



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 03:50 AM UTC

PDB ID : 3JB9 / pdb_00003jb9
EMDB ID : EMD-6413
Title : Cryo-EM structure of the yeast spliceosome at 3.6 angstrom resolution
Authors : Yan, C.; Hang, J.; Wan, R.; Huang, M.; Wong, C.; Shi, Y.
Deposited on : 2015-08-09
Resolution : 3.60 Å(reported)
Based on initial models : 3J7P, 3U1L, 2XL2, 2YTC, 4YVD, 3LRV, 4I43, 4WZJ, 1GV2, 2BAY

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:

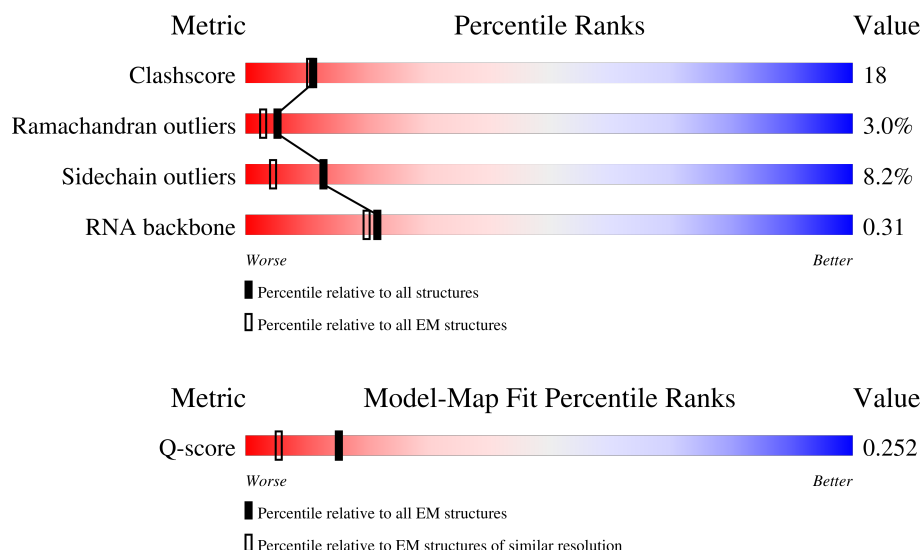
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data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



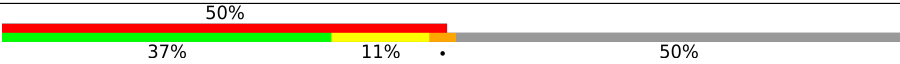
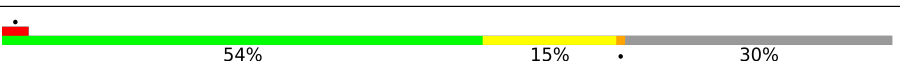
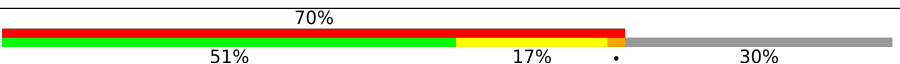
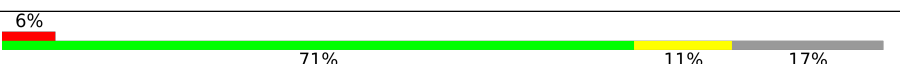
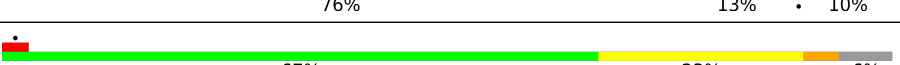
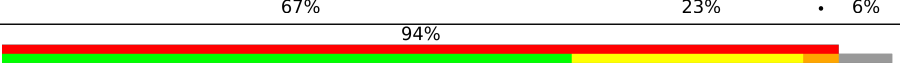
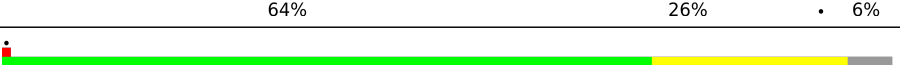
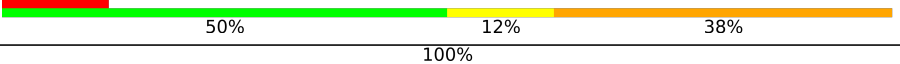
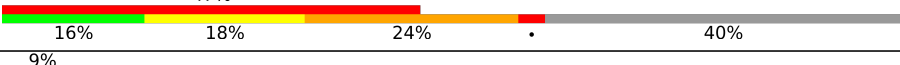
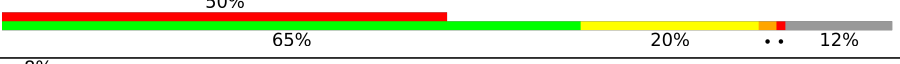
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	2363	
2	B	984	
3	C	120	

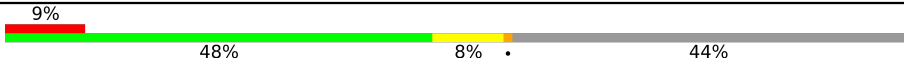
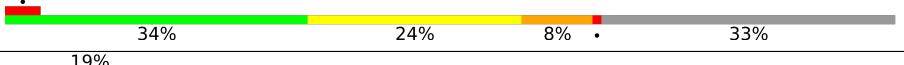
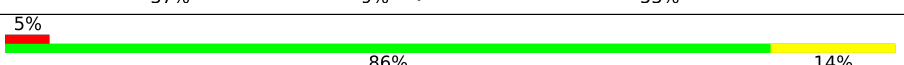
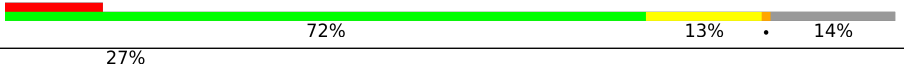
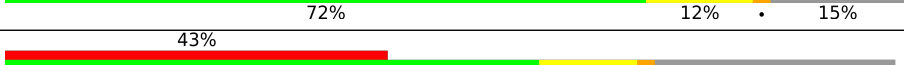
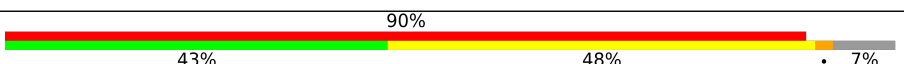
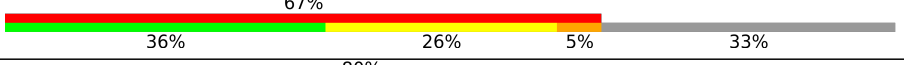
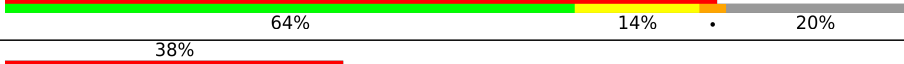
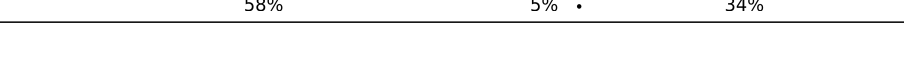
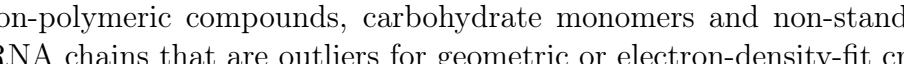
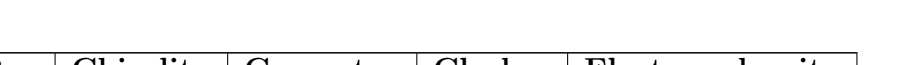
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Mol	Chain	Length	Quality of chain
4	D	97	
4	Z	97	
5	E	147	
5	b	147	
6	F	117	
6	f	117	
7	G	115	
7	l	115	
8	H	84	
8	m	84	
9	I	78	
9	n	78	
10	J	77	
10	o	77	
11	K	473	
12	L	340	
13	M	557	
14	N	99	
15	O	8	
16	Q	13	
17	P	186	
18	S	488	
18	T	488	
18	U	488	
18	V	488	

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Mol	Chain	Length	Quality of chain
19	W	757	
20	Y	388	
21	a	354	
22	c	639	
23	d	155	
24	e	146	
25	g	558	
26	h	265	
27	i	187	
28	R	674	
29	r	790	
30	X	1284	
31	j	239	
32	k	111	
33	x	412	

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
36	ZN	Y	501	-	-	X	-
36	ZN	a	402	-	-	X	-
36	ZN	e	201	-	-	X	-
36	ZN	e	202	-	-	X	-
36	ZN	e	203	-	-	X	-
37	ADP	X	1500	-	-	X	-

2 Entry composition

There are 37 unique types of molecules in this entry. The entry contains 86551 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-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1964	Total	C	N	O	S	0	0
			16230	10413	2859	2893	65		

- Molecule 2 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	904	Total	C	N	O	S	0	0
			7196	4586	1235	1340	35		

- Molecule 3 is a RNA chain called U5 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	105	Total	C	N	O	P	0	0
			2209	990	364	750	105		

- Molecule 4 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	96	Total	C	N	O	S	0	0
			760	470	147	136	7		
4	Z	80	Total	C	N	O	S	0	0
			639	396	118	118	7		

- Molecule 5 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	98	Total	C	N	O	S	0	0
			730	464	130	131	5		
5	b	74	Total	C	N	O	S	0	0
			576	365	99	107	5		

- Molecule 6 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	82	Total	C	N	O	S	0	0
			646	412	110	119	5		
6	f	82	Total	C	N	O	S	0	0
			646	412	110	119	5		

- Molecule 7 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	95	Total	C	N	O	S	0	0
			751	472	141	134	4		
7	l	87	Total	C	N	O	S	0	0
			696	440	128	124	4		

- Molecule 8 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	76	Total	C	N	O	S	0	0
			620	401	107	110	2		
8	m	76	Total	C	N	O	S	0	0
			620	401	107	110	2		

- Molecule 9 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	73	Total	C	N	O	S	0	0
			570	369	95	104	2		
9	n	73	Total	C	N	O	S	0	0
			570	369	95	104	2		

- Molecule 10 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	73	Total	C	N	O	S	0	0
			573	366	98	108	1		
10	o	73	Total	C	N	O	S	0	0
			573	366	98	108	1		

- Molecule 11 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	373	Total	C	N	O	S	0	0
			2730	1720	492	505	13		

- Molecule 12 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	293	Total	C	N	O	S	0	0
			2273	1425	407	430	11		

- Molecule 13 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	207	Total	C	N	O	S	0	0
			1661	1044	309	304	4		

- Molecule 14 is a RNA chain called U6 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	90	Total	C	N	O	P	0	0
			1928	863	357	618	90		

- Molecule 15 is a RNA chain called RNA (5'-R(P*GP*UP*AP*UP*GP*UP*AP*U)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	8	Total	C	N	O	P	0	0
			170	76	28	58	8		

- Molecule 16 is a RNA chain called RNA (5'-R(P*UP*UP*UP*AP*UP*AP*CP*UP*AP*A P*CP*AP*C)-3').

Mol	Chain	Residues	Atoms					AltConf	Trace
16	Q	13	Total	C	N	O	P	0	0
			270	122	44	91	13		

- Molecule 17 is a RNA chain called U2 snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	111	Total	C	N	O	P	0	0
			2323	1039	365	808	111		

- Molecule 18 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	132	Total	C	N	O	S	0	0
			1052	663	181	205	3		
18	T	134	Total	C	N	O	S	0	0
			1069	671	183	212	3		

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Mol	Chain	Residues	Atoms					AltConf	Trace
18	U	430	Total	C	N	O	S	0	0
			2864	1801	492	562	9		
18	V	131	Total	C	N	O	S	0	0
			1037	652	177	205	3		

- Molecule 19 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	W	426	Total	C	N	O	S	0	0
			3024	1881	562	574	7		

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Y	261	Total	C	N	O	S	0	0
			2008	1252	365	381	10		

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	a	255	Total	C	N	O	S	0	0
			1751	1088	324	325	14		

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf19.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	c	300	Total	C	N	O	S	0	0
			2425	1541	422	447	15		

- Molecule 23 is a protein called Peptidyl-prolyl cis-trans isomerase ppi1.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	d	155	Total	C	N	O	S	0	0
			1187	755	203	224	5		

- Molecule 24 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	e	144	Total	C	N	O	S	0	0
			1176	733	216	214	13		

- Molecule 25 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	g	148	Total	C	N	O	S	0	0
			1013	631	181	200	1		

- Molecule 26 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	h	90	Total	C	N	O	S	0	0
			752	467	146	138	1		

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	i	161	Total	C	N	O	S	0	0
			1218	758	219	238	3		

- Molecule 28 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	R	575	Total	C	N	O	S	0	0
			3800	2363	718	706	13		

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	r	573	Total	C	N	O	S	0	0
			3299	2039	619	640	1		

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	X	1195	Total	C	N	O	S	0	0
			9764	6282	1619	1820	43		

- Molecule 31 is a protein called U2 small nuclear ribonucleoprotein A'.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	j	160	Total	C	N	O	S	0	0
			1108	707	187	211	3		

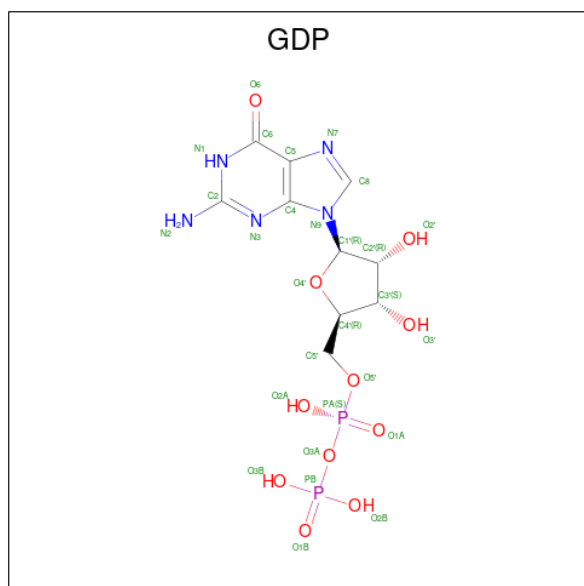
- Molecule 32 is a protein called Probable U2 small nuclear ribonucleoprotein B''.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	k	89	Total	C	N	O	S	0	0
			618	405	102	109	2		

- Molecule 33 is a protein called unknown chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
33	x	272	Total	C	N	O	0	0
			1360	816	272	272		

- Molecule 34 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
34	B	1	Total	C	N	O	P	0
			28	10	5	11	2	

- Molecule 35 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
35	N	4	Total	Mg	0
			4	4	

- Molecule 36 is ZINC ION (CCD ID: ZN) (formula: Zn).

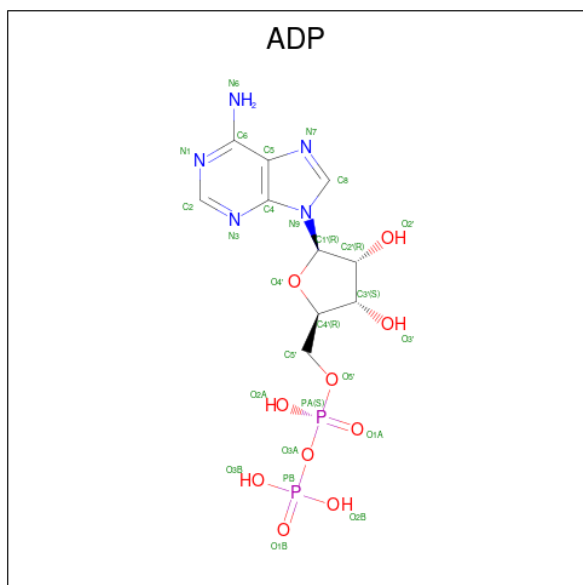
Mol	Chain	Residues	Atoms		AltConf
36	Y	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
36	a	2	Total	Zn	0
			2	2	
36	c	1	Total	Zn	0
			1	1	
36	e	3	Total	Zn	0
			3	3	

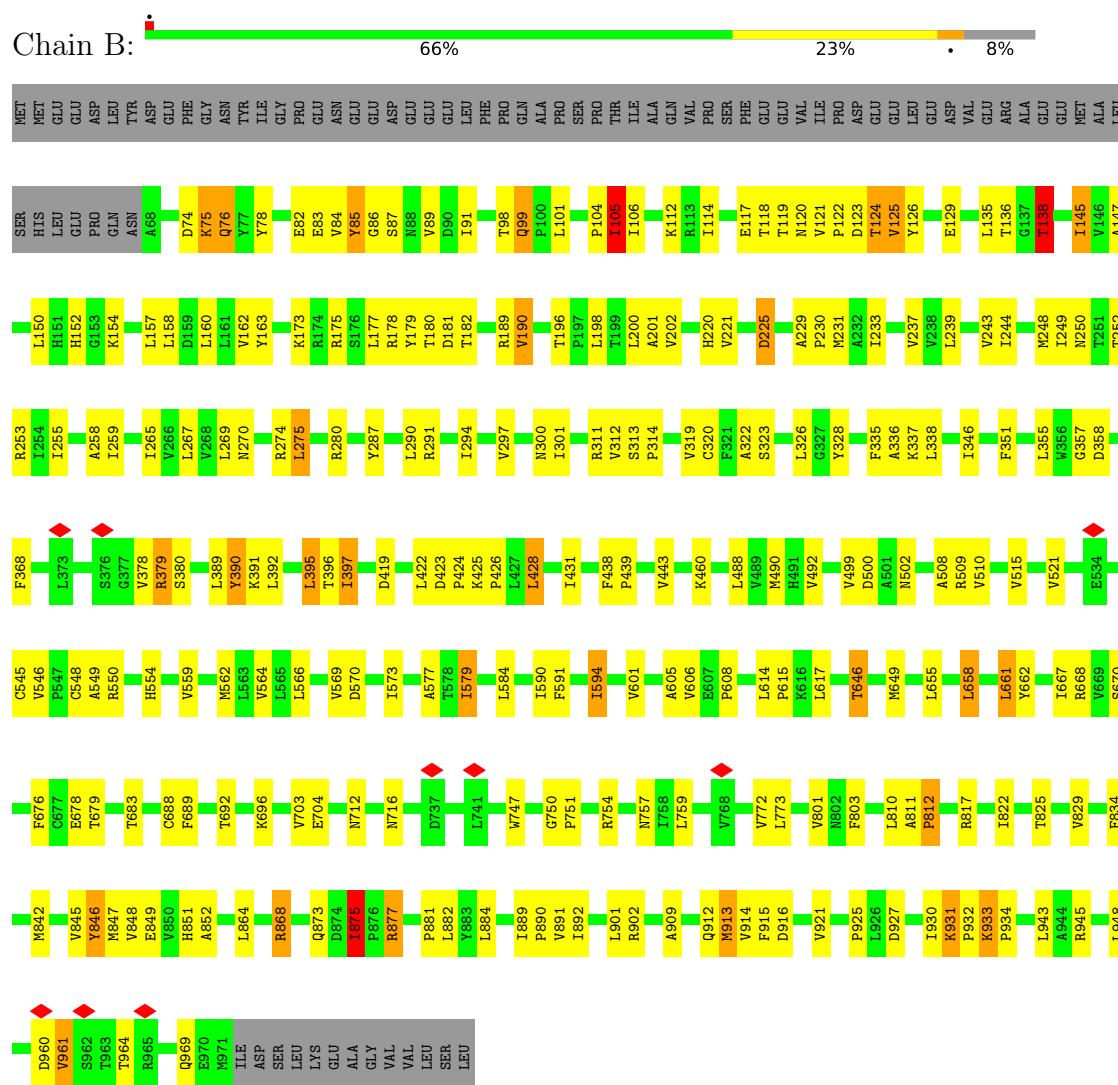
- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



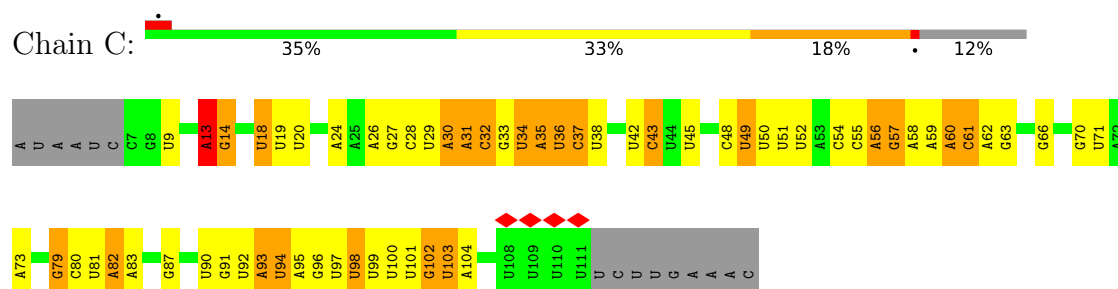
Mol	Chain	Residues	Atoms					AltConf
37	X	1	Total	C	N	O	P	0
			27	10	5	10	2	



- Molecule 2: Pre-mRNA-splicing factor cwf10

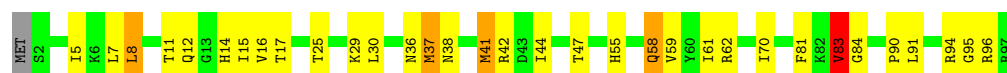


- Molecule 3: U5 snRNA



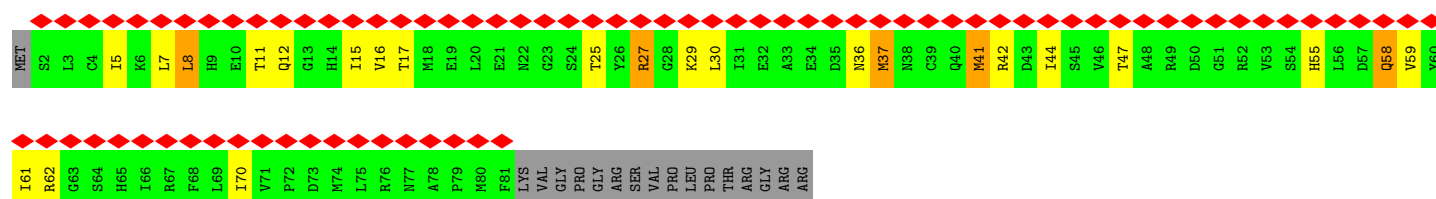
- Molecule 4: Small nuclear ribonucleoprotein Sm D3

Chain D: 



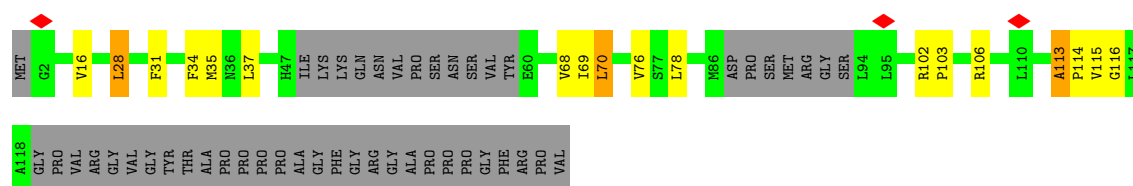
- Molecule 4: Small nuclear ribonucleoprotein Sm D3

Chain Z: 



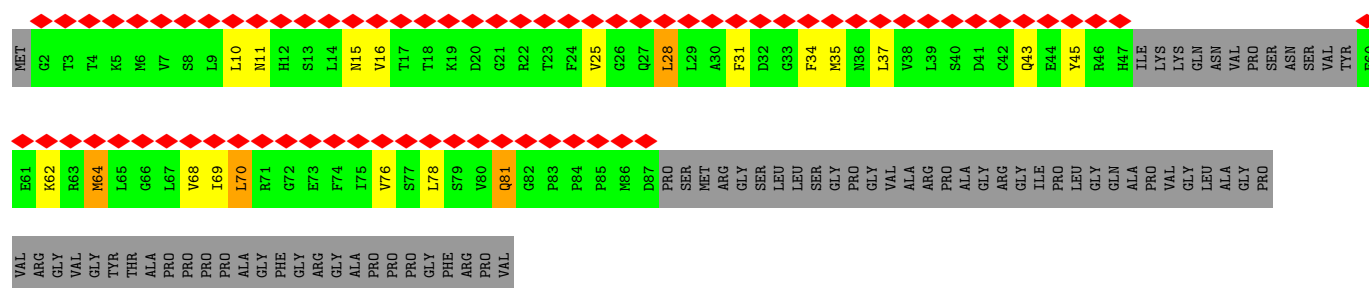
- Molecule 5: Small nuclear ribonucleoprotein-associated protein B

Chain E: 



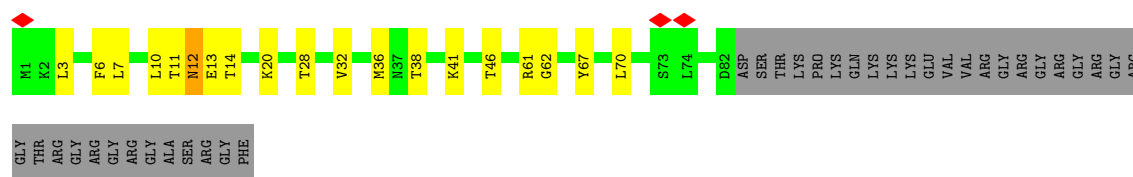
- Molecule 5: Small nuclear ribonucleoprotein-associated protein B

Chain b: 

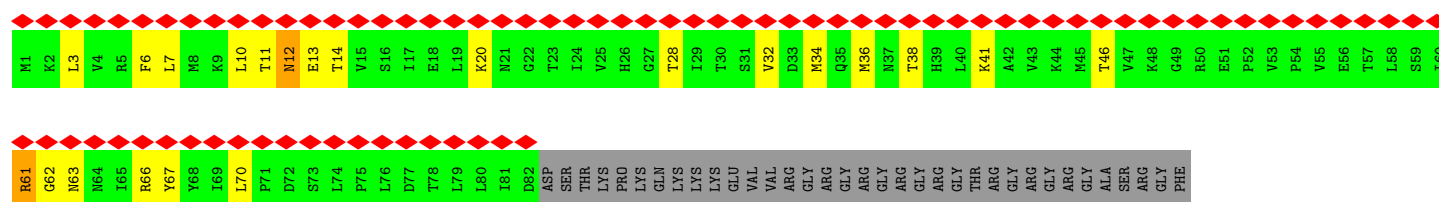


- Molecule 6: Small nuclear ribonucleoprotein Sm D1

Chain F: 



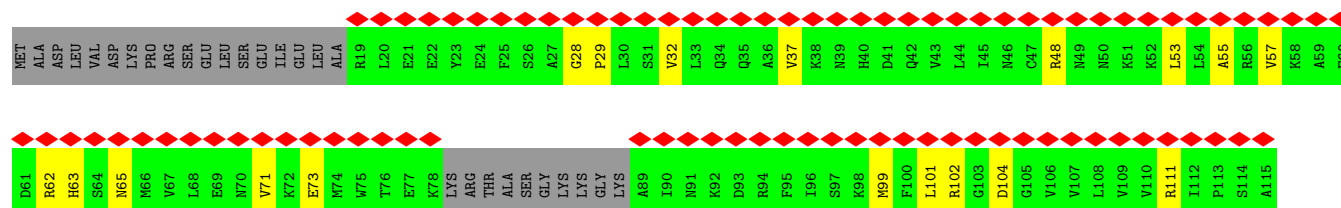
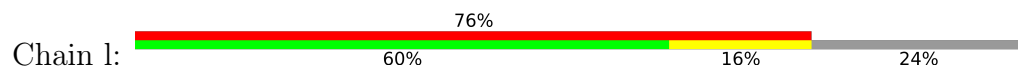
- Molecule 6: Small nuclear ribonucleoprotein Sm D1



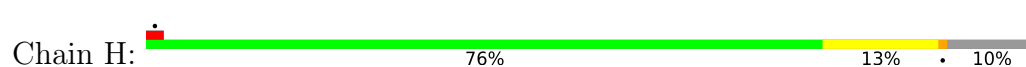
• Molecule 7: Small nuclear ribonucleoprotein Sm D2



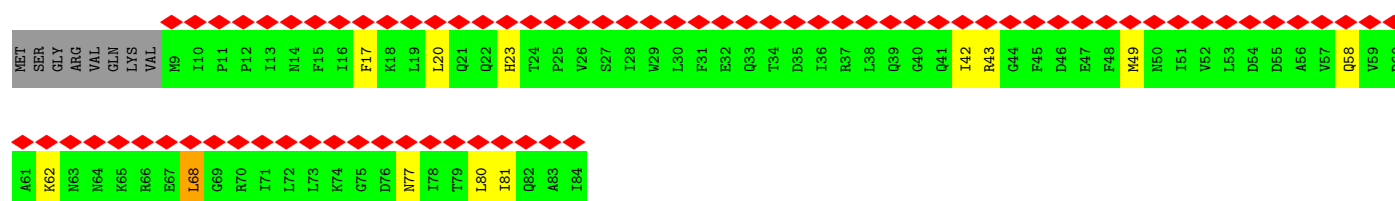
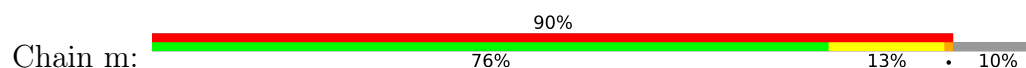
• Molecule 7: Small nuclear ribonucleoprotein Sm D2



• Molecule 8: Small nuclear ribonucleoprotein E

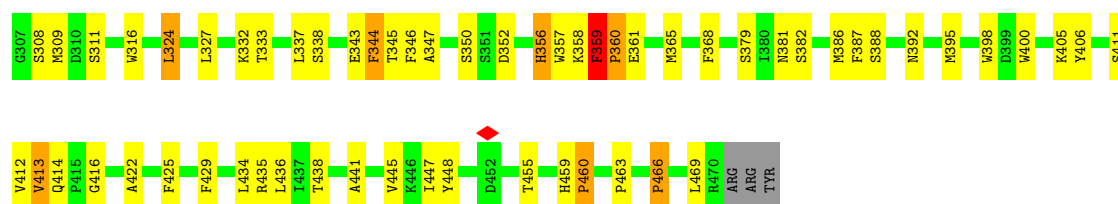


• Molecule 8: Small nuclear ribonucleoprotein E

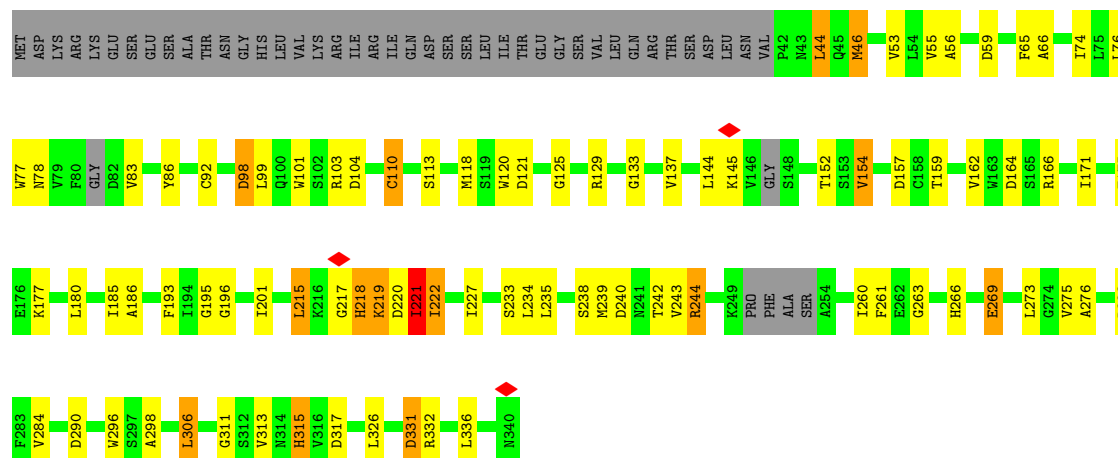


• Molecule 9: Small nuclear ribonucleoprotein F

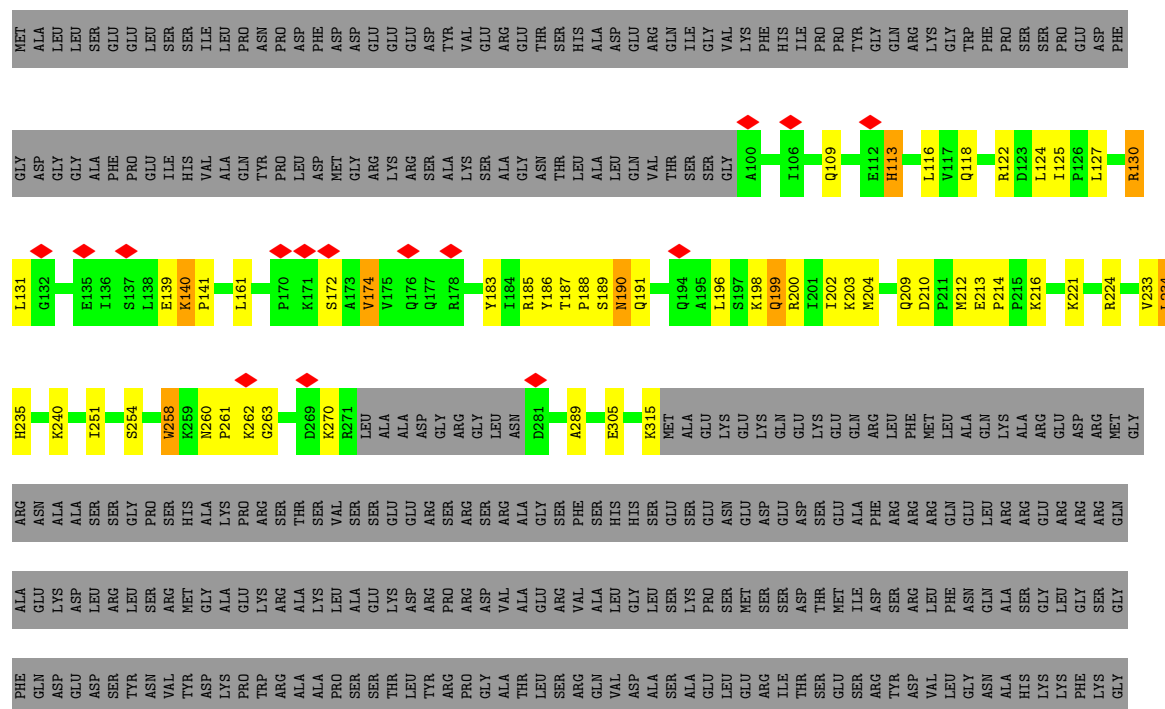




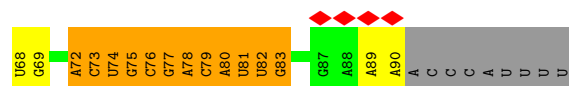
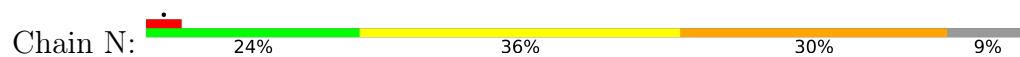
• Molecule 12: Pre-mRNA-splicing factor cwf17



• Molecule 13: Pre-mRNA-processing protein 45



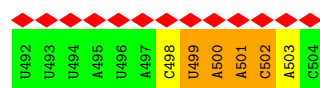
- Molecule 14: U6 snRNA



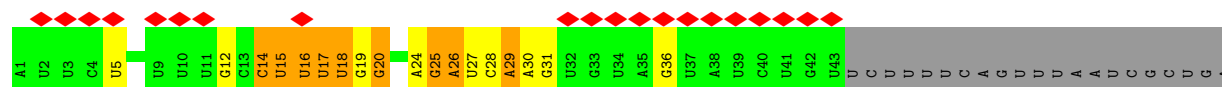
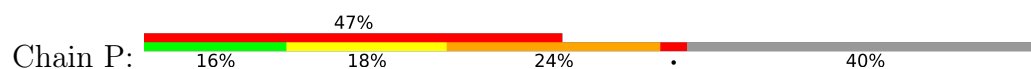
- Molecule 15: RNA (5'-R(P*GP*UP*AP*UP*GP*UP*AP*U)-3')



- Molecule 16: RNA (5'-R(P*UP*UP*UP*AP*UP*AP*CP*UP*AP*AP*CP*AP*C)-3')



- Molecule 17: U2 snRNA



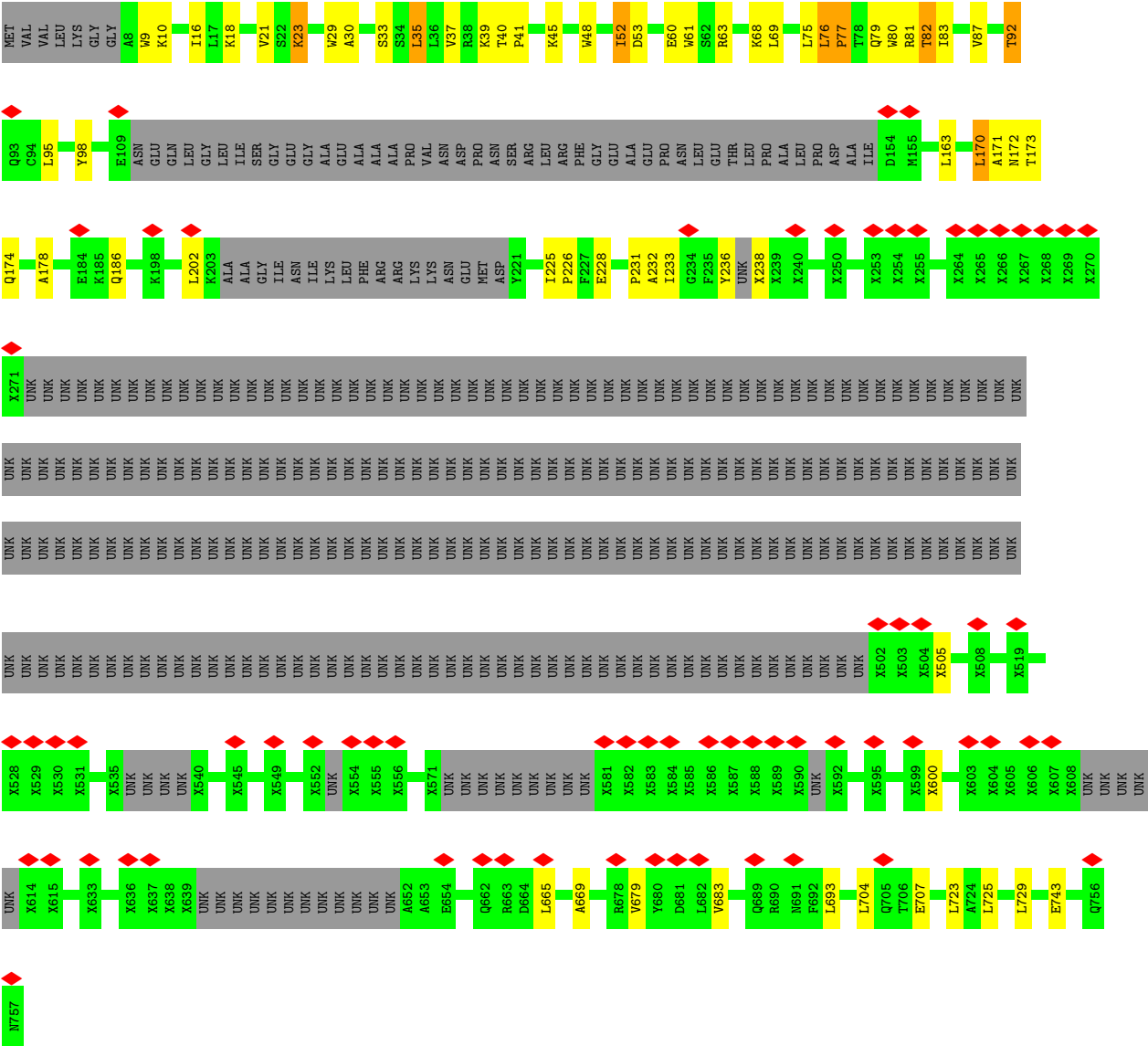
- Molecule 18: Pre-mRNA-processing factor 19



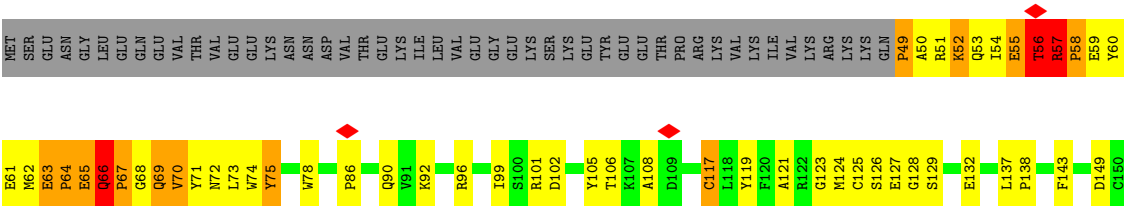
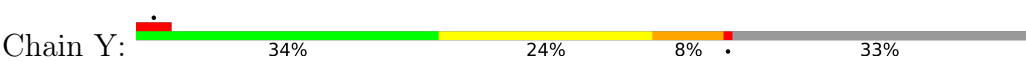


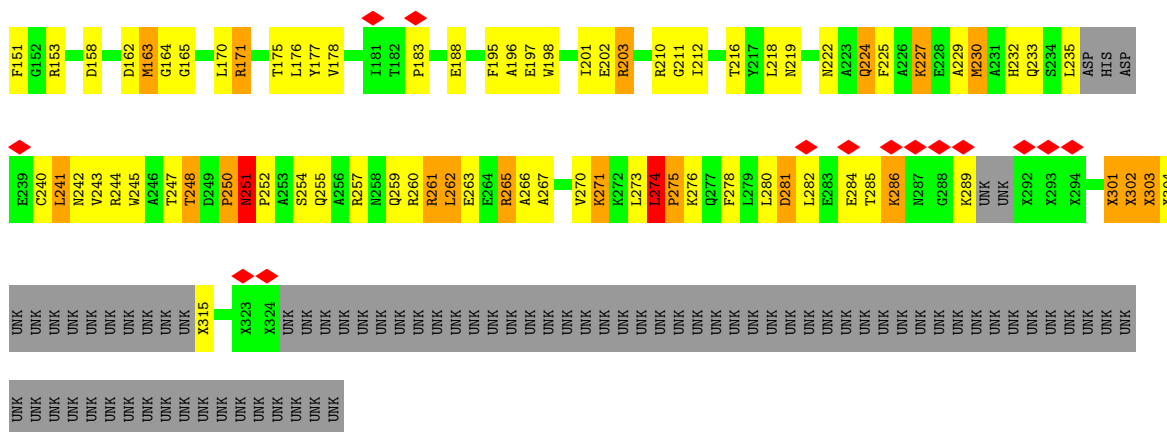
GLU
LEU
HIS
GLN
LEU
LEU
PHE
SER
THR
SER
ASN
GLY
ALA
ILE
LEU
ARG
LEU
GLY

• Molecule 19: Pre-mRNA-splicing factor cdc5

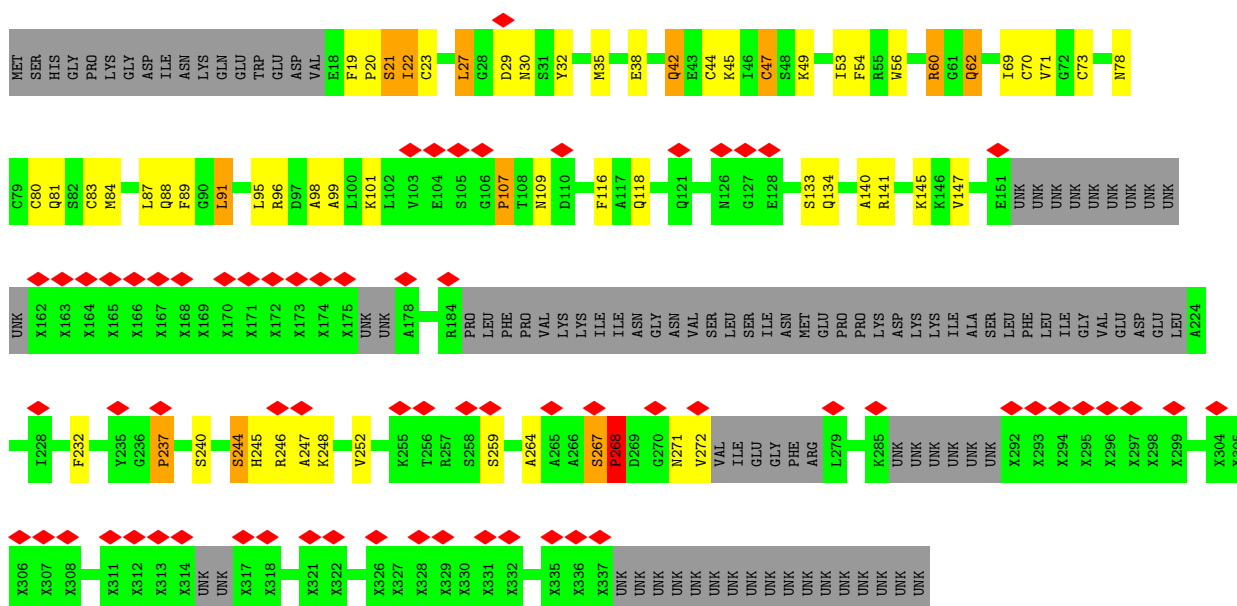


• Molecule 20: Pre-mRNA-splicing factor cwf2

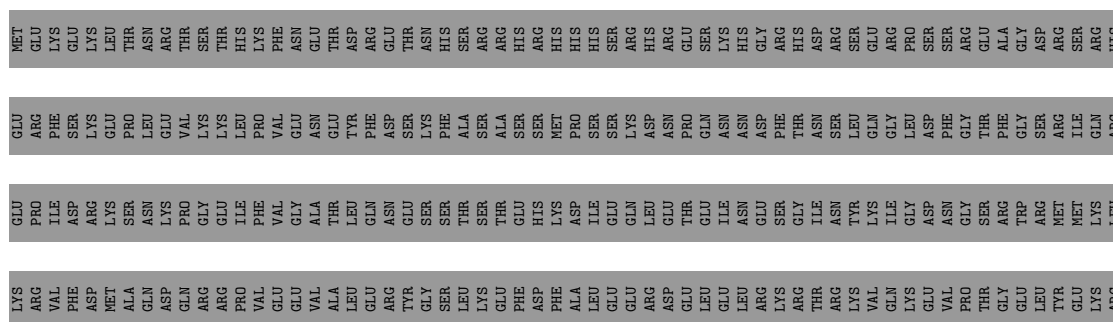
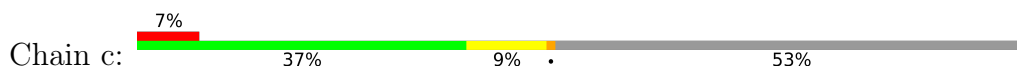


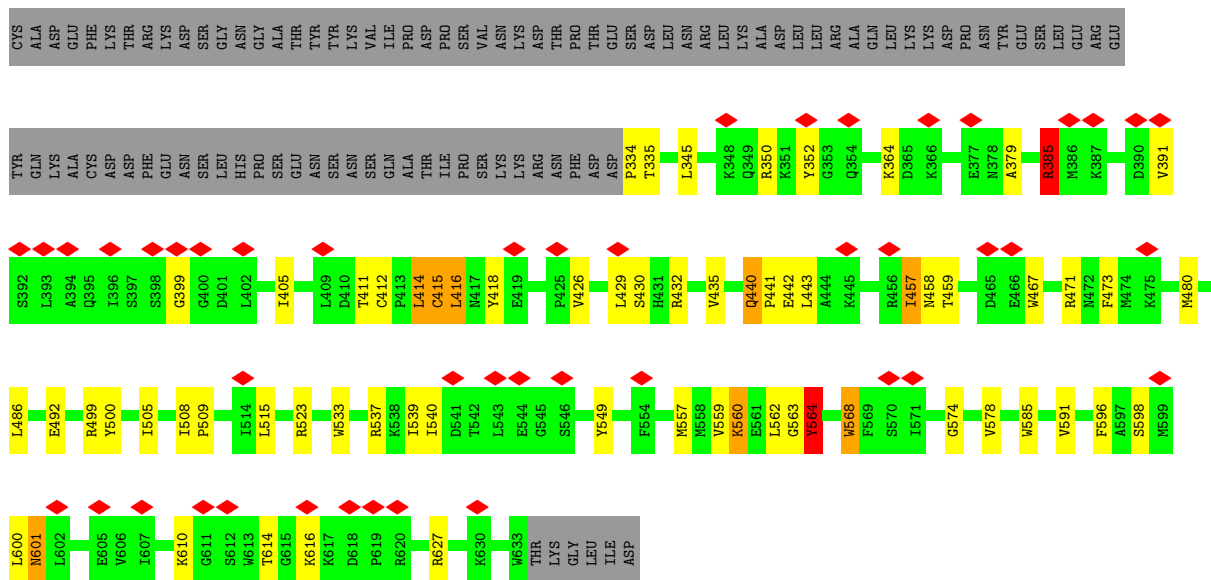


• Molecule 21: Pre-mRNA-splicing factor cwf5

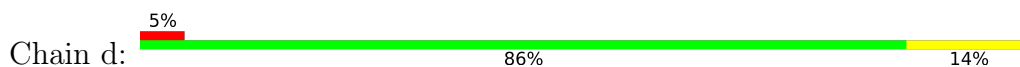


• Molecule 22: Pre-mRNA-splicing factor cwf19

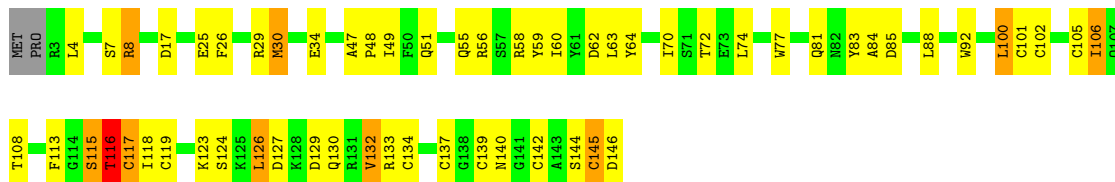




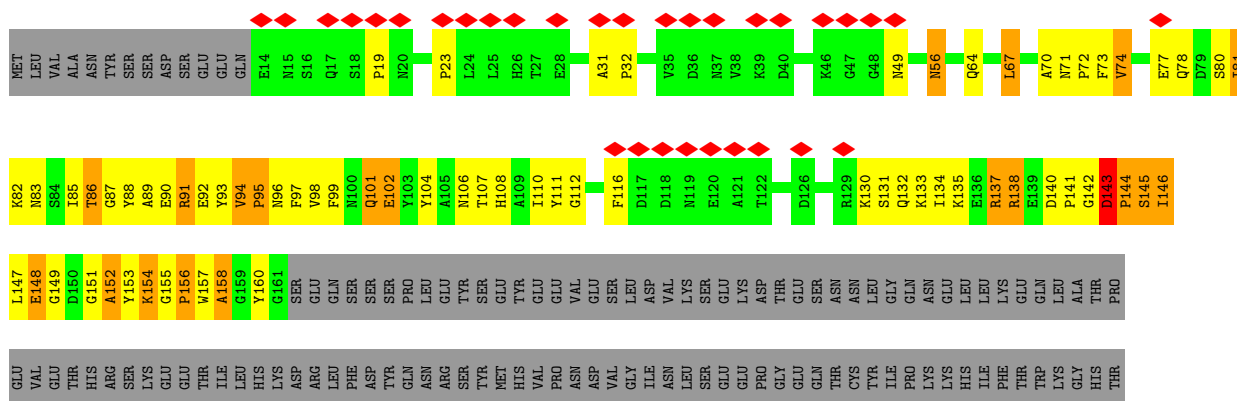
• Molecule 23: Peptidyl-prolyl cis-trans isomerase pp1l

