:U:H5'	1.46	0.95
1:A:1833:LEU:HD22	1:A:1833:LEU:H	1.28	0.95
39:q:60:PRO:C	39:s:93:ARG:CB	2.39	0.95
1:A:1386:TRP:HB3	25:Y:410:VAL:HG21	1.47	0.95
7:L:65:ARG:NH2	23:I:721:LYS:HZ1	1.58	0.95
20:H:156:U:H5''	20:H:156:U:C6	2.02	0.95
1:A:191:ILE:CG2	1:A:572:PHE:CE1	2.50	0.94
3:E:93:TRP:CZ3	21:b:105:GLY:O	2.20	0.94
7:L:124:LYS:HE2	7:L:129:ASP:OD2	1.68	0.94
1:A:166:PHE:HB3	1:A:167:PRO:CD	1.98	0.94
5:G:120:G:H5'	5:G:120:G:H8	1.33	0.94
23:I:661:ASP:HB2	23:I:694:ILE:HD11	1.50	0.94
1:A:1997:VAL:CG1	22:X:54:LEU:HD23	1.97	0.93
18:B:95:G:H5'	29:f:25:TRP:HH2	1.28	0.93
1:A:537:LYS:CD	19:F:37:C:N4	2.30	0.93
17:W:83:PRO:CB	17:W:87:THR:OG1	2.16	0.93
5:G:20:A:O2'	10:O:193:LEU:HD21	1.68	0.93
1:A:1495:PHE:CE2	1:A:1748:ARG:NE	2.35	0.93
20:H:40:C:O2'	20:H:41:U:C5'	2.16	0.93
5:G:27:U:O2'	5:G:28:A:O5'	1.84	0.93
17:W:264:ASN:HB2	30:l:16:GLN:OE1	1.67	0.93
1:A:861:ARG:HB3	1:A:861:ARG:NH1	1.84	0.92
14:T:216:ASN:OD1	14:T:472:GLN:HB2	1.69	0.92
1:A:1501:LEU:CD1	1:A:1753:LEU:HD13	1.99	0.92
1:A:1494:TYR:HB2	1:A:1744:ARG:HE	1.32	0.92
1:A:1089:CYS:O	1:A:1089:CYS:SG	2.28	0.92
5:G:27:U:C2'	5:G:28:A:O5'	2.15	0.92
23:I:691:CYS:SG	23:I:694:ILE:HG22	2.09	0.92
5:G:100:C:H2'	5:G:101:U:H6	1.29	0.92
1:A:1793:THR:HG21	19:F:43:A:C5'	1.99	0.92
2:C:667:VAL:H	2:C:824:THR:HG23	1.35	0.91
39:s:112:ALA:O	40:K:15:ALA:CB	2.18	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:ARG:NH1	1:A:1464:LEU:HA	1.84	0.91
2:C:666:VAL:HG13	2:C:823:ALA:O	1.70	0.91
20:H:40:C:O2'	20:H:41:U:O4'	1.87	0.91
20:H:30:A:C1'	22:X:73:PHE:HE1	1.83	0.91
17:W:73:ASP:OD2	17:W:74:PRO:CD	2.19	0.91
11:P:3:THR:HG23	19:F:79:C:C2	2.06	0.91
1:A:1471:ARG:HB3	1:A:1471:ARG:HH21	1.34	0.90
22:X:113:LYS:HZ2	22:X:113:LYS:HA	1.36	0.90
20:H:168:A:C1'	31:n:48:MET:HE1	2.00	0.90
20:H:39:U:O2'	20:H:40:C:OP1	1.87	0.90
36:Q:878:ARG:HA	36:Q:1036:ALA:O	1.70	0.90
1:A:1091:TYR:CE1	1:A:1190:CYS:SG	2.63	0.90
2:C:758:LEU:CD2	2:C:798:GLN:HA	2.00	0.90
13:S:72:ARG:HD2	17:W:71:HIS:HB3	1.53	0.90
1:A:613:TYR:HE2	41:A:3000:IHP:O45	1.52	0.90
7:L:5:MET:N	7:L:5:MET:SD	2.45	0.90
5:G:82:G:H4'	17:W:541:LYS:HZ1	1.34	0.90
20:H:168:A:H1'	31:n:48:MET:CE	2.01	0.90
2:C:852:ARG:NH2	4:4:-13:C:C2'	2.34	0.90
1:A:1997:VAL:HG13	22:X:54:LEU:HG	1.53	0.90
12:R:315:LYS:HA	12:R:315:LYS:HZ3	1.34	0.89
1:A:191:ILE:HG21	1:A:572:PHE:CE1	2.06	0.89
11:P:16:ARG:HH12	12:R:220:ARG:HA	1.37	0.89
20:H:168:A:H5''	20:H:168:A:H8	1.37	0.89
23:I:187:LEU:HA	23:I:196:ALA:CB	2.02	0.89
2:C:66:TYR:CD1	14:T:457:GLY:HA2	2.07	0.89
2:C:852:ARG:HH22	4:4:-13:C:H6	1.13	0.89
23:I:696:ASP:OD1	23:I:697:PRO:CD	2.18	0.89
14:T:297:HIS:NE2	14:T:340:ALA:HB2	1.88	0.89
1:A:1135:PRO:HD2	1:A:1138:ALA:CB	2.02	0.89
1:A:940:ILE:CD1	1:A:1090:ARG:NH1	2.36	0.89
2:C:68:THR:HG1	2:C:71:GLU:HB2	1.33	0.89
5:G:95:U:H2'	5:G:96:U:C5	2.07	0.89
5:G:20:A:O2'	5:G:21:A:OP2	1.91	0.89
8:M:133:ARG:HH22	19:F:88:G:H5''	1.37	0.89
11:P:212:ASN:HB3	14:T:458:SER:H	1.31	0.89
5:G:21:A:C1'	10:O:152:ARG:HH21	1.75	0.88
5:G:124:G:N3	5:G:124:G:O2'	2.05	0.88
20:H:39:U:H5''	20:H:39:U:C6	2.07	0.88
1:A:1045:GLY:CA	1:A:1090:ARG:HH22	1.84	0.88
1:A:1471:ARG:HH21	1:A:1471:ARG:CB	1.86	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:I:728:ARG:O	23:I:731:GLN:HB3	1.74	0.88
5:G:100:C:C2	5:G:101:U:C5	2.61	0.88
1:A:537:LYS:HD2	19:F:37:C:H42	1.39	0.88
2:C:852:ARG:CZ	4:4:-13:C:H2'	2.02	0.88
36:Q:849:THR:HA	36:Q:1058:ASN:O	1.73	0.88
23:I:688:TYR:O	23:I:703:PHE:HZ	1.56	0.88
1:A:1494:TYR:CB	1:A:1744:ARG:HE	1.86	0.88
8:M:133:ARG:HH22	19:F:88:G:C5'	1.86	0.88
1:A:1045:GLY:HA3	1:A:1090:ARG:HH22	0.93	0.88
23:I:731:GLN:O	23:I:731:GLN:NE2	2.07	0.88
1:A:1501:LEU:CD1	1:A:1753:LEU:HD11	2.02	0.88
1:A:1136:ARG:HG2	1:A:1136:ARG:HH11	1.35	0.88
18:B:95:G:H5''	28:d:47:ARG:HH22	1.38	0.88
1:A:775:ASN:O	1:A:775:ASN:ND2	2.07	0.87
7:L:4:ILE:CD1	22:X:78:MET:HE3	2.02	0.87
19:F:45:A:O2'	19:F:73:A:N3	2.05	0.87
20:H:154:C:O2	20:H:176:G:N2	2.07	0.87
1:A:1997:VAL:HG13	22:X:54:LEU:CG	2.03	0.87
21:b:46:ASP:OD2	21:b:64:LYS:HE3	1.75	0.87
22:X:72:GLN:NE2	22:X:72:GLN:O	2.08	0.87
1:A:1318:THR:HG22	1:A:1324:GLY:HA3	1.56	0.87
5:G:22:C:O2'	5:G:23:U:OP1	1.91	0.86
5:G:120:G:H5'	5:G:120:G:C8	2.09	0.86
23:I:276:ARG:CB	36:Q:357:ALA:HB3	2.04	0.86
1:A:166:PHE:CB	1:A:167:PRO:HD2	2.04	0.86
3:E:59:ILE:HD11	17:W:82:ASN:ND2	1.88	0.86
20:H:156:U:H6	20:H:156:U:C5'	1.88	0.86
13:S:85:GLU:O	13:S:127:THR:HG23	1.74	0.86
21:i:46:ASP:OD2	21:i:64:LYS:HE3	1.75	0.86
22:X:112:LEU:HD21	23:I:717:GLU:HB3	1.57	0.86
6:J:198:ALA:O	6:J:201:ARG:HB2	1.76	0.85
5:G:99:C:H2'	5:G:100:C:H5''	1.57	0.85
17:W:264:ASN:CB	30:l:16:GLN:OE1	2.24	0.85
19:F:33:G:H5''	19:F:33:G:H8	1.41	0.85
1:A:346:ASP:OD1	1:A:346:ASP:N	2.07	0.85
1:A:1798:LEU:HB2	5:G:96:U:C4'	2.07	0.85
1:A:858:GLN:CA	1:A:861:ARG:CD	2.52	0.85
14:T:385:TYR:CE2	14:T:401:PRO:HD2	2.11	0.85
20:H:98:G:N2	29:m:66:CYS:SG	2.50	0.85
2:C:96:PRO:HB3	14:T:276:GLU:OE2	1.77	0.85
20:H:154:C:OP2	38:p:19:LYS:CG	2.24	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:Q:851:ILE:HA	36:Q:1060:LEU:O	1.76	0.85
1:A:1134:TRP:HB3	1:A:1135:PRO:CD	2.06	0.85
18:B:95:G:H4'	18:B:96:A:O4'	1.77	0.85
13:S:37:LYS:NZ	13:S:37:LYS:HB2	1.92	0.84
23:I:273:GLU:CA	36:Q:357:ALA:CB	2.45	0.84
22:X:62:LYS:HE3	22:X:62:LYS:O	1.78	0.84
1:A:1793:THR:CG2	19:F:43:A:H5''	2.07	0.84
23:I:187:LEU:CA	23:I:196:ALA:HB1	2.08	0.84
1:A:109:PRO:O	1:A:190:ALA:HB1	1.75	0.84
36:Q:820:MET:O	36:Q:1130:THR:HA	1.76	0.84
2:C:85:ASP:OD1	2:C:85:ASP:N	2.08	0.84
12:R:307:GLN:HE21	12:R:307:GLN:HA	1.41	0.84
23:I:691:CYS:SG	23:I:694:ILE:HG21	2.16	0.84
23:I:272:PHE:CB	36:Q:356:VAL:H	1.91	0.84
8:M:221:LYS:NZ	20:H:18:U:OP2	2.10	0.84
14:T:402:ASP:OD1	14:T:402:ASP:N	2.11	0.83
1:A:293:TRP:NE1	1:A:1136:ARG:NH1	2.26	0.83
2:C:750:LEU:HD12	2:C:750:LEU:O	1.78	0.83
18:B:18:C:O2'	18:B:19:A:O5'	1.96	0.83
36:Q:877:LEU:O	36:Q:1036:ALA:N	2.09	0.83
6:J:205:LEU:HD12	6:J:205:LEU:O	1.77	0.83
20:H:152:G:N2	20:H:153:A:N7	2.27	0.83
23:I:84:HIS:CB	23:I:90:PRO:CA	2.56	0.83
23:I:692:SER:HA	23:I:703:PHE:CE2	2.13	0.83
2:C:852:ARG:HH22	4:4:-13:C:H2'	1.18	0.83
14:T:216:ASN:OD1	14:T:472:GLN:CB	2.26	0.83
14:T:400:PHE:HB3	14:T:401:PRO:HD2	1.58	0.83
19:F:8:C:H5''	19:F:8:C:C6	2.11	0.83
2:C:855:GLY:O	2:C:874:PHE:O	1.96	0.83
2:C:751:PRO:HG3	15:U:63:LYS:CB	2.07	0.83
3:E:266:PRO:CG	7:L:785:GLN:CB	2.54	0.83
17:W:259:GLN:OE1	31:n:13:MET:CG	2.26	0.83
11:P:16:ARG:NH1	12:R:220:ARG:HA	1.94	0.83
1:A:194:GLU:N	1:A:194:GLU:OE1	2.10	0.83
20:H:154:C:P	38:p:19:LYS:HD3	2.19	0.83
1:A:1793:THR:CG2	19:F:43:A:C5'	2.57	0.82
3:E:93:TRP:CH2	21:b:105:GLY:CA	2.63	0.82
14:T:197:TYR:CD2	14:T:488:VAL:HG12	2.13	0.82
17:W:233:LYS:HG3	17:W:355:TYR:OH	1.79	0.82
14:T:397:GLN:C	14:T:406:ILE:HG22	2.04	0.82
1:A:361:HIS:HE1	16:V:324:HIS:CA	1.92	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1258:LYS:CE	5:G:126:G:O2'	2.28	0.82
1:A:1135:PRO:O	1:A:1139:ARG:NE	2.12	0.82
20:H:40:C:O2'	20:H:41:U:C6	2.33	0.82
23:I:727:ARG:HH21	23:I:727:ARG:CB	1.92	0.82
1:A:1997:VAL:HG11	22:X:54:LEU:HD23	1.58	0.82
7:L:124:LYS:HE2	7:L:129:ASP:CG	2.04	0.82
17:W:130:ARG:HD3	19:F:22:A:N7	1.94	0.82
2:C:668:GLU:N	2:C:824:THR:HG21	1.94	0.82
23:I:725:ARG:O	23:I:725:ARG:HD2	1.79	0.82
7:L:62:GLU:OE2	22:X:104:ARG:CD	2.28	0.82
23:I:704:TRP:CZ3	23:I:727:ARG:CG	2.62	0.82
7:L:62:GLU:OE2	22:X:104:ARG:HD2	1.79	0.81
1:A:532:THR:OG1	5:G:3:A:O5'	1.98	0.81
1:A:1131:LYS:HD3	1:A:1174:PHE:CE2	2.14	0.81
3:E:192:ASN:ND2	3:E:196:VAL:HG22	1.95	0.81
5:G:82:G:C4'	17:W:541:LYS:HZ3	1.88	0.81
7:L:65:ARG:HH22	23:I:721:LYS:HZ1	1.23	0.81
14:T:342:GLU:HB3	14:T:343:PRO:HD2	1.61	0.81
20:H:105:G:C2'	20:H:106:G:H5''	2.10	0.81
23:I:109:MET:N	24:y:66:ASN:CB	2.43	0.81
39:r:112:ALA:HB1	40:K:36:VAL:O	1.79	0.81
5:G:126:G:H2'	5:G:126:G:N3	1.95	0.81
23:I:697:PRO:HD3	23:I:730:VAL:HG13	1.62	0.81
1:A:1258:LYS:HE2	5:G:126:G:HO2'	1.42	0.81
5:G:82:G:C4'	17:W:541:LYS:NZ	2.35	0.81
19:F:80:G:H5''	19:F:81:C:OP2	1.81	0.81
2:C:751:PRO:CG	15:U:63:LYS:CB	2.58	0.81
12:R:315:LYS:HA	12:R:315:LYS:NZ	1.95	0.81
1:A:188:LEU:HD13	1:A:188:LEU:N	1.96	0.81
12:R:332:ARG:HG2	12:R:332:ARG:NH1	1.92	0.81
1:A:1757:GLU:OE2	1:A:1758:PRO:HD2	1.80	0.81
20:H:40:C:C4'	20:H:41:U:OP1	2.27	0.81
5:G:20:A:C2	10:O:187:THR:OG1	2.33	0.81
5:G:120:G:H3'	5:G:120:G:OP2	1.81	0.81
12:R:131:ASP:OD1	12:R:131:ASP:N	2.14	0.80
1:A:940:ILE:HD11	1:A:1090:ARG:NH1	1.96	0.80
12:R:334:ARG:HB2	12:R:334:ARG:CZ	2.10	0.80
22:X:112:LEU:HD21	23:I:717:GLU:CB	2.11	0.80
6:J:247:LYS:HD2	19:F:83:A:OP2	1.81	0.80
17:W:84:THR:HG22	17:W:86:GLU:H	1.46	0.80
23:I:276:ARG:CB	36:Q:358:GLU:N	2.44	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:39:U:H3'	20:H:40:C:C5	2.16	0.80
14:T:385:TYR:O	14:T:400:PHE:HB2	1.82	0.80
19:F:45:A:N3	19:F:73:A:H1'	1.97	0.80
22:X:113:LYS:HA	22:X:113:LYS:NZ	1.96	0.80
1:A:1322:LEU:N	1:A:1322:LEU:HD23	1.96	0.80
5:G:83:A:O2'	5:G:84:U:OP2	1.99	0.80
22:X:116:ARG:CB	22:X:116:ARG:HH11	1.94	0.80
1:A:191:ILE:HG22	1:A:572:PHE:CE1	2.16	0.80
20:H:152:G:H5''	20:H:153:A:OP2	1.80	0.80
7:L:65:ARG:HH21	23:I:721:LYS:HZ2	1.27	0.80
12:R:325:ARG:O	12:R:325:ARG:HD3	1.82	0.80
6:J:239:ARG:HB2	6:J:239:ARG:HH11	1.46	0.79
23:I:681:ILE:HD13	23:I:714:HIS:HB3	1.63	0.79
2:C:673:LYS:HZ2	15:U:56:ASP:CB	1.92	0.79
20:H:40:C:H2'	20:H:41:U:C6	2.16	0.79
14:T:455:GLN:CG	14:T:456:PRO:HD2	2.05	0.79
20:H:101:U:H5''	20:H:102:U:H5'	1.64	0.79
22:X:96:GLN:HA	22:X:96:GLN:HE21	1.47	0.79
23:I:689:SER:HA	23:I:692:SER:HB3	1.64	0.79
1:A:1091:TYR:HE1	1:A:1190:CYS:SG	2.06	0.79
19:F:86:U:HO2'	19:F:87:C:P	2.03	0.79
14:T:197:TYR:CE2	14:T:488:VAL:HG11	2.18	0.79
1:A:1526:LEU:HD23	1:A:1526:LEU:O	1.81	0.79
1:A:1556:ASP:N	1:A:1556:ASP:OD1	2.14	0.79
23:I:692:SER:HB2	23:I:703:PHE:CZ	2.17	0.79
30:e:20:LEU:HD22	30:e:24:TYR:CE2	2.18	0.79
5:G:4:A:H61	19:F:43:A:H2	1.31	0.79
5:G:120:G:C5	19:F:45:A:N6	2.50	0.79
2:C:276:TYR:CE2	16:V:324:HIS:CB	2.66	0.79
7:L:124:LYS:HE3	7:L:129:ASP:OD2	1.83	0.79
23:I:726:ILE:O	23:I:726:ILE:HD13	1.82	0.79
1:A:1615:HIS:H	1:A:1618:LYS:HE3	1.46	0.78
5:G:21:A:OP2	10:O:193:LEU:CD2	2.30	0.78
23:I:723:MET:HA	23:I:726:ILE:HG22	1.64	0.78
23:I:728:ARG:O	23:I:731:GLN:CB	2.31	0.78
1:A:613:TYR:CE2	41:A:3000:IHP:O45	2.35	0.78
11:P:212:ASN:HB3	14:T:458:SER:CA	2.13	0.78
20:H:153:A:H2'	20:H:154:C:H5'	1.65	0.78
6:J:242:ILE:HG13	6:J:275:ASN:ND2	1.99	0.78
22:X:112:LEU:HD23	23:I:720:ILE:HG21	1.63	0.78
1:A:1275:ARG:NH2	1:A:1464:LEU:O	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:16:G:O2'	19:F:29:A:N6	2.16	0.78
30:l:20:LEU:HD22	30:l:24:TYR:CE2	2.18	0.78
14:T:397:GLN:HB3	14:T:406:ILE:CG2	2.13	0.78
11:P:16:ARG:HH21	11:P:16:ARG:HG3	1.49	0.78
25:Y:418:ASP:N	25:Y:418:ASP:OD1	2.17	0.78
3:E:174:GLY:O	3:E:192:ASN:N	2.16	0.78
39:q:60:PRO:CB	39:s:93:ARG:O	2.32	0.78
39:t:8:SER:O	39:t:9:ASN:CB	2.32	0.78
11:P:7:PRO:CB	20:H:20:G:O4'	2.32	0.77
26:h:47:THR:CB	37:o:65:ARG:NH2	2.47	0.77
39:q:106:ALA:HB1	39:t:106:ALA:CB	2.14	0.77
1:A:106:MET:CE	1:A:561:HIS:NE2	2.47	0.77
22:X:107:GLU:OE1	23:I:728:ARG:NH2	2.17	0.77
23:I:694:ILE:O	23:I:694:ILE:HD13	1.84	0.77
19:F:36:A:H2'	19:F:37:C:O5'	1.84	0.77
23:I:661:ASP:HB2	23:I:694:ILE:CD1	2.14	0.77
39:q:60:PRO:O	39:s:93:ARG:CB	2.32	0.77
22:X:113:LYS:HA	22:X:113:LYS:CE	2.14	0.77
29:f:70:LEU:HD22	29:f:71:TYR:HD2	1.50	0.77
2:C:95:LYS:NZ	2:C:95:LYS:HB3	1.98	0.77
20:H:177:A:H5''	20:H:178:A:OP1	1.84	0.77
29:m:70:LEU:HD22	29:m:71:TYR:HD2	1.49	0.77
3:E:192:ASN:HD22	3:E:196:VAL:CG2	1.98	0.77
22:X:72:GLN:HA	22:X:72:GLN:HE21	1.50	0.77
6:J:242:ILE:HG13	6:J:275:ASN:HD22	1.49	0.76
18:B:90:U:H5''	18:B:91:U:H5'	1.64	0.76
20:H:143:A:H3'	20:H:143:A:N3	2.00	0.76
19:F:45:A:O2'	19:F:73:A:C2	2.38	0.76
30:e:48:ILE:HD11	30:e:59:ASP:HB2	1.66	0.76
12:R:309:GLU:HA	12:R:309:GLU:OE2	1.86	0.76
20:H:39:U:H2'	20:H:40:C:C6	2.21	0.76
20:H:98:G:H1	29:m:41:ASN:HD21	1.33	0.76
1:A:191:ILE:CG2	1:A:572:PHE:CZ	2.67	0.76
1:A:1258:LYS:HE2	5:G:126:G:O3'	1.85	0.76
1:A:1371:TYR:OH	1:A:1473:ASP:OD2	2.02	0.76
30:l:48:ILE:HD11	30:l:59:ASP:HB2	1.66	0.76
31:n:35:ASP:HB2	31:n:36:PRO:HD2	1.68	0.76
1:A:178:TYR:CE2	1:A:183:LEU:HD12	2.21	0.76
12:R:311:LYS:HD2	12:R:311:LYS:C	2.10	0.76
17:W:130:ARG:NE	19:F:22:A:C8	2.53	0.76
22:X:57:ARG:HG3	22:X:57:ARG:NH2	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
39:q:106:ALA:HB1	39:t:106:ALA:HB1	1.64	0.76
3:E:266:PRO:HG2	7:L:785:GLN:CA	2.15	0.76
14:T:397:GLN:HB3	14:T:406:ILE:HG21	1.66	0.76
12:R:317:LYS:HA	12:R:317:LYS:CE	2.15	0.76
22:X:62:LYS:HE3	22:X:62:LYS:C	2.10	0.76
1:A:196:ASP:OD2	1:A:197:PRO:HD2	1.85	0.76
7:L:49:ARG:NH1	7:L:133:GLU:O	2.19	0.76
1:A:1908:LYS:NZ	17:W:449:ILE:HG13	2.01	0.76
2:C:672:LEU:O	2:C:822:MET:HG2	1.86	0.76
28:d:50:LYS:HG2	28:d:74:TRP:HB3	1.68	0.76
25:Y:416:PHE:CG	25:Y:425:ILE:HD11	2.20	0.76
26:h:45:ASN:OD1	37:o:16:THR:CB	2.34	0.76
39:q:8:SER:O	39:q:9:ASN:CB	2.34	0.76
31:g:35:ASP:HB2	31:g:36:PRO:HD2	1.68	0.75
28:k:50:LYS:HG2	28:k:74:TRP:HB3	1.68	0.75
1:A:178:TYR:CE2	1:A:183:LEU:CD1	2.69	0.75
1:A:1091:TYR:CD1	1:A:1190:CYS:SG	2.80	0.75
2:C:670:SER:HA	2:C:823:ALA:HB2	1.66	0.75
22:X:95:ARG:CZ	22:X:95:ARG:HB2	2.13	0.75
22:X:113:LYS:C	22:X:113:LYS:HD3	2.11	0.75
5:G:100:C:C2'	5:G:101:U:H6	1.98	0.75
1:A:470:ARG:HH21	1:A:470:ARG:HG2	1.52	0.75
2:C:670:SER:HA	2:C:823:ALA:CB	2.16	0.75
5:G:21:A:CI'	10:O:152:ARG:HH22	1.97	0.75
3:E:191:GLN:OE1	3:E:191:GLN:N	2.18	0.75
11:P:5:ALA:HB1	20:H:20:G:N7	2.02	0.75
11:P:6:ARG:HG3	19:F:78:A:C2	2.21	0.75
12:R:334:ARG:HB2	12:R:334:ARG:NH1	2.01	0.75
19:F:5:U:H3'	19:F:7:G:H5''	1.68	0.75
22:X:113:LYS:HZ2	22:X:113:LYS:CA	2.00	0.75
1:A:435:CYS:CB	4:4:-11:G:H22	1.99	0.75
1:A:1459:ARG:H	1:A:1459:ARG:HD2	1.51	0.75
7:L:65:ARG:NH2	23:I:721:LYS:HZ2	1.84	0.75
1:A:858:GLN:O	1:A:861:ARG:CG	2.30	0.75
1:A:1798:LEU:HD13	5:G:95:U:O2'	1.86	0.75
23:I:329:LEU:CB	36:Q:353:LEU:HA	2.16	0.75
23:I:698:ARG:HA	23:I:698:ARG:NE	2.02	0.75
5:G:20:A:HO2'	5:G:21:A:P	2.08	0.75
17:W:72:LEU:HD12	17:W:72:LEU:C	2.12	0.75
1:A:705:LYS:HG2	20:H:15:U:C5	2.22	0.74
1:A:1997:VAL:CG1	22:X:54:LEU:HG	2.17	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:I:273:GLU:HA	36:Q:357:ALA:HB3	1.67	0.74
39:s:8:SER:O	39:s:9:ASN:CB	2.35	0.74
40:K:90:PRO:CB	40:K:109:ASN:CB	2.64	0.74
5:G:27:U:H2'	5:G:28:A:O5'	1.86	0.74
28:d:110:LEU:HD11	29:f:59:LEU:HB3	1.70	0.74
20:H:30:A:H4'	22:X:73:PHE:HZ	1.52	0.74
25:Y:413:LYS:C	25:Y:419:PHE:CD1	2.64	0.74
1:A:106:MET:HE1	1:A:578:LEU:HD13	1.69	0.74
28:k:110:LEU:HD11	29:m:59:LEU:HB3	1.70	0.74
12:R:124:VAL:HG21	14:T:442:ARG:HH12	1.53	0.74
14:T:297:HIS:HE1	14:T:340:ALA:CB	1.91	0.74
9:N:42:LYS:HZ3	9:N:42:LYS:HB2	1.53	0.74
13:S:85:GLU:O	13:S:127:THR:CG2	2.36	0.74
20:H:40:C:C2'	20:H:41:U:C6	2.71	0.74
20:H:153:A:C2'	20:H:154:C:H5'	2.17	0.74
22:X:58:LEU:C	22:X:58:LEU:HD13	2.12	0.74
5:G:26:U:H2'	5:G:27:U:H5''	1.69	0.74
1:A:1134:TRP:HB3	1:A:1135:PRO:HD3	1.68	0.73
18:B:19:A:O2'	18:B:20:G:OP1	2.04	0.73
1:A:1491:LYS:HD2	1:A:1709:TYR:HD1	1.52	0.73
28:d:107:ILE:HG22	28:d:108:VAL:HG23	1.69	0.73
29:m:70:LEU:HD22	29:m:71:TYR:CD2	2.23	0.73
3:E:93:TRP:CH2	21:b:105:GLY:HA3	2.23	0.73
5:G:99:C:C2'	5:G:100:C:H5''	2.19	0.73
15:U:11:ARG:NH2	18:B:46:U:O2	2.20	0.73
28:k:107:ILE:HG22	28:k:108:VAL:HG23	1.69	0.73
6:J:241:VAL:HG13	6:J:244:ASN:HD21	1.51	0.73
11:P:16:ARG:HG3	11:P:16:ARG:NH2	2.02	0.73
20:H:179:C:H2'	20:H:180:G:H8	1.53	0.73
23:I:276:ARG:CB	36:Q:357:ALA:C	2.61	0.73
11:P:7:PRO:HB2	20:H:20:G:O4'	1.89	0.73
20:H:106:G:H4'	20:H:107:A:O4'	1.88	0.73
5:G:13:C:H2'	5:G:14:A:C8	2.24	0.73
8:M:198:ARG:NH2	20:H:11:G:N7	2.36	0.73
23:I:276:ARG:CB	36:Q:357:ALA:CB	2.67	0.73
23:I:685:ARG:NE	23:I:711:GLU:OE2	2.19	0.73
23:I:725:ARG:HD2	23:I:725:ARG:C	2.12	0.73
25:Y:413:LYS:C	25:Y:419:PHE:HD1	1.97	0.73
38:p:66:LEU:HD12	38:p:81:ILE:HG22	1.70	0.73
26:h:47:THR:CB	37:o:65:ARG:HH22	2.02	0.73
5:G:100:C:H5'	5:G:100:C:H6	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:102:G:C2'	5:G:103:U:H5'	2.19	0.72
5:G:102:G:H2'	5:G:103:U:H5'	1.70	0.72
14:T:345:ILE:HD11	14:T:359:LEU:HD13	1.71	0.72
25:Y:414:GLU:HG2	25:Y:419:PHE:CZ	2.23	0.72
36:Q:525:PRO:N	36:Q:525:PRO:C	2.47	0.72
14:T:455:GLN:CG	14:T:456:PRO:CD	2.64	0.72
17:W:233:LYS:HG3	17:W:355:TYR:CE2	2.24	0.72
22:X:113:LYS:HD3	22:X:113:LYS:O	1.90	0.72
29:f:70:LEU:HD22	29:f:71:TYR:CD2	2.23	0.72
4:4:-12:G:O2'	4:4:-11:G:O5'	2.07	0.72
14:T:385:TYR:CZ	14:T:401:PRO:HD2	2.23	0.72
23:I:575:ARG:O	23:I:579:LEU:HB2	1.90	0.72
5:G:91:A:H2	20:H:39:U:O2	1.71	0.72
14:T:197:TYR:HD2	14:T:488:VAL:HG12	1.53	0.72
25:Y:420:ASP:OD2	25:Y:420:ASP:N	2.22	0.72
1:A:203:VAL:O	1:A:205:ASP:N	2.22	0.72
2:C:682:LYS:HG3	2:C:803:ARG:HD2	1.72	0.72
14:T:385:TYR:CE2	14:T:400:PHE:HB3	2.24	0.72
19:F:59:G:O2'	19:F:60:C:OP1	2.07	0.72
5:G:6:A:C2	19:F:41:A:C2	2.78	0.72
5:G:20:A:H2	10:O:187:THR:HG1	1.29	0.72
14:T:216:ASN:OD1	14:T:472:GLN:CG	2.37	0.72
1:A:1468:ASN:OD1	5:G:130:G:C4'	2.37	0.72
1:A:1565:LYS:O	1:A:1567:PRO:CD	2.34	0.72
1:A:1833:LEU:HD22	1:A:1833:LEU:N	2.02	0.72
17:W:82:ASN:N	17:W:83:PRO:HD2	2.05	0.72
22:X:100:ILE:O	22:X:103:GLN:CB	2.21	0.72
5:G:7:G:O2'	5:G:8:C:H5'	1.90	0.72
1:A:1510:GLU:CB	5:G:124:G:H1	2.03	0.72
20:H:40:C:O2'	20:H:41:U:H6	1.73	0.72
23:I:723:MET:O	23:I:727:ARG:N	2.23	0.72
1:A:1258:LYS:HE2	5:G:126:G:C2'	2.20	0.71
14:T:282:ARG:HB2	14:T:320:LYS:HD3	1.72	0.71
19:F:31:U:C2'	19:F:32:U:H5'	2.19	0.71
1:A:609:LYS:NZ	41:A:3000:IHP:O31	2.23	0.71
5:G:90:C:C5	5:G:90:C:OP2	2.43	0.71
7:L:6:ILE:HD13	7:L:6:ILE:C	2.15	0.71
19:F:36:A:C2'	19:F:37:C:O5'	2.38	0.71
20:H:106:G:H21	20:H:107:A:N6	1.87	0.71
20:H:30:A:C1'	22:X:73:PHE:CE1	2.65	0.71
5:G:21:A:C4	10:O:152:ARG:NH2	2.58	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:45:A:H2	19:F:73:A:O4'	1.72	0.71
22:X:72:GLN:NE2	22:X:72:GLN:HA	2.05	0.71
7:L:7:LYS:HB3	7:L:40:ARG:C	2.16	0.71
9:N:42:LYS:HB2	9:N:42:LYS:NZ	2.06	0.71
19:F:34:G:C5'	19:F:34:G:H8	2.03	0.71
19:F:35:A:C5'	19:F:35:A:H8	2.03	0.71
25:Y:426:LEU:C	25:Y:426:LEU:HD23	2.15	0.71
1:A:178:TYR:HE2	1:A:183:LEU:CD1	2.04	0.71
1:A:1555:LEU:HD21	1:A:1574:ILE:HG13	1.72	0.71
23:I:727:ARG:HH21	23:I:727:ARG:CG	2.04	0.71
25:Y:413:LYS:H	25:Y:413:LYS:HD2	1.55	0.71
20:H:153:A:H2'	20:H:154:C:C5'	2.19	0.71
22:X:112:LEU:HD13	22:X:112:LEU:C	2.16	0.71
5:G:98:U:O2'	5:G:99:C:H6	1.73	0.71
2:C:758:LEU:HD12	2:C:758:LEU:O	1.90	0.70
6:J:277:THR:HG21	19:F:84:A:N3	2.06	0.70
13:S:98:LEU:HB3	13:S:130:GLY:CA	2.20	0.70
19:F:45:A:C2	19:F:73:A:H1'	2.26	0.70
22:X:101:GLU:HA	22:X:101:GLU:OE2	1.91	0.70
25:Y:426:LEU:HD23	25:Y:426:LEU:O	1.91	0.70
7:L:4:ILE:O	7:L:4:ILE:HD13	1.90	0.70
14:T:437:HIS:HD2	14:T:446:ASN:HD21	1.37	0.70
22:X:96:GLN:HE21	22:X:96:GLN:CA	2.04	0.70
1:A:186:GLU:HB3	1:A:187:PRO:HD3	1.71	0.70
1:A:1997:VAL:HG13	22:X:54:LEU:HD21	1.74	0.70
17:W:73:ASP:CG	17:W:74:PRO:HD2	2.16	0.70
1:A:163:ARG:NH2	41:A:3000:IHP:O35	2.22	0.70
17:W:83:PRO:CB	17:W:87:THR:HG1	1.97	0.70
1:A:684:GLU:HG2	14:T:308:ARG:HH12	1.56	0.70
1:A:1258:LYS:HD2	5:G:127:G:P	2.32	0.70
5:G:90:C:O2'	5:G:91:A:OP1	2.10	0.70
1:A:1495:PHE:HE2	1:A:1748:ARG:CD	2.04	0.70
5:G:6:A:H2	19:F:41:A:H2	1.38	0.70
6:J:244:ASN:H	6:J:244:ASN:ND2	1.89	0.70
7:L:7:LYS:CG	7:L:40:ARG:HA	2.22	0.70
23:I:272:PHE:CA	36:Q:355:ASN:CB	2.69	0.70
1:A:1494:TYR:CD1	1:A:1744:ARG:NH2	2.58	0.70
17:W:168:PHE:CE1	19:F:21:U:O2	2.44	0.70
20:H:154:C:H2'	20:H:155:C:C6	2.27	0.70
22:X:58:LEU:O	22:X:58:LEU:HD22	1.91	0.70
1:A:1428:HIS:HB2	25:Y:396:ASP:HB3	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1502:PHE:HE1	1:A:1754:TYR:HB2	1.57	0.70
1:A:1554:GLN:CA	1:A:1561:PHE:HB3	2.10	0.70
5:G:98:U:O2'	5:G:99:C:C6	2.43	0.70
23:I:109:MET:CA	24:y:66:ASN:CB	2.70	0.70
1:A:1132:LYS:CG	1:A:1139:ARG:HH12	2.05	0.69
1:A:1494:TYR:CG	1:A:1744:ARG:NE	2.60	0.69
2:C:666:VAL:CG1	2:C:823:ALA:O	2.39	0.69
2:C:850:LEU:HB3	2:C:855:GLY:HA3	1.74	0.69
12:R:325:ARG:HD3	12:R:325:ARG:C	2.16	0.69
23:I:187:LEU:CB	23:I:196:ALA:HB1	2.22	0.69
23:I:687:ILE:HA	23:I:690:PHE:HB2	1.74	0.69
7:L:7:LYS:HB3	7:L:40:ARG:O	1.92	0.69
19:F:31:U:O2'	19:F:32:U:H5'	1.92	0.69
23:I:272:PHE:HA	36:Q:355:ASN:CB	2.23	0.69
25:Y:416:PHE:CD2	25:Y:425:ILE:HD11	2.27	0.69
5:G:90:C:O2'	5:G:91:A:P	2.50	0.69
10:O:262:THR:HB	10:O:271:PHE:HB2	1.74	0.69
13:S:98:LEU:HD23	13:S:130:GLY:HA3	1.75	0.69
1:A:1131:LYS:NZ	1:A:1131:LYS:HB3	2.06	0.69
19:F:42:C:H3'	19:F:43:A:C8	2.28	0.69
20:H:101:U:O4'	26:h:66:SER:HB3	1.92	0.69
22:X:58:LEU:HD13	22:X:58:LEU:O	1.91	0.69
5:G:90:C:C5'	5:G:90:C:H6	2.04	0.69
13:S:37:LYS:HB2	13:S:37:LYS:HZ2	1.54	0.69
18:B:21:A:O3'	18:B:22:U:H4'	1.93	0.69
19:F:85:U:H3'	19:F:86:U:H5'	1.74	0.69
20:H:153:A:N6	20:H:177:A:C2	2.60	0.69
1:A:1793:THR:CG2	19:F:43:A:H5'	2.21	0.69
2:C:68:THR:HG1	2:C:71:GLU:CB	2.00	0.69
2:C:751:PRO:HG2	15:U:63:LYS:CB	2.22	0.69
8:M:198:ARG:HH12	20:H:10:C:N4	1.91	0.69
18:B:90:U:O4'	26:a:66:SER:HB3	1.92	0.69
7:L:6:ILE:HD13	7:L:6:ILE:O	1.93	0.69
8:M:198:ARG:NH1	20:H:10:C:N4	2.40	0.69
19:F:7:G:H5'	19:F:7:G:H8	1.58	0.69
23:I:109:MET:HA	24:y:66:ASN:CB	2.22	0.69
2:C:852:ARG:HH22	4:4:-13:C:C2'	2.01	0.69
11:P:7:PRO:HB3	20:H:20:G:O4'	1.93	0.69
23:I:725:ARG:O	23:I:728:ARG:HB3	1.92	0.69
1:A:850:TYR:OH	1:A:863:GLU:OE1	2.11	0.69
14:T:197:TYR:CE2	14:T:488:VAL:CG1	2.76	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1519:THR:CB	5:G:119:A:C2	2.76	0.68
23:I:724:LEU:HA	23:I:727:ARG:HB2	1.73	0.68
1:A:1645:LEU:HD22	1:A:1713:SER:HA	1.74	0.68
12:R:317:LYS:HA	12:R:317:LYS:HZ2	1.57	0.68
10:O:65:PHE:HE2	19:F:24:A:C6	2.11	0.68
19:F:39:A:O2'	19:F:40:U:H5'	1.93	0.68
1:A:186:GLU:CB	1:A:187:PRO:CD	2.70	0.68
1:A:1321:GLU:HG2	1:A:1322:LEU:HD23	1.74	0.68
1:A:1829:GLY:HA3	19:F:40:U:OP1	1.94	0.68
2:C:856:HIS:HE1	34:u:103:GLN:HA	1.57	0.68
1:A:1258:LYS:HB2	1:A:1258:LYS:NZ	2.08	0.68
13:S:71:GLY:C	13:S:111:GLN:HE22	2.00	0.68
14:T:442:ARG:HH11	14:T:442:ARG:HG3	1.57	0.68
20:H:106:G:C5'	28:k:47:ARG:HH22	2.05	0.68
20:H:150:U:H3	20:H:181:G:H1	1.41	0.68
20:H:152:G:O3'	20:H:153:A:O4'	2.11	0.68
22:X:57:ARG:HG3	22:X:57:ARG:HH21	1.56	0.68
1:A:1751:LEU:N	1:A:1751:LEU:HD23	2.08	0.68
1:A:1809:ILE:HB	1:A:1818:PHE:HB2	1.76	0.68
20:H:143:A:H2'	20:H:144:C:H6	1.59	0.68
23:I:727:ARG:HH21	23:I:727:ARG:HB3	1.58	0.68
1:A:663:ARG:NH2	1:A:663:ARG:HG3	2.08	0.68
7:L:65:ARG:HH21	23:I:721:LYS:NZ	1.77	0.68
14:T:342:GLU:OE1	14:T:342:GLU:HA	1.92	0.68
19:F:45:A:C2	19:F:73:A:C1'	2.76	0.68
20:H:40:C:H2'	20:H:41:U:C5	2.29	0.68
21:i:18:ARG:NH1	21:i:52:LYS:HB2	2.09	0.68
1:A:105:ASN:HD22	1:A:129:VAL:HG11	1.59	0.68
1:A:195:LEU:HD12	1:A:195:LEU:N	2.04	0.68
1:A:858:GLN:C	1:A:861:ARG:HG2	2.16	0.68
9:N:38:GLU:OE1	9:N:38:GLU:HA	1.94	0.68
25:Y:402:ILE:HG23	25:Y:411:LEU:HD11	1.75	0.68
36:Q:525:PRO:N	36:Q:525:PRO:CB	2.54	0.68
5:G:16:G:O2'	5:G:17:U:OP2	2.10	0.68
6:J:201:ARG:HG2	6:J:201:ARG:HH21	1.57	0.68
8:M:133:ARG:NH2	19:F:88:G:C5'	2.56	0.68
5:G:20:A:C2	10:O:187:THR:HG21	2.29	0.67
1:A:853:LYS:N	1:A:853:LYS:HD2	2.09	0.67
12:R:218:ILE:HG13	12:R:218:ILE:O	1.92	0.67
14:T:442:ARG:HH11	14:T:442:ARG:CG	2.07	0.67
1:A:1318:THR:CG2	1:A:1324:GLY:CA	2.71	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:673:LYS:HZ3	15:U:56:ASP:CB	2.05	0.67
5:G:120:G:C6	19:F:45:A:C6	2.83	0.67
14:T:339:GLN:HG3	14:T:339:GLN:O	1.93	0.67
1:A:1141:ARG:NH1	1:A:1183:PRO:HD2	2.09	0.67
1:A:1459:ARG:NH1	1:A:1459:ARG:HG2	2.08	0.67
9:N:41:ARG:O	9:N:41:ARG:HG2	1.94	0.67
39:q:53:ILE:CB	39:r:22:ASN:CB	2.73	0.67
1:A:1085:ILE:HG12	1:A:1099:PHE:HE1	1.59	0.67
7:L:62:GLU:OE2	22:X:104:ARG:NE	2.26	0.67
17:W:259:GLN:CD	31:n:13:MET:HG3	2.19	0.67
21:b:18:ARG:NH1	21:b:52:LYS:HB2	2.09	0.67
39:q:60:PRO:CB	39:s:94:GLN:N	2.57	0.67
1:A:1132:LYS:HG3	1:A:1139:ARG:HH12	1.60	0.67
2:C:114:TYR:HB3	26:a:79:ASN:HB3	1.76	0.67
11:P:3:THR:CG2	19:F:79:C:O2	2.42	0.67
13:S:98:LEU:HB3	13:S:130:GLY:HA3	1.76	0.67
1:A:200:ASP:OD1	1:A:200:ASP:N	2.28	0.67
5:G:26:U:H2'	5:G:27:U:C5'	2.24	0.67
14:T:213:GLU:CG	14:T:218:TRP:CZ2	2.77	0.67
5:G:17:U:H1'	10:O:46:LYS:NZ	2.10	0.67
10:O:243:ILE:HG12	10:O:294:ASN:HD22	1.60	0.67
14:T:261:LEU:HB2	14:T:273:TRP:HB2	1.76	0.67
15:U:23:LEU:H	16:V:474:HIS:HD2	1.42	0.67
23:I:692:SER:HB2	23:I:703:PHE:HZ	1.58	0.67
1:A:1829:GLY:CA	19:F:40:U:OP1	2.43	0.67
5:G:91:A:N1	20:H:39:U:O2	2.27	0.67
14:T:188:PRO:CG	14:T:443:THR:OG1	2.35	0.67
30:e:20:LEU:HD12	31:g:41:VAL:HG13	1.77	0.67
1:A:1459:ARG:HD2	1:A:1459:ARG:N	2.09	0.66
1:A:1793:THR:HG22	19:F:43:A:H5'	1.76	0.66
17:W:168:PHE:HE1	19:F:21:U:O2	1.77	0.66
20:H:75:A:H61	20:H:77:C:H42	1.44	0.66
1:A:1676:ILE:HD13	1:A:1706:ASP:HB2	1.77	0.66
19:F:85:U:H3'	19:F:86:U:C5'	2.25	0.66
20:H:67:C:H42	20:H:85:A:H61	1.44	0.66
1:A:698:PRO:HG2	1:A:701:ILE:HD13	1.75	0.66
1:A:1997:VAL:CG1	22:X:54:LEU:CG	2.71	0.66
22:X:85:ASP:N	22:X:85:ASP:OD1	2.21	0.66
23:I:681:ILE:HG23	23:I:710:PHE:CE2	2.30	0.66
1:A:1486:GLU:OE1	1:A:1674:HIS:NE2	2.29	0.66
5:G:95:U:H2'	5:G:96:U:C6	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:402:ILE:HG23	25:Y:411:LEU:CD1	2.25	0.66
19:F:33:G:H5''	19:F:33:G:C8	2.28	0.66
20:H:30:A:H4'	22:X:73:PHE:CZ	2.31	0.66
20:H:114:A:H61	20:H:142:C:H42	1.44	0.66
20:H:151:C:H2'	20:H:152:G:H8	1.59	0.66
21:i:18:ARG:NH1	21:i:52:LYS:CB	2.58	0.66
1:A:1515:TRP:CB	20:H:30:A:C6	2.78	0.66
5:G:17:U:O2'	10:O:46:LYS:NZ	2.28	0.66
20:H:151:C:C2	20:H:152:G:C8	2.83	0.66
22:X:104:ARG:HD3	23:I:728:ARG:HG2	1.78	0.66
1:A:381:PRO:HD2	2:C:334:ILE:HG22	1.78	0.66
22:X:107:GLU:CD	23:I:728:ARG:HH22	2.03	0.66
23:I:688:TYR:O	23:I:692:SER:CB	2.44	0.66
28:k:33:THR:HG22	28:k:37:LYS:HE2	1.76	0.66
1:A:658:ARG:NH2	19:F:65:G:OP2	2.29	0.66
1:A:1554:GLN:HB2	1:A:1561:PHE:HD1	1.61	0.66
5:G:91:A:N1	20:H:39:U:C2	2.64	0.66
12:R:132:LEU:HD12	12:R:132:LEU:O	1.96	0.66
18:B:95:G:H5'	29:f:25:TRP:CH2	2.21	0.66
22:X:116:ARG:N	22:X:116:ARG:HD2	2.10	0.66
10:O:223:LEU:HD22	10:O:285:GLU:HG2	1.78	0.66
23:I:273:GLU:O	36:Q:357:ALA:CB	2.44	0.66
1:A:1251:SER:OG	1:A:1259:ILE:HG12	1.96	0.65
20:H:40:C:O2'	20:H:41:U:C4'	2.44	0.65
20:H:41:U:H5''	20:H:41:U:H6	1.59	0.65
20:H:153:A:C3'	20:H:154:C:H5'	2.25	0.65
1:A:1251:SER:OG	1:A:1259:ILE:CG1	2.44	0.65
1:A:1494:TYR:CB	1:A:1744:ARG:NE	2.56	0.65
1:A:1833:LEU:H	1:A:1833:LEU:CD2	2.02	0.65
21:b:18:ARG:NH1	21:b:52:LYS:CB	2.58	0.65
28:d:33:THR:HG22	28:d:37:LYS:HE2	1.76	0.65
1:A:858:GLN:HA	1:A:861:ARG:CG	2.26	0.65
5:G:17:U:H1'	10:O:46:LYS:HZ3	1.62	0.65
20:H:151:C:O2	20:H:152:G:C8	2.48	0.65
1:A:1487:HIS:CE1	1:A:1671:TYR:CZ	2.85	0.65
5:G:90:C:OP2	5:G:90:C:H5	1.78	0.65
19:F:6:C:OP2	19:F:6:C:H4'	1.95	0.65
1:A:193:LEU:C	1:A:193:LEU:HD12	2.21	0.65
1:A:195:LEU:H	1:A:195:LEU:CD1	2.01	0.65
1:A:934:ARG:NH1	1:A:934:ARG:HG2	2.09	0.65
1:A:1193:GLU:HB3	1:A:1231:ARG:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:333:ASP:OD1	31:g:3:LYS:HB2	1.96	0.65
12:R:136:ASP:HB3	12:R:138:GLU:H	1.60	0.65
36:Q:943:ARG:CA	36:Q:969:PRO:CB	2.74	0.65
1:A:183:LEU:HG	1:A:183:LEU:O	1.97	0.65
1:A:186:GLU:N	1:A:186:GLU:OE2	2.30	0.65
2:C:476:CYS:HB3	2:C:565:ILE:HB	1.77	0.65
2:C:667:VAL:N	2:C:824:THR:HG23	2.09	0.65
14:T:307:SER:OG	14:T:308:ARG:N	2.29	0.65
10:O:250:ASN:OD1	13:S:91:LYS:NZ	2.26	0.65
5:G:101:U:O2	5:G:101:U:H2'	1.95	0.65
20:H:153:A:H3'	20:H:154:C:H5'	1.79	0.65
25:Y:413:LYS:HA	25:Y:416:PHE:CD2	2.32	0.65
37:o:5:THR:HG22	37:o:8:LEU:H	1.60	0.65
1:A:419:ARG:NH2	1:A:423:ASP:O	2.30	0.65
5:G:120:G:N7	19:F:45:A:N6	2.45	0.65
13:S:125:LYS:CB	13:S:126:HIS:CD2	2.80	0.65
17:W:341:ASN:OD1	17:W:388:GLN:NE2	2.29	0.65
1:A:537:LYS:HB2	19:F:37:C:H41	1.60	0.64
1:A:1258:LYS:CE	5:G:126:G:O3'	2.45	0.64
14:T:397:GLN:C	14:T:406:ILE:CG2	2.70	0.64
17:W:534:ILE:HD12	17:W:544:SER:HB3	1.79	0.64
3:E:307:ARG:HH22	21:b:115:PRO:HB3	1.61	0.64
14:T:213:GLU:HB2	14:T:218:TRP:CE3	2.32	0.64
19:F:45:A:C2	19:F:73:A:O4'	2.51	0.64
20:H:156:U:C6	20:H:156:U:C5'	2.72	0.64
30:l:20:LEU:HD12	31:n:41:VAL:HG13	1.77	0.64
1:A:1141:ARG:HB2	1:A:1182:ASN:OD1	1.98	0.64
20:H:168:A:C8	20:H:168:A:C5'	2.76	0.64
22:X:112:LEU:HD23	23:I:720:ILE:CG2	2.26	0.64
2:C:129:ILE:HG22	2:C:199:LEU:HB3	1.79	0.64
28:d:32:LEU:HD22	28:d:65:MET:HE3	1.80	0.64
1:A:523:ASN:OD1	1:A:552:ARG:NH2	2.31	0.64
2:C:137:HIS:HD2	2:C:238:ASN:H	1.44	0.64
3:E:93:TRP:HH2	21:b:105:GLY:CA	2.10	0.64
17:W:130:ARG:HH21	19:F:22:A:H2'	1.62	0.64
17:W:233:LYS:HG3	17:W:355:TYR:CZ	2.32	0.64
23:I:442:LEU:O	23:I:446:HIS:N	2.30	0.64
1:A:1134:TRP:CB	1:A:1135:PRO:CD	2.76	0.64
5:G:120:G:C5	19:F:45:A:C6	2.86	0.64
16:V:544:LEU:HD11	16:V:578:SER:HB3	1.79	0.64
20:H:41:U:H2'	20:H:42:G:C8	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:PRO:N	1:A:345:PRO:C	2.52	0.64
2:C:753:GLU:HG3	2:C:753:GLU:O	1.97	0.64
13:S:102:ASN:ND2	13:S:108:ASN:OD1	2.30	0.64
