



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 14, 2025 – 05:01 PM JST

PDB ID : 8KAJ / pdb\_00008kaj  
Title : Crystal structure of SpyCas9-crRNA-tracrRNA complex bound to 16nt target DNA  
Authors : Chen, Y.; Chen, J.; Liu, L.  
Deposited on : 2023-08-03  
Resolution : 3.42 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

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>.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	2.0rc1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.42

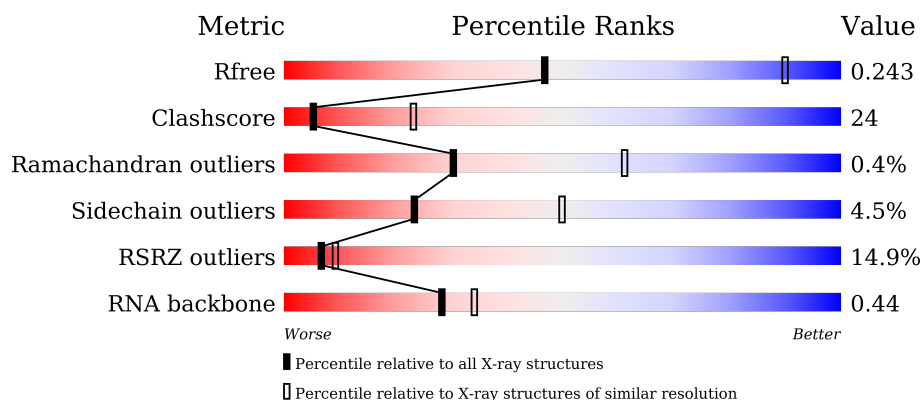
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.42 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)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	164625	1112 (3.48-3.36)
Clashscore	180529	1144 (3.48-3.36)
Ramachandran outliers	177936	1146 (3.48-3.36)
Sidechain outliers	177891	1146 (3.48-3.36)
RSRZ outliers	164620	1112 (3.48-3.36)
RNA backbone	3690	1038 (3.84-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	34	<div> <div>9%</div> <div>12% 44% 32% 12%</div> </div>
1	E	34	<div> <div>9%</div> <div>24% 44% 21% 9%</div> </div>
2	B	1368	<div> <div>10%</div> <div>54% 41%</div> </div>
2	F	1368	<div> <div>20%</div> <div>51% 43%</div> </div>

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Mol	Chain	Length	Quality of chain
3	C	24	<div><div></div><div>8%</div><div>25%</div><div>63%</div><div>12%</div></div>
3	G	24	<div><div></div><div>4%</div><div>50%</div><div>38%</div><div>12%</div></div>
4	D	11	<div><div></div><div>18%</div><div>45%</div><div>45%</div><div>9%</div></div>
4	H	11	<div><div></div><div>18%</div><div>64%</div><div>36%</div><div></div></div>
5	I	65	<div><div></div><div>5%</div><div>15%</div><div>49%</div><div>28%</div><div>5%</div><div></div></div>
5	J	65	<div><div></div><div>6%</div><div>17%</div><div>45%</div><div>29%</div><div>6%</div><div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 26963 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (34-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	34	Total	C	N	O	P	0	0	0
			725	325	127	239	34			
1	E	31	Total	C	N	O	P	0	0	0
			663	297	118	217	31			

- Molecule 2 is a protein called CRISPR-associated endonuclease Cas9/Csn1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1326	Total	C	N	O	S	0	0	0
			10769	6854	1869	2024	22			
2	F	1327	Total	C	N	O	S	0	0	0
			10698	6816	1845	2014	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	10	ALA	ASP	engineered mutation	UNP Q99ZW2
B	840	ALA	HIS	engineered mutation	UNP Q99ZW2
F	10	ALA	ASP	engineered mutation	UNP Q99ZW2
F	840	ALA	HIS	engineered mutation	UNP Q99ZW2

- Molecule 3 is a DNA chain called DNA (5'-D(\*CP\*AP\*AP\*TP\*AP\*CP\*CP\*TP\*TP\*TP\*TP\*AP\*TP\*CP\*CP\*AP\*TP\*AP\*AP\*AP\*TP\*TP\*CP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	24	Total	C	N	O	P	0	0	0
			481	234	81	143	23			
3	G	24	Total	C	N	O	P	0	0	0
			481	234	81	143	23			

- Molecule 4 is a DNA chain called DNA (5'-D(\*TP\*TP\*TP\*AP\*GP\*GP\*TP\*AP\*TP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	11	Total 225	C 110	N 37	O 68	P 10	0	0	0
4	H	11	Total 225	C 110	N 37	O 68	P 10	0	0	0

- Molecule 5 is a RNA chain called RNA (65-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	63	Total 1348	C 603	N 245	O 437	P 63	0	0	0
5	J	63	Total 1348	C 603	N 245	O 437	P 63	0	0	0