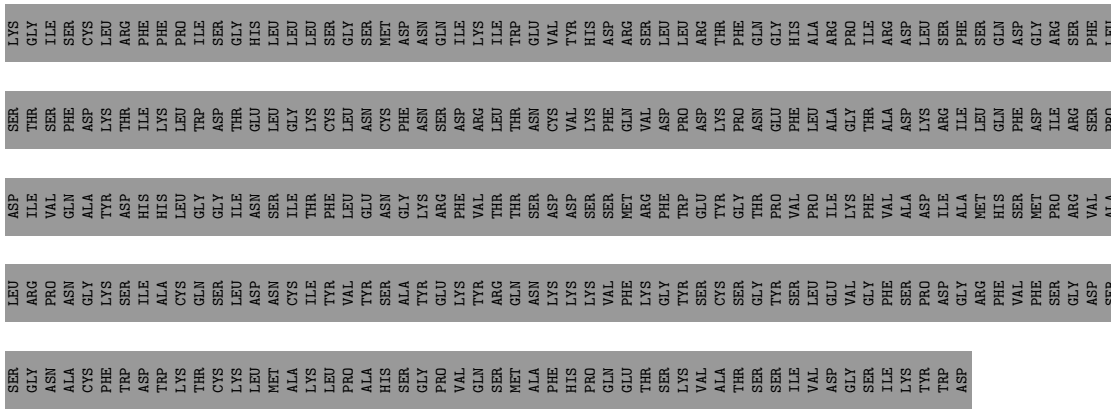


• Molecule 24: Pre-mRNA-splicing factor cwf14

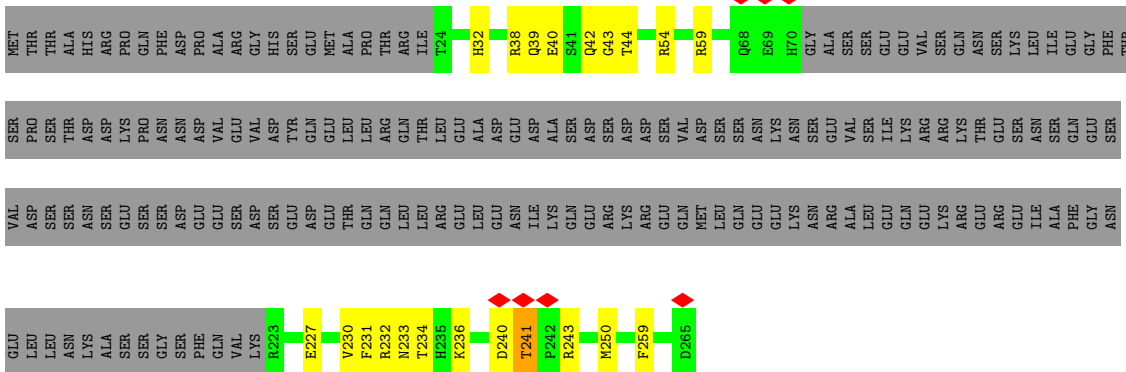


• Molecule 25: Pre-mRNA-processing factor 17

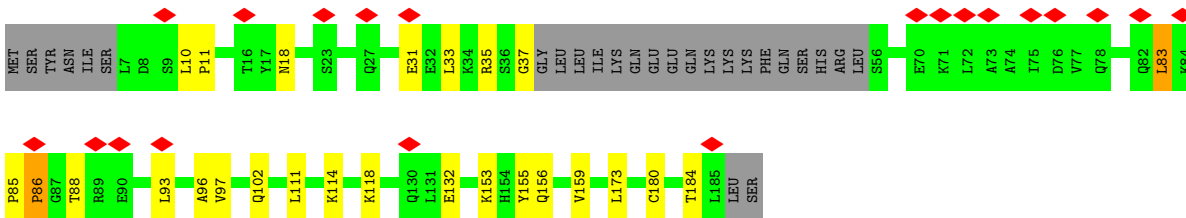




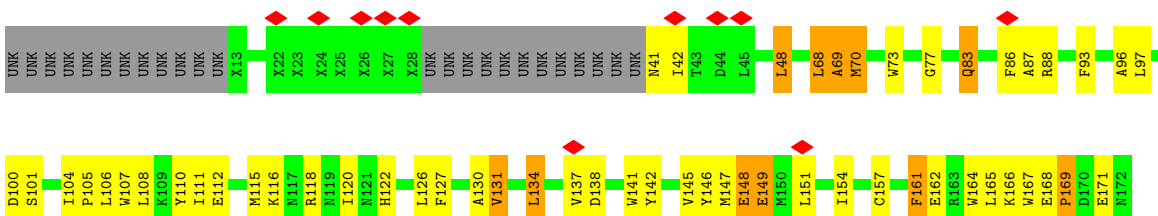
- Molecule 26: Pre-mRNA-splicing factor cwf15

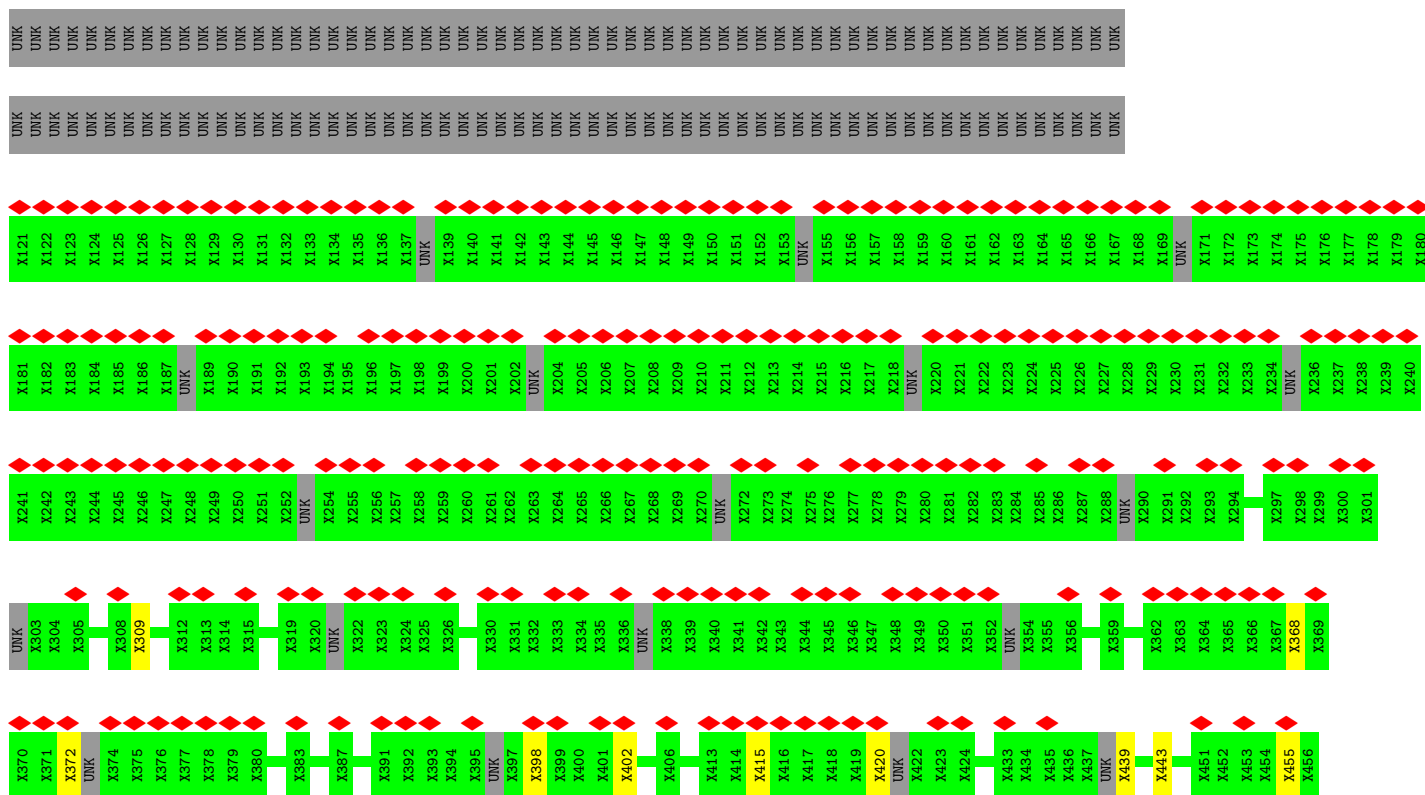


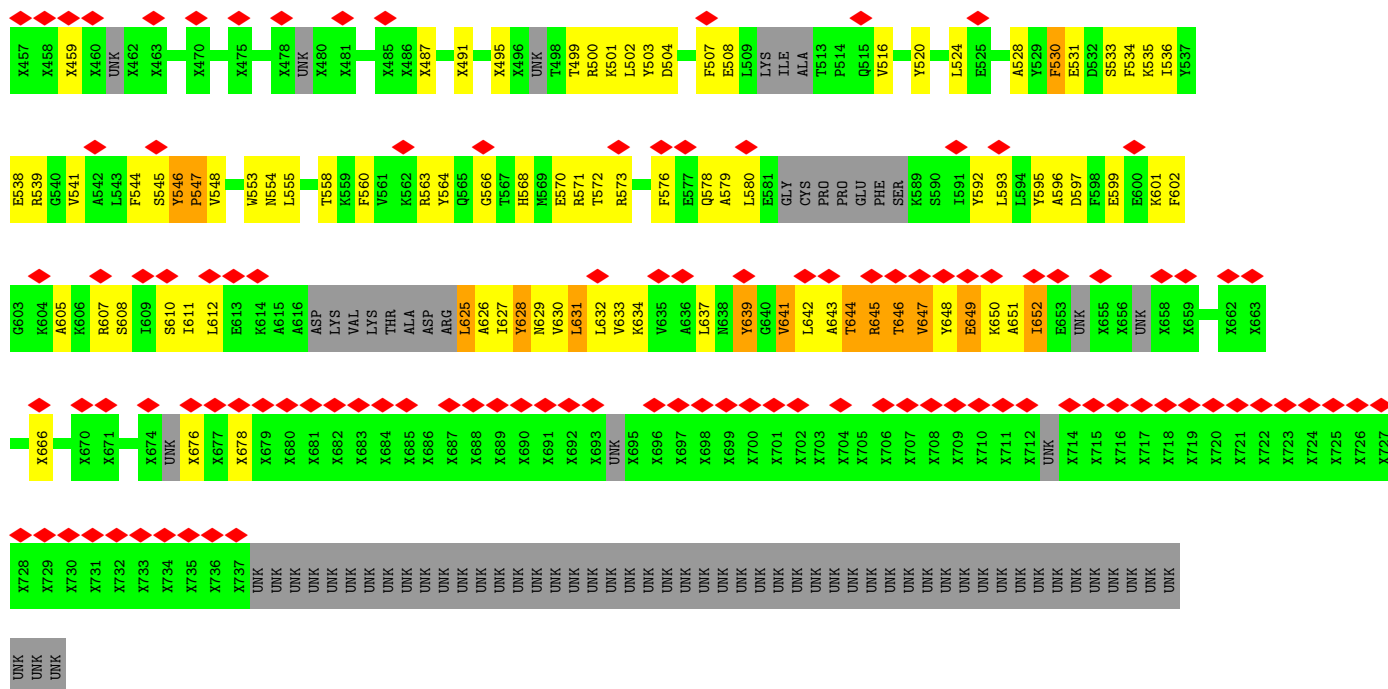
- Molecule 27: Pre-mRNA-splicing factor cwf7



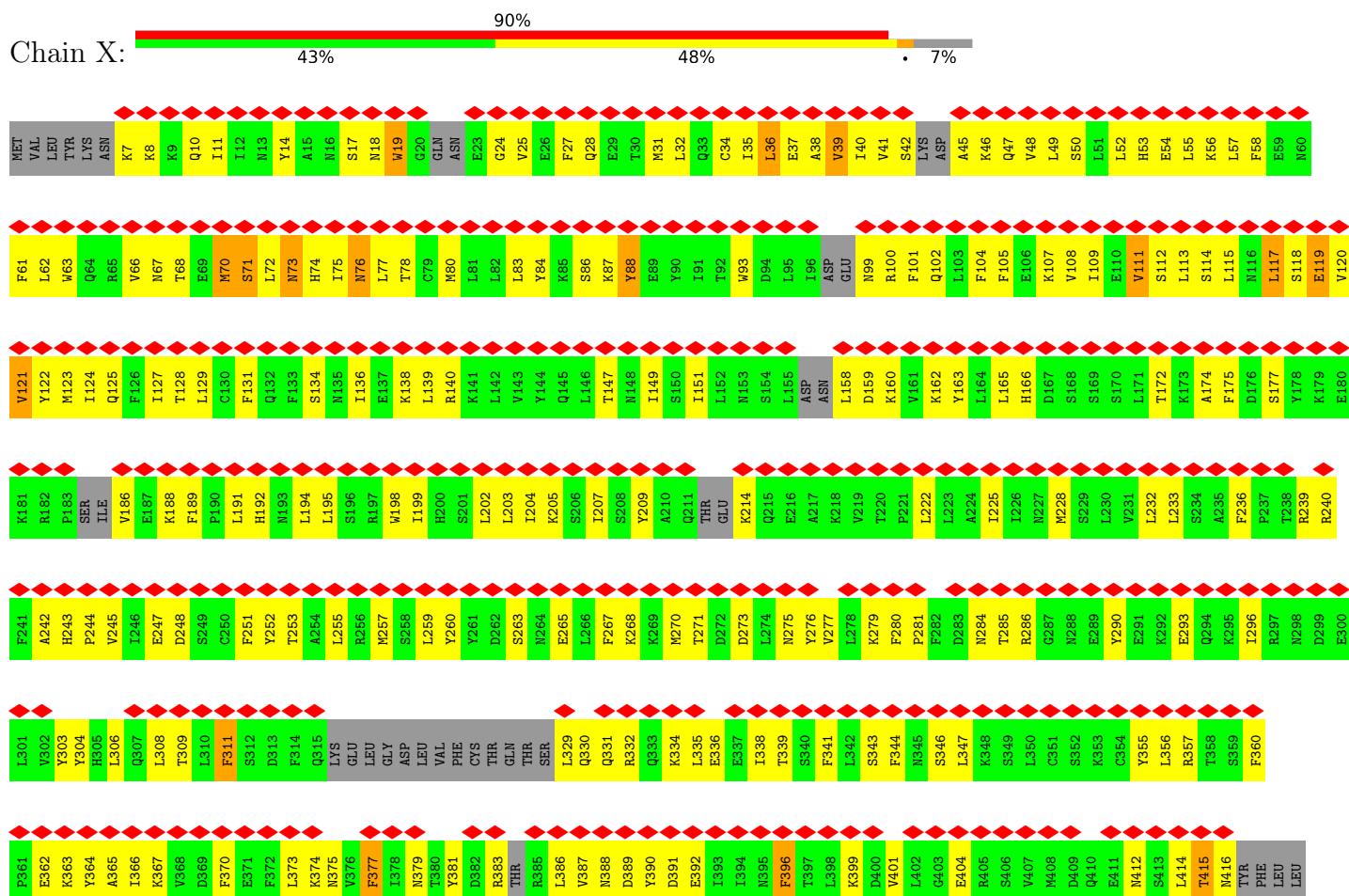
- Molecule 28: Pre-mRNA-splicing factor cwf4



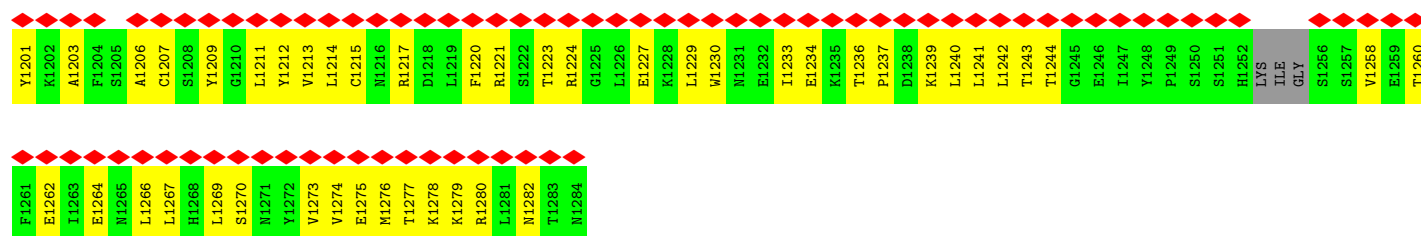




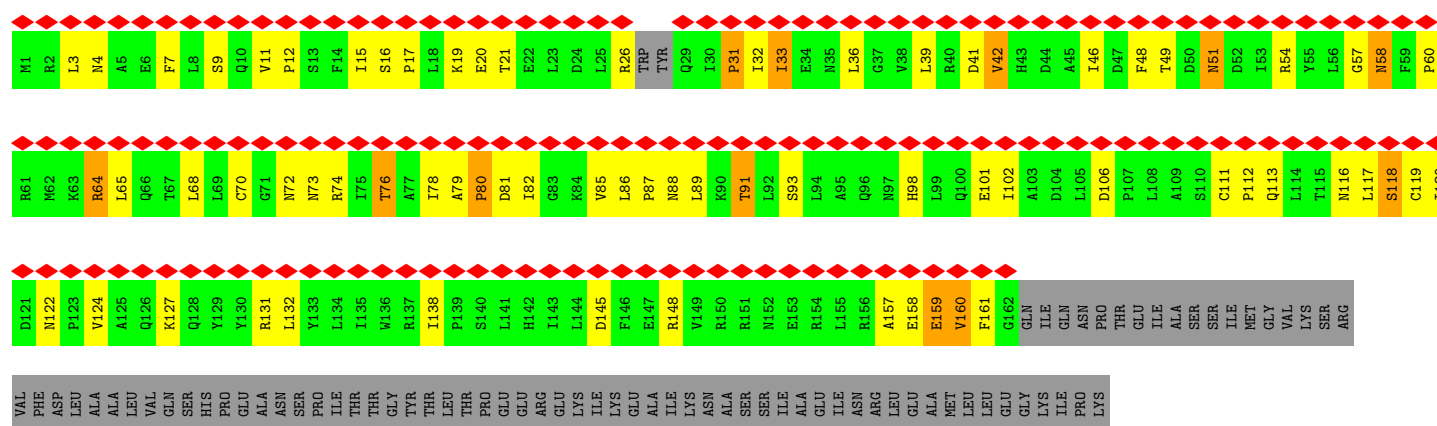
• Molecule 30: Pre-mRNA-splicing factor cwf11



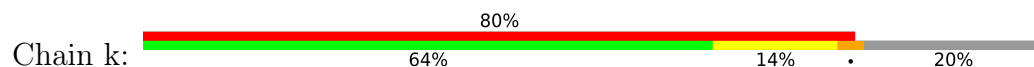
S1141	G1081	ASN	T961	T901	I641	W761	S721	GLY	Y601	K541	N481	GLN
Q1142	F1082	ASN	R962	Y902	Q842	F782	N722	LEU	R602	L542	N482	ASN
V1143	A1083	THR	L963	N903	A843	S783	R723		P603	L543	F483	
S1144	H1084		G964	K904	P844	M784	L724		K604	H544	K484	
L1145	E1085		T965	D905	G845	W785	Y725		Q605	G545	V485	
L1146	V1086		L966	N906	S846	W786	Y726		L606	N546	T486	
M1147	Q1087		K967	F907	H847	L787	Y727		K607	A547	S487	
E1148	F1088		E968	F908	D848	F788	N728		F608	L548	V488	
I1149	N1089		K969	D909	A849	W789	N729		N609	L549	A489	
I1150	K1090		E970	Y910	S850	L790	K730		F610	P550	P490	
S1151	V1091		F971	A911	P851	L791	Q731		A611	L551	PRG	
V1152	C972		D952	T912	D852	W792	L732		L612	E552	GLN	
A1153	F973		T853	K913	T853	K793	E733		V613	GLY	ILE	
F1094	N874		A854	L914	A854	A794	S734		L614	V554	GLY	
K1095	N875		L855	Y915	L855	R795	I735		S615	T555	VAL	
G1096	L876		Y856	G916	F856	C796	L736		PRG	D556	L497	
S1097	I877		F857	E917	F857	W797	R737		GLU	F557	Q499	
Q1098	V878		R858	L918	H798	H798	G738		ALA	T558	F501	
E1099	N879		D859	E919	D859	GLN	S739		N619	I559	F501	
T1100	N880		A860	Y920	A860	GLY	Q740		K620	A560	V501	
E1101	S981		Y861	N921	Y861	H801	P741		W622	T561	K502	
P1102	Q882		L862	F922	L862	L802	G742		L623	I562	C503	
V1103	N883		K863	Q923	K863	L803	L743		D624	C563	Q504	
S1104	I884		A864	Q924	A864	Y804	T744		L625	N564	M505	
G1105	Y1046		L865	L925	L865	L805	T745		N626	D565	G506	
V1106	E886		Y866	E926	Y866	S806	W746		I627	D566	L507	
K1107	S887		E867	E927	E867	D807	N747		V627	V567	R447	
Q1108	S888		K868	I928	K868	E808	G748		W629	G568	S508	
N1109	E1050		Y869	R929	Y869	GLY	P749		S630	M569	R509	
L1110	S1051		L870	P930	L870	LYS	T750		L631	P510	P510	
G1111	I1052		N871	F931	N871	GLU	R751		L632	GLY	PRG	
E1112	S1053		L872	G932	L872	LEU	C752		N633	ASP	PHE	
A1113	L993		D873	L933	D873	L814	G753		E693	M574	HIS	
E1114	S1054		K874	L934	K874	E815	K754		R634	A516	S515	
Y1115	C1056		ASP	R835	ASP	R816	H755		A635	Q575	A516	
A1116	S1057		K876	Y936	K876	Y817	V756		K636	S576	L517	
V1117	S1058		D877	Y937	D877	G818	L757		E637	D577	R518	
A1118	E1059		S878	Y938	S878	T819	V758		F638	S578	D519	
L1119	Y1060		V879	D939	V879	L820	C759		P639	L520	L520	
F1180	P1061		D880	E940	D880	S821	K760		W641	K521	K521	
V1181	L1062		A881	E941	A881	S822	L761		F642	N522	N522	
I1182	D1063		Y882	L942	Y882	W823	L762		E643	K581	I523	
F1183	I1064		N883	Y943	N883	L824	E763		L583	ILE	LYS	
R1184	K1065		R884	A944	R884	S825	V764		D644	S526	S526	
M1125	L1066		F885	L945	F885	W826	L765		L545	P527	I465	
L1126	V1067		P886	C946	P886	L827	Q766		F646	F528	K466	
G1127	D1068		F887	Q947	F887	P828	D767		L547	L529	N467	
Y1128	S1069		S888	Q948	S888	G829	T768		G648	C530	A468	
P1129	K1070		S889	S949	S889	L830	S769		F649	L631	T469	
T1130	N1071		Y890	R950	Y890	L831	W770		G650	I532	K470	
N1131	M1072		F891	P951	F891	R832	P770		T651	Y591	N471	
E1132	K1073		G892	I952	G892	E833	N771		P652	Y592	I534	
I1133	L1074		D893	G953	D893	T834	D772		D653	H593	THR	
V1134	S1075		K894	C954	K894	G835	R773		I654	S594	ASP	
I1135	L1076		S895	T955	S895	R836	T774		C655	L595	N475	
C1136	G1077		K896	Y956	K896	L837	W775		A656	A596	F478	
Y1077	Y1077		R897	T957	R897	A838	V776		F657	G597	F477	
G1078	N1078		P898	T958	P898	A839	L777		P658	L597	M538	
N1079	S1080		T899	S960	T899	S840	S778		N659	G599	Y540	
F1200	E1140		E900		E900		S780		A660	E600	L480	



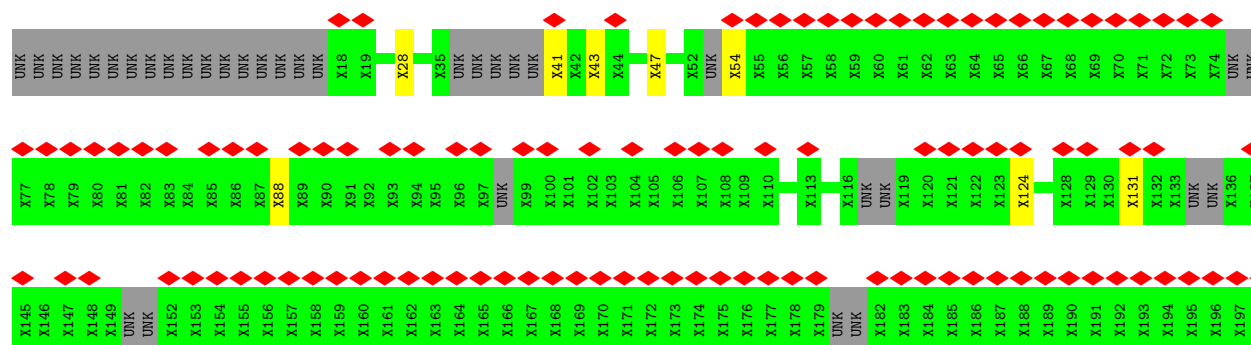
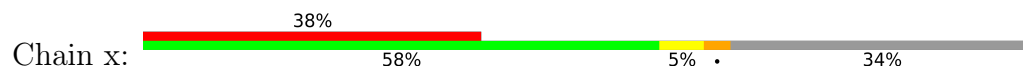
• Molecule 31: U2 small nuclear ribonucleoprotein A'

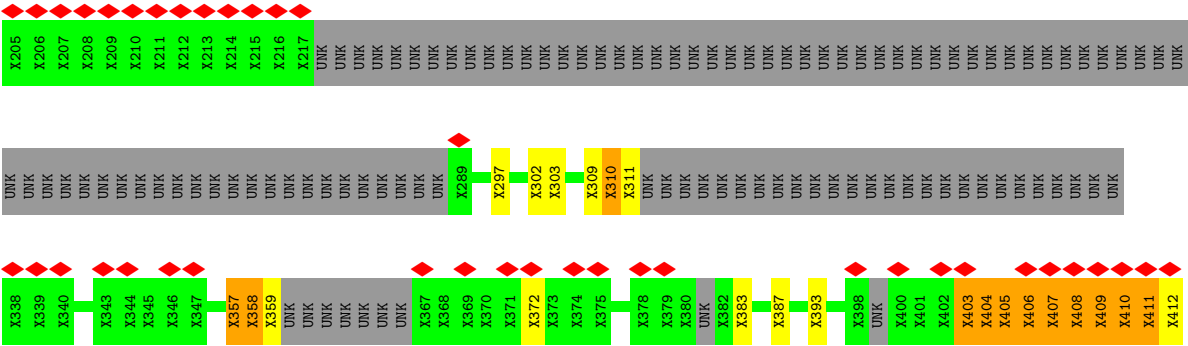


• Molecule 32: Probable U2 small nuclear ribonucleoprotein B'



• Molecule 33: unknown chain





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	112795	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	Not provided	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	Not provided	
Minimum defocus (nm)	3.0	Depositor
Maximum defocus (nm)	1.5	Depositor
Magnification	Not provided	
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum map value	0.189	Depositor
Minimum map value	-0.087	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.0203	Depositor
Map size ($\text{\AA}$)	475.2, 475.2, 475.2	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.47	0/16654	0.79	13/22571 (0.1%)
2	B	0.46	0/7357	0.79	6/9980 (0.1%)
3	C	0.41	0/2463	0.79	2/3829 (0.1%)
4	D	0.39	0/772	0.71	0/1038
4	Z	0.37	0/648	0.69	0/871
5	E	0.42	0/741	0.75	1/998 (0.1%)
5	b	0.43	0/584	0.80	2/785 (0.3%)
6	F	0.40	0/654	0.67	0/885
6	f	0.40	0/654	0.67	0/885
7	G	0.39	0/760	0.71	2/1016 (0.2%)
7	l	0.39	0/705	0.71	2/945 (0.2%)
8	H	0.42	0/630	0.64	0/851
8	m	0.42	0/630	0.64	0/851
9	I	0.42	0/579	0.62	0/785
9	n	0.42	0/579	0.63	0/785
10	J	0.36	0/578	0.71	0/774
10	o	0.36	0/578	0.71	0/774
11	K	0.53	0/2539	0.93	10/3453 (0.3%)
12	L	0.40	0/2317	0.74	2/3130 (0.1%)
13	M	0.48	0/1698	0.79	2/2295 (0.1%)
14	N	0.39	0/2160	0.73	1/3365 (0.0%)
15	O	0.37	0/189	0.59	0/292
16	Q	0.36	0/300	0.63	0/463
17	P	0.85	23/2580 (0.9%)	1.25	34/4000 (0.8%)
18	S	0.45	0/1069	0.68	0/1449
18	T	0.44	0/1086	0.74	0/1472
18	U	1.24	32/2888 (1.1%)	1.01	10/3898 (0.3%)
18	V	0.45	0/1053	0.71	0/1429
19	W	0.42	0/2300	0.76	3/3087 (0.1%)
20	Y	0.55	7/1934 (0.4%)	0.91	8/2609 (0.3%)
21	a	0.57	3/1479 (0.2%)	0.89	2/1980 (0.1%)
22	c	0.44	0/2486	0.75	1/3360 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
23	d	0.46	0/1214	0.70	0/1646
24	e	0.47	0/1199	0.80	1/1609 (0.1%)
25	g	0.63	6/1033 (0.6%)	1.07	9/1412 (0.6%)
26	h	0.45	0/767	0.71	0/1028
27	i	0.44	0/1231	0.74	0/1657
28	R	0.41	0/2243	0.79	0/3016
29	r	0.50	0/1161	0.86	2/1565 (0.1%)
30	X	0.40	0/9957	0.83	10/13430 (0.1%)
31	j	1.49	14/1118 (1.3%)	2.25	61/1513 (4.0%)
32	k	0.98	3/624 (0.5%)	1.85	13/838 (1.6%)
All	All	0.55	88/82191 (0.1%)	0.86	197/112619 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5
11	K	0	2
20	Y	0	3
33	x	0	12
All	All	0	22

All (88) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	j	76	THR	CB-OG1	21.45	1.78	1.43
31	j	118	SER	CB-OG	20.24	1.82	1.42
31	j	58	ASN	CA-CB	-10.64	1.38	1.53
18	U	318	CYS	CB-SG	-9.93	1.48	1.81
18	U	227	CYS	CB-SG	-9.71	1.49	1.81
31	j	70	CYS	CB-SG	-8.93	1.51	1.81
18	U	219	PRO	CA-CB	-8.78	1.41	1.53
18	U	193	SER	CA-CB	-8.77	1.39	1.53
31	j	111	CYS	CB-SG	-8.72	1.52	1.81
18	U	254	CYS	CB-SG	-8.61	1.52	1.81
18	U	235	CYS	CB-SG	-8.51	1.53	1.81
31	j	119	CYS	CB-SG	-8.36	1.53	1.81
31	j	81	ASP	CA-CB	-8.14	1.41	1.53
18	U	454	CYS	CB-SG	-8.05	1.54	1.81
17	P	153	U	O3'-P	-8.05	1.49	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	U	255	CYS	CB-SG	-7.82	1.55	1.81
17	P	141	C	C1'-N1	7.71	1.60	1.48
18	U	202	THR	CB-OG1	7.49	1.55	1.43
32	k	68	ASN	CA-CB	-7.21	1.42	1.53
17	P	138	U	C1'-N1	7.14	1.59	1.48
17	P	112	U	C1'-N1	7.08	1.59	1.48
17	P	153	U	C1'-N1	7.08	1.59	1.48
17	P	122	U	C1'-N1	7.08	1.59	1.48
17	P	113	U	C1'-N1	7.07	1.59	1.48
17	P	132	U	C1'-N1	7.05	1.59	1.48
17	P	134	U	C1'-N1	7.05	1.59	1.48
17	P	139	U	C1'-N1	7.05	1.59	1.48
18	U	180	THR	CB-OG1	7.02	1.54	1.43
17	P	124	U	C1'-N1	7.02	1.58	1.48
17	P	158	C	C1'-N1	6.96	1.58	1.48
18	U	335	HIS	CB-CG	-6.96	1.40	1.50
17	P	166	C	C1'-N1	6.85	1.57	1.47
17	P	172	G	C1'-N9	-6.80	1.37	1.48
18	U	188	THR	CB-OG1	6.78	1.54	1.43
18	U	199	THR	CB-OG1	6.67	1.54	1.43
17	P	154	C	C1'-N1	6.57	1.58	1.48
17	P	123	C	C1'-N1	6.57	1.58	1.48
18	U	418	THR	CB-OG1	6.57	1.54	1.43
17	P	121	C	C1'-N1	6.54	1.58	1.48
18	U	211	SER	CB-OG	6.54	1.55	1.42
17	P	120	C	C1'-N1	6.54	1.58	1.48
17	P	140	C	C1'-N1	6.50	1.58	1.48
18	U	362	THR	CB-OG1	6.50	1.54	1.43
31	j	98	HIS	CB-CG	-6.48	1.41	1.50
17	P	131	C	C1'-N1	6.46	1.58	1.48
18	U	222	SER	CB-OG	6.38	1.54	1.42
31	j	93	SER	CB-OG	6.35	1.54	1.42
32	k	93	ALA	CA-CB	-6.34	1.31	1.52
18	U	196	LEU	CB-CG	-6.25	1.41	1.53
20	Y	63	GLU	C-N	6.21	1.41	1.33
18	U	376	SER	CA-CB	-6.11	1.43	1.53
25	g	143	ASP	C-N	6.09	1.40	1.33
18	U	480	SER	CA-CB	-6.08	1.42	1.54
18	U	333	ALA	CA-CB	-5.93	1.43	1.53
18	U	364	SER	CB-OG	5.92	1.53	1.42
18	U	408	SER	CB-OG	5.90	1.53	1.42
18	U	250	SER	CB-OG	5.82	1.53	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	j	79	ALA	CA-CB	-5.78	1.44	1.53
20	Y	274	LEU	C-N	5.76	1.41	1.33
25	g	155	GLY	C-N	5.76	1.40	1.33
25	g	94	VAL	C-N	5.72	1.41	1.33
31	j	91	THR	CB-OG1	5.64	1.52	1.43
20	Y	67	PRO	N-CD	5.45	1.55	1.47
18	U	201	SER	CA-CB	-5.41	1.44	1.53
32	k	22	THR	CB-OG1	5.38	1.52	1.43
20	Y	64	PRO	N-CD	5.37	1.55	1.47
18	U	428	THR	CB-OG1	5.34	1.52	1.43
25	g	144	PRO	N-CD	5.30	1.55	1.47
17	P	107	U	C1'-N1	5.30	1.56	1.48
18	U	279	SER	CB-OG	5.29	1.52	1.42
21	a	267	SER	CB-OG	5.28	1.52	1.42
31	j	21	THR	CB-OG1	5.22	1.52	1.43
31	j	15	ILE	CB-CG1	-5.21	1.43	1.53
25	g	156	PRO	N-CD	5.21	1.55	1.47
17	P	97	U	C1'-N1	5.20	1.56	1.48
20	Y	275	PRO	N-CD	5.19	1.55	1.47
18	U	365	GLY	CA-C	5.18	1.56	1.51
17	P	93	A	C1'-N9	-5.18	1.40	1.48
20	Y	252	PRO	N-CD	5.17	1.54	1.47
21	a	240	SER	CB-OG	5.14	1.52	1.42
21	a	259	SER	CB-OG	5.13	1.52	1.42
18	U	214	SER	CB-OG	5.12	1.52	1.42
20	Y	250	PRO	N-CD	5.12	1.54	1.47
18	U	284	SER	CB-OG	5.08	1.52	1.42
18	U	260	SER	CB-OG	5.07	1.52	1.42
25	g	95	PRO	N-CD	5.06	1.54	1.47
18	U	431	LEU	CB-CG	-5.05	1.43	1.53
31	j	9	SER	CB-OG	5.04	1.52	1.42

All (197) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	j	54	ARG	CD-NE-CZ	13.19	142.87	124.40
31	j	70	CYS	CA-C-N	12.14	131.63	120.10
31	j	70	CYS	C-N-CA	12.14	131.63	120.10
31	j	48	PHE	CA-CB-CG	11.44	125.23	113.80
21	a	237	PRO	N-CA-CB	11.26	110.77	103.23
20	Y	56	THR	N-CA-C	9.85	121.78	111.14
20	Y	57	ARG	C-N-CD	-9.82	84.75	125.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Y	49	PRO	CA-N-CD	-9.78	98.31	112.00
30	X	892	GLY	N-CA-C	-9.69	102.63	115.32
21	a	268	PRO	N-CA-CB	9.62	110.99	103.30
31	j	12	PRO	N-CA-CB	9.03	111.32	103.19
18	U	217	PRO	N-CA-CB	9.00	112.70	103.25
31	j	98	HIS	CA-CB-CG	-8.74	105.06	113.80
17	P	112	U	O3'-P-O5'	-8.63	91.06	104.00
17	P	121	C	O3'-P-O5'	-8.63	91.05	104.00
17	P	124	U	O3'-P-O5'	-8.61	91.08	104.00
17	P	125	G	O3'-P-O5'	-8.60	91.10	104.00
17	P	139	U	O3'-P-O5'	-8.59	91.11	104.00
17	P	119	G	O3'-P-O5'	-8.59	91.12	104.00
17	P	140	C	O3'-P-O5'	-8.59	91.12	104.00
17	P	113	U	O3'-P-O5'	-8.59	91.12	104.00
17	P	132	U	O3'-P-O5'	-8.58	91.13	104.00
17	P	138	U	O3'-P-O5'	-8.58	91.13	104.00
17	P	120	C	O3'-P-O5'	-8.58	91.13	104.00
17	P	114	G	O3'-P-O5'	-8.58	91.13	104.00
17	P	123	C	O3'-P-O5'	-8.58	91.13	104.00
17	P	131	C	O3'-P-O5'	-8.58	91.13	104.00
17	P	133	A	O3'-P-O5'	-8.58	91.13	104.00
17	P	134	U	O3'-P-O5'	-8.57	91.15	104.00
17	P	122	U	O3'-P-O5'	-8.56	91.16	104.00
31	j	7	PHE	CA-CB-CG	8.55	122.35	113.80
17	P	115	G	O3'-P-O5'	-8.54	91.19	104.00
3	C	36	U	C4'-C3'-O3'	8.54	125.81	113.00
31	j	4	ASN	N-CA-CB	-8.51	98.29	111.05
18	U	268	ASP	CA-CB-CG	-8.46	104.14	112.60
1	A	1808	ASN	N-CA-C	8.32	120.43	111.36
18	U	415	PRO	N-CA-CB	8.13	111.79	103.25
31	j	15	ILE	CA-C-O	-8.04	111.82	120.59
31	j	98	HIS	N-CA-C	7.92	122.72	112.26
19	W	77	PRO	N-CA-CB	7.92	111.56	103.25
11	K	359	PHE	CA-C-N	7.91	129.72	119.84
11	K	359	PHE	C-N-CA	7.91	129.72	119.84
29	r	547	PRO	N-CA-CB	7.90	111.54	103.25
31	j	46	ILE	N-CA-CB	7.86	122.99	111.52
29	r	641	VAL	N-CA-C	7.67	118.44	110.62
31	j	116	ASN	CA-C-O	7.62	128.40	120.40
17	P	168	A	P-O5'-C5'	-7.54	109.58	120.90
1	A	647	GLY	CA-C-N	7.53	129.26	119.84
1	A	647	GLY	C-N-CA	7.53	129.26	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	k	56	PRO	CA-CB-CG	7.48	118.72	104.50
17	P	167	U	O3'-P-O5'	-7.33	93.01	104.00
25	g	143	ASP	CA-C-N	-7.20	112.90	120.03
25	g	143	ASP	C-N-CA	-7.20	112.90	120.03
5	b	81	GLN	N-CA-C	7.17	118.89	111.14
31	j	16	SER	CA-C-N	7.16	126.87	119.56
31	j	16	SER	C-N-CA	7.16	126.87	119.56
11	K	463	PRO	N-CA-CB	7.14	109.28	103.36
11	K	460	PRO	N-CA-CB	7.12	110.73	103.25
17	P	170	U	C3'-C2'-O2'	-7.03	104.06	114.60
18	U	184	PRO	N-CA-CB	7.00	108.94	101.88
17	P	154	C	O3'-P-O5'	-6.97	93.55	104.00
31	j	106	ASP	CA-CB-CG	6.95	119.55	112.60
31	j	3	LEU	N-CA-C	-6.88	98.00	108.67
31	j	74	ARG	NE-CZ-NH1	-6.88	114.62	121.50
32	k	50	HIS	CA-C-O	-6.82	112.82	120.32
20	Y	63	GLU	CA-C-N	-6.78	113.32	120.03
20	Y	63	GLU	C-N-CA	-6.78	113.32	120.03
25	g	94	VAL	CA-C-N	-6.74	112.82	119.76
25	g	94	VAL	C-N-CA	-6.74	112.82	119.76
11	K	414	GLN	CA-C-N	6.70	128.21	119.84
11	K	414	GLN	C-N-CA	6.70	128.21	119.84
31	j	80	PRO	N-CA-CB	6.69	110.28	103.25
18	U	276	PRO	N-CA-CB	6.65	110.23	103.25
25	g	32	PRO	N-CA-CB	6.65	110.23	103.25
11	K	466	PRO	N-CA-CB	6.62	110.20	103.25
17	P	164	C	C5'-C4'-O4'	-6.62	99.17	109.10
24	e	115	SER	N-CA-C	6.61	118.19	108.14
1	A	325	HIS	CA-C-N	6.60	128.09	119.84
1	A	325	HIS	C-N-CA	6.60	128.09	119.84
25	g	155	GLY	CA-C-N	-6.57	112.86	119.56
25	g	155	GLY	C-N-CA	-6.57	112.86	119.56
25	g	23	PRO	N-CA-CB	6.54	110.45	103.39
20	Y	86	PRO	N-CA-CB	6.54	110.11	103.25
31	j	120	ILE	CA-C-O	6.51	128.91	120.78
32	k	55	ASP	CA-C-N	6.50	125.94	118.85
32	k	55	ASP	C-N-CA	6.50	125.94	118.85
2	B	852	ALA	N-CA-C	6.50	113.98	108.13
31	j	17	PRO	N-CA-CB	6.42	109.91	103.48
22	c	334	PRO	N-CA-CB	6.42	110.06	103.00
20	Y	274	LEU	CA-C-N	-6.32	113.47	119.85
20	Y	274	LEU	C-N-CA	-6.32	113.47	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	j	86	LEU	CA-C-N	6.31	126.22	119.28
31	j	86	LEU	C-N-CA	6.31	126.22	119.28
17	P	169	C	P-O3'-C3'	6.30	129.66	120.20
31	j	11	VAL	N-CA-C	6.28	114.86	109.02
31	j	54	ARG	NE-CZ-NH1	6.27	127.77	121.50
2	B	646	THR	N-CA-C	6.25	119.75	111.75
31	j	39	LEU	CA-C-N	6.25	131.46	122.40
31	j	39	LEU	C-N-CA	6.25	131.46	122.40
7	l	28	GLY	CA-C-N	6.24	125.72	119.24
7	l	28	GLY	C-N-CA	6.24	125.72	119.24
1	A	971	PRO	N-CA-C	6.23	118.30	110.70
25	g	19	PRO	N-CA-CB	6.23	110.12	103.52
13	M	140	LYS	CA-C-N	6.22	127.61	119.84
13	M	140	LYS	C-N-CA	6.22	127.61	119.84
7	G	28	GLY	CA-C-N	6.21	125.70	119.24
7	G	28	GLY	C-N-CA	6.21	125.70	119.24
17	P	168	A	C5'-C4'-C3'	-6.20	106.69	116.00
1	A	207	PRO	N-CA-C	6.17	121.67	113.40
31	j	72	ASN	N-CA-C	6.14	119.82	111.17
18	U	305	PRO	N-CA-CB	6.12	110.23	103.26
31	j	51	ASN	CA-CB-CG	6.09	118.69	112.60
11	K	308	SER	N-CA-C	6.08	117.43	108.86
31	j	82	ILE	N-CA-C	6.08	117.55	110.62
32	k	43	PRO	N-CA-C	-6.06	104.80	113.47
31	j	26	ARG	CB-CA-C	-6.03	98.65	110.10
31	j	74	ARG	N-CA-CB	-6.00	102.62	111.51
12	L	221	ILE	N-CA-C	5.97	121.76	109.34
31	j	122	ASN	OD1-CG-ND2	5.97	128.57	122.60
30	X	1044	THR	N-CA-C	5.96	117.76	107.93
32	k	22	THR	CA-CB-OG1	5.90	118.45	109.60
30	X	888	HIS	N-CA-C	-5.89	105.69	114.64
31	j	117	LEU	CA-C-N	-5.88	114.47	122.77
31	j	117	LEU	C-N-CA	-5.88	114.47	122.77
18	U	216	PHE	CA-CB-CG	5.84	119.64	113.80
17	P	163	G	O3'-P-O5'	-5.83	95.26	104.00
31	j	49	THR	CA-C-O	5.78	127.67	121.55
1	A	210	ALA	N-CA-C	5.73	117.98	108.13
2	B	875	ILE	CB-CA-C	-5.71	103.73	109.33
19	W	171	ALA	N-CA-C	5.71	117.50	111.28
17	P	164	C	P-O3'-C3'	5.70	128.74	120.20
1	A	147	ILE	CB-CA-C	-5.68	106.40	111.74
31	j	148	ARG	CB-CA-C	-5.63	102.05	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	P	168	A	O4'-C1'-C2'	-5.63	101.97	107.60
2	B	138	THR	N-CA-C	5.63	117.17	109.18
11	K	240	ILE	CB-CA-C	-5.62	106.05	111.05
31	j	102	ILE	CA-CB-CG1	5.62	119.95	110.40
32	k	70	ILE	N-CA-CB	-5.62	104.59	110.82
17	P	14	C	C2'-C3'-O3'	5.61	117.92	109.50
5	b	76	VAL	CB-CA-C	-5.59	106.96	111.71
5	E	76	VAL	CB-CA-C	-5.58	106.97	111.71
31	j	112	PRO	N-CA-CB	5.57	109.61	103.26
1	A	781	ARG	N-CA-C	-5.55	106.51	113.28
30	X	1167	GLY	N-CA-C	5.55	117.48	110.38
17	P	165	A	N9-C1'-C2'	5.54	120.31	112.00
19	W	52	ILE	N-CA-C	5.54	116.94	110.62
14	N	44	A	C4'-C3'-O3'	-5.53	104.71	113.00
31	j	85	VAL	CA-C-O	5.51	124.20	118.96
31	j	91	THR	CA-CB-OG1	5.51	117.86	109.60
32	k	56	PRO	N-CA-CB	5.50	109.60	103.44
17	P	157	G	P-O5'-C5'	-5.49	112.66	120.90
31	j	33	ILE	CA-C-O	-5.48	114.28	120.74
31	j	158	GLU	N-CA-C	-5.48	104.95	111.69
30	X	88	TYR	N-CA-C	-5.45	106.58	113.18
30	X	1081	GLY	N-CA-C	-5.42	107.84	115.32
31	j	39	LEU	N-CA-C	-5.41	106.18	112.89
12	L	244	ARG	N-CA-C	5.39	118.10	110.50
31	j	131	ARG	CD-NE-CZ	5.39	131.95	124.40
31	j	31	PRO	CA-C-N	5.39	130.48	122.99
31	j	31	PRO	C-N-CA	5.39	130.48	122.99
31	j	54	ARG	NE-CZ-NH2	-5.34	114.40	119.20
32	k	17	LYS	N-CA-C	5.32	117.50	111.11
30	X	526	SER	CA-C-N	5.32	125.23	119.76
30	X	526	SER	C-N-CA	5.32	125.23	119.76
11	K	368	PHE	N-CA-C	-5.31	101.99	109.96
31	j	160	VAL	O-C-N	-5.30	117.65	122.79
31	j	145	ASP	CA-C-N	5.30	130.08	122.40
31	j	145	ASP	C-N-CA	5.30	130.08	122.40
31	j	32	ILE	N-CA-CB	-5.29	103.79	111.52
31	j	87	PRO	CB-CA-C	-5.27	103.98	112.21
30	X	470	LYS	N-CA-C	5.27	117.00	108.41
3	C	13	A	C2'-C3'-O3'	5.26	121.58	113.70
32	k	43	PRO	CA-CB-CG	5.25	114.48	104.50
31	j	124	VAL	CA-C-N	5.25	127.84	120.28
31	j	124	VAL	C-N-CA	5.25	127.84	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1043	LYS	CB-CA-C	-5.24	110.56	116.63
30	X	638	PHE	N-CA-C	-5.22	102.11	110.10
32	k	48	GLN	N-CA-C	5.18	117.54	109.52
17	P	170	U	O4'-C1'-C2'	-5.14	100.66	105.80
17	P	156	U	C4'-C3'-C2'	5.12	107.72	102.60
31	j	76	THR	CA-CB-OG1	5.11	117.26	109.60
31	j	138	ILE	CA-C-N	5.10	124.76	119.56
31	j	138	ILE	C-N-CA	5.10	124.76	119.56
1	A	766	VAL	N-CA-C	-5.10	105.87	110.82
18	U	373	PRO	N-CA-CB	5.09	108.60	103.25
31	j	89	LEU	CA-C-O	-5.08	113.24	120.51
18	U	415	PRO	CA-CB-CG	5.08	114.16	104.50
32	k	45	MET	N-CA-C	5.08	119.48	113.28
18	U	179	ARG	CA-CB-CG	-5.07	103.96	114.10
32	k	35	VAL	O-C-N	5.06	127.05	121.83
2	B	569	VAL	N-CA-C	5.04	111.61	106.21
31	j	98	HIS	N-CA-CB	-5.04	102.90	111.17
17	P	155	U	P-O3'-C3'	5.04	127.76	120.20
31	j	42	VAL	N-CA-C	5.03	118.58	112.80
2	B	124	THR	N-CA-C	5.02	116.07	107.28
1	A	1826	PRO	CA-N-CD	-5.01	104.99	112.00
31	j	80	PRO	CA-CB-CG	5.00	114.00	104.50

There are no chirality outliers.

All (22) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1191	THR	Peptide
1	A	1440	ILE	Peptide
1	A	187	PHE	Peptide
1	A	457	HIS	Peptide
1	A	964	LYS	Peptide
11	K	301	ASP	Peptide
11	K	359	PHE	Peptide
20	Y	301	UNK	Mainchain
20	Y	302	UNK	Mainchain
20	Y	303	UNK	Mainchain
33	x	310	UNK	Mainchain
33	x	357	UNK	Mainchain
33	x	358	UNK	Mainchain
33	x	403	UNK	Mainchain
33	x	404	UNK	Mainchain

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Mol	Chain	Res	Type	Group
33	x	405	UNK	Mainchain
33	x	406	UNK	Mainchain
33	x	407	UNK	Mainchain
33	x	408	UNK	Mainchain
33	x	409	UNK	Mainchain
33	x	410	UNK	Mainchain
33	x	411	UNK	Mainchain

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	16230	0	16208	413	0
2	B	7196	0	7229	150	0
3	C	2209	0	1115	27	0
4	D	760	0	776	16	0
4	Z	639	0	640	19	0
5	E	730	0	753	16	0
5	b	576	0	584	33	0
6	F	646	0	694	7	0
6	f	646	0	694	27	0
7	G	751	0	772	9	0
7	l	696	0	710	56	0
8	H	620	0	641	8	0
8	m	620	0	641	8	0
9	I	570	0	590	16	0
9	n	570	0	590	25	0
10	J	573	0	602	7	0
10	o	573	0	602	7	0
11	K	2730	0	2435	87	0
12	L	2273	0	2226	117	0
13	M	1661	0	1689	63	0
14	N	1928	0	971	161	0
15	O	170	0	85	13	0
16	Q	270	0	138	23	0
17	P	2323	0	1178	219	0
18	S	1052	0	1073	19	0
18	T	1069	0	1084	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	U	2864	0	2384	56	0
18	V	1037	0	1052	15	0
19	W	3024	0	2433	48	0
20	Y	2008	0	1817	358	0
21	a	1751	0	1463	110	0
22	c	2425	0	2346	27	0
23	d	1187	0	1181	22	0
24	e	1176	0	1171	98	0
25	g	1013	0	826	194	0
26	h	752	0	729	8	0
27	i	1218	0	1163	22	0
28	R	3800	0	2469	128	0
29	r	3299	0	1614	154	0
30	X	9764	0	9707	608	0
31	j	1108	0	951	36	0
32	k	618	0	558	11	0
33	x	1360	0	300	59	0
34	B	28	0	12	0	0
35	N	4	0	0	0	0
36	Y	1	0	0	2	0
36	a	2	0	0	6	0
36	c	1	0	0	0	0
36	e	3	0	0	7	0
37	X	27	0	12	23	0
All	All	86551	0	76908	2967	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 18.