18:B:23:C:O2'	18:B:24:G:O5'	2.15	0.64
20:H:154:C:H2'	20:H:155:C:H6	1.63	0.64
1:A:1135:PRO:CD	1:A:1138:ALA:HB3	2.16	0.64
1:A:1835:GLN:OE1	1:A:1835:GLN:HA	1.97	0.64
5:G:100:C:C2	5:G:101:U:C6	2.86	0.64
10:O:133:PRO:HG2	10:O:137:LEU:HB2	1.80	0.64
19:F:42:C:H5''	19:F:43:A:OP2	1.97	0.64
23:I:704:TRP:CH2	23:I:727:ARG:HG3	2.31	0.64
3:E:93:TRP:HH2	21:b:105:GLY:HA2	1.63	0.64
8:M:133:ARG:NH2	19:F:88:G:H5'	2.13	0.64
14:T:409:LEU:HD12	14:T:409:LEU:N	2.13	0.64
2:C:680:ASN:HD21	2:C:803:ARG:NH1	1.96	0.63
20:H:39:U:H2'	20:H:40:C:C5	2.32	0.63
1:A:1090:ARG:HD2	1:A:1095:ILE:HD11	1.80	0.63
11:P:3:THR:HG22	19:F:79:C:O2	1.98	0.63
20:H:147:G:H2'	20:H:148:C:H6	1.62	0.63
28:k:32:LEU:HD22	28:k:65:MET:HE3	1.79	0.63
2:C:750:LEU:HA	2:C:753:GLU:HB3	1.79	0.63
3:E:307:ARG:NH2	21:b:115:PRO:HB3	2.12	0.63
5:G:21:A:OP2	10:O:193:LEU:HD11	1.98	0.63
14:T:197:TYR:CD2	14:T:488:VAL:CG1	2.81	0.63
14:T:216:ASN:OD1	14:T:472:GLN:HG2	1.98	0.63
14:T:250:ARG:NH1	14:T:266:GLU:OE2	2.30	0.63
23:I:681:ILE:HG23	23:I:710:PHE:HZ	1.56	0.63
23:I:698:ARG:HG3	23:I:698:ARG:O	1.98	0.63
39:r:8:SER:CB	39:s:86:MET:CB	2.77	0.63
23:I:726:ILE:HD13	23:I:726:ILE:C	2.24	0.63
1:A:1798:LEU:HB2	5:G:96:U:H4'	1.77	0.63
10:O:166:SER:OG	19:F:29:A:N3	2.29	0.63
20:H:164:C:H6	20:H:164:C:H5'	1.63	0.63
5:G:18:A:C2	10:O:196:GLN:O	2.52	0.63
12:R:317:LYS:HA	12:R:317:LYS:HZ1	1.63	0.63
30:l:74:LEU:HB3	30:l:77:ILE:HD11	1.81	0.63
1:A:1020:LYS:NZ	20:H:26:A:OP1	2.32	0.63
18:B:95:G:C5'	28:d:47:ARG:HH22	2.12	0.63
25:Y:413:LYS:HA	25:Y:416:PHE:HD2	1.63	0.63
1:A:196:ASP:OD2	1:A:197:PRO:CD	2.47	0.63
2:C:531:TRP:HB2	2:C:551:LEU:HB2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:95:U:H4'	5:G:96:U:OP1	1.98	0.63
10:O:27:CYS:SG	10:O:83:THR:OG1	2.57	0.63
14:T:191:HIS:HE1	14:T:440:ASP:CG	2.07	0.63
17:W:253:SER:HB3	17:W:256:HIS:HB2	1.80	0.63
5:G:6:A:C2	19:F:41:A:H2	2.16	0.62
9:N:139:CYS:SG	9:N:140:ARG:N	2.72	0.62
13:S:125:LYS:HB3	13:S:126:HIS:CD2	2.33	0.62
1:A:1091:TYR:HD2	1:A:1091:TYR:C	2.07	0.62
2:C:668:GLU:H	2:C:824:THR:HG21	1.64	0.62
5:G:5:G:O5'	5:G:5:G:H8	1.81	0.62
5:G:20:A:H2	10:O:187:THR:HG21	1.64	0.62
5:G:73:G:C2'	5:G:74:G:O4'	2.46	0.62
6:J:239:ARG:HH11	6:J:239:ARG:CB	2.12	0.62
12:R:123:GLU:HA	12:R:123:GLU:OE2	1.98	0.62
20:H:152:G:C2	20:H:153:A:C5	2.87	0.62
2:C:177:ARG:NH2	2:C:638:ASP:OD2	2.32	0.62
5:G:100:C:H6	5:G:100:C:C5'	2.12	0.62
14:T:397:GLN:CB	14:T:406:ILE:CG2	2.77	0.62
23:I:692:SER:HA	23:I:703:PHE:CZ	2.33	0.62
1:A:1494:TYR:HB2	1:A:1744:ARG:NE	2.09	0.62
7:L:123:LEU:HD22	7:L:125:PRO:HD2	1.81	0.62
18:B:19:A:H2'	18:B:20:G:H5''	1.81	0.62
23:I:698:ARG:HA	23:I:698:ARG:HE	1.62	0.62
23:I:728:ARG:O	23:I:731:GLN:N	2.33	0.62
1:A:1798:LEU:HD13	5:G:96:U:H5'	1.82	0.62
39:r:8:SER:O	39:r:9:ASN:CB	2.47	0.62
5:G:18:A:N1	10:O:196:GLN:O	2.32	0.62
14:T:187:LYS:N	14:T:188:PRO:CD	2.63	0.62
23:I:273:GLU:CB	36:Q:357:ALA:HB2	2.29	0.62
6:J:238:ASN:HB3	6:J:241:VAL:HG12	1.82	0.62
7:L:106:LYS:CD	22:X:105:ARG:HH22	2.13	0.62
14:T:459:LEU:HB3	14:T:462:GLU:CG	2.30	0.62
20:H:15:U:C2'	20:H:16:U:OP2	2.48	0.62
20:H:153:A:N6	20:H:177:A:H2	1.98	0.62
22:X:64:ARG:NH1	22:X:64:ARG:HG3	2.13	0.62
1:A:1494:TYR:HD1	1:A:1710:ASN:ND2	1.98	0.62
1:A:1809:ILE:HD11	1:A:1845:VAL:HG22	1.82	0.62
2:C:506:PRO:HA	2:C:526:THR:HA	1.82	0.62
2:C:750:LEU:HD12	2:C:750:LEU:C	2.24	0.62
3:E:274:VAL:HG12	3:E:275:LYS:HG3	1.82	0.62
2:C:94:ILE:O	2:C:94:ILE:HG22	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:61:MET:HE2	13:S:63:GLN:HB2	1.82	0.62
14:T:327:SER:O	14:T:357:TRP:CH2	2.53	0.62
1:A:858:GLN:O	1:A:858:GLN:NE2	2.32	0.61
2:C:711:ARG:NH2	2:C:730:ARG:O	2.33	0.61
19:F:43:A:O5'	19:F:43:A:H8	1.82	0.61
25:Y:401:GLU:O	25:Y:405:MET:HG2	2.00	0.61
1:A:856:LEU:O	1:A:860:GLN:OE1	2.18	0.61
1:A:1433:ASP:OD1	1:A:1439:ARG:NH2	2.33	0.61
19:F:35:A:H5''	19:F:35:A:H8	1.64	0.61
7:L:62:GLU:OE2	22:X:104:ARG:CZ	2.49	0.61
10:O:78:LYS:O	10:O:97:ARG:NH2	2.32	0.61
19:F:27:A:O2'	19:F:28:A:C8	2.51	0.61
10:O:26:THR:OG1	10:O:159:ARG:NH2	2.34	0.61
17:W:247:TYR:HB3	17:W:251:GLY:HA2	1.83	0.61
18:B:12:U:O2'	18:B:13:C:O5'	2.19	0.61
20:H:39:U:H6	20:H:39:U:C5'	2.07	0.61
20:H:142:C:C2'	20:H:143:A:H5'	2.30	0.61
20:H:157:G:H5''	20:H:157:G:H8	1.65	0.61
1:A:942:PRO:HB3	1:A:1091:TYR:CE2	2.35	0.61
1:A:1639:VAL:H	1:A:1656:THR:HA	1.65	0.61
3:E:307:ARG:HH22	21:b:115:PRO:HG3	1.65	0.61
7:L:4:ILE:O	7:L:4:ILE:HG23	1.99	0.61
1:A:1468:ASN:ND2	5:G:130:G:H5'	2.14	0.61
2:C:68:THR:OG1	2:C:71:GLU:HB3	1.99	0.61
20:H:112:G:H2'	20:H:113:G:H8	1.65	0.61
22:X:95:ARG:HB2	22:X:95:ARG:NH1	2.15	0.61
37:o:123:ASN:O	37:o:126:THR:HB	1.99	0.61
2:C:853:ARG:NH1	2:C:879:ASP:O	2.33	0.61
3:E:104:THR:OG1	21:b:103:GLY:HA3	2.00	0.61
17:W:71:HIS:CD2	17:W:71:HIS:N	2.69	0.61
20:H:33:G:H2'	20:H:34:U:C6	2.35	0.61
22:X:116:ARG:HH11	22:X:116:ARG:HB3	1.64	0.61
36:Q:823:GLY:O	36:Q:1096:ASP:CB	2.48	0.61
2:C:853:ARG:NH2	2:C:886:ASP:OD2	2.33	0.61
7:L:6:ILE:O	7:L:6:ILE:HG23	2.00	0.61
9:N:36:PRO:C	9:N:38:GLU:H	2.08	0.61
20:H:143:A:H2'	20:H:144:C:C6	2.35	0.61
2:C:65:TYR:H	2:C:65:TYR:HD2	1.49	0.61
2:C:779:LEU:HB3	2:C:934:MET:HE1	1.83	0.61
12:R:315:LYS:O	12:R:319:LYS:HG2	2.01	0.61
14:T:345:ILE:HG22	14:T:345:ILE:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:X:100:ILE:C	22:X:103:GLN:HB2	2.17	0.61
5:G:13:C:H2'	5:G:14:A:H8	1.65	0.61
6:J:206:LEU:HD22	7:L:175:GLN:HE21	1.65	0.61
17:W:70:VAL:HG22	17:W:70:VAL:O	2.01	0.61
17:W:384:ASP:OD2	17:W:430:ASN:ND2	2.34	0.61
22:X:116:ARG:HH11	22:X:116:ARG:HA	1.66	0.61
1:A:532:THR:HG1	5:G:3:A:P	2.24	0.60
3:E:162:ARG:HH21	3:E:203:ASP:HB3	1.66	0.60
11:P:13:ARG:HG3	11:P:13:ARG:NH1	2.14	0.60
14:T:187:LYS:N	14:T:188:PRO:HD2	2.16	0.60
24:y:43:THR:C	24:y:45:LYS:H	2.09	0.60
1:A:186:GLU:CB	1:A:187:PRO:HD3	2.26	0.60
11:P:3:THR:O	11:P:3:THR:OG1	2.19	0.60
23:I:608:LEU:HB2	23:I:611:HIS:HB2	1.83	0.60
1:A:191:ILE:HG21	1:A:572:PHE:CD1	2.35	0.60
5:G:21:A:O2'	5:G:22:C:P	2.59	0.60
12:R:64:PHE:O	12:R:71:GLN:NE2	2.29	0.60
13:S:98:LEU:HB3	13:S:130:GLY:C	2.26	0.60
20:H:106:G:H5'	28:k:47:ARG:HH22	1.65	0.60
23:I:688:TYR:O	23:I:692:SER:HB2	2.00	0.60
30:e:74:LEU:HB3	30:e:77:ILE:HD11	1.81	0.60
1:A:1131:LYS:HD3	1:A:1174:PHE:CZ	2.35	0.60
2:C:668:GLU:H	2:C:824:THR:CG2	2.14	0.60
3:E:81:LEU:HB2	3:E:93:TRP:HB2	1.83	0.60
2:C:693:GLU:H	2:C:696:LEU:HD12	1.65	0.60
20:H:106:G:N2	20:H:107:A:C6	2.67	0.60
23:I:692:SER:HB2	23:I:703:PHE:CE2	2.35	0.60
2:C:221:ILE:HG23	2:C:495:ARG:HB2	1.82	0.60
2:C:829:GLU:HB2	2:C:907:VAL:HG22	1.84	0.60
5:G:90:C:H6	5:G:90:C:O5'	1.85	0.60
1:A:1136:ARG:HH11	1:A:1136:ARG:CG	2.10	0.60
1:A:150:MET:HG2	1:A:193:LEU:HB3	1.83	0.60
1:A:252:ASP:O	1:A:332:TYR:OH	2.19	0.60
1:A:1495:PHE:CE2	1:A:1748:ARG:CD	2.83	0.60
1:A:1787:ARG:HH21	1:A:1805:GLY:HA2	1.67	0.60
2:C:277:LYS:NZ	2:C:864:PRO:O	2.35	0.60
5:G:83:A:O2'	5:G:84:U:P	2.60	0.60
7:L:62:GLU:OE1	23:I:725:ARG:HD3	2.01	0.60
17:W:354:ARG:NH1	17:W:373:ARG:O	2.35	0.60
1:A:435:CYS:HB3	4:4:-11:G:H22	1.65	0.60
2:C:749:THR:HG23	2:C:749:THR:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:197:TYR:HE2	14:T:488:VAL:HG11	1.64	0.60
17:W:82:ASN:N	17:W:83:PRO:CD	2.65	0.60
1:A:1094:ARG:H	1:A:1094:ARG:HD2	1.67	0.60
1:A:1561:PHE:O	1:A:1561:PHE:HD2	1.84	0.60
17:W:565:LYS:HD2	17:W:577:LEU:HD21	1.83	0.60
19:F:34:G:C5'	19:F:34:G:C8	2.85	0.60
19:F:85:U:O2'	19:F:86:U:H5''	2.02	0.60
23:I:272:PHE:CB	36:Q:356:VAL:N	2.64	0.60
1:A:1318:THR:HG21	1:A:1324:GLY:CA	2.32	0.59
14:T:438:LEU:HD12	14:T:448:GLN:HB3	1.84	0.59
14:T:459:LEU:HB3	14:T:462:GLU:HG3	1.82	0.59
2:C:667:VAL:H	2:C:824:THR:CG2	2.12	0.59
1:A:193:LEU:HG	1:A:193:LEU:O	2.02	0.59
1:A:915:GLU:OE1	1:A:1012:LYS:NZ	2.36	0.59
1:A:940:ILE:HD11	1:A:1090:ARG:HH12	1.65	0.59
3:E:248:SER:HB3	3:E:265:ARG:HE	1.67	0.59
17:W:347:PHE:HD2	17:W:359:TRP:HB2	1.68	0.59
1:A:293:TRP:CD1	1:A:1136:ARG:CZ	2.85	0.59
5:G:23:U:C6	5:G:23:U:H5''	2.37	0.59
39:r:7:ILE:O	39:s:90:PHE:CB	2.50	0.59
1:A:203:VAL:HG12	1:A:206:TRP:CZ2	2.37	0.59
1:A:293:TRP:NE1	1:A:1136:ARG:HH12	2.01	0.59
1:A:761:ILE:CD1	1:A:772:CYS:SG	2.90	0.59
1:A:1908:LYS:HZ3	17:W:449:ILE:HG13	1.66	0.59
5:G:6:A:H2'	5:G:7:G:C8	2.37	0.59
23:I:688:TYR:O	23:I:703:PHE:CZ	2.47	0.59
19:F:35:A:C5'	19:F:35:A:C8	2.85	0.59
1:A:58:LYS:NZ	1:A:477:LYS:O	2.35	0.59
5:G:19:G:H21	10:O:196:GLN:HG3	1.66	0.59
5:G:20:A:O2'	5:G:21:A:P	2.59	0.59
1:A:977:LEU:HB3	1:A:1097:ILE:HB	1.85	0.59
5:G:121:C:H4'	5:G:121:C:OP1	2.03	0.59
14:T:188:PRO:HG3	14:T:443:THR:HG1	1.64	0.59
19:F:27:A:O2'	19:F:28:A:N7	2.35	0.59
19:F:85:U:O2'	19:F:86:U:OP1	2.20	0.59
22:X:79:VAL:HG13	22:X:79:VAL:O	2.01	0.59
1:A:186:GLU:HB3	1:A:187:PRO:CD	2.32	0.59
1:A:1459:ARG:HG2	1:A:1459:ARG:HH11	1.68	0.59
3:E:102:TYR:O	21:b:102:GLY:HA2	2.03	0.59
7:L:4:ILE:HD11	22:X:78:MET:CE	2.17	0.59
11:P:2:THR:O	11:P:2:THR:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:127:ALA:O	14:T:384:HIS:CE1	2.55	0.59
23:I:731:GLN:NE2	23:I:731:GLN:HA	2.18	0.59
1:A:1941:ARG:NH2	1:A:2012:LEU:O	2.35	0.59
2:C:824:THR:HG23	2:C:824:THR:O	2.02	0.59
5:G:12:G:H2'	5:G:13:C:C5	2.38	0.59
5:G:87:U:C5'	5:G:88:G:OP2	2.51	0.59
6:J:344:GLN:HG2	8:M:132:LEU:HD21	1.83	0.59
17:W:70:VAL:O	17:W:70:VAL:HG13	2.03	0.59
2:C:196:LYS:HD2	26:a:14:GLU:OE1	2.02	0.58
2:C:802:HIS:H	2:C:802:HIS:CD2	2.18	0.58
17:W:72:LEU:HD12	17:W:72:LEU:O	2.02	0.58
22:X:79:VAL:O	22:X:79:VAL:HG22	2.02	0.58
1:A:850:TYR:HD2	1:A:864:LEU:HD21	1.67	0.58
1:A:1318:THR:HG22	1:A:1318:THR:O	2.03	0.58
2:C:758:LEU:HD21	2:C:797:ALA:O	2.03	0.58
5:G:87:U:C5	5:G:88:G:N2	2.71	0.58
16:V:503:TYR:HB2	16:V:546:ASN:HA	1.84	0.58
29:f:70:LEU:CD2	29:f:71:TYR:HD2	2.16	0.58
1:A:1393:ARG:HH11	25:Y:405:MET:HE2	1.68	0.58
2:C:65:TYR:N	2:C:65:TYR:CD2	2.71	0.58
5:G:22:C:O2	5:G:22:C:H2'	2.02	0.58
14:T:244:GLY:O	14:T:271:LYS:NZ	2.34	0.58
20:H:40:C:HO2'	20:H:41:U:C1'	2.16	0.58
23:I:272:PHE:CB	36:Q:355:ASN:CB	2.81	0.58
1:A:182:ILE:O	1:A:182:ILE:HG22	2.02	0.58
14:T:314:ILE:HD12	14:T:324:HIS:HB2	1.86	0.58
1:A:1318:THR:HG21	1:A:1324:GLY:HA3	1.79	0.58
2:C:224:GLY:HA3	2:C:438:ILE:HD12	1.84	0.58
14:T:185:MET:HG3	14:T:186:PRO:HD3	0.76	0.58
23:I:692:SER:CA	23:I:703:PHE:CZ	2.86	0.58
37:o:133:LEU:HD12	37:o:158:ALA:HB2	1.84	0.58
1:A:347:LEU:HD22	1:A:348:PRO:HD3	1.84	0.58
3:E:93:TRP:CH2	21:b:105:GLY:HA2	2.38	0.58
10:O:276:THR:HG23	10:O:279:ALA:H	1.67	0.58
14:T:186:PRO:HG2	14:T:188:PRO:HD3	1.84	0.58
20:H:154:C:OP1	38:p:19:LYS:HD3	2.03	0.58
36:Q:828:GLY:HA2	45:Q:1501:ATP:O1B	2.04	0.58
1:A:1460:HIS:CD2	1:A:1460:HIS:N	2.71	0.58
5:G:22:C:HO2'	5:G:23:U:P	2.27	0.58
7:L:5:MET:HE2	7:L:39:HIS:ND1	2.19	0.58
12:R:310:ARG:HA	12:R:310:ARG:HE	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:I:694:ILE:HD13	23:I:694:ILE:C	2.28	0.58
1:A:955:TRP:CD1	1:A:1189:MET:HE1	2.39	0.58
7:L:135:LYS:HD2	7:L:135:LYS:N	2.17	0.58
10:O:239:LEU:O	10:O:296:ARG:NH1	2.34	0.58
12:R:307:GLN:HA	12:R:307:GLN:NE2	2.14	0.58
19:F:77:C:H2'	19:F:78:A:H5'	1.86	0.58
36:Q:944:TRP:HA	36:Q:947:TYR:CB	2.33	0.58
1:A:1321:GLU:C	1:A:1323:GLY:H	2.11	0.58
1:A:1601:LEU:HA	1:A:1606:ILE:HD12	1.86	0.58
29:m:70:LEU:CD2	29:m:71:TYR:HD2	2.16	0.58
2:C:776:GLU:OE1	2:C:813:ARG:NH2	2.37	0.58
8:M:198:ARG:NH2	20:H:10:C:C4	2.72	0.58
10:O:84:CYS:SG	10:O:159:ARG:NH2	2.77	0.58
25:Y:405:MET:HB3	25:Y:411:LEU:HG	1.85	0.58
25:Y:414:GLU:HG2	25:Y:419:PHE:HZ	1.67	0.58
1:A:873:ASN:ND2	1:A:876:GLU:OE1	2.36	0.57
3:E:209:ILE:HG12	3:E:219:VAL:HG22	1.85	0.57
6:J:266:GLU:OE2	6:J:301:ARG:NH1	2.31	0.57
6:J:285:MET:O	6:J:289:ASN:ND2	2.37	0.57
13:S:83:GLU:HA	13:S:106:ASP:HB2	1.84	0.57
19:F:39:A:C3'	19:F:40:U:H5'	2.34	0.57
23:I:272:PHE:O	36:Q:355:ASN:CB	2.52	0.57
36:Q:828:GLY:CA	45:Q:1501:ATP:O1B	2.52	0.57
1:A:344:ASP:OD1	1:A:344:ASP:N	2.37	0.57
7:L:699:ASN:CB	40:K:110:SER:CB	2.81	0.57
16:V:608:LEU:HB3	16:V:611:PHE:HB3	1.86	0.57
20:H:24:A:H3'	20:H:25:G:H5''	1.86	0.57
1:A:73:HIS:ND1	1:A:88:TYR:OH	2.34	0.57
1:A:300:ASN:HB3	2:C:939:ARG:HH22	1.69	0.57
1:A:1495:PHE:CE2	1:A:1748:ARG:CZ	2.86	0.57
11:P:3:THR:HG22	19:F:79:C:C2	2.39	0.57
1:A:1553:VAL:HG13	1:A:1553:VAL:O	2.04	0.57
12:R:315:LYS:HA	12:R:315:LYS:CE	2.30	0.57
22:X:66:GLN:OE1	22:X:66:GLN:HA	2.04	0.57
26:h:45:ASN:HB3	37:o:22:ARG:NH1	2.18	0.57
31:n:19:LEU:O	31:n:26:HIS:HD2	1.88	0.57
1:A:347:LEU:HD22	1:A:348:PRO:CD	2.35	0.57
10:O:76:LYS:HG2	17:W:111:LEU:HD22	1.85	0.57
14:T:223:SER:OG	14:T:224:ALA:N	2.37	0.57
20:H:154:C:O2'	20:H:155:C:H5'	2.04	0.57
22:X:84:GLU:HA	22:X:84:GLU:OE2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1253:SER:O	1:A:1253:SER:OG	2.07	0.57
14:T:327:SER:O	14:T:357:TRP:HH2	1.88	0.57
17:W:404:ASP:OD2	17:W:406:ARG:NH1	2.38	0.57
22:X:64:ARG:HG3	22:X:64:ARG:HH11	1.68	0.57
3:E:194:TYR:HD2	3:E:214:ASP:HB3	1.70	0.57
22:X:116:ARG:HH11	22:X:116:ARG:CA	2.16	0.57
40:K:181:MET:O	40:K:185:TRP:N	2.36	0.57
1:A:415:SER:OG	1:A:416:GLY:N	2.37	0.57
1:A:1258:LYS:HD2	5:G:126:G:O3'	2.04	0.57
1:A:1560:ILE:O	1:A:1560:ILE:HG22	2.05	0.57
6:J:205:LEU:HD12	6:J:205:LEU:C	2.29	0.57
7:L:256:GLU:OE2	7:L:260:ARG:NH2	2.38	0.57
20:H:152:G:N2	20:H:153:A:C5	2.73	0.57
2:C:758:LEU:HD21	2:C:798:GLN:HA	1.83	0.57
5:G:89:U:OP2	5:G:89:U:H6	1.88	0.57
1:A:480:LYS:NZ	9:N:112:ASN:OD1	2.37	0.57
13:S:11:PRO:O	13:S:29:TRP:NE1	2.36	0.57
19:F:38:G:H2'	19:F:39:A:C8	2.40	0.57
20:H:36:G:O2'	20:H:37:U:H5'	2.04	0.57
25:Y:686:GLU:HA	25:Y:716:THR:O	2.05	0.57
37:o:101:VAL:HG23	37:o:102:GLU:HG3	1.86	0.57
6:J:180:LYS:HE3	7:L:145:ASP:HB3	1.86	0.56
20:H:54:U:H2'	20:H:55:U:H6	1.70	0.56
20:H:73:C:H2'	20:H:74:U:H6	1.70	0.56
20:H:141:C:C2	20:H:142:C:C5	2.93	0.56
36:Q:95:CYS:O	36:Q:98:VAL:N	2.37	0.56
30:l:20:LEU:HD22	30:l:24:TYR:CZ	2.40	0.56
37:o:2:VAL:HG11	37:o:29:TYR:O	2.05	0.56
1:A:761:ILE:HD13	1:A:772:CYS:SG	2.45	0.56
1:A:1515:TRP:CB	20:H:30:A:N3	2.64	0.56
3:E:91:LEU:HD22	3:E:101:ASN:HD21	1.70	0.56
3:E:324:PRO:O	21:b:112:ARG:NH1	2.38	0.56
11:P:10:GLU:HG2	11:P:10:GLU:O	2.05	0.56
17:W:532:LEU:HD11	17:W:568:THR:HG21	1.87	0.56
19:F:39:A:H2'	19:F:40:U:C5'	2.29	0.56
20:H:39:U:C3'	20:H:40:C:C5	2.87	0.56
20:H:70:C:C2	20:H:71:C:C5	2.93	0.56
20:H:149:A:H2'	20:H:150:U:H6	1.71	0.56
1:A:1091:TYR:C	1:A:1091:TYR:CD2	2.83	0.56
1:A:1908:LYS:NZ	17:W:447:TRP:O	2.38	0.56
5:G:83:A:HO2'	5:G:84:U:P	2.28	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:385:TYR:OH	14:T:401:PRO:CD	2.53	0.56
18:B:47:A:O2'	18:B:48:A:H5''	2.06	0.56
20:H:40:C:H5''	20:H:41:U:OP1	2.05	0.56
20:H:88:A:H2'	20:H:89:U:H6	1.70	0.56
20:H:91:U:H2'	20:H:92:U:H6	1.70	0.56
20:H:150:U:H2'	20:H:151:C:H6	1.71	0.56
29:f:11:LEU:CD1	29:f:40:MET:HE2	2.35	0.56
1:A:940:ILE:CD1	1:A:1090:ARG:HH11	2.16	0.56
1:A:1595:GLN:HA	1:A:1598:ASP:HB2	1.86	0.56
1:A:1908:LYS:HZ1	17:W:449:ILE:HG13	1.70	0.56
3:E:307:ARG:HH22	21:b:115:PRO:CB	2.17	0.56
22:X:104:ARG:CZ	22:X:104:ARG:HB2	2.34	0.56
1:A:623:LYS:HB3	41:A:3000:IHP:P4	2.45	0.56
5:G:124:G:N3	5:G:124:G:C2'	2.68	0.56
7:L:106:LYS:HD3	22:X:105:ARG:HH22	1.69	0.56
1:A:1472:THR:O	1:A:1472:THR:HG22	2.05	0.56
3:E:268:ALA:HB2	3:E:272:ARG:HH21	1.69	0.56
11:P:16:ARG:HH12	12:R:220:ARG:CA	2.16	0.56
13:S:66:ASP:CG	13:S:73:GLY:O	2.48	0.56
19:F:45:A:H5'	19:F:46:G:OP2	2.05	0.56
29:m:70:LEU:HD23	29:m:70:LEU:C	2.31	0.56
1:A:537:LYS:CB	19:F:37:C:H41	2.19	0.56
2:C:82:GLN:HG3	14:T:238:LEU:HB2	1.87	0.56
5:G:20:A:H2	10:O:187:THR:CB	2.19	0.56
20:H:69:U:H2'	20:H:70:C:H6	1.71	0.56
20:H:77:C:C2	20:H:78:C:C5	2.94	0.56
1:A:1328:LEU:HB3	1:A:1368:LEU:HD11	1.88	0.56
2:C:196:LYS:HE3	26:a:14:GLU:HB2	1.87	0.56
20:H:83:A:H2'	20:H:84:C:H6	1.71	0.56
23:I:697:PRO:HD3	23:I:730:VAL:CG1	2.35	0.56
31:g:19:LEU:O	31:g:26:HIS:HD2	1.88	0.56
1:A:1265:THR:O	1:A:1265:THR:OG1	2.21	0.56
1:A:1555:LEU:CD2	1:A:1574:ILE:HG13	2.36	0.56
20:H:70:C:H2'	20:H:71:C:H6	1.71	0.56
20:H:77:C:H2'	20:H:78:C:H6	1.71	0.56
20:H:183:G:H2'	20:H:184:C:H6	1.71	0.56
21:b:52:LYS:HE3	27:c:53:VAL:HG21	1.88	0.56
22:X:56:GLU:OE1	22:X:56:GLU:HA	2.05	0.56
30:e:20:LEU:HD22	30:e:24:TYR:CZ	2.40	0.56
21:i:52:LYS:HE3	27:j:53:VAL:HG21	1.88	0.56
1:A:425:PRO:HD3	18:B:26:A:H5'	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:66:TYR:HB3	2:C:67:PRO:CD	2.36	0.56
2:C:750:LEU:HD23	15:U:67:GLU:HA	1.88	0.56
13:S:54:HIS:CD2	13:S:71:GLY:HA3	2.41	0.56
17:W:264:ASN:HD22	30:l:16:GLN:HE22	1.54	0.56
19:F:34:G:H8	19:F:34:G:O5'	1.89	0.56
20:H:68:G:H2'	20:H:69:U:H6	1.70	0.56
23:I:697:PRO:CD	23:I:730:VAL:HG13	2.35	0.56
1:A:293:TRP:CD1	1:A:1136:ARG:NH1	2.74	0.55
1:A:1131:LYS:CD	1:A:1174:PHE:CZ	2.88	0.55
2:C:62:ASP:OD1	2:C:62:ASP:N	2.35	0.55
2:C:233:GLU:OE1	2:C:837:GLN:NE2	2.39	0.55
3:E:101:ASN:HD22	21:b:104:PRO:C	2.13	0.55
1:A:1540:PRO:HB3	1:A:1670:ASP:HA	1.88	0.55
1:A:1592:ASP:O	1:A:1596:VAL:N	2.39	0.55
3:E:307:ARG:HH22	21:b:115:PRO:CG	2.18	0.55
10:O:45:CYS:SG	10:O:48:CYS:N	2.76	0.55
20:H:57:A:H2'	20:H:58:U:H6	1.71	0.55
20:H:150:U:C2	20:H:151:C:C5	2.94	0.55
20:H:152:G:N2	20:H:153:A:C8	2.73	0.55
39:r:127:ALA:HB1	39:s:127:ALA:HB3	1.87	0.55
1:A:537:LYS:CD	19:F:37:C:H41	2.17	0.55
1:A:774:LYS:HD2	20:H:23:A:N7	2.21	0.55
3:E:101:ASN:ND2	21:b:104:PRO:O	2.39	0.55
5:G:120:G:C6	19:F:45:A:C5	2.94	0.55
14:T:397:GLN:CB	14:T:406:ILE:HG23	2.36	0.55
19:F:25:C:H4'	19:F:26:U:O5'	2.05	0.55
20:H:59:A:H2'	20:H:60:U:H6	1.71	0.55
20:H:90:A:H2'	20:H:91:U:H6	1.71	0.55
20:H:181:G:H2'	20:H:182:U:H6	1.70	0.55
24:y:43:THR:C	24:y:45:LYS:N	2.64	0.55
25:Y:419:PHE:C	25:Y:419:PHE:CD2	2.83	0.55
29:m:8:LYS:HB3	29:m:9:PRO:HD3	1.88	0.55
1:A:1252:GLY:HA3	5:G:122:U:O4	2.05	0.55
1:A:1829:GLY:N	19:F:40:U:OP1	2.40	0.55
18:B:94:U:H2'	18:B:95:G:H5''	1.89	0.55
20:H:72:U:C2	20:H:73:C:C5	2.94	0.55
21:b:56:SER:HB2	21:b:59:ALA:O	2.07	0.55
28:d:50:LYS:HG2	28:d:74:TRP:CB	2.36	0.55
29:m:11:LEU:CD1	29:m:40:MET:HE2	2.35	0.55
1:A:377:GLU:O	2:C:342:ARG:NH2	2.38	0.55
1:A:1520:ASN:O	1:A:1523:ARG:CB	2.55	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:6:A:C2	19:F:41:A:N1	2.75	0.55
10:O:34:ILE:HB	12:R:197:ILE:HG12	1.89	0.55
20:H:141:C:H2'	20:H:142:C:H6	1.71	0.55
28:d:94:ARG:HE	28:d:96:ILE:HD11	1.72	0.55
37:o:14:GLN:HG2	37:o:22:ARG:NH2	2.21	0.55
1:A:347:LEU:CD2	1:A:348:PRO:HD3	2.37	0.55
1:A:1095:ILE:O	1:A:1095:ILE:HG22	2.05	0.55
1:A:1979:VAL:HA	1:A:1982:GLN:HB2	1.87	0.55
7:L:124:LYS:N	7:L:125:PRO:HD2	2.21	0.55
13:S:84:ASP:OD1	13:S:108:ASN:ND2	2.38	0.55
19:F:45:A:N3	19:F:73:A:C1'	2.68	0.55
20:H:71:C:C2	20:H:72:U:C5	2.94	0.55
1:A:1184:ASN:OD1	1:A:1195:ARG:NH1	2.40	0.55
6:J:222:ASP:O	6:J:226:ARG:NH1	2.39	0.55
6:J:502:GLU:O	6:J:506:GLU:N	2.39	0.55
14:T:188:PRO:HG3	14:T:443:THR:CB	2.34	0.55
14:T:354:ILE:HB	14:T:368:LEU:HB2	1.88	0.55
19:F:81:C:H4'	19:F:82:A:OP2	2.07	0.55
1:A:470:ARG:HG2	1:A:470:ARG:NH2	2.20	0.55
1:A:603:ARG:NH2	4:4:-6:C:O2	2.38	0.55
1:A:762:ARG:HH22	11:P:226:LYS:HZ3	1.55	0.55
1:A:776:LEU:HD12	1:A:776:LEU:O	2.07	0.55
1:A:1501:LEU:HD12	1:A:1753:LEU:CD2	2.36	0.55
5:G:120:G:C8	5:G:120:G:C5'	2.87	0.55
12:R:97:LYS:NZ	13:S:146:GLU:OE1	2.40	0.55
20:H:69:U:C2	20:H:70:C:C5	2.94	0.55
20:H:73:C:C2	20:H:74:U:C5	2.94	0.55
20:H:83:A:C4	20:H:84:C:C5	2.95	0.55
23:I:692:SER:CB	23:I:703:PHE:CE2	2.90	0.55
29:f:70:LEU:HD23	29:f:70:LEU:C	2.31	0.55
1:A:36:LYS:NZ	17:W:163:GLN:O	2.40	0.55
2:C:846:VAL:HG22	2:C:887:LEU:HD11	1.88	0.55
12:R:312:MET:O	12:R:312:MET:HE3	2.07	0.55
20:H:54:U:C2	20:H:55:U:C5	2.94	0.55
20:H:91:U:C2	20:H:92:U:C5	2.95	0.55
20:H:147:G:C4	20:H:148:C:C5	2.94	0.55
20:H:149:A:C4	20:H:150:U:C5	2.95	0.55
20:H:179:C:H2'	20:H:180:G:C8	2.38	0.55
1:A:1553:VAL:O	1:A:1553:VAL:HG22	2.07	0.55
2:C:561:LYS:NZ	2:C:614:TYR:O	2.40	0.55
14:T:343:PRO:HB3	14:T:356:LEU:HD23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:183:G:C4	20:H:184:C:C5	2.94	0.55
21:i:56:SER:HB2	21:i:59:ALA:O	2.07	0.55
1:A:110:TRP:O	1:A:190:ALA:HB3	2.07	0.54
1:A:178:TYR:CE2	1:A:183:LEU:HD13	2.41	0.54
1:A:939:TRP:NE1	1:A:1049:ASP:OD2	2.39	0.54
1:A:1555:LEU:HD21	1:A:1574:ILE:CG1	2.37	0.54
5:G:22:C:O2'	5:G:23:U:P	2.66	0.54
20:H:68:G:C4	20:H:69:U:C5	2.95	0.54
20:H:71:C:H2'	20:H:72:U:H6	1.70	0.54
23:I:443:GLU:O	23:I:448:ASN:N	2.40	0.54
23:I:692:SER:CB	23:I:703:PHE:CZ	2.88	0.54
23:I:704:TRP:CH2	23:I:727:ARG:CG	2.90	0.54
1:A:461:HIS:NE2	18:B:26:A:N6	2.55	0.54
1:A:1827:TRP:HZ3	1:A:1836:LEU:HB3	1.72	0.54
9:N:126:LEU:CD2	19:F:22:A:C2	2.90	0.54
17:W:233:LYS:HG3	17:W:355:TYR:HE2	1.72	0.54
19:F:34:G:H8	19:F:34:G:H5''	1.70	0.54
1:A:105:ASN:HD22	1:A:129:VAL:CG1	2.20	0.54
1:A:579:GLN:HG3	1:A:629:PHE:H	1.73	0.54
3:E:145:LYS:NZ	3:E:181:ILE:O	2.39	0.54
6:J:201:ARG:HG2	6:J:201:ARG:NH2	2.21	0.54
20:H:59:A:C4	20:H:60:U:C5	2.95	0.54
20:H:105:G:C6	27:j:20:LYS:HD3	2.42	0.54
20:H:153:A:C3'	20:H:154:C:C5'	2.85	0.54
20:H:181:G:C4	20:H:182:U:C5	2.95	0.54
28:k:94:ARG:HE	28:k:96:ILE:HD11	1.72	0.54
1:A:453:TYR:O	1:A:457:ASN:ND2	2.40	0.54
1:A:1501:LEU:HD11	1:A:1753:LEU:HD13	1.87	0.54
1:A:1533:ARG:HG3	1:A:1751:LEU:HA	1.90	0.54
1:A:1838:LYS:HG2	1:A:1871:PRO:HG2	1.88	0.54
2:C:64:LYS:HE3	2:C:64:LYS:O	2.07	0.54
8:M:133:ARG:NH1	19:F:88:G:H5'	2.22	0.54
8:M:198:ARG:HH12	20:H:10:C:H41	1.54	0.54
14:T:210:ILE:HG12	14:T:221:THR:HG22	1.89	0.54
14:T:353:THR:HG22	14:T:369:THR:HG22	1.90	0.54
29:f:8:LYS:HB3	29:f:9:PRO:HD3	1.88	0.54
1:A:182:ILE:HD11	1:A:562:VAL:HG13	1.90	0.54
1:A:714:SER:O	1:A:718:ARG:NH1	2.40	0.54
5:G:17:U:O2	10:O:198:ILE:HD11	2.07	0.54
12:R:111:VAL:HG21	14:T:402:ASP:HB3	1.89	0.54
17:W:326:ARG:NH1	17:W:363:THR:O	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:465:PRO:HG2	17:W:481:MET:HE3	1.89	0.54
20:H:72:U:H2'	20:H:73:C:H6	1.71	0.54
20:H:88:A:C4	20:H:89:U:C5	2.95	0.54
20:H:90:A:C4	20:H:91:U:C5	2.95	0.54
23:I:624:GLU:O	23:I:628:GLN:N	2.41	0.54
23:I:699:THR:HG23	23:I:700:THR:HG23	1.89	0.54
1:A:108:MET:HB3	1:A:109:PRO:HD2	1.90	0.54
2:C:65:TYR:HB2	2:C:66:TYR:CD2	2.42	0.54
5:G:21:A:O2'	5:G:22:C:C5'	2.55	0.54
23:I:273:GLU:C	36:Q:357:ALA:CB	2.80	0.54
1:A:67:ARG:HD3	1:A:179:ALA:HB2	1.89	0.54
1:A:1787:ARG:NH2	1:A:1804:ASN:O	2.41	0.54
3:E:62:LEU:HD23	21:b:107:GLY:HA2	1.88	0.54
3:E:155:ASN:ND2	3:E:172:ASP:OD1	2.40	0.54
7:L:782:LYS:O	7:L:786:HIS:N	2.39	0.54
9:N:2:PRO:HG2	9:N:4:VAL:HA	1.90	0.54
14:T:345:ILE:CD1	14:T:359:LEU:HD13	2.38	0.54
23:I:661:ASP:CB	23:I:694:ILE:HD11	2.29	0.54
23:I:704:TRP:CE3	23:I:727:ARG:CG	2.83	0.54
23:I:723:MET:O	23:I:727:ARG:HB2	2.07	0.54
23:I:727:ARG:HB3	23:I:727:ARG:NH2	2.21	0.54
39:q:106:ALA:HB1	39:t:106:ALA:HB3	1.89	0.54
1:A:425:PRO:CD	18:B:26:A:H5'	2.38	0.54
1:A:1094:ARG:H	1:A:1094:ARG:CD	2.21	0.54
12:R:170:LYS:HE3	18:B:16:U:OP1	2.08	0.54
22:X:72:GLN:NE2	22:X:72:GLN:CA	2.70	0.54
25:Y:402:ILE:O	25:Y:406:ILE:HD12	2.07	0.54
28:d:88:LYS:HG3	28:d:89:PRO:HD2	1.89	0.54
1:A:189:GLU:O	1:A:571:ALA:HB2	2.08	0.54
1:A:1144:LYS:O	1:A:1148:ASN:ND2	2.41	0.54
1:A:1318:THR:HG22	1:A:1324:GLY:CA	2.31	0.54
1:A:1390:ALA:HB2	25:Y:410:VAL:CG1	2.38	0.54
2:C:66:TYR:CE1	14:T:457:GLY:HA2	2.43	0.54
24:y:43:THR:O	24:y:45:LYS:N	2.41	0.54
1:A:955:TRP:HE1	1:A:976:MET:HE1	1.73	0.54
2:C:704:VAL:HG23	2:C:705:VAL:HG13	1.89	0.54
14:T:397:GLN:O	14:T:406:ILE:HG22	2.08	0.54
19:F:80:G:H5''	19:F:81:C:P	2.48	0.54
20:H:40:C:C5'	20:H:41:U:OP1	2.56	0.54
20:H:57:A:C4	20:H:58:U:C5	2.95	0.54
3:E:128:SER:OG	3:E:129:THR:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:190:PHE:N	3:E:190:PHE:CD2	2.76	0.53
5:G:5:G:H2'	5:G:6:A:C8	2.44	0.53
20:H:147:G:H2'	20:H:148:C:C6	2.43	0.53
27:j:68:PHE:HB2	28:k:100:PHE:HB3	1.90	0.53
1:A:1468:ASN:OD1	5:G:130:G:H5''	2.04	0.53
2:C:259:LYS:HG2	42:C:1500:GTP:C6	2.43	0.53
2:C:343:LEU:HD13	2:C:373:ILE:HD11	1.91	0.53
7:L:264:LYS:O	7:L:268:LYS:N	2.36	0.53
13:S:126:HIS:CD2	13:S:126:HIS:N	2.76	0.53
14:T:213:GLU:HG3	14:T:218:TRP:CD2	2.39	0.53
15:U:77:MET:O	15:U:81:GLY:N	2.40	0.53
17:W:449:ILE:HG22	17:W:451:VAL:H	1.73	0.53
1:A:1087:LEU:HB2	1:A:1098:PHE:HB3	1.89	0.53
1:A:1632:PHE:HE1	1:A:1659:LYS:HG2	1.73	0.53
5:G:100:C:N1	5:G:101:U:C5	2.77	0.53
9:N:40:LYS:CE	9:N:40:LYS:HA	2.38	0.53
14:T:442:ARG:HG2	14:T:443:THR:HG23	1.90	0.53
17:W:103:GLN:O	17:W:108:ARG:NH2	2.40	0.53
22:X:95:ARG:NH1	22:X:95:ARG:CB	2.72	0.53
1:A:941:LYS:HG3	1:A:941:LYS:O	2.09	0.53
9:N:42:LYS:O	9:N:42:LYS:HG3	2.08	0.53
12:R:301:ALA:O	12:R:304:MET:HB3	2.08	0.53
14:T:185:MET:N	14:T:186:PRO:CD	2.71	0.53
22:X:114:GLU:N	22:X:114:GLU:OE2	2.41	0.53
23:I:273:GLU:O	36:Q:357:ALA:HB3	2.07	0.53
14:T:409:LEU:N	14:T:409:LEU:CD1	2.72	0.53
20:H:153:A:H3'	20:H:154:C:C5'	2.38	0.53
20:H:164:C:H5'	20:H:164:C:C6	2.44	0.53
23:I:310:LYS:O	23:I:311:MET:C	2.51	0.53
1:A:1501:LEU:CD2	1:A:1501:LEU:N	2.71	0.53
1:A:1519:THR:CB	5:G:119:A:N1	2.72	0.53
2:C:137:HIS:HB2	2:C:239:THR:HG23	1.91	0.53
7:L:65:ARG:NH2	23:I:721:LYS:CE	2.70	0.53
7:L:569:GLN:HA	39:q:114:CYS:O	2.07	0.53
10:O:81:CYS:HB3	10:O:84:CYS:HB2	1.90	0.53
11:P:13:ARG:HG3	11:P:13:ARG:HH11	1.72	0.53
14:T:405:PHE:CD1	14:T:405:PHE:C	2.84	0.53
20:H:15:U:H2'	20:H:16:U:OP2	2.08	0.53
23:I:102:ALA:O	36:Q:934:TYR:HA	2.08	0.53
1:A:762:ARG:NH2	11:P:227:TYR:OH	2.42	0.53
1:A:1664:ILE:HD13	1:A:1703:ILE:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:677:GLU:OE1	2:C:681:LYS:NZ	2.38	0.53
3:E:133:VAL:HG21	3:E:169:THR:HG21	1.90	0.53
12:R:315:LYS:CE	12:R:315:LYS:CA	2.85	0.53
14:T:270:VAL:HG21	14:T:305:THR:HG21	1.89	0.53
14:T:314:ILE:HD11	14:T:326:LEU:HD11	1.90	0.53
19:F:58:G:O2'	19:F:59:G:OP1	2.20	0.53
19:F:58:G:O2'	19:F:59:G:P	2.66	0.53
1:A:856:LEU:H	1:A:856:LEU:HD12	1.74	0.53
6:J:497:TYR:HA	6:J:537:TRP:N	2.24	0.53
17:W:209:SER:O	17:W:213:GLN:N	2.41	0.53
17:W:443:ARG:NH1	17:W:452:ASP:OD2	2.41	0.53
22:X:116:ARG:N	22:X:116:ARG:CD	2.72	0.53
31:n:17:LEU:HD23	31:n:72:ALA:HA	1.91	0.53
1:A:1257:THR:HB	1:A:1320:LYS:HE2	1.91	0.53
3:E:243:LEU:HD23	3:E:250:LEU:HD12	1.91	0.53
6:J:242:ILE:O	6:J:242:ILE:HG22	2.08	0.53
12:R:334:ARG:NH1	12:R:334:ARG:CB	2.71	0.53
13:S:125:LYS:C	13:S:126:HIS:CD2	2.87	0.53
23:I:727:ARG:CG	23:I:727:ARG:NH2	2.70	0.53
1:A:974:ASN:HD22	1:A:1178:TYR:HD2	1.57	0.53
1:A:1491:LYS:HD2	1:A:1709:TYR:CD1	2.37	0.53
5:G:95:U:O2'	5:G:96:U:C5'	2.49	0.53
5:G:130:G:C2'	5:G:130:G:N3	2.72	0.53
12:R:60:ASP:N	12:R:60:ASP:OD1	2.42	0.53
19:F:40:U:H2'	19:F:41:A:C8	2.44	0.53
20:H:39:U:C4	20:H:40:C:N4	2.77	0.52
20:H:154:C:OP2	38:p:19:LYS:CD	2.56	0.52
1:A:623:LYS:O	41:A:3000:IHP:O24	2.26	0.52
1:A:1091:TYR:CD2	1:A:1092:ILE:HG13	2.45	0.52
2:C:92:PRO:HB3	14:T:276:GLU:O	2.09	0.52
2:C:801:LEU:CD2	2:C:801:LEU:N	2.72	0.52
3:E:171:SER:OG	3:E:173:ASP:OD1	2.26	0.52
16:V:584:LYS:HG3	16:V:634:ILE:HG12	1.91	0.52
19:F:26:U:O2'	19:F:27:A:P	2.67	0.52
19:F:42:C:H2'	19:F:43:A:C1'	2.40	0.52
1:A:1251:SER:O	1:A:1298:ARG:NH2	2.41	0.52
2:C:758:LEU:HD12	2:C:761:SER:HB2	1.90	0.52
22:X:57:ARG:HH21	22:X:57:ARG:CG	2.20	0.52
22:X:113:LYS:HZ2	22:X:113:LYS:CB	2.23	0.52
5:G:20:A:O2'	10:O:193:LEU:CD2	2.50	0.52
5:G:20:A:H2	10:O:187:THR:CG2	2.21	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:39:U:H3'	20:H:40:C:H5	1.72	0.52
22:X:68:GLU:OE2	22:X:68:GLU:HA	2.05	0.52
23:I:592:ALA:HB3	23:I:623:VAL:HG12	1.91	0.52
1:A:94:TYR:HB2	12:R:207:MET:HE1	1.91	0.52
1:A:300:ASN:HB3	2:C:939:ARG:HH12	1.74	0.52
1:A:850:TYR:CD2	1:A:864:LEU:HD21	2.43	0.52
1:A:1468:ASN:OD1	5:G:130:G:H4'	2.08	0.52
1:A:1593:LEU:HA	1:A:1596:VAL:HB	1.91	0.52
18:B:27:U:O2'	18:B:28:A:O5'	2.25	0.52
19:F:58:G:H2'	19:F:59:G:C8	2.44	0.52
20:H:154:C:OP2	38:p:19:LYS:HD3	2.09	0.52
22:X:114:GLU:HB2	22:X:115:TYR:CD2	2.44	0.52
28:k:107:ILE:HG22	28:k:108:VAL:CG2	2.39	0.52
30:l:87:LEU:HB2	31:n:61:VAL:HB	1.92	0.52
11:P:49:ASP:OD2	14:T:215:GLY:HA3	2.10	0.52
17:W:305:LEU:HD21	17:W:313:ILE:HG23	1.92	0.52
20:H:33:G:H3'	20:H:33:G:OP2	2.10	0.52
20:H:153:A:C2'	20:H:154:C:C5'	2.86	0.52
23:I:309:ALA:O	23:I:310:LYS:C	2.52	0.52
2:C:938:ARG:O	2:C:942:GLY:N	2.42	0.52
5:G:21:A:HO2'	5:G:22:C:P	2.32	0.52
6:J:206:LEU:HD22	7:L:175:GLN:NE2	2.25	0.52
13:S:15:TYR:HB3	13:S:163:TYR:HB2	1.91	0.52
27:c:68:PHE:HB2	28:d:100:PHE:HB3	1.90	0.52
1:A:1501:LEU:CD1	1:A:1753:LEU:CD2	2.88	0.52
5:G:82:G:C4'	17:W:541:LYS:HZ1	2.10	0.52
7:L:7:LYS:CB	7:L:40:ARG:HA	2.39	0.52
12:R:307:GLN:NE2	12:R:307:GLN:CA	2.72	0.52
14:T:185:MET:N	14:T:186:PRO:HD2	2.25	0.52
14:T:294:LEU:HD12	14:T:303:LEU:HD11	1.92	0.52
22:X:119:LEU:HD13	23:I:712:VAL:HG13	1.92	0.52
23:I:728:ARG:O	23:I:731:GLN:CA	2.58	0.52
36:Q:531:TRP:CB	36:Q:635:GLN:CB	2.88	0.52
28:k:50:LYS:HG2	28:k:74:TRP:CB	2.36	0.52
1:A:1354:ARG:HG3	15:U:19:VAL:HG22	1.92	0.52
2:C:799:GLU:OE1	2:C:799:GLU:N	2.43	0.52
5:G:100:C:C6	5:G:101:U:H5	2.28	0.52
9:N:41:ARG:HA	19:F:28:A:O4'	2.08	0.52
14:T:213:GLU:HB2	14:T:218:TRP:CZ3	2.45	0.52
17:W:243:VAL:HG13	17:W:245:GLU:H	1.74	0.52
18:B:22:U:O2	18:B:22:U:H2'	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:77:C:C2'	19:F:78:A:H5'	2.40	0.52