### 3 Residue-property plots [i](#)

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

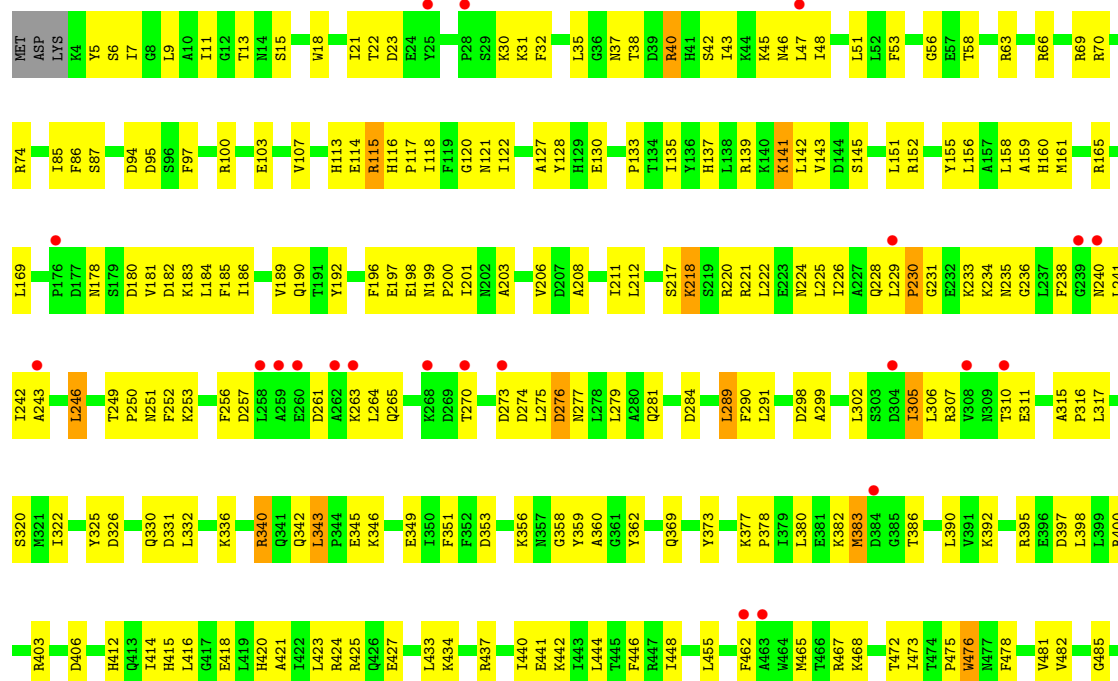
- Molecule 1: RNA (34-MER)