All (2967) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:278:PHE:CE2	21:a:141:ARG:HB2	1.24	1.60
14:N:26:U:H5	20:Y:244:ARG:CZ	1.03	1.57
12:L:195:GLY:CA	12:L:222:ILE:CD1	1.84	1.54
14:N:26:U:C5	20:Y:244:ARG:CZ	1.90	1.54
29:r:637:LEU:CD2	29:r:644:THR:HG21	1.15	1.54
20:Y:278:PHE:CZ	21:a:141:ARG:HB2	1.38	1.52
28:R:120:ILE:HD13	28:R:151:LEU:CD2	1.41	1.51
24:e:51:GLN:HG3	25:g:157:TRP:CE2	1.44	1.49
12:L:195:GLY:C	12:L:222:ILE:HD11	1.09	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:r:637:LEU:CD2	29:r:644:THR:CG2	1.95	1.41
20:Y:165:GLY:HA2	20:Y:227:LYS:NZ	1.30	1.41
28:R:142:TYR:CE2	33:x:387:UNK:HA	1.53	1.41
29:r:648:TYR:CZ	29:r:666:UNK:CB	2.03	1.40
12:L:196:GLY:N	12:L:222:ILE:HD11	1.34	1.40
12:L:195:GLY:C	12:L:222:ILE:CD1	1.85	1.39
14:N:26:U:C5	20:Y:244:ARG:NE	1.90	1.39
28:R:146:TYR:CE2	33:x:393:UNK:CB	2.08	1.37
24:e:7:SER:O	24:e:8:ARG:HG3	1.25	1.36
20:Y:278:PHE:CE2	21:a:141:ARG:CB	2.08	1.35
14:N:23:A:H2'	20:Y:119:TYR:OH	1.24	1.33
30:X:120:VAL:CG1	30:X:124:ILE:HG13	1.58	1.32
31:j:76:THR:OG1	31:j:76:THR:CB	1.78	1.31
14:N:23:A:N7	20:Y:119:TYR:CD2	1.98	1.31
29:r:648:TYR:CE1	29:r:666:UNK:CB	2.14	1.31
20:Y:69:GLN:HB2	20:Y:78:TRP:CE3	1.66	1.31
17:P:102:U:H5'	6:f:63:ASN:OD1	1.17	1.30
20:Y:304:UNK:HA	23:d:110:PRO:CB	1.62	1.30
24:e:51:GLN:HG3	25:g:157:TRP:NE1	1.44	1.30
29:r:637:LEU:CG	29:r:644:THR:HG21	1.61	1.29
30:X:753:GLY:CA	37:X:1500:ADP:O5'	1.80	1.29
14:N:76:C:C6	14:N:77:G:C8	2.20	1.29
31:j:19:LYS:CG	5:b:64:MET:HG3	1.62	1.28
1:A:1810:TYR:CE2	1:A:1857:LEU:HD12	1.68	1.27
12:L:195:GLY:HA3	12:L:222:ILE:CD1	1.52	1.26
1:A:1844:LYS:CD	1:A:1938:MET:HE1	1.62	1.26
31:j:118:SER:OG	31:j:118:SER:CB	1.82	1.25
30:X:753:GLY:CA	37:X:1500:ADP:C5'	2.14	1.24
17:P:105:G:H5''	7:l:48:ARG:NH2	1.51	1.24
30:X:725:TYR:CD2	37:X:1500:ADP:C8	2.24	1.24
25:g:142:GLY:CA	25:g:153:TYR:HA	1.65	1.24
24:e:117:CYS:SG	36:e:203:ZN:ZN	1.25	1.23
18:U:408:SER:CB	27:i:35:ARG:HG3	1.67	1.22
20:Y:50:ALA:CB	20:Y:129:SER:HA	1.69	1.22
25:g:142:GLY:HA3	25:g:153:TYR:CA	1.68	1.22
20:Y:230:MET:CE	20:Y:241:LEU:HD12	1.68	1.22
30:X:725:TYR:CE2	37:X:1500:ADP:H8	1.57	1.21
28:R:120:ILE:CG2	28:R:151:LEU:HD11	1.70	1.21
14:N:23:A:N7	20:Y:119:TYR:CG	2.10	1.20
17:P:105:G:C5'	7:l:48:ARG:NH2	2.06	1.19
30:X:115:LEU:HD12	30:X:119:GLU:CB	1.72	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:282:LEU:CD1	21:a:145:LYS:CG	2.20	1.19
20:Y:171:ARG:HH12	20:Y:248:THR:HG23	1.02	1.18
20:Y:195:PHE:CZ	20:Y:230:MET:HG3	1.78	1.18
14:N:73:C:O2'	14:N:74:U:OP2	1.62	1.17
21:a:19:PHE:CE2	25:g:89:ALA:CB	2.27	1.17
25:g:149:GLY:HA2	25:g:152:ALA:HB2	1.20	1.17
13:M:191:GLN:CD	25:g:86:THR:HG22	1.69	1.16
12:L:201:ILE:HB	12:L:215:LEU:CD1	1.75	1.16
20:Y:105:TYR:CE1	20:Y:106:THR:O	1.98	1.16
21:a:19:PHE:CE2	25:g:89:ALA:HB1	1.80	1.16
28:R:120:ILE:CD1	28:R:151:LEU:HD21	1.74	1.16
30:X:753:GLY:HA2	37:X:1500:ADP:O5'	0.98	1.16
18:V:100:GLU:OE1	33:x:28:UNK:O	1.64	1.16
12:L:195:GLY:CA	12:L:222:ILE:HD13	1.59	1.15
25:g:138:ARG:HB2	25:g:160:TYR:CD1	1.80	1.15
30:X:753:GLY:HA3	37:X:1500:ADP:H5'1	1.29	1.14
20:Y:52:LYS:HG3	20:Y:127:GLU:O	1.46	1.14
12:L:220:ASP:OD1	12:L:239:MET:HB2	1.47	1.14
29:r:637:LEU:HD21	29:r:644:THR:CG2	1.67	1.14
20:Y:50:ALA:HB3	20:Y:129:SER:HA	1.14	1.13
20:Y:66:GLN:NE2	20:Y:67:PRO:CA	2.11	1.13
17:P:104:G:H5'	7:l:104:ASP:CG	1.73	1.13
20:Y:195:PHE:CE2	20:Y:230:MET:HE3	1.84	1.12
30:X:725:TYR:CD2	37:X:1500:ADP:N7	2.16	1.12
28:R:116:LYS:HZ2	33:x:303:UNK:HA	1.02	1.12
14:N:23:A:H2'	20:Y:119:TYR:CZ	1.83	1.12
20:Y:282:LEU:CD1	21:a:145:LYS:HG3	1.72	1.12
30:X:120:VAL:HG12	30:X:124:ILE:CG1	1.78	1.12
17:P:166:C:N4	32:k:86:LYS:H	1.48	1.12
28:R:120:ILE:HG21	28:R:151:LEU:CD1	1.80	1.12
1:A:1810:TYR:HE2	1:A:1857:LEU:HD12	0.96	1.12
29:r:648:TYR:CE2	29:r:666:UNK:CB	2.33	1.11
18:S:86:GLU:OE2	33:x:41:UNK:HA	1.47	1.11
30:X:107:LYS:O	30:X:111:VAL:HG23	1.51	1.11
28:R:116:LYS:HZ2	33:x:303:UNK:CA	1.64	1.11
30:X:725:TYR:CG	37:X:1500:ADP:N7	2.19	1.11
20:Y:250:PRO:O	20:Y:251:ASN:ND2	1.82	1.11
30:X:725:TYR:CE2	37:X:1500:ADP:C8	2.39	1.11
1:A:1844:LYS:HD3	1:A:1938:MET:HE1	1.26	1.11
14:N:23:A:C8	20:Y:119:TYR:CD1	2.38	1.11
29:r:592:TYR:HB2	29:r:628:TYR:OH	1.50	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:19:PHE:HE2	25:g:89:ALA:HB1	1.02	1.10
30:X:115:LEU:HD12	30:X:119:GLU:HB2	1.22	1.10
20:Y:315:UNK:N	25:g:72:PRO:O	1.83	1.09
1:A:1844:LYS:HD2	1:A:1938:MET:SD	1.91	1.09
18:U:408:SER:HB3	27:i:35:ARG:HG3	1.23	1.09
20:Y:278:PHE:CZ	21:a:141:ARG:CB	2.29	1.09
17:P:104:G:C2	6:f:20:LYS:HG2	1.88	1.09
20:Y:66:GLN:HE22	20:Y:67:PRO:HB3	1.11	1.09
20:Y:282:LEU:HD11	21:a:145:LYS:HG3	1.20	1.09
1:A:1844:LYS:CD	1:A:1938:MET:CE	2.29	1.08
24:e:51:GLN:CG	25:g:157:TRP:CE2	2.36	1.08
17:P:156:U:H6	17:P:156:U:H5''	1.10	1.08
20:Y:50:ALA:HB3	20:Y:129:SER:CA	1.83	1.08
20:Y:251:ASN:HD21	20:Y:254:SER:HB3	1.16	1.07
16:Q:500:A:H4'	16:Q:501:A:H5''	1.35	1.07
20:Y:227:LYS:HG2	20:Y:243:VAL:HG11	1.37	1.07
24:e:142:CYS:SG	36:e:202:ZN:ZN	1.41	1.07
20:Y:304:UNK:C	23:d:110:PRO:HB3	1.84	1.07
28:R:142:TYR:HE2	33:x:387:UNK:CA	1.66	1.07
28:R:288:LYS:NZ	29:r:578:GLN:HE22	1.53	1.07
29:r:309:UNK:CB	30:X:329:LEU:HG	1.84	1.07
14:N:23:A:C8	20:Y:119:TYR:CG	2.42	1.06
14:N:24:A:C2	20:Y:60:TYR:HE2	1.72	1.06
14:N:76:C:C6	14:N:77:G:H8	1.61	1.06
20:Y:60:TYR:CE1	20:Y:62:MET:SD	2.48	1.06
24:e:129:ASP:OD2	25:g:111:TYR:CE2	2.09	1.06
28:R:120:ILE:CD1	28:R:151:LEU:CD2	2.31	1.06
28:R:115:MET:SD	28:R:147:MET:HE2	1.95	1.06
14:N:26:U:H5	20:Y:244:ARG:NE	1.37	1.05
31:j:19:LYS:CG	5:b:64:MET:CG	2.34	1.05
14:N:76:C:H6	14:N:77:G:C8	1.66	1.05
17:P:104:G:H5'	7:l:104:ASP:OD2	1.57	1.05
28:R:142:TYR:CE2	33:x:387:UNK:CA	2.37	1.05
29:r:628:TYR:HA	29:r:631:LEU:HD11	1.36	1.05
28:R:120:ILE:HD13	28:R:151:LEU:HD22	1.34	1.04
14:N:76:C:C5	14:N:77:G:C8	2.45	1.04
20:Y:230:MET:CE	20:Y:241:LEU:CD1	2.34	1.04
25:g:138:ARG:HA	25:g:160:TYR:HA	1.37	1.04
20:Y:165:GLY:CA	20:Y:227:LYS:NZ	2.20	1.04
25:g:138:ARG:HB2	25:g:160:TYR:HD1	1.15	1.04
20:Y:69:GLN:HB3	20:Y:78:TRP:HB3	1.08	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:r:637:LEU:HD23	29:r:644:THR:CG2	1.83	1.03
13:M:263:GLY:N	19:W:173:THR:HG21	1.73	1.03
20:Y:69:GLN:HB2	20:Y:78:TRP:HE3	1.01	1.03
20:Y:175:THR:HG22	20:Y:216:THR:HG22	1.39	1.03
29:r:649:GLU:HA	29:r:652:ILE:HD11	1.37	1.03
20:Y:171:ARG:NH1	20:Y:248:THR:HG23	1.73	1.03
20:Y:278:PHE:CE2	21:a:141:ARG:NE	2.27	1.02
28:R:116:LYS:NZ	33:x:303:UNK:CA	2.21	1.02
18:S:86:GLU:CD	33:x:41:UNK:HA	1.84	1.02
20:Y:69:GLN:CB	20:Y:78:TRP:HE3	1.71	1.02
1:A:1844:LYS:CD	1:A:1938:MET:SD	2.47	1.02
1:A:1844:LYS:HD3	1:A:1938:MET:CE	1.87	1.02
24:e:129:ASP:CG	25:g:111:TYR:HE2	1.66	1.02
14:N:23:A:C8	20:Y:119:TYR:CE1	2.47	1.02
14:N:26:U:C4	20:Y:244:ARG:NE	2.28	1.02
12:L:201:ILE:HB	12:L:215:LEU:HD12	1.38	1.01
28:R:120:ILE:HG21	28:R:151:LEU:HD11	1.04	1.01
24:e:51:GLN:CG	25:g:157:TRP:NE1	2.23	1.01
21:a:244:SER:HB3	21:a:247:ALA:HB3	1.43	1.01
28:R:120:ILE:HD13	28:R:151:LEU:HD21	1.03	1.00
20:Y:304:UNK:CA	23:d:110:PRO:CB	2.39	1.00
17:P:171:G:O6	32:k:14:LYS:NZ	1.95	1.00
20:Y:230:MET:HE1	20:Y:241:LEU:CD1	1.91	1.00
28:R:288:LYS:HZ3	29:r:578:GLN:HE22	1.10	1.00
1:A:1819:GLU:OE1	1:A:1819:GLU:N	1.95	0.99
14:N:26:U:C5	20:Y:244:ARG:NH2	2.29	0.99
25:g:83:ASN:HB2	25:g:88:TYR:CD1	1.97	0.99
20:Y:165:GLY:HA2	20:Y:227:LYS:HZ1	1.25	0.99
20:Y:138:PRO:HD3	20:Y:225:PHE:HD2	1.27	0.99
17:P:97:U:O4	7:l:62:ARG:HD3	1.61	0.99
20:Y:66:GLN:HE22	20:Y:67:PRO:CB	1.74	0.99
20:Y:105:TYR:CD1	20:Y:106:THR:N	2.31	0.99
17:P:102:U:C5'	6:f:63:ASN:OD1	2.10	0.99
12:L:201:ILE:CG2	12:L:215:LEU:HD11	1.93	0.98
20:Y:304:UNK:HA	23:d:110:PRO:CG	1.93	0.98
30:X:117:LEU:HD23	30:X:205:LYS:NZ	1.78	0.98
28:R:146:TYR:HE2	33:x:393:UNK:CB	1.76	0.98
30:X:117:LEU:HD13	30:X:118:SER:H	1.28	0.98
20:Y:195:PHE:HE2	20:Y:230:MET:HE3	1.23	0.98
20:Y:55:GLU:OE1	20:Y:56:THR:N	1.97	0.97
14:N:23:A:C8	20:Y:119:TYR:CD2	2.52	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:7:SER:O	24:e:8:ARG:CG	2.12	0.97
30:X:115:LEU:HD12	30:X:119:GLU:CG	1.95	0.97
17:P:168:A:H5'	17:P:168:A:C8	1.98	0.97
28:R:288:LYS:CD	29:r:538:GLU:HB3	1.94	0.97
21:a:19:PHE:CZ	25:g:89:ALA:HB2	1.99	0.97
21:a:19:PHE:HE2	25:g:89:ALA:CB	1.68	0.97
28:R:116:LYS:NZ	33:x:303:UNK:HA	1.80	0.97
30:X:753:GLY:CA	37:X:1500:ADP:H5'1	1.89	0.97
1:A:1832:PHE:CZ	1:A:1843:LEU:HD11	2.00	0.96
17:P:104:G:N1	6:f:20:LYS:CG	2.28	0.96
20:Y:304:UNK:CA	23:d:110:PRO:HB3	1.95	0.96
17:P:159:U:H2'	17:P:160:A:H8	1.30	0.96
12:L:195:GLY:CA	12:L:222:ILE:HD11	1.70	0.96
13:M:189:SER:HB3	25:g:82:LYS:HG2	1.48	0.96
25:g:133:LYS:O	25:g:137:ARG:NH1	1.97	0.96
24:e:117:CYS:SG	24:e:134:CYS:SG	2.64	0.96
20:Y:53:GLN:OE1	20:Y:123:GLY:C	2.09	0.95
30:X:753:GLY:HA2	37:X:1500:ADP:C5'	1.84	0.95
1:A:100:ARG:HD2	14:N:24:A:C5	2.01	0.95
17:P:97:U:C6	7:l:63:HIS:NE2	2.35	0.95
29:r:637:LEU:HG	29:r:644:THR:CG2	1.96	0.95
12:L:195:GLY:HA3	12:L:222:ILE:HD13	1.18	0.95
15:O:100:G:H8	15:O:101:U:H3	1.12	0.95
17:P:103:U:O4'	7:l:102:ARG:NH2	1.99	0.95
17:P:159:U:H2'	17:P:160:A:C8	2.01	0.95
24:e:25:GLU:HG2	25:g:147:LEU:HD13	1.48	0.95
30:X:120:VAL:CG1	30:X:124:ILE:CG1	2.40	0.95
17:P:156:U:H5'	17:P:156:U:C6	2.02	0.94
14:N:75:G:H5'	14:N:76:C:O2	1.68	0.94
24:e:29:ARG:HG3	25:g:147:LEU:HD23	1.47	0.94
25:g:91:ARG:HG2	25:g:91:ARG:HH21	1.32	0.94
13:M:270:LYS:HZ1	33:x:372:UNK:HA	1.33	0.94
30:X:205:LYS:CE	30:X:209:TYR:OH	2.16	0.94
1:A:1817:THR:OG1	1:A:1821:ASN:O	1.85	0.94
12:L:195:GLY:HA3	12:L:222:ILE:HD12	1.47	0.94
30:X:115:LEU:CD1	30:X:119:GLU:HB2	1.97	0.94
13:M:189:SER:N	25:g:86:THR:O	2.00	0.94
17:P:158:C:N4	32:k:14:LYS:HZ3	1.64	0.94
21:a:19:PHE:CE2	25:g:89:ALA:HB2	2.03	0.93
20:Y:66:GLN:NE2	20:Y:67:PRO:CB	2.30	0.93
20:Y:125:CYS:SG	36:Y:501:ZN:ZN	1.57	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:81:ILE:H	25:g:81:ILE:HD12	1.29	0.93
29:r:625:LEU:O	29:r:629:ASN:ND2	2.02	0.93
29:r:637:LEU:HD21	29:r:644:THR:HG21	0.95	0.93
29:r:648:TYR:CD1	29:r:666:UNK:CB	2.52	0.93
18:U:408:SER:HB2	27:i:35:ARG:HG3	1.50	0.93
25:g:142:GLY:HA3	25:g:153:TYR:HA	0.93	0.93
30:X:117:LEU:HD23	30:X:205:LYS:HZ2	1.32	0.93
28:R:288:LYS:NZ	29:r:578:GLN:NE2	2.17	0.93
20:Y:203:ARG:HH22	20:Y:257:ARG:HH11	1.15	0.93
17:P:97:U:O4'	7:l:63:HIS:NE2	2.02	0.92
20:Y:195:PHE:CZ	20:Y:230:MET:CG	2.52	0.92
17:P:104:G:N1	6:f:20:LYS:HG2	1.84	0.92
20:Y:66:GLN:NE2	20:Y:67:PRO:HB3	1.83	0.92
28:R:288:LYS:HB3	29:r:538:GLU:CB	2.00	0.92
14:N:23:A:C8	20:Y:119:TYR:CZ	2.57	0.92
30:X:117:LEU:HB3	30:X:205:LYS:HD3	1.51	0.92
12:L:201:ILE:CB	12:L:215:LEU:CD1	2.47	0.92
20:Y:92:LYS:HA	20:Y:240:CYS:SG	2.09	0.92
20:Y:69:GLN:CB	20:Y:78:TRP:CE3	2.48	0.92
20:Y:230:MET:HE2	20:Y:241:LEU:HD12	1.50	0.91
14:N:23:A:H8	20:Y:119:TYR:CD1	1.78	0.91
25:g:143:ASP:O	25:g:153:TYR:HB2	1.71	0.91
12:L:218:HIS:CE1	12:L:244:ARG:HD2	2.04	0.91
12:L:201:ILE:HB	12:L:215:LEU:CG	2.01	0.91
17:P:104:G:O2'	17:P:105:G:O5'	1.89	0.91
16:Q:499:U:H3'	16:Q:500:A:H5'	1.51	0.91
20:Y:163:MET:HE3	20:Y:245:TRP:HB2	1.53	0.91
13:M:270:LYS:NZ	33:x:372:UNK:HA	1.85	0.90
14:N:38:G:O2'	15:O:102:A:N6	2.04	0.90
25:g:130:LYS:O	25:g:134:ILE:HG13	1.72	0.90
20:Y:227:LYS:HG2	20:Y:243:VAL:CG1	2.02	0.90
18:U:408:SER:HB2	27:i:35:ARG:CG	2.01	0.90
24:e:29:ARG:HG3	25:g:147:LEU:CD2	2.00	0.90
17:P:103:U:O3'	7:l:104:ASP:OD1	1.88	0.90
19:W:172:ASN:HD21	19:W:174:GLN:HG2	1.36	0.90
25:g:146:ILE:HG22	25:g:152:ALA:HA	1.54	0.90
25:g:148:GLU:OE1	25:g:148:GLU:N	2.03	0.90
29:r:645:ARG:NH2	29:r:678:UNK:CB	2.35	0.90
14:N:23:A:C8	20:Y:119:TYR:CE2	2.60	0.90
20:Y:278:PHE:CD2	21:a:141:ARG:NE	2.39	0.90
30:X:1118:ALA:HB1	30:X:1273:VAL:HG21	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:278:PHE:HE2	21:a:141:ARG:HE	1.11	0.90
18:U:376:SER:CB	18:U:395:ASN:HB2	2.01	0.90
20:Y:280:LEU:O	20:Y:284:GLU:HG3	1.70	0.90
17:P:168:A:H5'	17:P:168:A:H8	1.36	0.89
1:A:1844:LYS:HD2	1:A:1938:MET:CE	2.01	0.89
29:r:649:GLU:HA	29:r:652:ILE:CD1	2.03	0.89
12:L:201:ILE:O	12:L:215:LEU:HG	1.72	0.89
20:Y:66:GLN:NE2	20:Y:67:PRO:HA	1.87	0.89
30:X:751:ARG:HH21	30:X:1177:ARG:HB3	1.36	0.89
12:L:195:GLY:HA2	12:L:222:ILE:HD13	1.55	0.89
25:g:148:GLU:O	25:g:152:ALA:HA	1.72	0.89
20:Y:105:TYR:HD1	20:Y:106:THR:H	1.14	0.89
20:Y:304:UNK:HA	23:d:110:PRO:HB2	1.54	0.89
1:A:168:MET:HE1	1:A:211:ILE:HG21	1.54	0.89
12:L:221:ILE:HB	12:L:239:MET:CG	2.02	0.89
17:P:5:U:OP1	33:x:297:UNK:CB	2.21	0.89
20:Y:66:GLN:NE2	20:Y:67:PRO:N	2.21	0.89
17:P:105:G:H5'	7:l:48:ARG:NH2	1.87	0.88
18:U:408:SER:CB	27:i:35:ARG:CG	2.49	0.88
20:Y:53:GLN:O	20:Y:54:ILE:HD13	1.74	0.88
24:e:7:SER:C	24:e:8:ARG:HG3	1.99	0.88
2:B:249:ILE:HG21	2:B:914:VAL:HG21	1.54	0.88
20:Y:195:PHE:CE1	20:Y:230:MET:HG3	2.07	0.88
13:M:191:GLN:NE2	25:g:86:THR:CG2	2.37	0.88
1:A:1815:HIS:NE2	1:A:1825:LYS:HB3	1.87	0.88
17:P:97:U:C4	7:l:62:ARG:HD3	2.08	0.88
12:L:242:THR:HB	12:L:244:ARG:HE	1.37	0.88
20:Y:121:ALA:HB2	20:Y:225:PHE:CE1	2.09	0.88
20:Y:69:GLN:CB	20:Y:78:TRP:HB3	2.00	0.88
1:A:1872:LEU:HD21	1:A:1938:MET:HE2	1.56	0.87
24:e:127:ASP:OD1	25:g:108:HIS:ND1	2.08	0.87
17:P:154:C:O2	17:P:176:G:N2	2.07	0.87
25:g:146:ILE:HG21	25:g:152:ALA:H	1.39	0.87
31:j:20:GLU:CG	5:b:62:LYS:NZ	2.36	0.87
20:Y:177:TYR:HD2	20:Y:244:ARG:HB2	1.37	0.87
24:e:129:ASP:CG	25:g:111:TYR:CE2	2.52	0.87
25:g:142:GLY:CA	25:g:152:ALA:O	2.23	0.87
31:j:42:VAL:CB	5:b:81:GLN:O	2.23	0.87
13:M:263:GLY:CA	19:W:173:THR:HG21	2.04	0.87
30:X:117:LEU:H	30:X:117:LEU:HD12	1.40	0.87
13:M:191:GLN:CD	25:g:86:THR:CG2	2.47	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:24:A:N3	20:Y:60:TYR:HE2	1.73	0.87
24:e:117:CYS:HG	36:e:203:ZN:ZN	0.57	0.86
24:e:129:ASP:OD2	25:g:111:TYR:HE2	1.47	0.86
14:N:26:U:O4	20:Y:242:ASN:ND2	2.09	0.86
30:X:35:ILE:HG21	30:X:74:HIS:NE2	1.89	0.86
12:L:201:ILE:CB	12:L:215:LEU:HD12	2.06	0.86
29:r:628:TYR:HA	29:r:631:LEU:CD1	2.05	0.86
12:L:201:ILE:HG21	12:L:215:LEU:HD11	1.56	0.86
17:P:98:G:O6	9:n:40:TYR:HA	1.74	0.86
20:Y:61:GLU:OE1	20:Y:62:MET:N	2.09	0.86
20:Y:105:TYR:HE1	20:Y:106:THR:O	1.58	0.86
28:R:288:LYS:HD3	29:r:538:GLU:HB3	1.57	0.86
31:j:42:VAL:CB	5:b:81:GLN:HG2	2.06	0.86
12:L:315:HIS:CE1	12:L:317:ASP:OD1	2.29	0.86
15:O:100:G:OP2	22:c:364:LYS:HE3	1.74	0.86
20:Y:60:TYR:HE1	20:Y:62:MET:SD	1.94	0.86
21:a:83:CYS:SG	36:a:402:ZN:ZN	1.64	0.86
20:Y:278:PHE:CE2	21:a:141:ARG:CG	2.58	0.86
20:Y:202:GLU:CD	20:Y:261:ARG:HH22	1.83	0.85
14:N:80:A:N3	14:N:80:A:H5''	1.91	0.85
20:Y:203:ARG:HH22	20:Y:257:ARG:NH1	1.74	0.85
25:g:83:ASN:HB2	25:g:88:TYR:HD1	1.40	0.85
20:Y:66:GLN:HE21	20:Y:67:PRO:HA	1.41	0.85
19:W:172:ASN:HD21	19:W:174:GLN:CG	1.89	0.85
1:A:100:ARG:HD2	14:N:24:A:C4	2.11	0.85
29:r:637:LEU:HD21	29:r:644:THR:CB	2.06	0.85
21:a:23:CYS:HG	36:a:402:ZN:ZN	0.90	0.85
30:X:71:SER:HA	30:X:75:ILE:HD11	1.59	0.85
30:X:117:LEU:CD2	30:X:205:LYS:NZ	2.39	0.85
20:Y:61:GLU:O	20:Y:62:MET:HG3	1.76	0.85
29:r:649:GLU:O	29:r:652:ILE:HD12	1.76	0.85
1:A:1844:LYS:NZ	1:A:1844:LYS:HB3	1.90	0.85
12:L:219:LYS:HA	12:L:219:LYS:CE	2.07	0.85
17:P:156:U:H6	17:P:156:U:C5'	1.89	0.85
24:e:101:CYS:SG	24:e:142:CYS:SG	2.75	0.85
30:X:1088:PHE:HB2	30:X:1217:ARG:HH21	1.42	0.85
17:P:166:C:H41	32:k:86:LYS:H	1.21	0.84
20:Y:227:LYS:CG	20:Y:243:VAL:HG11	2.06	0.84
20:Y:250:PRO:C	20:Y:251:ASN:HD22	1.84	0.84
28:R:146:TYR:HE2	33:x:393:UNK:C	1.88	0.84
13:M:187:THR:O	25:g:87:GLY:CA	2.25	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:205:GLU:HB3	18:U:466:LEU:CB	2.08	0.84
20:Y:230:MET:HE1	20:Y:241:LEU:HD13	1.57	0.84
13:M:187:THR:O	25:g:87:GLY:HA3	1.78	0.84
18:V:100:GLU:OE1	33:x:28:UNK:C	2.25	0.84
20:Y:262:LEU:HD11	21:a:98:ALA:HB3	1.58	0.84
24:e:101:CYS:SG	24:e:139:CYS:SG	2.74	0.84
20:Y:282:LEU:HD13	21:a:145:LYS:CG	2.08	0.84
30:X:120:VAL:HG12	30:X:124:ILE:HG13	0.85	0.84
14:N:24:A:N1	20:Y:71:TYR:OH	2.09	0.84
1:A:1817:THR:O	1:A:1820:GLY:HA3	1.77	0.83
19:W:172:ASN:HD22	19:W:173:THR:N	1.75	0.83
20:Y:125:CYS:HG	36:Y:501:ZN:ZN	0.56	0.83
20:Y:69:GLN:HB3	20:Y:78:TRP:CB	2.02	0.83
17:P:104:G:N1	6:f:20:LYS:HG3	1.92	0.83
1:A:1984:ILE:HD13	1:A:1995:LEU:HD23	1.61	0.83
14:N:77:G:H1	14:N:79:C:H41	1.26	0.83
1:A:1844:LYS:CG	1:A:1938:MET:HE1	2.09	0.83
30:X:205:LYS:HE3	30:X:209:TYR:CZ	2.13	0.83
17:P:25:G:H2'	17:P:26:A:H5'	1.61	0.83
20:Y:165:GLY:HA2	20:Y:227:LYS:HZ2	0.96	0.83
24:e:127:ASP:OD1	25:g:108:HIS:CE1	2.31	0.83
30:X:257:MET:SD	30:X:375:ASN:ND2	2.51	0.83
14:N:23:A:C2'	20:Y:119:TYR:OH	2.20	0.83
17:P:125:G:H1	17:P:130:G:H22	1.23	0.83
12:L:219:LYS:HB3	12:L:240:ASP:OD2	1.78	0.82
13:M:189:SER:HB2	25:g:80:SER:OG	1.79	0.82
14:N:23:A:C5	20:Y:119:TYR:CD2	2.67	0.82
20:Y:52:LYS:HE2	20:Y:129:SER:CB	2.08	0.82
20:Y:138:PRO:HD3	20:Y:225:PHE:CD2	2.14	0.82
24:e:51:GLN:HA	25:g:157:TRP:CZ2	2.13	0.82
30:X:401:VAL:O	30:X:450:TYR:OH	1.95	0.82
30:X:726:THR:O	37:X:1500:ADP:N6	2.13	0.82
13:M:187:THR:N	25:g:88:TYR:O	2.11	0.82
20:Y:203:ARG:NH2	20:Y:257:ARG:HH11	1.77	0.82
20:Y:262:LEU:O	20:Y:262:LEU:HD22	1.80	0.82
1:A:731:THR:HA	17:P:16:U:N3	1.94	0.82
24:e:102:CYS:HG	36:e:201:ZN:ZN	0.89	0.82
17:P:104:G:C2'	17:P:105:G:O5'	2.26	0.82
29:r:644:THR:HA	29:r:647:VAL:HG23	1.60	0.82
13:M:262:LYS:C	19:W:173:THR:HG21	2.04	0.82
13:M:189:SER:OG	25:g:86:THR:O	1.96	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:191:GLN:NE2	25:g:86:THR:HG22	1.95	0.82
14:N:78:A:H4'	28:R:108:LEU:CD1	2.09	0.82
20:Y:165:GLY:CA	20:Y:227:LYS:HZ1	1.85	0.82
2:B:104:PRO:O	2:B:105:ILE:HB	1.80	0.82
17:P:105:G:H5''	7:l:48:ARG:CZ	2.10	0.82
20:Y:178:VAL:HA	20:Y:242:ASN:O	1.78	0.82
25:g:145:SER:C	25:g:146:ILE:HD12	2.05	0.82
12:L:195:GLY:C	12:L:222:ILE:HD12	2.01	0.81
14:N:24:A:C2	20:Y:60:TYR:CE2	2.64	0.81
30:X:74:HIS:O	30:X:77:LEU:N	2.12	0.81
20:Y:227:LYS:CG	20:Y:243:VAL:CG1	2.58	0.81
24:e:51:GLN:HG3	25:g:157:TRP:CD1	2.14	0.81
15:O:100:G:H5'	16:Q:501:A:H1'	1.61	0.81
20:Y:62:MET:O	20:Y:78:TRP:CZ2	2.33	0.81
20:Y:203:ARG:NH2	20:Y:257:ARG:HD3	1.95	0.81
20:Y:278:PHE:HE2	21:a:141:ARG:CG	1.91	0.81
15:O:100:G:H8	15:O:101:U:N3	1.78	0.81
20:Y:242:ASN:HD21	20:Y:244:ARG:HE	1.28	0.81
24:e:137:CYS:SG	24:e:139:CYS:SG	2.79	0.81
24:e:102:CYS:SG	36:e:201:ZN:ZN	1.70	0.81
25:g:95:PRO:HG2	25:g:98:VAL:HG23	1.61	0.81
25:g:156:PRO:HG2	25:g:157:TRP:CE3	2.15	0.81
14:N:78:A:H2	28:R:104:ILE:HG13	1.46	0.81
17:P:135:G:H2'	17:P:136:C:O4'	1.81	0.81
1:A:100:ARG:CD	14:N:24:A:C8	2.64	0.81
17:P:177:C:H6	17:P:177:C:H5''	1.46	0.81
30:X:73:ASN:O	30:X:76:ASN:HB2	1.81	0.81
20:Y:304:UNK:C	23:d:110:PRO:CB	2.58	0.80
1:A:1817:THR:C	1:A:1820:GLY:HA3	2.06	0.80
24:e:26:PHE:CE1	24:e:55:GLN:HG2	2.15	0.80
1:A:1825:LYS:HD2	22:c:418:TYR:HE2	1.46	0.80
12:L:217:GLY:O	12:L:244:ARG:NH1	2.14	0.80
17:P:97:U:C5	7:l:62:ARG:CD	2.65	0.80
20:Y:62:MET:O	20:Y:78:TRP:CH2	2.34	0.80
25:g:142:GLY:C	25:g:152:ALA:O	2.24	0.80
24:e:129:ASP:OD2	25:g:111:TYR:CD2	2.35	0.80
12:L:221:ILE:O	12:L:238:SER:HA	1.81	0.80
20:Y:261:ARG:HH21	20:Y:261:ARG:HG3	1.46	0.80
17:P:104:G:C5'	7:l:104:ASP:OD2	2.29	0.79
17:P:137:U:H2'	17:P:138:U:H6	1.47	0.79
24:e:51:GLN:HG3	25:g:157:TRP:CD2	2.15	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:82:LYS:HD2	25:g:85:ILE:O	1.81	0.79
30:X:725:TYR:HB3	37:X:1500:ADP:HN61	1.46	0.79
17:P:100:U:H5''	17:P:101:U:H5'	1.64	0.79
20:Y:195:PHE:CZ	20:Y:230:MET:SD	2.75	0.79
30:X:1046:TYR:CD1	37:X:1500:ADP:N3	2.50	0.79
1:A:1825:LYS:HG3	1:A:1826:PRO:CD	2.12	0.79
17:P:166:C:N4	32:k:86:LYS:N	2.30	0.79
28:R:289:GLN:HB3	29:r:539:ARG:HH21	1.46	0.79
28:R:116:LYS:NZ	33:x:303:UNK:N	2.29	0.79
30:X:1124:ARG:HH22	30:X:1163:PRO:HB3	1.48	0.79
1:A:100:ARG:CD	14:N:24:A:N7	2.46	0.79
15:O:100:G:H2'	15:O:100:G:N3	1.98	0.79
2:B:492:VAL:HG22	2:B:508:ALA:HB2	1.65	0.79
20:Y:177:TYR:CD2	20:Y:244:ARG:HB2	2.18	0.79
29:r:646:THR:HA	29:r:649:GLU:OE2	1.82	0.79
17:P:105:G:C5'	7:l:48:ARG:HH22	1.93	0.79
21:a:22:ILE:HG21	21:a:27:LEU:HD13	1.63	0.79
30:X:753:GLY:N	37:X:1500:ADP:C5'	2.46	0.78
13:M:188:PRO:HA	25:g:87:GLY:HA3	1.63	0.78
30:X:117:LEU:CB	30:X:205:LYS:HD3	2.13	0.78
6:f:14:THR:HG22	6:f:28:THR:HG22	1.65	0.78
1:A:1817:THR:HB	1:A:1820:GLY:CA	2.13	0.78
12:L:201:ILE:HB	12:L:215:LEU:HG	1.63	0.78
17:P:97:U:C5	7:l:62:ARG:HD2	2.18	0.78
17:P:97:U:N1	7:l:63:HIS:CD2	2.51	0.78
28:R:138:ASP:OD2	33:x:383:UNK:CB	2.32	0.78
14:N:77:G:H2'	14:N:77:G:N3	1.97	0.78
30:X:117:LEU:CD2	30:X:205:LYS:HZ2	1.95	0.78
18:U:372:GLY:O	18:U:373:PRO:CB	2.30	0.78
20:Y:273:LEU:HD12	21:a:89:PHE:HD1	1.48	0.78
12:L:164:ASP:HB2	12:L:171:ILE:HD11	1.66	0.78
20:Y:53:GLN:OE1	20:Y:123:GLY:HA2	1.83	0.78
30:X:204:ILE:HD11	30:X:364:TYR:HA	1.64	0.77
14:N:78:A:H3'	14:N:78:A:OP2	1.84	0.77
20:Y:61:GLU:C	20:Y:62:MET:HG3	2.09	0.77
25:g:146:ILE:HG21	25:g:152:ALA:N	1.99	0.77
18:U:200:PRO:O	18:U:201:SER:CB	2.32	0.77
20:Y:53:GLN:OE1	20:Y:123:GLY:CA	2.32	0.77
20:Y:203:ARG:HH22	20:Y:257:ARG:CD	1.97	0.77
21:a:244:SER:HB3	21:a:247:ALA:CB	2.13	0.77
11:K:233:ASP:HB2	11:K:240:ILE:HD11	1.66	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:421:ALA:H	18:U:438:GLU:CG	1.97	0.77
20:Y:49:PRO:HD2	20:Y:129:SER:HG	1.49	0.77
2:B:229:ALA:HB3	2:B:230:PRO:HD3	1.67	0.77
20:Y:49:PRO:O	20:Y:129:SER:OG	2.02	0.77
20:Y:52:LYS:CG	20:Y:127:GLU:O	2.32	0.77
30:X:528:PHE:H	30:X:559:ILE:HB	1.49	0.77
30:X:1135:ILE:HB	30:X:1166:VAL:HG22	1.67	0.77
1:A:1825:LYS:HD2	22:c:418:TYR:CE2	2.19	0.77
12:L:221:ILE:HB	12:L:239:MET:HG2	1.64	0.77
6:F:14:THR:HG22	6:F:28:THR:HG22	1.65	0.77
31:j:42:VAL:CA	5:b:81:GLN:HG2	2.15	0.77
14:N:23:A:H2	20:Y:57:ARG:HH21	1.29	0.77
14:N:73:C:H1'	14:N:74:U:C2	2.20	0.77
20:Y:195:PHE:HZ	20:Y:230:MET:SD	2.08	0.77
1:A:100:ARG:HD3	14:N:24:A:C8	2.20	0.76
3:C:59:A:H2'	3:C:60:A:H5'	1.66	0.76
20:Y:66:GLN:HE21	20:Y:67:PRO:CA	1.92	0.76
24:e:101:CYS:SG	36:e:202:ZN:ZN	1.73	0.76
14:N:78:A:OP1	28:R:105:PRO:HB3	1.85	0.76
13:M:187:THR:O	25:g:88:TYR:N	2.18	0.76
20:Y:121:ALA:HB2	20:Y:225:PHE:HE1	1.47	0.76
30:X:117:LEU:CD1	30:X:118:SER:H	1.99	0.76
2:B:253:ARG:NH2	2:B:914:VAL:HG13	2.00	0.76
3:C:59:A:C2'	3:C:60:A:H5'	2.15	0.76
14:N:77:G:H1	14:N:79:C:N4	1.82	0.76
18:U:374:HIS:NE2	18:U:392:VAL:HG13	2.01	0.76
30:X:73:ASN:H	30:X:73:ASN:ND2	1.84	0.76
13:M:189:SER:CB	25:g:82:LYS:HG2	2.15	0.76
17:P:106:U:C5	17:P:107:U:C5	2.74	0.76
19:W:172:ASN:ND2	19:W:174:GLN:H	1.84	0.76
29:r:645:ARG:HH22	29:r:678:UNK:CB	1.97	0.76
24:e:102:CYS:SG	24:e:137:CYS:SG	2.73	0.76
30:X:115:LEU:HD12	30:X:119:GLU:HG3	1.66	0.76
1:A:537:THR:HG22	20:Y:70:VAL:HG11	1.67	0.75
1:A:1832:PHE:CZ	1:A:1920:ILE:HG21	2.21	0.75
14:N:23:A:C2	20:Y:57:ARG:NH2	2.53	0.75
1:A:100:ARG:HD3	14:N:24:A:N7	2.01	0.75
29:r:309:UNK:CB	30:X:329:LEU:CG	2.64	0.75
30:X:163:TYR:HA	30:X:166:HIS:HD2	1.52	0.75
14:N:24:A:N3	20:Y:60:TYR:CE2	2.54	0.75
20:Y:241:LEU:N	20:Y:241:LEU:HD23	2.02	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R:115:MET:SD	28:R:147:MET:CE	2.74	0.75
17:P:102:U:C4	6:f:61:ARG:NE	2.55	0.75
19:W:505:UNK:CB	29:r:528:ALA:O	2.35	0.75
28:R:288:LYS:HD2	29:r:538:GLU:HB3	1.69	0.75
1:A:1663:VAL:HG11	1:A:1741:ASN:HB3	1.68	0.75
14:N:23:A:C2'	20:Y:119:TYR:CZ	2.66	0.75
30:X:99:ASN:OD1	30:X:138:LYS:NZ	2.19	0.75
20:Y:92:LYS:HG2	20:Y:240:CYS:SG	2.26	0.75
11:K:274:TRP:CZ3	11:K:281:ASN:HB3	2.21	0.75
19:W:725:LEU:HD12	27:i:159:VAL:HG11	1.67	0.75
20:Y:266:ALA:CB	21:a:99:ALA:CB	2.65	0.75
29:r:592:TYR:CB	29:r:628:TYR:OH	2.34	0.75
1:A:100:ARG:CD	14:N:24:A:C5	2.69	0.75
17:P:137:U:H2'	17:P:138:U:C6	2.21	0.75
25:g:142:GLY:O	25:g:152:ALA:O	2.04	0.75
30:X:117:LEU:HD12	30:X:117:LEU:N	2.01	0.75
24:e:105:CYS:C	24:e:106:ILE:HD12	2.12	0.75
24:e:117:CYS:SG	24:e:119:CYS:SG	2.85	0.75
28:R:149:GLU:OE1	28:R:180:MET:SD	2.45	0.75
30:X:108:VAL:HG13	30:X:123:MET:HE3	1.69	0.75
1:A:1287:TRP:HB2	1:A:1319:ILE:HD13	1.69	0.74
20:Y:230:MET:SD	20:Y:241:LEU:HD12	2.26	0.74
19:W:725:LEU:HD11	27:i:10:LEU:HD21	1.70	0.74
20:Y:64:PRO:O	20:Y:69:GLN:HG2	1.87	0.74
24:e:139:CYS:HB3	24:e:142:CYS:SG	2.26	0.74
28:R:288:LYS:HD3	29:r:538:GLU:CD	2.13	0.74
29:r:648:TYR:CD2	29:r:666:UNK:CB	2.69	0.74
30:X:222:LEU:HA	30:X:225:ILE:HD12	1.68	0.74
12:L:201:ILE:CG2	12:L:215:LEU:CD1	2.63	0.74
14:N:81:U:C2'	14:N:82:U:H5'	2.18	0.74
20:Y:242:ASN:HD22	20:Y:243:VAL:N	1.85	0.74
29:r:644:THR:HA	29:r:647:VAL:CG2	2.16	0.74
17:P:166:C:H41	32:k:86:LYS:N	1.84	0.74
29:r:637:LEU:HD23	29:r:644:THR:HG23	1.70	0.74
5:E:116:GLY:HA2	25:g:94:VAL:HG11	1.69	0.74
14:N:15:U:H2'	25:g:104:TYR:OH	1.87	0.74
17:P:158:C:H41	32:k:14:LYS:HZ3	1.33	0.74
20:Y:251:ASN:ND2	20:Y:254:SER:HB3	1.99	0.74
25:g:146:ILE:HG22	25:g:148:GLU:O	1.88	0.74
1:A:731:THR:HA	17:P:16:U:C4	2.23	0.73
12:L:244:ARG:HG2	12:L:260:ILE:HG12	1.68	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:r:637:LEU:CG	29:r:644:THR:CG2	2.38	0.73
30:X:28:GLN:HB2	30:X:31:MET:HG2	1.70	0.73
30:X:463:LEU:HB2	30:X:471:ASN:HB2	1.69	0.73
1:A:1268:ILE:HD13	1:A:1315:CYS:HB3	1.70	0.73
21:a:83:CYS:HG	36:a:402:ZN:ZN	1.01	0.73
25:g:83:ASN:HB2	25:g:88:TYR:CE1	2.22	0.73
14:N:76:C:H6	14:N:77:G:H8	1.06	0.73
20:Y:282:LEU:HD11	21:a:145:LYS:CG	1.99	0.73
21:a:80:CYS:SG	36:a:402:ZN:ZN	1.76	0.73
29:r:595:TYR:HE2	29:r:611:ILE:HG13	1.53	0.73
30:X:531:LEU:HB2	30:X:615:SER:HA	1.69	0.73
20:Y:278:PHE:HE2	21:a:141:ARG:NE	1.72	0.73
12:L:196:GLY:N	12:L:222:ILE:CD1	2.30	0.73
25:g:95:PRO:HG2	25:g:98:VAL:CG2	2.18	0.73
29:r:560:PHE:HE2	29:r:572:THR:HG22	1.52	0.73
30:X:63:TRP:HH2	30:X:101:PHE:HB3	1.53	0.73
30:X:195:LEU:HA	30:X:198:TRP:HD1	1.53	0.73
2:B:249:ILE:HD11	2:B:849:GLU:HB3	1.70	0.73
24:e:140:ASN:O	25:g:138:ARG:NH2	2.21	0.73
30:X:74:HIS:O	30:X:77:LEU:HB2	1.89	0.73
30:X:74:HIS:ND1	30:X:77:LEU:HD12	2.04	0.73
14:N:23:A:H8	20:Y:119:TYR:CE1	1.97	0.73
17:P:158:C:N4	32:k:14:LYS:NZ	2.36	0.73
20:Y:242:ASN:HD21	20:Y:244:ARG:NE	1.87	0.73
24:e:29:ARG:CG	25:g:147:LEU:HD23	2.18	0.73
1:A:100:ARG:HD2	14:N:24:A:C8	2.23	0.73
1:A:1209:ASN:HB3	1:A:1222:LEU:HD12	1.71	0.73
14:N:80:A:H4'	14:N:80:A:OP1	1.88	0.73
20:Y:52:LYS:HE2	20:Y:129:SER:HB3	1.71	0.73
25:g:81:ILE:HD12	25:g:81:ILE:N	2.04	0.73
30:X:878:SER:HB3	30:X:904:LYS:HG2	1.70	0.73
30:X:36:LEU:HD21	30:X:74:HIS:HB2	1.71	0.72
16:Q:500:A:H3'	16:Q:500:A:OP2	1.89	0.72
20:Y:196:ALA:HA	20:Y:201:ILE:HD11	1.71	0.72
25:g:140:ASP:CG	25:g:141:PRO:HD2	2.14	0.72
20:Y:304:UNK:O	23:d:110:PRO:CB	2.38	0.72
11:K:263:VAL:HG22	11:K:273:VAL:HG22	1.71	0.72
20:Y:273:LEU:CD1	21:a:89:PHE:HA	2.19	0.72
31:j:64:ARG:HH21	5:b:45:TYR:HE2	1.36	0.72
1:A:1817:THR:HG22	1:A:1819:GLU:OE1	1.89	0.72
12:L:220:ASP:HB3	12:L:240:ASP:OD1	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:236:PHE:HA	30:X:239:ARG:HB3	1.70	0.72
17:P:98:G:C8	9:n:40:TYR:CE2	2.78	0.72
30:X:117:LEU:HD13	30:X:118:SER:N	2.05	0.72
1:A:1810:TYR:CZ	1:A:1857:LEU:HD12	2.24	0.72
4:Z:17:THR:HG23	4:Z:27:ARG:NE	2.05	0.72
17:P:25:G:C2'	17:P:26:A:H5'	2.20	0.72
20:Y:262:LEU:HD13	20:Y:262:LEU:C	2.15	0.72
1:A:1810:TYR:HE1	1:A:1812:VAL:HG13	1.55	0.71
20:Y:304:UNK:HA	23:d:110:PRO:HG2	1.70	0.71
28:R:288:LYS:HB3	29:r:538:GLU:HB2	1.71	0.71
30:X:1136:CYS:HB2	30:X:1183:PHE:HE1	1.55	0.71
12:L:282:ARG:O	12:L:298:ALA:CB	2.38	0.71
16:Q:500:A:C4'	16:Q:501:A:H5''	2.19	0.71
25:g:142:GLY:C	25:g:153:TYR:HA	2.15	0.71
1:A:1810:TYR:HE2	1:A:1857:LEU:CD1	1.90	0.71
20:Y:218:LEU:O	20:Y:265:ARG:NH2	2.23	0.71
20:Y:270:VAL:HG11	21:a:140:ALA:HB1	1.71	0.71
29:r:637:LEU:CD2	29:r:644:THR:CB	2.66	0.71
30:X:1126:LEU:HD23	30:X:1280:ARG:HH12	1.53	0.71
30:X:396:PHE:HA	30:X:622:TRP:HH2	1.56	0.71
30:X:591:TYR:HB3	30:X:607:LYS:HE2	1.71	0.71
1:A:74:TYR:CD1	24:e:108:THR:HG21	2.26	0.71
12:L:221:ILE:HB	12:L:239:MET:HG3	1.72	0.71
30:X:35:ILE:CG2	30:X:74:HIS:NE2	2.54	0.71
17:P:125:G:H1	17:P:130:G:N2	1.89	0.71
20:Y:285:THR:O	20:Y:289:LYS:HG3	1.90	0.71
21:a:29:ASP:CG	25:g:110:ILE:HD13	2.16	0.71
1:A:510:ILE:HD11	1:A:515:ALA:HB2	1.71	0.71
1:A:978:TRP:CD1	1:A:1095:LEU:HD11	2.25	0.71
25:g:91:ARG:HG2	25:g:91:ARG:NH2	2.02	0.71
17:P:98:G:N7	9:n:40:TYR:CE2	2.58	0.71
30:X:754:LYS:NZ	30:X:1010:ASN:OD1	2.22	0.71
14:N:80:A:H3'	14:N:81:U:O4'	1.91	0.70
20:Y:50:ALA:CB	20:Y:129:SER:CA	2.55	0.70
14:N:25:U:O2	20:Y:90:GLN:HB3	1.91	0.70
14:N:26:U:H5	20:Y:244:ARG:NH1	1.82	0.70
30:X:47:GLN:O	30:X:50:SER:OG	2.06	0.70
30:X:205:LYS:HE3	30:X:209:TYR:OH	1.87	0.70
30:X:723:ARG:HH21	30:X:763:GLU:HB2	1.55	0.70
1:A:1815:HIS:CD2	1:A:1825:LYS:HB3	2.27	0.70
1:A:1841:LEU:HB3	1:A:1843:LEU:CD2	2.20	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:97:U:C5	7:l:62:ARG:HD3	2.26	0.70
20:Y:49:PRO:O	20:Y:129:SER:CB	2.39	0.70
25:g:149:GLY:CA	25:g:152:ALA:HB2	2.10	0.70
14:N:26:U:C4	20:Y:244:ARG:CZ	2.70	0.70
14:N:81:U:H2'	14:N:82:U:H5'	1.72	0.70
1:A:1832:PHE:CE1	1:A:1843:LEU:CD1	2.75	0.70
20:Y:121:ALA:CB	20:Y:225:PHE:HE1	2.05	0.70
20:Y:304:UNK:O	23:d:110:PRO:HB3	1.91	0.70
20:Y:266:ALA:HB3	21:a:99:ALA:CB	2.21	0.70
1:A:1810:TYR:HE1	1:A:1812:VAL:CG1	2.04	0.70
30:X:1243:THR:HB	30:X:1258:VAL:HB	1.74	0.70
1:A:1851:TRP:CE3	1:A:1851:TRP:HA	2.27	0.70
12:L:201:ILE:CD1	12:L:215:LEU:HD12	2.22	0.70
1:A:1850:VAL:CG1	1:A:1864:LYS:NZ	2.54	0.70
14:N:24:A:C4	20:Y:60:TYR:CE2	2.79	0.70
21:a:80:CYS:HG	36:a:402:ZN:ZN	1.02	0.70
30:X:1124:ARG:HD3	30:X:1130:THR:HG22	1.74	0.69
31:j:19:LYS:CG	5:b:64:MET:HB2	2.22	0.69
20:Y:230:MET:HE2	20:Y:241:LEU:CD1	2.13	0.69
30:X:532:ILE:O	30:X:555:THR:OG1	2.08	0.69
29:r:634:LYS:HZ2	33:x:124:UNK:C	2.05	0.69
31:j:20:GLU:CG	5:b:62:LYS:HZ3	2.05	0.69
1:A:720:ILE:O	11:K:332:LYS:NZ	2.21	0.69
2:B:873:GLN:HG2	2:B:875:ILE:HD11	1.74	0.69
20:Y:203:ARG:HH22	20:Y:257:ARG:HD3	1.54	0.69
30:X:207:ILE:HG12	30:X:367:LYS:HD2	1.74	0.69
30:X:563:CYS:H	30:X:583:ILE:HA	1.57	0.69
20:Y:266:ALA:CB	21:a:99:ALA:HB2	2.20	0.69
1:A:803:THR:HG23	1:A:921:PHE:CD1	2.28	0.69
30:X:74:HIS:O	30:X:77:LEU:CB	2.41	0.69
1:A:1851:TRP:HA	1:A:1851:TRP:HE3	1.57	0.69
17:P:177:C:H6	17:P:177:C:C5'	2.05	0.69
20:Y:251:ASN:O	20:Y:255:GLN:HG3	1.91	0.69
11:K:359:PHE:HB3	11:K:360:PRO:CD	2.23	0.69
13:M:185:ARG:HG3	25:g:90:GLU:HG3	1.75	0.69
17:P:96:U:C4	6:f:34:MET:HE1	2.28	0.69
18:V:34:GLU:OE1	33:x:43:UNK:CB	2.41	0.69
25:g:148:GLU:O	25:g:152:ALA:CA	2.40	0.69
30:X:233:LEU:O	30:X:239:ARG:NH2	2.26	0.69
30:X:595:LEU:HD23	30:X:605:GLN:HE22	1.58	0.69
30:X:880:ASP:O	30:X:884:ARG:N	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:48:TRP:HA	19:W:52:ILE:HG22	1.75	0.69
29:r:531:GLU:HA	29:r:534:PHE:HD2	1.57	0.69
30:X:1191:ALA:HB1	30:X:1194:HIS:HB2	1.74	0.69
21:a:30:ASN:CG	25:g:106:ASN:OD1	2.36	0.69
28:R:288:LYS:HB3	29:r:538:GLU:CG	2.23	0.69
30:X:1091:VAL:HG21	30:X:1214:LEU:HB3	1.74	0.69
12:L:201:ILE:HD12	12:L:215:LEU:HD12	1.73	0.68
17:P:168:A:C8	17:P:168:A:C5'	2.75	0.68
20:Y:262:LEU:HD11	21:a:98:ALA:CB	2.21	0.68
28:R:120:ILE:CG1	28:R:151:LEU:HD21	2.23	0.68
30:X:46:LYS:NZ	30:X:412:ASN:O	2.26	0.68
1:A:1966:ALA:HB1	1:A:2007:LEU:HD22	1.75	0.68
20:Y:52:LYS:HE2	20:Y:129:SER:H	1.58	0.68
30:X:668:ARG:HG2	30:X:699:PHE:HB3	1.75	0.68
12:L:195:GLY:HA2	12:L:222:ILE:CD1	2.09	0.68
20:Y:49:PRO:HD2	20:Y:129:SER:OG	1.92	0.68
12:L:215:LEU:N	12:L:215:LEU:HD23	2.08	0.68
20:Y:282:LEU:HD13	21:a:145:LYS:HG2	1.69	0.68
29:r:634:LYS:NZ	33:x:124:UNK:C	2.56	0.68
30:X:147:THR:HA	30:X:151:ILE:HD11	1.76	0.68
31:j:19:LYS:CG	5:b:64:MET:CB	2.71	0.68
17:P:135:G:C2	17:P:136:C:C2	2.82	0.68
20:Y:203:ARG:NH2	20:Y:257:ARG:NH1	2.38	0.68
21:a:29:ASP:HB3	25:g:110:ILE:HD13	1.74	0.68
29:r:439:UNK:O	29:r:443:UNK:N	2.26	0.68
30:X:815:GLU:O	30:X:819:THR:N	2.18	0.68
2:B:692:THR:HA	2:B:825:THR:HG21	1.75	0.68
30:X:462:ARG:HD3	30:X:470:LYS:HD3	1.76	0.68
30:X:74:HIS:HD1	30:X:77:LEU:HB2	1.58	0.68
30:X:741:PRO:HA	30:X:1004:ARG:HG2	1.75	0.68
31:j:64:ARG:NH2	5:b:45:TYR:HE2	1.91	0.68
2:B:181:ASP:C	2:B:182:THR:HG1	2.02	0.67
11:K:206:ALA:HB3	11:K:226:ASP:OD1	1.94	0.67
14:N:25:U:C2	20:Y:232:HIS:CE1	2.81	0.67
25:g:141:PRO:HA	25:g:154:LYS:O	1.94	0.67
31:j:42:VAL:O	5:b:81:GLN:CD	2.37	0.67
19:W:174:GLN:HB3	19:W:178:ALA:HB3	1.76	0.67
5:E:113:ALA:HB1	5:E:114:PRO:CD	2.23	0.67
12:L:154:VAL:HG12	12:L:180:LEU:HB2	1.74	0.67
29:r:644:THR:CA	29:r:647:VAL:HG23	2.23	0.67
1:A:84:PRO:HA	1:A:508:THR:HG21	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:g:146:ILE:CG2	25:g:152:ALA:HA	2.25	0.67
25:g:156:PRO:HG2	25:g:157:TRP:CZ3	2.29	0.67
11:K:305:VAL:HG12	11:K:337:LEU:HD13	1.77	0.67
20:Y:55:GLU:OE1	20:Y:55:GLU:N	2.28	0.67
20:Y:92:LYS:CG	20:Y:240:CYS:SG	2.83	0.67
28:R:288:LYS:HB3	29:r:538:GLU:HG3	1.76	0.67
30:X:57:LEU:HD23	30:X:61:PHE:HD2	1.58	0.67
30:X:396:PHE:HA	30:X:622:TRP:CH2	2.30	0.67
4:Z:17:THR:HG23	4:Z:27:ARG:HE	1.59	0.67
17:P:135:G:H2'	17:P:136:C:H6	1.59	0.67
25:g:151:GLY:O	25:g:152:ALA:O	2.11	0.67
30:X:1125:MET:HG3	30:X:1277:THR:HB	1.77	0.67
30:X:17:SER:O	30:X:25:VAL:N	2.26	0.67
2:B:490:MET:HE3	2:B:566:LEU:HD11	1.76	0.67
21:a:244:SER:CB	21:a:247:ALA:HB3	2.22	0.67
29:r:637:LEU:HG	29:r:644:THR:HG21	1.54	0.67
30:X:653:ASP:O	30:X:659:ASN:ND2	2.28	0.67
11:K:413:VAL:HG21	11:K:422:ALA:HB2	1.77	0.67
16:Q:500:A:O2'	16:Q:501:A:OP2	2.11	0.67
17:P:104:G:C2	6:f:20:LYS:CG	2.72	0.66
28:R:149:GLU:OE1	28:R:180:MET:CE	2.43	0.66
17:P:104:G:C5'	7:l:104:ASP:CG	2.60	0.66
20:Y:53:GLN:C	20:Y:54:ILE:HD13	2.20	0.66
20:Y:202:GLU:OE1	20:Y:261:ARG:NH2	2.29	0.66
28:R:116:LYS:NZ	33:x:303:UNK:CB	2.58	0.66
30:X:189:PHE:HA	30:X:192:HIS:HD2	1.59	0.66
24:e:106:ILE:O	24:e:106:ILE:HG22	1.93	0.66
30:X:745:MET:HE1	30:X:1029:PHE:HA	1.78	0.66
31:j:42:VAL:HA	5:b:81:GLN:HG2	1.78	0.66
17:P:159:U:O5'	17:P:159:U:H6	1.78	0.66
17:P:168:A:H1'	4:Z:27:ARG:HH11	1.61	0.66
20:Y:270:VAL:HG12	20:Y:274:LEU:CD2	2.26	0.66
30:X:74:HIS:CG	30:X:77:LEU:HD12	2.30	0.66
30:X:120:VAL:O	30:X:123:MET:N	2.28	0.66
20:Y:52:LYS:N	20:Y:52:LYS:HD2	2.11	0.66
25:g:112:GLY:O	25:g:116:PHE:N	2.28	0.66
29:r:544:PHE:HB3	29:r:548:VAL:HB	1.78	0.66
30:X:1122:TYR:OH	30:X:1269:LEU:O	2.11	0.66
5:E:113:ALA:HB1	5:E:114:PRO:HD2	1.77	0.66
18:U:392:VAL:CG1	18:U:403:TRP:HE1	2.08	0.66
21:a:23:CYS:SG	36:a:402:ZN:ZN	1.84	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:d:45:ARG:NH1	23:d:47:ILE:HD11	2.11	0.66
30:X:332:ARG:NH2	30:X:383:ARG:O	2.29	0.66
11:K:201:LEU:HB3	11:K:232:TRP:CZ3	2.30	0.66
1:A:169:TRP:CH2	1:A:639:PHE:HB2	2.30	0.65
2:B:145:ILE:HD11	2:B:230:PRO:HB2	1.79	0.65
12:L:152:THR:HG23	12:L:185:ILE:HD11	1.77	0.65
17:P:104:G:C6	6:f:20:LYS:HG3	2.31	0.65
30:X:699:PHE:HD2	30:X:717:PHE:HA	1.61	0.65
30:X:754:LYS:HB3	30:X:1008:LEU:HD13	1.78	0.65
12:L:220:ASP:OD1	12:L:239:MET:CB	2.35	0.65
14:N:81:U:H6	14:N:81:U:H5''	1.61	0.65
1:A:1850:VAL:HG12	1:A:1864:LYS:HZ2	1.61	0.65
14:N:57:C:H2'	14:N:58:U:H5'	1.77	0.65
16:Q:501:A:H4'	16:Q:502:C:OP2	1.96	0.65
20:Y:276:LYS:O	20:Y:280:LEU:N	2.27	0.65
17:P:97:U:C4	7:l:62:ARG:CD	2.80	0.65
30:X:441:TYR:HB2	30:X:625:LEU:HD21	1.77	0.65
30:X:627:ILE:HD13	30:X:963:LEU:HD12	1.79	0.65
17:P:137:U:O5'	17:P:137:U:H6	1.78	0.65
20:Y:227:LYS:HG3	20:Y:243:VAL:HG12	1.78	0.65
1:A:1850:VAL:HG11	1:A:1864:LYS:HZ3	1.62	0.65
11:K:172:GLU:HG3	11:K:177:TRP:CZ2	2.32	0.65
17:P:97:U:C1'	7:l:63:HIS:HE2	2.09	0.65
18:T:90:LEU:HD12	18:U:90:LEU:HD23	1.79	0.65
30:X:1119:LEU:HA	30:X:1122:TYR:HD2	1.62	0.65
30:X:1233:ILE:O	30:X:1236:THR:OG1	2.15	0.65
30:X:248:ASP:O	30:X:357:ARG:NH2	2.30	0.65
14:N:78:A:C2	28:R:104:ILE:HG13	2.31	0.65
16:Q:500:A:H4'	16:Q:501:A:C5'	2.19	0.65
22:c:540:ILE:HG22	22:c:557:MET:HE3	1.78	0.65
30:X:1119:LEU:HD21	30:X:1269:LEU:HD13	1.77	0.65
14:N:25:U:C2	20:Y:232:HIS:HE1	2.15	0.64
29:r:648:TYR:CG	29:r:666:UNK:CB	2.79	0.64
30:X:743:LEU:HD23	30:X:1005:LEU:HB2	1.79	0.64
14:N:57:C:C2'	14:N:58:U:H5'	2.28	0.64
24:e:29:ARG:NH2	25:g:148:GLU:OE2	2.30	0.64
30:X:120:VAL:HG11	30:X:124:ILE:CG1	2.24	0.64
30:X:1066:THR:HG21	37:X:1500:ADP:C2	2.33	0.64
31:j:64:ARG:NH2	5:b:45:TYR:CE2	2.65	0.64
28:R:149:GLU:OE1	28:R:180:MET:HE1	1.97	0.64
20:Y:108:ALA:HB2	20:Y:132:GLU:O	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R:289:GLN:HB3	29:r:539:ARG:NH2	2.13	0.64
29:r:503:TYR:OH	29:r:516:VAL:HG12	1.97	0.64
30:X:268:LYS:O	30:X:271:THR:OG1	2.16	0.64
20:Y:243:VAL:O	20:Y:244:ARG:HD3	1.98	0.64
29:r:530:PHE:O	29:r:533:SER:OG	2.09	0.64
30:X:1051:SER:O	30:X:1054:SER:OG	2.15	0.64
12:L:282:ARG:O	12:L:298:ALA:HB2	1.98	0.64
14:N:78:A:H4'	28:R:108:LEU:HD12	1.78	0.64
17:P:164:C:H6	17:P:164:C:H5'	1.63	0.64
29:r:641:VAL:O	29:r:644:THR:OG1	2.15	0.64
30:X:71:SER:HA	30:X:75:ILE:CD1	2.27	0.64
30:X:534:ILE:HD11	30:X:610:PHE:HA	1.80	0.64
30:X:1044:THR:HG23	30:X:1065:LYS:HA	1.78	0.64
1:A:1832:PHE:CZ	1:A:1843:LEU:CD1	2.79	0.64
1:A:1841:LEU:HB3	1:A:1843:LEU:HD21	1.78	0.64
3:C:55:C:C2'	3:C:56:A:H5'	2.28	0.64
12:L:55:VAL:HG21	12:L:98:ASP:HA	1.79	0.64
14:N:76:C:H2'	14:N:77:G:O4'	1.98	0.64
17:P:103:U:C2	7:l:102:ARG:CZ	2.81	0.64
20:Y:69:GLN:HA	20:Y:69:GLN:NE2	2.12	0.64
20:Y:202:GLU:CD	20:Y:261:ARG:NH2	2.56	0.64
1:A:1825:LYS:HG3	1:A:1826:PRO:HD2	1.80	0.64
17:P:106:U:C6	17:P:107:U:H5	2.15	0.64
20:Y:250:PRO:O	20:Y:251:ASN:CG	2.41	0.64
24:e:25:GLU:HG2	25:g:147:LEU:CD1	2.25	0.64
1:A:840:LEU:HD12	1:A:845:PHE:CD2	2.32	0.64
17:P:135:G:H2'	17:P:136:C:C6	2.32	0.64
30:X:117:LEU:CD2	30:X:205:LYS:HZ3	2.10	0.64
12:L:152:THR:CG2	12:L:185:ILE:HD11	2.27	0.63
13:M:186:TYR:OH	25:g:86:THR:HB	1.98	0.63
17:P:97:U:C1'	7:l:63:HIS:CD2	2.80	0.63
17:P:103:U:C1'	7:l:102:ARG:NH2	2.61	0.63
20:Y:266:ALA:HB3	21:a:99:ALA:HB2	1.81	0.63
20:Y:195:PHE:CE2	20:Y:230:MET:CE	2.74	0.63
20:Y:276:LYS:O	20:Y:280:LEU:HG	1.96	0.63
28:R:288:LYS:HD3	29:r:538:GLU:CB	2.28	0.63
1:A:74:TYR:CE1	24:e:108:THR:HG21	2.33	0.63
12:L:219:LYS:HA	12:L:219:LYS:NZ	2.13	0.63
13:M:204:MET:SD	21:a:35:MET:HE2	2.38	0.63
12:L:242:THR:CB	12:L:244:ARG:HE	2.09	0.63
30:X:725:TYR:CB	37:X:1500:ADP:N7	2.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:775:VAL:HB	30:X:976:LEU:HD23	1.80	0.63
11:K:327:LEU:HD13	11:K:357:TRP:CZ3	2.34	0.63
20:Y:203:ARG:HH12	20:Y:257:ARG:NH1	1.97	0.63
30:X:667:ALA:HB1	30:X:670:LEU:HD12	1.80	0.63
17:P:118:A:H2'	17:P:119:G:H8	1.64	0.63
29:r:531:GLU:HA	29:r:534:PHE:CD2	2.33	0.63
30:X:594:SER:HB2	30:X:605:GLN:HG2	1.80	0.63
30:X:646:PHE:O	30:X:1031:ARG:NH1	2.32	0.63
14:N:9:G:H2'	14:N:10:A:O4'	1.97	0.63
28:R:83:GLN:N	28:R:83:GLN:HE21	1.95	0.63
28:R:146:TYR:CE2	33:x:393:UNK:C	2.76	0.63
29:r:628:TYR:CA	29:r:631:LEU:HD11	2.21	0.63
30:X:273:ASP:HA	30:X:276:TYR:HD2	1.64	0.63
1:A:1844:LYS:HB3	1:A:1844:LYS:HZ1	1.64	0.63
25:g:142:GLY:O	25:g:143:ASP:HB2	1.97	0.63
28:R:284:THR:O	28:R:288:LYS:HG3	1.97	0.63
30:X:668:ARG:N	30:X:700:TYR:O	2.32	0.63
28:R:146:TYR:CD2	33:x:393:UNK:CB	2.79	0.63
2:B:136:THR:HG23	2:B:559:VAL:HG21	1.81	0.62
24:e:26:PHE:HE1	24:e:55:GLN:HG2	1.64	0.62
30:X:982:GLN:HB2	30:X:1030:LYS:HE3	1.80	0.62
16:Q:500:A:H1'	16:Q:501:A:OP2	1.99	0.62
24:e:119:CYS:SG	24:e:139:CYS:SG	2.98	0.62
21:a:60:ARG:HH22	25:g:107:THR:HG23	1.64	0.62
1:A:1819:GLU:H	1:A:1819:GLU:CD	2.00	0.62
17:P:97:U:N1	7:l:63:HIS:NE2	2.46	0.62
18:U:392:VAL:HG12	18:U:403:TRP:HE1	1.65	0.62
20:Y:227:LYS:CG	20:Y:243:VAL:HG12	2.28	0.62
23:d:82:HIS:CD2	23:d:118:ILE:HD11	2.35	0.62
1:A:1292:ILE:HD12	22:c:533:TRP:HH2	1.65	0.62
12:L:220:ASP:CG	12:L:221:ILE:HG13	2.24	0.62
17:P:104:G:P	7:l:104:ASP:OD1	2.57	0.62
14:N:26:U:C5	20:Y:244:ARG:CD	2.81	0.62
18:S:86:GLU:OE2	33:x:41:UNK:CA	2.37	0.62
20:Y:138:PRO:CD	20:Y:225:PHE:HD2	2.08	0.62
25:g:140:ASP:OD1	25:g:141:PRO:HD2	1.99	0.62
30:X:194:LEU:HB3	30:X:198:TRP:HE1	1.64	0.62
19:W:61:TRP:CD1	19:W:98:TYR:CZ	2.88	0.62
25:g:146:ILE:HD12	25:g:146:ILE:N	2.14	0.62
30:X:854:ALA:O	30:X:858:ARG:HG3	2.00	0.62
17:P:104:G:H5'	7:l:104:ASP:OD1	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:r:580:LEU:HD11	29:r:592:TYR:CZ	2.35	0.62
30:X:502:LYS:HE2	30:X:586:TYR:HE1	1.65	0.62
13:M:109:GLN:HE22	19:W:233:ILE:HG21	1.64	0.61
18:U:205:GLU:CB	18:U:466:LEU:CB	2.76	0.61
20:Y:92:LYS:CA	20:Y:240:CYS:SG	2.86	0.61
30:X:189:PHE:HA	30:X:192:HIS:CD2	2.35	0.61
30:X:463:LEU:O	30:X:470:LYS:HA	1.99	0.61
1:A:945:LEU:HD23	1:A:1059:PHE:CE2	2.35	0.61
30:X:83:LEU:HA	30:X:129:LEU:HD11	1.82	0.61
30:X:1173:PRO:O	30:X:1176:LYS:N	2.33	0.61
12:L:269:GLU:HG2	25:g:95:PRO:CD	2.31	0.61
17:P:103:U:C2	7:l:102:ARG:NH1	2.68	0.61
20:Y:227:LYS:HG3	20:Y:243:VAL:CG1	2.30	0.61
30:X:774:THR:HG22	30:X:975:ASN:HB2	1.83	0.61
17:P:104:G:C6	6:f:20:LYS:CG	2.83	0.61
29:r:643:ALA:O	29:r:647:VAL:HG23	2.00	0.61
30:X:1031:ARG:HG3	30:X:1032:LEU:HD12	1.82	0.61
1:A:1850:VAL:CG1	1:A:1864:LYS:HZ3	2.13	0.61
12:L:44:LEU:HD22	12:L:83:VAL:HG11	1.83	0.61
14:N:23:A:H2	20:Y:57:ARG:NH2	1.92	0.61
17:P:118:A:H8	17:P:118:A:O5'	1.83	0.61
30:X:509:ARG:HH21	30:X:581:LYS:NZ	1.98	0.61
30:X:1011:GLN:CD	30:X:1033:ARG:HD3	2.26	0.61
1:A:667:ILE:O	1:A:668:VAL:C	2.43	0.61
12:L:220:ASP:OD1	12:L:221:ILE:HG13	1.98	0.61
17:P:97:U:C1'	7:l:63:HIS:NE2	2.63	0.61
20:Y:273:LEU:HD12	21:a:89:PHE:CD1	2.33	0.61
21:a:29:ASP:CB	25:g:110:ILE:HD13	2.30	0.61
25:g:96:ASN:OD1	25:g:97:PHE:N	2.34	0.61
28:R:255:LYS:HE3	29:r:508:GLU:OE2	1.99	0.61
30:X:149:ILE:HG21	30:X:175:PHE:CD1	2.35	0.61
30:X:807:ASP:OD1	30:X:962:ARG:NH2	2.27	0.61
30:X:1079:ASN:ND2	30:X:1209:TYR:O	2.32	0.61
14:N:73:C:O2'	14:N:74:U:P	2.59	0.61
24:e:137:CYS:SG	36:e:201:ZN:ZN	1.88	0.61
14:N:26:U:C4	20:Y:244:ARG:NH2	2.69	0.61
29:r:627:ILE:O	29:r:631:LEU:HG	1.99	0.61
31:j:42:VAL:HA	5:b:81:GLN:CG	2.30	0.61
1:A:1819:GLU:HB2	1:A:1820:GLY:HA2	1.83	0.61
20:Y:278:PHE:CZ	21:a:141:ARG:CA	2.84	0.61
1:A:208:LEU:C	24:e:8:ARG:NH1	2.59	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:TYR:HD1	1:A:818:LEU:HD12	1.65	0.60
1:A:1844:LYS:HD3	1:A:1938:MET:SD	2.27	0.60
2:B:679:THR:HG21	2:B:842:MET:HE3	1.83	0.60
20:Y:242:ASN:HD22	20:Y:242:ASN:C	2.06	0.60
20:Y:278:PHE:HD2	21:a:141:ARG:NE	1.95	0.60
30:X:388:ASN:O	30:X:392:GLU:N	2.29	0.60
1:A:1847:HIS:CE1	1:A:1934:THR:C	2.79	0.60
20:Y:203:ARG:HH12	20:Y:257:ARG:HH11	1.49	0.60
28:R:142:TYR:HE2	33:x:387:UNK:N	1.99	0.60
1:A:456:GLU:O	1:A:457:HIS:CG	2.54	0.60
2:B:960:ASP:O	2:B:961:VAL:HG12	2.01	0.60
30:X:817:TYR:HD1	30:X:820:LEU:HD12	1.66	0.60
14:N:78:A:C5'	28:R:105:PRO:HG3	2.31	0.60
17:P:116:A:C6	17:P:117:A:N6	2.70	0.60
29:r:524:LEU:HD22	29:r:536:ILE:HD11	1.82	0.60
30:X:533:TYR:HD1	30:X:554:VAL:HA	1.65	0.60
30:X:747:ASN:ND2	30:X:1041:ASP:OD1	2.33	0.60
21:a:80:CYS:SG	21:a:83:CYS:SG	2.88	0.60
30:X:117:LEU:HD23	30:X:205:LYS:CD	2.32	0.60
1:A:1832:PHE:CE1	1:A:1843:LEU:HD13	2.37	0.60
17:P:136:C:C4	17:P:137:U:O4	2.54	0.60
30:X:561:THR:OG1	30:X:569:MET:SD	2.59	0.60
30:X:1049:ARG:NH1	30:X:1085:GLU:OE2	2.34	0.60
4:D:8:LEU:O	4:D:11:THR:HG22	2.01	0.60
14:N:78:A:H2	28:R:104:ILE:CG1	2.14	0.60
25:g:138:ARG:HB2	25:g:160:TYR:CE1	2.35	0.60
30:X:120:VAL:CG1	30:X:124:ILE:CD1	2.80	0.60
30:X:163:TYR:HA	30:X:166:HIS:CD2	2.35	0.60
24:e:106:ILE:HD12	24:e:106:ILE:N	2.16	0.60
28:R:146:TYR:CZ	33:x:393:UNK:CB	2.80	0.60
30:X:462:ARG:HH21	30:X:612:LEU:HB2	1.65	0.60
2:B:490:MET:SD	2:B:510:VAL:HG22	2.41	0.60
17:P:105:G:H4'	17:P:106:U:O5'	2.00	0.60
17:P:157:G:H5''	17:P:157:G:H8	1.65	0.60
20:Y:278:PHE:HE2	21:a:141:ARG:CD	2.14	0.60
30:X:753:GLY:N	37:X:1500:ADP:O5'	2.33	0.60
21:a:44:CYS:HB2	21:a:70:CYS:HB3	1.84	0.60
29:r:500:ARG:HG3	29:r:520:TYR:OH	2.01	0.60
30:X:1141:SER:O	30:X:1144:SER:OG	2.18	0.60
1:A:1832:PHE:CE1	1:A:1843:LEU:HD11	2.37	0.59
12:L:282:ARG:O	12:L:298:ALA:HB3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:262:LYS:HB2	17:P:18:U:C6	2.37	0.59
17:P:97:U:H5	7:l:62:ARG:HD2	1.64	0.59
29:r:415:UNK:O	29:r:420:UNK:N	2.35	0.59
30:X:306:LEU:O	30:X:309:THR:OG1	2.14	0.59
30:X:1066:THR:O	30:X:1069:SER:OG	2.17	0.59
1:A:265:LEU:HD13	1:A:434:PHE:CD2	2.37	0.59
2:B:811:ALA:HB1	2:B:812:PRO:HD2	1.83	0.59
14:N:76:C:H3'	14:N:77:G:C8	2.37	0.59
20:Y:263:GLU:HG3	21:a:99:ALA:HA	1.83	0.59
25:g:156:PRO:CG	25:g:157:TRP:CZ3	2.85	0.59
29:r:541:VAL:HG21	29:r:553:TRP:CE3	2.37	0.59
29:r:568:HIS:HD2	29:r:571:ARG:HB3	1.65	0.59
30:X:497:LEU:HD22	30:X:589:PRO:HB2	1.84	0.59
1:A:1663:VAL:HG13	1:A:1742:TRP:O	2.02	0.59
17:P:153:U:C2	17:P:154:C:C5	2.91	0.59
28:R:288:LYS:O	29:r:535:LYS:HB3	2.02	0.59
30:X:195:LEU:HA	30:X:198:TRP:CD1	2.37	0.59
1:A:718:ASP:OD1	11:K:333:THR:HG23	2.02	0.59
13:M:251:ILE:O	13:M:251:ILE:HG23	2.02	0.59
29:r:612:LEU:HD23	29:r:632:LEU:HA	1.84	0.59
30:X:1091:VAL:N	30:X:1215:CYS:O	2.33	0.59
14:N:76:C:C6	14:N:77:G:C1'	2.86	0.59
30:X:56:LYS:H	30:X:1224:ARG:NE	2.01	0.59
30:X:205:LYS:HE3	30:X:209:TYR:CE2	2.37	0.59
30:X:693:GLU:HA	30:X:696:LEU:HG	1.84	0.59
14:N:24:A:C4	20:Y:60:TYR:CD2	2.91	0.59
17:P:160:A:C2	17:P:161:U:N3	2.70	0.59
19:W:172:ASN:ND2	19:W:174:GLN:HG2	2.14	0.59
23:d:132:MET:HG3	23:d:147:LEU:HD13	1.83	0.59
14:N:23:A:N7	20:Y:119:TYR:CE2	2.60	0.59
17:P:105:G:C5'	7:l:48:ARG:HH21	2.12	0.59
18:S:20:GLY:HA3	18:T:53:VAL:HG12	1.84	0.59
18:U:368:LEU:O	27:i:37:GLY:HA3	2.02	0.59
21:a:244:SER:O	21:a:248:LYS:N	2.34	0.59
28:R:288:LYS:CB	29:r:538:GLU:CB	2.79	0.59
30:X:979:MET:SD	30:X:1008:LEU:HD12	2.43	0.59
14:N:8:G:C3'	14:N:9:G:H5'	2.33	0.59
17:P:156:U:C6	17:P:156:U:C5'	2.72	0.59
21:a:32:TYR:HB3	25:g:99:PHE:CE2	2.37	0.59
30:X:204:ILE:HG12	30:X:365:ALA:H	1.67	0.59
1:A:658:ARG:O	1:A:659:VAL:C	2.43	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:28:C:O2'	17:P:29:A:O5'	2.18	0.59
30:X:753:GLY:N	37:X:1500:ADP:H5'2	2.18	0.59
4:Z:8:LEU:O	4:Z:11:THR:HG22	2.01	0.59
1:A:121:LEU:HD13	1:A:664:LEU:HB2	1.84	0.59