23:I:681:ILE:HD11	23:I:714:HIS:ND1	2.25	0.52
37:o:5:THR:CG2	37:o:8:LEU:H	2.23	0.52
1:A:776:LEU:HD22	1:A:900:ASP:HB2	1.92	0.52
1:A:1056:HIS:NE2	1:A:1060:GLU:OE2	2.43	0.52
2:C:207:GLY:O	2:C:238:ASN:ND2	2.42	0.52
3:E:93:TRP:CZ3	21:b:105:GLY:C	2.87	0.52
5:G:81:U:O2'	5:G:82:G:OP2	2.24	0.52
6:J:239:ARG:HB2	6:J:239:ARG:NH1	2.22	0.52
8:M:236:ASN:ND2	8:M:242:ALA:O	2.43	0.52
16:V:590:LEU:HD22	16:V:599:LEU:HD13	1.90	0.52
16:V:620:ASN:HB3	16:V:623:ASN:HB2	1.92	0.52
19:F:5:U:H5'	19:F:6:C:OP2	2.10	0.52
30:e:87:LEU:HB2	31:g:61:VAL:HB	1.92	0.52
32:v:53:HIS:CB	33:w:149:CYS:O	2.58	0.52
2:C:797:ALA:HB3	2:C:800:PRO:HB3	1.92	0.51
2:C:801:LEU:N	2:C:801:LEU:HD22	2.24	0.51
6:J:427:LYS:HE2	23:I:512:ASP:OD2	2.10	0.51
8:M:133:ARG:CZ	19:F:88:G:H5'	2.40	0.51
8:M:224:ARG:HD2	20:H:14:C:N4	2.24	0.51
16:V:549:LYS:O	16:V:553:HIS:ND1	2.43	0.51
18:B:18:C:C2'	18:B:19:A:O5'	2.58	0.51
36:Q:809:ALA:HB2	36:Q:1131:VAL:CB	2.40	0.51
11:P:66:ARG:O	11:P:69:ALA:N	2.43	0.51
12:R:334:ARG:HH11	12:R:334:ARG:CG	2.23	0.51
18:B:89:U:O2'	26:a:64:ARG:NH2	2.43	0.51
19:F:43:A:C6	19:F:44:G:O6	2.64	0.51
28:d:85:LYS:HG2	28:d:85:LYS:O	2.09	0.51
1:A:976:MET:HG2	1:A:1187:PHE:HB3	1.92	0.51
1:A:977:LEU:HD23	1:A:1097:ILE:HD12	1.91	0.51
5:G:89:U:OP2	5:G:89:U:C6	2.62	0.51
13:S:25:LEU:HD23	13:S:98:LEU:HD22	1.93	0.51
14:T:418:THR:HG21	14:T:468:CYS:H	1.75	0.51
20:H:107:A:C6	20:H:108:G:C5	2.99	0.51
23:I:731:GLN:NE2	23:I:731:GLN:CA	2.71	0.51
31:g:17:LEU:HD23	31:g:72:ALA:HA	1.91	0.51
1:A:312:TYR:OH	2:C:886:ASP:OD2	2.27	0.51
1:A:1793:THR:HG22	19:F:43:A:C5'	2.34	0.51
7:L:222:LEU:HD12	12:R:84:ASN:HB3	1.93	0.51
39:s:112:ALA:C	40:K:15:ALA:CB	2.82	0.51
1:A:461:HIS:CD2	18:B:26:A:N6	2.78	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1070:ASP:OD1	1:A:1073:SER:OG	2.24	0.51
5:G:100:C:C2'	5:G:101:U:C6	2.77	0.51
20:H:143:A:N3	20:H:143:A:C3'	2.73	0.51
22:X:115:TYR:CD2	22:X:115:TYR:N	2.78	0.51
23:I:84:HIS:O	23:I:85:ARG:C	2.52	0.51
39:q:106:ALA:CB	39:t:106:ALA:CB	2.87	0.51
1:A:181:ASN:N	1:A:181:ASN:ND2	2.59	0.51
2:C:682:LYS:HG3	2:C:803:ARG:CD	2.40	0.51
3:E:174:GLY:O	3:E:191:GLN:HA	2.11	0.51
14:T:399:LYS:O	14:T:403:GLY:HA2	2.10	0.51
17:W:72:LEU:C	17:W:72:LEU:CD1	2.84	0.51
23:I:83:LYS:O	23:I:84:HIS:C	2.51	0.51
39:r:112:ALA:CB	40:K:36:VAL:O	2.55	0.51
1:A:361:HIS:HE1	16:V:324:HIS:CB	2.24	0.51
1:A:888:GLN:O	1:A:889:ARG:NH1	2.39	0.51
2:C:476:CYS:SG	2:C:477:HIS:N	2.83	0.51
9:N:36:PRO:C	9:N:38:GLU:N	2.69	0.51
16:V:570:LEU:HD13	16:V:611:PHE:HA	1.93	0.51
17:W:341:ASN:ND2	17:W:345:THR:OG1	2.37	0.51
40:K:90:PRO:CB	40:K:109:ASN:C	2.83	0.51
1:A:641:MET:HA	1:A:644:ILE:HG22	1.93	0.51
17:W:392:VAL:HG12	17:W:424:ILE:HD13	1.92	0.51
23:I:698:ARG:HE	23:I:698:ARG:CA	2.24	0.51
3:E:124:LEU:HB3	3:E:136:TRP:HB2	1.93	0.51
10:O:235:TYR:HB3	10:O:301:LYS:HB2	1.93	0.51
11:P:7:PRO:O	11:P:7:PRO:HG2	2.11	0.51
11:P:16:ARG:NH1	12:R:220:ARG:CA	2.72	0.51
11:P:38:HIS:HB3	14:T:282:ARG:HH21	1.75	0.51
23:I:692:SER:CA	23:I:703:PHE:CE2	2.88	0.51
21:i:50:LYS:HG2	21:i:51:ILE:HG13	1.93	0.51
1:A:858:GLN:OE1	1:A:861:ARG:HG3	2.11	0.51
1:A:1312:PRO:HG2	1:A:1314:VAL:HG12	1.93	0.51
1:A:1828:ALA:C	19:F:40:U:OP1	2.54	0.51
2:C:95:LYS:HB3	2:C:95:LYS:HZ1	1.73	0.51
10:O:50:ARG:NH1	10:O:122:GLU:OE1	2.44	0.51
16:V:535:THR:HA	16:V:538:ARG:HB2	1.92	0.51
18:B:94:U:H5	28:d:104:ASP:O	1.94	0.51
29:m:51:ILE:HG22	29:m:56:SER:HB2	1.93	0.51
2:C:66:TYR:HB3	2:C:67:PRO:HD2	1.91	0.50
14:T:190:TRP:CE3	14:T:190:TRP:O	2.64	0.50
19:F:50:A:O2'	19:F:51:U:P	2.69	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:111:G:O3'	20:H:112:G:O4'	2.29	0.50
22:X:96:GLN:CA	22:X:96:GLN:NE2	2.72	0.50
1:A:139:VAL:O	1:A:143:GLN:N	2.40	0.50
1:A:934:ARG:NH1	1:A:934:ARG:CG	2.72	0.50
5:G:130:G:N3	5:G:130:G:H2'	2.22	0.50
17:W:249:TYR:CD2	31:n:11:LYS:HG2	2.45	0.50
19:F:85:U:C3'	19:F:86:U:C5'	2.90	0.50
20:H:106:G:H5'	29:m:25:TRP:HH2	1.76	0.50
23:I:668:CYS:SG	23:I:669:LEU:N	2.83	0.50
36:Q:929:CYS:O	36:Q:930:GLU:C	2.54	0.50
1:A:266:SER:OG	1:A:271:MET:O	2.28	0.50
1:A:766:THR:HG1	18:B:39:C:N4	2.09	0.50
1:A:856:LEU:HD12	1:A:856:LEU:N	2.27	0.50
2:C:300:LEU:HA	2:C:306:ASN:HD22	1.76	0.50
3:E:93:TRP:CZ3	21:b:105:GLY:HA3	2.46	0.50
5:G:2:U:O2	19:F:45:A:C6	2.61	0.50
5:G:7:G:H2'	5:G:8:C:C6	2.46	0.50
5:G:20:A:C2	10:O:187:THR:CG2	2.94	0.50
9:N:51:ARG:NH2	17:W:192:PHE:O	2.45	0.50
14:T:289:SER:OG	14:T:308:ARG:NH2	2.44	0.50
17:W:130:ARG:CD	19:F:22:A:N7	2.72	0.50
23:I:727:ARG:HH21	23:I:727:ARG:C	2.18	0.50
29:m:20:MET:HE2	29:m:30:LYS:HB2	1.94	0.50
40:K:18:TYR:CB	40:K:171:GLN:CB	2.90	0.50
1:A:1798:LEU:HB2	5:G:96:U:O4'	2.10	0.50
5:G:98:U:H2'	5:G:99:C:C6	2.45	0.50
22:X:64:ARG:N	22:X:64:ARG:HD2	2.24	0.50
25:Y:405:MET:HE1	25:Y:410:VAL:HG11	1.93	0.50
37:o:92:GLU:OE1	38:p:25:ARG:NE	2.39	0.50
37:o:102:GLU:HG2	37:o:128:LYS:HZ1	1.75	0.50
1:A:92:LEU:HG	1:A:652:LEU:HD13	1.93	0.50
1:A:856:LEU:C	1:A:856:LEU:CD1	2.84	0.50
1:A:858:GLN:C	1:A:858:GLN:NE2	2.70	0.50
1:A:944:ASP:HB3	1:A:1436:TRP:NE1	2.27	0.50
2:C:210:ASN:HB3	2:C:636:TYR:HB2	1.93	0.50
5:G:21:A:OP2	10:O:193:LEU:CG	2.58	0.50
13:S:55:ARG:HH21	13:S:57:ILE:HD11	1.77	0.50
14:T:398:TRP:N	14:T:406:ILE:HG22	2.27	0.50
20:H:100:U:O2'	26:h:64:ARG:NH2	2.43	0.50
21:b:50:LYS:HG2	21:b:51:ILE:HG13	1.93	0.50
22:X:113:LYS:C	22:X:113:LYS:CD	2.84	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:Y:413:LYS:H	25:Y:413:LYS:CD	2.18	0.50
29:f:20:MET:HE2	29:f:30:LYS:HB2	1.94	0.50
1:A:1700:GLY:H	1:A:1717:ASN:HB2	1.77	0.50
2:C:607:LEU:O	2:C:611:ASN:ND2	2.45	0.50
12:R:316:GLU:OE1	12:R:320:HIS:CD2	2.64	0.50
14:T:347:THR:HG21	14:T:357:TRP:HE1	1.76	0.50
17:W:445:TRP:HE1	17:W:452:ASP:HB3	1.77	0.50
18:B:100:C:H2'	18:B:101:U:C6	2.47	0.50
22:X:116:ARG:HG3	23:I:717:GLU:CD	2.36	0.50
1:A:705:LYS:HG2	20:H:15:U:C4	2.47	0.50
1:A:1214:TRP:NE1	1:A:1276:GLU:OE1	2.45	0.50
1:A:1321:GLU:C	1:A:1323:GLY:N	2.68	0.50
2:C:700:ILE:O	2:C:740:THR:OG1	2.28	0.50
12:R:124:VAL:HG21	14:T:442:ARG:NH1	2.25	0.50
22:X:116:ARG:HH11	22:X:116:ARG:CG	2.24	0.50
23:I:511:LEU:HD12	23:I:543:ARG:HD2	1.92	0.50
26:h:55:VAL:HG21	37:o:67:LYS:NZ	2.25	0.50
26:h:75:ASP:O	26:h:78:LYS:HG2	2.12	0.50
1:A:658:ARG:HD3	19:F:67:G:OP1	2.12	0.50
1:A:862:GLU:O	1:A:862:GLU:HG2	2.11	0.50
1:A:978:GLU:OE2	1:A:1188:ASN:N	2.36	0.50
2:C:183:SER:OG	2:C:480:LYS:NZ	2.44	0.50
5:G:6:A:H2	19:F:41:A:C2	2.16	0.50
17:W:130:ARG:HD3	19:F:22:A:C5	2.46	0.50
19:F:43:A:N6	19:F:44:G:O6	2.44	0.50
19:F:45:A:H1'	19:F:73:A:C2	2.47	0.50
36:Q:1005:PHE:O	36:Q:1008:LEU:N	2.44	0.50
3:E:253:ASN:HD21	3:E:302:ALA:HB1	1.76	0.50
6:J:239:ARG:C	6:J:239:ARG:CD	2.82	0.50
6:J:440:LEU:HG	6:J:445:LYS:HD2	1.93	0.50
7:L:145:ASP:OD1	7:L:145:ASP:N	2.40	0.50
10:O:116:TYR:O	10:O:120:ASN:ND2	2.45	0.50
18:B:20:G:OP1	18:B:20:G:H4'	2.12	0.50
23:I:265:TYR:CA	23:I:274:LYS:CB	2.80	0.50
23:I:311:MET:O	23:I:312:GLU:C	2.52	0.50
1:A:880:ARG:HG3	1:A:884:HIS:CD2	2.47	0.49
1:A:1459:ARG:HH11	1:A:1459:ARG:CG	2.23	0.49
5:G:100:C:N1	5:G:101:U:H5	2.10	0.49
13:S:72:ARG:CD	17:W:71:HIS:HB3	2.35	0.49
28:k:41:GLN:H	28:k:115:ILE:HB	1.76	0.49
1:A:1761:PRO:HG2	1:A:1761:PRO:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:340:PRO:HB2	3:E:356:ILE:HB	1.94	0.49
5:G:8:C:H2'	5:G:9:C:C6	2.46	0.49
5:G:27:U:HO2'	5:G:28:A:C5'	2.26	0.49
10:O:22:ILE:HD13	17:W:111:LEU:HD23	1.94	0.49
12:R:332:ARG:HH11	12:R:332:ARG:CG	2.05	0.49
17:W:527:ASP:OD1	17:W:531:LYS:N	2.44	0.49
29:f:51:ILE:HG22	29:f:56:SER:HB2	1.93	0.49
30:e:15:VAL:O	31:g:33:GLY:HA3	2.12	0.49
30:e:20:LEU:HD13	31:g:61:VAL:CG2	2.43	0.49
1:A:409:ARG:NH1	18:B:25:C:C6	2.81	0.49
1:A:435:CYS:HB3	4:4:-11:G:N2	2.27	0.49
1:A:790:ARG:NH1	1:A:986:GLU:O	2.44	0.49
1:A:1286:ASP:OD1	1:A:1354:ARG:NH2	2.45	0.49
1:A:1386:TRP:CB	25:Y:410:VAL:CG2	2.80	0.49
2:C:673:LYS:HG3	2:C:686:THR:HG23	1.95	0.49
3:E:107:GLY:O	3:E:143:ARG:NH1	2.45	0.49
5:G:21:A:OP2	10:O:193:LEU:CD1	2.60	0.49
10:O:132:ARG:HD3	10:O:133:PRO:HD2	1.95	0.49
18:B:23:C:O2'	18:B:24:G:H3'	2.11	0.49
20:H:104:U:O2'	29:m:65:ARG:NH2	2.45	0.49
22:X:60:GLU:OE1	22:X:60:GLU:HA	2.11	0.49
23:I:272:PHE:CB	36:Q:355:ASN:CA	2.90	0.49
1:A:467:GLN:CG	18:B:19:A:C5	2.95	0.49
1:A:1493:THR:C	1:A:1495:PHE:N	2.69	0.49
1:A:1555:LEU:HD23	1:A:1556:ASP:H	1.77	0.49
6:J:247:LYS:CD	19:F:83:A:OP2	2.58	0.49
12:R:321:GLU:HA	12:R:324:LEU:HD23	1.94	0.49
14:T:392:PRO:HG3	14:T:415:ILE:HA	1.93	0.49
25:Y:397:PRO:O	25:Y:400:TRP:HB3	2.13	0.49
28:d:41:GLN:H	28:d:115:ILE:HB	1.76	0.49
1:A:1136:ARG:NH1	1:A:1136:ARG:CG	2.72	0.49
1:A:1494:TYR:CE1	1:A:1744:ARG:NH2	2.80	0.49
2:C:682:LYS:HB3	2:C:797:ALA:HB2	1.95	0.49
5:G:100:C:C2	5:G:101:U:H5	2.22	0.49
10:O:68:THR:HA	10:O:83:THR:HG22	1.93	0.49
18:B:57:G:H2'	18:B:58:U:H5'	1.95	0.49
18:B:93:U:O2'	29:f:65:ARG:NH2	2.45	0.49
22:X:77:ASN:N	22:X:77:ASN:OD1	2.45	0.49
30:l:15:VAL:O	31:n:33:GLY:HA3	2.12	0.49
1:A:209:ASP:HB3	1:A:212:PRO:HA	1.93	0.49
1:A:425:PRO:HG3	18:B:26:A:H5''	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:J:263:SER:O	6:J:267:ARG:N	2.45	0.49
12:R:124:VAL:CG2	14:T:442:ARG:NH1	2.75	0.49
12:R:124:VAL:CG2	14:T:442:ARG:HH12	2.24	0.49
17:W:103:GLN:NE2	17:W:111:LEU:O	2.46	0.49
18:B:87:A:H2'	29:f:39:TYR:CE2	2.47	0.49
19:F:8:C:C6	19:F:8:C:C5'	2.91	0.49
19:F:45:A:H2	19:F:73:A:C1'	2.19	0.49
23:I:681:ILE:CD1	23:I:714:HIS:ND1	2.76	0.49
37:o:66:LEU:HD21	37:o:69:LEU:HG	1.94	0.49
1:A:193:LEU:C	1:A:193:LEU:CD1	2.85	0.49
2:C:857:VAL:HG22	2:C:873:ALA:HB2	1.95	0.49
5:G:7:G:OP2	5:G:7:G:H8	1.95	0.49
5:G:90:C:C5'	5:G:90:C:C6	2.90	0.49
6:J:237:LYS:NZ	19:F:79:C:P	2.84	0.49
19:F:50:A:HO2'	19:F:51:U:P	2.35	0.49
20:H:98:G:H2'	29:m:39:TYR:CE2	2.47	0.49
39:q:60:PRO:CB	39:s:93:ARG:CB	2.91	0.49
39:t:72:PRO:CB	40:K:81:LEU:CB	2.90	0.49
1:A:1252:GLY:O	5:G:123:C:N4	2.46	0.49
5:G:8:C:H42	19:F:39:A:H61	1.59	0.49
7:L:51:TYR:O	7:L:58:ILE:HD11	2.12	0.49
14:T:400:PHE:HB3	14:T:401:PRO:CD	2.35	0.49
19:F:42:C:H2'	19:F:43:A:H1'	1.94	0.49
23:I:273:GLU:C	36:Q:357:ALA:HB2	2.38	0.49
26:a:75:ASP:O	26:a:78:LYS:HG2	2.12	0.49
1:A:66:VAL:HG11	1:A:487:LEU:HD11	1.94	0.49
1:A:609:LYS:CE	41:A:3000:IHP:O31	2.61	0.49
1:A:642:ARG:NE	18:B:55:C:O2	2.31	0.49
1:A:1201:ARG:O	1:A:1203:SER:N	2.45	0.49
2:C:259:LYS:HD2	2:C:262:ARG:HD2	1.93	0.49
5:G:120:G:C6	19:F:45:A:N6	2.81	0.49
6:J:204:GLU:HG2	6:J:204:GLU:O	2.13	0.49
7:L:569:GLN:CB	39:q:114:CYS:C	2.86	0.49
17:W:82:ASN:H	17:W:83:PRO:HD2	1.76	0.49
19:F:34:G:C8	19:F:34:G:H5''	2.47	0.49
25:Y:412:SER:OG	25:Y:415:GLU:HG3	2.13	0.49
1:A:1011:ALA:HB2	7:L:80:THR:HB	1.95	0.49
1:A:1275:ARG:NH1	1:A:1373:GLN:O	2.40	0.49
1:A:1563:HIS:ND1	1:A:1563:HIS:N	2.60	0.49
3:E:214:ASP:OD1	3:E:214:ASP:N	2.46	0.49
3:E:215:ASN:O	3:E:232:ARG:NH1	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:N:35:GLU:HG2	9:N:35:GLU:O	2.12	0.49
16:V:528:ILE:HA	16:V:531:GLU:HB2	1.93	0.49
16:V:620:ASN:O	16:V:624:THR:N	2.43	0.49
19:F:37:C:H3'	19:F:37:C:H6	1.78	0.49
22:X:89:PHE:CD2	22:X:90:LEU:HD23	2.48	0.49
28:d:107:ILE:HG22	28:d:108:VAL:CG2	2.39	0.49
1:A:1275:ARG:HD2	1:A:1375:TRP:CE2	2.47	0.48
1:A:1456:THR:OG1	1:A:1457:HIS:N	2.46	0.48
1:A:1798:LEU:HB2	5:G:96:U:C5'	2.43	0.48
7:L:192:ARG:NH2	7:L:198:ILE:O	2.46	0.48
13:S:20:MET:HE2	13:S:141:ARG:HB3	1.95	0.48
22:X:114:GLU:HB2	22:X:115:TYR:CE2	2.48	0.48
1:A:435:CYS:SG	4:4:-11:G:N2	2.78	0.48
1:A:1588:SER:O	1:A:1592:ASP:N	2.36	0.48
1:A:1891:LEU:HD22	1:A:1937:ILE:HD12	1.94	0.48
1:A:1910:THR:HG22	17:W:412:GLN:OE1	2.13	0.48
2:C:440:SER:HB2	2:C:443:VAL:H	1.77	0.48
37:o:2:VAL:O	37:o:2:VAL:HG13	2.13	0.48
1:A:1418:ARG:HB2	1:A:1461:ASP:O	2.13	0.48
1:A:1501:LEU:H	1:A:1501:LEU:HD23	1.78	0.48
3:E:60:MET:HA	21:b:109:ALA:HA	1.94	0.48
7:L:29:ASN:HB3	20:H:24:A:H2	1.78	0.48
10:O:229:LYS:HD3	10:O:277:ARG:HH12	1.78	0.48
11:P:212:ASN:CB	14:T:458:SER:H	2.13	0.48
14:T:427:LEU:HB3	14:T:439:TRP:HB2	1.95	0.48
19:F:50:A:O2'	19:F:51:U:OP1	2.27	0.48
1:A:1502:PHE:O	1:A:1502:PHE:CD1	2.67	0.48
2:C:856:HIS:CE1	34:u:103:GLN:HA	2.44	0.48
3:E:93:TRP:CZ3	21:b:105:GLY:CA	2.97	0.48
7:L:191:LEU:HD21	17:W:352:TYR:CE1	2.49	0.48
14:T:247:SER:OG	14:T:248:THR:N	2.46	0.48
20:H:107:A:C2	20:H:108:G:C4	3.01	0.48
22:X:100:ILE:HA	22:X:103:GLN:HG3	1.95	0.48
22:X:112:LEU:HD21	23:I:717:GLU:HB2	1.95	0.48
23:I:681:ILE:CG2	23:I:710:PHE:CZ	2.80	0.48
30:l:20:LEU:HD13	31:n:61:VAL:CG2	2.42	0.48
1:A:975:VAL:HB	1:A:1099:PHE:HB2	1.96	0.48
1:A:1096:HIS:CD2	1:A:1096:HIS:N	2.80	0.48
1:A:1258:LYS:HB2	1:A:1258:LYS:HZ1	1.77	0.48
1:A:1699:THR:HA	1:A:1717:ASN:HD22	1.78	0.48
9:N:126:LEU:HD23	19:F:22:A:C2	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:39:U:C2'	20:H:40:C:C6	2.92	0.48
23:I:699:THR:HG23	23:I:699:THR:O	2.12	0.48
1:A:532:THR:CB	5:G:3:A:O5'	2.61	0.48
1:A:1921:ASP:OD2	1:A:1968:TRP:N	2.46	0.48
2:C:560:VAL:HG12	2:C:561:LYS:H	1.79	0.48
5:G:12:G:H2'	5:G:13:C:C6	2.49	0.48
7:L:18:ILE:O	7:L:22:ALA:N	2.47	0.48
7:L:55:ASP:HB3	7:L:58:ILE:HG13	1.95	0.48
14:T:405:PHE:C	14:T:405:PHE:HD1	2.22	0.48
19:F:31:U:H2'	19:F:32:U:H5'	1.95	0.48
39:q:60:PRO:CB	39:s:94:GLN:HA	2.43	0.48
3:E:75:HIS:ND1	3:E:77:ASN:OD1	2.46	0.48
5:G:6:A:N1	19:F:41:A:C2	2.79	0.48
5:G:90:C:OP2	5:G:90:C:C6	2.66	0.48
10:O:245:GLU:OE1	10:O:249:ARG:NH1	2.46	0.48
11:P:13:ARG:HH11	11:P:13:ARG:CG	2.26	0.48
18:B:92:U:O4	21:b:38:MET:HG3	2.14	0.48
22:X:119:LEU:HD13	23:I:712:VAL:CG1	2.43	0.48
23:I:694:ILE:CD1	23:I:694:ILE:C	2.86	0.48
23:I:727:ARG:NH2	23:I:727:ARG:C	2.72	0.48
1:A:702:LYS:NZ	8:M:127:TYR:OH	2.47	0.48
1:A:850:TYR:OH	1:A:863:GLU:CD	2.56	0.48
1:A:1498:TRP:CD1	1:A:1498:TRP:C	2.85	0.48
3:E:78:GLY:O	3:E:336:HIS:NE2	2.45	0.48
6:J:201:ARG:NH2	6:J:201:ARG:CG	2.73	0.48
23:I:725:ARG:C	23:I:725:ARG:CD	2.85	0.48
32:v:140:HIS:O	33:w:70:VAL:CB	2.62	0.48
1:A:668:VAL:O	1:A:668:VAL:HG12	2.14	0.48
2:C:749:THR:OG1	2:C:792:LEU:O	2.30	0.48
5:G:19:G:H21	10:O:196:GLN:CG	2.27	0.48
19:F:43:A:C6	19:F:44:G:C6	3.02	0.48
20:H:39:U:C2'	20:H:40:C:C5	2.97	0.48
22:X:72:GLN:NE2	22:X:72:GLN:C	2.72	0.48
25:Y:426:LEU:HG	25:Y:427:PRO:HD2	1.96	0.48
36:Q:943:ARG:O	36:Q:947:TYR:CB	2.61	0.48
1:A:1265:THR:O	1:A:1265:THR:HG23	2.12	0.48
1:A:1471:ARG:CB	1:A:1471:ARG:NH2	2.68	0.48
1:A:1521:ALA:CB	5:G:120:G:H5''	2.44	0.48
3:E:191:GLN:N	3:E:191:GLN:CD	2.71	0.48
10:O:147:LEU:O	10:O:151:ALA:N	2.47	0.48
12:R:265:ASP:N	12:R:265:ASP:OD1	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:264:ASN:HD22	30:l:16:GLN:NE2	2.12	0.48
22:X:116:ARG:CG	22:X:116:ARG:NH1	2.73	0.48
23:I:71:TRP:N	24:y:29:PHE:O	2.47	0.48
23:I:661:ASP:HA	23:I:664:ALA:HB3	1.95	0.48
31:g:35:ASP:HB2	31:g:36:PRO:CD	2.42	0.48
39:r:127:ALA:HB1	39:s:127:ALA:CB	2.44	0.48
1:A:681:PHE:HE2	1:A:746:LYS:HG3	1.78	0.47
1:A:818:GLU:O	1:A:818:GLU:HG2	2.13	0.47
1:A:1716:GLY:O	1:A:1718:TRP:NE1	2.47	0.47
6:J:183:ALA:HB3	7:L:142:ILE:HG12	1.96	0.47
14:T:186:PRO:HG3	14:T:442:ARG:NH2	2.29	0.47
17:W:523:VAL:HB	17:W:535:TRP:HB2	1.96	0.47
20:H:44:U:H2'	20:H:45:C:C6	2.48	0.47
22:X:100:ILE:HA	22:X:103:GLN:CG	2.44	0.47
22:X:112:LEU:C	22:X:112:LEU:CD1	2.87	0.47
1:A:280:GLU:HG2	18:B:48:A:O4'	2.14	0.47
1:A:824:PRO:O	1:A:933:ARG:NH1	2.45	0.47
1:A:1657:THR:OG1	1:A:1659:LYS:O	2.28	0.47
2:C:82:GLN:OE1	2:C:82:GLN:HA	2.03	0.47
2:C:114:TYR:O	2:C:117:ASP:HB2	2.13	0.47
3:E:294:SER:HB3	3:E:299:LYS:HB2	1.96	0.47
7:L:6:ILE:C	7:L:6:ILE:CD1	2.82	0.47
14:T:190:TRP:O	14:T:190:TRP:CD2	2.67	0.47
23:I:329:LEU:CB	36:Q:353:LEU:CA	2.90	0.47
23:I:555:ASP:OD1	23:I:555:ASP:N	2.46	0.47
23:I:593:LYS:HE2	23:I:631:MET:HG3	1.95	0.47
37:o:153:LYS:O	37:o:157:GLU:HG3	2.14	0.47
39:q:61:ILE:N	39:s:93:ARG:CB	2.75	0.47
1:A:347:LEU:HA	1:A:347:LEU:HD23	1.54	0.47
1:A:1248:LEU:HD21	1:A:1295:ILE:HG22	1.95	0.47
1:A:1537:TRP:HE3	1:A:1751:LEU:HD13	1.79	0.47
2:C:800:PRO:CB	2:C:803:ARG:HB2	2.44	0.47
9:N:51:ARG:HH21	17:W:193:LEU:HD23	1.78	0.47
10:O:88:LEU:O	12:R:183:GLN:NE2	2.47	0.47
14:T:267:ASP:OD2	14:T:269:GLN:NE2	2.47	0.47
14:T:459:LEU:HB3	14:T:462:GLU:HG2	1.96	0.47
14:T:471:ASP:OD1	14:T:471:ASP:N	2.46	0.47
19:F:8:C:H6	19:F:8:C:C5'	2.09	0.47
29:m:10:PHE:CE2	30:l:78:MET:HB2	2.49	0.47
29:m:36:VAL:HG12	29:m:37:ASP:N	2.29	0.47
1:A:53:PHE:HE2	1:A:55:ASP:HB3	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:ASP:O	9:N:4:VAL:HG21	2.15	0.47
1:A:589:THR:OG1	1:A:590:GLY:N	2.46	0.47
1:A:761:ILE:HD11	1:A:772:CYS:SG	2.54	0.47
2:C:114:TYR:CB	26:a:79:ASN:HB3	2.43	0.47
9:N:126:LEU:HD23	19:F:22:A:N1	2.29	0.47
12:R:334:ARG:HH11	12:R:334:ARG:HG3	1.80	0.47
20:H:42:G:H8	20:H:42:G:O5'	1.98	0.47
22:X:80:ARG:HD2	22:X:80:ARG:O	2.14	0.47
29:f:10:PHE:CE2	30:e:78:MET:HB2	2.48	0.47
36:Q:929:CYS:O	36:Q:931:THR:N	2.47	0.47
1:A:1091:TYR:CE2	1:A:1092:ILE:HG13	2.49	0.47
1:A:1132:LYS:HG3	1:A:1139:ARG:NH1	2.27	0.47
2:C:453:TYR:CZ	2:C:575:GLN:HB2	2.49	0.47
18:B:20:G:H1'	18:B:21:A:OP1	2.14	0.47
20:H:30:A:O4'	22:X:73:PHE:HE1	1.96	0.47
20:H:77:C:H2'	20:H:78:C:C6	2.49	0.47
20:H:151:C:C2	20:H:152:G:N7	2.82	0.47
22:X:55:TYR:CD1	22:X:56:GLU:HG2	2.48	0.47
23:I:272:PHE:C	36:Q:355:ASN:CB	2.88	0.47
32:v:24:PHE:HA	32:v:33:ARG:O	2.14	0.47
1:A:467:GLN:HG2	18:B:19:A:C5	2.49	0.47
1:A:704:ASN:ND2	20:H:16:U:OP2	2.48	0.47
1:A:1386:TRP:HB3	25:Y:410:VAL:HG23	1.88	0.47
1:A:1555:LEU:CD2	1:A:1574:ILE:CG1	2.91	0.47
6:J:239:ARG:NH1	6:J:239:ARG:CG	2.72	0.47
7:L:15:GLU:HG2	7:L:151:MET:HE1	1.96	0.47
12:R:315:LYS:NZ	12:R:315:LYS:CA	2.72	0.47
20:H:68:G:H2'	20:H:69:U:C6	2.50	0.47
20:H:103:U:O4	21:i:38:MET:HG3	2.14	0.47
23:I:727:ARG:HH21	23:I:727:ARG:HG2	1.76	0.47
1:A:439:GLN:O	1:A:444:ARG:NH1	2.48	0.47
1:A:711:GLN:HE22	20:H:18:U:H3'	1.79	0.47
1:A:1108:ASP:OD2	1:A:1112:ARG:NH1	2.48	0.47
1:A:1494:TYR:CD2	1:A:1494:TYR:O	2.68	0.47
1:A:1515:TRP:CB	20:H:30:A:N9	2.75	0.47
2:C:750:LEU:N	2:C:751:PRO:CD	2.78	0.47
3:E:69:VAL:O	3:E:331:ASN:ND2	2.38	0.47
5:G:17:U:O2	10:O:198:ILE:CD1	2.63	0.47
8:M:211:ILE:HD12	8:M:212:ASN:HB2	1.95	0.47
14:T:335:THR:OG1	14:T:336:VAL:N	2.47	0.47
20:H:33:G:O2'	20:H:34:U:O4'	2.23	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:39:U:C3'	20:H:40:C:C6	2.97	0.47
20:H:72:U:H2'	20:H:73:C:C6	2.49	0.47
22:X:59:GLN:CD	22:X:59:GLN:C	2.83	0.47
27:c:20:LYS:HE2	27:c:63:ASN:O	2.15	0.47
28:d:108:VAL:CG1	29:f:62:VAL:HG13	2.44	0.47
26:h:43:MET:HB3	26:h:46:ILE:HD11	1.97	0.47
1:A:127:SER:OG	1:A:495:GLN:NE2	2.45	0.47
1:A:857:ASN:C	1:A:861:ARG:HD2	2.13	0.47
1:A:1258:LYS:CD	5:G:126:G:O3'	2.63	0.47
1:A:1465:TRP:O	1:A:1465:TRP:CD1	2.67	0.47
1:A:1471:ARG:NH2	1:A:1471:ARG:CG	2.78	0.47
1:A:1515:TRP:CB	20:H:30:A:C2	2.97	0.47
1:A:1615:HIS:HB3	1:A:1618:LYS:HB2	1.96	0.47
7:L:123:LEU:HD22	7:L:125:PRO:CD	2.44	0.47
12:R:325:ARG:C	12:R:325:ARG:CD	2.84	0.47
13:S:97:ILE:CG2	13:S:128:ILE:HG23	2.45	0.47
19:F:25:C:O4'	19:F:26:U:OP2	2.33	0.47
20:H:59:A:H2'	20:H:60:U:C6	2.50	0.47
20:H:181:G:H2'	20:H:182:U:C6	2.50	0.47
22:X:64:ARG:HH11	22:X:64:ARG:CG	2.28	0.47
22:X:95:ARG:CZ	22:X:95:ARG:CB	2.88	0.47
1:A:1034:LEU:HB2	1:A:1037:ALA:HB2	1.97	0.47
1:A:1136:ARG:HG2	1:A:1136:ARG:NH1	2.13	0.47
1:A:1471:ARG:HH21	1:A:1471:ARG:CG	2.26	0.47
2:C:852:ARG:NH1	4:4:-13:C:H2'	2.27	0.47
7:L:135:LYS:N	7:L:135:LYS:CD	2.78	0.47
10:O:65:PHE:CE2	19:F:24:A:C6	2.97	0.47
10:O:196:GLN:HE21	10:O:208:PRO:HG2	1.80	0.47
12:R:318:GLU:HA	12:R:318:GLU:OE2	2.13	0.47
13:S:125:LYS:HB2	13:S:126:HIS:CD2	2.48	0.47
20:H:83:A:H2'	20:H:84:C:C6	2.49	0.47
25:Y:644:TYR:HA	25:Y:660:TYR:O	2.14	0.47
31:g:64:GLY:HA2	31:g:67:ILE:HD12	1.97	0.47
27:j:6:PHE:CD1	27:j:6:PHE:C	2.93	0.47
1:A:702:LYS:HD2	8:M:124:PHE:HE2	1.80	0.47
1:A:1470:TYR:CD2	1:A:1470:TYR:O	2.69	0.47
2:C:785:ARG:HG2	2:C:786:ASN:HB2	1.97	0.47
7:L:54:LEU:O	7:L:55:ASP:C	2.58	0.47
20:H:54:U:H2'	20:H:55:U:C6	2.50	0.47
20:H:91:U:H2'	20:H:92:U:C6	2.50	0.47
20:H:183:G:H2'	20:H:184:C:C6	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:a:24:THR:O	26:a:51:ARG:NH1	2.46	0.47
26:a:43:MET:HB3	26:a:46:ILE:HD11	1.97	0.47
30:e:18:ILE:HA	30:e:21:ILE:HD12	1.97	0.47
26:h:45:ASN:HB3	37:o:22:ARG:HH11	1.79	0.47
3:E:266:PRO:CB	7:L:788:TYR:CB	2.92	0.46
5:G:27:U:HO2'	5:G:28:A:C4'	2.27	0.46
6:J:523:PRO:O	6:J:527:LYS:N	2.46	0.46
14:T:329:HIS:HB3	14:T:351:ASP:OD2	2.15	0.46
27:c:6:PHE:CD1	27:c:6:PHE:C	2.93	0.46
29:f:36:VAL:HG12	29:f:37:ASP:N	2.29	0.46
1:A:58:LYS:HB2	1:A:477:LYS:HE2	1.97	0.46
1:A:832:TYR:HD2	1:A:835:ASP:HB3	1.79	0.46
1:A:1310:ARG:NH2	1:A:1563:HIS:O	2.42	0.46
1:A:2015:GLU:CD	22:X:55:TYR:HE2	2.24	0.46
5:G:98:U:C2'	5:G:99:C:C6	2.98	0.46
7:L:7:LYS:HG3	7:L:40:ARG:HA	1.97	0.46
12:R:124:VAL:HG22	12:R:126:ASN:N	2.30	0.46
13:S:66:ASP:OD1	13:S:73:GLY:O	2.32	0.46
14:T:186:PRO:HG3	14:T:442:ARG:HH22	1.81	0.46
1:A:53:PHE:CE1	18:B:65:G:C5'	2.98	0.46
1:A:663:ARG:NH1	19:F:64:U:OP2	2.49	0.46
1:A:1070:ASP:OD1	1:A:1070:ASP:N	2.39	0.46
1:A:1798:LEU:HD22	5:G:96:U:O4'	2.16	0.46
1:A:1860:GLN:HG2	1:A:1883:VAL:HB	1.97	0.46
12:R:147:THR:HG23	14:T:360:VAL:HG12	1.96	0.46
20:H:30:A:C4'	22:X:73:PHE:CZ	2.98	0.46
20:H:78:C:H2'	20:H:79:G:H8	1.81	0.46
39:s:65:PRO:O	39:s:66:PRO:C	2.59	0.46
1:A:372:PRO:HG2	2:C:342:ARG:HG2	1.97	0.46
1:A:435:CYS:CB	4:4:-11:G:N2	2.74	0.46
1:A:467:GLN:NE2	18:B:19:A:C6	2.84	0.46
1:A:1543:ASN:HB2	1:A:1569:LEU:CD2	2.45	0.46
1:A:1760:GLU:HG2	1:A:1761:PRO:HD2	1.98	0.46
2:C:843:VAL:HG13	2:C:871:ILE:HD11	1.97	0.46
3:E:114:GLU:OE2	3:E:116:HIS:NE2	2.43	0.46
6:J:195:LEU:HD22	7:L:24:MET:HE1	1.96	0.46
6:J:196:ARG:HA	8:M:208:ILE:HD11	1.98	0.46
6:J:454:ASN:O	6:J:458:PHE:N	2.46	0.46
7:L:216:PHE:CE1	12:R:219:PRO:HG3	2.51	0.46
19:F:36:A:O2'	19:F:37:C:P	2.74	0.46
20:H:70:C:H2'	20:H:71:C:C6	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:81:G:H2'	20:H:82:G:H8	1.81	0.46
20:H:142:C:H2'	20:H:143:A:H5'	1.98	0.46
20:H:153:A:C8	20:H:154:C:H5'	2.50	0.46
22:X:108:GLU:HG2	23:I:724:LEU:HD21	1.97	0.46
27:c:61:ARG:HB3	27:c:64:ASN:HD22	1.80	0.46
27:j:61:ARG:HB3	27:j:64:ASN:HD22	1.80	0.46
37:o:56:LYS:HG2	37:o:58:ASP:HB2	1.97	0.46
1:A:345:PRO:N	1:A:346:ASP:N	2.64	0.46
1:A:1418:ARG:O	1:A:1420:ASN:N	2.49	0.46
1:A:1771:LEU:HD22	1:A:1812:PRO:HG2	1.97	0.46
1:A:2015:GLU:CD	22:X:55:TYR:CE2	2.94	0.46
2:C:174:GLU:OE2	2:C:182:LYS:N	2.44	0.46
2:C:221:ILE:O	2:C:495:ARG:NH1	2.48	0.46
5:G:7:G:H2'	5:G:8:C:H6	1.80	0.46
16:V:498:ALA:HB1	16:V:543:LYS:HB3	1.97	0.46
17:W:420:ALA:O	17:W:438:ASP:N	2.48	0.46
20:H:69:U:H2'	20:H:70:C:C6	2.49	0.46
20:H:107:A:C6	20:H:108:G:C6	3.04	0.46
23:I:725:ARG:NH1	23:I:729:SER:HB2	2.30	0.46
28:k:108:VAL:CG1	29:m:62:VAL:HG13	2.45	0.46
1:A:1494:TYR:OH	1:A:1735:LYS:HG2	2.16	0.46
2:C:750:LEU:C	2:C:750:LEU:CD1	2.87	0.46
6:J:224:LYS:HE2	6:J:255:LEU:HD13	1.96	0.46
7:L:5:MET:HE2	7:L:39:HIS:CE1	2.51	0.46
20:H:141:C:H2'	20:H:142:C:C6	2.50	0.46
23:I:624:GLU:HB3	23:I:627:GLN:HB2	1.98	0.46
30:l:18:ILE:HA	30:l:21:ILE:HD12	1.98	0.46
1:A:942:PRO:HG2	1:A:1438:VAL:HG12	1.96	0.46
1:A:1560:ILE:HD11	1:A:1668:TRP:CD2	2.51	0.46
1:A:1797:ASN:OD1	5:G:96:U:H5''	2.16	0.46
8:M:133:ARG:HH12	19:F:88:G:H5'	1.81	0.46
8:M:198:ARG:NH1	20:H:10:C:H41	2.10	0.46
13:S:125:LYS:HB2	13:S:126:HIS:HD2	1.80	0.46
14:T:210:ILE:HG13	14:T:480:ALA:HB2	1.97	0.46
17:W:497:ASN:OD1	17:W:497:ASN:N	2.49	0.46
30:e:16:GLN:HB3	30:e:19:ASN:OD1	2.16	0.46
37:o:61:PRO:O	37:o:86:ALA:HB1	2.16	0.46
1:A:1131:LYS:NZ	1:A:1131:LYS:CB	2.73	0.46
1:A:1501:LEU:HD13	1:A:1753:LEU:HD22	1.98	0.46
1:A:1700:GLY:O	1:A:1717:ASN:N	2.49	0.46
7:L:77:LEU:HD22	12:R:285:ALA:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:R:310:ARG:HE	12:R:310:ARG:CA	2.28	0.46
20:H:39:U:N3	20:H:40:C:N4	2.63	0.46
22:X:62:LYS:C	22:X:62:LYS:CE	2.85	0.46
22:X:71:GLU:C	22:X:71:GLU:CD	2.84	0.46
1:A:1562:MET:HE2	1:A:1562:MET:HB2	1.54	0.46
2:C:508:LYS:HA	2:C:524:ILE:HG22	1.98	0.46
11:P:77:ASP:O	11:P:78:ARG:NE	2.47	0.46
14:T:191:HIS:ND1	14:T:191:HIS:N	2.58	0.46
14:T:397:GLN:HB2	14:T:406:ILE:HG23	1.98	0.46
17:W:525:SER:OG	17:W:526:GLY:N	2.49	0.46
27:j:20:LYS:HE2	27:j:63:ASN:O	2.15	0.46
1:A:464:PRO:HD2	18:B:20:G:O2'	2.16	0.46
1:A:773:LYS:HB3	20:H:23:A:N3	2.31	0.46
1:A:829:PRO:HG2	1:A:832:TYR:HB2	1.96	0.46
1:A:1493:THR:C	1:A:1495:PHE:H	2.23	0.46
1:A:1640:SER:HB2	1:A:1650:ASP:HB3	1.98	0.46
2:C:66:TYR:CD2	2:C:66:TYR:N	2.83	0.46
3:E:90:ILE:HB	3:E:105:LEU:HB2	1.98	0.46
12:R:233:PRO:HB2	12:R:234:SER:H	1.62	0.46
20:H:152:G:O2'	20:H:153:A:H1'	2.16	0.46
21:b:17:MET:HE1	21:b:82:VAL:HG22	1.98	0.46
22:X:116:ARG:CB	22:X:116:ARG:NH1	2.72	0.46
23:I:668:CYS:SG	23:I:691:CYS:HB3	2.56	0.46
23:I:668:CYS:SG	23:I:691:CYS:CB	3.04	0.46
30:e:68:THR:O	30:e:68:THR:HG22	2.15	0.46
30:l:68:THR:HG22	30:l:68:THR:O	2.15	0.46
37:o:14:GLN:HG3	37:o:44:PHE:HE1	1.80	0.46
37:o:120:ILE:HG22	37:o:120:ILE:O	2.16	0.46
1:A:843:LEU:HD22	1:A:867:ILE:HG23	1.98	0.45
1:A:1258:LYS:HE2	5:G:126:G:C3'	2.46	0.45
1:A:1453:PHE:CE1	1:A:1465:TRP:CH2	3.03	0.45
1:A:1801:LYS:HD2	19:F:42:C:OP1	2.16	0.45
1:A:1827:TRP:CE3	1:A:1833:LEU:HD12	2.51	0.45
5:G:87:U:H5''	5:G:88:G:OP2	2.15	0.45
14:T:193:PRO:HD2	14:T:495:ALA:HB1	1.98	0.45
18:B:23:C:HO2'	18:B:24:G:P	2.38	0.45
20:H:79:G:H2'	20:H:80:A:H8	1.81	0.45
20:H:114:A:H2'	20:H:115:G:H8	1.81	0.45
23:I:516:ALA:HA	23:I:520:ILE:HD11	1.98	0.45
28:d:46:CYS:HB3	28:d:48:ASN:OD1	2.15	0.45
28:k:46:CYS:HB3	28:k:48:ASN:OD1	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:TRP:O	1:A:190:ALA:CB	2.64	0.45
1:A:1116:GLU:OE2	11:P:196:ASN:ND2	2.47	0.45
1:A:1470:TYR:CD2	1:A:1470:TYR:C	2.91	0.45
1:A:1940:LEU:HD23	1:A:1943:LEU:HD12	1.97	0.45
8:M:125:SER:HB3	12:R:239:VAL:HG22	1.97	0.45
10:O:131:THR:HG23	17:W:111:LEU:H	1.81	0.45
13:S:142:VAL:HG13	13:S:157:VAL:HG11	1.99	0.45
18:B:93:U:O4	28:d:64:ASN:ND2	2.42	0.45
20:H:71:C:H2'	20:H:72:U:C6	2.50	0.45
20:H:150:U:H2'	20:H:151:C:C6	2.50	0.45
38:p:72:PHE:HA	38:p:73:PRO:HD3	1.83	0.45
39:t:65:PRO:O	39:t:66:PRO:C	2.58	0.45
1:A:53:PHE:CE1	18:B:65:G:H5''	2.52	0.45
1:A:1418:ARG:HH12	1:A:1464:LEU:CA	2.15	0.45
1:A:1697:SER:OG	1:A:1699:THR:O	2.32	0.45
1:A:1892:PRO:HD3	1:A:1941:ARG:HH21	1.81	0.45
20:H:74:U:H2'	20:H:75:A:H8	1.81	0.45
22:X:92:GLU:C	22:X:92:GLU:CD	2.84	0.45
23:I:599:TYR:HA	23:I:602:LEU:HG	1.99	0.45
21:i:17:MET:HE1	21:i:82:VAL:HG22	1.99	0.45
30:l:16:GLN:HB3	30:l:19:ASN:OD1	2.16	0.45
31:n:64:GLY:HA2	31:n:67:ILE:HD12	1.97	0.45
1:A:344:ASP:HA	1:A:345:PRO:HD2	1.46	0.45
1:A:537:LYS:HB2	19:F:37:C:N4	2.30	0.45
1:A:1418:ARG:NH1	1:A:1463:LYS:O	2.50	0.45
2:C:725:ASP:HB3	2:C:728:ALA:HB3	1.98	0.45
5:G:90:C:O2'	5:G:91:A:O5'	2.35	0.45
5:G:94:C:H2'	5:G:95:U:C6	2.51	0.45
20:H:80:A:H2'	20:H:81:G:H8	1.81	0.45
20:H:89:U:H2'	20:H:90:A:H8	1.82	0.45
20:H:92:U:H2'	20:H:93:A:H8	1.82	0.45
20:H:112:G:H2'	20:H:113:G:C8	2.50	0.45
1:A:26:SER:H	1:A:29:LYS:HD2	1.81	0.45
1:A:803:ALA:HB2	12:R:287:LEU:HA	1.98	0.45
1:A:1430:LEU:HB2	25:Y:400:TRP:CZ3	2.52	0.45
1:A:1487:HIS:NE2	1:A:1671:TYR:CZ	2.84	0.45
1:A:1495:PHE:HE2	1:A:1748:ARG:HE	1.55	0.45
6:J:267:ARG:HH11	7:L:216:PHE:HB2	1.82	0.45
7:L:699:ASN:O	7:L:703:MET:N	2.50	0.45
8:M:224:ARG:CD	20:H:14:C:N4	2.79	0.45
20:H:67:C:H2'	20:H:68:G:H8	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:90:A:H2'	20:H:91:U:C6	2.50	0.45
20:H:182:U:H2'	20:H:183:G:H8	1.81	0.45
23:I:242:ALA:HB1	36:Q:527:ILE:HA	1.98	0.45
26:a:77:LEU:HD12	26:a:77:LEU:N	2.32	0.45
28:d:72:GLU:HG2	28:d:74:TRP:CE3	2.51	0.45
1:A:540:PHE:HB3	1:A:544:PHE:HB3	1.98	0.45
1:A:1510:GLU:CB	5:G:124:G:N1	2.75	0.45
1:A:2001:SER:OG	22:X:54:LEU:HD22	2.12	0.45
2:C:750:LEU:HD12	2:C:753:GLU:HG2	1.98	0.45
6:J:197:GLU:O	6:J:201:ARG:HG2	2.17	0.45
6:J:308:ARG:HH21	6:J:339:TRP:HE3	1.64	0.45
14:T:477:LEU:HB3	14:T:489:TYR:HB2	1.98	0.45
19:F:58:G:HO2'	19:F:59:G:P	2.34	0.45
20:H:56:A:H2'	20:H:57:A:H8	1.82	0.45
28:k:22:GLU:OE1	28:k:22:GLU:HA	2.17	0.45
28:k:72:GLU:HG2	28:k:74:TRP:CE3	2.51	0.45
39:s:65:PRO:O	39:s:67:SER:N	2.49	0.45
1:A:299:ILE:HG12	1:A:1346:THR:HG21	1.99	0.45
1:A:1066:GLN:NE2	25:Y:426:LEU:HD13	2.32	0.45
10:O:258:ILE:HD13	10:O:261:ILE:HD11	1.99	0.45
20:H:57:A:H2'	20:H:58:U:C6	2.50	0.45
20:H:148:C:H2'	20:H:149:A:H8	1.82	0.45
28:d:22:GLU:OE1	28:d:22:GLU:HA	2.17	0.45
31:g:38:MET:HE2	31:g:67:ILE:HG21	1.98	0.45
1:A:53:PHE:HE1	18:B:65:G:H5''	1.81	0.45
1:A:211:GLN:OE1	1:A:214:ARG:NH1	2.48	0.45
1:A:1146:ASP:OD2	1:A:1182:ASN:ND2	2.50	0.45
1:A:1400:ASN:CG	25:Y:1034:LYS:CB	2.90	0.45
2:C:348:TYR:HE1	2:C:367:ARG:HG2	1.82	0.45
2:C:663:CYS:HB2	2:C:828:MET:HB2	1.98	0.45
8:M:148:THR:HA	8:M:151:ARG:HB2	1.99	0.45
11:P:41:ILE:HD11	14:T:318:ARG:HB3	1.99	0.45
13:S:41:GLU:OE2	13:S:44:ARG:NH2	2.38	0.45
14:T:191:HIS:CE1	14:T:440:ASP:CG	2.90	0.45
19:F:12:G:H2'	19:F:13:G:O4'	2.17	0.45
22:X:55:TYR:HD1	22:X:56:GLU:HG2	1.82	0.45
22:X:67:GLN:CD	22:X:67:GLN:C	2.85	0.45