1:A:1023:LEU:HD11	1:A:1066:PHE:CD1	2.37	0.59
1:A:1872:LEU:HD21	1:A:1938:MET:CE	2.32	0.59
13:M:124:LEU:HD21	13:M:234:LEU:O	2.03	0.59
13:M:262:LYS:C	19:W:173:THR:CG2	2.76	0.59
17:P:104:G:H2'	17:P:105:G:O5'	2.00	0.59
20:Y:177:TYR:HB3	20:Y:244:ARG:O	2.03	0.59
9:I:40:TYR:O	9:I:67:CYS:SG	2.59	0.58
14:N:23:A:C5	20:Y:119:TYR:CE2	2.91	0.58
21:a:19:PHE:HZ	25:g:89:ALA:HB2	1.64	0.58
21:a:47:CYS:SG	21:a:73:CYS:SG	2.97	0.58
25:g:101:GLN:OE1	25:g:102:GLU:N	2.36	0.58
30:X:1177:ARG:HG2	30:X:1206:ALA:HA	1.85	0.58
1:A:91:MET:HA	1:A:91:MET:HE3	1.86	0.58
14:N:15:U:OP1	24:e:116:THR:OG1	2.21	0.58
20:Y:53:GLN:NE2	20:Y:102:ASP:OD2	2.36	0.58
28:R:329:UNK:CB	29:r:570:GLU:HG3	2.33	0.58
29:r:487:UNK:O	29:r:491:UNK:N	2.35	0.58
30:X:53:HIS:O	30:X:1224:ARG:NE	2.37	0.58
33:x:407:UNK:O	33:x:408:UNK:C	2.51	0.58
33:x:408:UNK:O	33:x:409:UNK:C	2.52	0.58
20:Y:262:LEU:HD22	20:Y:262:LEU:C	2.27	0.58
20:Y:281:ASP:O	20:Y:284:GLU:N	2.37	0.58
30:X:83:LEU:O	30:X:86:SER:OG	2.14	0.58
4:Z:17:THR:CG2	4:Z:27:ARG:NE	2.66	0.58
11:K:151:ALA:HB1	11:K:152:PRO:HD2	1.85	0.58
12:L:159:THR:HG22	12:L:175:GLU:HG2	1.84	0.58
17:P:102:U:N3	6:f:61:ARG:HD3	2.17	0.58
19:W:170:LEU:N	19:W:170:LEU:HD23	2.17	0.58
29:r:560:PHE:CE2	29:r:572:THR:HG22	2.36	0.58
30:X:505:MET:H	30:X:583:ILE:H	1.50	0.58
30:X:888:HIS:O	30:X:892:GLY:N	2.37	0.58
30:X:976:LEU:HB2	30:X:1005:LEU:HD23	1.85	0.58
31:j:64:ARG:HH22	5:b:25:VAL:HG21	1.68	0.58
31:j:88:ASN:HA	31:j:113:GLN:CG	2.34	0.58
2:B:89:VAL:HG22	11:K:155:LEU:O	2.03	0.58
2:B:873:GLN:CG	2:B:875:ILE:HD11	2.33	0.58
12:L:65:PHE:HD1	12:L:326:LEU:HD11	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:W:172:ASN:HD22	19:W:172:ASN:C	2.10	0.58
24:e:8:ARG:HG3	24:e:8:ARG:HH21	1.68	0.58
25:g:142:GLY:HA3	25:g:152:ALA:C	2.28	0.58
14:N:73:C:N1	14:N:74:U:N3	2.48	0.58
17:P:106:U:C6	17:P:107:U:C5	2.90	0.58
20:Y:278:PHE:CE2	21:a:141:ARG:CD	2.87	0.58
30:X:260:TYR:HB3	30:X:267:PHE:CZ	2.38	0.58
30:X:339:THR:HB	30:X:374:LYS:HG2	1.84	0.58
30:X:390:TYR:HE2	30:X:435:ARG:HD3	1.68	0.58
8:H:58:GLN:HB2	8:H:68:LEU:HD21	1.86	0.58
12:L:219:LYS:HA	12:L:219:LYS:HZ1	1.67	0.58
30:X:67:ASN:H	30:X:70:MET:HB2	1.68	0.58
31:j:132:LEU:HD12	31:j:157:ALA:HB2	1.84	0.58
1:A:422:ALA:O	1:A:426:ILE:HD12	2.02	0.58
1:A:839:TRP:CD1	1:A:1073:LEU:HD13	2.37	0.58
12:L:46:MET:HE1	12:L:336:LEU:HG	1.86	0.58
20:Y:302:UNK:O	20:Y:303:UNK:C	2.51	0.58
1:A:456:GLU:O	1:A:457:HIS:CD2	2.57	0.58
2:B:772:VAL:HG12	2:B:810:LEU:HD13	1.86	0.58
14:N:73:C:C1'	14:N:74:U:C4	2.86	0.58
28:R:97:LEU:HD21	28:R:107:TRP:CH2	2.38	0.58
28:R:194:TYR:O	28:R:198:VAL:HG23	2.04	0.58
30:X:46:LYS:HD3	30:X:414:LEU:HD12	1.85	0.58
30:X:115:LEU:CD1	30:X:119:GLU:HG3	2.34	0.58
33:x:410:UNK:O	33:x:411:UNK:C	2.51	0.58
1:A:832:ILE:HD13	1:A:1190:LEU:HD11	1.85	0.58
14:N:25:U:O2'	20:Y:90:GLN:OE1	2.21	0.58
15:O:100:G:C8	15:O:101:U:N3	2.67	0.58
17:P:97:U:H5	7:l:62:ARG:CD	2.17	0.58
20:Y:49:PRO:O	20:Y:50:ALA:HB3	2.04	0.58
20:Y:203:ARG:NH1	20:Y:257:ARG:HH11	2.01	0.58
30:X:507:LEU:HD12	30:X:583:ILE:HD12	1.86	0.58
33:x:310:UNK:O	33:x:311:UNK:C	2.51	0.58
1:A:1392:LEU:HD21	1:A:1491:LEU:HD21	1.85	0.57
20:Y:56:THR:O	20:Y:57:ARG:CB	2.52	0.57
20:Y:301:UNK:O	20:Y:302:UNK:C	2.52	0.57
30:X:1217:ARG:HB3	30:X:1221:ARG:HH21	1.67	0.57
2:B:881:PRO:C	2:B:882:LEU:HD22	2.29	0.57
3:C:56:A:O2'	3:C:57:G:O5'	2.22	0.57
11:K:413:VAL:CG2	11:K:422:ALA:HB2	2.35	0.57
12:L:315:HIS:ND1	12:L:317:ASP:OD1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:e:126:LEU:HD23	24:e:130:GLN:HG3	1.86	0.57
30:X:1267:LEU:O	30:X:1270:SER:OG	2.14	0.57
1:A:714:ASN:ND2	11:K:309:MET:SD	2.77	0.57
17:P:104:G:O6	6:f:66:ARG:NE	2.27	0.57
24:e:70:ILE:HG23	24:e:74:LEU:HD23	1.84	0.57
28:R:289:GLN:CB	29:r:539:ARG:NH2	2.67	0.57
30:X:19:TRP:HB2	30:X:61:PHE:HE1	1.68	0.57
12:L:218:HIS:NE2	12:L:238:SER:HB3	2.19	0.57
13:M:187:THR:O	25:g:87:GLY:C	2.47	0.57
28:R:130:ALA:O	28:R:134:LEU:HD12	2.04	0.57
30:X:509:ARG:HH21	30:X:581:LYS:HZ1	1.52	0.57
30:X:728:ASN:ND2	30:X:1044:THR:OG1	2.37	0.57
30:X:944:ALA:HA	30:X:948:GLN:HB3	1.85	0.57
7:G:55:ALA:HB2	7:G:71:VAL:HA	1.85	0.57
8:H:68:LEU:HD22	9:I:72:TRP:HH2	1.70	0.57
18:U:352:LEU:CG	18:U:356:GLU:H	2.17	0.57
21:a:23:CYS:SG	21:a:80:CYS:SG	2.94	0.57
24:e:116:THR:O	24:e:117:CYS:C	2.47	0.57
25:g:83:ASN:CB	25:g:88:TYR:HD1	2.15	0.57
30:X:125:GLN:O	30:X:128:THR:OG1	2.17	0.57
30:X:881:ALA:O	30:X:888:HIS:NE2	2.36	0.57
30:X:1191:ALA:HB3	30:X:1195:TRP:CD1	2.40	0.57
2:B:253:ARG:CZ	2:B:914:VAL:HG13	2.34	0.57
17:P:160:A:C8	17:P:171:G:N2	2.73	0.57
19:W:174:GLN:HB3	19:W:178:ALA:CB	2.35	0.57
20:Y:69:GLN:C	20:Y:70:VAL:HG23	2.30	0.57
21:a:42:GLN:HG3	21:a:53:ILE:HD11	1.85	0.57
33:x:409:UNK:O	33:x:410:UNK:C	2.51	0.57
5:E:116:GLY:HA2	25:g:94:VAL:CG1	2.34	0.57
20:Y:176:LEU:HD21	20:Y:227:LYS:HB2	1.87	0.57
21:a:71:VAL:HG23	21:a:81:GLN:HE22	1.70	0.57
30:X:57:LEU:HD23	30:X:61:PHE:CD2	2.39	0.57
30:X:1070:SER:H	30:X:1071:PRO:HD2	1.70	0.57
11:K:180:THR:HG21	11:K:445:VAL:HG21	1.85	0.57
17:P:104:G:C8	7:l:104:ASP:HB3	2.40	0.57
20:Y:203:ARG:CZ	20:Y:257:ARG:HH11	2.17	0.57
25:g:56:ASN:HD22	25:g:56:ASN:N	2.02	0.57
25:g:140:ASP:OD1	25:g:141:PRO:CD	2.53	0.57
28:R:225:GLN:HA	28:R:228:LEU:HD12	1.87	0.57
30:X:736:LEU:O	30:X:739:SER:OG	2.12	0.57
33:x:403:UNK:O	33:x:404:UNK:C	2.51	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:76:C:H3'	14:N:77:G:H8	1.70	0.57
18:U:300:PHE:CB	18:U:338:SER:HA	2.35	0.57
29:r:626:ALA:O	29:r:630:VAL:HG23	2.04	0.57
30:X:188:LYS:HA	30:X:191:LEU:HD12	1.86	0.57
30:X:205:LYS:HE2	30:X:209:TYR:OH	2.03	0.57
33:x:404:UNK:O	33:x:405:UNK:C	2.51	0.57
1:A:1850:VAL:HG11	1:A:1864:LYS:NZ	2.20	0.57
14:N:73:C:O4'	14:N:74:U:C5	2.58	0.57
18:U:300:PHE:CB	18:U:339:LEU:N	2.68	0.57
18:V:72:LEU:HD23	18:V:75:LEU:HD12	1.87	0.57
20:Y:278:PHE:HZ	21:a:141:ARG:O	1.87	0.57
30:X:109:ILE:O	30:X:112:SER:OG	2.21	0.57
30:X:347:LEU:HD11	30:X:370:PHE:CD1	2.40	0.57
7:l:55:ALA:HB2	7:l:71:VAL:HA	1.85	0.57
1:A:427:LEU:O	1:A:428:LEU:C	2.48	0.56
2:B:221:VAL:HG21	2:B:914:VAL:HG22	1.87	0.56
2:B:287:TYR:OH	2:B:357:GLY:HA3	2.05	0.56
16:Q:500:A:H1'	16:Q:501:A:P	2.45	0.56
18:U:379:LYS:CG	18:U:422:ALA:O	2.53	0.56
20:Y:63:GLU:N	20:Y:63:GLU:OE2	2.38	0.56
20:Y:242:ASN:ND2	20:Y:244:ARG:HE	2.02	0.56
25:g:142:GLY:HA3	25:g:153:TYR:N	2.17	0.56
25:g:142:GLY:HA3	25:g:152:ALA:O	2.02	0.56
29:r:633:VAL:O	29:r:637:LEU:HG	2.05	0.56
30:X:1269:LEU:O	30:X:1273:VAL:HG23	2.05	0.56
2:B:221:VAL:HG23	2:B:250:ASN:OD1	2.05	0.56
11:K:233:ASP:HB2	11:K:240:ILE:CD1	2.34	0.56
13:M:183:TYR:CZ	13:M:203:LYS:HD2	2.39	0.56
17:P:122:U:H2'	17:P:123:C:H6	1.71	0.56
21:a:60:ARG:NH2	25:g:107:THR:HG23	2.19	0.56
24:e:105:CYS:SG	24:e:117:CYS:SG	3.03	0.56
29:r:646:THR:HA	29:r:649:GLU:CD	2.29	0.56
30:X:1122:TYR:O	30:X:1126:LEU:HG	2.05	0.56
1:A:485:ALA:O	1:A:486:HIS:HB3	2.04	0.56
1:A:1802:LEU:HD22	1:A:1833:ILE:HG22	1.87	0.56
1:A:1808:ASN:HB2	1:A:1830:ALA:O	2.04	0.56
1:A:1815:HIS:HA	1:A:1816:LYS:HE3	1.87	0.56
1:A:1832:PHE:CE2	1:A:1920:ILE:HG21	2.40	0.56
2:B:249:ILE:HD11	2:B:849:GLU:CB	2.35	0.56
2:B:614:LEU:N	2:B:615:PRO:HD2	2.20	0.56
12:L:219:LYS:HA	12:L:219:LYS:HE3	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:97:U:C2	7:l:63:HIS:CD2	2.92	0.56
17:P:139:U:H2'	17:P:140:C:H6	1.71	0.56
18:U:317:LYS:O	18:U:328:TYR:CG	2.59	0.56
20:Y:261:ARG:HG3	20:Y:261:ARG:NH2	2.19	0.56
29:r:625:LEU:HG	29:r:629:ASN:HD21	1.69	0.56
29:r:628:TYR:HA	29:r:631:LEU:CG	2.34	0.56
30:X:49:LEU:HD23	30:X:52:LEU:HD12	1.87	0.56
8:m:58:GLN:HB2	8:m:68:LEU:HD21	1.86	0.56
17:P:102:U:H3	6:f:61:ARG:HD3	1.68	0.56
25:g:138:ARG:CB	25:g:160:TYR:HD1	2.04	0.56
25:g:157:TRP:O	25:g:158:ALA:C	2.47	0.56
28:R:146:TYR:HE2	33:x:393:UNK:CA	2.17	0.56
30:X:441:TYR:HD1	30:X:621:TYR:HH	1.54	0.56
30:X:639:PRO:O	30:X:643:GLU:HG3	2.04	0.56
30:X:681:LEU:HB3	30:X:684:CYS:HB2	1.87	0.56
30:X:820:LEU:HA	30:X:823:TRP:HD1	1.70	0.56
14:N:75:G:N3	14:N:75:G:H2'	2.20	0.56
17:P:131:C:H2'	17:P:132:U:H6	1.71	0.56
17:P:140:C:C2	17:P:141:C:C5	2.93	0.56
20:Y:261:ARG:O	20:Y:261:ARG:HD3	2.05	0.56
25:g:147:LEU:C	25:g:148:GLU:OE1	2.48	0.56
30:X:19:TRP:HA	30:X:24:GLY:HA3	1.88	0.56
30:X:236:PHE:O	30:X:240:ARG:HG3	2.05	0.56
30:X:259:LEU:O	30:X:263:SER:N	2.38	0.56
30:X:306:LEU:HD11	30:X:381:TYR:CE1	2.40	0.56
31:j:57:GLY:O	31:j:58:ASN:CB	2.54	0.56
12:L:144:LEU:HD21	12:L:185:ILE:HG21	1.88	0.56
17:P:119:G:H2'	17:P:120:C:H6	1.71	0.56
17:P:120:C:C2	17:P:121:C:C5	2.94	0.56
17:P:123:C:C2	17:P:124:U:C5	2.94	0.56
17:P:139:U:C2	17:P:140:C:C5	2.94	0.56
22:c:568:TRP:HA	22:c:574:GLY:HA2	1.88	0.56
30:X:50:SER:HA	30:X:53:HIS:HD2	1.70	0.56
30:X:562:ILE:HA	30:X:583:ILE:HG23	1.86	0.56
8:m:68:LEU:HD22	9:n:72:TRP:HH2	1.70	0.56
33:x:405:UNK:O	33:x:406:UNK:C	2.51	0.56
1:A:168:MET:CE	1:A:211:ILE:HG21	2.32	0.56
1:A:1110:LEU:HD12	1:A:1121:MET:HB2	1.87	0.56
14:N:77:G:H22	14:N:79:C:N4	2.03	0.56
17:P:120:C:H2'	17:P:121:C:H6	1.71	0.56
30:X:1136:CYS:HB2	30:X:1183:PHE:CE1	2.37	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:1273:VAL:O	30:X:1277:THR:OG1	2.11	0.56
1:A:1405:ASP:O	1:A:1409:VAL:HG23	2.06	0.56
1:A:1663:VAL:HG12	1:A:1664:SER:N	2.20	0.56
3:C:49:U:O2	3:C:49:U:O2'	2.24	0.56
13:M:191:GLN:HE22	21:a:23:CYS:HA	1.70	0.56
17:P:133:A:H2'	17:P:134:U:H6	1.70	0.56
20:Y:61:GLU:O	20:Y:62:MET:CG	2.50	0.56
20:Y:303:UNK:O	20:Y:304:UNK:C	2.52	0.56
30:X:117:LEU:HD22	30:X:205:LYS:HZ3	1.71	0.56
13:M:189:SER:O	13:M:190:ASN:C	2.48	0.56
17:P:104:G:C5	6:f:20:LYS:HE2	2.41	0.56
30:X:84:TYR:O	30:X:88:TYR:N	2.30	0.56
30:X:517:LEU:HD13	30:X:562:ILE:HD13	1.88	0.56
31:j:33:ILE:O	31:j:58:ASN:CB	2.54	0.56
33:x:358:UNK:O	33:x:359:UNK:C	2.52	0.56
1:A:1847:HIS:HE1	1:A:1934:THR:C	2.14	0.56
12:L:195:GLY:CA	12:L:222:ILE:HD12	2.03	0.56
18:S:86:GLU:OE1	33:x:41:UNK:HA	2.04	0.56
18:S:95:THR:HG21	18:U:58:PHE:CD1	2.41	0.56
18:V:85:LEU:HD11	27:i:96:ALA:HB3	1.87	0.56
30:X:1192:SER:OG	30:X:1193:ASP:N	2.34	0.56
13:M:189:SER:OG	25:g:82:LYS:HD2	2.07	0.55
17:P:121:C:H2'	17:P:122:U:H6	1.71	0.55
17:P:138:U:C2	17:P:139:U:C5	2.94	0.55
19:W:236:TYR:C	19:W:238:UNK:H2	2.13	0.55
14:N:73:C:O2'	14:N:73:C:O2	2.23	0.55
17:P:112:U:H2'	17:P:113:U:H6	1.70	0.55
17:P:119:G:C4	17:P:120:C:C5	2.94	0.55
20:Y:281:ASP:O	20:Y:282:LEU:C	2.50	0.55
22:c:457:ILE:HD11	22:c:500:TYR:CE1	2.40	0.55
30:X:1095:LYS:NZ	30:X:1114:GLU:OE1	2.39	0.55
1:A:1214:MET:HG2	1:A:1215:THR:HG23	1.87	0.55
12:L:315:HIS:CE1	12:L:317:ASP:CG	2.83	0.55
17:P:18:U:C6	17:P:18:U:H5''	2.41	0.55
17:P:122:U:C2	17:P:123:C:C5	2.94	0.55
24:e:25:GLU:HG3	25:g:147:LEU:HD22	1.88	0.55
28:R:116:LYS:HZ1	33:x:303:UNK:CA	2.15	0.55
30:X:344:PHE:CZ	30:X:370:PHE:HB2	2.41	0.55
30:X:627:ILE:O	30:X:630:SER:OG	2.20	0.55
17:P:121:C:C2	17:P:122:U:C5	2.94	0.55
17:P:131:C:C2	17:P:132:U:C5	2.94	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:138:U:H2'	17:P:139:U:H6	1.71	0.55
29:r:597:ASP:O	29:r:601:LYS:NZ	2.39	0.55
30:X:595:LEU:HA	30:X:598:LEU:HG	1.88	0.55
30:X:669:ASN:HB2	30:X:723:ARG:HD2	1.87	0.55
30:X:986:GLU:HG2	30:X:1028:LEU:HG	1.89	0.55
33:x:411:UNK:O	33:x:412:UNK:C	2.51	0.55
1:A:1352:LEU:HD13	1:A:1491:LEU:HD11	1.89	0.55
2:B:438:PHE:CG	2:B:439:PRO:HD2	2.42	0.55
2:B:617:LEU:HD23	2:B:617:LEU:C	2.31	0.55
17:P:123:C:H2'	17:P:124:U:H6	1.70	0.55
29:r:504:ASP:HA	29:r:507:PHE:HD2	1.71	0.55
30:X:50:SER:HA	30:X:53:HIS:CD2	2.41	0.55
14:N:78:A:H5'	28:R:105:PRO:HG3	1.88	0.55
17:P:112:U:C2	17:P:113:U:C5	2.94	0.55
17:P:168:A:H1'	4:Z:27:ARG:NH1	2.22	0.55
30:X:461:ARG:HD3	30:X:545:GLY:H	1.71	0.55
30:X:1139:TYR:OH	30:X:1187:GLU:OE2	2.23	0.55
17:P:140:C:H2'	17:P:141:C:H6	1.71	0.55
20:Y:203:ARG:NH1	20:Y:257:ARG:NH1	2.55	0.55
28:R:288:LYS:NZ	29:r:578:GLN:CD	2.65	0.55
30:X:958:SER:O	30:X:961:THR:OG1	2.19	0.55
11:K:398:TRP:CE3	11:K:405:LYS:HB3	2.42	0.55
12:L:74:ILE:HD11	12:L:110:CYS:SG	2.46	0.55
14:N:15:U:C4	25:g:104:TYR:CD2	2.95	0.55
20:Y:55:GLU:CD	20:Y:56:THR:H	2.09	0.55
25:g:81:ILE:H	25:g:81:ILE:CD1	2.09	0.55
30:X:1142:GLN:HE22	30:X:1186:VAL:HG13	1.72	0.55
1:A:147:ILE:HD11	13:M:212:MET:CE	2.36	0.55
1:A:1843:LEU:N	1:A:1843:LEU:HD23	2.22	0.55
11:K:429:PHE:HA	11:K:435:ARG:O	2.07	0.55
14:N:22:A:O2'	14:N:23:A:OP1	2.21	0.55
17:P:102:U:N3	6:f:61:ARG:CD	2.70	0.55
20:Y:105:TYR:HD1	20:Y:106:THR:N	1.83	0.55
23:d:101:GLN:CD	25:g:67:LEU:HD11	2.31	0.55
29:r:612:LEU:HB3	29:r:632:LEU:HG	1.88	0.55
1:A:1850:VAL:CG1	1:A:1864:LYS:HZ2	2.19	0.55
14:N:77:G:N2	14:N:79:C:C4	2.73	0.55
24:e:29:ARG:CD	25:g:147:LEU:HD23	2.37	0.55
24:e:100:LEU:HD23	24:e:100:LEU:C	2.32	0.55
28:R:118:ARG:HE	33:x:309:UNK:CB	2.19	0.55
30:X:205:LYS:NZ	30:X:209:TYR:OH	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:253:THR:O	30:X:257:MET:HG2	2.07	0.55
30:X:534:ILE:HD12	30:X:606:LEU:HD22	1.89	0.55
30:X:1117:VAL:HA	30:X:1120:PHE:HD2	1.71	0.55
33:x:357:UNK:O	33:x:358:UNK:C	2.51	0.55
33:x:406:UNK:O	33:x:407:UNK:C	2.51	0.55
1:A:570:MET:CG	1:A:675:LEU:HD21	2.36	0.54
10:J:13:LEU:HD23	10:J:31:LEU:HD12	1.89	0.54
14:N:23:A:H2'	20:Y:119:TYR:CE1	2.41	0.54
17:P:104:G:C5'	7:l:104:ASP:OD1	2.55	0.54
21:a:245:HIS:O	21:a:248:LYS:HG3	2.07	0.54
29:r:645:ARG:HA	29:r:648:TYR:CD2	2.42	0.54
30:X:308:LEU:HA	30:X:311:PHE:HD2	1.73	0.54
30:X:735:ILE:HA	30:X:761:LEU:HD21	1.88	0.54
6:f:10:LEU:HD11	6:f:70:LEU:HD22	1.88	0.54
1:A:1298:TYR:O	1:A:1299:ARG:C	2.51	0.54
14:N:76:C:H5	14:N:77:G:C8	2.20	0.54
20:Y:164:GLY:O	20:Y:227:LYS:NZ	2.39	0.54
24:e:132:VAL:HG22	24:e:133:ARG:H	1.73	0.54
9:n:40:TYR:O	9:n:41:MET:HB2	2.06	0.54
1:A:724:ILE:O	1:A:724:ILE:HG22	2.05	0.54
14:N:82:U:O4	14:N:83:G:O6	2.25	0.54
17:P:97:U:C6	7:l:63:HIS:CD2	2.92	0.54
30:X:158:LEU:O	30:X:162:LYS:HG3	2.07	0.54
30:X:749:PRO:HG2	30:X:752:CYS:SG	2.46	0.54
4:Z:42:ARG:HE	4:Z:58:GLN:HE22	1.55	0.54
4:D:83:VAL:HG12	4:D:84:GLY:H	1.73	0.54
9:I:22:VAL:HG12	9:I:73:VAL:HA	1.90	0.54
13:M:185:ARG:HG2	25:g:92:GLU:HG2	1.89	0.54
17:P:133:A:C4	17:P:134:U:C5	2.95	0.54
29:r:639:TYR:CD1	29:r:639:TYR:C	2.86	0.54
2:B:82:GLU:O	2:B:86:GLY:N	2.41	0.54
2:B:294:ILE:HD13	2:B:314:PRO:HD3	1.88	0.54
4:D:61:ILE:HG22	4:D:62:ARG:N	2.22	0.54
12:L:201:ILE:CB	12:L:215:LEU:HG	2.37	0.54
13:M:183:TYR:CE2	13:M:203:LYS:HD2	2.42	0.54
17:P:103:U:O2	7:l:102:ARG:HG2	2.07	0.54
17:P:177:C:C5'	17:P:177:C:C6	2.88	0.54
20:Y:60:TYR:CD1	20:Y:62:MET:SD	3.01	0.54
25:g:157:TRP:O	25:g:158:ALA:O	2.26	0.54
30:X:562:ILE:HG23	30:X:583:ILE:HG12	1.90	0.54
30:X:731:GLN:O	30:X:734:SER:OG	2.14	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:805:LEU:HB3	30:X:962:ARG:NH1	2.23	0.54
11:K:256:HIS:CD2	11:K:257:PRO:HD2	2.43	0.54
12:L:235:LEU:HD11	12:L:284:VAL:HG22	1.88	0.54
12:L:315:HIS:HD1	12:L:315:HIS:C	2.16	0.54
17:P:171:G:H2'	17:P:172:G:C8	2.43	0.54
18:U:368:LEU:O	27:i:37:GLY:CA	2.55	0.54
20:Y:198:TRP:HZ3	20:Y:230:MET:CG	2.20	0.54
20:Y:262:LEU:CD1	21:a:98:ALA:CB	2.84	0.54
25:g:146:ILE:CG2	25:g:152:ALA:CA	2.86	0.54
29:r:495:UNK:HA	29:r:499:THR:HG21	1.89	0.54
1:A:1844:LYS:HG2	1:A:1938:MET:HE1	1.86	0.54
2:B:248:MET:HE1	2:B:851:HIS:NE2	2.22	0.54
20:Y:50:ALA:HB3	20:Y:129:SER:CB	2.37	0.54
20:Y:121:ALA:CB	20:Y:225:PHE:CE1	2.84	0.54
20:Y:278:PHE:C	20:Y:278:PHE:CD1	2.86	0.54
24:e:51:GLN:CG	25:g:157:TRP:CZ2	2.89	0.54
25:g:99:PHE:CD1	25:g:99:PHE:C	2.85	0.54
30:X:71:SER:O	30:X:72:LEU:HD23	2.07	0.54
30:X:962:ARG:O	30:X:965:THR:OG1	2.20	0.54
30:X:1100:THR:N	30:X:1108:GLN:O	2.25	0.54
10:o:13:LEU:HD23	10:o:31:LEU:HD12	1.89	0.54
1:A:792:LYS:O	1:A:793:THR:C	2.51	0.54
17:P:105:G:H5'	7:l:48:ARG:HH22	1.58	0.54
20:Y:99:ILE:HD12	20:Y:197:GLU:HB3	1.89	0.54
20:Y:262:LEU:HD13	20:Y:263:GLU:N	2.22	0.54
25:g:143:ASP:O	25:g:153:TYR:CB	2.49	0.54
25:g:146:ILE:CG2	25:g:148:GLU:O	2.56	0.54
2:B:846:TYR:CZ	2:B:891:VAL:HG22	2.43	0.54
12:L:242:THR:HG21	12:L:244:ARG:HH21	1.73	0.54
13:M:263:GLY:HA2	19:W:23:LYS:HE2	1.89	0.54
14:N:82:U:C5	14:N:83:G:N7	2.76	0.54
18:V:115:ILE:HD11	19:W:600:UNK:CB	2.38	0.54
20:Y:273:LEU:HD13	21:a:89:PHE:HA	1.89	0.54
25:g:157:TRP:HE3	25:g:157:TRP:H	1.56	0.54
28:R:131:VAL:HG13	28:R:141:TRP:CZ2	2.43	0.54
1:A:612:THR:O	1:A:613:GLY:C	2.50	0.54
1:A:1850:VAL:HG12	1:A:1864:LYS:NZ	2.22	0.54
13:M:198:LYS:O	13:M:199:GLN:HB2	2.07	0.54
18:S:86:GLU:CD	33:x:41:UNK:CA	2.72	0.54
20:Y:52:LYS:CE	20:Y:129:SER:CB	2.83	0.54
30:X:696:LEU:HB3	30:X:715:ARG:HH12	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:61:ILE:HG22	4:Z:62:ARG:N	2.22	0.54
1:A:699:ARG:NH2	14:N:64:A:OP2	2.39	0.53
1:A:760:ASN:O	1:A:761:MET:C	2.51	0.53
1:A:1810:TYR:HD1	1:A:1810:TYR:C	2.16	0.53
2:B:488:LEU:HD11	2:B:515:VAL:HG22	1.90	0.53
2:B:548:CYS:O	2:B:550:ARG:N	2.41	0.53
2:B:845:VAL:HG12	2:B:890:PRO:HA	1.90	0.53
19:W:69:LEU:HD22	19:W:87:VAL:CB	2.38	0.53
29:r:535:LYS:HA	29:r:538:GLU:CG	2.37	0.53
30:X:151:ILE:HG22	30:X:245:VAL:HG21	1.88	0.53
7:l:37:VAL:HG22	7:l:57:VAL:HB	1.90	0.53
2:B:267:LEU:HD13	2:B:269:LEU:HD21	1.91	0.53
3:C:34:U:H3'	3:C:35:A:H5''	1.89	0.53
14:N:60:C:H6	14:N:60:C:C5'	2.22	0.53
20:Y:137:LEU:HD22	20:Y:198:TRP:O	2.09	0.53
25:g:154:LYS:HG3	25:g:158:ALA:HA	1.89	0.53
30:X:104:PHE:O	30:X:108:VAL:HG23	2.09	0.53
30:X:191:LEU:HD23	30:X:194:LEU:HD11	1.90	0.53
30:X:563:CYS:SG	30:X:584:ASN:N	2.81	0.53
1:A:1007:VAL:O	1:A:1011:VAL:HG23	2.08	0.53
1:A:1490:GLN:HE21	1:A:1492:ASN:HB2	1.73	0.53
4:D:44:ILE:HD12	4:D:59:VAL:CG2	2.38	0.53
6:F:10:LEU:HD11	6:F:70:LEU:HD22	1.88	0.53
11:K:183:GLY:CA	11:K:207:THR:HG22	2.38	0.53
16:Q:499:U:O2	16:Q:499:U:H2'	2.07	0.53
21:a:264:ALA:O	21:a:268:PRO:CG	2.56	0.53
29:r:637:LEU:CD2	29:r:644:THR:OG1	2.57	0.53
29:r:643:ALA:O	29:r:646:THR:OG1	2.27	0.53
30:X:489:ALA:HB3	30:X:499:GLN:HB2	1.90	0.53
30:X:591:TYR:O	30:X:594:SER:OG	2.23	0.53
4:Z:44:ILE:HD12	4:Z:59:VAL:CG2	2.38	0.53
1:A:1287:TRP:CZ2	1:A:1291:LEU:HD13	2.43	0.53
1:A:1692:PHE:CG	1:A:1732:CYS:SG	3.02	0.53
12:L:235:LEU:HD13	12:L:275:VAL:HG12	1.90	0.53
14:N:76:C:C5	14:N:77:G:N9	2.77	0.53
18:S:89:GLU:OE2	33:x:41:UNK:N	2.42	0.53
28:R:146:TYR:CE2	33:x:393:UNK:CA	2.86	0.53
28:R:289:GLN:HA	29:r:539:ARG:NH2	2.23	0.53
30:X:343:SER:N	30:X:346:SER:OG	2.42	0.53
30:X:866:TRP:HB3	30:X:915:TYR:HE1	1.73	0.53
30:X:1200:PHE:HA	30:X:1203:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:252:THR:HG22	2:B:300:ASN:ND2	2.24	0.53
14:N:23:A:C2'	20:Y:119:TYR:CE1	2.92	0.53
17:P:164:C:H5'	17:P:164:C:C6	2.44	0.53
20:Y:65:GLU:O	20:Y:67:PRO:HD2	2.09	0.53
20:Y:278:PHE:HD2	21:a:141:ARG:CZ	2.21	0.53
28:R:288:LYS:HD3	29:r:538:GLU:CG	2.38	0.53
30:X:831:LEU:HD23	30:X:834:ILE:HD12	1.91	0.53
1:A:1565:THR:O	1:A:1568:ARG:HD3	2.08	0.53
4:D:44:ILE:HD12	4:D:59:VAL:HG21	1.90	0.53
12:L:219:LYS:CE	12:L:219:LYS:CA	2.86	0.53
14:N:76:C:C6	14:N:77:G:N9	2.73	0.53
14:N:78:A:C2	28:R:104:ILE:CG1	2.90	0.53
18:T:115:ILE:O	18:T:119:THR:HG23	2.08	0.53
19:W:729:LEU:HD21	27:i:159:VAL:HG13	1.89	0.53
20:Y:52:LYS:HE2	20:Y:129:SER:HB2	1.87	0.53
20:Y:225:PHE:O	20:Y:225:PHE:HD1	1.90	0.53
20:Y:233:GLN:O	20:Y:241:LEU:CD2	2.56	0.53
21:a:29:ASP:HB3	25:g:110:ILE:CD1	2.39	0.53
24:e:51:GLN:CD	25:g:157:TRP:CD1	2.87	0.53
29:r:564:TYR:O	29:r:566:GLY:N	2.35	0.53
1:A:668:VAL:HB	1:A:669:PRO:HD3	1.90	0.53
2:B:243:VAL:O	2:B:243:VAL:HG12	2.09	0.53
2:B:396:THR:OG1	2:B:397:ILE:N	2.42	0.53
16:Q:501:A:H5'	16:Q:502:C:O5'	2.09	0.53
25:g:97:PHE:CD1	25:g:97:PHE:C	2.86	0.53
30:X:370:PHE:CE2	30:X:374:LYS:HE3	2.44	0.53
30:X:461:ARG:HG2	30:X:545:GLY:HA3	1.91	0.53
9:n:22:VAL:HG12	9:n:73:VAL:HA	1.89	0.53
1:A:624:GLN:HG2	1:A:663:PHE:HB2	1.90	0.53
1:A:835:THR:HG21	26:h:230:VAL:HG11	1.91	0.53
1:A:970:PRO:C	1:A:972:PRO:HD2	2.34	0.53
1:A:1003:ARG:HB3	1:A:1197:ASP:HB3	1.91	0.53
4:Z:44:ILE:HD12	4:Z:59:VAL:HG21	1.90	0.53
1:A:1815:HIS:CD2	1:A:1825:LYS:CB	2.91	0.53
2:B:521:VAL:CG1	2:B:579:ILE:HG23	2.38	0.53
19:W:48:TRP:CE2	19:W:53:ASP:HB3	2.44	0.53
20:Y:278:PHE:HE1	20:Y:282:LEU:CD1	2.22	0.53
28:R:289:GLN:CA	29:r:539:ARG:NH2	2.72	0.53
30:X:194:LEU:HB3	30:X:198:TRP:NE1	2.23	0.53
30:X:480:LEU:HD12	30:X:611:ALA:C	2.34	0.53
30:X:529:LEU:O	30:X:615:SER:HB2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:819:THR:O	30:X:822:SER:OG	2.15	0.53
30:X:942:LEU:HD21	30:X:969:LYS:HD2	1.91	0.53
30:X:964:GLY:HA2	30:X:967:LYS:HD2	1.91	0.53
1:A:997:ASN:HB2	1:A:1203:TYR:HB3	1.91	0.53
7:G:37:VAL:HG22	7:G:57:VAL:HB	1.90	0.53
17:P:15:U:O2	17:P:15:U:O4'	2.22	0.53
30:X:39:VAL:O	30:X:42:SER:OG	2.21	0.53
30:X:388:ASN:HA	30:X:391:ASP:HB2	1.91	0.53
1:A:495:LEU:HD23	1:A:496:LEU:N	2.23	0.52
1:A:592:ILE:HG22	1:A:596:GLN:HB2	1.90	0.52
1:A:1522:TRP:O	1:A:1523:GLU:C	2.52	0.52
1:A:1810:TYR:OH	1:A:1857:LEU:CD1	2.57	0.52
1:A:1887:VAL:HG11	1:A:1892:MET:CB	2.39	0.52
4:D:42:ARG:HE	4:D:58:GLN:HE22	1.55	0.52
5:E:16:VAL:HG22	5:E:78:LEU:HD23	1.91	0.52
12:L:220:ASP:O	12:L:238:SER:HB2	2.08	0.52
20:Y:52:LYS:CE	20:Y:129:SER:HB3	2.39	0.52
20:Y:198:TRP:CH2	20:Y:230:MET:HA	2.45	0.52
24:e:129:ASP:OD1	25:g:111:TYR:HE2	1.91	0.52
30:X:46:LYS:O	30:X:49:LEU:HB2	2.08	0.52
30:X:465:ILE:HB	30:X:469:THR:OG1	2.08	0.52
1:A:783:ARG:NH1	1:A:789:THR:HG22	2.24	0.52
3:C:34:U:C3'	3:C:35:A:H5''	2.39	0.52
17:P:153:U:H2'	17:P:154:C:H6	1.74	0.52
18:U:461:SER:O	18:U:462:SER:CB	2.56	0.52
28:R:463:UNK:CB	33:x:88:UNK:CB	2.88	0.52
30:X:590:PHE:HA	30:X:593:HIS:HD2	1.73	0.52
31:j:20:GLU:CG	5:b:62:LYS:HZ1	2.20	0.52
1:A:778:HIS:HA	26:h:259:PHE:CE2	2.43	0.52
1:A:909:LEU:HD23	1:A:1027:ASN:ND2	2.24	0.52
1:A:973:LEU:HD11	1:A:1403:PHE:CD1	2.44	0.52
12:L:269:GLU:HG2	25:g:95:PRO:HD2	1.91	0.52
20:Y:52:LYS:HG3	20:Y:127:GLU:C	2.27	0.52
20:Y:60:TYR:CD1	20:Y:60:TYR:C	2.88	0.52
29:r:607:ARG:O	29:r:611:ILE:HG12	2.08	0.52
30:X:260:TYR:HB3	30:X:267:PHE:CE2	2.44	0.52
30:X:751:ARG:HG3	30:X:1177:ARG:HH11	1.75	0.52
31:j:42:VAL:CB	5:b:81:GLN:C	2.82	0.52
7:l:29:PRO:HB3	9:n:64:LEU:HD12	1.91	0.52
2:B:490:MET:HB2	2:B:579:ILE:HB	1.90	0.52
12:L:218:HIS:CE1	12:L:238:SER:HB3	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:c:480:MET:HE3	22:c:627:ARG:HB3	1.91	0.52
30:X:1137:THR:N	30:X:1167:GLY:O	2.34	0.52
1:A:168:MET:HE1	1:A:211:ILE:CG2	2.34	0.52
2:B:233:ILE:HG23	2:B:509:ARG:HB2	1.90	0.52
16:Q:499:U:H3'	16:Q:500:A:C5'	2.33	0.52
17:P:159:U:O2'	17:P:160:A:H5'	2.10	0.52
17:P:160:A:C2	17:P:161:U:C2	2.97	0.52
28:R:70:MET:HE2	28:R:100:ASP:HB3	1.92	0.52
30:X:111:VAL:O	30:X:114:SER:OG	2.27	0.52
1:A:691:VAL:O	1:A:692:ALA:HB2	2.09	0.52
1:A:695:ILE:HG22	1:A:696:THR:N	2.24	0.52
1:A:1816:LYS:N	1:A:1816:LYS:CE	2.73	0.52
2:B:117:GLU:HG2	2:B:499:VAL:HG21	1.92	0.52
11:K:151:ALA:HB1	11:K:152:PRO:CD	2.39	0.52
12:L:215:LEU:HD23	12:L:215:LEU:H	1.73	0.52
20:Y:69:GLN:NE2	20:Y:69:GLN:CA	2.73	0.52
25:g:146:ILE:N	25:g:146:ILE:CD1	2.73	0.52
1:A:112:ALA:O	1:A:113:LEU:C	2.53	0.52
1:A:740:TRP:CE2	1:A:769:LYS:HD3	2.44	0.52
1:A:1810:TYR:C	1:A:1810:TYR:CD1	2.85	0.52
12:L:193:PHE:CE1	12:L:227:ILE:HD11	2.44	0.52
12:L:261:PHE:HB3	12:L:296:TRP:CZ2	2.45	0.52
14:N:26:U:O4	20:Y:244:ARG:NE	2.27	0.52
17:P:171:G:H8	17:P:171:G:O5'	1.91	0.52
30:X:74:HIS:CE1	30:X:77:LEU:HD12	2.45	0.52
30:X:360:PHE:HD2	30:X:366:ILE:HG12	1.74	0.52
30:X:414:LEU:H	30:X:416:ASN:ND2	2.08	0.52
5:b:16:VAL:HG22	5:b:78:LEU:HD23	1.91	0.52
2:B:248:MET:HE1	2:B:851:HIS:CD2	2.45	0.52
2:B:846:TYR:HB3	2:B:915:PHE:HA	1.92	0.52
14:N:38:G:HO2'	15:O:102:A:N6	2.07	0.52
14:N:78:A:C2	28:R:104:ILE:CB	2.93	0.52
21:a:22:ILE:CG2	21:a:27:LEU:HD13	2.37	0.52
24:e:60:ILE:HD12	24:e:84:ALA:HB2	1.91	0.52
30:X:1091:VAL:HG13	30:X:1094:PHE:HE2	1.74	0.52
17:P:105:G:N2	17:P:106:U:N3	2.55	0.52
20:Y:219:ASN:HB2	20:Y:222:ASN:HD22	1.74	0.52
20:Y:280:LEU:O	20:Y:284:GLU:CG	2.51	0.52
24:e:51:GLN:CG	25:g:157:TRP:CD1	2.85	0.52
25:g:138:ARG:HG3	25:g:138:ARG:NH1	2.25	0.52
28:R:110:TYR:CE2	28:R:126:LEU:HD21	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:532:ILE:HG21	30:X:610:PHE:HB3	1.92	0.52
1:A:126:ASN:O	1:A:135:ARG:NH2	2.43	0.52
1:A:620:ARG:O	1:A:622:MET:N	2.42	0.52
1:A:1817:THR:HB	1:A:1820:GLY:HA2	1.90	0.52
2:B:147:ALA:C	2:B:154:LYS:HD3	2.35	0.52
2:B:608:PRO:HD3	2:B:617:LEU:HD13	1.91	0.52
2:B:811:ALA:O	2:B:817:ARG:NH2	2.41	0.52
3:C:32:C:O2	3:C:32:C:H3'	2.10	0.52
17:P:103:U:H3	7:l:65:ASN:HD21	1.56	0.52
17:P:104:G:N7	7:l:104:ASP:HB3	2.24	0.52
17:P:135:G:C2'	17:P:136:C:O4'	2.57	0.52
30:X:732:LEU:O	30:X:736:LEU:HG	2.10	0.52
1:A:1819:GLU:N	1:A:1820:GLY:HA2	2.24	0.51
12:L:221:ILE:HD12	12:L:239:MET:HG3	1.93	0.51
30:X:1049:ARG:HH12	30:X:1078:GLY:HA2	1.75	0.51
1:A:1215:THR:OG1	1:A:1216:GLY:N	2.43	0.51
29:r:607:ARG:O	29:r:610:SER:OG	2.18	0.51
1:A:537:THR:HG22	20:Y:70:VAL:CG1	2.36	0.51
11:K:201:LEU:HD13	11:K:232:TRP:CE3	2.45	0.51
11:K:361:GLU:HA	13:M:116:LEU:HD22	1.92	0.51
19:W:92:THR:HA	19:W:95:LEU:HD12	1.91	0.51
19:W:18:LYS:HB2	19:W:52:ILE:HD11	1.92	0.51
20:Y:68:GLY:C	20:Y:69:GLN:HE21	2.18	0.51
20:Y:176:LEU:CD2	20:Y:227:LYS:HB2	2.40	0.51
30:X:74:HIS:ND1	30:X:77:LEU:HB2	2.23	0.51
30:X:172:THR:HA	30:X:175:PHE:CZ	2.45	0.51
30:X:497:LEU:HD21	30:X:593:HIS:NE2	2.26	0.51
1:A:614:MET:O	1:A:616:ARG:N	2.44	0.51
1:A:1287:TRP:CE3	1:A:1319:ILE:HD12	2.45	0.51
7:G:29:PRO:HB3	9:I:64:LEU:HD12	1.91	0.51
17:P:102:U:O4	5:b:35:MET:HG3	2.11	0.51
29:r:629:ASN:O	29:r:633:VAL:HG23	2.10	0.51
30:X:136:ILE:HB	30:X:139:LEU:HD12	1.91	0.51
30:X:727:TYR:HB3	30:X:731:GLN:HB2	1.93	0.51
30:X:769:SER:HB2	30:X:772:ASP:HB2	1.92	0.51
30:X:1227:GLU:HA	30:X:1230:TRP:HD1	1.76	0.51
1:A:1409:VAL:CG1	1:A:1443:ILE:HD11	2.40	0.51
1:A:1819:GLU:N	1:A:1820:GLY:CA	2.73	0.51
2:B:158:LEU:HD13	2:B:198:LEU:HD12	1.93	0.51
4:D:41:MET:HB2	4:D:44:ILE:HD11	1.93	0.51
5:E:115:VAL:HG13	25:g:94:VAL:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:48:ALA:HB3	9:I:63:ILE:HD12	1.93	0.51
15:O:100:G:N3	15:O:100:G:C2'	2.73	0.51
20:Y:233:GLN:O	20:Y:241:LEU:HD23	2.11	0.51
30:X:251:PHE:CE2	30:X:255:LEU:HD11	2.46	0.51
30:X:817:TYR:CE1	30:X:937:TYR:HB3	2.46	0.51
1:A:100:ARG:HD2	14:N:24:A:N9	2.25	0.51
25:g:153:TYR:C	25:g:153:TYR:CD1	2.86	0.51
27:i:85:PRO:CB	27:i:86:PRO:HD2	2.40	0.51
29:r:541:VAL:HG21	29:r:553:TRP:HE3	1.76	0.51
1:A:1843:LEU:CD2	1:A:1843:LEU:N	2.73	0.51
11:K:216:ARG:C	26:h:38:ARG:HG3	2.36	0.51
1:A:583:SER:O	1:A:597:LEU:HD12	2.11	0.51
11:K:169:VAL:CG2	11:K:180:THR:HG22	2.41	0.51
18:S:86:GLU:OE1	33:x:41:UNK:CA	2.59	0.51
30:X:590:PHE:HA	30:X:593:HIS:CD2	2.46	0.51
30:X:1109:ASN:HB3	30:X:1112:GLU:HB2	1.92	0.51
1:A:1237:VAL:HG12	1:A:1253:PHE:HA	1.93	0.51
1:A:1297:TYR:CD2	1:A:1298:TYR:CE1	2.99	0.51
1:A:1825:LYS:HG3	1:A:1826:PRO:N	2.26	0.51
2:B:124:THR:O	2:B:126:TYR:N	2.43	0.51
2:B:231:MET:HE1	2:B:258:ALA:HA	1.93	0.51
2:B:239:LEU:HD11	2:B:255:ILE:HG13	1.93	0.51
12:L:221:ILE:CB	12:L:239:MET:HG3	2.40	0.51
18:T:31:VAL:HG22	18:U:85:LEU:HD11	1.93	0.51
20:Y:50:ALA:HB2	20:Y:129:SER:HA	1.78	0.51
29:r:643:ALA:HA	29:r:646:THR:OG1	2.11	0.51
30:X:827:LEU:HD21	30:X:928:ILE:HG21	1.92	0.51
31:j:42:VAL:O	5:b:81:GLN:OE1	2.29	0.51
1:A:979:CYS:SG	1:A:1219:VAL:HG11	2.50	0.50
3:C:93:A:O2'	3:C:94:U:OP2	2.27	0.50
17:P:136:C:O2	17:P:136:C:H2'	2.10	0.50
17:P:159:U:C2'	17:P:160:A:H8	2.11	0.50
19:W:21:VAL:HG21	19:W:48:TRP:CZ3	2.47	0.50
28:R:110:TYR:CD2	28:R:126:LEU:HD21	2.46	0.50
30:X:701:THR:OG1	30:X:714:ASP:O	2.19	0.50
30:X:820:LEU:HA	30:X:823:TRP:CD1	2.46	0.50
1:A:316:ASN:HD22	1:A:317:ASP:H	1.59	0.50
11:K:157:ARG:NH2	11:K:193:ALA:O	2.45	0.50
20:Y:198:TRP:CZ3	20:Y:230:MET:CG	2.93	0.50
25:g:156:PRO:CG	25:g:157:TRP:CE3	2.90	0.50
27:i:173:LEU:HD13	27:i:173:LEU:C	2.36	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:r:535:LYS:HA	29:r:538:GLU:HG3	1.94	0.50
30:X:120:VAL:HG11	30:X:124:ILE:HD11	1.93	0.50
30:X:677:LEU:HD13	30:X:715:ARG:HH22	1.75	0.50
30:X:1115:TYR:HB2	30:X:1266:LEU:HD23	1.93	0.50
20:Y:195:PHE:CZ	20:Y:230:MET:HE3	2.43	0.50
30:X:58:PHE:HA	30:X:62:LEU:HB2	1.93	0.50
30:X:120:VAL:HG11	30:X:124:ILE:CD1	2.42	0.50
30:X:823:TRP:CE3	30:X:928:ILE:HG12	2.46	0.50
30:X:924:GLN:O	30:X:928:ILE:HG13	2.12	0.50
7:G:111:ARG:NH2	9:I:64:LEU:HD13	2.26	0.50
12:L:92:CYS:SG	12:L:118:MET:HG3	2.50	0.50
13:M:270:LYS:NZ	33:x:372:UNK:CA	2.69	0.50
20:Y:50:ALA:HB1	20:Y:128:GLY:C	2.37	0.50
20:Y:52:LYS:N	20:Y:52:LYS:CD	2.73	0.50
21:a:60:ARG:NH2	25:g:107:THR:CG2	2.75	0.50
24:e:51:GLN:CA	25:g:157:TRP:CZ2	2.91	0.50
30:X:202:LEU:HD13	30:X:225:ILE:HG12	1.93	0.50
30:X:749:PRO:HD2	30:X:1042:LEU:HB2	1.93	0.50
30:X:773:ARG:NH2	30:X:947:GLN:HA	2.27	0.50
30:X:1115:TYR:O	30:X:1119:LEU:HG	2.11	0.50
1:A:1392:LEU:CD2	1:A:1491:LEU:HD21	2.41	0.50
1:A:1526:PHE:O	1:A:1777:LEU:HD12	2.11	0.50
11:K:114:UNK:HA	28:R:225:GLN:HE21	1.77	0.50
11:K:231:CYS:O	11:K:232:TRP:C	2.54	0.50
18:U:228:LEU:HB3	18:U:231:ASP:CG	2.36	0.50
19:W:35:LEU:C	19:W:35:LEU:HD23	2.36	0.50
30:X:202:LEU:O	30:X:205:LYS:HB3	2.11	0.50
30:X:401:VAL:HG11	30:X:446:LEU:HD22	1.93	0.50
30:X:430:ILE:O	30:X:434:MET:HG2	2.11	0.50
30:X:892:GLY:HA2	30:X:898:PRO:HG3	1.92	0.50
30:X:1197:PRO:HA	30:X:1200:PHE:HD2	1.77	0.50
1:A:1810:TYR:OH	1:A:1857:LEU:HD11	2.11	0.50
1:A:1851:TRP:HH2	1:A:1861:ALA:HA	1.75	0.50
12:L:193:PHE:CD2	12:L:234:LEU:HD11	2.47	0.50
13:M:260:ASN:C	13:M:260:ASN:HD22	2.19	0.50
13:M:261:PRO:HA	14:N:42:A:C5	2.46	0.50
17:P:104:G:H1	6:f:20:LYS:HG3	1.73	0.50
18:S:109:ASP:HA	18:S:112:LEU:HD22	1.92	0.50
18:U:51:VAL:HG11	18:V:15:ILE:HD11	1.93	0.50
30:X:17:SER:OG	30:X:18:ASN:N	2.43	0.50
30:X:539:GLU:HB3	30:X:543:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:41:MET:HB2	4:Z:44:ILE:HD11	1.93	0.50
3:C:70:G:H2'	3:C:71:U:O4'	2.12	0.50
5:E:106:ARG:CZ	12:L:306:LEU:HD13	2.42	0.50
14:N:8:G:H3'	14:N:9:G:H5'	1.93	0.50
18:S:125:ALA:HB1	18:V:125:ALA:HB1	1.92	0.50
18:V:87:GLN:HE21	18:V:87:GLN:C	2.20	0.50
20:Y:266:ALA:HB2	21:a:95:LEU:HD23	1.93	0.50
21:a:271:ASN:CG	21:a:272:VAL:H	2.20	0.50
30:X:303:TYR:HE1	30:X:381:TYR:HD1	1.59	0.50
30:X:1114:GLU:HA	30:X:1149:ILE:HD13	1.93	0.50
30:X:1117:VAL:HG21	30:X:1149:ILE:HB	1.93	0.50
31:j:101:GLU:HG2	31:j:127:LYS:HZ1	1.77	0.50
2:B:545:CYS:SG	2:B:554:HIS:ND1	2.85	0.50
8:H:68:LEU:HD22	9:I:72:TRP:CH2	2.47	0.50
11:K:187:ILE:HG12	11:K:211:LEU:HD21	1.93	0.50
19:W:172:ASN:HD22	19:W:174:GLN:H	1.58	0.50
28:R:289:GLN:CB	29:r:539:ARG:HH21	2.18	0.50
30:X:404:GLU:HB2	30:X:450:TYR:OH	2.11	0.50
30:X:977:ILE:HG23	30:X:1006:VAL:HB	1.93	0.50
30:X:1244:THR:O	30:X:1280:ARG:NH2	2.35	0.50
1:A:510:ILE:HD12	1:A:514:GLU:HG2	1.93	0.50
2:B:104:PRO:O	2:B:105:ILE:CB	2.58	0.50
20:Y:235:LEU:HG	20:Y:241:LEU:HD11	1.92	0.50
30:X:75:ILE:C	30:X:77:LEU:N	2.69	0.50
30:X:750:THR:HB	30:X:1177:ARG:NH1	2.27	0.50
30:X:844:PRO:HD2	30:X:861:TYR:HE1	1.77	0.50
30:X:1087:GLN:HE21	30:X:1240:LEU:HA	1.76	0.50
9:n:40:TYR:O	9:n:67:CYS:SG	2.58	0.50
1:A:1815:HIS:NE2	1:A:1825:LYS:CB	2.69	0.49
14:N:73:C:C1'	14:N:74:U:N3	2.75	0.49
18:U:239:GLN:O	18:U:240:SER:CB	2.60	0.49
30:X:45:ALA:O	30:X:49:LEU:HG	2.11	0.49
30:X:214:LYS:NZ	30:X:259:LEU:H	2.10	0.49
30:X:1134:VAL:HG22	30:X:1164:ALA:HB3	1.94	0.49
1:A:146:ALA:O	1:A:147:ILE:HG23	2.12	0.49
1:A:377:PRO:O	1:A:378:ILE:HG22	2.13	0.49
1:A:440:ALA:O	1:A:441:THR:CB	2.60	0.49
1:A:754:LEU:HD11	1:A:759:GLU:HG2	1.94	0.49
9:I:40:TYR:O	9:I:42:ASN:N	2.45	0.49
13:M:189:SER:CB	25:g:86:THR:O	2.60	0.49
13:M:270:LYS:HZ3	33:x:372:UNK:HA	1.73	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:135:G:N2	17:P:136:C:C2	2.80	0.49
18:U:296:GLU:CG	18:U:316:GLU:N	2.76	0.49
25:g:143:ASP:N	25:g:153:TYR:CD1	2.78	0.49
30:X:222:LEU:HD23	30:X:225:ILE:HD12	1.93	0.49
30:X:330:GLN:O	30:X:383:ARG:NE	2.45	0.49
30:X:504:GLN:HG2	30:X:563:CYS:SG	2.52	0.49
30:X:1046:TYR:O	30:X:1066:THR:OG1	2.30	0.49
30:X:1059:ILE:HG21	30:X:1201:TYR:OH	2.12	0.49
1:A:1390:PRO:HG2	1:A:1498:VAL:HG22	1.94	0.49
2:B:326:LEU:HD22	2:B:428:LEU:HB3	1.94	0.49
18:S:95:THR:HG21	18:U:58:PHE:CE1	2.48	0.49
20:Y:267:ALA:CB	21:a:147:VAL:HG21	2.42	0.49
21:a:32:TYR:HB3	25:g:99:PHE:CZ	2.47	0.49
30:X:239:ARG:HA	30:X:242:ALA:HB3	1.93	0.49
30:X:831:LEU:HA	30:X:834:ILE:HD12	1.94	0.49
30:X:930:PRO:HA	30:X:933:LEU:HD12	1.94	0.49
1:A:207:PRO:O	1:A:208:LEU:HB3	2.13	0.49
1:A:1004:LEU:HB2	1:A:1007:VAL:CG2	2.42	0.49
1:A:1816:LYS:H	1:A:1816:LYS:CD	2.25	0.49
2:B:114:ILE:CG1	2:B:661:LEU:HD11	2.43	0.49
16:Q:500:A:C1'	16:Q:501:A:P	3.00	0.49
17:P:103:U:N3	7:l:102:ARG:NH1	2.60	0.49
17:P:104:G:P	9:n:68:ASN:HD21	2.35	0.49
17:P:166:C:N4	32:k:85:SER:HA	2.28	0.49
18:U:408:SER:HB2	27:i:35:ARG:HG2	1.92	0.49
25:g:146:ILE:CG2	25:g:152:ALA:N	2.74	0.49
30:X:63:TRP:HE3	30:X:100:ARG:NH2	2.09	0.49
30:X:204:ILE:HD11	30:X:364:TYR:HD1	1.77	0.49
7:l:111:ARG:NH2	9:n:64:LEU:HD13	2.26	0.49
1:A:1661:TRP:CE3	1:A:1743:ILE:HD13	2.47	0.49
12:L:154:VAL:HG12	12:L:180:LEU:CB	2.42	0.49
18:T:90:LEU:HD21	18:U:94:LEU:HD12	1.95	0.49
21:a:133:SER:HB3	25:g:78:GLN:HE21	1.77	0.49
30:X:191:LEU:HA	30:X:194:LEU:HG	1.95	0.49
9:n:48:ALA:HB3	9:n:63:ILE:HD12	1.93	0.49
1:A:1037:ASN:O	1:A:1049:ASN:HB3	2.12	0.49
14:N:78:A:H5''	28:R:105:PRO:HA	1.93	0.49
14:N:82:U:O5'	14:N:82:U:H6	1.95	0.49
24:e:59:TYR:HA	25:g:144:PRO:HB2	1.95	0.49
30:X:36:LEU:HD21	30:X:74:HIS:CB	2.39	0.49
30:X:120:VAL:O	30:X:122:TYR:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:240:ARG:HG2	30:X:284:ASN:O	2.12	0.49
1:A:570:MET:HG2	1:A:675:LEU:HD21	1.95	0.49
1:A:673:ARG:O	1:A:677:ASN:HB2	2.13	0.49
1:A:798:ASN:CG	1:A:798:ASN:O	2.55	0.49
1:A:1264:PHE:CG	1:A:1294:LEU:HD13	2.48	0.49
1:A:1816:LYS:N	1:A:1816:LYS:CD	2.75	0.49
1:A:1844:LYS:HB3	1:A:1844:LYS:HZ2	1.73	0.49
2:B:389:LEU:O	2:B:392:LEU:N	2.45	0.49
13:M:189:SER:OG	25:g:82:LYS:CD	2.60	0.49
14:N:77:G:H4'	14:N:78:A:OP1	2.13	0.49
30:X:73:ASN:H	30:X:73:ASN:HD22	1.56	0.49
30:X:160:LYS:NZ	30:X:356:LEU:O	2.38	0.49
30:X:638:PHE:CG	30:X:639:PRO:HD2	2.48	0.49
31:j:65:LEU:HD21	31:j:68:LEU:HG	1.94	0.49
2:B:389:LEU:O	2:B:390:TYR:C	2.56	0.49
5:E:115:VAL:O	25:g:94:VAL:CG1	2.61	0.49
11:K:275:ASP:O	11:K:276:MET:C	2.56	0.49
14:N:78:A:C2	28:R:104:ILE:HB	2.47	0.49
1:A:586:GLN:HB3	1:A:592:ILE:HD11	1.94	0.49
1:A:833:TYR:O	1:A:837:VAL:HG23	2.13	0.49
1:A:974:LEU:HD12	1:A:1214:MET:SD	2.53	0.49
11:K:425:PHE:CE2	11:K:441:ALA:HB2	2.48	0.49
14:N:25:U:O2	20:Y:232:HIS:HE1	1.95	0.49
14:N:74:U:O2	14:N:74:U:H3'	2.12	0.49
20:Y:49:PRO:HD2	20:Y:49:PRO:O	2.12	0.49
20:Y:164:GLY:C	20:Y:227:LYS:HZ1	2.20	0.49
21:a:19:PHE:HB2	21:a:20:PRO:CD	2.43	0.49
25:g:151:GLY:C	25:g:152:ALA:O	2.56	0.49
29:r:649:GLU:C	29:r:652:ILE:HD12	2.38	0.49
10:o:42:LEU:HD12	10:o:62:ILE:HD11	1.95	0.49
1:A:85:GLU:HG3	24:e:30:MET:HE2	1.94	0.49
1:A:265:LEU:HD13	1:A:434:PHE:CE2	2.47	0.49
1:A:692:ALA:HB3	11:K:244:HIS:NE2	2.27	0.49
1:A:791:ASP:O	1:A:792:LYS:C	2.55	0.49
1:A:985:LEU:HB2	1:A:988:VAL:CG2	2.43	0.49
29:r:554:ASN:O	29:r:558:THR:HG23	2.12	0.49
1:A:244:TYR:O	1:A:441:THR:HG21	2.13	0.48
1:A:1825:LYS:CD	22:c:418:TYR:HE2	2.20	0.48
11:K:188:LYS:HD3	11:K:197:LEU:HD21	1.94	0.48
14:N:24:A:C4	20:Y:60:TYR:HE2	2.19	0.48
15:O:102:A:H2'	15:O:102:A:N3	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:U:375:SER:O	18:U:376:SER:CB	2.60	0.48
20:Y:52:LYS:CE	20:Y:129:SER:HB2	2.43	0.48
20:Y:66:GLN:HE21	20:Y:66:GLN:C	2.21	0.48
20:Y:286:LYS:HA	20:Y:289:LYS:HD2	1.95	0.48
20:Y:304:UNK:O	23:d:110:PRO:HB2	2.13	0.48
30:X:741:PRO:HA	30:X:1004:ARG:CG	2.43	0.48
30:X:902:TYR:HB3	30:X:906:ASN:HD22	1.78	0.48
1:A:569:LEU:HD22	1:A:573:ILE:HD12	1.95	0.48
1:A:1491:LEU:O	1:A:1492:ASN:C	2.56	0.48
1:A:1898:VAL:O	1:A:1901:LEU:HD22	2.13	0.48
2:B:683:THR:HG22	2:B:704:GLU:HG2	1.95	0.48
11:K:295:LEU:HD23	11:K:305:VAL:O	2.12	0.48
30:X:558:THR:O	30:X:585:VAL:HG13	2.13	0.48
30:X:1047:ASN:HA	30:X:1069:SER:HA	1.95	0.48
5:b:37:LEU:HD11	5:b:78:LEU:HD21	1.95	0.48
1:A:208:LEU:C	24:e:8:ARG:HH11	2.19	0.48
2:B:835:LEU:HD13	2:B:964:THR:HB	1.95	0.48
3:C:34:U:H3'	3:C:35:A:C5'	2.42	0.48
4:D:16:VAL:HG21	4:D:30:LEU:HD12	1.95	0.48
11:K:169:VAL:HG23	11:K:180:THR:HG22	1.95	0.48
18:S:20:GLY:CA	18:T:53:VAL:HG12	2.43	0.48
29:r:309:UNK:CB	30:X:329:LEU:CD2	2.91	0.48
30:X:8:LYS:HA	30:X:11:ILE:HD12	1.95	0.48
30:X:872:THR:OG1	30:X:884:ARG:HB3	2.13	0.48
30:X:1095:LYS:HD2	30:X:1111:GLY:HA3	1.96	0.48
30:X:1109:ASN:ND2	30:X:1112:GLU:OE1	2.45	0.48
30:X:1266:LEU:HG	30:X:1269:LEU:HD12	1.95	0.48
1:A:1238:TRP:CH2	1:A:1254:ILE:CD1	2.97	0.48
2:B:78:TYR:CD1	11:K:416:GLY:HA2	2.48	0.48
3:C:60:A:H2'	3:C:61:C:O4'	2.13	0.48
5:E:37:LEU:HD11	5:E:78:LEU:HD21	1.95	0.48
10:J:13:LEU:HD23	10:J:31:LEU:CD1	2.43	0.48
18:V:30:GLN:OE1	33:x:47:UNK:CB	2.61	0.48
22:c:486:LEU:HD21	22:c:509:PRO:HB2	1.95	0.48
29:r:648:TYR:O	29:r:651:ALA:HB3	2.12	0.48
30:X:414:LEU:O	30:X:416:ASN:N	2.47	0.48
30:X:1086:VAL:HA	30:X:1211:LEU:O	2.13	0.48
1:A:741:ARG:HB3	13:M:258:TRP:CZ2	2.48	0.48
1:A:826:ALA:O	1:A:830:VAL:HG23	2.14	0.48
1:A:1563:SER:N	1:A:1564:PRO:CD	2.77	0.48
25:g:156:PRO:HD2	25:g:157:TRP:CZ3	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ASP:HB2	1:A:507:SER:O	2.14	0.48
2:B:114:ILE:HG13	2:B:661:LEU:HD11	1.95	0.48
2:B:119:THR:OG1	2:B:120:ASN:ND2	2.47	0.48
28:R:148:GLU:HB3	28:R:157:CYS:SG	2.54	0.48
30:X:453:LEU:HD21	30:X:533:TYR:CG	2.49	0.48
30:X:519:ASP:HA	30:X:522:ASN:ND2	2.28	0.48
30:X:562:ILE:HA	30:X:583:ILE:HG12	1.93	0.48
31:j:42:VAL:CA	5:b:81:GLN:CG	2.88	0.48
31:j:64:ARG:NH2	5:b:25:VAL:HG21	2.28	0.48
4:Z:16:VAL:HG21	4:Z:30:LEU:HD12	1.95	0.48
1:A:495:LEU:HD23	1:A:495:LEU:C	2.38	0.48
1:A:668:VAL:HG12	1:A:669:PRO:N	2.28	0.48
1:A:1784:GLU:O	1:A:1785:GLN:C	2.56	0.48
3:C:55:C:H2'	3:C:56:A:H5'	1.94	0.48
12:L:331:ASP:OD1	25:g:93:TYR:CD2	2.66	0.48
16:Q:502:C:N4	16:Q:503:A:N6	2.60	0.48
17:P:136:C:C4	17:P:137:U:C4	3.02	0.48
18:T:69:LEU:HB2	18:T:70:PRO:HD3	1.95	0.48
22:c:435:VAL:HG23	22:c:473:PHE:CE2	2.48	0.48
29:r:645:ARG:HA	29:r:648:TYR:CE2	2.48	0.48
30:X:75:ILE:O	30:X:78:THR:N	2.47	0.48
8:m:68:LEU:HD22	9:n:72:TRP:CH2	2.47	0.48
10:o:13:LEU:HD23	10:o:31:LEU:CD1	2.44	0.48
1:A:886:GLU:O	1:A:890:VAL:HG23	2.13	0.48
2:B:74:ASP:O	2:B:75:LYS:C	2.57	0.48
2:B:747:TRP:HB2	2:B:759:LEU:HB2	1.96	0.48
2:B:851:HIS:O	2:B:909:ALA:HA	2.13	0.48
17:P:104:G:C5	6:f:20:LYS:CE	2.97	0.48
20:Y:262:LEU:CD1	21:a:98:ALA:HB1	2.42	0.48
29:r:568:HIS:CD2	29:r:571:ARG:HB3	2.47	0.48
30:X:105:PHE:O	30:X:108:VAL:HB	2.13	0.48
30:X:1241:LEU:HB3	30:X:1260:THR:HB	1.96	0.48
30:X:1274:VAL:HG13	30:X:1278:LYS:HD2	1.95	0.48
1:A:437:ARG:O	1:A:438:SER:CB	2.62	0.48
1:A:1784:GLU:OE1	1:A:1907:THR:HB	2.14	0.48
1:A:1817:THR:HB	1:A:1820:GLY:C	2.38	0.48
10:J:42:LEU:HD12	10:J:62:ILE:HD11	1.95	0.48
11:K:305:VAL:HG12	11:K:337:LEU:CD1	2.41	0.48
14:N:29:A:C8	20:Y:75:TYR:OH	2.61	0.48
18:U:482:GLY:O	18:U:483:ALA:HB3	2.13	0.48
28:R:77:GLY:HA3	28:R:93:PHE:CZ	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:r:605:ALA:O	29:r:608:SER:OG	2.22	0.48
1:A:608:VAL:HG11	1:A:660:TRP:CZ2	2.49	0.48
1:A:1802:LEU:HD22	1:A:1833:ILE:CG2	2.44	0.48
1:A:1960:LEU:HD12	1:A:1960:LEU:C	2.39	0.48
6:F:7:LEU:HD12	6:F:36:MET:HE1	1.96	0.48
28:R:48:LEU:C	28:R:48:LEU:HD12	2.39	0.48
30:X:869:TYR:HB3	30:X:884:ARG:O	2.14	0.48
30:X:917:GLU:HA	30:X:920:TYR:HD2	1.78	0.48
30:X:1124:ARG:HH12	30:X:1163:PRO:HD3	1.78	0.48
1:A:208:LEU:HD23	1:A:209:GLU:O	2.14	0.47
1:A:1409:VAL:HG12	1:A:1443:ILE:HD11	1.95	0.47
1:A:1669:LEU:HD21	1:A:1742:TRP:CH2	2.49	0.47
2:B:121:VAL:HG13	2:B:122:PRO:HD2	1.96	0.47
2:B:267:LEU:HD11	2:B:297:VAL:HG21	1.96	0.47
28:R:234:LEU:HD23	28:R:239:LEU:HA	1.96	0.47
30:X:62:LEU:HD13	30:X:78:THR:HG22	1.96	0.47
30:X:555:THR:HB	30:X:557:PHE:CE1	2.49	0.47
30:X:601:TYR:HB2	30:X:603:PRO:HD3	1.95	0.47
1:A:437:ARG:O	1:A:438:SER:OG	2.23	0.47
1:A:1133:ILE:HG22	1:A:1137:LEU:HD12	1.94	0.47
1:A:1816:LYS:CE	1:A:1816:LYS:H	2.28	0.47
5:E:68:VAL:HG12	5:E:70:LEU:HD23	1.96	0.47
11:K:183:GLY:HA3	11:K:207:THR:HG22	1.96	0.47
20:Y:105:TYR:CD1	20:Y:105:TYR:C	2.86	0.47
20:Y:273:LEU:HD11	21:a:89:PHE:CA	2.43	0.47
21:a:232:PHE:CD2	21:a:252:VAL:HG11	2.49	0.47
25:g:147:LEU:CB	25:g:148:GLU:OE1	2.62	0.47
28:R:214:GLU:HB3	28:R:223:VAL:HG22	1.96	0.47
29:r:573:ARG:NE	29:r:595:TYR:OH	2.48	0.47
1:A:243:THR:HG23	3:C:18:U:H5''	1.97	0.47
1:A:289:ASN:ND2	1:A:289:ASN:O	2.47	0.47
2:B:252:THR:OG1	2:B:253:ARG:N	2.48	0.47
2:B:817:ARG:HB3	2:B:822:ILE:HD11	1.97	0.47
11:K:395:MET:HE1	11:K:448:TYR:OH	2.14	0.47
18:T:132:PHE:CZ	18:U:132:PHE:HB3	2.49	0.47
18:V:85:LEU:HD12	27:i:93:LEU:HD13	1.96	0.47
20:Y:105:TYR:CD1	20:Y:106:THR:O	2.59	0.47
30:X:214:LYS:HZ3	30:X:259:LEU:H	1.62	0.47
30:X:532:ILE:HB	30:X:557:PHE:CE2	2.49	0.47
1:A:1494:TYR:O	1:A:1498:VAL:HG23	2.14	0.47
2:B:335:PHE:O	2:B:338:LEU:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:391:LYS:O	2:B:395:LEU:N	2.46	0.47
2:B:848:VAL:HA	2:B:912:GLN:O	2.14	0.47
18:U:299:ASN:CG	18:U:336:ILE:O	2.57	0.47
20:Y:72:ASN:O	20:Y:74:TRP:N	2.46	0.47
24:e:51:GLN:CB	25:g:157:TRP:NE1	2.77	0.47
30:X:68:THR:O	30:X:107:LYS:NZ	2.43	0.47
30:X:162:LYS:HA	30:X:165:LEU:HG	1.95	0.47
30:X:755:HIS:CE1	30:X:979:MET:HE2	2.50	0.47
30:X:1086:VAL:HG22	30:X:1211:LEU:HB2	1.96	0.47
1:A:745:ALA:O	1:A:746:ASN:CB	2.63	0.47
3:C:79:G:O2'	3:C:82:A:N3	2.39	0.47
17:P:122:U:H2'	17:P:123:C:C6	2.50	0.47
18:U:302:GLN:CG	18:U:341:VAL:H	2.26	0.47
30:X:117:LEU:CD1	30:X:117:LEU:N	2.73	0.47
1:A:300:PRO:O	1:A:301:LEU:CB	2.63	0.47
1:A:614:MET:HG2	1:A:621:LEU:HD22	1.96	0.47
1:A:1256:VAL:HG13	1:A:1298:TYR:CE2	2.49	0.47
2:B:126:TYR:CD2	2:B:201:ALA:HB3	2.49	0.47
2:B:126:TYR:CG	2:B:201:ALA:HB3	2.50	0.47
17:P:105:G:H5''	7:l:48:ARG:HH21	1.66	0.47
17:P:117:A:H2'	17:P:118:A:C8	2.50	0.47
20:Y:66:GLN:CD	20:Y:67:PRO:N	2.73	0.47
20:Y:250:PRO:O	20:Y:251:ASN:CB	2.62	0.47
20:Y:304:UNK:CA	23:d:110:PRO:CG	2.81	0.47
28:R:198:VAL:HA	28:R:206:ASN:ND2	2.30	0.47
28:R:288:LYS:HZ1	29:r:578:GLN:CD	2.21	0.47
29:r:541:VAL:HG11	29:r:553:TRP:CZ3	2.49	0.47
30:X:279:LYS:HB2	30:X:386:LEU:HD11	1.96	0.47
30:X:362:GLU:O	30:X:364:TYR:N	2.35	0.47
30:X:1119:LEU:HA	30:X:1122:TYR:CD2	2.46	0.47
10:o:17:VAL:HG12	10:o:18:PHE:N	2.30	0.47
1:A:299:GLU:HB3	1:A:300:PRO:CD	2.44	0.47
1:A:736:LEU:O	1:A:739:ALA:HB3	2.14	0.47
1:A:1966:ALA:CB	1:A:2007:LEU:HD22	2.44	0.47
2:B:82:GLU:O	2:B:84:VAL:N	2.48	0.47
2:B:425:LYS:HB3	2:B:426:PRO:HD3	1.97	0.47
2:B:864:LEU:CD2	2:B:889:ILE:HD11	2.45	0.47
2:B:927:ASP:HB3	2:B:930:ILE:HD12	1.95	0.47
11:K:260:ASP:O	11:K:261:VAL:HG23	2.15	0.47
12:L:219:LYS:HE3	12:L:219:LYS:CA	2.44	0.47
12:L:311:GLY:N	12:L:331:ASP:OD2	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:23:A:O2'	20:Y:119:TYR:CE1	2.68	0.47
14:N:73:C:H1'	14:N:74:U:N3	2.28	0.47
17:P:116:A:N6	17:P:117:A:N6	2.62	0.47
17:P:131:C:H2'	17:P:132:U:C6	2.50	0.47
20:Y:53:GLN:OE1	20:Y:124:MET:N	2.48	0.47
20:Y:66:GLN:NE2	20:Y:66:GLN:C	2.73	0.47
20:Y:278:PHE:CE1	20:Y:282:LEU:HD11	2.50	0.47
22:c:352:TYR:OH	22:c:385:ARG:NH2	2.48	0.47
23:d:53:GLN:HG2	23:d:103:PHE:HB3	1.96	0.47
25:g:138:ARG:HH11	25:g:138:ARG:CG	2.27	0.47
28:R:145:VAL:HG21	28:R:161:PHE:CE2	2.49	0.47
30:X:32:LEU:HD23	30:X:35:ILE:HD12	1.96	0.47
30:X:459:GLN:O	30:X:461:ARG:HG3	2.15	0.47
30:X:462:ARG:HA	30:X:471:ASN:O	2.14	0.47
30:X:910:TYR:O	30:X:914:LEU:HG	2.15	0.47
4:Z:17:THR:HB	4:Z:70:ILE:HB	1.97	0.47
5:b:68:VAL:HG12	5:b:70:LEU:HD23	1.96	0.47
1:A:590:GLY:O	1:A:591:ASN:C	2.58	0.47
1:A:621:LEU:C	1:A:623:ARG:H	2.23	0.47
1:A:708:LEU:C	1:A:708:LEU:HD23	2.40	0.47
1:A:1002:THR:HG22	1:A:1198:THR:HB	1.96	0.47
2:B:91:ILE:HD12	2:B:91:ILE:N	2.30	0.47
2:B:243:VAL:HG12	2:B:275:LEU:HD13	1.97	0.47
7:G:111:ARG:HH22	9:I:64:LEU:HD13	1.80	0.47
11:K:172:GLU:HG3	11:K:177:TRP:CE2	2.49	0.47
11:K:229:VAL:HB	11:K:243:TYR:HB2	1.96	0.47
12:L:219:LYS:HE3	12:L:219:LYS:O	2.13	0.47
14:N:25:U:O2'	14:N:26:U:OP1	2.31	0.47
17:P:140:C:H2'	17:P:141:C:C6	2.50	0.47
24:e:8:ARG:CG	24:e:8:ARG:HH21	2.27	0.47
25:g:131:SER:O	25:g:135:LYS:N	2.44	0.47
30:X:386:LEU:HA	30:X:389:ASP:HB2	1.96	0.47
30:X:845:GLY:O	30:X:847:HIS:N	2.47	0.47
1:A:393:GLU:HG2	2:B:358:ASP:HB3	1.95	0.47
1:A:435:ASN:ND2	1:A:435:ASN:C	2.73	0.47
1:A:641:THR:O	1:A:642:GLY:C	2.58	0.47
1:A:1661:TRP:HB3	1:A:1743:ILE:HD11	1.97	0.47
17:P:138:U:H2'	17:P:139:U:C6	2.50	0.47
20:Y:64:PRO:HG2	20:Y:69:GLN:HG3	1.97	0.47
28:R:68:LEU:O	28:R:69:ALA:HB2	2.15	0.47
30:X:481:ASN:HB2	30:X:506:GLY:HA3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:909:ASP:O	30:X:913:LYS:HG3	2.15	0.47
30:X:959:LEU:O	30:X:963:LEU:HG	2.14	0.47
30:X:1198:LYS:HA	30:X:1201:TYR:HD2	1.80	0.47
1:A:1734:ASN:HD21	1:A:1768:ARG:NH2	2.13	0.47
2:B:244:ILE:HD12	2:B:274:ARG:NH1	2.30	0.47
11:K:324:LEU:HD23	13:M:113:HIS:CE1	2.50	0.47
13:M:289:ALA:HA	19:W:75:LEU:HD22	1.97	0.47
21:a:22:ILE:HG21	21:a:27:LEU:CD1	2.39	0.47
29:r:628:TYR:CG	29:r:631:LEU:HD11	2.50	0.47
30:X:62:LEU:O	30:X:66:VAL:N	2.29	0.47
30:X:344:PHE:HA	30:X:347:LEU:HD12	1.97	0.47
30:X:723:ARG:HH22	30:X:764:VAL:HG23	1.80	0.47
30:X:855:LEU:HD11	30:X:929:ARG:HH22	1.80	0.47
6:f:7:LEU:HD12	6:f:36:MET:HE1	1.96	0.47
1:A:147:ILE:HD12	1:A:149:PHE:CE2	2.50	0.46
1:A:1579:LEU:HD13	1:A:1584:ILE:CD1	2.45	0.46
1:A:1579:LEU:HD23	1:A:1580:ASP:N	2.29	0.46
12:L:110:CYS:SG	12:L:120:TRP:NE1	2.88	0.46
19:W:48:TRP:CD1	19:W:48:TRP:C	2.92	0.46
20:Y:49:PRO:O	20:Y:129:SER:HB2	2.15	0.46
24:e:88:LEU:HD21	24:e:92:TRP:CZ2	2.50	0.46
28:R:164:TRP:CD2	28:R:173:CYS:SG	3.01	0.46
29:r:631:LEU:O	29:r:632:LEU:C	2.57	0.46
30:X:11:ILE:HA	30:X:14:TYR:HD2	1.80	0.46
30:X:159:ASP:O	30:X:162:LYS:HB2	2.15	0.46
30:X:777:LEU:HA	30:X:954:CYS:O	2.14	0.46