23:I:272:PHE:CB	36:Q:355:ASN:HA	2.46	0.45
1:A:197:PRO:HA	1:A:204:LEU:HD13	1.98	0.45
1:A:857:ASN:O	1:A:861:ARG:HD3	1.61	0.45
1:A:1557:LEU:HA	1:A:1557:LEU:HD23	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:121:ASP:OD2	26:a:76:MET:SD	2.75	0.45
3:E:62:LEU:HB2	3:E:351:LEU:HB2	1.97	0.45
5:G:23:U:H5''	5:G:23:U:H6	1.82	0.45
12:R:62:GLY:N	13:S:132:VAL:O	2.41	0.45
14:T:197:TYR:O	14:T:197:TYR:CD1	2.70	0.45
17:W:79:VAL:CG2	21:b:114:ILE:CD1	2.72	0.45
18:B:12:U:H3	18:B:65:G:H1	1.63	0.45
23:I:725:ARG:O	23:I:728:ARG:CB	2.62	0.45
28:d:48:ASN:O	28:d:49:ASN:HB2	2.17	0.45
1:A:53:PHE:CE2	1:A:55:ASP:HB3	2.52	0.45
5:G:73:G:O2'	5:G:74:G:C1'	2.59	0.45
7:L:6:ILE:HD12	22:X:80:ARG:HG2	1.99	0.45
10:O:229:LYS:HA	10:O:277:ARG:HH12	1.82	0.45
22:X:90:LEU:HD23	22:X:90:LEU:N	2.32	0.45
28:d:43:LEU:HD11	28:d:51:LYS:HB3	1.99	0.45
30:e:25:LEU:C	30:e:25:LEU:HD23	2.42	0.45
1:A:858:GLN:CA	1:A:861:ARG:CG	2.92	0.44
1:A:984:MET:HG3	1:A:1048:MET:HE1	1.99	0.44
1:A:1306:LYS:NZ	18:B:38:C:O2'	2.49	0.44
1:A:1416:ILE:HD13	1:A:1416:ILE:HA	1.76	0.44
1:A:1921:ASP:HB3	1:A:1966:HIS:HB3	1.99	0.44
3:E:70:TYR:HE2	3:E:86:PHE:HB2	1.81	0.44
17:W:84:THR:O	17:W:87:THR:N	2.50	0.44
20:H:58:U:H2'	20:H:59:A:H8	1.82	0.44
20:H:149:A:H2'	20:H:150:U:C6	2.50	0.44
21:b:37:HIS:O	21:b:38:MET:HB2	2.17	0.44
1:A:185:VAL:HG21	1:A:565:ARG:O	2.17	0.44
1:A:193:LEU:HD12	1:A:194:GLU:N	2.32	0.44
1:A:1076:ASP:O	1:A:1079:THR:OG1	2.34	0.44
1:A:1366:PRO:HG2	1:A:1473:ASP:O	2.17	0.44
1:A:1468:ASN:HD22	1:A:1468:ASN:HA	1.46	0.44
2:C:323:PHE:CD2	2:C:373:ILE:HG12	2.53	0.44
6:J:210:PRO:O	6:J:210:PRO:HG2	2.17	0.44
8:M:218:PHE:HE2	12:R:262:ILE:HD11	1.81	0.44
12:R:185:GLY:O	12:R:187:ALA:N	2.51	0.44
13:S:35:THR:HG22	13:S:82:PHE:HE2	1.82	0.44
20:H:180:G:H2'	20:H:181:G:H8	1.81	0.44
36:Q:929:CYS:CB	36:Q:1012:ARG:HA	2.47	0.44
28:k:43:LEU:HD11	28:k:51:LYS:HB3	1.99	0.44
31:n:32:ARG:HG3	31:n:43:ASP:HB2	1.99	0.44
1:A:193:LEU:O	1:A:193:LEU:CG	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1095:ILE:HG23	1:A:1095:ILE:HD12	1.80	0.44
1:A:1976:TRP:O	1:A:1980:GLU:N	2.43	0.44
2:C:834:VAL:HG11	2:C:883:PHE:HE2	1.82	0.44
8:M:118:LYS:HD2	19:F:89:U:OP1	2.16	0.44
17:W:82:ASN:N	17:W:82:ASN:HD22	2.15	0.44
17:W:341:ASN:HB3	17:W:345:THR:H	1.81	0.44
17:W:475:TRP:HA	17:W:490:ALA:H	1.82	0.44
20:H:84:C:H2'	20:H:85:A:H8	1.82	0.44
20:H:93:A:H2'	20:H:94:A:H8	1.82	0.44
20:H:104:U:O4	28:k:64:ASN:ND2	2.42	0.44
20:H:113:G:H2'	20:H:114:A:H8	1.82	0.44
20:H:168:A:C2'	31:n:48:MET:HE1	2.46	0.44
26:h:77:LEU:N	26:h:77:LEU:HD12	2.32	0.44
30:l:20:LEU:CD2	30:l:24:TYR:CZ	3.00	0.44
1:A:1125:ILE:HG22	1:A:1147:VAL:HG21	1.99	0.44
1:A:1241:HIS:ND1	1:A:1291:CYS:SG	2.89	0.44
1:A:1263:TRP:CZ2	1:A:1292:GLU:HG2	2.53	0.44
1:A:1607:GLU:HB3	1:A:1632:PHE:HB3	1.99	0.44
2:C:856:HIS:O	2:C:856:HIS:CG	2.69	0.44
11:P:12:ALA:HB2	19:F:58:G:O3'	2.17	0.44
17:W:338:ILE:HG22	17:W:349:SER:HA	1.99	0.44
17:W:436:THR:HG21	17:W:464:MET:HB2	1.98	0.44
19:F:34:G:C3'	19:F:35:A:H5''	2.46	0.44
23:I:71:TRP:N	24:y:29:PHE:HA	2.33	0.44
23:I:649:ARG:HG2	23:I:674:MET:HE1	2.00	0.44
25:Y:419:PHE:C	25:Y:419:PHE:HD2	2.25	0.44
30:e:20:LEU:CD2	30:e:24:TYR:CZ	3.00	0.44
34:u:82:SER:O	34:u:219:ALA:HA	2.17	0.44
30:l:25:LEU:HD23	30:l:25:LEU:C	2.42	0.44
1:A:488:ASP:OD1	1:A:489:TRP:N	2.51	0.44
1:A:858:GLN:C	1:A:858:GLN:CD	2.84	0.44
1:A:1132:LYS:HG2	1:A:1139:ARG:HH12	1.82	0.44
1:A:1317:TYR:HB3	1:A:1474:MET:HE3	1.98	0.44
1:A:1949:ARG:HG2	1:A:1986:LEU:HD11	1.99	0.44
2:C:130:ARG:HE	2:C:435:VAL:HA	1.83	0.44
5:G:98:U:H2'	5:G:99:C:C5	2.52	0.44
12:R:307:GLN:HE21	12:R:307:GLN:CA	2.19	0.44
20:H:154:C:O2'	20:H:155:C:C5'	2.66	0.44
21:b:18:ARG:NH1	21:b:52:LYS:HB3	2.31	0.44
1:A:57:GLN:NE2	18:B:13:C:O2'	2.51	0.44
1:A:201:ALA:N	1:A:202:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:TYR:O	2:C:645:ARG:NH1	2.50	0.44
1:A:1498:TRP:O	1:A:1498:TRP:CG	2.69	0.44
1:A:1941:ARG:HH22	1:A:2013:GLY:HA2	1.82	0.44
2:C:95:LYS:H	2:C:95:LYS:HG2	1.45	0.44
2:C:605:ASP:OD1	2:C:608:ARG:NH1	2.41	0.44
3:E:266:PRO:CD	7:L:785:GLN:CB	2.96	0.44
18:B:99:C:H2'	18:B:100:C:C6	2.53	0.44
20:H:143:A:OP2	20:H:143:A:C2	2.71	0.44
23:I:509:ARG:HD3	23:I:509:ARG:HA	1.79	0.44
25:Y:413:LYS:HD2	25:Y:413:LYS:N	2.27	0.44
1:A:186:GLU:N	1:A:186:GLU:CD	2.73	0.44
1:A:701:ILE:O	1:A:703:GLN:NE2	2.50	0.44
2:C:114:TYR:CG	26:a:79:ASN:HB3	2.52	0.44
8:M:137:ARG:NH2	19:F:87:C:OP1	2.42	0.44
9:N:115:THR:OG1	9:N:116:ASN:N	2.51	0.44
12:R:74:LEU:HD12	13:S:136:ILE:HG23	1.99	0.44
13:S:37:LYS:HB2	13:S:37:LYS:HZ3	1.78	0.44
17:W:79:VAL:HG23	21:b:114:ILE:HG12	2.00	0.44
19:F:40:U:O4	19:F:41:A:N6	2.50	0.44
21:b:52:LYS:HG3	21:b:52:LYS:O	2.18	0.44
23:I:651:ILE:HD12	23:I:654:LYS:HE2	2.00	0.44
26:a:5:VAL:HB	26:a:6:PRO:HD3	2.00	0.44
32:v:53:HIS:N	33:w:149:CYS:O	2.34	0.44
1:A:940:ILE:O	1:A:940:ILE:HG22	2.17	0.44
2:C:532:ILE:HD13	2:C:532:ILE:HA	1.87	0.44
5:G:26:U:C2'	5:G:27:U:H5''	2.43	0.44
7:L:56:PRO:HG2	12:R:268:LEU:HD11	1.98	0.44
9:N:121:VAL:HG21	19:F:22:A:O4'	2.18	0.44
10:O:261:ILE:HG23	10:O:272:ILE:HG13	1.99	0.44
14:T:248:THR:HB	14:T:266:GLU:HG3	2.00	0.44
17:W:79:VAL:CG2	21:b:114:ILE:CG1	2.96	0.44
17:W:313:ILE:HB	17:W:328:PHE:HB2	1.99	0.44
20:H:55:U:H2'	20:H:56:A:H8	1.82	0.44
20:H:178:A:N3	20:H:178:A:H2'	2.33	0.44
22:X:58:LEU:HA	22:X:61:GLN:HE21	1.83	0.44
22:X:112:LEU:HD13	22:X:116:ARG:HG2	2.00	0.44
26:h:5:VAL:HB	26:h:6:PRO:HD3	2.00	0.44
21:i:37:HIS:O	21:i:38:MET:HB2	2.17	0.44
1:A:1776:ILE:HB	1:A:1858:PRO:HA	1.98	0.44
2:C:115:GLU:O	2:C:119:LEU:N	2.50	0.44
3:E:150:HIS:CG	3:E:171:SER:HG	2.34	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:5:G:C5'	5:G:5:G:C8	3.01	0.44
6:J:225:LEU:HD23	6:J:225:LEU:HA	1.88	0.44
6:J:239:ARG:HH11	6:J:239:ARG:CG	2.28	0.44
12:R:95:LYS:H	12:R:95:LYS:HD2	1.82	0.44
12:R:312:MET:HE1	12:R:315:LYS:HB3	2.00	0.44
14:T:270:VAL:HB	14:T:284:TYR:HB2	1.98	0.44
18:B:27:U:HO2'	18:B:28:A:P	2.41	0.44
19:F:25:C:C4'	19:F:26:U:OP2	2.65	0.44
19:F:26:U:H4'	19:F:27:A:OP2	2.17	0.44
23:I:548:PHE:HD1	23:I:553:VAL:HG22	1.82	0.44
31:n:38:MET:HE2	31:n:67:ILE:HG21	1.99	0.44
1:A:1792:LYS:HG2	1:A:1798:LEU:HG	1.99	0.43
3:E:94:ASN:HB3	3:E:100:ASP:H	1.83	0.43
5:G:7:G:C8	5:G:7:G:OP2	2.71	0.43
9:N:40:LYS:HA	9:N:40:LYS:HE2	2.00	0.43
12:R:158:LYS:NZ	14:T:322:SER:O	2.51	0.43
20:H:73:C:H2'	20:H:74:U:C6	2.50	0.43
31:g:32:ARG:HG3	31:g:43:ASP:HB2	1.99	0.43
28:k:48:ASN:O	28:k:49:ASN:HB2	2.17	0.43
30:l:20:LEU:HD13	31:n:61:VAL:HG22	2.00	0.43
1:A:1192:PHE:CD2	1:A:1192:PHE:N	2.86	0.43
12:R:333:GLU:OE1	12:R:333:GLU:HA	2.18	0.43
19:F:35:A:H8	19:F:35:A:H5'	1.82	0.43
21:b:18:ARG:HB2	21:b:83:GLU:HG2	1.99	0.43
25:Y:419:PHE:CD2	25:Y:419:PHE:O	2.71	0.43
1:A:766:THR:OG1	18:B:39:C:N4	2.51	0.43
1:A:1187:PHE:CD2	1:A:1189:MET:HE3	2.53	0.43
1:A:1465:TRP:O	1:A:1465:TRP:CG	2.71	0.43
1:A:1937:ILE:HG21	1:A:2012:LEU:HA	2.00	0.43
3:E:259:VAL:HB	3:E:277:PHE:HB2	1.99	0.43
6:J:506:GLU:O	6:J:510:VAL:N	2.47	0.43
10:O:254:GLN:NE2	13:S:120:GLN:OE1	2.51	0.43
17:W:391:PHE:HB2	17:W:403:TRP:HB2	1.99	0.43
20:H:82:G:H2'	20:H:83:A:H8	1.81	0.43
20:H:142:C:O2'	20:H:143:A:H5'	2.18	0.43
20:H:153:A:H62	20:H:177:A:H2	1.67	0.43
22:X:116:ARG:HB3	22:X:116:ARG:NH1	2.30	0.43
36:Q:931:THR:HA	36:Q:934:TYR:CB	2.47	0.43
37:o:37:LEU:HB2	37:o:61:PRO:HD3	2.00	0.43
1:A:293:TRP:HE1	1:A:1136:ARG:NH1	2.11	0.43
1:A:1751:LEU:N	1:A:1751:LEU:CD2	2.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:L:646:GLY:O	7:L:650:GLY:N	2.52	0.43
17:W:250:GLN:HE21	31:n:15:LYS:CE	2.31	0.43
19:F:7:G:H5'	19:F:7:G:C8	2.45	0.43
23:I:518:PRO:HA	23:I:521:VAL:HG12	2.00	0.43
27:c:67:TYR:HB2	28:d:100:PHE:O	2.19	0.43
30:e:20:LEU:HD13	31:g:61:VAL:HG22	2.00	0.43
1:A:1318:THR:HG21	1:A:1324:GLY:N	2.33	0.43
1:A:1764:SER:OG	1:A:1766:GLN:NE2	2.49	0.43
3:E:99:CYS:O	21:b:107:GLY:HA3	2.18	0.43
5:G:121:C:O2	5:G:121:C:C2'	2.66	0.43
7:L:7:LYS:HB3	7:L:40:ARG:HA	2.00	0.43
10:O:239:LEU:HD22	10:O:270:ALA:HB2	2.00	0.43
12:R:301:ALA:O	12:R:304:MET:CB	2.65	0.43
14:T:442:ARG:CG	14:T:442:ARG:NH1	2.73	0.43
17:W:248:ASP:HB2	17:W:252:ARG:HG2	2.00	0.43
17:W:551:LYS:HB3	17:W:572:ASP:HB3	2.00	0.43
19:F:42:C:C5'	19:F:43:A:OP2	2.65	0.43
23:I:442:LEU:O	23:I:446:HIS:CB	2.66	0.43
21:i:18:ARG:HB2	21:i:83:GLU:HG2	1.99	0.43
21:i:52:LYS:HG3	21:i:52:LYS:O	2.18	0.43
39:q:106:ALA:CB	39:t:106:ALA:HB1	2.43	0.43
3:E:346:SER:OG	3:E:348:ASP:OD1	2.31	0.43
12:R:312:MET:O	12:R:312:MET:SD	2.76	0.43
17:W:84:THR:N	17:W:87:THR:OG1	2.52	0.43
17:W:416:ARG:HB3	17:W:443:ARG:HH12	1.84	0.43
25:Y:412:SER:HG	25:Y:415:GLU:HG3	1.84	0.43
29:f:65:ARG:HH11	29:f:65:ARG:HG3	1.83	0.43
1:A:693:ILE:HD12	1:A:706:ALA:HA	2.01	0.43
1:A:1543:ASN:HB2	1:A:1569:LEU:HD21	1.99	0.43
1:A:1686:ASP:O	1:A:1690:ASP:N	2.51	0.43
2:C:501:ILE:HG22	2:C:530:LEU:HD11	2.00	0.43
2:C:756:LYS:HE2	2:C:756:LYS:HB3	1.49	0.43
3:E:266:PRO:HB3	7:L:788:TYR:CB	2.49	0.43
5:G:92:U:H2'	5:G:93:A:O4'	2.18	0.43
11:P:6:ARG:N	11:P:6:ARG:HD2	2.29	0.43
17:W:504:GLY:H	17:W:535:TRP:HZ2	1.65	0.43
18:B:40:U:H6	18:B:40:U:O5'	2.01	0.43
19:F:45:A:C2'	19:F:73:A:C2	3.02	0.43
22:X:112:LEU:HD11	23:I:717:GLU:CB	2.49	0.43
39:q:106:ALA:CB	39:t:106:ALA:HB3	2.48	0.43
2:C:750:LEU:N	2:C:751:PRO:HD2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:21:A:N6	10:O:91:GLY:O	2.51	0.43
19:F:39:A:H2'	19:F:40:U:O4'	2.19	0.43
20:H:88:A:H2'	20:H:89:U:C6	2.50	0.43
20:H:98:G:H5'	20:H:104:U:OP2	2.19	0.43
23:I:673:ASP:OD1	23:I:677:LYS:HE3	2.19	0.43
32:v:51:TYR:CB	33:w:151:VAL:O	2.66	0.43
1:A:99:VAL:HG13	1:A:554:THR:HG21	1.99	0.43
1:A:331:TRP:HZ3	2:C:179:VAL:HG11	1.83	0.43
1:A:1611:LYS:HA	1:A:1629:ILE:HG12	2.01	0.43
17:W:552:VAL:HG13	17:W:571:TRP:CD1	2.54	0.43
22:X:101:GLU:C	22:X:103:GLN:N	2.76	0.43
23:I:273:GLU:CA	36:Q:357:ALA:HB3	2.37	0.43
23:I:685:ARG:HH21	23:I:711:GLU:CD	2.26	0.43
30:l:51:ASP:C	30:l:51:ASP:OD1	2.61	0.43
1:A:369:GLU:O	1:A:371:LEU:N	2.51	0.43
7:L:126:GLY:HA2	22:X:82:LEU:O	2.19	0.43
14:T:459:LEU:CB	14:T:462:GLU:HG3	2.48	0.43
17:W:341:ASN:HB2	17:W:346:GLN:H	1.84	0.43
19:F:36:A:HO2'	19:F:37:C:P	2.42	0.43
20:H:157:G:H2'	20:H:158:G:O4'	2.19	0.43
27:j:66:ARG:CZ	28:k:48:ASN:HB3	2.49	0.43
1:A:73:HIS:HD1	1:A:88:TYR:HH	1.54	0.42
1:A:856:LEU:C	1:A:860:GLN:OE1	2.62	0.42
1:A:1124:ASN:ND2	1:A:1148:ASN:OD1	2.52	0.42
1:A:1393:ARG:NH1	25:Y:405:MET:HG3	2.33	0.42
3:E:307:ARG:HH12	21:b:115:PRO:CG	2.32	0.42
6:J:486:ALA:O	6:J:490:ASN:N	2.52	0.42
7:L:6:ILE:HD11	22:X:80:ARG:HG3	2.01	0.42
17:W:77:LYS:NZ	17:W:77:LYS:HB3	2.34	0.42
17:W:250:GLN:HE21	31:n:15:LYS:HE2	1.83	0.42
17:W:296:LEU:HB3	17:W:297:PHE:H	1.62	0.42
17:W:417:HIS:ND1	17:W:437:SER:HB3	2.34	0.42
20:H:106:G:H5'	28:k:47:ARG:NH2	2.34	0.42
22:X:112:LEU:CG	23:I:717:GLU:HB2	2.48	0.42
36:Q:826:GLY:O	36:Q:1136:GLN:HA	2.18	0.42
1:A:1418:ARG:HB2	1:A:1462:GLY:HA3	2.01	0.42
1:A:1643:SER:H	1:A:1718:TRP:HE1	1.67	0.42
1:A:1807:ILE:HG23	1:A:1841:THR:HG23	2.00	0.42
2:C:566:THR:OG1	2:C:567:GLU:N	2.51	0.42
2:C:769:GLY:O	2:C:773:GLY:N	2.52	0.42
5:G:87:U:H3'	5:G:88:G:H21	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:W:315:LEU:O	17:W:325:LEU:N	2.47	0.42
17:W:553:CYS:HA	17:W:570:GLY:HA2	2.01	0.42
18:B:94:U:O2'	18:B:95:G:H3'	2.19	0.42
20:H:33:G:OP2	20:H:33:G:H8	2.01	0.42
20:H:43:U:H2'	20:H:44:U:C6	2.53	0.42
22:X:104:ARG:O	22:X:108:GLU:CD	2.62	0.42
28:d:33:THR:CG2	28:d:37:LYS:HE2	2.46	0.42
1:A:80:LYS:NZ	9:N:37:HIS:O	2.53	0.42
1:A:980:ARG:HG2	1:A:1094:ARG:HG3	2.01	0.42
1:A:980:ARG:HA	1:A:1094:ARG:HA	2.01	0.42
1:A:1072:LEU:HD22	1:A:1087:LEU:HD22	2.01	0.42
2:C:261:ASP:OD2	42:C:1500:GTP:N1	2.46	0.42
2:C:750:LEU:CD1	2:C:753:GLU:HG2	2.49	0.42
5:G:124:G:N3	5:G:124:G:H2'	2.32	0.42
6:J:526:GLU:O	6:J:530:TRP:N	2.48	0.42
7:L:176:LEU:HD22	17:W:440:LYS:HE3	2.00	0.42
11:P:6:ARG:N	11:P:6:ARG:CD	2.80	0.42
11:P:13:ARG:HA	14:T:309:ASP:O	2.19	0.42
12:R:222:PRO:O	12:R:222:PRO:CG	2.68	0.42
14:T:342:GLU:OE1	14:T:342:GLU:CA	2.65	0.42
14:T:465:ILE:HG12	14:T:481:GLU:HG2	2.01	0.42
18:B:57:G:C2'	18:B:58:U:H5'	2.49	0.42
37:o:56:LYS:HE2	37:o:58:ASP:CG	2.45	0.42
1:A:191:ILE:H	1:A:191:ILE:HG12	1.40	0.42
1:A:331:TRP:CZ3	2:C:179:VAL:HG21	2.54	0.42
5:G:126:G:N3	5:G:126:G:C2'	2.72	0.42
6:J:216:ASP:O	6:J:218:GLU:N	2.53	0.42
18:B:95:G:C6	30:e:36:TYR:O	2.72	0.42
20:H:107:A:N1	20:H:108:G:C5	2.88	0.42
23:I:661:ASP:HB2	23:I:694:ILE:CG1	2.48	0.42
27:c:63:ASN:HA	28:d:102:ARG:CZ	2.50	0.42
28:k:68:GLU:HA	28:k:97:SER:O	2.19	0.42
1:A:772:CYS:SG	1:A:1249:MET:HE1	2.60	0.42
1:A:1467:LEU:HA	1:A:1467:LEU:HD23	1.56	0.42
1:A:1631:LEU:HD23	1:A:1631:LEU:HA	1.85	0.42
1:A:1631:LEU:HB3	1:A:1637:TRP:HZ3	1.84	0.42
2:C:667:VAL:N	2:C:824:THR:CG2	2.78	0.42
3:E:103:ALA:HA	21:b:101:ALA:O	2.20	0.42
5:G:14:A:C8	5:G:14:A:OP2	2.72	0.42
8:M:212:ASN:HB3	8:M:215:ASN:H	1.84	0.42
13:S:72:ARG:NH2	17:W:73:ASP:O	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:101:U:H4'	21:i:73:ARG:NH2	2.35	0.42
21:b:9:MET:HE2	27:c:39:HIS:HE1	1.85	0.42
22:X:112:LEU:CD1	22:X:116:ARG:HG2	2.49	0.42
23:I:491:ALA:HB2	23:I:510:ILE:HD11	2.00	0.42
23:I:697:PRO:HG3	23:I:730:VAL:HG13	2.01	0.42
23:I:699:THR:CG2	23:I:700:THR:HG23	2.49	0.42
23:I:727:ARG:NH2	23:I:727:ARG:HG2	2.33	0.42
27:c:66:ARG:CZ	28:d:48:ASN:HB3	2.49	0.42
30:e:51:ASP:C	30:e:51:ASP:OD1	2.61	0.42
33:w:137:GLN:O	33:w:143:PRO:HA	2.19	0.42
27:j:67:TYR:HB2	28:k:100:PHE:O	2.19	0.42
1:A:1976:TRP:HA	1:A:1979:VAL:HG22	2.00	0.42
2:C:64:LYS:H	2:C:64:LYS:HG3	1.67	0.42
2:C:534:VAL:HB	2:C:537:TYR:HB2	2.00	0.42
2:C:750:LEU:HA	2:C:753:GLU:CB	2.48	0.42
10:O:247:ASP:HA	10:O:250:ASN:HD22	1.84	0.42
17:W:84:THR:C	17:W:86:GLU:N	2.74	0.42
17:W:264:ASN:HB3	30:l:16:GLN:OE1	2.17	0.42
17:W:304:LEU:HD11	17:W:567:ILE:HG21	2.02	0.42
21:b:50:LYS:C	21:b:51:ILE:HG13	2.45	0.42
22:X:62:LYS:CE	22:X:66:GLN:HB2	2.49	0.42
36:Q:93:SER:HA	36:Q:96:CYS:CB	2.49	0.42
29:m:65:ARG:HG3	29:m:65:ARG:HH11	1.83	0.42
1:A:150:MET:SD	1:A:153:ARG:NH2	2.84	0.42
1:A:258:PHE:CE2	1:A:434:HIS:HA	2.55	0.42
1:A:612:ILE:O	1:A:616:PHE:N	2.46	0.42
1:A:1333:VAL:HG11	16:V:467:LEU:HD12	2.02	0.42
1:A:1528:GLN:O	1:A:1528:GLN:CG	2.68	0.42
2:C:264:ILE:HG12	2:C:378:TYR:CE1	2.55	0.42
5:G:100:C:N3	5:G:101:U:C5	2.88	0.42
7:L:5:MET:SD	7:L:5:MET:O	2.78	0.42
8:M:182:MET:HE2	8:M:182:MET:HB3	1.97	0.42
9:N:117:CYS:SG	9:N:119:CYS:HB3	2.60	0.42
14:T:213:GLU:OE1	14:T:215:GLY:N	2.51	0.42
17:W:265:LEU:HD12	17:W:300:SER:HB2	2.02	0.42
17:W:398:LYS:HG2	17:W:419:GLY:H	1.84	0.42
17:W:462:HIS:ND1	17:W:482:ASP:HB3	2.35	0.42
19:F:43:A:O2'	19:F:44:G:H5'	2.19	0.42
23:I:688:TYR:O	23:I:692:SER:N	2.52	0.42
23:I:693:GLN:CD	23:I:693:GLN:C	2.88	0.42
34:u:254:PHE:HA	34:u:401:ASP:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:i:18:ARG:NH1	21:i:52:LYS:HB3	2.31	0.42
27:j:63:ASN:HA	28:k:102:ARG:CZ	2.50	0.42
30:l:34:TRP:CD1	30:l:34:TRP:N	2.86	0.42
1:A:881:ILE:HG23	1:A:918:THR:HG23	2.02	0.42
1:A:2003:THR:H	1:A:2006:GLU:HB2	1.85	0.42
2:C:589:LYS:HG3	2:C:628:VAL:HG13	2.02	0.42
8:M:138:LEU:HD23	8:M:138:LEU:HA	1.89	0.42
14:T:385:TYR:CZ	14:T:400:PHE:HB3	2.54	0.42
14:T:418:THR:OG1	14:T:466:PHE:O	2.38	0.42
18:B:87:A:H5'	18:B:93:U:OP2	2.19	0.42
22:X:69:TYR:CD1	22:X:69:TYR:C	2.97	0.42
21:i:50:LYS:C	21:i:51:ILE:HG13	2.45	0.42
38:p:74:PHE:CG	38:p:79:MET:HE3	2.55	0.42
1:A:150:MET:CG	1:A:193:LEU:HB3	2.49	0.42
1:A:310:THR:OG1	15:U:2:TYR:O	2.37	0.42
1:A:940:ILE:CD1	1:A:1090:ARG:HH12	2.20	0.42
1:A:1091:TYR:HD1	1:A:1190:CYS:SG	2.39	0.42
1:A:1160:ARG:HD3	11:P:192:VAL:HG11	2.01	0.42
1:A:1260:VAL:HG22	1:A:1327:MET:HE2	2.01	0.42
1:A:1497:THR:O	1:A:1497:THR:HG23	2.18	0.42
5:G:7:G:C2'	5:G:8:C:H5'	2.50	0.42
6:J:313:TRP:CE3	6:J:336:TRP:HB2	2.55	0.42
7:L:633:GLN:O	7:L:637:VAL:N	2.50	0.42
20:H:43:U:OP2	20:H:43:U:C6	2.73	0.42
23:I:590:LYS:HA	23:I:590:LYS:HD3	1.84	0.42
23:I:731:GLN:NE2	23:I:731:GLN:C	2.74	0.42
28:d:28:PRO:HD2	29:f:37:ASP:HB3	2.02	0.42
37:o:161:MET:O	37:o:162:PHE:HB2	2.19	0.42
1:A:451:LEU:HD23	1:A:451:LEU:HA	1.84	0.42
1:A:663:ARG:HG3	1:A:663:ARG:HH21	1.81	0.42
1:A:764:GLY:HA2	1:A:1245:ARG:NH1	2.35	0.42
1:A:1136:ARG:H	1:A:1345:GLN:HA	1.85	0.42
1:A:1430:LEU:CB	25:Y:400:TRP:CZ3	3.03	0.42
1:A:1501:LEU:CD2	1:A:1501:LEU:H	2.33	0.42
1:A:1528:GLN:HE21	1:A:1528:GLN:HB2	1.40	0.42
2:C:136:GLY:O	2:C:142:LYS:NZ	2.38	0.42
7:L:7:LYS:HB3	7:L:40:ARG:CA	2.49	0.42
9:N:118:ILE:HG23	19:F:23:U:C6	2.55	0.42
20:H:157:G:H5''	20:H:157:G:C8	2.50	0.42
22:X:112:LEU:HD13	22:X:112:LEU:O	2.20	0.42
23:I:84:HIS:CB	23:I:90:PRO:CB	2.97	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:e:34:TRP:N	30:e:34:TRP:CD1	2.86	0.42
1:A:975:VAL:HG22	1:A:1177:VAL:HG22	2.01	0.41
1:A:1494:TYR:HB3	1:A:1744:ARG:HD3	2.02	0.41
6:J:527:LYS:O	6:J:531:LYS:N	2.48	0.41
7:L:29:ASN:HB3	20:H:24:A:C2	2.53	0.41
8:M:165:ASN:HB2	12:R:95:LYS:HA	2.02	0.41
9:N:102:CYS:HB3	9:N:104:ARG:H	1.84	0.41
28:d:68:GLU:HA	28:d:97:SER:O	2.19	0.41
21:i:9:MET:HE2	27:j:39:HIS:HE1	1.84	0.41
1:A:470:ARG:NH2	1:A:470:ARG:CG	2.81	0.41
1:A:1470:TYR:O	1:A:1470:TYR:CG	2.68	0.41
1:A:1930:TYR:HA	1:A:1933:PHE:HB3	2.02	0.41
2:C:140:HIS:CD2	2:C:230:ASP:HB2	2.56	0.41
2:C:680:ASN:HD21	2:C:803:ARG:HH11	1.66	0.41
3:E:266:PRO:HG2	7:L:785:GLN:HA	1.96	0.41
3:E:266:PRO:HB3	7:L:788:TYR:C	2.46	0.41
5:G:21:A:C8	10:O:152:ARG:NH2	2.86	0.41
10:O:39:GLU:OE1	19:F:25:C:N4	2.53	0.41
14:T:186:PRO:CG	14:T:442:ARG:NH2	2.83	0.41
18:B:90:U:H4'	21:b:73:ARG:NH2	2.35	0.41
19:F:37:C:C3'	19:F:37:C:C6	3.02	0.41
20:H:155:C:H2'	20:H:156:U:H5''	2.01	0.41
23:I:511:LEU:HD11	23:I:521:VAL:HG23	2.01	0.41
23:I:581:GLU:HA	23:I:584:LEU:HD12	2.01	0.41
23:I:687:ILE:HA	23:I:690:PHE:CB	2.46	0.41
1:A:191:ILE:CG2	1:A:572:PHE:CD1	2.95	0.41
1:A:773:LYS:HA	1:A:773:LYS:HD2	1.67	0.41
1:A:1090:ARG:HH11	1:A:1090:ARG:HD3	1.69	0.41
17:W:130:ARG:CD	19:F:22:A:C8	3.03	0.41
20:H:39:U:C6	20:H:39:U:C5'	2.90	0.41
23:I:273:GLU:HA	36:Q:357:ALA:H	1.85	0.41
29:m:65:ARG:HG3	29:m:65:ARG:NH1	2.35	0.41
1:A:274:PRO:HB3	4:4:-11:G:C8	2.56	0.41
1:A:1095:ILE:HD13	1:A:1095:ILE:HA	1.54	0.41
1:A:1130:ASN:HA	1:A:1174:PHE:HE1	1.85	0.41
1:A:1156:ASP:OD2	1:A:1160:ARG:NH2	2.53	0.41
2:C:756:LYS:HA	2:C:759:LEU:HB3	2.03	0.41
3:E:61:LEU:O	21:b:108:ARG:O	2.38	0.41
5:G:100:C:C5'	5:G:100:C:C6	3.00	0.41
11:P:72:ARG:O	11:P:76:ARG:N	2.53	0.41
12:R:334:ARG:NH1	12:R:334:ARG:CG	2.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:H:103:U:C3'	20:H:104:U:H5'	2.51	0.41
23:I:729:SER:C	23:I:731:GLN:N	2.77	0.41
26:h:24:THR:O	26:h:51:ARG:NH1	2.46	0.41
26:h:58:LEU:HD22	31:n:71:GLU:CD	2.45	0.41
28:k:103:GLY:O	28:k:106:VAL:HG23	2.20	0.41
38:p:13:ASN:HB2	38:p:80:ARG:HH21	1.86	0.41
39:q:60:PRO:CB	39:s:94:GLN:CA	2.97	0.41
1:A:199:GLU:CA	1:A:199:GLU:OE1	2.68	0.41
1:A:599:MET:HE3	1:A:599:MET:HB3	1.89	0.41
1:A:1400:ASN:ND2	25:Y:1034:LYS:CB	2.84	0.41
2:C:604:LEU:HD23	2:C:604:LEU:HA	1.88	0.41
2:C:801:LEU:HD22	2:C:801:LEU:H	1.84	0.41
3:E:310:TYR:CE1	3:E:322:LYS:HE2	2.55	0.41
7:L:30:GLN:HE22	19:F:48:A:H61	1.68	0.41
9:N:37:HIS:O	9:N:37:HIS:CG	2.68	0.41
11:P:6:ARG:CG	19:F:78:A:C2	2.99	0.41
13:S:11:PRO:HA	13:S:12:PRO:HD3	1.89	0.41
16:V:171:ASN:CB	34:u:277:ILE:HA	2.51	0.41
17:W:82:ASN:ND2	17:W:82:ASN:N	2.69	0.41
18:B:20:G:C1'	18:B:21:A:OP1	2.69	0.41
18:B:92:U:C3'	18:B:93:U:H5'	2.50	0.41
19:F:43:A:N1	19:F:44:G:C6	2.89	0.41
23:I:329:LEU:CB	36:Q:353:LEU:CB	2.98	0.41
23:I:717:GLU:HA	23:I:720:ILE:HB	2.02	0.41
30:e:24:TYR:CD1	30:e:31:ILE:HD11	2.56	0.41
36:Q:95:CYS:O	36:Q:99:ASN:N	2.47	0.41
1:A:467:GLN:HG2	18:B:19:A:C4	2.55	0.41
1:A:1310:ARG:NH1	1:A:1566:ILE:HD11	2.36	0.41
9:N:41:ARG:NE	9:N:44:GLU:OE1	2.54	0.41
9:N:124:SER:OG	9:N:125:LYS:NZ	2.47	0.41
11:P:3:THR:HG21	19:F:79:C:C2	2.47	0.41
17:W:140:ASP:OD1	17:W:140:ASP:N	2.50	0.41
20:H:102:U:O2'	27:j:61:ARG:NH1	2.51	0.41
22:X:104:ARG:HB2	22:X:104:ARG:NH1	2.35	0.41
22:X:120:LYS:HD3	22:X:120:LYS:HA	1.87	0.41
28:d:39:ASN:OD1	28:d:55:ARG:HD3	2.21	0.41
1:A:273:ILE:H	1:A:273:ILE:HG13	1.56	0.41
1:A:1298:ARG:HA	1:A:1298:ARG:HD2	1.89	0.41
1:A:1611:LYS:HA	1:A:1629:ILE:HA	2.03	0.41
2:C:307:VAL:HG12	2:C:308:CYS:O	2.20	0.41
2:C:366:GLN:HB3	2:C:370:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:561:LYS:NZ	2:C:611:ASN:O	2.38	0.41
2:C:666:VAL:CG1	2:C:824:THR:HG22	2.49	0.41
2:C:803:ARG:HA	2:C:803:ARG:HD3	1.94	0.41
3:E:231:MET:HB3	3:E:262:TRP:CZ3	2.55	0.41
12:R:222:PRO:O	12:R:222:PRO:HG2	2.20	0.41
20:H:24:A:H3'	20:H:25:G:C5'	2.50	0.41
29:f:65:ARG:HB3	29:f:68:ASN:HD22	1.85	0.41
30:e:21:ILE:HA	30:e:24:TYR:HD2	1.86	0.41
1:A:779:LEU:HD23	1:A:782:LEU:HD12	2.02	0.41
1:A:1951:LYS:O	1:A:1955:LYS:N	2.53	0.41
2:C:131:ASN:HA	2:C:201:ASN:HB2	2.03	0.41
2:C:151:GLU:OE1	2:C:417:ARG:NH2	2.53	0.41
6:J:239:ARG:CD	6:J:239:ARG:O	2.69	0.41
6:J:529:HIS:O	6:J:533:TYR:N	2.42	0.41
12:R:99:ASP:OD2	12:R:103:ARG:NE	2.42	0.41
14:T:312:ALA:HB3	14:T:326:LEU:HB2	2.02	0.41
20:H:30:A:O4'	22:X:73:PHE:CE1	2.74	0.41
20:H:152:G:H2'	20:H:153:A:C1'	2.51	0.41
20:H:171:U:H2'	20:H:172:C:O4'	2.21	0.41
22:X:114:GLU:OE2	22:X:114:GLU:CA	2.69	0.41
23:I:681:ILE:HA	23:I:710:PHE:HZ	1.86	0.41
28:k:62:HIS:O	28:k:103:GLY:HA3	2.21	0.41
1:A:198:GLU:OE1	1:A:198:GLU:CA	2.69	0.41
1:A:591:MET:HE2	1:A:591:MET:HB3	1.84	0.41
1:A:1259:ILE:HD13	1:A:1259:ILE:HG21	1.68	0.41
1:A:1561:PHE:O	1:A:1561:PHE:CD2	2.69	0.41
2:C:134:LEU:O	2:C:205:THR:OG1	2.29	0.41
5:G:20:A:OP2	10:O:159:ARG:HG3	2.21	0.41
5:G:92:U:H3	20:H:38:A:H61	1.69	0.41
5:G:129:U:O2	5:G:129:U:C2'	2.67	0.41
6:J:204:GLU:O	6:J:204:GLU:CG	2.69	0.41
6:J:258:ILE:O	6:J:262:ARG:N	2.51	0.41
8:M:165:ASN:OD1	8:M:166:SER:N	2.54	0.41
9:N:132:ILE:HD13	9:N:132:ILE:HA	1.88	0.41
10:O:81:CYS:SG	10:O:82:GLN:N	2.94	0.41
10:O:292:ILE:HG12	10:O:297:ARG:HA	2.03	0.41
11:P:9:PHE:HD1	11:P:9:PHE:HA	1.68	0.41
16:V:623:ASN:HA	16:V:626:PHE:HB3	2.03	0.41
17:W:72:LEU:O	17:W:72:LEU:CG	2.67	0.41
17:W:79:VAL:HG21	21:b:114:ILE:CG1	2.49	0.41
17:W:458:GLU:HB3	17:W:460:SER:H	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:F:7:G:H4'	19:F:7:G:OP1	2.20	0.41
20:H:40:C:C2'	20:H:41:U:H5''	2.47	0.41
20:H:90:A:C6	20:H:91:U:C4	3.09	0.41
20:H:168:A:C2	31:n:54:GLN:CB	3.04	0.41
20:H:183:G:C6	20:H:184:C:N4	2.89	0.41
22:X:105:ARG:HA	22:X:108:GLU:OE1	2.20	0.41
23:I:631:MET:HA	23:I:634:ILE:HB	2.03	0.41
26:a:58:LEU:HD22	31:g:71:GLU:CD	2.46	0.41
28:d:103:GLY:O	28:d:106:VAL:HG23	2.20	0.41
29:f:65:ARG:HG3	29:f:65:ARG:NH1	2.35	0.41
36:Q:875:HIS:O	36:Q:1034:ILE:N	2.49	0.41
27:j:3:LEU:O	27:j:6:PHE:HB3	2.21	0.41
37:o:37:LEU:HB2	37:o:61:PRO:CD	2.51	0.41
1:A:196:ASP:OD2	1:A:196:ASP:C	2.63	0.41
1:A:461:HIS:CD2	18:B:26:A:H61	2.39	0.41
1:A:516:LEU:HD11	1:A:538:SER:HB2	2.03	0.41
1:A:940:ILE:HD11	1:A:1090:ARG:HH11	1.79	0.41
1:A:1899:VAL:HB	1:A:1902:PHE:HD2	1.86	0.41
2:C:604:LEU:HD21	2:C:627:HIS:CE1	2.56	0.41
9:N:131:ILE:HG21	10:O:177:GLU:HG2	2.03	0.41
11:P:10:GLU:O	11:P:10:GLU:CG	2.69	0.41
20:H:149:A:C6	20:H:150:U:C4	3.09	0.41
22:X:71:GLU:CD	22:X:71:GLU:O	2.64	0.41
28:d:110:LEU:CD1	29:f:59:LEU:HB3	2.46	0.41
38:p:3:ILE:HG22	38:p:83:TYR:HB2	2.02	0.41
1:A:274:PRO:HG3	15:U:1:MET:HB3	2.02	0.40
1:A:1562:MET:H	1:A:1562:MET:HG3	1.69	0.40
2:C:458:ASP:OD1	2:C:458:ASP:N	2.54	0.40
2:C:935:ILE:HG22	2:C:939:ARG:HE	1.87	0.40
3:E:144:VAL:HG12	3:E:145:LYS:HG3	2.02	0.40
6:J:215:THR:OG1	6:J:216:ASP:N	2.47	0.40
12:R:126:ASN:O	14:T:442:ARG:NH1	2.54	0.40
14:T:331:ASN:HB3	14:T:332:ALA:H	1.77	0.40
19:F:26:U:HO2'	19:F:27:A:P	2.42	0.40
20:H:59:A:C6	20:H:60:U:C4	3.10	0.40
20:H:153:A:C8	20:H:154:C:O4'	2.75	0.40
22:X:83:ASP:HB2	22:X:84:GLU:H	1.75	0.40
23:I:521:VAL:HG21	23:I:544:GLY:HA3	2.03	0.40
27:c:20:LYS:O	27:c:66:ARG:NH2	2.55	0.40
28:k:33:THR:CG2	28:k:37:LYS:HE2	2.45	0.40
37:o:52:ASN:HB2	37:o:74:ASN:OD1	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:LEU:HD23	1:A:89:LEU:HA	1.89	0.40
1:A:260:LEU:HA	1:A:260:LEU:HD23	1.91	0.40
1:A:496:VAL:O	1:A:500:GLY:N	2.52	0.40
1:A:638:LEU:HA	1:A:638:LEU:HD23	1.77	0.40
1:A:641:MET:HE3	1:A:641:MET:HB3	1.94	0.40
1:A:801:ILE:O	1:A:805:GLU:HB3	2.21	0.40
1:A:885:LEU:HD23	1:A:885:LEU:HA	1.88	0.40
1:A:940:ILE:HD13	1:A:1090:ARG:NH1	2.29	0.40
1:A:1386:TRP:CD1	25:Y:408:ALA:HB1	2.56	0.40
5:G:9:C:H2'	5:G:10:U:O4'	2.22	0.40
5:G:129:U:O2	5:G:129:U:O2'	2.30	0.40
10:O:174:LYS:HB2	19:F:28:A:C2	2.55	0.40
14:T:297:HIS:NE2	14:T:340:ALA:CB	2.73	0.40
14:T:427:LEU:O	14:T:439:TRP:N	2.50	0.40
17:W:233:LYS:HG3	17:W:355:TYR:HH	1.82	0.40
17:W:357:LYS:HE2	17:W:369:ARG:HD3	2.03	0.40
18:B:12:U:O2'	18:B:13:C:P	2.79	0.40
22:X:80:ARG:O	22:X:80:ARG:CG	2.70	0.40
27:j:20:LYS:O	27:j:66:ARG:NH2	2.55	0.40
37:o:160:LYS:O	37:o:161:MET:C	2.63	0.40
1:A:185:VAL:CG2	1:A:565:ARG:O	2.70	0.40
1:A:1318:THR:CG2	1:A:1324:GLY:N	2.84	0.40
3:E:167:VAL:HB	3:E:179:TRP:HB2	2.03	0.40
7:L:169:ARG:HH22	19:F:45:A:H5'	1.85	0.40
7:L:190:GLU:OE1	17:W:352:TYR:OH	2.38	0.40
13:S:71:GLY:O	13:S:111:GLN:NE2	2.50	0.40
17:W:101:THR:HG23	17:W:104:MET:H	1.86	0.40
19:F:33:G:O2'	19:F:34:G:P	2.79	0.40
20:H:33:G:OP2	20:H:33:G:C8	2.73	0.40
20:H:36:G:C3'	20:H:37:U:H5'	2.47	0.40
22:X:54:LEU:N	22:X:54:LEU:HD12	2.37	0.40
29:m:65:ARG:HB3	29:m:68:ASN:HD22	1.85	0.40
1:A:91:ALA:HA	12:R:207:MET:HE3	2.04	0.40
3:E:305:ALA:HA	3:E:329:SER:HB2	2.04	0.40
11:P:3:THR:HG23	19:F:79:C:N3	2.34	0.40
18:B:24:G:O2'	18:B:26:A:C5	2.73	0.40
20:H:39:U:HO2'	20:H:40:C:P	2.28	0.40
26:a:63:ILE:HG12	31:g:69:MET:HG3	2.03	0.40
28:d:62:HIS:O	28:d:103:GLY:HA3	2.21	0.40
26:h:63:ILE:HG12	31:n:69:MET:HG3	2.03	0.40
28:k:28:PRO:HD2	29:m:37:ASP:HB3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:VAL:O	1:A:854:SER:N	2.54	0.40
1:A:1392:LYS:NZ	1:A:1407:ASP:O	2.39	0.40
2:C:63:LYS:O	2:C:63:LYS:HG2	2.22	0.40
2:C:95:LYS:NZ	2:C:95:LYS:CB	2.73	0.40
2:C:304:LEU:HD23	2:C:304:LEU:HA	1.90	0.40
2:C:750:LEU:HA	2:C:753:GLU:CG	2.51	0.40
12:R:122:LYS:HB3	12:R:122:LYS:HE3	1.89	0.40
12:R:224:SEP:HA	12:R:225:PRO:HD3	1.88	0.40
12:R:312:MET:O	12:R:312:MET:CE	2.70	0.40
17:W:308:SER:HB3	17:W:312:LYS:H	1.86	0.40
22:X:120:LYS:HE3	22:X:120:LYS:CA	2.51	0.40
25:Y:402:ILE:O	25:Y:405:MET:HB2	2.22	0.40
36:Q:876:LEU:HA	36:Q:1034:ILE:O	2.22	0.40
28:k:39:ASN:OD1	28:k:55:ARG:HD3	2.21	0.40
29:m:5:LEU:O	30:l:49:GLY:HA3	2.22	0.40
31:n:35:ASP:HB2	31:n:36:PRO:CD	2.42	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	1980/2335 (85%)	1807 (91%)	160 (8%)	13 (1%)	18	51
2	C	856/972 (88%)	790 (92%)	64 (8%)	2 (0%)	43	72
3	E	297/357 (83%)	276 (93%)	20 (7%)	1 (0%)	36	65
6	J	529/848 (62%)	491 (93%)	31 (6%)	7 (1%)	9	39
7	L	425/802 (53%)	408 (96%)	15 (4%)	2 (0%)	24	57
8	M	128/243 (53%)	117 (91%)	11 (9%)	0	100	100
9	N	141/144 (98%)	125 (89%)	14 (10%)	2 (1%)	9	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	O	283/420 (67%)	259 (92%)	23 (8%)	1 (0%)	30	61
11	P	107/229 (47%)	88 (82%)	16 (15%)	3 (3%)	4	26
12	R	274/536 (51%)	247 (90%)	23 (8%)	4 (2%)	8	37
13	S	157/166 (95%)	148 (94%)	9 (6%)	0	100	100
14	T	310/514 (60%)	278 (90%)	25 (8%)	7 (2%)	5	30
15	U	68/2752 (2%)	60 (88%)	8 (12%)	0	100	100
16	V	444/908 (49%)	431 (97%)	12 (3%)	1 (0%)	43	72
17	W	507/579 (88%)	433 (85%)	68 (13%)	6 (1%)	10	41
21	b	98/240 (41%)	93 (95%)	2 (2%)	3 (3%)	3	25
21	i	84/240 (35%)	82 (98%)	2 (2%)	0	100	100
22	X	67/254 (26%)	64 (96%)	3 (4%)	0	100	100
23	I	575/855 (67%)	562 (98%)	11 (2%)	2 (0%)	36	65
24	y	77/301 (26%)	74 (96%)	1 (1%)	2 (3%)	4	27
25	Y	667/1220 (55%)	642 (96%)	23 (3%)	2 (0%)	36	65
26	a	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
26	h	77/126 (61%)	76 (99%)	1 (1%)	0	100	100
27	c	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
27	j	80/119 (67%)	77 (96%)	3 (4%)	0	100	100
28	d	95/118 (80%)	91 (96%)	4 (4%)	0	100	100
28	k	81/118 (69%)	78 (96%)	3 (4%)	0	100	100
29	f	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
29	m	72/86 (84%)	69 (96%)	3 (4%)	0	100	100
30	e	77/92 (84%)	76 (99%)	1 (1%)	0	100	100
30	l	76/92 (83%)	75 (99%)	1 (1%)	0	100	100
31	g	72/76 (95%)	70 (97%)	2 (3%)	0	100	100
31	n	65/76 (86%)	63 (97%)	2 (3%)	0	100	100
32	v	142/146 (97%)	138 (97%)	4 (3%)	0	100	100
33	w	89/174 (51%)	87 (98%)	1 (1%)	1 (1%)	11	43
34	u	384/411 (93%)	372 (97%)	9 (2%)	3 (1%)	16	49
35	x	23/703 (3%)	22 (96%)	1 (4%)	0	100	100
36	Q	1308/1485 (88%)	1278 (98%)	27 (2%)	3 (0%)	43	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
37	o	160/255 (63%)	146 (91%)	12 (8%)	2 (1%)	9	39
38	p	92/225 (41%)	90 (98%)	2 (2%)	0	100	100
39	q	130/504 (26%)	117 (90%)	7 (5%)	6 (5%)	2	17
39	r	129/504 (26%)	118 (92%)	9 (7%)	2 (2%)	7	36
39	s	130/504 (26%)	114 (88%)	8 (6%)	8 (6%)	1	12
39	t	129/504 (26%)	116 (90%)	9 (7%)	4 (3%)	3	25
40	K	147/225 (65%)	139 (95%)	5 (3%)	3 (2%)	6	32
All	All	11861/21789 (54%)	11109 (94%)	662 (6%)	90 (1%)	18	49

All (90) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	167	PRO
1	A	857	ASN
1	A	942	PRO
1	A	1831	LYS
6	J	217	GLU
7	L	10	VAL
7	L	125	PRO
9	N	41	ARG
9	N	43	VAL
11	P	7	PRO
11	P	8	THR
12	R	233	PRO
14	T	187	LYS
14	T	188	PRO
14	T	341	ALA
14	T	343	PRO
14	T	401	PRO
17	W	82	ASN
17	W	83	PRO
17	W	259	GLN
23	I	532	LYS
24	y	44	GLU
34	u	383	ASN
36	Q	934	TYR
39	q	24	VAL
39	q	59	HIS
39	q	60	PRO
39	s	9	ASN

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Mol	Chain	Res	Type
39	s	55	ILE
39	s	60	PRO
39	s	66	PRO
39	s	71	ILE
39	t	9	ASN
39	t	69	THR
40	K	78	PRO
1	A	204	LEU
1	A	1092	ILE
2	C	439	PRO
6	J	709	VAL
14	T	344	GLN
25	Y	1185	ASP
33	w	115	GLY
34	u	340	GLY
34	u	385	ASP
37	o	160	LYS
39	q	9	ASN
39	q	19	PRO
39	s	24	VAL
1	A	1515	TRP
2	C	63	LYS
6	J	188	GLN
12	R	52	PRO
12	R	186	VAL
16	V	597	PRO
24	y	41	TYR
39	q	23	HIS
39	r	9	ASN
39	t	67	SER
1	A	570	ASP
1	A	1134	TRP
1	A	1135	PRO
3	E	193	THR
6	J	206	LEU
6	J	341	PRO
6	J	604	PRO
11	P	205	LYS
12	R	73	PRO
14	T	407	GLN
17	W	74	PRO
17	W	258	PRO