30:X:1086:VAL:HG13	30:X:1211:LEU:HB2	1.96	0.46
1:A:275:TYR:CD2	1:A:276:LEU:HD13	2.50	0.46
1:A:561:SER:O	1:A:563:PHE:N	2.48	0.46
1:A:631:PHE:O	1:A:632:LYS:C	2.56	0.46
1:A:740:TRP:CE2	1:A:744:LYS:HD2	2.51	0.46
1:A:1812:VAL:HA	1:A:1825:LYS:O	2.15	0.46
2:B:877:ARG:HB3	2:B:884:LEU:HD13	1.97	0.46
3:C:30:A:O2'	3:C:31:A:OP2	2.31	0.46
12:L:129:ARG:HH12	12:L:166:ARG:C	2.24	0.46
12:L:201:ILE:HG21	12:L:215:LEU:CD1	2.33	0.46
17:P:136:C:C5	17:P:137:U:O4	2.68	0.46
18:S:69:LEU:HD11	18:T:80:TRP:CE2	2.50	0.46
18:U:470:ASN:CB	18:U:475:LEU:CG	2.92	0.46
19:W:16:ILE:HD11	19:W:163:LEU:HD23	1.96	0.46
20:Y:55:GLU:N	20:Y:55:GLU:CD	2.73	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
29:r:601:LYS:HG3	29:r:602:PHE:CD2	2.50	0.46
29:r:637:LEU:HD23	29:r:644:THR:OG1	2.15	0.46
30:X:865:LEU:O	30:X:869:TYR:HD2	1.99	0.46
30:X:988:SER:O	30:X:991:SER:OG	2.25	0.46
1:A:508:THR:HG22	1:A:509:SER:N	2.31	0.46
9:I:35:GLN:CG	9:I:46:LEU:HD23	2.46	0.46
11:K:186:THR:HG22	11:K:202:THR:HG22	1.96	0.46
12:L:315:HIS:ND1	12:L:315:HIS:C	2.73	0.46
18:T:90:LEU:HD12	18:U:90:LEU:CD2	2.43	0.46
28:R:145:VAL:O	28:R:148:GLU:N	2.48	0.46
28:R:271:MET:N	28:R:272:PRO:CD	2.79	0.46
30:X:58:PHE:HA	30:X:62:LEU:HD12	1.97	0.46
30:X:120:VAL:O	30:X:121:VAL:C	2.57	0.46
30:X:399:LYS:HE3	30:X:606:LEU:HD11	1.97	0.46
30:X:1050:GLU:HA	30:X:1065:LYS:HZ1	1.80	0.46
1:A:388:LEU:N	1:A:388:LEU:HD23	2.31	0.46
1:A:1301:ALA:O	1:A:1302:ALA:C	2.58	0.46
1:A:1819:GLU:CB	1:A:1820:GLY:HA2	2.41	0.46
14:N:30:A:H1'	14:N:31:C:O4'	2.15	0.46
18:U:202:THR:O	18:U:465:ASN:CG	2.59	0.46
24:e:51:GLN:HG3	25:g:157:TRP:CG	2.51	0.46
28:R:180:MET:HA	28:R:180:MET:HE3	1.97	0.46
30:X:117:LEU:HD23	30:X:205:LYS:CE	2.42	0.46
30:X:280:PHE:HE1	30:X:435:ARG:NH1	2.13	0.46
30:X:684:CYS:SG	30:X:709:ASP:HB3	2.55	0.46
7:l:111:ARG:HH22	9:n:64:LEU:HD13	1.80	0.46
9:n:35:GLN:CD	9:n:46:LEU:HD23	2.41	0.46
10:J:40:ILE:HD11	10:J:70:ILE:HD11	1.98	0.46
14:N:30:A:H1'	14:N:31:C:C6	2.50	0.46
17:P:104:G:OP2	9:n:66:ARG:NH1	2.49	0.46
17:P:121:C:H2'	17:P:122:U:C6	2.50	0.46
20:Y:70:VAL:O	20:Y:71:TYR:CB	2.63	0.46
20:Y:304:UNK:CA	23:d:110:PRO:HB2	2.28	0.46
1:A:869:LEU:HD22	1:A:940:ILE:HD13	1.97	0.46
3:C:58:A:H2'	3:C:59:A:C8	2.51	0.46
9:I:35:GLN:CD	9:I:46:LEU:HD23	2.41	0.46
12:L:193:PHE:CD1	12:L:227:ILE:HD11	2.50	0.46
13:M:189:SER:CB	25:g:82:LYS:CG	2.91	0.46
14:N:25:U:H6	14:N:25:U:H5''	1.81	0.46
15:O:101:U:O2'	15:O:102:A:O5'	2.31	0.46
16:Q:499:U:H5'	16:Q:500:A:OP2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:102:U:O4	5:b:35:MET:CG	2.63	0.46
17:P:114:G:H2'	17:P:115:G:H8	1.81	0.46
18:U:55:VAL:N	18:U:56:PRO:CD	2.79	0.46
18:V:63:PRO:O	18:V:64:PRO:C	2.58	0.46
20:Y:241:LEU:HD23	20:Y:241:LEU:H	1.76	0.46
24:e:29:ARG:HG3	25:g:147:LEU:HD21	1.93	0.46
29:r:535:LYS:HA	29:r:538:GLU:HG2	1.98	0.46
30:X:477:PHE:HB3	30:X:613:VAL:HG12	1.98	0.46
30:X:666:TYR:HB2	30:X:767:ASP:HB3	1.98	0.46
5:b:35:MET:HE1	5:b:78:LEU:HD11	1.97	0.46
1:A:128:PRO:O	1:A:129:MET:CB	2.64	0.46
1:A:1605:LEU:HD22	1:A:1609:ILE:HD11	1.97	0.46
2:B:179:TYR:O	2:B:180:THR:OG1	2.22	0.46
2:B:655:LEU:HA	2:B:658:LEU:HD23	1.97	0.46
8:H:80:LEU:O	8:H:81:ILE:HD12	2.16	0.46
22:c:564:TYR:HA	22:c:578:VAL:HA	1.98	0.46
24:e:132:VAL:HG13	24:e:133:ARG:N	2.30	0.46
30:X:19:TRP:HZ2	30:X:27:PHE:CZ	2.34	0.46
7:l:53:LEU:HD22	7:l:71:VAL:HG11	1.97	0.46
1:A:116:LEU:N	1:A:117:PRO:CD	2.79	0.46
1:A:587:TYR:O	1:A:587:TYR:CG	2.69	0.46
1:A:1579:LEU:HD13	1:A:1584:ILE:HD11	1.96	0.46
2:B:925:PRO:HB2	2:B:948:LEU:HD22	1.98	0.46
12:L:59:ASP:OD1	12:L:101:TRP:CE2	2.68	0.46
12:L:65:PHE:CZ	12:L:336:LEU:HD21	2.51	0.46
18:U:296:GLU:CG	18:U:316:GLU:HB3	2.46	0.46
19:W:16:ILE:HG22	19:W:35:LEU:HD21	1.98	0.46
19:W:29:TRP:NE1	19:W:45:LYS:HG3	2.31	0.46
30:X:34:CYS:O	30:X:39:VAL:HG23	2.15	0.46
30:X:243:HIS:HB3	30:X:244:PRO:HD3	1.98	0.46
30:X:275:ASN:O	30:X:279:LYS:N	2.39	0.46
30:X:972:CYS:HB3	30:X:999:PRO:HG3	1.98	0.46
1:A:251:LEU:N	1:A:252:PRO:HD2	2.31	0.46
1:A:290:VAL:HG21	1:A:329:THR:HB	1.98	0.46
1:A:1038:VAL:HG12	1:A:1039:VAL:N	2.31	0.46
1:A:1245:THR:HG22	1:A:1247:GLN:HG3	1.97	0.46
1:A:1817:THR:HB	1:A:1820:GLY:HA3	1.97	0.46
2:B:351:PHE:HE1	2:B:355:LEU:HD21	1.81	0.46
4:D:17:THR:HB	4:D:70:ILE:HB	1.97	0.46
16:Q:498:C:H2'	16:Q:499:U:O4'	2.16	0.46
18:U:63:PRO:O	18:U:65:SER:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:57:ARG:HG2	20:Y:58:PRO:N	2.31	0.46
20:Y:177:TYR:HD2	20:Y:244:ARG:CB	2.20	0.46
20:Y:233:GLN:O	20:Y:241:LEU:HG	2.15	0.46
20:Y:271:LYS:O	20:Y:271:LYS:HD3	2.15	0.46
23:d:46:VAL:HG13	23:d:52:ILE:HG22	1.96	0.46
25:g:83:ASN:H	25:g:88:TYR:HA	1.81	0.46
30:X:54:GLU:C	30:X:1224:ARG:HE	2.23	0.46
1:A:517:LEU:HD21	1:A:585:VAL:HG21	1.97	0.46
1:A:999:LEU:C	1:A:999:LEU:HD23	2.41	0.46
2:B:389:LEU:O	2:B:391:LYS:N	2.49	0.46
5:E:35:MET:HE1	5:E:78:LEU:HD11	1.97	0.46
10:J:17:VAL:HG12	10:J:18:PHE:N	2.30	0.46
18:U:276:PRO:CG	18:U:279:SER:HB2	2.46	0.46
24:e:102:CYS:SG	24:e:105:CYS:SG	3.13	0.46
30:X:127:ILE:HG22	30:X:131:PHE:CE2	2.51	0.46
30:X:685:HIS:O	30:X:710:VAL:HG13	2.16	0.46
1:A:187:PHE:HB3	1:A:188:PRO:CD	2.46	0.45
1:A:1919:ALA:HB1	1:A:1967:LEU:HB2	1.98	0.45
2:B:696:LYS:HB3	2:B:811:ALA:HB2	1.98	0.45
7:G:32:VAL:HB	7:G:111:ARG:HH11	1.81	0.45
17:P:94:U:H2'	17:P:95:C:C6	2.51	0.45
20:Y:225:PHE:CD1	20:Y:225:PHE:C	2.93	0.45
20:Y:229:ALA:O	20:Y:233:GLN:OE1	2.34	0.45
20:Y:262:LEU:HD12	21:a:98:ALA:HB1	1.99	0.45
21:a:69:ILE:HD11	21:a:84:MET:SD	2.56	0.45
6:f:67:TYR:CG	7:l:99:MET:HE3	2.51	0.45
8:m:80:LEU:O	8:m:81:ILE:HD12	2.16	0.45
10:o:40:ILE:HD11	10:o:70:ILE:HD11	1.98	0.45
1:A:1043:LYS:NZ	17:P:26:A:OP1	2.49	0.45
1:A:1556:ARG:HD3	1:A:1596:SER:OG	2.16	0.45
2:B:106:ILE:HG21	11:K:218:PRO:HB3	1.98	0.45
2:B:323:SER:OG	2:B:328:TYR:CZ	2.68	0.45
2:B:759:LEU:HD23	2:B:803:PHE:HB2	1.97	0.45
3:C:55:C:O2'	3:C:56:A:H5'	2.16	0.45
6:F:67:TYR:CG	7:G:99:MET:HE3	2.51	0.45
11:K:187:ILE:HD11	11:K:222:SER:HB3	1.98	0.45
14:N:22:A:N6	20:Y:151:PHE:O	2.48	0.45
30:X:267:PHE:HA	30:X:270:MET:HG2	1.98	0.45
9:n:35:GLN:CG	9:n:46:LEU:HD23	2.46	0.45
1:A:768:SER:O	1:A:769:LYS:C	2.58	0.45
1:A:1291:LEU:HD23	1:A:1291:LEU:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1851:TRP:CE3	1:A:1851:TRP:CA	2.99	0.45
2:B:202:VAL:HG11	2:B:443:VAL:HG22	1.98	0.45
17:P:106:U:H5	17:P:107:U:C4	2.34	0.45
17:P:134:U:H2'	17:P:135:G:H8	1.81	0.45
18:U:392:VAL:HG11	18:U:403:TRP:HE1	1.78	0.45
19:W:236:TYR:O	19:W:238:UNK:N	2.46	0.45
21:a:69:ILE:HD11	21:a:84:MET:HG2	1.98	0.45
24:e:62:ASP:OD2	25:g:144:PRO:HG3	2.16	0.45
30:X:251:PHE:O	30:X:255:LEU:HG	2.15	0.45
30:X:669:ASN:OD1	30:X:698:LYS:HD3	2.17	0.45
30:X:671:PHE:CZ	30:X:680:VAL:HG22	2.52	0.45
30:X:863:LYS:O	30:X:867:GLU:HG3	2.16	0.45
30:X:868:LYS:O	30:X:872:THR:HG23	2.16	0.45
5:b:34:PHE:O	5:b:35:MET:HB2	2.17	0.45
7:l:32:VAL:HB	7:l:111:ARG:HH11	1.81	0.45
1:A:274:PHE:O	1:A:275:TYR:C	2.60	0.45
2:B:378:VAL:O	2:B:379:ARG:CB	2.65	0.45
2:B:676:PHE:CZ	2:B:892:ILE:HD11	2.52	0.45
14:N:26:U:O2	14:N:26:U:C2'	2.65	0.45
17:P:113:U:H2'	17:P:114:G:H8	1.81	0.45
17:P:119:G:H2'	17:P:120:C:C6	2.50	0.45
30:X:117:LEU:HD22	30:X:205:LYS:NZ	2.24	0.45
30:X:199:ILE:O	30:X:203:LEU:HG	2.17	0.45
30:X:560:ALA:HB1	30:X:569:MET:HE1	1.97	0.45
30:X:1087:GLN:HB2	30:X:1212:TYR:HD1	1.81	0.45
1:A:632:LYS:O	1:A:633:HIS:C	2.59	0.45
1:A:1887:VAL:HG11	1:A:1892:MET:HB2	1.97	0.45
17:P:139:U:H2'	17:P:140:C:C6	2.49	0.45
18:U:63:PRO:O	18:U:64:PRO:C	2.59	0.45
1:A:608:VAL:HG11	1:A:660:TRP:CH2	2.52	0.45
12:L:103:ARG:HD2	12:L:145:LYS:HA	1.99	0.45
24:e:146:ASP:OD1	25:g:131:SER:HB2	2.15	0.45
30:X:8:LYS:HE2	30:X:48:VAL:HG22	1.97	0.45
30:X:117:LEU:CD1	30:X:118:SER:N	2.73	0.45
30:X:910:TYR:HA	30:X:913:LYS:HD2	1.99	0.45
30:X:1089:ILE:HD13	30:X:1214:LEU:HD23	1.97	0.45
1:A:376:ASN:HB3	1:A:377:PRO:HD2	1.99	0.45
1:A:735:HIS:O	1:A:736:LEU:C	2.59	0.45
1:A:1324:LYS:HG2	1:A:1332:PRO:HD2	1.97	0.45
1:A:1667:SER:O	1:A:1739:TYR:HA	2.17	0.45
14:N:26:U:C5	20:Y:244:ARG:NH1	2.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:125:G:H2'	17:P:126:G:H8	1.81	0.45
25:g:142:GLY:H	25:g:154:LYS:N	2.15	0.45
28:R:181:GLU:HB3	28:R:190:ALA:HB2	1.98	0.45
30:X:239:ARG:HH22	30:X:277:VAL:HG12	1.82	0.45
30:X:749:PRO:HG3	30:X:1063:ASP:OD2	2.16	0.45
30:X:805:LEU:HB2	30:X:954:CYS:SG	2.57	0.45
1:A:231:LYS:O	1:A:232:ALA:C	2.60	0.45
1:A:333:ILE:HG22	1:A:333:ILE:O	2.17	0.45
1:A:983:ASN:ND2	1:A:1249:THR:OG1	2.49	0.45
2:B:930:ILE:O	2:B:931:LYS:C	2.59	0.45
7:G:53:LEU:HD22	7:G:71:VAL:HG11	1.97	0.45
11:K:243:TYR:CE1	11:K:279:ARG:HA	2.52	0.45
12:L:201:ILE:CG1	12:L:215:LEU:HD12	2.47	0.45
17:P:124:U:H2'	17:P:125:G:H8	1.81	0.45
17:P:168:A:C1'	4:Z:27:ARG:HH11	2.28	0.45
20:Y:273:LEU:HD11	21:a:89:PHE:HA	1.93	0.45
24:e:123:LYS:O	24:e:124:SER:C	2.60	0.45
28:R:288:LYS:HB3	29:r:538:GLU:HB3	1.94	0.45
29:r:368:UNK:O	29:r:372:UNK:N	2.50	0.45
29:r:599:GLU:CB	29:r:608:SER:HB3	2.47	0.45
29:r:631:LEU:O	29:r:634:LYS:N	2.49	0.45
30:X:332:ARG:HE	30:X:383:ARG:N	2.14	0.45
30:X:486:THR:OG1	30:X:502:LYS:O	2.25	0.45
30:X:758:VAL:O	30:X:762:LEU:HG	2.17	0.45
30:X:816:ARG:O	30:X:820:LEU:HG	2.17	0.45
30:X:1150:ILE:O	30:X:1154:CYS:HB2	2.17	0.45
1:A:258:HIS:CE1	1:A:265:LEU:HD11	2.51	0.45
1:A:275:TYR:CE2	1:A:276:LEU:HD13	2.52	0.45
1:A:1743:ILE:HG23	1:A:1744:PRO:HD2	1.99	0.45
2:B:921:VAL:HG13	2:B:943:LEU:HD11	1.98	0.45
11:K:153:TRP:NE1	11:K:406:TYR:OH	2.48	0.45
12:L:74:ILE:HG23	12:L:99:LEU:HD11	1.98	0.45
16:Q:500:A:C4'	16:Q:501:A:C5'	2.86	0.45
20:Y:278:PHE:HE2	21:a:141:ARG:HG3	1.78	0.45
30:X:470:LYS:HD2	30:X:611:ALA:HB2	1.98	0.45
30:X:558:THR:OG1	30:X:586:TYR:HB2	2.17	0.45
30:X:865:LEU:HB3	30:X:886:PRO:HB3	1.99	0.45
30:X:894:LYS:HE3	30:X:914:LEU:HD21	1.98	0.45
1:A:300:PRO:O	1:A:301:LEU:HB3	2.17	0.45
1:A:635:ILE:O	1:A:636:TYR:C	2.60	0.45
1:A:1847:HIS:HE1	1:A:1934:THR:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:201:ILE:HG22	12:L:215:LEU:HD11	1.94	0.45
14:N:80:A:N3	14:N:80:A:C5'	2.73	0.45
17:P:123:C:H2'	17:P:124:U:C6	2.50	0.45
20:Y:278:PHE:CE1	20:Y:282:LEU:CD1	3.00	0.45
30:X:446:LEU:HD23	30:X:449:LEU:HD12	1.98	0.45
30:X:738:GLY:O	30:X:1004:ARG:NH1	2.50	0.45
1:A:129:MET:HG2	1:A:131:TRP:CH2	2.52	0.44
1:A:570:MET:HG3	1:A:675:LEU:HD21	1.98	0.44
1:A:928:LEU:CD1	1:A:928:LEU:N	2.80	0.44
1:A:1007:VAL:HG11	1:A:1064:TRP:CH2	2.53	0.44
1:A:1841:LEU:HB3	1:A:1843:LEU:HD23	1.98	0.44
6:F:11:THR:O	6:F:12:ASN:CB	2.65	0.44
9:I:4:VAL:HG12	9:I:5:PRO:HD2	1.99	0.44
11:K:387:PHE:CD2	11:K:436:LEU:HD21	2.51	0.44
16:Q:502:C:O2'	16:Q:503:A:H5'	2.16	0.44
17:P:135:G:N2	17:P:136:C:O2	2.50	0.44
20:Y:149:ASP:OD2	20:Y:224:GLN:HG2	2.17	0.44
30:X:516:ALA:O	30:X:519:ASP:HB2	2.18	0.44
30:X:1126:LEU:HD23	30:X:1280:ARG:NH1	2.27	0.44
1:A:126:ASN:O	1:A:127:MET:C	2.59	0.44
1:A:649:GLY:O	1:A:650:CYS:C	2.60	0.44
2:B:243:VAL:O	2:B:243:VAL:CG1	2.65	0.44
3:C:42:U:C4	3:C:43:C:C5	3.05	0.44
12:L:76:LEU:HB2	12:L:86:TYR:HB2	1.99	0.44
14:N:21:C:O3'	14:N:22:A:H3'	2.18	0.44
19:W:48:TRP:HA	19:W:52:ILE:CG2	2.45	0.44
20:Y:56:THR:O	20:Y:57:ARG:HB3	2.16	0.44
20:Y:203:ARG:CZ	20:Y:257:ARG:NH1	2.79	0.44
22:c:458:ASN:ND2	22:c:560:LYS:O	2.50	0.44
28:R:165:LEU:HD22	28:R:174:TRP:CE2	2.53	0.44
30:X:87:LYS:NZ	30:X:415:THR:O	2.47	0.44
30:X:93:TRP:CZ3	30:X:139:LEU:HD11	2.52	0.44
30:X:121:VAL:O	30:X:125:GLN:HG3	2.18	0.44
30:X:1028:LEU:O	30:X:1032:LEU:HB2	2.17	0.44
1:A:451:LYS:HA	1:A:454:TYR:CE2	2.52	0.44
1:A:792:LYS:O	1:A:796:LYS:N	2.49	0.44
2:B:104:PRO:HB3	11:K:235:GLU:O	2.18	0.44
2:B:270:ASN:HA	2:B:322:ALA:O	2.17	0.44
5:E:28:LEU:C	5:E:28:LEU:HD12	2.42	0.44
12:L:65:PHE:HD2	12:L:77:TRP:HB2	1.82	0.44
12:L:78:ASN:ND2	12:L:86:TYR:OH	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:N:23:A:N9	20:Y:119:TYR:CZ	2.84	0.44
17:P:97:U:C2	7:l:63:HIS:HD2	2.35	0.44
20:Y:96:ARG:HE	20:Y:233:GLN:HG2	1.82	0.44
20:Y:273:LEU:CD1	21:a:89:PHE:CA	2.92	0.44
21:a:134:GLN:CG	25:g:78:GLN:HE22	2.30	0.44
22:c:601:ASN:O	22:c:601:ASN:CG	2.59	0.44
30:X:76:ASN:O	30:X:80:MET:HG2	2.16	0.44
30:X:280:PHE:HE1	30:X:435:ARG:HH11	1.65	0.44
30:X:1082:PHE:HD1	30:X:1242:LEU:HD22	1.83	0.44
1:A:377:PRO:O	1:A:378:ILE:CB	2.65	0.44
2:B:490:MET:CE	2:B:566:LEU:HD11	2.44	0.44
11:K:345:THR:HG21	11:K:400:TRP:HH2	1.83	0.44
11:K:381:ASN:OD1	11:K:382:SER:N	2.45	0.44
12:L:219:LYS:CB	12:L:240:ASP:OD2	2.59	0.44
14:N:31:C:H2'	14:N:32:G:O4'	2.16	0.44
17:P:132:U:H2'	17:P:133:A:H8	1.82	0.44
20:Y:62:MET:C	20:Y:63:GLU:CD	2.85	0.44
21:a:53:ILE:C	21:a:54:PHE:HD1	2.25	0.44
24:e:62:ASP:OD2	25:g:144:PRO:CG	2.66	0.44
25:g:143:ASP:H	25:g:153:TYR:HD1	1.60	0.44
29:r:503:TYR:CZ	29:r:520:TYR:HB2	2.52	0.44
29:r:593:LEU:HB3	33:x:131:UNK:CB	2.47	0.44
29:r:648:TYR:O	29:r:652:ILE:HG13	2.17	0.44
30:X:134:SER:O	30:X:140:ARG:HG3	2.17	0.44
30:X:931:PHE:O	30:X:940:GLN:NE2	2.50	0.44
6:f:11:THR:O	6:f:12:ASN:CB	2.65	0.44
1:A:1399:TRP:O	1:A:1400:GLU:C	2.61	0.44
1:A:1811:ARG:O	1:A:1826:PRO:HA	2.17	0.44
2:B:772:VAL:CG1	2:B:810:LEU:HD13	2.48	0.44
4:D:36:ASN:O	4:D:37:MET:HB2	2.18	0.44
17:P:120:C:H2'	17:P:121:C:C6	2.50	0.44
17:P:133:A:H2'	17:P:134:U:C6	2.50	0.44
18:U:69:LEU:HA	18:U:72:LEU:HD13	2.00	0.44
18:U:371:PHE:HB3	18:U:403:TRP:CH2	2.53	0.44
20:Y:55:GLU:CD	20:Y:55:GLU:H	2.24	0.44
21:a:35:MET:HE1	21:a:54:PHE:CD2	2.53	0.44
25:g:138:ARG:CB	25:g:160:TYR:CD1	2.74	0.44
29:r:553:TRP:HE1	29:r:579:ALA:CB	2.30	0.44
30:X:37:GLU:HA	30:X:41:VAL:HB	1.98	0.44
5:b:28:LEU:C	5:b:28:LEU:HD12	2.42	0.44
1:A:1865:THR:O	1:A:1869:VAL:HG23	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:U:O2	3:C:49:U:C2'	2.66	0.44
11:K:295:LEU:HA	11:K:305:VAL:O	2.17	0.44
11:K:434:LEU:HD11	26:h:54:ARG:HG3	2.00	0.44
12:L:235:LEU:HD13	12:L:275:VAL:CG1	2.47	0.44
14:N:67:A:OP1	14:N:69:G:O2'	2.27	0.44
17:P:115:G:H2'	17:P:116:A:H8	1.82	0.44
19:W:16:ILE:CG2	19:W:35:LEU:HD21	2.47	0.44
24:e:106:ILE:N	24:e:106:ILE:CD1	2.78	0.44
28:R:151:LEU:HD23	28:R:151:LEU:HA	1.85	0.44
30:X:755:HIS:HE1	30:X:783:SER:HB2	1.83	0.44
30:X:852:ASP:O	30:X:855:LEU:HB2	2.17	0.44
4:Z:36:ASN:O	4:Z:37:MET:HB2	2.18	0.44
1:A:274:PHE:O	1:A:276:LEU:N	2.51	0.44
1:A:561:SER:O	1:A:562:ARG:C	2.60	0.44
1:A:920:GLU:O	1:A:931:VAL:N	2.47	0.44
1:A:1692:PHE:CD2	1:A:1732:CYS:SG	3.10	0.44
14:N:77:G:N3	14:N:77:G:C2'	2.73	0.44
15:O:100:G:H4'	15:O:101:U:OP1	2.17	0.44
17:P:102:U:C4	6:f:61:ARG:CD	3.01	0.44
18:U:14:VAL:HG12	18:U:52:PRO:HA	1.99	0.44
22:c:411:THR:O	22:c:412:CYS:C	2.61	0.44
24:e:51:GLN:HB2	25:g:157:TRP:HE1	1.82	0.44
24:e:117:CYS:SG	24:e:134:CYS:HB2	2.58	0.44
28:R:198:VAL:HG11	28:R:207:TRP:CH2	2.53	0.44
30:X:75:ILE:O	30:X:76:ASN:C	2.60	0.44
30:X:202:LEU:HD22	30:X:225:ILE:HD11	2.00	0.44
30:X:243:HIS:CE1	30:X:247:GLU:OE2	2.70	0.44
30:X:1196:ASN:HA	30:X:1197:PRO:HD2	1.81	0.44
9:n:4:VAL:HG12	9:n:5:PRO:HD2	1.99	0.44
1:A:274:PHE:O	1:A:277:PHE:N	2.51	0.44
1:A:1035:LYS:O	1:A:1038:VAL:CG2	2.66	0.44
1:A:1514:PHE:O	1:A:1517:THR:OG1	2.33	0.44
2:B:606:VAL:HG12	2:B:617:LEU:HD11	2.00	0.44
11:K:221:PHE:N	11:K:221:PHE:CD1	2.86	0.44
11:K:267:ARG:C	11:K:269:ALA:N	2.75	0.44
11:K:343:GLU:O	11:K:344:PHE:HB3	2.18	0.44
14:N:76:C:H6	14:N:77:G:C1'	2.29	0.44
14:N:78:A:O5'	28:R:105:PRO:HG3	2.18	0.44
20:Y:203:ARG:HH22	20:Y:257:ARG:CZ	2.30	0.44
22:c:585:TRP:CH2	22:c:591:VAL:HG11	2.53	0.44
28:R:288:LYS:CB	29:r:538:GLU:HB2	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R:288:LYS:CB	29:r:538:GLU:HB3	2.48	0.44
29:r:633:VAL:HG13	29:r:644:THR:HG22	2.00	0.44
30:X:162:LYS:O	30:X:165:LEU:HB2	2.17	0.44
30:X:362:GLU:C	30:X:364:TYR:H	2.21	0.44
30:X:963:LEU:O	30:X:967:LYS:HG3	2.18	0.44
30:X:992:ILE:O	30:X:995:SER:OG	2.27	0.44
30:X:1196:ASN:O	30:X:1199:THR:OG1	2.24	0.44
1:A:708:LEU:HD23	1:A:709:ARG:N	2.33	0.44
1:A:1075:ILE:HG13	1:A:1186:LEU:HD21	2.00	0.44
2:B:243:VAL:CG1	2:B:275:LEU:HD13	2.47	0.44
2:B:396:THR:HG22	2:B:431:ILE:HD12	1.99	0.44
19:W:665:LEU:O	19:W:669:ALA:HB3	2.18	0.44
20:Y:195:PHE:CZ	20:Y:230:MET:CE	3.01	0.44
24:e:26:PHE:CZ	24:e:55:GLN:HG2	2.52	0.44
29:r:631:LEU:HG	29:r:631:LEU:H	1.55	0.44
30:X:921:MET:O	30:X:925:LEU:HG	2.18	0.44
30:X:1240:LEU:O	30:X:1262:GLU:HA	2.17	0.44
1:A:207:PRO:O	1:A:208:LEU:CB	2.66	0.43
2:B:225:ASP:OD1	2:B:225:ASP:N	2.34	0.43
14:N:72:A:O2'	14:N:73:C:OP1	2.33	0.43
17:P:98:G:O6	9:n:40:TYR:CA	2.57	0.43
17:P:112:U:H2'	17:P:113:U:C6	2.50	0.43
21:a:44:CYS:SG	21:a:70:CYS:N	2.82	0.43
28:R:198:VAL:HA	28:R:206:ASN:HD21	1.82	0.43
30:X:293:GLU:HA	30:X:296:ILE:HD12	2.00	0.43
30:X:338:ILE:HA	30:X:341:PHE:HD2	1.82	0.43
30:X:725:TYR:HB3	37:X:1500:ADP:N6	2.25	0.43
30:X:725:TYR:HB3	37:X:1500:ADP:N7	2.33	0.43
30:X:1055:LEU:O	30:X:1229:LEU:HD22	2.18	0.43
30:X:1157:ASN:HB2	30:X:1160:PHE:HD2	1.83	0.43
1:A:372:ASP:HB3	1:A:375:ILE:HD12	1.99	0.43
1:A:756:ALA:N	1:A:757:PRO:HD2	2.32	0.43
1:A:1008:PHE:HD1	1:A:1053:LEU:HD12	1.83	0.43
1:A:1817:THR:HB	1:A:1821:ASN:N	2.33	0.43
8:H:17:PHE:HA	8:H:20:LEU:HD12	1.99	0.43
10:J:9:LEU:HD11	10:J:38:LEU:CD1	2.48	0.43
13:M:251:ILE:O	13:M:251:ILE:CG2	2.66	0.43
14:N:1:G:C8	24:e:145:CYS:HB3	2.53	0.43
14:N:80:A:H5'	14:N:81:U:OP2	2.19	0.43
17:P:103:U:N1	7:l:102:ARG:NH2	2.65	0.43
17:P:157:G:H5''	17:P:157:G:C8	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:T:121:GLU:HG2	18:U:122:ARG:HD2	2.00	0.43
19:W:679:VAL:O	19:W:683:VAL:N	2.48	0.43
22:c:508:ILE:HD12	22:c:596:PHE:CZ	2.52	0.43
24:e:56:ARG:HD2	24:e:83:TYR:O	2.18	0.43
30:X:72:LEU:H	30:X:75:ILE:HD12	1.83	0.43
30:X:74:HIS:C	30:X:77:LEU:H	2.20	0.43
30:X:253:THR:OG1	30:X:379:ASN:ND2	2.50	0.43
30:X:281:PRO:HB2	30:X:290:TYR:CD2	2.52	0.43
30:X:387:VAL:HG22	30:X:435:ARG:CZ	2.48	0.43
30:X:650:GLY:HA3	30:X:654:ILE:HD11	1.99	0.43
30:X:765:LEU:O	30:X:769:SER:OG	2.23	0.43
30:X:1139:TYR:CE2	30:X:1186:VAL:HG11	2.53	0.43
30:X:1227:GLU:HA	30:X:1230:TRP:CD1	2.52	0.43
8:m:77:ASN:ND2	9:n:71:LEU:HD22	2.34	0.43
1:A:566:ALA:O	1:A:567:PHE:C	2.61	0.43
4:D:5:ILE:HD12	4:D:5:ILE:N	2.33	0.43
5:E:34:PHE:O	5:E:35:MET:HB2	2.17	0.43
14:N:75:G:O3'	14:N:76:C:C2	2.71	0.43
17:P:20:G:H2'	17:P:20:G:N3	2.33	0.43
18:V:115:ILE:O	18:V:119:THR:HG23	2.18	0.43
20:Y:55:GLU:CD	20:Y:56:THR:N	2.74	0.43
20:Y:175:THR:HA	20:Y:216:THR:HA	2.01	0.43
20:Y:274:LEU:HD12	20:Y:275:PRO:HD3	2.00	0.43
20:Y:278:PHE:HE1	20:Y:282:LEU:HD11	1.82	0.43
21:a:271:ASN:CG	21:a:272:VAL:N	2.74	0.43
25:g:147:LEU:HB2	25:g:148:GLU:OE1	2.18	0.43
30:X:50:SER:HB3	30:X:88:TYR:OH	2.17	0.43
30:X:83:LEU:HD21	30:X:125:GLN:C	2.43	0.43
30:X:462:ARG:HH12	30:X:533:TYR:C	2.27	0.43
30:X:1191:ALA:CB	30:X:1194:HIS:HB2	2.45	0.43
1:A:133:GLU:OE2	24:e:8:ARG:NE	2.52	0.43
1:A:270:ASP:O	1:A:271:ASP:CB	2.65	0.43
2:B:335:PHE:HA	2:B:338:LEU:HD12	2.00	0.43
2:B:389:LEU:HD23	2:B:389:LEU:HA	1.92	0.43
3:C:103:U:H4'	3:C:104:A:O4'	2.17	0.43
12:L:121:ASP:O	12:L:125:GLY:N	2.48	0.43
14:N:76:C:C6	14:N:77:G:H1'	2.53	0.43
17:P:106:U:H5	17:P:107:U:C5	2.32	0.43
20:Y:262:LEU:C	20:Y:262:LEU:CD1	2.86	0.43
29:r:628:TYR:CA	29:r:631:LEU:CD1	2.88	0.43
30:X:131:PHE:HE2	30:X:228:MET:HE1	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:253:THR:HA	30:X:379:ASN:HD21	1.82	0.43
30:X:504:GLN:NE2	30:X:567:VAL:HG22	2.33	0.43
30:X:1055:LEU:HD21	30:X:1236:THR:HG21	2.01	0.43
1:A:217:GLU:HA	1:A:224:MET:HE3	2.00	0.43
1:A:1297:TYR:CE2	1:A:1298:TYR:HE1	2.36	0.43
1:A:1810:TYR:CE2	1:A:1857:LEU:CD1	2.64	0.43
13:M:186:TYR:CD1	21:a:19:PHE:CZ	3.07	0.43
19:W:80:TRP:HB3	19:W:92:THR:CG2	2.49	0.43
20:Y:278:PHE:HZ	21:a:141:ARG:C	2.26	0.43
21:a:22:ILE:HD11	21:a:56:TRP:CZ3	2.53	0.43
30:X:40:ILE:HD12	30:X:77:LEU:HD13	2.01	0.43
30:X:54:GLU:HA	30:X:1224:ARG:HG3	2.00	0.43
30:X:115:LEU:CD1	30:X:119:GLU:CG	2.82	0.43
30:X:174:ALA:O	30:X:177:SER:OG	2.33	0.43
30:X:339:THR:C	30:X:374:LYS:HE2	2.43	0.43
30:X:689:ASN:ND2	30:X:714:ASP:OD1	2.50	0.43
1:A:377:PRO:O	1:A:378:ILE:HB	2.19	0.43
1:A:754:LEU:CD1	1:A:759:GLU:HG2	2.48	0.43
1:A:1449:LYS:O	22:c:598:SER:CB	2.66	0.43
1:A:1817:THR:HG22	1:A:1819:GLU:CD	2.44	0.43
1:A:1843:LEU:HD23	1:A:1843:LEU:H	1.84	0.43
14:N:76:C:C6	14:N:76:C:OP2	2.71	0.43
17:P:97:U:O4	7:l:62:ARG:HB2	2.17	0.43
19:W:21:VAL:HG11	19:W:48:TRP:CH2	2.53	0.43
21:a:60:ARG:NE	24:e:130:GLN:OE1	2.51	0.43
24:e:77:TRP:O	24:e:81:GLN:HB2	2.18	0.43
30:X:332:ARG:O	30:X:336:GLU:HG3	2.18	0.43
30:X:504:GLN:HE22	30:X:567:VAL:HG22	1.83	0.43
30:X:879:VAL:HA	30:X:882:TYR:CD2	2.54	0.43
30:X:1135:ILE:O	30:X:1166:VAL:HA	2.19	0.43
1:A:1174:LEU:O	1:A:1178:VAL:HG23	2.17	0.43
2:B:961:VAL:O	2:B:961:VAL:HG13	2.17	0.43
3:C:102:G:C2	3:C:104:A:H4'	2.54	0.43
3:C:102:G:C6	6:F:20:LYS:HG2	2.54	0.43
11:K:209:ARG:HG2	11:K:251:TYR:HA	2.00	0.43
11:K:240:ILE:HG23	26:h:32:HIS:CE1	2.54	0.43
11:K:287:GLY:O	11:K:288:HIS:C	2.62	0.43
17:P:118:A:H2'	17:P:119:G:C8	2.50	0.43
22:c:459:THR:HG21	22:c:505:ILE:HD11	1.99	0.43
30:X:502:LYS:HE2	30:X:586:TYR:CE1	2.52	0.43
30:X:671:PHE:HD1	30:X:676:GLN:HB3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:828:PRO:O	30:X:832:ARG:HG3	2.18	0.43
31:j:36:LEU:HB2	31:j:60:PRO:HD3	2.00	0.43
8:m:17:PHE:HA	8:m:20:LEU:HD12	1.99	0.43
1:A:667:ILE:HD12	1:A:667:ILE:HA	1.85	0.43
1:A:774:THR:O	1:A:775:SER:C	2.60	0.43
1:A:774:THR:HG23	1:A:805:LEU:CD1	2.49	0.43
2:B:259:ILE:HD13	2:B:301:ILE:HG23	2.00	0.43
11:K:172:GLU:CG	11:K:177:TRP:CZ2	3.01	0.43
11:K:258:THR:O	11:K:259:LEU:C	2.61	0.43
12:L:220:ASP:OD2	12:L:221:ILE:HG13	2.19	0.43
13:M:122:ARG:HA	13:M:125:ILE:HD12	2.00	0.43
20:Y:241:LEU:N	20:Y:241:LEU:CD2	2.73	0.43
21:a:19:PHE:HD1	21:a:20:PRO:HD2	1.84	0.43
23:d:50:PHE:HD2	23:d:51:VAL:HG22	1.84	0.43
25:g:73:PHE:O	25:g:74:VAL:C	2.62	0.43
25:g:97:PHE:CD1	25:g:98:VAL:N	2.87	0.43
30:X:276:TYR:HD1	30:X:386:LEU:HD13	1.83	0.43
30:X:727:TYR:HE2	30:X:760:LYS:NZ	2.16	0.43
30:X:1061:PRO:HG2	30:X:1063:ASP:OD1	2.18	0.43
30:X:1115:TYR:CG	30:X:1266:LEU:HB3	2.53	0.43
30:X:1140:GLU:OE2	30:X:1171:LYS:NZ	2.39	0.43
4:Z:5:ILE:HD12	4:Z:5:ILE:N	2.33	0.43
8:m:68:LEU:HD13	9:n:72:TRP:CZ2	2.54	0.43
1:A:619:TYR:O	1:A:620:ARG:C	2.62	0.43
11:K:206:ALA:O	11:K:207:THR:C	2.61	0.43
14:N:52:G:O2'	14:N:53:G:OP1	2.36	0.43
14:N:60:C:C5'	14:N:60:C:C6	3.01	0.43
20:Y:52:LYS:HE2	20:Y:129:SER:N	2.29	0.43
25:g:143:ASP:O	25:g:153:TYR:CG	2.72	0.43
29:r:503:TYR:HE2	29:r:507:PHE:CE2	2.37	0.43
29:r:628:TYR:O	29:r:631:LEU:HD12	2.18	0.43
30:X:466:LYS:HE3	30:X:541:LYS:NZ	2.33	0.43
30:X:624:ASP:O	30:X:628:LEU:HG	2.19	0.43
30:X:915:TYR:O	30:X:919:GLU:HG3	2.19	0.43
30:X:1046:TYR:HD1	30:X:1066:THR:HG21	1.82	0.43
31:j:160:VAL:O	31:j:161:PHE:HB2	2.19	0.43
32:k:67:LYS:O	32:k:68:ASN:CB	2.67	0.43
1:A:326:PRO:O	1:A:327:ILE:HB	2.18	0.43
1:A:639:PHE:CE2	1:A:650:CYS:HA	2.54	0.43
1:A:1005:SER:OG	1:A:1006:LYS:N	2.51	0.43
1:A:1320:GLN:HG3	1:A:1351:MET:HE1	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:74:ASP:O	2:B:76:GLN:N	2.51	0.43
2:B:178:ARG:O	2:B:179:TYR:C	2.62	0.43
8:H:68:LEU:HD13	9:I:72:TRP:CZ2	2.54	0.43
20:Y:162:ASP:O	20:Y:244:ARG:NH1	2.44	0.43
25:g:111:TYR:CD1	25:g:111:TYR:C	2.96	0.43
25:g:142:GLY:HA3	25:g:153:TYR:C	2.37	0.43
25:g:153:TYR:CG	25:g:153:TYR:O	2.70	0.43
28:R:288:LYS:HZ2	29:r:578:GLN:NE2	2.13	0.43
30:X:84:TYR:HA	30:X:87:LYS:HB2	2.01	0.43
30:X:109:ILE:HA	30:X:112:SER:OG	2.18	0.43
30:X:727:TYR:HE2	30:X:760:LYS:HZ2	1.66	0.43
30:X:912:THR:HA	30:X:915:TYR:HD2	1.83	0.43
30:X:1068:ASP:HA	30:X:1072:ASN:ND2	2.34	0.43
4:Z:7:LEU:HD22	5:b:69:ILE:HD11	2.01	0.43
10:o:9:LEU:HD11	10:o:38:LEU:CD1	2.49	0.43
1:A:68:VAL:HG13	1:A:69:LYS:N	2.33	0.42
1:A:1901:LEU:HD23	1:A:1902:ASP:N	2.34	0.42
2:B:98:THR:O	2:B:99:GLN:HG3	2.19	0.42
2:B:221:VAL:CG2	2:B:914:VAL:HG22	2.49	0.42
2:B:379:ARG:O	2:B:380:SER:C	2.61	0.42
9:I:21:LEU:HD22	9:I:78:VAL:HG22	2.01	0.42
11:K:253:LEU:HD21	11:K:262:LEU:HD11	2.00	0.42
17:P:16:U:H2'	17:P:17:U:H5'	2.00	0.42
17:P:104:G:OP2	9:n:66:ARG:NH2	2.51	0.42
19:W:33:SER:OG	19:W:39:LYS:O	2.29	0.42
20:Y:63:GLU:N	20:Y:63:GLU:CD	2.77	0.42
20:Y:163:MET:HB2	20:Y:244:ARG:HB3	2.01	0.42
20:Y:196:ALA:CA	20:Y:201:ILE:HD11	2.46	0.42
24:e:51:GLN:HA	25:g:157:TRP:HZ2	1.72	0.42
27:i:33:LEU:HD13	27:i:33:LEU:O	2.18	0.42
28:R:104:ILE:N	28:R:105:PRO:CD	2.82	0.42
29:r:649:GLU:CA	29:r:652:ILE:CD1	2.86	0.42
30:X:159:ASP:HA	30:X:162:LYS:HD2	2.01	0.42
30:X:429:SER:O	30:X:432:PHE:HB3	2.19	0.42
9:n:21:LEU:HD22	9:n:78:VAL:HG22	2.01	0.42
1:A:906:ARG:HA	1:A:909:LEU:HD12	2.01	0.42
1:A:1693:GLY:N	1:A:1732:CYS:SG	2.91	0.42
2:B:124:THR:O	2:B:124:THR:HG23	2.19	0.42
2:B:688:CYS:SG	2:B:689:PHE:N	2.92	0.42
8:H:77:ASN:ND2	9:I:71:LEU:HD22	2.34	0.42
14:N:57:C:C2	14:N:66:G:N2	2.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:98:G:C8	9:n:40:TYR:CZ	3.07	0.42
17:P:135:G:C4	17:P:136:C:C6	3.07	0.42
24:e:58:ARG:HD3	24:e:92:TRP:CZ2	2.54	0.42
24:e:115:SER:OG	24:e:116:THR:N	2.52	0.42
30:X:31:MET:O	30:X:35:ILE:HG13	2.19	0.42
30:X:1033:ARG:HG3	30:X:1039:ILE:HD13	2.01	0.42
30:X:1279:LYS:HA	30:X:1282:ASN:ND2	2.34	0.42
1:A:405:ILE:HD12	2:B:368:PHE:CZ	2.54	0.42
1:A:742:CYS:SG	1:A:747:ILE:HG13	2.59	0.42
11:K:183:GLY:HA2	11:K:207:THR:HG22	2.00	0.42
12:L:186:ALA:HA	12:L:227:ILE:HD13	2.00	0.42
17:P:116:A:C2	17:P:117:A:C5	3.08	0.42
20:Y:251:ASN:O	20:Y:255:GLN:CG	2.66	0.42
21:a:107:PRO:HG3	21:a:116:PHE:CD1	2.54	0.42
24:e:4:LEU:HD12	24:e:4:LEU:O	2.18	0.42
30:X:56:LYS:H	30:X:1224:ARG:CZ	2.31	0.42
30:X:729:ASP:O	30:X:733:GLU:HG3	2.19	0.42
30:X:866:TRP:CZ3	30:X:886:PRO:HD2	2.54	0.42
30:X:1150:ILE:HA	30:X:1154:CYS:HB2	2.00	0.42
31:j:64:ARG:NH1	5:b:15:ASN:OD1	2.48	0.42
4:Z:17:THR:OG1	4:Z:27:ARG:HD3	2.19	0.42
1:A:636:TYR:C	1:A:638:ARG:H	2.27	0.42
1:A:668:VAL:CB	1:A:669:PRO:HD3	2.50	0.42
1:A:1339:VAL:HG22	1:A:1562:TRP:CD2	2.55	0.42
2:B:438:PHE:CD1	2:B:439:PRO:HD2	2.55	0.42
2:B:500:ASP:HB2	2:B:502:ASN:ND2	2.34	0.42
2:B:703:VAL:HG13	2:B:801:VAL:HG13	2.01	0.42
11:K:252:ALA:O	11:K:264:THR:HA	2.19	0.42
11:K:356:HIS:O	11:K:365:MET:HB2	2.19	0.42
11:K:411:SER:C	11:K:412:VAL:HG23	2.44	0.42
18:U:376:SER:CB	18:U:377:PRO:CD	2.98	0.42
28:R:154:ILE:C	28:R:154:ILE:HD12	2.44	0.42
30:X:102:GLN:HA	30:X:105:PHE:HB3	2.01	0.42
30:X:773:ARG:NH2	30:X:946:CYS:O	2.41	0.42
30:X:817:TYR:HA	30:X:820:LEU:HB2	2.01	0.42
30:X:957:THR:O	30:X:960:SER:OG	2.27	0.42
1:A:515:ALA:HA	1:A:518:GLN:HB2	2.02	0.42
1:A:778:HIS:HA	26:h:259:PHE:CZ	2.55	0.42
1:A:1050:SER:HB3	19:W:82:THR:HG21	2.02	0.42
13:M:198:LYS:O	13:M:199:GLN:CB	2.67	0.42
17:P:97:U:H5'	17:P:103:U:OP2	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:Y:261:ARG:NH2	20:Y:261:ARG:CG	2.76	0.42
21:a:88:GLN:NE2	21:a:133:SER:OG	2.53	0.42
27:i:85:PRO:HB2	27:i:86:PRO:HD2	2.02	0.42
28:R:70:MET:HE3	28:R:106:LEU:HD12	2.00	0.42
28:R:111:ILE:HG22	28:R:115:MET:HE2	2.02	0.42
30:X:57:LEU:HG	30:X:1224:ARG:HH22	1.84	0.42
30:X:561:THR:OG1	30:X:569:MET:HA	2.20	0.42
30:X:679:SER:C	30:X:682:PRO:HD3	2.44	0.42
30:X:1276:MET:O	30:X:1280:ARG:HG3	2.19	0.42
1:A:177:ARG:HD2	1:A:644:VAL:HG11	2.01	0.42
1:A:1663:VAL:HG11	1:A:1741:ASN:CB	2.46	0.42
1:A:1836:PRO:HA	1:A:1957:PHE:CE2	2.55	0.42
9:I:7:ASN:HB3	9:I:8:PRO:HD2	2.02	0.42
11:K:346:PHE:CD2	11:K:346:PHE:O	2.72	0.42
21:a:23:CYS:HB3	21:a:80:CYS:HB2	2.01	0.42
22:c:416:LEU:N	22:c:416:LEU:HD23	2.34	0.42
24:e:59:TYR:CZ	24:e:63:LEU:HD11	2.55	0.42
25:g:138:ARG:NH1	25:g:158:ALA:O	2.48	0.42
29:r:398:UNK:O	29:r:402:UNK:N	2.53	0.42
29:r:639:TYR:CD1	29:r:639:TYR:O	2.73	0.42
30:X:32:LEU:HD11	30:X:70:MET:HE1	2.01	0.42
30:X:858:ARG:HB3	30:X:863:LYS:HE3	2.01	0.42
30:X:1140:GLU:O	30:X:1143:VAL:HB	2.19	0.42
1:A:354:PRO:O	1:A:355:SER:HB3	2.19	0.42
1:A:574:LEU:HD22	1:A:574:LEU:HA	1.95	0.42
1:A:1806:ASP:O	1:A:1889:ARG:NH1	2.52	0.42
1:A:1848:THR:O	1:A:1851:TRP:HB2	2.20	0.42
2:B:82:GLU:O	2:B:85:TYR:N	2.42	0.42
2:B:138:THR:HG21	4:D:14:HIS:CE1	2.55	0.42
2:B:312:VAL:HG12	2:B:319:VAL:HG22	2.02	0.42
4:D:15:ILE:HD12	4:D:15:ILE:N	2.35	0.42
12:L:273:LEU:HD22	12:L:313:VAL:O	2.20	0.42
14:N:28:A:H3'	14:N:28:A:N3	2.35	0.42
14:N:82:U:H2'	14:N:83:G:C8	2.55	0.42
17:P:160:A:N9	17:P:171:G:N2	2.67	0.42
18:U:466:LEU:CB	18:U:479:THR:OG1	2.68	0.42
25:g:148:GLU:O	25:g:152:ALA:CB	2.68	0.42
28:R:204:VAL:HG21	28:R:240:ASN:CG	2.45	0.42
29:r:534:PHE:O	29:r:538:GLU:HG2	2.20	0.42
30:X:335:LEU:HD22	30:X:377:PHE:CE2	2.54	0.42
30:X:472:LEU:HD22	30:X:612:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:480:LEU:HD22	30:X:483:PHE:CZ	2.55	0.42
30:X:797:PHE:HD2	30:X:801:HIS:NE2	2.18	0.42
30:X:1056:CYS:HB3	30:X:1060:TYR:HE2	1.84	0.42
30:X:1081:GLY:HA2	30:X:1243:THR:O	2.20	0.42
30:X:1185:THR:O	30:X:1187:GLU:N	2.52	0.42
1:A:354:PRO:O	1:A:355:SER:CB	2.67	0.42
1:A:704:GLN:HG2	1:A:772:TRP:CZ3	2.55	0.42
2:B:125:VAL:CG1	4:D:81:PHE:HE1	2.32	0.42
2:B:688:CYS:SG	2:B:829:VAL:HG13	2.60	0.42
13:M:186:TYR:CD1	21:a:19:PHE:HZ	2.36	0.42
14:N:77:G:N1	14:N:79:C:N4	2.60	0.42
14:N:79:C:H42	17:P:12:G:H21	1.68	0.42
16:Q:500:A:H1'	16:Q:501:A:O5'	2.20	0.42
18:T:98:LYS:HE3	18:U:97:THR:HG21	2.01	0.42
20:Y:54:ILE:O	20:Y:126:SER:HA	2.19	0.42
20:Y:235:LEU:CD1	20:Y:241:LEU:HD11	2.50	0.42
22:c:440:GLN:N	22:c:441:PRO:CD	2.83	0.42
25:g:138:ARG:HG3	25:g:138:ARG:HH11	1.83	0.42
25:g:138:ARG:NH1	25:g:138:ARG:CG	2.83	0.42
25:g:142:GLY:N	25:g:154:LYS:O	2.44	0.42
30:X:74:HIS:O	30:X:77:LEU:CA	2.66	0.42
30:X:882:TYR:OH	30:X:899:ILE:HG23	2.19	0.42
30:X:1067:VAL:O	30:X:1071:PRO:HG2	2.19	0.42
30:X:1239:LYS:HD3	30:X:1264:GLU:HG2	2.02	0.42
31:j:159:GLU:O	31:j:160:VAL:C	2.63	0.42
1:A:1815:HIS:HA	1:A:1816:LYS:CE	2.48	0.42
2:B:573:ILE:HG23	2:B:577:ALA:CB	2.49	0.42
4:D:7:LEU:HD22	5:E:69:ILE:HD11	2.01	0.42
11:K:268:ASP:O	11:K:269:ALA:HB3	2.20	0.42
12:L:218:HIS:HE1	12:L:242:THR:O	2.02	0.42
13:M:270:LYS:HZ3	33:x:372:UNK:CA	2.32	0.42
16:Q:501:A:H4'	16:Q:501:A:OP1	2.20	0.42
17:P:98:G:N7	9:n:40:TYR:CD2	2.88	0.42
17:P:108:U:H6	17:P:108:U:H5''	1.85	0.42
20:Y:164:GLY:C	20:Y:227:LYS:NZ	2.78	0.42
22:c:399:GLY:O	22:c:405:ILE:HD12	2.20	0.42
30:X:414:LEU:HB3	30:X:415:THR:H	1.50	0.42
30:X:462:ARG:NH1	30:X:533:TYR:O	2.53	0.42
30:X:466:LYS:HA	30:X:467:ASN:HA	1.67	0.42
30:X:1113:ALA:O	30:X:1117:VAL:HG23	2.20	0.42
30:X:1196:ASN:HB2	30:X:1199:THR:HG23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:1220:PHE:HB2	30:X:1230:TRP:CZ2	2.55	0.42
30:X:1223:THR:O	30:X:1227:GLU:HG3	2.19	0.42
32:k:71:PHE:CG	32:k:76:MET:HE3	2.55	0.42
2:B:145:ILE:HD11	2:B:230:PRO:C	2.45	0.42
2:B:419:ASP:O	2:B:422:LEU:HB2	2.20	0.42
11:K:347:ALA:CB	11:K:386:MET:HE1	2.50	0.42
17:P:157:G:H2'	17:P:158:C:O4'	2.19	0.42
18:S:64:PRO:HG3	18:T:9:THR:HG21	2.02	0.42
25:g:132:GLN:HA	25:g:135:LYS:HB3	2.02	0.42
30:X:304:TYR:O	30:X:308:LEU:HG	2.20	0.42
30:X:481:ASN:HB2	30:X:506:GLY:C	2.45	0.42
30:X:530:CYS:HB2	30:X:557:PHE:HB2	2.01	0.42
30:X:1100:THR:OG1	30:X:1110:LEU:HG	2.20	0.42
30:X:1157:ASN:HB2	30:X:1160:PHE:CD2	2.55	0.42
1:A:100:ARG:HG3	14:N:24:A:C6	2.54	0.41
1:A:240:ASN:OD1	1:A:245:ARG:O	2.38	0.41
1:A:450:ILE:HD12	1:A:450:ILE:O	2.20	0.41
5:E:35:MET:HE1	5:E:78:LEU:CD1	2.50	0.41
11:K:278:THR:C	11:K:279:ARG:HG2	2.45	0.41
11:K:345:THR:HG22	11:K:358:LYS:HA	2.01	0.41
13:M:183:TYR:OH	25:g:96:ASN:HB2	2.20	0.41
21:a:62:GLN:CA	21:a:62:GLN:HE21	2.32	0.41
28:R:116:LYS:HZ1	33:x:303:UNK:CB	2.31	0.41
28:R:120:ILE:HG21	28:R:151:LEU:HD21	2.02	0.41
29:r:534:PHE:CE1	29:r:560:PHE:HD1	2.37	0.41
29:r:676:UNK:CB	33:x:54:UNK:H2	2.33	0.41
30:X:57:LEU:HG	30:X:1224:ARG:NH2	2.34	0.41
30:X:99:ASN:C	30:X:102:GLN:HE22	2.28	0.41
30:X:748:GLY:HA2	30:X:749:PRO:HD2	1.97	0.41
8:m:20:LEU:HD23	8:m:42:ILE:HG22	2.02	0.41
1:A:221:ALA:N	1:A:222:PRO:CD	2.83	0.41
1:A:504:PHE:CE2	13:M:210:ASP:HB2	2.55	0.41
1:A:921:PHE:HA	1:A:929:ILE:O	2.21	0.41
2:B:667:ILE:CG2	2:B:668:ARG:N	2.83	0.41
2:B:848:VAL:HG22	2:B:913:MET:SD	2.60	0.41
3:C:37:C:H2'	3:C:38:U:C6	2.55	0.41
11:K:287:GLY:C	11:K:288:HIS:O	2.62	0.41
11:K:304:VAL:HB	11:K:316:TRP:HB2	2.02	0.41
12:L:53:VAL:HG23	12:L:332:ARG:HA	2.02	0.41
13:M:233:VAL:CG1	13:M:235:HIS:CD2	3.03	0.41
25:g:156:PRO:CD	25:g:157:TRP:CE3	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:R:120:ILE:CD1	28:R:151:LEU:HD22	2.24	0.41
30:X:820:LEU:O	30:X:823:TRP:HB2	2.20	0.41
30:X:986:GLU:O	30:X:990:THR:HG23	2.20	0.41
1:A:817:TYR:CD1	1:A:817:TYR:C	2.96	0.41
1:A:1053:LEU:HD13	1:A:1053:LEU:C	2.45	0.41
2:B:667:ILE:HG22	2:B:668:ARG:N	2.35	0.41
2:B:933:LYS:HA	2:B:934:PRO:HD3	1.96	0.41
14:N:81:U:O2'	14:N:82:U:H5'	2.20	0.41
19:W:76:LEU:HD12	19:W:83:ILE:HG13	2.02	0.41
20:Y:225:PHE:O	20:Y:225:PHE:CD1	2.70	0.41
21:a:91:LEU:HD13	21:a:96:ARG:HB2	2.02	0.41
25:g:141:PRO:CA	25:g:154:LYS:O	2.66	0.41
29:r:501:LYS:HG3	29:r:502:LEU:HD12	2.02	0.41
29:r:627:ILE:HG22	29:r:631:LEU:HD21	2.02	0.41
1:A:427:LEU:O	1:A:430:ALA:N	2.54	0.41
1:A:1917:PHE:HD1	1:A:1920:ILE:HD11	1.85	0.41
2:B:336:ALA:O	2:B:337:LYS:C	2.63	0.41
8:H:20:LEU:HD23	8:H:42:ILE:HG22	2.02	0.41
11:K:425:PHE:HE2	11:K:441:ALA:HB2	1.85	0.41
18:S:79:GLU:O	18:S:83:VAL:HG23	2.20	0.41
20:Y:198:TRP:HZ3	20:Y:230:MET:HG3	1.82	0.41
23:d:107:ALA:HB1	23:d:108:PRO:HD2	2.03	0.41
24:e:88:LEU:CD2	24:e:92:TRP:CZ2	3.04	0.41
28:R:120:ILE:HG21	28:R:151:LEU:CD2	2.51	0.41
29:r:595:TYR:CE2	29:r:611:ILE:HG13	2.43	0.41
30:X:425:ILE:HG23	30:X:1031:ARG:HD2	2.02	0.41
30:X:594:SER:C	30:X:605:GLN:HE21	2.28	0.41
30:X:815:GLU:HB2	30:X:818:GLY:H	1.84	0.41
30:X:1230:TRP:O	30:X:1234:GLU:HG3	2.21	0.41
1:A:495:LEU:HD23	1:A:496:LEU:CA	2.50	0.41
1:A:495:LEU:HD23	1:A:496:LEU:HA	2.03	0.41
1:A:521:ARG:O	1:A:522:GLN:C	2.62	0.41
11:K:162:HIS:CE1	11:K:182:ALA:HB2	2.56	0.41
11:K:306:THR:O	11:K:337:LEU:HD11	2.20	0.41
17:P:102:U:C3'	17:P:103:U:H5'	2.50	0.41
17:P:104:G:O2'	17:P:105:G:H3'	2.20	0.41
18:S:115:ILE:HG13	18:V:115:ILE:HG22	2.01	0.41
20:Y:49:PRO:O	20:Y:50:ALA:CB	2.68	0.41
30:X:751:ARG:HE	30:X:1177:ARG:HD3	1.86	0.41
30:X:1050:GLU:HG2	30:X:1065:LYS:HD2	2.01	0.41
30:X:1181:VAL:HB	30:X:1207:CYS:SG	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Z:15:ILE:HD12	4:Z:15:ILE:N	2.35	0.41
1:A:511:ASP:OD1	1:A:513:VAL:N	2.48	0.41
2:B:244:ILE:CD1	2:B:274:ARG:HG2	2.51	0.41
3:C:32:C:O2	3:C:32:C:C3'	2.68	0.41
3:C:98:U:H3	4:D:38:ASN:HD21	1.68	0.41
5:E:113:ALA:CB	5:E:114:PRO:CD	2.96	0.41
11:K:183:GLY:HA2	11:K:207:THR:HA	2.03	0.41
11:K:199:LEU:HD13	11:K:201:LEU:HD21	2.02	0.41
12:L:113:SER:HA	12:L:137:VAL:HG13	2.03	0.41
17:P:155:U:H2'	17:P:156:U:H5''	2.02	0.41
24:e:47:ALA:N	24:e:48:PRO:CD	2.83	0.41
25:g:156:PRO:HD2	25:g:157:TRP:CE3	2.55	0.41
26:h:230:VAL:HG23	26:h:231:PHE:CD1	2.55	0.41
28:R:104:ILE:HB	28:R:105:PRO:HD3	2.02	0.41
28:R:130:ALA:O	28:R:131:VAL:C	2.62	0.41
28:R:134:LEU:O	28:R:137:VAL:HG22	2.20	0.41
28:R:174:TRP:O	28:R:177:TYR:HB3	2.20	0.41
29:r:633:VAL:HG22	29:r:647:VAL:HG11	2.03	0.41
30:X:19:TRP:HB2	30:X:61:PHE:CE1	2.51	0.41
30:X:34:CYS:O	30:X:38:ALA:HB3	2.20	0.41
30:X:476:ASN:HB3	30:X:477:PHE:CD2	2.56	0.41
30:X:1066:THR:HG21	37:X:1500:ADP:H2	1.83	0.41
1:A:128:PRO:O	1:A:129:MET:HB2	2.19	0.41
1:A:183:LYS:NZ	1:A:1709:LEU:O	2.45	0.41
1:A:980:GLN:HA	1:A:980:GLN:HE21	1.85	0.41
1:A:1691:ARG:O	1:A:1730:ASP:HA	2.21	0.41
6:F:32:VAL:HG22	6:F:38:THR:HG22	2.03	0.41
10:J:19:VAL:HG12	10:J:20:GLN:N	2.36	0.41
12:L:240:ASP:OD1	12:L:240:ASP:N	2.53	0.41
13:M:127:LEU:HD12	13:M:130:ARG:HD3	2.03	0.41
17:P:99:U:C2	10:o:63:ARG:CZ	3.04	0.41
18:U:180:THR:O	18:U:183:GLN:CG	2.69	0.41
21:a:42:GLN:OE1	21:a:42:GLN:O	2.38	0.41
27:i:180:CYS:O	27:i:184:THR:HG23	2.21	0.41
28:R:116:LYS:HE3	33:x:302:UNK:CB	2.51	0.41
30:X:55:LEU:H	30:X:1224:ARG:HH21	1.67	0.41
30:X:131:PHE:CZ	30:X:232:LEU:HD21	2.55	0.41
30:X:666:TYR:HA	30:X:701:THR:HG22	2.03	0.41
5:b:35:MET:HE1	5:b:78:LEU:CD1	2.50	0.41
1:A:1175:GLY:O	1:A:1176:ARG:C	2.63	0.41
1:A:1449:LYS:O	22:c:598:SER:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:676:PHE:CE1	2:B:892:ILE:HD11	2.55	0.41
11:K:172:GLU:HG2	11:K:213:VAL:HG11	2.02	0.41
12:L:275:VAL:HG12	12:L:276:ALA:N	2.35	0.41
16:Q:503:A:H8	16:Q:503:A:O5'	2.04	0.41
18:S:69:LEU:HD11	18:T:80:TRP:CZ2	2.55	0.41
18:U:65:SER:HB3	18:U:68:SER:HB2	2.02	0.41
20:Y:242:ASN:ND2	20:Y:242:ASN:C	2.73	0.41
25:g:151:GLY:O	25:g:152:ALA:C	2.64	0.41
29:r:545:SER:OG	29:r:546:TYR:N	2.53	0.41
29:r:596:ALA:CB	29:r:612:LEU:HD11	2.51	0.41
30:X:77:LEU:O	30:X:80:MET:HB2	2.21	0.41
30:X:209:TYR:HB3	30:X:214:LYS:HG2	2.03	0.41
30:X:668:ARG:HA	30:X:699:PHE:HB3	2.02	0.41
30:X:941:GLU:HG2	30:X:942:LEU:N	2.35	0.41
1:A:139:VAL:O	1:A:507:SER:HA	2.21	0.41
1:A:576:LEU:HD13	1:A:608:VAL:CG2	2.50	0.41
1:A:803:THR:HG23	1:A:921:PHE:CE1	2.54	0.41
1:A:1018:ARG:O	1:A:1021:SER:OG	2.32	0.41
1:A:1122:PHE:CE2	1:A:1178:VAL:HG11	2.55	0.41
1:A:1271:ILE:HG23	1:A:1286:LYS:HE2	2.03	0.41
1:A:1542:LEU:O	1:A:1546:GLN:NE2	2.42	0.41
2:B:135:LEU:HB3	2:B:562:MET:SD	2.61	0.41
2:B:160:LEU:HD21	2:B:439:PRO:HB3	2.02	0.41
2:B:189:ARG:O	2:B:190:VAL:HB	2.21	0.41
2:B:515:VAL:HG12	2:B:544:ILE:HD11	2.02	0.41
2:B:605:ALA:HB3	2:B:670:SER:HB3	2.02	0.41
7:G:53:LEU:HD23	7:G:73:GLU:HG2	2.02	0.41
11:K:438:THR:O	11:K:445:VAL:HG22	2.21	0.41
12:L:152:THR:HG22	12:L:162:VAL:HG22	2.03	0.41
12:L:215:LEU:H	12:L:215:LEU:CD2	2.30	0.41
12:L:243:VAL:O	12:L:243:VAL:HG12	2.21	0.41
12:L:266:HIS:CD2	12:L:273:LEU:HD12	2.54	0.41
13:M:189:SER:CB	25:g:82:LYS:CD	2.98	0.41
13:M:213:GLU:HA	13:M:214:PRO:HD3	1.94	0.41
14:N:57:C:N3	14:N:66:G:C2	2.88	0.41
14:N:76:C:C5	14:N:77:G:H1'	2.56	0.41
17:P:103:U:N1	7:l:102:ARG:CZ	2.84	0.41
17:P:105:G:OP2	7:l:48:ARG:NH2	2.47	0.41
18:S:91:ARG:O	18:S:95:THR:HG23	2.20	0.41
20:Y:163:MET:CE	20:Y:245:TRP:HB2	2.35	0.41
20:Y:210:ARG:O	20:Y:212:ILE:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:a:30:ASN:OD1	25:g:106:ASN:OD1	2.38	0.41
21:a:134:GLN:HG3	25:g:78:GLN:HE22	1.86	0.41
24:e:64:TYR:OH	24:e:72:THR:HG22	2.20	0.41
24:e:144:SER:O	24:e:145:CYS:CB	2.68	0.41
28:R:142:TYR:CZ	33:x:387:UNK:HA	2.36	0.41
28:R:149:GLU:OE2	28:R:149:GLU:HA	2.21	0.41
28:R:169:PRO:HG2	28:R:173:CYS:SG	2.61	0.41
28:R:407:UNK:C	28:R:409:UNK:H2	2.33	0.41
29:r:576:PHE:CD1	29:r:595:TYR:HB2	2.55	0.41
29:r:580:LEU:HD11	29:r:592:TYR:CE1	2.56	0.41
29:r:644:THR:HA	29:r:647:VAL:HG21	1.97	0.41
30:X:7:LYS:HD3	30:X:10:GLN:NE2	2.35	0.41
30:X:32:LEU:HA	30:X:35:ILE:HD12	2.02	0.41
30:X:252:TYR:OH	30:X:275:ASN:ND2	2.49	0.41
30:X:331:GLN:HB2	30:X:334:LYS:HG3	2.03	0.41
30:X:480:LEU:HB3	30:X:483:PHE:HZ	1.86	0.41
30:X:532:ILE:HD12	30:X:557:PHE:HE2	1.86	0.41
30:X:752:CYS:N	37:X:1500:ADP:O2B	2.54	0.41
30:X:1084:HIS:CD2	30:X:1237:PRO:HG3	2.56	0.41
7:l:53:LEU:HD23	7:l:73:GLU:HG2	2.02	0.41
1:A:1301:ALA:O	1:A:1304:SER:N	2.52	0.41
2:B:220:HIS:CD2	2:B:649:MET:HG2	2.56	0.41
14:N:78:A:C2	28:R:104:ILE:HG21	2.56	0.41
18:U:376:SER:CB	18:U:377:PRO:HD2	2.51	0.41
22:c:486:LEU:HD21	22:c:509:PRO:CB	2.51	0.41
24:e:8:ARG:CG	24:e:8:ARG:NH2	2.83	0.41
27:i:85:PRO:O	27:i:86:PRO:C	2.64	0.41
29:r:455:UNK:O	29:r:459:UNK:N	2.54	0.41
30:X:806:SER:C	30:X:962:ARG:HH22	2.29	0.41
30:X:1087:GLN:HB2	30:X:1212:TYR:CD1	2.56	0.41
1:A:403:PHE:CD1	1:A:403:PHE:C	3.00	0.40
1:A:1346:LEU:HD12	1:A:1508:ILE:HD13	2.03	0.40
1:A:1625:LEU:HD12	1:A:1625:LEU:C	2.46	0.40
1:A:1625:LEU:HA	1:A:1630:ILE:HD12	2.02	0.40
1:A:1661:TRP:CD2	1:A:1743:ILE:HD13	2.56	0.40
2:B:162:VAL:O	2:B:163:TYR:C	2.65	0.40
2:B:290:LEU:O	2:B:291:ARG:C	2.63	0.40
11:K:171:VAL:HG22	11:K:178:PHE:CB	2.50	0.40
11:K:327:LEU:HB3	11:K:357:TRP:CH2	2.56	0.40
16:Q:499:U:O2	17:P:36:G:C2	2.74	0.40
17:P:104:G:H2'	17:P:105:G:C5'	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:P:119:G:C6	17:P:120:C:N4	2.89	0.40
18:V:1:MET:HE2	18:V:58:PHE:CE1	2.56	0.40
20:Y:163:MET:HE3	20:Y:245:TRP:CB	2.39	0.40
26:h:232:ARG:O	26:h:234:THR:N	2.54	0.40
28:R:145:VAL:O	28:R:148:GLU:HB2	2.21	0.40
30:X:46:LYS:HD3	30:X:414:LEU:CD1	2.50	0.40
30:X:265:GLU:HB3	30:X:267:PHE:CE1	2.56	0.40
30:X:285:THR:OG1	30:X:286:ARG:N	2.54	0.40
30:X:486:THR:OG1	30:X:487:SER:N	2.54	0.40
30:X:747:ASN:CG	30:X:1033:ARG:HE	2.29	0.40
30:X:1183:PHE:H	30:X:1213:VAL:HG22	1.85	0.40
9:n:7:ASN:HB3	9:n:8:PRO:HD2	2.02	0.40
1:A:179:ARG:O	1:A:180:LYS:HB3	2.22	0.40
1:A:790:VAL:HG22	1:A:791:ASP:H	1.86	0.40
1:A:1947:TRP:O	1:A:1951:VAL:N	2.54	0.40
2:B:712:ASN:O	2:B:716:ASN:ND2	2.55	0.40
13:M:189:SER:OG	25:g:86:THR:C	2.64	0.40
14:N:22:A:N1	20:Y:117:CYS:HA	2.36	0.40
17:P:102:U:OP1	6:f:63:ASN:OD1	2.40	0.40
19:W:30:ALA:HA	19:W:41:PRO:HG3	2.04	0.40
20:Y:51:ARG:HH12	20:Y:101:ARG:HB3	1.86	0.40
21:a:47:CYS:CB	21:a:73:CYS:HG	2.34	0.40
29:r:503:TYR:CE2	29:r:507:PHE:CE2	3.09	0.40
30:X:784:MET:HE3	30:X:788:PHE:HE2	1.86	0.40
5:b:10:LEU:HD23	5:b:11:ASN:N	2.37	0.40
1:A:408:ASP:OD1	1:A:408:ASP:C	2.65	0.40
1:A:536:LEU:HD12	1:A:539:LEU:CD1	2.51	0.40
1:A:732:ILE:HG22	1:A:762:ILE:HD11	2.02	0.40
1:A:799:LEU:HD23	1:A:799:LEU:C	2.47	0.40
1:A:913:THR:HB	19:W:81:ARG:NH1	2.36	0.40
1:A:1251:GLN:HE21	1:A:1251:GLN:HA	1.86	0.40
2:B:845:VAL:O	2:B:916:ASP:O	2.38	0.40
2:B:875:ILE:N	2:B:875:ILE:HD12	2.36	0.40
14:N:38:G:N1	15:O:100:G:O2'	2.52	0.40
14:N:77:G:N1	14:N:79:C:C5	2.89	0.40
27:i:85:PRO:CB	27:i:86:PRO:CD	3.00	0.40
27:i:93:LEU:O	27:i:97:VAL:HG23	2.21	0.40
28:R:73:TRP:CE3	28:R:96:ALA:HB2	2.56	0.40
29:r:634:LYS:HD2	33:x:124:UNK:HA	1.96	0.40
30:X:722:ASN:OD1	30:X:795:ARG:HG3	2.21	0.40
30:X:762:LEU:HB3	30:X:951:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:929:ARG:N	30:X:930:PRO:HD2	2.36	0.40
31:j:41:ASP:OD1	31:j:64:ARG:HB2	2.21	0.40
31:j:51:ASN:HB2	31:j:73:ASN:OD1	2.20	0.40
1:A:1526:PHE:CE1	22:c:559:VAL:HG11	2.56	0.40
1:A:1810:TYR:HD1	1:A:1811:ARG:N	2.19	0.40
2:B:590:ILE:HG22	2:B:591:PHE:N	2.36	0.40
3:C:13:A:H2'	3:C:14:G:H4'	2.04	0.40
12:L:56:ALA:HA	12:L:66:ALA:O	2.22	0.40
13:M:172:SER:C	13:M:174:VAL:H	2.30	0.40
14:N:76:C:C5	14:N:76:C:OP2	2.74	0.40
17:P:104:G:C6	6:f:20:LYS:CE	3.05	0.40
17:P:133:A:C6	17:P:134:U:C4	3.09	0.40
23:d:107:ALA:HB1	23:d:108:PRO:CD	2.52	0.40
24:e:51:GLN:CB	25:g:157:TRP:CZ2	3.04	0.40
29:r:564:TYR:CD1	29:r:568:HIS:HE1	2.39	0.40
30:X:665:ILE:HB	30:X:702:ASN:O	2.21	0.40
31:j:36:LEU:HB2	31:j:60:PRO:CD	2.51	0.40
1:A:89:LYS:HG3	24:e:34:GLU:HA	2.03	0.40
1:A:187:PHE:CE2	1:A:603:TYR:CD1	3.10	0.40
1:A:273:TYR:CD1	1:A:273:TYR:C	2.98	0.40
1:A:363:ASP:OD1	1:A:363:ASP:N	2.50	0.40
1:A:1020:MET:HE2	1:A:1063:ILE:HG12	2.03	0.40
1:A:1216:GLY:O	1:A:1217:PHE:O	2.40	0.40
1:A:1280:PHE:CE2	1:A:1323:VAL:HG13	2.56	0.40
1:A:1471:LEU:O	1:A:1471:LEU:HD12	2.21	0.40
2:B:751:PRO:HD3	2:B:757:ASN:HD22	1.86	0.40
11:K:309:MET:C	11:K:311:SER:H	2.30	0.40
13:M:188:PRO:HA	25:g:87:GLY:CA	2.43	0.40
19:W:725:LEU:HD12	27:i:159:VAL:CG1	2.45	0.40
20:Y:69:GLN:HE21	20:Y:69:GLN:N	2.20	0.40
20:Y:158:ASP:OD1	20:Y:170:LEU:HD12	2.22	0.40
20:Y:203:ARG:NH2	20:Y:257:ARG:CD	2.63	0.40
20:Y:265:ARG:HH11	20:Y:265:ARG:HG2	1.86	0.40
21:a:47:CYS:HG	21:a:73:CYS:HG	1.52	0.40
22:c:414:LEU:O	22:c:415:CYS:C	2.65	0.40
25:g:95:PRO:CG	25:g:98:VAL:HG23	2.43	0.40
28:R:167:TRP:C	28:R:168:GLU:HG3	2.47	0.40
29:r:612:LEU:CB	29:r:632:LEU:HG	2.52	0.40
30:X:186:VAL:HA	30:X:189:PHE:HD2	1.87	0.40
30:X:306:LEU:HD21	30:X:381:TYR:CZ	2.56	0.40
30:X:347:LEU:HD13	30:X:373:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:X:773:ARG:HB2	30:X:973:PHE:HA	2.04	0.40
30:X:830:LEU:O	30:X:834:ILE:HG13	2.22	0.40
30:X:858:ARG:NH1	30:X:926:GLU:OE2	2.54	0.40
30:X:1049:ARG:HG2	30:X:1209:TYR:HD1	1.87	0.40
30:X:1053:SER:O	30:X:1057:SER:N	2.55	0.40
6:f:32:VAL:HG22	6:f:38:THR:HG22	2.03	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	1956/2363 (83%)	1657 (85%)	220 (11%)	79 (4%)	2	20
2	B	902/984 (92%)	783 (87%)	97 (11%)	22 (2%)	4	29
4	D	94/97 (97%)	80 (85%)	8 (8%)	6 (6%)	1	12
4	Z	78/97 (80%)	71 (91%)	6 (8%)	1 (1%)	9	39
5	E	92/147 (63%)	81 (88%)	9 (10%)	2 (2%)	5	30
5	b	70/147 (48%)	67 (96%)	3 (4%)	0	100	100
6	F	80/117 (68%)	72 (90%)	6 (8%)	2 (2%)	4	28
6	f	80/117 (68%)	72 (90%)	6 (8%)	2 (2%)	4	28
7	G	91/115 (79%)	88 (97%)	3 (3%)	0	100	100
7	l	83/115 (72%)	81 (98%)	2 (2%)	0	100	100
8	H	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
8	m	74/84 (88%)	69 (93%)	5 (7%)	0	100	100
9	I	70/78 (90%)	64 (91%)	4 (6%)	2 (3%)	3	26
9	n	70/78 (90%)	65 (93%)	3 (4%)	2 (3%)	3	26
10	J	71/77 (92%)	66 (93%)	5 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	o	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
11	K	320/473 (68%)	246 (77%)	50 (16%)	24 (8%)	1	9
12	L	285/340 (84%)	239 (84%)	41 (14%)	5 (2%)	6	34
13	M	203/557 (36%)	172 (85%)	22 (11%)	9 (4%)	2	18
18	S	130/488 (27%)	122 (94%)	7 (5%)	1 (1%)	16	49
18	T	132/488 (27%)	123 (93%)	8 (6%)	1 (1%)	16	49
18	U	414/488 (85%)	383 (92%)	20 (5%)	11 (3%)	4	27
18	V	129/488 (26%)	121 (94%)	4 (3%)	4 (3%)	3	25
19	W	266/757 (35%)	244 (92%)	13 (5%)	9 (3%)	3	23
20	Y	234/388 (60%)	200 (86%)	24 (10%)	10 (4%)	2	18
21	a	189/354 (53%)	167 (88%)	18 (10%)	4 (2%)	5	31
22	c	298/639 (47%)	254 (85%)	31 (10%)	13 (4%)	2	18
23	d	153/155 (99%)	137 (90%)	13 (8%)	3 (2%)	6	32
24	e	142/146 (97%)	120 (84%)	17 (12%)	5 (4%)	3	23
25	g	146/558 (26%)	123 (84%)	15 (10%)	8 (6%)	1	14
26	h	86/265 (32%)	75 (87%)	7 (8%)	4 (5%)	2	17
27	i	157/187 (84%)	144 (92%)	10 (6%)	3 (2%)	6	33
28	R	248/674 (37%)	219 (88%)	20 (8%)	9 (4%)	2	22
29	r	130/790 (16%)	120 (92%)	6 (5%)	4 (3%)	3	25
30	X	1143/1284 (89%)	1032 (90%)	87 (8%)	24 (2%)	5	31
31	j	156/239 (65%)	140 (90%)	14 (9%)	2 (1%)	9	39
32	k	87/111 (78%)	85 (98%)	2 (2%)	0	100	100
All	All	9004/14646 (62%)	7917 (88%)	816 (9%)	271 (3%)	5	25

All (271) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	GLY
1	A	68	VAL
1	A	155	ARG
1	A	188	PRO
1	A	232	ALA
1	A	275	TYR
1	A	378	ILE

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Mol	Chain	Res	Type
1	A	438	SER
1	A	441	THR
1	A	562	ARG
1	A	615	TYR
1	A	621	LEU
1	A	648	PRO
1	A	650	CYS
1	A	695	ILE
1	A	965	PRO
1	A	1005	SER
1	A	1038	VAL
1	A	1299	ARG
1	A	1492	ASN
1	A	1523	GLU
1	A	1971	THR
2	B	75	LYS
2	B	105	ILE
2	B	190	VAL
2	B	379	ARG
2	B	932	PRO
4	D	83	VAL
11	K	207	THR
11	K	276	MET
11	K	288	HIS
11	K	302	PRO
11	K	360	PRO
11	K	460	PRO
12	L	221	ILE
13	M	113	HIS
13	M	141	PRO
13	M	190	ASN
13	M	200	ARG
13	M	209	GLN
18	U	53	VAL
18	U	64	PRO
18	U	69	LEU
18	U	201	SER
18	U	217	PRO
18	U	373	PRO
18	V	67	THR
19	W	77	PRO
20	Y	66	GLN

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Mol	Chain	Res	Type
20	Y	73	LEU
21	a	22	ILE
21	a	107	PRO
22	c	391	VAL
22	c	415	CYS
22	c	563	GLY
22	c	564	TYR
24	e	145	CYS
25	g	74	VAL
25	g	158	ALA
27	i	86	PRO
28	R	69	ALA
28	R	169	PRO
28	R	272	PRO
29	r	546	TYR
29	r	547	PRO
30	X	396	PHE
30	X	935	ARG
30	X	1070	SER
30	X	1098	GLN
1	A	73	GLY
1	A	301	LEU
1	A	317	ASP
1	A	415	ASP
1	A	444	ALA
1	A	457	HIS
1	A	691	VAL
1	A	692	ALA
1	A	749	TRP
1	A	753	GLY
1	A	790	VAL
1	A	1115	ILE
1	A	1217	PHE
1	A	1663	VAL
2	B	125	VAL
2	B	150	LEU
2	B	311	ARG
2	B	390	TYR
2	B	549	ALA
2	B	594	ILE
4	D	37	MET
5	E	103	PRO