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Mol	Chain	Res	Type
25	Y	1182	LYS
36	Q	525	PRO
37	o	32	PRO
39	t	65	PRO
40	K	65	ILE
1	A	364	SER
1	A	1494	TYR
1	A	1758	PRO
21	b	105	GLY
21	b	106	ILE
39	s	62	ARG
6	J	216	ASP
10	O	20	PHE
23	I	372	ARG
36	Q	532	PRO
21	b	115	PRO
17	W	271	PRO
40	K	17	PRO
39	s	38	GLY
39	r	60	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	1780/2108 (84%)	1705 (96%)	75 (4%)	26	53
2	C	761/866 (88%)	746 (98%)	15 (2%)	48	66
3	E	256/300 (85%)	254 (99%)	2 (1%)	73	77
6	J	241/751 (32%)	236 (98%)	5 (2%)	47	65
7	L	218/709 (31%)	211 (97%)	7 (3%)	34	58
8	M	117/209 (56%)	116 (99%)	1 (1%)	70	76
9	N	130/130 (100%)	122 (94%)	8 (6%)	16	44
10	O	255/361 (71%)	253 (99%)	2 (1%)	73	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	P	101/203 (50%)	96 (95%)	5 (5%)	22	49
12	R	236/457 (52%)	213 (90%)	23 (10%)	8	31
13	S	129/134 (96%)	127 (98%)	2 (2%)	55	69
14	T	268/441 (61%)	250 (93%)	18 (7%)	15	42
15	U	21/2432 (1%)	19 (90%)	2 (10%)	8	32
16	V	98/838 (12%)	95 (97%)	3 (3%)	35	59
17	W	448/502 (89%)	435 (97%)	13 (3%)	37	60
21	b	83/177 (47%)	80 (96%)	3 (4%)	31	56
21	i	77/177 (44%)	74 (96%)	3 (4%)	28	54
22	X	68/230 (30%)	45 (66%)	23 (34%)	0	1
23	I	198/749 (26%)	183 (92%)	15 (8%)	12	39
25	Y	32/1085 (3%)	26 (81%)	6 (19%)	1	10
26	a	72/101 (71%)	72 (100%)	0	100	100
26	h	70/101 (69%)	70 (100%)	0	100	100
27	c	77/101 (76%)	75 (97%)	2 (3%)	40	62
27	j	77/101 (76%)	75 (97%)	2 (3%)	40	62
28	d	90/110 (82%)	89 (99%)	1 (1%)	65	74
28	k	80/110 (73%)	79 (99%)	1 (1%)	61	72
29	f	63/74 (85%)	61 (97%)	2 (3%)	34	58
29	m	63/74 (85%)	61 (97%)	2 (3%)	34	58
30	e	74/84 (88%)	74 (100%)	0	100	100
30	l	73/84 (87%)	73 (100%)	0	100	100
31	g	64/66 (97%)	63 (98%)	1 (2%)	55	69
31	n	59/66 (89%)	58 (98%)	1 (2%)	53	69
37	o	139/218 (64%)	133 (96%)	6 (4%)	26	52
38	p	82/195 (42%)	79 (96%)	3 (4%)	30	56
All	All	6600/14344 (46%)	6348 (96%)	252 (4%)	30	55