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Mol	Chain	Res	Type
6	F	12	ASN
9	I	41	MET
11	K	232	TRP
11	K	350	SER
11	K	413	VAL
11	K	459	HIS
11	K	469	LEU
12	L	263	GLY
12	L	331	ASP
13	M	199	GLN
18	S	57	ASP
18	U	270	ILE
19	W	232	ALA
20	Y	58	PRO
20	Y	211	GLY
22	c	379	ALA
22	c	426	VAL
24	e	118	ILE
24	e	132	VAL
25	g	49	ASN
25	g	152	ALA
26	h	233	ASN
27	i	83	LEU
28	R	42	ILE
30	X	36	LEU
30	X	121	VAL
30	X	621	TYR
30	X	1275	GLU
31	j	159	GLU
4	Z	37	MET
6	f	12	ASN
1	A	71	LYS
1	A	205	LEU
1	A	211	ILE
1	A	240	ASN
1	A	246	ARG
1	A	271	ASP
1	A	316	ASN
1	A	494	SER
1	A	618	LYS
1	A	641	THR
1	A	721	PRO

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Mol	Chain	Res	Type
1	A	725	ARG
1	A	791	ASP
1	A	2022	ASN
2	B	87	SER
2	B	123	ASP
11	K	249	GLY
11	K	338	SER
11	K	344	PHE
12	L	133	GLY
18	V	65	SER
19	W	226	PRO
20	Y	57	ARG
20	Y	143	PHE
20	Y	183	PRO
21	a	21	SER
22	c	335	THR
22	c	457	ILE
22	c	614	THR
26	h	43	GLY
28	R	86	PHE
28	R	185	HIS
28	R	202	PRO
29	r	530	PHE
29	r	563	ARG
30	X	363	LYS
30	X	428	LEU
30	X	1186	VAL
1	A	135	ARG
1	A	352	HIS
1	A	355	SER
1	A	391	SER
1	A	486	HIS
1	A	552	THR
1	A	613	GLY
1	A	1324	LYS
1	A	1331	MET
1	A	1543	THR
1	A	1664	SER
2	B	754	ARG
2	B	868	ARG
4	D	96	ARG
11	K	173	PRO

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Mol	Chain	Res	Type
11	K	359	PHE
11	K	466	PRO
12	L	177	LYS
13	M	174	VAL
18	V	63	PRO
19	W	63	ARG
19	W	92	THR
20	Y	251	ASN
20	Y	281	ASP
22	c	385	ARG
22	c	442	GLU
22	c	537	ARG
22	c	539	ILE
23	d	95	PRO
24	e	116	THR
24	e	117	CYS
25	g	70	ALA
26	h	240	ASP
30	X	19	TRP
30	X	311	PHE
30	X	355	TYR
30	X	567	VAL
30	X	1004	ARG
31	j	31	PRO
1	A	269	ARG
1	A	325	HIS
1	A	327	ILE
1	A	622	MET
1	A	643	PRO
1	A	761	MET
2	B	83	GLU
2	B	177	LEU
2	B	662	TYR
2	B	750	GLY
4	D	90	PRO
6	F	62	GLY
9	I	42	ASN
11	K	150	HIS
11	K	161	GLY
11	K	257	PRO
11	K	455	THR
13	M	140	LYS

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Mol	Chain	Res	Type
13	M	196	LEU
18	U	60	ARG
19	W	9	TRP
19	W	37	VAL
20	Y	163	MET
25	g	31	ALA
28	R	87	ALA
30	X	76	ASN
30	X	415	THR
30	X	846	SER
6	f	62	GLY
9	n	41	MET
9	n	42	ASN
1	A	187	PHE
1	A	432	HIS
1	A	793	THR
1	A	825	THR
2	B	812	PRO
4	D	91	LEU
11	K	287	GLY
11	K	324	LEU
18	U	415	PRO
21	a	267	SER
25	g	143	ASP
30	X	465	ILE
30	X	528	PHE
30	X	970	GLY
30	X	1192	SER
1	A	723	GLY
5	E	113	ALA
11	K	203	GLY
25	g	64	GLN
30	X	39	VAL
1	A	326	PRO
1	A	1720	PRO
2	B	424	PRO
4	D	95	GLY
18	U	219	PRO
27	i	11	PRO
1	A	642	GLY
1	A	1143	PRO
18	T	20	GLY

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Mol	Chain	Res	Type
19	W	231	PRO
26	h	241	THR
28	R	201	HIS
1	A	129	MET
18	V	20	GLY
19	W	225	ILE
23	d	86	GLY
1	A	206	GLU
1	A	668	VAL
2	B	601	VAL
18	U	376	SER
23	d	69	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1775/2138 (83%)	1557 (88%)	218 (12%)	4	23
2	B	809/881 (92%)	755 (93%)	54 (7%)	15	42
4	D	85/86 (99%)	75 (88%)	10 (12%)	5	24
4	Z	72/86 (84%)	63 (88%)	9 (12%)	4	22
5	E	80/118 (68%)	76 (95%)	4 (5%)	22	49
5	b	66/118 (56%)	61 (92%)	5 (8%)	12	39
6	F	77/102 (76%)	71 (92%)	6 (8%)	11	38
6	f	77/102 (76%)	71 (92%)	6 (8%)	11	38
7	G	81/101 (80%)	79 (98%)	2 (2%)	42	63
7	l	76/101 (75%)	75 (99%)	1 (1%)	61	72
8	H	69/76 (91%)	64 (93%)	5 (7%)	13	40
8	m	69/76 (91%)	64 (93%)	5 (7%)	13	40
9	I	64/69 (93%)	60 (94%)	4 (6%)	16	44
9	n	64/69 (93%)	60 (94%)	4 (6%)	16	44

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
10	J	63/67 (94%)	58 (92%)	5 (8%)	11	37
10	o	63/67 (94%)	58 (92%)	5 (8%)	11	37
11	K	261/278 (94%)	239 (92%)	22 (8%)	10	35
12	L	251/292 (86%)	235 (94%)	16 (6%)	16	43
13	M	182/477 (38%)	167 (92%)	15 (8%)	10	36
18	S	120/443 (27%)	112 (93%)	8 (7%)	15	42
18	T	123/443 (28%)	111 (90%)	12 (10%)	7	31
18	U	223/443 (50%)	205 (92%)	18 (8%)	11	36
18	V	118/443 (27%)	111 (94%)	7 (6%)	18	45
19	W	234/294 (80%)	216 (92%)	18 (8%)	12	38
20	Y	194/253 (77%)	165 (85%)	29 (15%)	3	17
21	a	142/222 (64%)	123 (87%)	19 (13%)	4	21
22	c	259/579 (45%)	234 (90%)	25 (10%)	8	31
23	d	129/129 (100%)	126 (98%)	3 (2%)	44	64
24	e	130/132 (98%)	120 (92%)	10 (8%)	12	38
25	g	78/496 (16%)	62 (80%)	16 (20%)	1	8
26	h	79/240 (33%)	69 (87%)	10 (13%)	4	22
27	i	118/163 (72%)	106 (90%)	12 (10%)	7	30
28	R	224/224 (100%)	196 (88%)	28 (12%)	4	22
29	r	117/136 (86%)	104 (89%)	13 (11%)	6	27
30	X	1106/1188 (93%)	1098 (99%)	8 (1%)	76	78
31	j	87/214 (41%)	83 (95%)	4 (5%)	24	51
32	k	49/96 (51%)	47 (96%)	2 (4%)	27	53
All	All	7814/11442 (68%)	7176 (92%)	638 (8%)	13	36

All (638) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	65	LYS
1	A	69	LYS
1	A	77	THR
1	A	85	GLU
1	A	87	LEU
1	A	91	MET

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Mol	Chain	Res	Type
1	A	108	SER
1	A	110	LEU
1	A	124	LEU
1	A	127	MET
1	A	129	MET
1	A	137	VAL
1	A	139	VAL
1	A	147	ILE
1	A	148	THR
1	A	153	SER
1	A	156	VAL
1	A	167	THR
1	A	183	LYS
1	A	197	PHE
1	A	206	GLU
1	A	211	ILE
1	A	229	GLU
1	A	239	VAL
1	A	246	ARG
1	A	249	LEU
1	A	250	ASN
1	A	254	MET
1	A	263	GLN
1	A	269	ARG
1	A	277	PHE
1	A	280	ASN
1	A	284	THR
1	A	292	ILE
1	A	301	LEU
1	A	316	ASN
1	A	319	TYR
1	A	328	LYS
1	A	331	TYR
1	A	344	ARG
1	A	365	ASP
1	A	366	LEU
1	A	387	GLU
1	A	388	LEU
1	A	403	PHE
1	A	404	GLU
1	A	408	ASP
1	A	414	GLU

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Mol	Chain	Res	Type
1	A	428	LEU
1	A	435	ASN
1	A	436	LYS
1	A	443	ARG
1	A	445	GLN
1	A	465	LYS
1	A	467	ARG
1	A	469	SER
1	A	473	LEU
1	A	474	LEU
1	A	478	VAL
1	A	484	MET
1	A	494	SER
1	A	495	LEU
1	A	497	ARG
1	A	500	LYS
1	A	503	LYS
1	A	507	SER
1	A	518	GLN
1	A	522	GLN
1	A	529	LEU
1	A	536	LEU
1	A	537	THR
1	A	547	LEU
1	A	553	LEU
1	A	569	LEU
1	A	570	MET
1	A	572	GLU
1	A	573	ILE
1	A	574	LEU
1	A	575	ARG
1	A	578	LYS
1	A	580	ILE
1	A	587	TYR
1	A	588	ARG
1	A	589	LEU
1	A	593	ASP
1	A	597	LEU
1	A	608	VAL
1	A	616	ARG
1	A	618	LYS
1	A	622	MET

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Mol	Chain	Res	Type
1	A	628	CYS
1	A	646	LYS
1	A	656	SER
1	A	667	ILE
1	A	668	VAL
1	A	670	LEU
1	A	671	LEU
1	A	675	LEU
1	A	678	LEU
1	A	693	LYS
1	A	705	ASP
1	A	708	LEU
1	A	713	MET
1	A	714	ASN
1	A	720	ILE
1	A	728	LYS
1	A	751	VAL
1	A	754	LEU
1	A	759	GLU
1	A	761	MET
1	A	768	SER
1	A	781	ARG
1	A	792	LYS
1	A	808	LYS
1	A	810	GLU
1	A	812	GLU
1	A	814	GLN
1	A	817	TYR
1	A	839	TRP
1	A	856	LYS
1	A	860	LYS
1	A	862	LEU
1	A	879	LEU
1	A	884	ARG
1	A	900	MET
1	A	912	ARG
1	A	920	GLU
1	A	937	MET
1	A	949	LEU
1	A	952	GLU
1	A	969	GLU
1	A	974	LEU

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Mol	Chain	Res	Type
1	A	978	TRP
1	A	980	GLN
1	A	996	CYS
1	A	1001	GLU
1	A	1010	LYS
1	A	1015	LEU
1	A	1050	SER
1	A	1053	LEU
1	A	1055	ARG
1	A	1066	PHE
1	A	1069	LEU
1	A	1076	LEU
1	A	1078	LEU
1	A	1080	ARG
1	A	1110	LEU
1	A	1113	ARG
1	A	1120	ILE
1	A	1121	MET
1	A	1130	ARG
1	A	1153	LYS
1	A	1174	LEU
1	A	1188	ARG
1	A	1196	GLU
1	A	1210	LEU
1	A	1221	ILE
1	A	1222	LEU
1	A	1226	ARG
1	A	1228	ASN
1	A	1230	GLU
1	A	1233	LEU
1	A	1251	GLN
1	A	1270	GLN
1	A	1282	LYS
1	A	1283	ILE
1	A	1289	THR
1	A	1305	THR
1	A	1308	LEU
1	A	1318	LYS
1	A	1329	SER
1	A	1334	ARG
1	A	1352	LEU
1	A	1358	LEU

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Mol	Chain	Res	Type
1	A	1392	LEU
1	A	1412	GLU
1	A	1440	ILE
1	A	1465	GLU
1	A	1472	LEU
1	A	1480	THR
1	A	1482	GLN
1	A	1546	GLN
1	A	1550	LEU
1	A	1560	LEU
1	A	1576	GLN
1	A	1590	ILE
1	A	1593	LEU
1	A	1605	LEU
1	A	1684	TYR
1	A	1710	ASP
1	A	1737	SER
1	A	1767	LEU
1	A	1784	GLU
1	A	1811	ARG
1	A	1816	LYS
1	A	1817	THR
1	A	1818	PHE
1	A	1819	GLU
1	A	1828	ASN
1	A	1843	LEU
1	A	1844	LYS
1	A	1845	VAL
1	A	1846	ILE
1	A	1847	HIS
1	A	1848	THR
1	A	1849	SER
1	A	1850	VAL
1	A	1851	TRP
1	A	1855	LYS
1	A	1857	LEU
1	A	1883	ARG
1	A	1901	LEU
1	A	1960	LEU
1	A	1962	LEU
1	A	1973	LYS
1	A	1974	THR

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Mol	Chain	Res	Type
1	A	1975	LYS
1	A	1976	LEU
2	B	76	GLN
2	B	85	TYR
2	B	99	GLN
2	B	101	LEU
2	B	105	ILE
2	B	112	LYS
2	B	118	THR
2	B	129	GLU
2	B	138	THR
2	B	145	ILE
2	B	152	HIS
2	B	157	LEU
2	B	173	LYS
2	B	175	ARG
2	B	196	THR
2	B	200	LEU
2	B	225	ASP
2	B	237	VAL
2	B	265	ILE
2	B	275	LEU
2	B	280	ARG
2	B	313	SER
2	B	320	CYS
2	B	346	ILE
2	B	395	LEU
2	B	397	ILE
2	B	423	ASP
2	B	428	LEU
2	B	460	LYS
2	B	546	VAL
2	B	564	VAL
2	B	570	ASP
2	B	579	ILE
2	B	584	LEU
2	B	594	ILE
2	B	646	THR
2	B	658	LEU
2	B	661	LEU
2	B	678	GLU
2	B	773	LEU

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Mol	Chain	Res	Type
2	B	834	PHE
2	B	846	TYR
2	B	847	MET
2	B	868	ARG
2	B	875	ILE
2	B	877	ARG
2	B	901	LEU
2	B	902	ARG
2	B	913	MET
2	B	931	LYS
2	B	933	LYS
2	B	945	ARG
2	B	961	VAL
2	B	969	GLN
4	D	8	LEU
4	D	12	GLN
4	D	25	THR
4	D	29	LYS
4	D	41	MET
4	D	47	THR
4	D	55	HIS
4	D	58	GLN
4	D	83	VAL
4	D	94	ARG
5	E	28	LEU
5	E	31	PHE
5	E	70	LEU
5	E	102	ARG
6	F	3	LEU
6	F	6	PHE
6	F	13	GLU
6	F	41	LYS
6	F	46	THR
6	F	61	ARG
7	G	101	LEU
7	G	104	ASP
8	H	23	HIS
8	H	43	ARG
8	H	49	MET
8	H	62	LYS
8	H	68	LEU
9	I	15	LEU

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Mol	Chain	Res	Type
9	I	34	LEU
9	I	35	GLN
9	I	72	TRP
10	J	3	LYS
10	J	26	LYS
10	J	48	GLU
10	J	63	ARG
10	J	75	LYS
11	K	154	THR
11	K	169	VAL
11	K	170	ASP
11	K	191	ASP
11	K	200	THR
11	K	205	ILE
11	K	216	ARG
11	K	217	HIS
11	K	231	CYS
11	K	248	SER
11	K	253	LEU
11	K	261	VAL
11	K	273	VAL
11	K	282	VAL
11	K	291	THR
11	K	297	VAL
11	K	352	ASP
11	K	356	HIS
11	K	379	SER
11	K	388	SER
11	K	392	ASN
11	K	447	ILE
12	L	44	LEU
12	L	46	MET
12	L	98	ASP
12	L	104	ASP
12	L	110	CYS
12	L	154	VAL
12	L	157	ASP
12	L	215	LEU
12	L	218	HIS
12	L	219	LYS
12	L	222	ILE
12	L	233	SER

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Mol	Chain	Res	Type
12	L	269	GLU
12	L	290	ASP
12	L	306	LEU
12	L	315	HIS
13	M	118	GLN
13	M	130	ARG
13	M	131	LEU
13	M	139	GLU
13	M	161	LEU
13	M	202	ILE
13	M	216	LYS
13	M	221	LYS
13	M	224	ARG
13	M	234	LEU
13	M	240	LYS
13	M	254	SER
13	M	258	TRP
13	M	305	GLU
13	M	315	LYS
18	S	11	LYS
18	S	26	ARG
18	S	54	LYS
18	S	62	ARG
18	S	69	LEU
18	S	101	LEU
18	S	105	LEU
18	S	112	LEU
18	T	11	LYS
18	T	37	LYS
18	T	55	VAL
18	T	60	ARG
18	T	72	LEU
18	T	76	PHE
18	T	77	GLN
18	T	85	LEU
18	T	90	LEU
18	T	91	ARG
18	T	99	GLN
18	T	101	LEU
18	U	11	LYS
18	U	14	VAL
18	U	54	LYS

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Mol	Chain	Res	Type
18	U	76	PHE
18	U	87	GLN
18	U	94	LEU
18	U	118	LEU
18	U	127	GLU
18	U	175	SER
18	U	184	PRO
18	U	209	THR
18	U	217	PRO
18	U	258	THR
18	U	276	PRO
18	U	278	SER
18	U	279	SER
18	U	341	VAL
18	U	415	PRO
18	V	11	LYS
18	V	62	ARG
18	V	85	LEU
18	V	87	GLN
18	V	92	ARG
18	V	101	LEU
18	V	105	LEU
19	W	10	LYS
19	W	23	LYS
19	W	35	LEU
19	W	40	THR
19	W	60	GLU
19	W	68	LYS
19	W	76	LEU
19	W	79	GLN
19	W	82	THR
19	W	170	LEU
19	W	186	GLN
19	W	202	LEU
19	W	228	GLU
19	W	693	LEU
19	W	704	LEU
19	W	707	GLU
19	W	723	LEU
19	W	743	GLU
20	Y	52	LYS
20	Y	55	GLU

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Mol	Chain	Res	Type
20	Y	56	THR
20	Y	59	GLU
20	Y	65	GLU
20	Y	66	GLN
20	Y	69	GLN
20	Y	70	VAL
20	Y	75	TYR
20	Y	117	CYS
20	Y	153	ARG
20	Y	171	ARG
20	Y	188	GLU
20	Y	203	ARG
20	Y	224	GLN
20	Y	227	LYS
20	Y	230	MET
20	Y	241	LEU
20	Y	247	THR
20	Y	248	THR
20	Y	251	ASN
20	Y	259	GLN
20	Y	260	ARG
20	Y	261	ARG
20	Y	262	LEU
20	Y	265	ARG
20	Y	271	LYS
20	Y	274	LEU
20	Y	286	LYS
21	a	21	SER
21	a	27	LEU
21	a	38	GLU
21	a	42	GLN
21	a	45	LYS
21	a	47	CYS
21	a	49	LYS
21	a	60	ARG
21	a	62	GLN
21	a	78	ASN
21	a	87	LEU
21	a	91	LEU
21	a	101	LYS
21	a	109	ASN
21	a	118	GLN

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Mol	Chain	Res	Type
21	a	237	PRO
21	a	244	SER
21	a	246	ARG
21	a	268	PRO
22	c	345	LEU
22	c	350	ARG
22	c	385	ARG
22	c	414	LEU
22	c	416	LEU
22	c	429	LEU
22	c	430	SER
22	c	432	ARG
22	c	440	GLN
22	c	443	LEU
22	c	467	TRP
22	c	471	ARG
22	c	492	GLU
22	c	499	ARG
22	c	515	LEU
22	c	523	ARG
22	c	549	TYR
22	c	560	LYS
22	c	562	LEU
22	c	564	TYR
22	c	568	TRP
22	c	600	LEU
22	c	601	ASN
22	c	610	LYS
22	c	616	LYS
23	d	71	LYS
23	d	115	LYS
23	d	151	LYS
24	e	8	ARG
24	e	17	ASP
24	e	30	MET
24	e	49	ILE
24	e	85	ASP
24	e	100	LEU
24	e	106	ILE
24	e	113	PHE
24	e	116	THR
24	e	126	LEU

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Mol	Chain	Res	Type
25	g	56	ASN
25	g	67	LEU
25	g	71	ASN
25	g	77	GLU
25	g	81	ILE
25	g	86	THR
25	g	91	ARG
25	g	101	GLN
25	g	102	GLU
25	g	137	ARG
25	g	138	ARG
25	g	143	ASP
25	g	145	SER
25	g	146	ILE
25	g	148	GLU
25	g	154	LYS
26	h	39	GLN
26	h	40	GLU
26	h	42	GLN
26	h	44	THR
26	h	59	ARG
26	h	227	GLU
26	h	236	LYS
26	h	241	THR
26	h	243	ARG
26	h	250	MET
27	i	18	ASN
27	i	31	GLU
27	i	83	LEU
27	i	88	THR
27	i	102	GLN
27	i	111	LEU
27	i	114	LYS
27	i	118	LYS
27	i	132	GLU
27	i	153	LYS
27	i	155	TYR
27	i	156	GLN
28	R	41	ASN
28	R	48	LEU
28	R	68	LEU
28	R	70	MET

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Mol	Chain	Res	Type
28	R	83	GLN
28	R	88	ARG
28	R	101	SER
28	R	112	GLU
28	R	122	HIS
28	R	127	PHE
28	R	131	VAL
28	R	134	LEU
28	R	148	GLU
28	R	149	GLU
28	R	161	PHE
28	R	162	GLU
28	R	166	LYS
28	R	171	GLU
28	R	180	MET
28	R	194	TYR
28	R	201	HIS
28	R	203	GLU
28	R	238	PHE
28	R	258	GLU
28	R	272	PRO
28	R	273	ARG
28	R	275	LYS
28	R	279	LEU
29	r	555	LEU
29	r	625	LEU
29	r	628	TYR
29	r	631	LEU
29	r	639	TYR
29	r	642	LEU
29	r	644	THR
29	r	645	ARG
29	r	646	THR
29	r	647	VAL
29	r	649	GLU
29	r	650	LYS
29	r	652	ILE
30	X	70	MET
30	X	71	SER
30	X	73	ASN
30	X	111	VAL
30	X	113	LEU

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Mol	Chain	Res	Type
30	X	117	LEU
30	X	119	GLU
30	X	377	PHE
31	j	64	ARG
31	j	78	ILE
31	j	80	PRO
31	j	91	THR
32	k	43	PRO
32	k	56	PRO
4	Z	8	LEU
4	Z	12	GLN
4	Z	25	THR
4	Z	27	ARG
4	Z	29	LYS
4	Z	41	MET
4	Z	47	THR
4	Z	55	HIS
4	Z	58	GLN
5	b	28	LEU
5	b	31	PHE
5	b	43	GLN
5	b	64	MET
5	b	70	LEU
6	f	3	LEU
6	f	6	PHE
6	f	13	GLU
6	f	41	LYS
6	f	46	THR
6	f	61	ARG
7	l	101	LEU
8	m	23	HIS
8	m	43	ARG
8	m	49	MET
8	m	62	LYS
8	m	68	LEU
9	n	15	LEU
9	n	34	LEU
9	n	35	GLN
9	n	72	TRP
10	o	3	LYS
10	o	26	LYS
10	o	48	GLU

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Mol	Chain	Res	Type
10	o	63	ARG
10	o	75	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (181) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	86	HIS
1	A	151	ASN
1	A	240	ASN
1	A	250	ASN
1	A	253	GLN
1	A	263	GLN
1	A	272	ASN
1	A	289	ASN
1	A	316	ASN
1	A	356	ASN
1	A	376	ASN
1	A	420	HIS
1	A	435	ASN
1	A	457	HIS
1	A	483	HIS
1	A	518	GLN
1	A	532	HIS
1	A	586	GLN
1	A	591	ASN
1	A	596	GLN
1	A	677	ASN
1	A	698	GLN
1	A	714	ASN
1	A	947	GLN
1	A	980	GLN
1	A	983	ASN
1	A	1017	ASN
1	A	1027	ASN
1	A	1049	ASN
1	A	1140	ASN
1	A	1150	ASN
1	A	1227	GLN
1	A	1251	GLN
1	A	1407	GLN
1	A	1422	GLN
1	A	1424	ASN

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Mol	Chain	Res	Type
1	A	1475	ASN
1	A	1490	GLN
1	A	1552	GLN
1	A	1576	GLN
1	A	1578	GLN
1	A	1629	GLN
1	A	1734	ASN
1	A	1815	HIS
1	A	1847	HIS
1	A	1854	GLN
2	B	76	GLN
2	B	99	GLN
2	B	111	HIS
2	B	120	ASN
2	B	166	HIS
2	B	220	HIS
2	B	261	HIS
2	B	371	GLN
2	B	449	HIS
2	B	694	ASN
2	B	821	GLN
2	B	917	HIS
2	B	919	GLN
4	D	9	HIS
4	D	14	HIS
4	D	38	ASN
4	D	40	GLN
4	D	58	GLN
4	D	65	HIS
6	F	12	ASN
6	F	63	ASN
7	G	34	GLN
7	G	35	GLN
7	G	40	HIS
8	H	33	GLN
8	H	64	ASN
8	H	77	ASN
9	I	13	GLN
9	I	28	GLN
9	I	44	GLN
11	K	217	HIS
11	K	246	HIS

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Mol	Chain	Res	Type
11	K	329	HIS
11	K	376	ASN
11	K	414	GLN
12	L	187	GLN
12	L	209	ASN
12	L	213	HIS
12	L	218	HIS
12	L	266	HIS
12	L	292	ASN
12	L	322	GLN
13	M	118	GLN
13	M	158	GLN
13	M	167	GLN
13	M	177	GLN
13	M	191	GLN
13	M	219	HIS
13	M	246	GLN
13	M	247	GLN
18	S	43	GLN
18	V	87	GLN
19	W	28	GLN
19	W	172	ASN
19	W	186	GLN
20	Y	66	GLN
20	Y	69	GLN
20	Y	172	GLN
20	Y	194	HIS
20	Y	208	ASN
20	Y	222	ASN
20	Y	232	HIS
20	Y	233	GLN
20	Y	242	ASN
20	Y	251	ASN
20	Y	259	GLN
21	a	62	GLN
21	a	81	GLN
21	a	88	GLN
21	a	118	GLN
21	a	121	GLN
21	a	134	GLN
22	c	347	ASN
22	c	349	GLN

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Mol	Chain	Res	Type
22	c	601	ASN
23	d	3	ASN
23	d	21	HIS
23	d	116	HIS
24	e	107	GLN
25	g	56	ASN
25	g	78	GLN
26	h	32	HIS
26	h	39	GLN
27	i	82	GLN
27	i	130	GLN
27	i	156	GLN
28	R	41	ASN
28	R	83	GLN
28	R	117	ASN
28	R	119	ASN
28	R	122	HIS
28	R	125	ASN
28	R	159	GLN
28	R	187	ASN
28	R	219	ASN
28	R	225	GLN
28	R	240	ASN
29	r	629	ASN
30	X	53	HIS
30	X	73	ASN
30	X	166	HIS
30	X	192	HIS
30	X	243	HIS
30	X	305	HIS
30	X	416	ASN
30	X	522	ASN
30	X	544	HIS
30	X	564	ASN
30	X	593	HIS
30	X	605	GLN
30	X	740	GLN
30	X	755	HIS
30	X	766	GLN
30	X	798	HIS
30	X	847	HIS
30	X	906	ASN

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Mol	Chain	Res	Type
30	X	983	ASN
30	X	1084	HIS
30	X	1108	GLN
30	X	1156	HIS
30	X	1252	HIS
30	X	1282	ASN
4	Z	9	HIS
4	Z	38	ASN
4	Z	40	GLN
4	Z	58	GLN
5	b	27	GLN
6	f	12	ASN
7	l	34	GLN
7	l	35	GLN
7	l	40	HIS
8	m	33	GLN
8	m	77	ASN
9	n	13	GLN
9	n	44	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
14	N	89/99 (89%)	53 (59%)	12 (13%)
15	O	8/8 (100%)	3 (37%)	1 (12%)
16	Q	12/13 (92%)	4 (33%)	2 (16%)
17	P	106/186 (56%)	28 (26%)	8 (7%)
3	C	104/120 (86%)	54 (51%)	13 (12%)
All	All	319/426 (74%)	142 (44%)	36 (11%)

All (142) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	C	9	U
3	C	14	G
3	C	18	U
3	C	19	U
3	C	20	U
3	C	24	A
3	C	26	A
3	C	27	G

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Mol	Chain	Res	Type
3	C	28	C
3	C	29	U
3	C	30	A
3	C	31	A
3	C	32	C
3	C	33	G
3	C	34	U
3	C	35	A
3	C	36	U
3	C	37	C
3	C	43	C
3	C	45	U
3	C	48	C
3	C	49	U
3	C	50	U
3	C	51	U
3	C	52	U
3	C	54	C
3	C	56	A
3	C	57	G
3	C	60	A
3	C	61	C
3	C	62	A
3	C	63	G
3	C	66	G
3	C	73	A
3	C	79	G
3	C	80	C
3	C	81	U
3	C	82	A
3	C	83	A
3	C	87	G
3	C	90	U
3	C	91	G
3	C	92	U
3	C	93	A
3	C	94	U
3	C	95	A
3	C	96	G
3	C	97	U
3	C	98	U
3	C	99	U

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Mol	Chain	Res	Type
3	C	100	U
3	C	101	U
3	C	102	G
3	C	103	U
14	N	5	U
14	N	6	U
14	N	7	C
14	N	8	G
14	N	9	G
14	N	11	U
14	N	14	C
14	N	18	G
14	N	19	G
14	N	21	C
14	N	22	A
14	N	23	A
14	N	24	A
14	N	25	U
14	N	26	U
14	N	27	G
14	N	28	A
14	N	29	A
14	N	30	A
14	N	31	C
14	N	40	G
14	N	43	G
14	N	45	U
14	N	47	A
14	N	48	G
14	N	50	A
14	N	52	G
14	N	53	G
14	N	54	C
14	N	55	C
14	N	56	C
14	N	58	U
14	N	60	C
14	N	61	A
14	N	62	C
14	N	63	A
14	N	64	A
14	N	65	G

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Mol	Chain	Res	Type
14	N	68	U
14	N	72	A
14	N	73	C
14	N	74	U
14	N	75	G
14	N	76	C
14	N	77	G
14	N	78	A
14	N	79	C
14	N	80	A
14	N	81	U
14	N	82	U
14	N	83	G
14	N	89	A
14	N	90	A
15	O	101	U
15	O	102	A
15	O	104	G
16	Q	499	U
16	Q	500	A
16	Q	501	A
16	Q	502	C
17	P	14	C
17	P	15	U
17	P	16	U
17	P	17	U
17	P	18	U
17	P	19	G
17	P	20	G
17	P	24	A
17	P	25	G
17	P	26	A
17	P	27	U
17	P	29	A
17	P	30	A
17	P	31	G
17	P	104	G
17	P	105	G
17	P	107	U
17	P	108	U
17	P	117	A
17	P	118	A

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Mol	Chain	Res	Type
17	P	156	U
17	P	157	G
17	P	164	C
17	P	165	A
17	P	168	A
17	P	169	C
17	P	171	G
17	P	177	C

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	C	13	A
3	C	27	G
3	C	28	C
3	C	30	A
3	C	31	A
3	C	36	U
3	C	50	U
3	C	60	A
3	C	90	U
3	C	91	G
3	C	94	U
3	C	96	G
3	C	100	U
14	N	10	A
14	N	14	C
14	N	17	U
14	N	21	C
14	N	22	A
14	N	24	A
14	N	30	A
14	N	39	A
14	N	52	G
14	N	60	C
14	N	72	A
14	N	77	G
15	O	100	G
16	Q	500	A
16	Q	501	A
17	P	14	C
17	P	17	U

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Mol	Chain	Res	Type
17	P	18	U
17	P	24	A
17	P	104	G
17	P	156	U
17	P	164	C
17	P	168	A

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	ADP	X	1500	-	28,29,29	1.42	4 (14%)	43,45,45	1.85	9 (20%)
34	GDP	B	1000	-	29,30,30	1.44	4 (13%)	45,47,47	1.76	5 (11%)

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
37	ADP	X	1500	-	-	7/16/32/32	0/3/3/3
34	GDP	B	1000	-	-	5/16/32/32	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	X	1500	ADP	C5-C4	4.75	1.47	1.39
34	B	1000	GDP	PA-O3A	4.52	1.64	1.59
34	B	1000	GDP	C5-C4	3.03	1.47	1.38
37	X	1500	ADP	C5-C6	2.77	1.48	1.41
34	B	1000	GDP	C5-N7	-2.63	1.33	1.39
34	B	1000	GDP	C6-N1	-2.50	1.34	1.38
37	X	1500	ADP	C8-N7	2.36	1.36	1.31
37	X	1500	ADP	C5-N7	-2.22	1.35	1.39

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	1000	GDP	C5-C4-N3	-6.19	118.54	128.39
37	X	1500	ADP	C5-C4-N3	-5.84	118.68	126.72
34	B	1000	GDP	N9-C4-N3	5.22	136.40	125.95
37	X	1500	ADP	N3-C4-N9	4.63	135.04	127.17
34	B	1000	GDP	C2-N3-C4	4.60	120.23	112.30
37	X	1500	ADP	C2-N3-C4	3.70	120.86	111.83
37	X	1500	ADP	C4-C5-N7	-3.49	106.59	110.58
37	X	1500	ADP	N3-C2-N1	-3.18	123.77	128.58
37	X	1500	ADP	C4-N9-C8	2.64	108.51	105.74
34	B	1000	GDP	O6-C6-C5	-2.56	119.77	126.53
37	X	1500	ADP	C5-N7-C8	2.55	107.45	103.45
37	X	1500	ADP	C3'-C2'-C1'	2.53	106.25	101.46
34	B	1000	GDP	C6-C5-N7	2.11	134.13	130.29
37	X	1500	ADP	C6-C5-N7	2.11	136.15	132.09

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	B	1000	GDP	C5'-O5'-PA-O3A
37	X	1500	ADP	C5'-O5'-PA-O3A
37	X	1500	ADP	C4'-C5'-O5'-PA
34	B	1000	GDP	C3'-C4'-C5'-O5'
37	X	1500	ADP	O4'-C1'-N9-C8
37	X	1500	ADP	O4'-C1'-N9-C4
34	B	1000	GDP	O4'-C4'-C5'-O5'
37	X	1500	ADP	PB-O3A-PA-O1A
34	B	1000	GDP	C5'-O5'-PA-O1A
37	X	1500	ADP	C5'-O5'-PA-O1A

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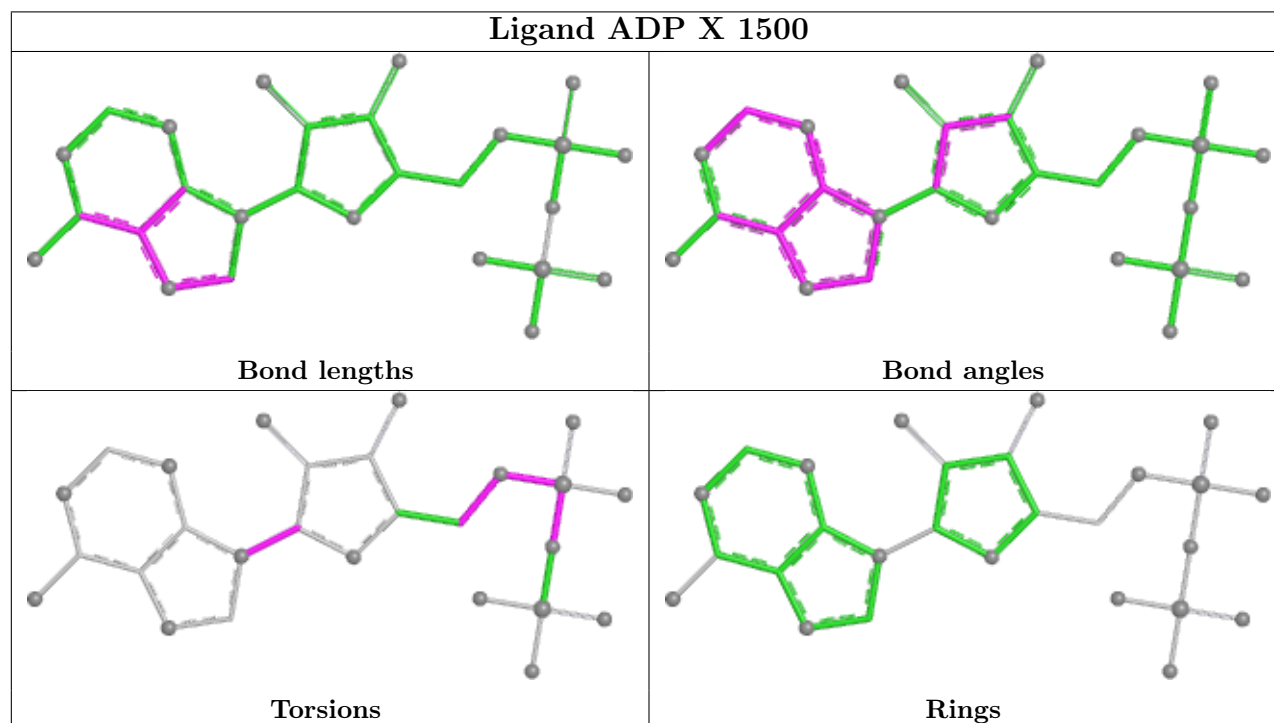
Mol	Chain	Res	Type	Atoms
37	X	1500	ADP	PB-O3A-PA-O2A
34	B	1000	GDP	PA-O3A-PB-O2B

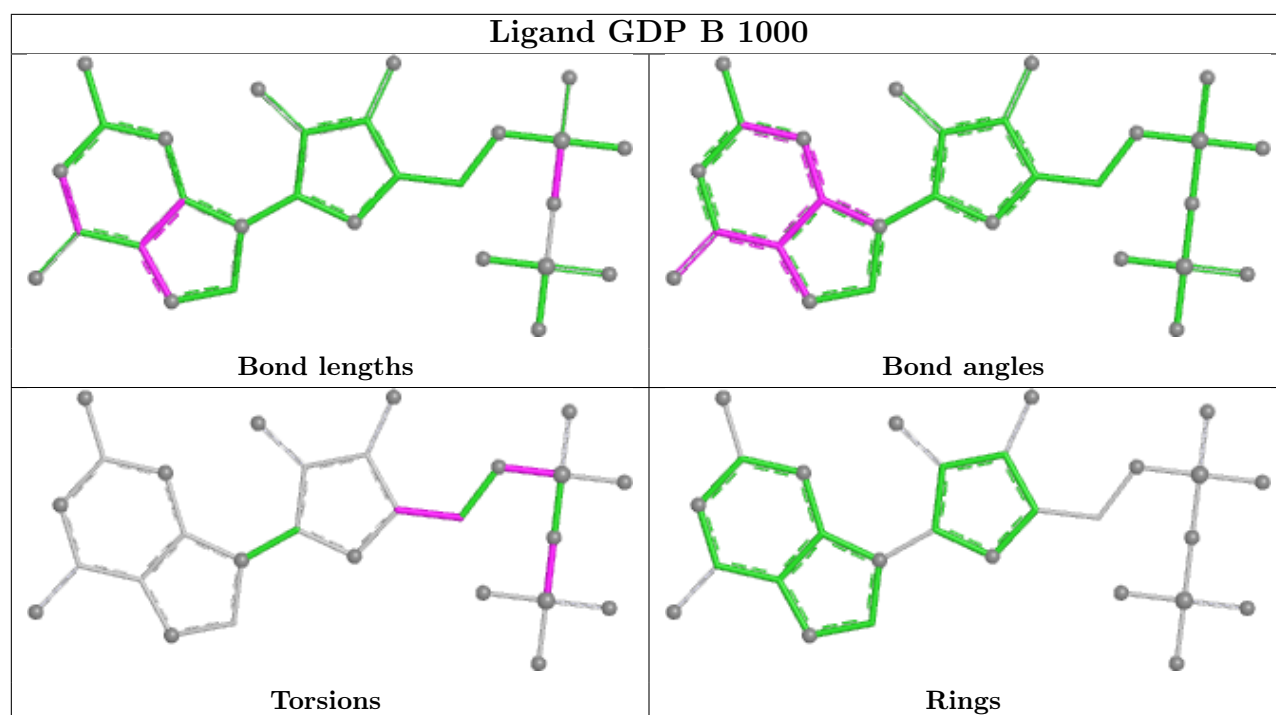
There are no ring outliers.

1 monomer is involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
37	X	1500	ADP	23	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.

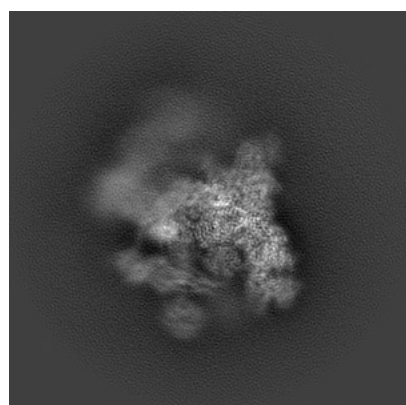
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6413. These allow visual inspection of the internal detail of the map and identification of artifacts.

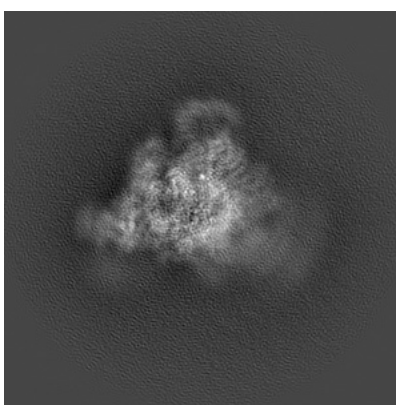
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

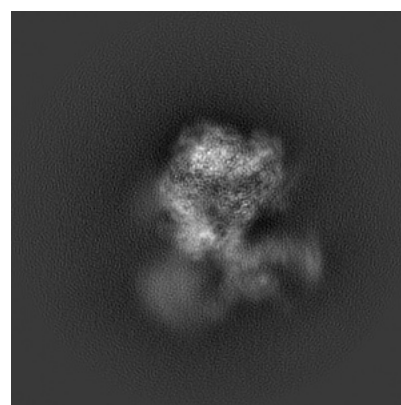
6.1.1 Primary map



X



Y

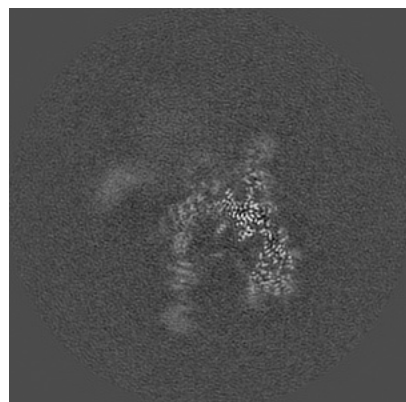


Z

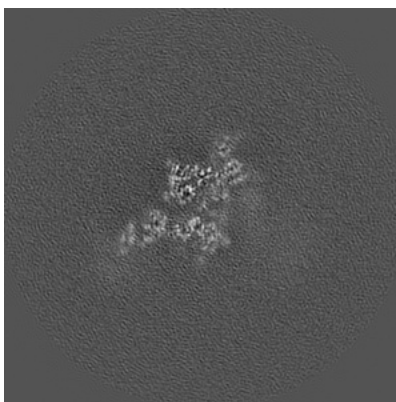
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

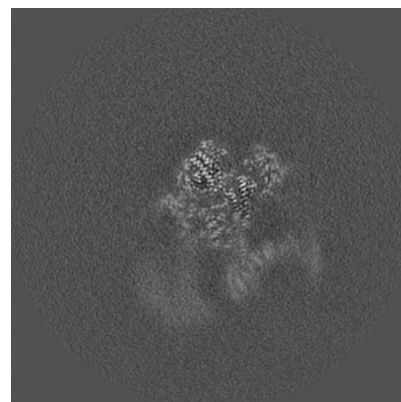
6.2.1 Primary map



X Index: 180



Y Index: 180

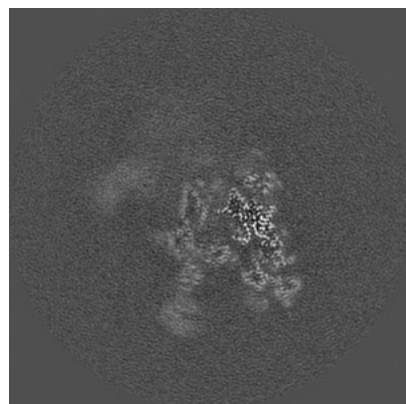


Z Index: 180

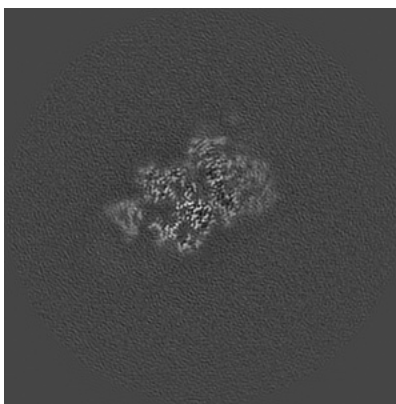
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

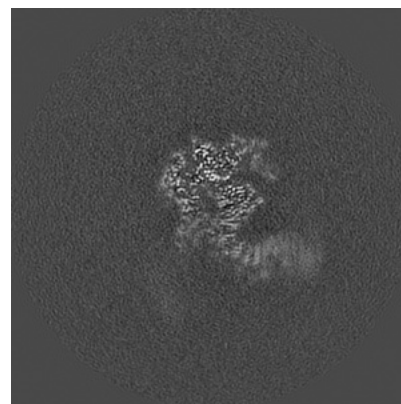
6.3.1 Primary map



X Index: 174



Y Index: 217

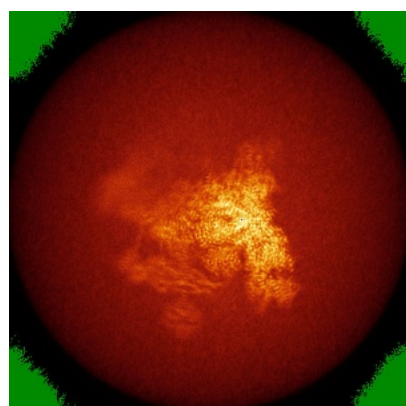


Z Index: 165

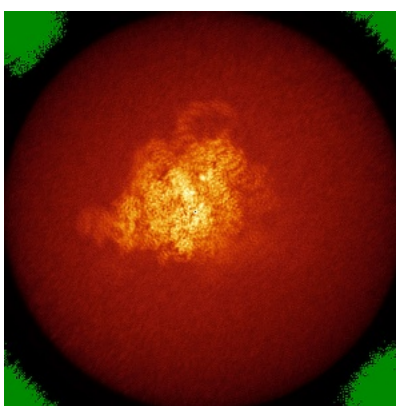
The images above show the largest variance slices of the map in three orthogonal directions.

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

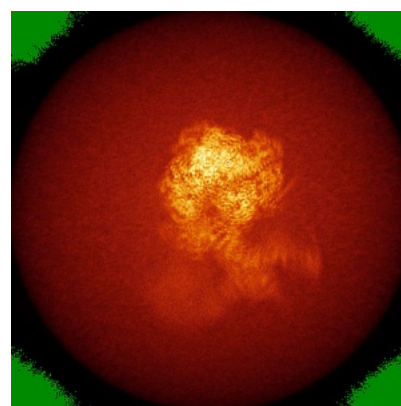
6.4.1 Primary map



X



Y

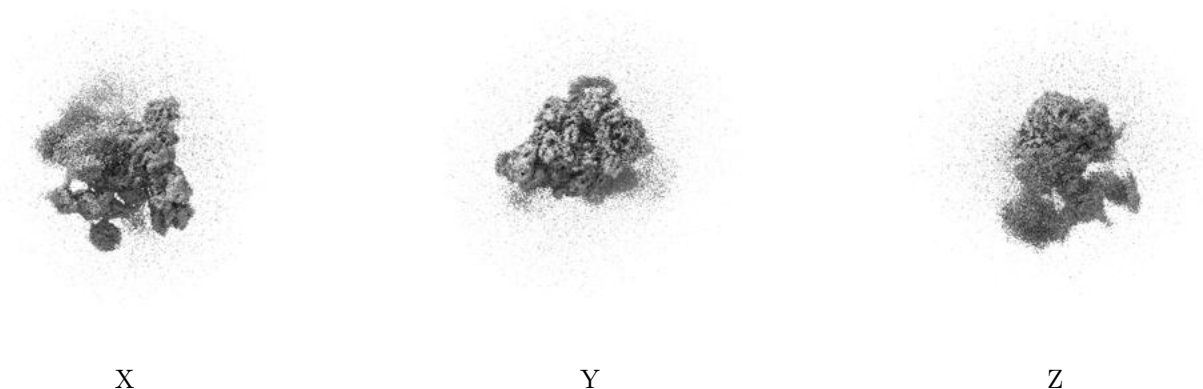


Z

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 0.0203. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

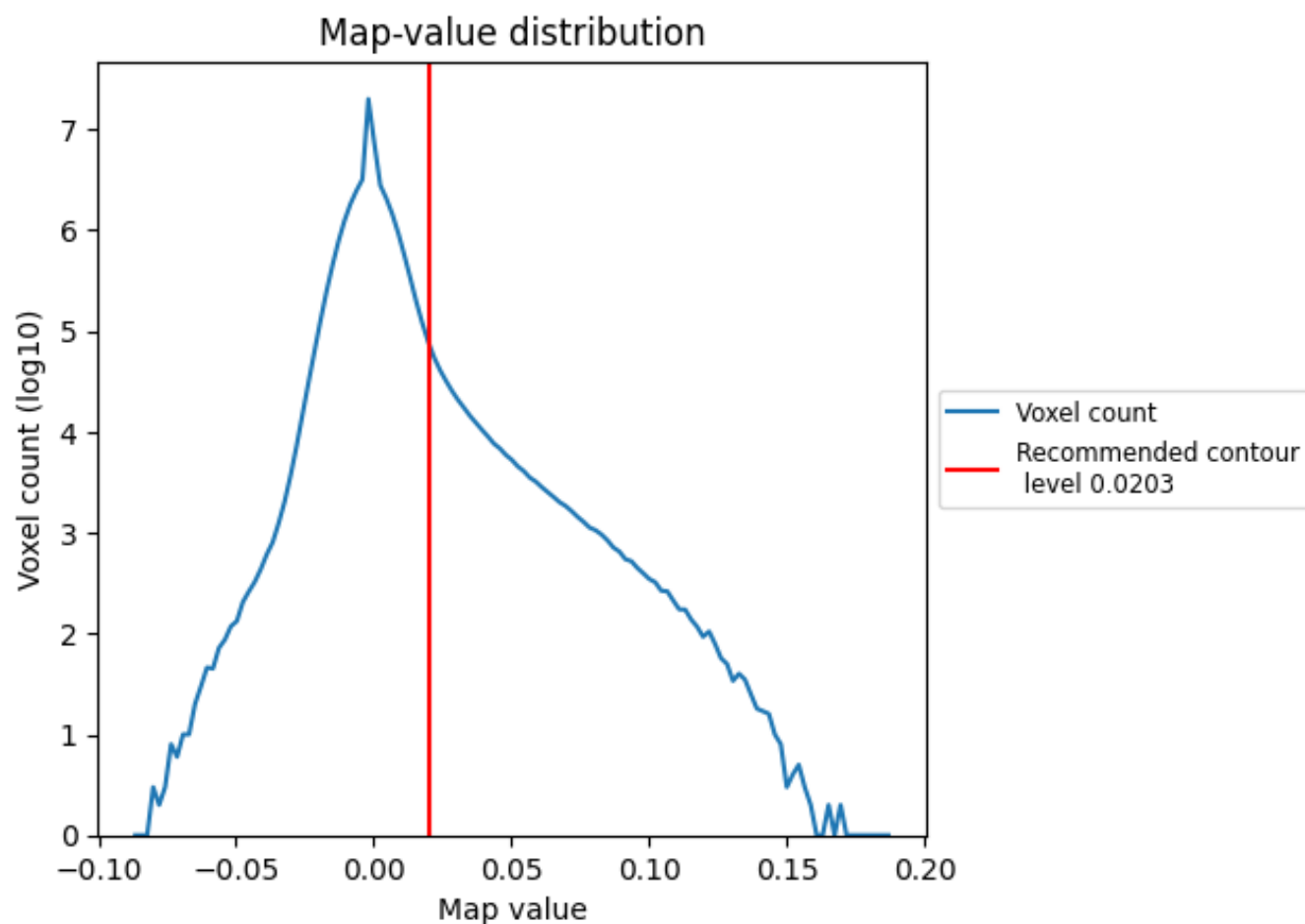
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

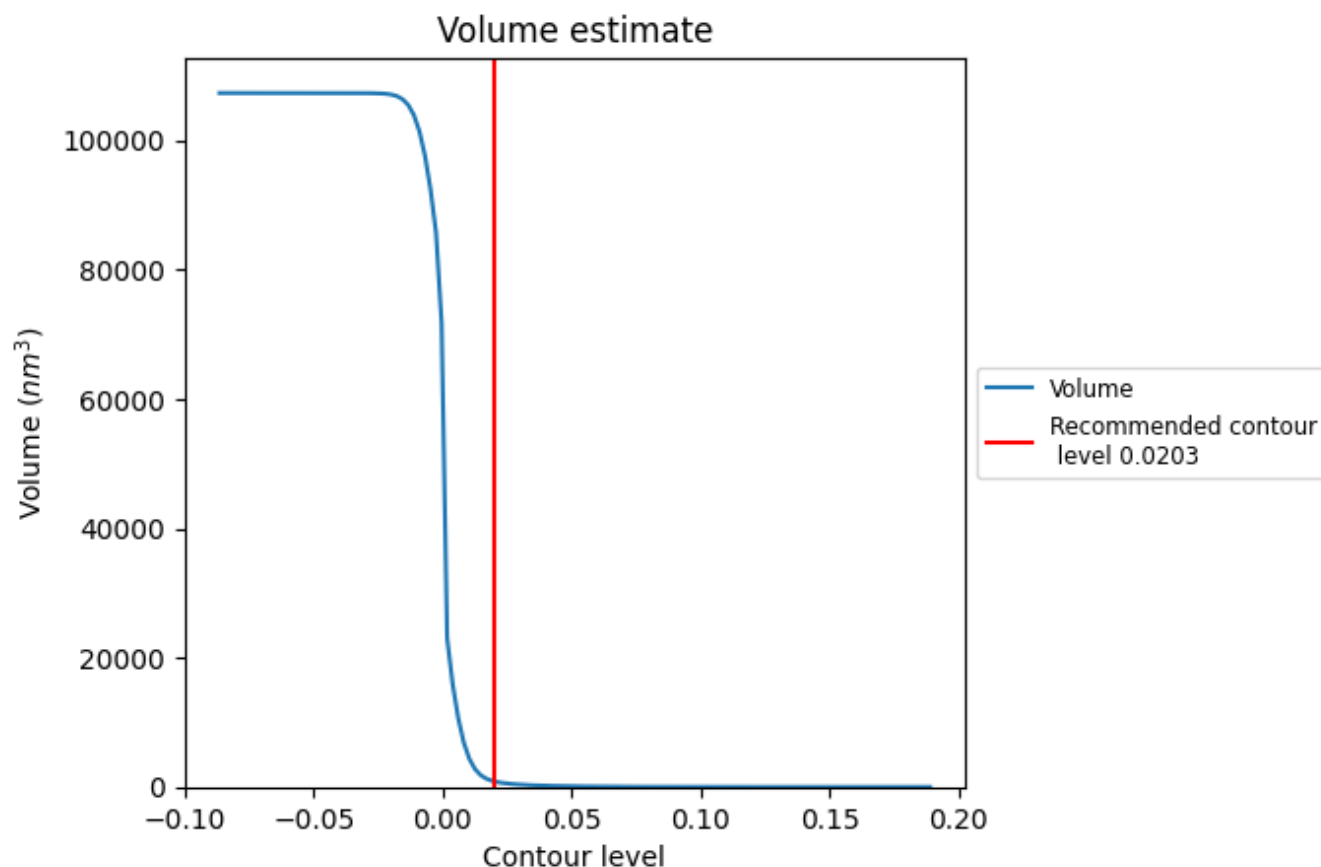
This section contains the results of statistical analysis of the map.

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.

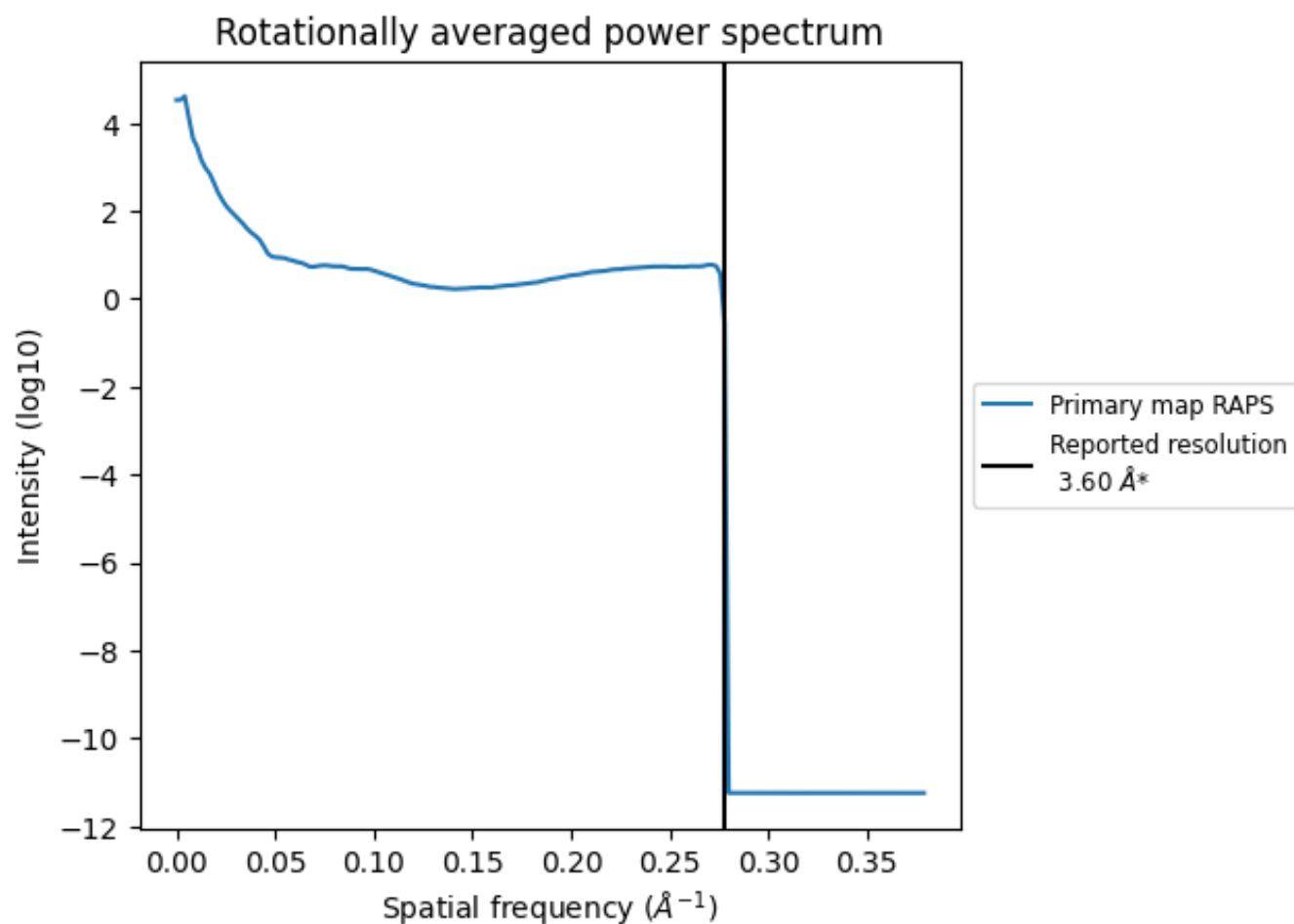
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 836 nm^3 ; this corresponds to an approximate mass of 755 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

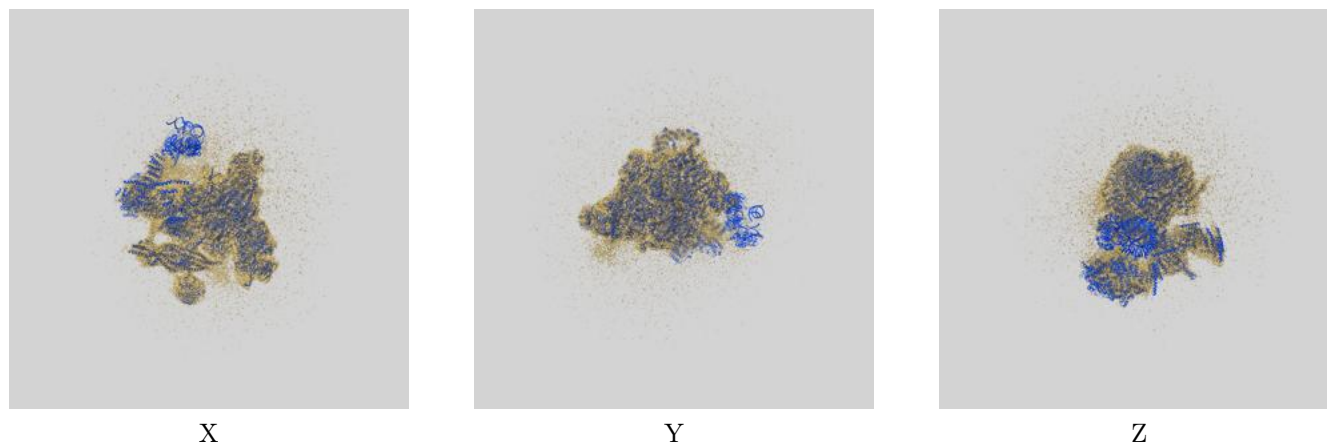
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

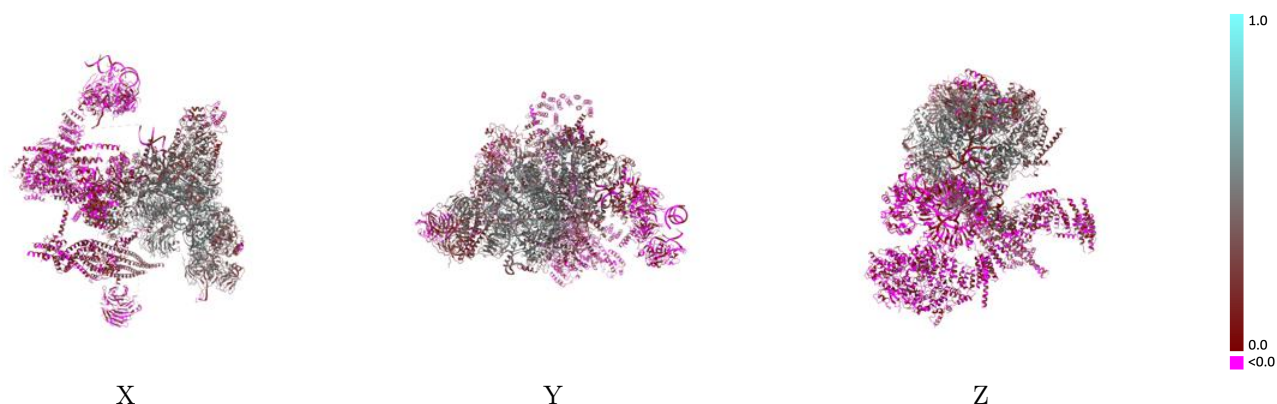
This section contains information regarding the fit between EMDB map EMD-6413 and PDB model 3JB9. Per-residue inclusion information can be found in section [3](#) on page [12](#).

9.1 Map-model overlay [i](#)



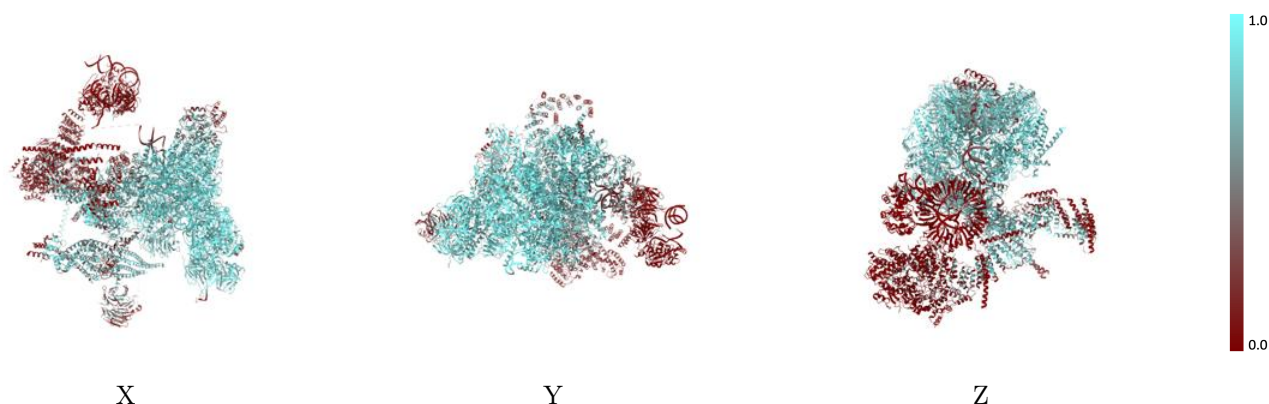
The images above show the 3D surface view of the map at the recommended contour level 0.0203 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



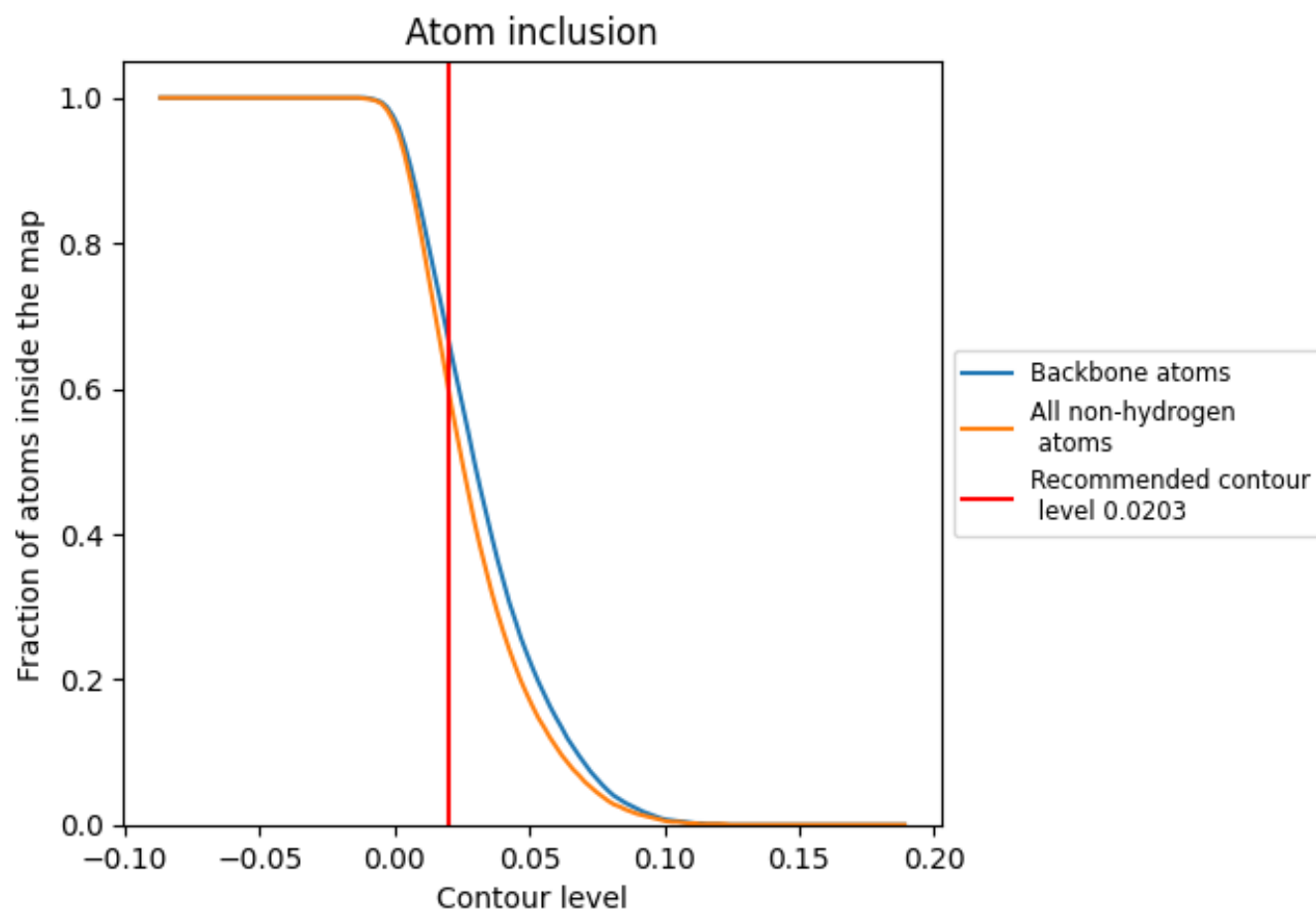
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0203).

9.4 Atom inclusion [i](#)



At the recommended contour level, 66% of all backbone atoms, 59% 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 (0.0203) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5930	 0.2520
A	 0.8040	 0.4010
B	 0.8680	 0.4180
C	 0.9290	 0.4420
D	 0.8890	 0.4500
E	 0.8480	 0.3960
F	 0.7740	 0.3100
G	 0.7330	 0.2220
H	 0.8070	 0.3130
I	 0.7740	 0.2540
J	 0.8220	 0.3800
K	 0.8760	 0.4390
L	 0.8580	 0.4210
M	 0.7380	 0.3490
N	 0.8110	 0.3390
O	 0.7120	 0.2310
P	 0.1830	 0.0590
Q	 0.2220	 0.0640
R	 0.6470	 0.2420
S	 0.5140	 0.1110
T	 0.6350	 0.1600
U	 0.3930	 0.0610
V	 0.5480	 0.1070
W	 0.6940	 0.2420
X	 0.0760	 0.0030
Y	 0.7700	 0.2860
Z	 0.0080	 0.0210
a	 0.6500	 0.2880
b	 0.0050	 0.0380
c	 0.6500	 0.3140
d	 0.7450	 0.3010
e	 0.8980	 0.4560
f	 0.0030	 0.0210
g	 0.7290	 0.3180
h	 0.7500	 0.4070



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Chain	Atom inclusion	Q-score
i	 0.6580	 0.1600
j	 0.0040	 -0.0160
k	 0.0050	 0.0040
l	 0.0030	 -0.0040
m	 0.0000	 -0.0030
n	 0.0020	 -0.0110
o	 0.0040	 -0.0400
r	 0.4200	 0.0610
x	 0.4110	 0.0850