All (252) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	164	MET
1	A	181	ASN

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Mol	Chain	Res	Type
1	A	185	VAL
1	A	186	GLU
1	A	188	LEU
1	A	189	GLU
1	A	191	ILE
1	A	193	LEU
1	A	194	GLU
1	A	195	LEU
1	A	199	GLU
1	A	202	PRO
1	A	338	VAL
1	A	346	ASP
1	A	387	PHE
1	A	413	LEU
1	A	664	HIS
1	A	666	LYS
1	A	701	ILE
1	A	771	VAL
1	A	773	LYS
1	A	774	LYS
1	A	818	GLU
1	A	847	LYS
1	A	852	VAL
1	A	853	LYS
1	A	855	ARG
1	A	856	LEU
1	A	858	GLN
1	A	861	ARG
1	A	880	ARG
1	A	944	ASP
1	A	1089	CYS
1	A	1091	TYR
1	A	1092	ILE
1	A	1093	ASP
1	A	1095	ILE
1	A	1131	LYS
1	A	1136	ARG
1	A	1189	MET
1	A	1249	MET
1	A	1251	SER
1	A	1257	THR
1	A	1258	LYS

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Mol	Chain	Res	Type
1	A	1261	ASN
1	A	1263	TRP
1	A	1318	THR
1	A	1319	PRO
1	A	1322	LEU
1	A	1416	ILE
1	A	1460	HIS
1	A	1468	ASN
1	A	1471	ARG
1	A	1496	PRO
1	A	1501	LEU
1	A	1502	PHE
1	A	1504	GLU
1	A	1505	LYS
1	A	1528	GLN
1	A	1553	VAL
1	A	1554	GLN
1	A	1555	LEU
1	A	1556	ASP
1	A	1560	ILE
1	A	1561	PHE
1	A	1562	MET
1	A	1565	LYS
1	A	1749	LYS
1	A	1751	LEU
1	A	1752	GLN
1	A	1753	LEU
1	A	1755	SER
1	A	1757	GLU
1	A	1763	LEU
1	A	1833	LEU
2	C	64	LYS
2	C	82	GLN
2	C	84	GLU
2	C	85	ASP
2	C	93	ILE
2	C	95	LYS
2	C	513	ASN
2	C	572	GLU
2	C	573	GLU
2	C	748	ASP
2	C	749	THR

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Mol	Chain	Res	Type
2	C	750	LEU
2	C	756	LYS
2	C	799	GLU
2	C	802	HIS
3	E	190	PHE
3	E	243	LEU
6	J	201	ARG
6	J	205	LEU
6	J	214	ILE
6	J	239	ARG
6	J	244	ASN
7	L	4	ILE
7	L	5	MET
7	L	6	ILE
7	L	7	LYS
7	L	10	VAL
7	L	123	LEU
7	L	133	GLU
8	M	152	LEU
9	N	33	GLU
9	N	35	GLU
9	N	38	GLU
9	N	40	LYS
9	N	41	ARG
9	N	42	LYS
9	N	43	VAL
9	N	119	CYS
10	O	150	LEU
10	O	272	ILE
11	P	3	THR
11	P	7	PRO
11	P	8	THR
11	P	10	GLU
11	P	18	LYS
12	R	95	LYS
12	R	123	GLU
12	R	124	VAL
12	R	128	ASP
12	R	131	ASP
12	R	217	LYS
12	R	262	ILE
12	R	303	GLU

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Mol	Chain	Res	Type
12	R	307	GLN
12	R	308	VAL
12	R	310	ARG
12	R	311	LYS
12	R	312	MET
12	R	314	GLN
12	R	315	LYS
12	R	316	GLU
12	R	317	LYS
12	R	324	LEU
12	R	325	ARG
12	R	329	GLN
12	R	332	ARG
12	R	334	ARG
12	R	335	ARG
13	S	37	LYS
13	S	126	HIS
14	T	189	GLN
14	T	191	HIS
14	T	197	TYR
14	T	338	CYS
14	T	342	GLU
14	T	343	PRO
14	T	345	ILE
14	T	399	LYS
14	T	400	PHE
14	T	401	PRO
14	T	402	ASP
14	T	407	GLN
14	T	408	ASN
14	T	412	HIS
14	T	416	ILE
14	T	442	ARG
14	T	454	VAL
14	T	462	GLU
15	U	23	LEU
15	U	25	LEU
16	V	458	THR
16	V	535	THR
16	V	597	PRO
17	W	71	HIS
17	W	72	LEU

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Mol	Chain	Res	Type
17	W	74	PRO
17	W	76	VAL
17	W	82	ASN
17	W	200	VAL
17	W	205	VAL
17	W	233	LYS
17	W	243	VAL
17	W	257	ILE
17	W	259	GLN
17	W	294	VAL
17	W	552	VAL
21	b	13	ILE
21	b	57	LYS
21	b	58	GLN
22	X	57	ARG
22	X	59	GLN
22	X	62	LYS
22	X	72	GLN
22	X	78	MET
22	X	79	VAL
22	X	84	GLU
22	X	86	GLU
22	X	87	THR
22	X	92	GLU
22	X	93	VAL
22	X	96	GLN
22	X	97	GLN
22	X	99	LEU
22	X	101	GLU
22	X	102	LYS
22	X	104	ARG
22	X	106	GLU
22	X	109	LEU
22	X	113	LYS
22	X	114	GLU
22	X	116	ARG
22	X	120	LYS
23	I	528	LEU
23	I	532	LYS
23	I	548	PHE
23	I	645	VAL
23	I	668	CYS

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Mol	Chain	Res	Type
23	I	691	CYS
23	I	694	ILE
23	I	699	THR
23	I	724	LEU
23	I	725	ARG
23	I	726	ILE
23	I	727	ARG
23	I	730	VAL
23	I	731	GLN
23	I	733	THR
25	Y	413	LYS
25	Y	418	ASP
25	Y	419	PHE
25	Y	420	ASP
25	Y	421	GLU
25	Y	425	ILE
27	c	4	VAL
27	c	40	LEU
28	d	112	ASN
29	f	27	MET
29	f	55	LEU
31	g	65	ASN
21	i	13	ILE
21	i	57	LYS
21	i	58	GLN
27	j	4	VAL
27	j	40	LEU
28	k	112	ASN
29	m	27	MET
29	m	55	LEU
31	n	65	ASN
37	o	5	THR
37	o	71	VAL
37	o	79	ILE
37	o	101	VAL
37	o	114	SER
37	o	126	THR
38	p	46	MET
38	p	66	LEU
38	p	87	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (121) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	105	ASN
1	A	181	ASN
1	A	321	ASN
1	A	361	HIS
1	A	368	GLN
1	A	457	ASN
1	A	467	GLN
1	A	584	HIS
1	A	703	GLN
1	A	711	GLN
1	A	792	HIS
1	A	834	HIS
1	A	904	HIS
1	A	974	ASN
1	A	994	ASN
1	A	1013	ASN
1	A	1014	ASN
1	A	1023	ASN
1	A	1066	GLN
1	A	1096	HIS
1	A	1117	HIS
1	A	1124	ASN
1	A	1359	HIS
1	A	1373	GLN
1	A	1460	HIS
1	A	1487	HIS
1	A	1528	GLN
1	A	1710	ASN
1	A	1717	ASN
1	A	1766	GLN
1	A	1791	HIS
1	A	1830	GLN
1	A	1894	GLN
2	C	137	HIS
2	C	154	HIS
2	C	208	HIS
2	C	245	HIS
2	C	280	HIS
2	C	297	ASN
2	C	411	ASN
2	C	451	HIS
2	C	513	ASN

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Mol	Chain	Res	Type
2	C	538	HIS
2	C	680	ASN
2	C	702	ASN
2	C	802	HIS
2	C	856	HIS
2	C	892	GLN
3	E	101	ASN
3	E	192	ASN
3	E	253	ASN
6	J	212	GLN
6	J	221	ASN
6	J	244	ASN
6	J	250	GLN
6	J	259	GLN
6	J	275	ASN
6	J	373	HIS
7	L	175	GLN
7	L	186	GLN
7	L	245	GLN
7	L	266	HIS
8	M	212	ASN
10	O	113	ASN
10	O	120	ASN
10	O	196	GLN
10	O	251	HIS
10	O	294	ASN
11	P	29	GLN
11	P	48	GLN
12	R	133	GLN
12	R	183	GLN
12	R	189	ASN
12	R	279	HIS
12	R	307	GLN
12	R	314	GLN
13	S	10	GLN
13	S	38	ASN
13	S	87	HIS
13	S	126	HIS
14	T	283	HIS
14	T	297	HIS
14	T	384	HIS
14	T	437	HIS

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Mol	Chain	Res	Type
14	T	455	GLN
15	U	3	ASN
15	U	20	GLN
16	V	474	HIS
17	W	82	ASN
17	W	128	GLN
17	W	147	GLN
17	W	250	GLN
17	W	264	ASN
17	W	388	GLN
17	W	492	ASN
17	W	529	ASN
21	b	22	GLN
21	b	76	ASN
22	X	61	GLN
22	X	72	GLN
22	X	96	GLN
23	I	531	HIS
23	I	601	GLN
23	I	705	GLN
26	a	60	GLN
27	c	64	ASN
28	d	34	GLN
29	f	58	HIS
30	e	65	HIS
31	g	65	ASN
26	h	60	GLN
21	i	22	GLN
21	i	76	ASN
27	j	64	ASN
28	k	34	GLN
29	m	58	HIS
30	l	65	HIS
31	n	65	ASN
37	o	156	GLN
38	p	7	HIS

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
18	B	82/117 (70%)	17 (20%)	4 (4%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
19	F	96/107 (89%)	46 (47%)	16 (16%)
20	H	133/188 (70%)	34 (25%)	10 (7%)
4	4	13/46 (28%)	8 (61%)	3 (23%)
5	G	80/174 (45%)	63 (78%)	19 (23%)
All	All	404/632 (63%)	168 (41%)	52 (12%)

All (168) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
4	4	-12	G
4	4	-11	G
4	4	-10	C
4	4	-9	C
4	4	-7	C
4	4	-6	C
4	4	-4	A
4	4	-1	G
5	G	2	U
5	G	3	A
5	G	5	G
5	G	6	A
5	G	7	G
5	G	8	C
5	G	10	U
5	G	11	A
5	G	12	G
5	G	13	C
5	G	14	A
5	G	17	U
5	G	21	A
5	G	22	C
5	G	23	U
5	G	24	G
5	G	25	G
5	G	26	U
5	G	27	U
5	G	28	A
5	G	29	C
5	G	30	C
5	G	31	U
5	G	73	G
5	G	74	G

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Mol	Chain	Res	Type
5	G	75	U
5	G	76	U
5	G	77	U
5	G	78	C
5	G	79	C
5	G	80	U
5	G	81	U
5	G	82	G
5	G	83	A
5	G	84	U
5	G	87	U
5	G	88	G
5	G	89	U
5	G	90	C
5	G	91	A
5	G	92	U
5	G	93	A
5	G	96	U
5	G	97	A
5	G	98	U
5	G	99	C
5	G	100	C
5	G	101	U
5	G	102	G
5	G	103	U
5	G	119	A
5	G	120	G
5	G	121	C
5	G	122	U
5	G	123	C
5	G	124	G
5	G	125	C
5	G	126	G
5	G	127	G
5	G	128	U
5	G	129	U
5	G	130	G
5	G	132	G
18	B	12	U
18	B	13	C
18	B	19	A
18	B	20	G

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Mol	Chain	Res	Type
18	B	21	A
18	B	22	U
18	B	23	C
18	B	24	G
18	B	25	C
18	B	26	A
18	B	28	A
18	B	36	C
18	B	38	C
18	B	45	C
18	B	57	G
18	B	70	A
18	B	71	C
19	F	5	U
19	F	6	C
19	F	7	G
19	F	8	C
19	F	9	U
19	F	10	U
19	F	12	G
19	F	25	C
19	F	26	U
19	F	27	A
19	F	28	A
19	F	29	A
19	F	31	U
19	F	33	G
19	F	34	G
19	F	35	A
19	F	36	A
19	F	37	C
19	F	38	G
19	F	40	U
19	F	43	A
19	F	45	A
19	F	46	G
19	F	47	A
19	F	48	A
19	F	49	G
19	F	51	U
19	F	54	G
19	F	56	A

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Mol	Chain	Res	Type
19	F	59	G
19	F	60	C
19	F	61	C
19	F	62	C
19	F	68	C
19	F	73	A
19	F	74	U
19	F	78	A
19	F	79	C
19	F	80	G
19	F	81	C
19	F	82	A
19	F	83	A
19	F	84	A
19	F	85	U
19	F	86	U
19	F	87	C
20	H	13	C
20	H	14	C
20	H	15	U
20	H	16	U
20	H	17	U
20	H	19	G
20	H	24	A
20	H	25	G
20	H	28	C
20	H	29	A
20	H	30	A
20	H	31	G
20	H	33	G
20	H	37	U
20	H	39	U
20	H	40	C
20	H	41	U
20	H	42	G
20	H	43	U
20	H	112	G
20	H	143	A
20	H	147	G
20	H	152	G
20	H	153	A
20	H	154	C

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Mol	Chain	Res	Type
20	H	156	U
20	H	157	G
20	H	164	C
20	H	165	A
20	H	168	A
20	H	169	C
20	H	177	A
20	H	178	A
20	H	179	C

All (52) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
4	4	-13	C
4	4	-12	G
4	4	-11	G
5	G	1	G
5	G	16	G
5	G	20	A
5	G	21	A
5	G	22	C
5	G	23	U
5	G	90	C
5	G	95	U
5	G	96	U
5	G	97	A
5	G	98	U
5	G	100	C
5	G	119	A
5	G	120	G
5	G	124	G
5	G	125	C
5	G	126	G
5	G	128	U
5	G	129	U
18	B	18	C
18	B	19	A
18	B	20	G
18	B	27	U
19	F	5	U
19	F	7	G
19	F	25	C

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Mol	Chain	Res	Type
19	F	26	U
19	F	33	G
19	F	34	G
19	F	35	A
19	F	36	A
19	F	45	A
19	F	50	A
19	F	58	G
19	F	59	G
19	F	73	A
19	F	81	C
19	F	84	A
19	F	86	U
20	H	15	U
20	H	28	C
20	H	29	A
20	H	30	A
20	H	38	A
20	H	39	U
20	H	40	C
20	H	156	U
20	H	164	C
20	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	$\# Z > 2$
12	SEP	R	224	12	8,9,10	1.74	3 (37%)	7,12,14	2.15	3 (42%)
12	SEP	R	232	12	8,9,10	1.61	1 (12%)	7,12,14	0.99	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
12	SEP	R	224	12	-	0/6/8/10	-
12	SEP	R	232	12	-	2/6/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	R	232	SEP	P-O1P	3.54	1.61	1.50
12	R	224	SEP	P-OG	-2.93	1.51	1.60
12	R	224	SEP	CB-CA	-2.23	1.45	1.52
12	R	224	SEP	P-O2P	-2.11	1.46	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	R	224	SEP	OG-CB-CA	-4.52	103.74	108.14
12	R	232	SEP	OG-CB-CA	2.34	110.42	108.14
12	R	224	SEP	O3P-P-O2P	2.30	116.42	107.80
12	R	224	SEP	O3P-P-OG	-2.16	101.03	106.67

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
12	R	232	SEP	N-CA-CB-OG
12	R	232	SEP	C-CA-CB-OG

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	R	224	SEP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
41	IHP	A	3000	-	36,36,36	0.72	0	60,60,60	1.09	0
42	GTP	C	1500	43	33,34,34	1.07	2 (6%)	50,54,54	1.77	11 (22%)
45	ATP	Q	1501	43	32,33,33	2.04	8 (25%)	48,52,52	1.87	16 (33%)

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
41	IHP	A	3000	-	-	3/30/54/54	0/1/1/1
42	GTP	C	1500	43	-	2/22/38/38	0/3/3/3
45	ATP	Q	1501	43	-	4/22/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	Q	1501	ATP	PB-O3B	7.23	1.67	1.59
45	Q	1501	ATP	C6-N6	4.71	1.46	1.34
45	Q	1501	ATP	C4-N3	3.22	1.40	1.34
45	Q	1501	ATP	C2'-C3'	-2.80	1.45	1.53
42	C	1500	GTP	C5-N7	-2.33	1.34	1.39
42	C	1500	GTP	O4'-C4'	-2.26	1.40	1.45
45	Q	1501	ATP	C8-N7	2.20	1.35	1.31
45	Q	1501	ATP	C3'-C4'	-2.17	1.47	1.53
45	Q	1501	ATP	O2'-C2'	-2.12	1.37	1.43
45	Q	1501	ATP	O3'-C3'	-2.06	1.37	1.43

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
42	C	1500	GTP	C5-C4-N3	-5.15	120.20	128.39
45	Q	1501	ATP	C5-C4-N3	-4.90	119.97	126.72
42	C	1500	GTP	C2-N3-C4	4.46	119.98	112.30
45	Q	1501	ATP	N3-C2-N1	-4.24	122.16	128.58
45	Q	1501	ATP	N3-C4-N9	3.73	133.52	127.17
42	C	1500	GTP	C2'-C1'-N9	-3.60	103.23	113.25
42	C	1500	GTP	N9-C4-N3	3.57	133.08	125.95
42	C	1500	GTP	C2-N1-C6	-3.54	118.70	125.11
45	Q	1501	ATP	N9-C8-N7	-3.40	109.12	113.94
45	Q	1501	ATP	C2-N3-C4	3.23	119.72	111.83
42	C	1500	GTP	N9-C8-N7	-2.99	107.86	113.40
45	Q	1501	ATP	C5-N7-C8	2.93	108.06	103.45
45	Q	1501	ATP	C4-N9-C8	2.90	108.79	105.74
42	C	1500	GTP	C5-C6-N1	2.85	120.52	113.25
45	Q	1501	ATP	C4-C5-N7	-2.68	107.52	110.58
45	Q	1501	ATP	O2A-PA-O1A	-2.54	100.62	112.44
42	C	1500	GTP	O2B-PB-O3B	2.48	113.98	107.27
42	C	1500	GTP	O6-C6-C5	-2.46	120.05	126.53
45	Q	1501	ATP	O2G-PG-O1G	-2.45	101.27	110.83
42	C	1500	GTP	C8-N7-C5	2.32	108.39	104.26
45	Q	1501	ATP	O2A-PA-O3A	2.29	113.47	107.27
42	C	1500	GTP	C3'-C2'-C1'	2.29	105.80	101.46
45	Q	1501	ATP	O2B-PB-O1B	-2.26	101.95	112.44
45	Q	1501	ATP	O2G-PG-O3B	2.25	112.19	104.64
45	Q	1501	ATP	O5'-C5'-C4'	2.10	116.13	108.99
45	Q	1501	ATP	O3G-PG-O3B	2.04	111.49	104.64
45	Q	1501	ATP	O4'-C1'-N9	2.04	112.01	108.09

There are no chirality outliers.

All (9) torsion outliers are listed below:

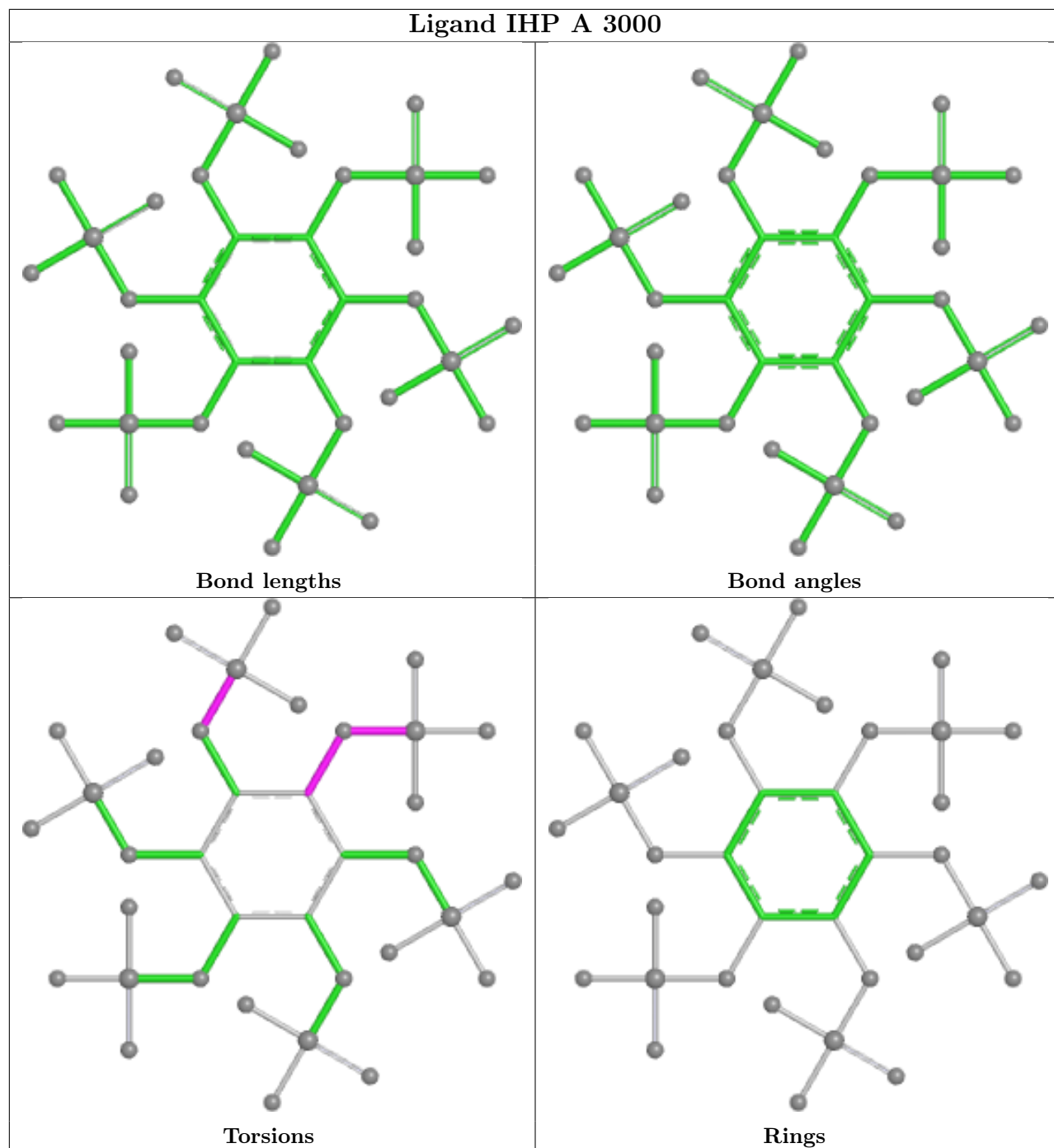
Mol	Chain	Res	Type	Atoms
45	Q	1501	ATP	C5'-O5'-PA-O1A
45	Q	1501	ATP	C5'-O5'-PA-O2A
45	Q	1501	ATP	C5'-O5'-PA-O3A
42	C	1500	GTP	O4'-C4'-C5'-O5'
42	C	1500	GTP	C5'-O5'-PA-O1A
41	A	3000	IHP	C3-O13-P3-O43
41	A	3000	IHP	C3-C4-O14-P4
41	A	3000	IHP	C4-O14-P4-O24
45	Q	1501	ATP	PB-O3A-PA-O2A

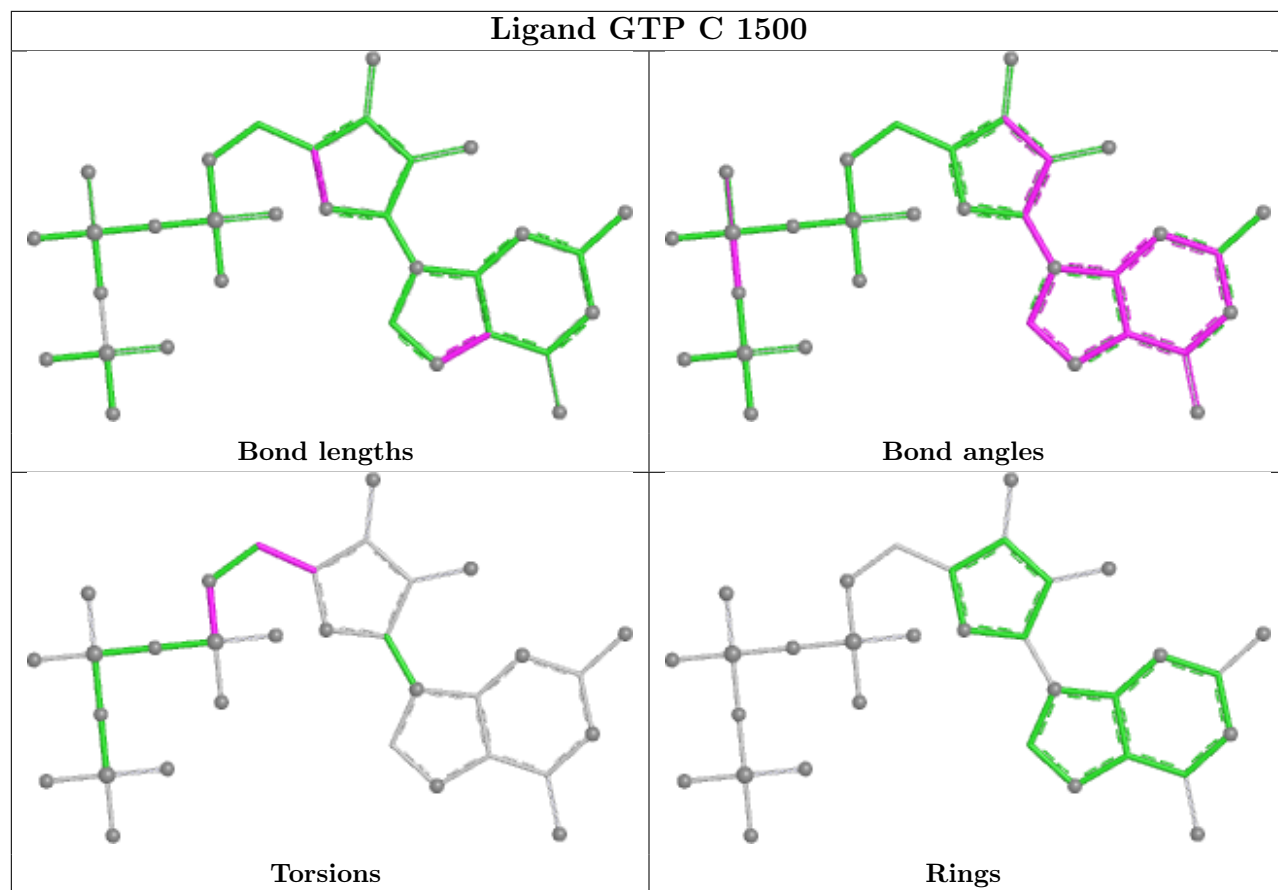
There are no ring outliers.

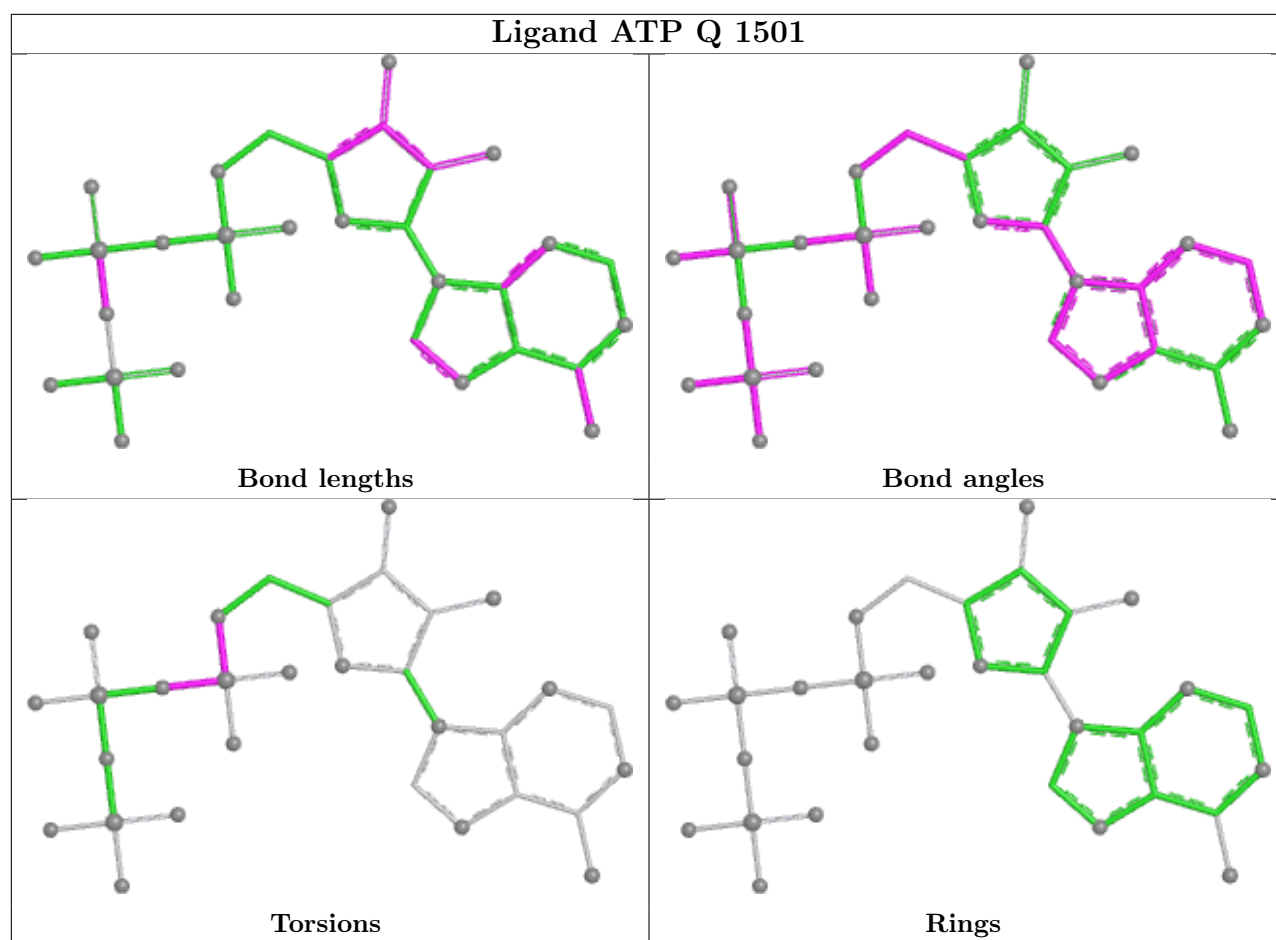
3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
41	A	3000	IHP	9	0
42	C	1500	GTP	2	0
45	Q	1501	ATP	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

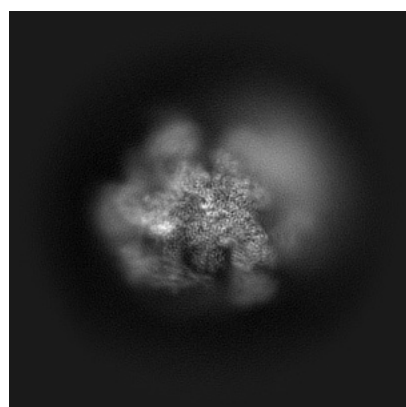
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32317. These allow visual inspection of the internal detail of the map and identification of artifacts.

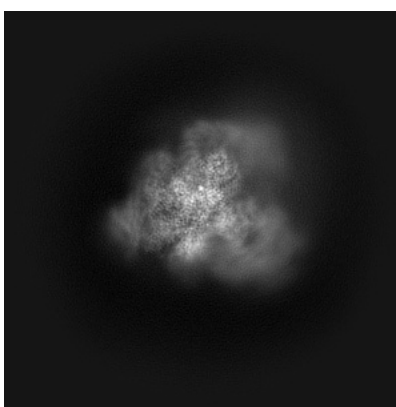
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

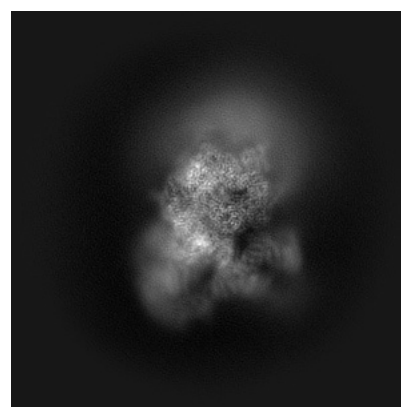
6.1.1 Primary map



X



Y

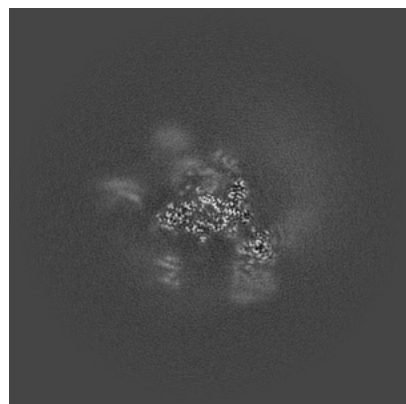


Z

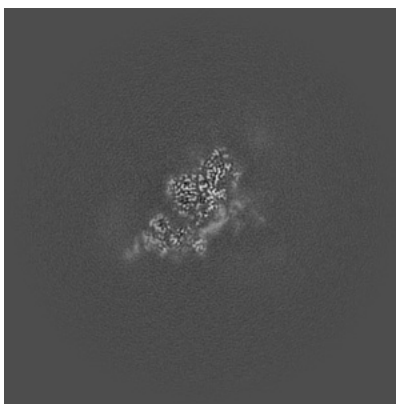
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

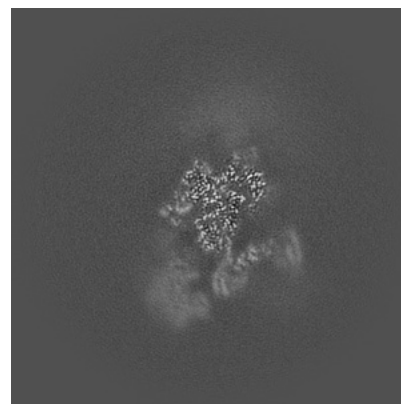
6.2.1 Primary map



X Index: 200



Y Index: 200

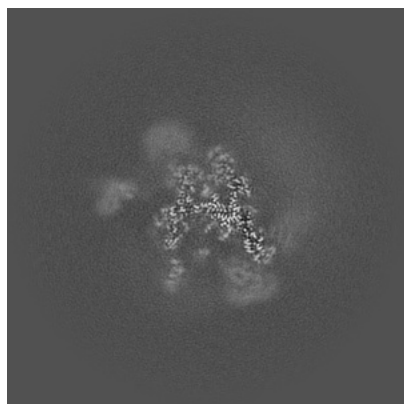


Z Index: 200

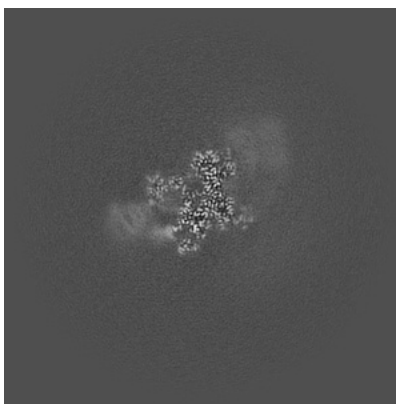
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

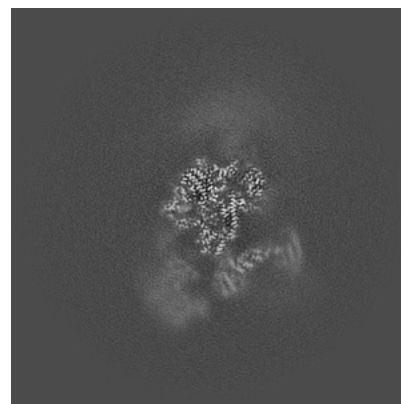
6.3.1 Primary map



X Index: 193



Y Index: 227

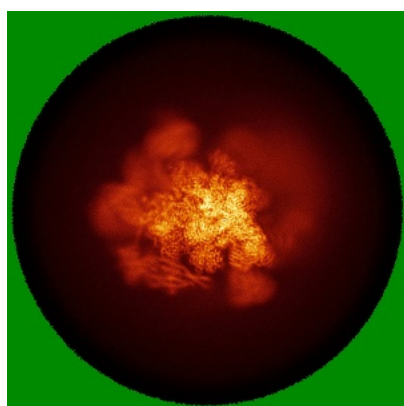


Z Index: 197

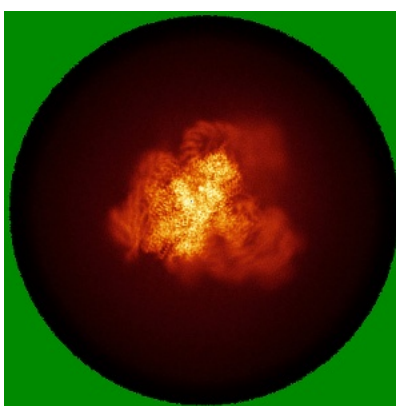
The images above show the largest variance slices of the map in three orthogonal directions.

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

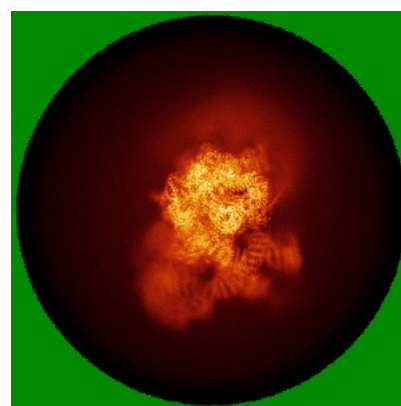
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.38. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

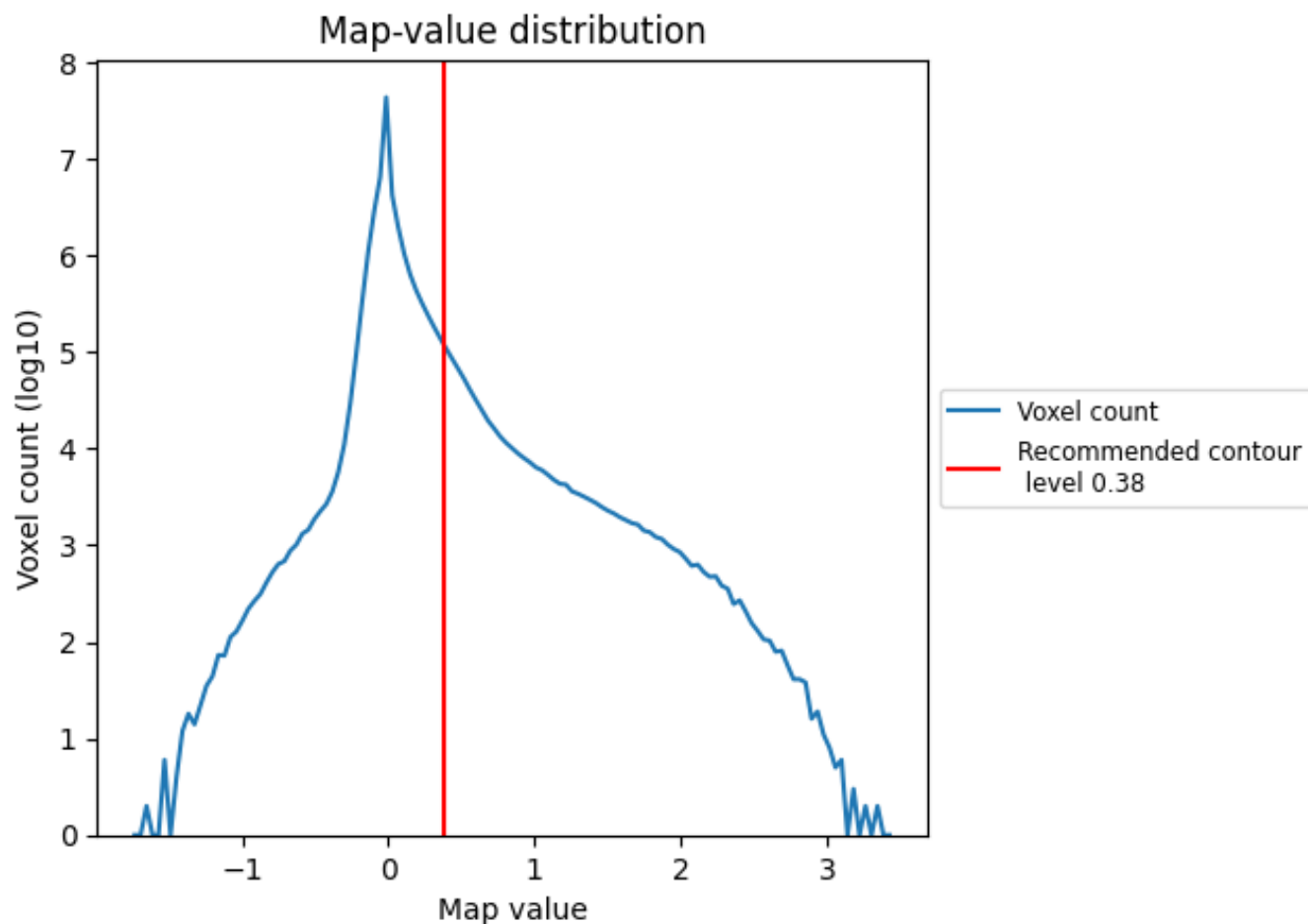
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

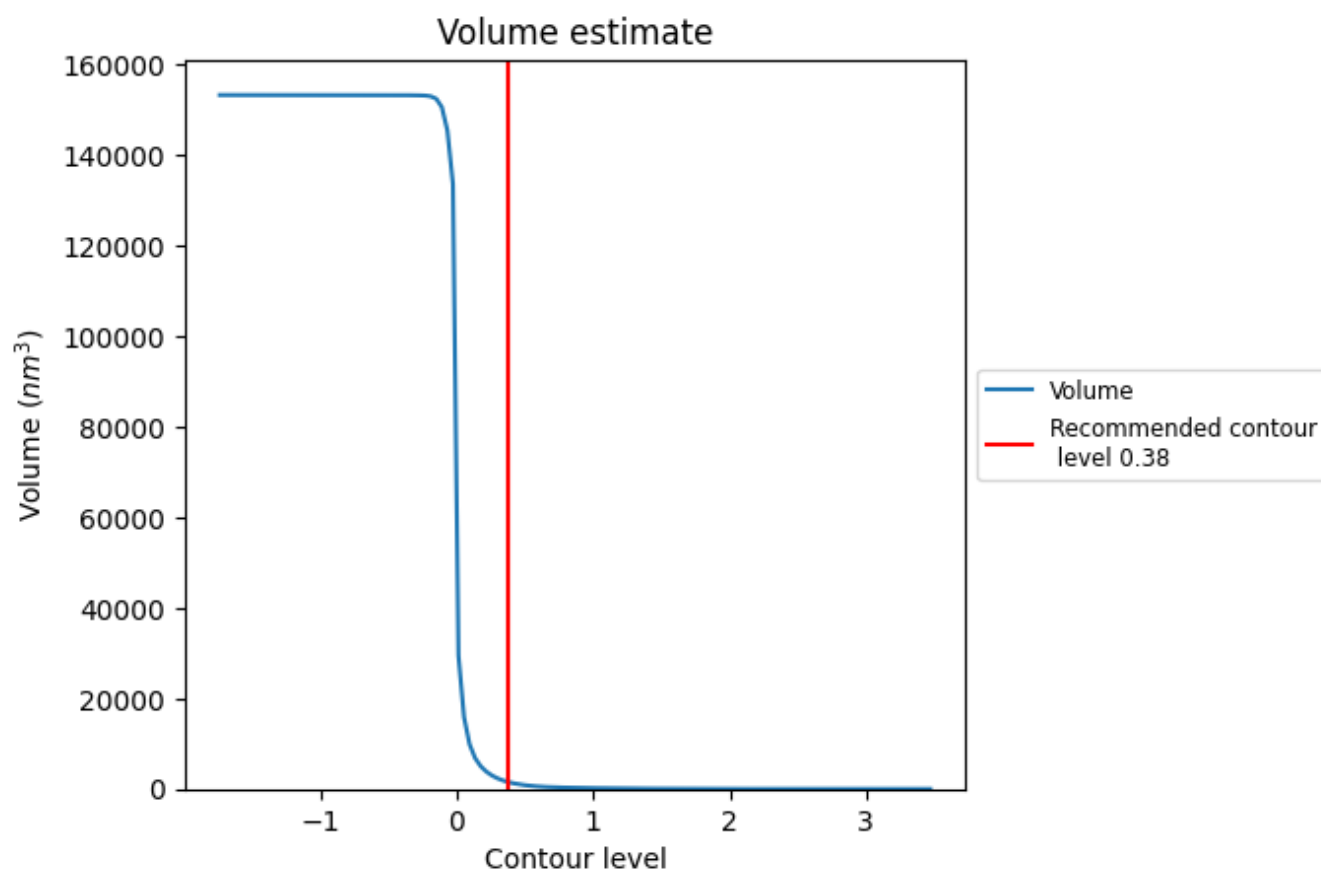
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

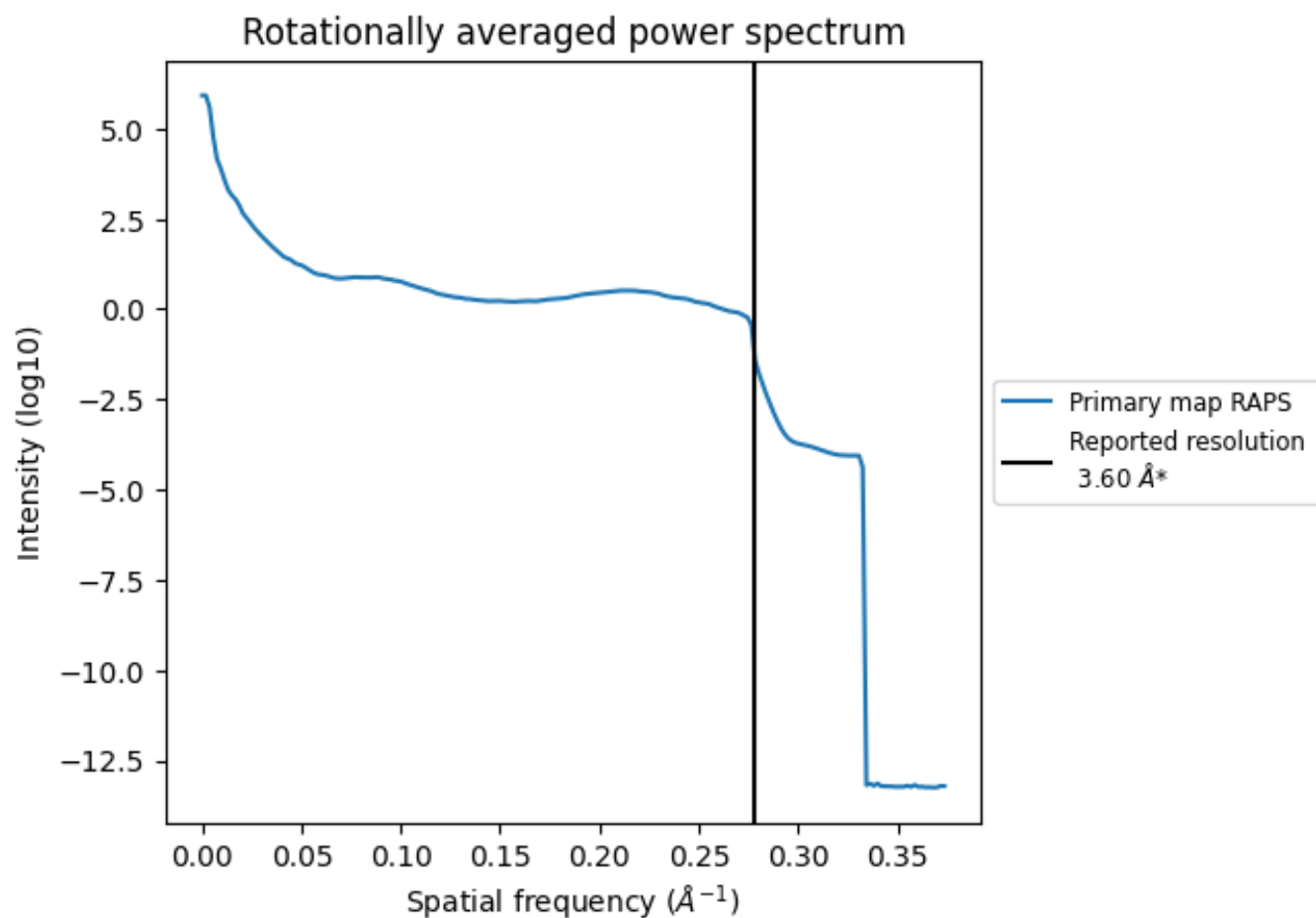
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1511 nm³; this corresponds to an approximate mass of 1365 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 0.278 Å⁻¹

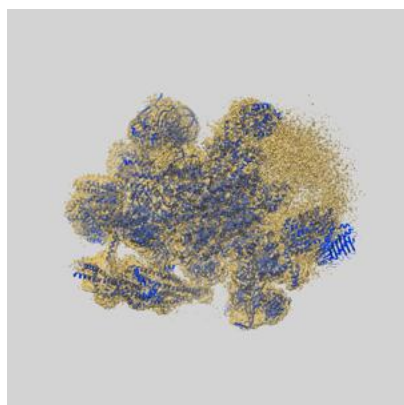
8 Fourier-Shell correlation ⓘ

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

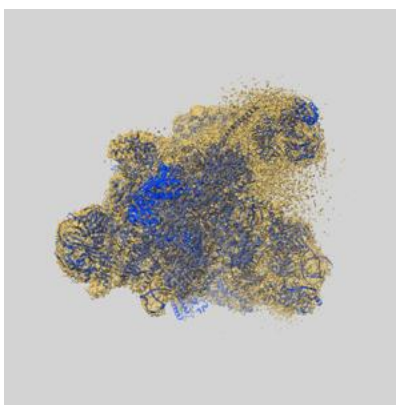
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32317 and PDB model 7W59. Per-residue inclusion information can be found in section 3 on page 15.

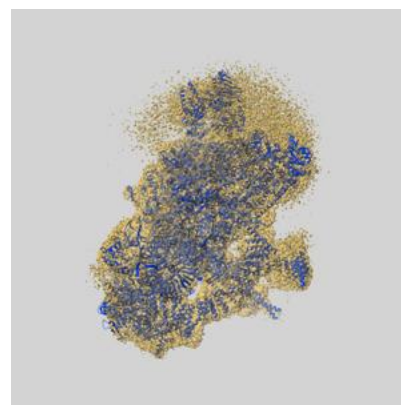
9.1 Map-model overlay [i](#)



X



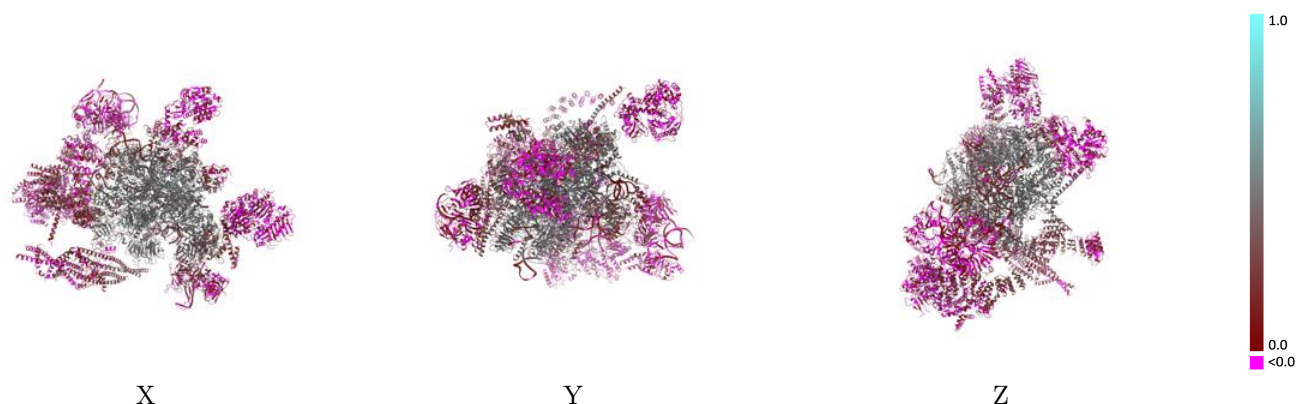
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.38 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](#)

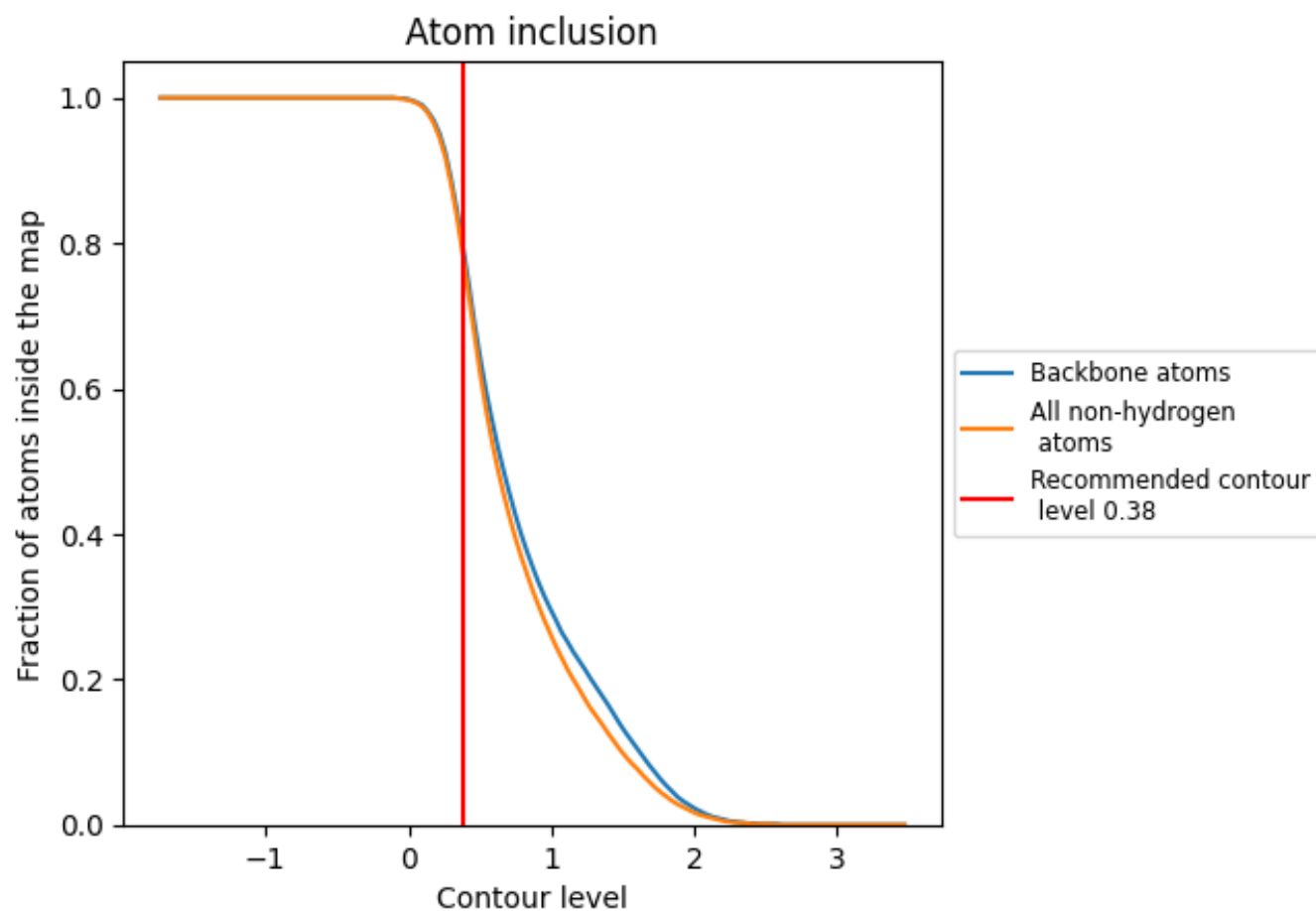


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 80% of all backbone atoms, 78% 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 (0.38) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7840	 0.2680
4	 0.9930	 0.4660
A	 0.9080	 0.4360
B	 0.9410	 0.3070
C	 0.9120	 0.4070
E	 0.9420	 0.4320
F	 0.9510	 0.3510
G	 0.7400	 0.1590
H	 0.7980	 0.1190
I	 0.9150	 0.2190
J	 0.9070	 0.3200
K	 0.9470	 0.1950
L	 0.8990	 0.3480
M	 0.8760	 0.4000
N	 0.9380	 0.4560
O	 0.8940	 0.3870
P	 0.8340	 0.4200
Q	 0.5800	 0.0360
R	 0.8750	 0.4190
S	 0.9270	 0.4120
T	 0.9660	 0.5060
U	 0.8800	 0.3190
V	 0.5730	 0.1630
W	 0.8580	 0.3230
X	 0.9320	 0.4390
Y	 0.2980	 0.0460
a	 0.7690	 0.1890
b	 0.7540	 0.1470
c	 0.8630	 0.0820
d	 0.7680	 0.0280
e	 0.6850	 0.1080
f	 0.7670	 0.0650
g	 0.5850	 0.0950
h	 0.7070	 0.0390
i	 0.5380	 0.0180



Continued on next page...

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Chain	Atom inclusion	Q-score
j	 0.6140	 0.0150
k	 0.6200	 0.0240
l	 0.7020	 0.0070
m	 0.7990	 0.0160
n	 0.7580	 0.0690
o	 0.5350	 0.0260
p	 0.7860	 0.0300
q	 0.6090	 0.0490
r	 0.9330	 0.1960
s	 0.4960	 0.1310
t	 0.4140	 0.0610
u	 0.1990	 0.0220
v	 0.0070	 -0.0000
w	 0.0130	 -0.0170
x	 0.0650	 0.0020
y	 0.8000	 0.1020