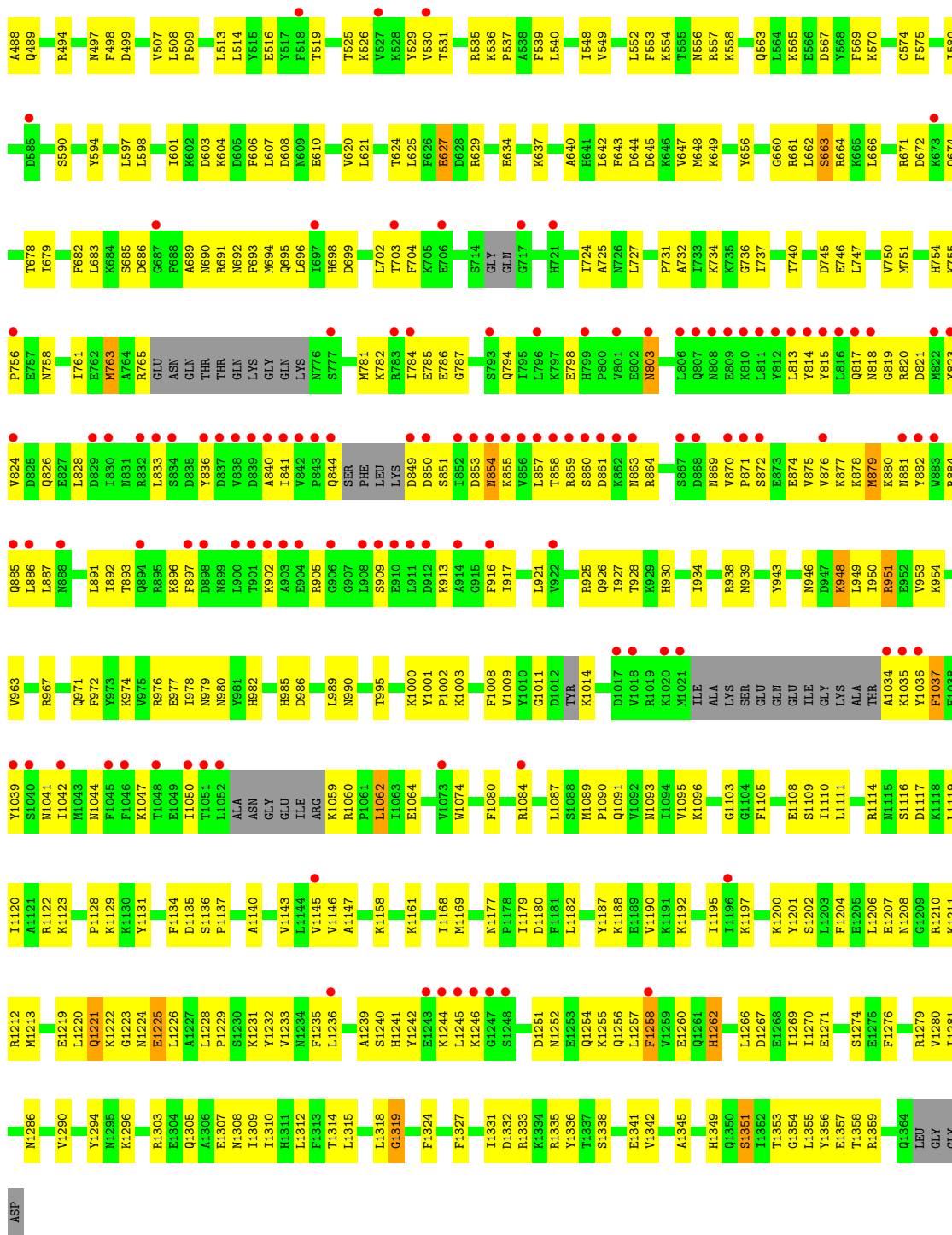


- Molecule 1: RNA (34-MER)



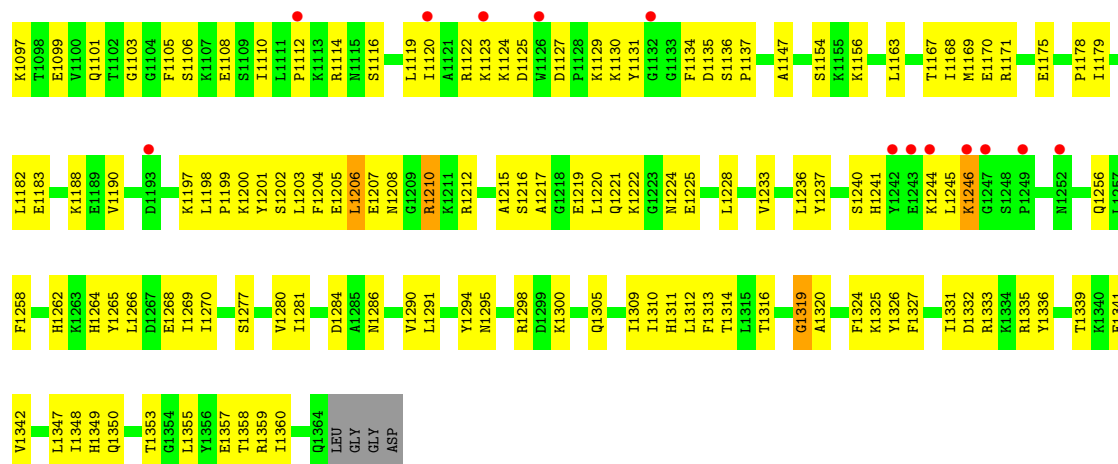
- Molecule 2: CRISPR-associated endonuclease Cas9/Csn1



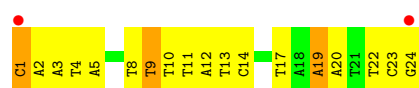


• Molecule 2: CRISPR-associated endonuclease Cas9/Csn1

R1019	M939	R859	I795	I724	F643	Y484	I414	A337	D973	T211	L142	I79
K1020	N940	S860	L796	L727	D644	G485	H415	L338	D274	L212	V143	C80
I1021	Y943	N863	E797	L727	D645	Q489	L416	V339	D275	ALA	D144	F81
A1023		R864	K646	P731	K647	S490	G417	Q342	D276	ARG	S145	L82
LYS	D947	S867	H799	K734	M648	F491	E418	Y347	N277	LEU	A149	Q83
SER	K948	D868	P800	K734	K649	R494	A421	K348	L278	SER	D150	F84
GLN	L949	N869	E802	K737	Q650	R494	L422	E349	L279	LYS	D151	I85
GLU	P950	N870	L651	I737	L651	D499	L423	F349	Q280	S219	R152	F86
ILE	R951	E873	T804	L738	K652	D499	R425	F350	I282	R220	I151	S87
GLY	E952	E873	Q805	Q739	R653	E584	R425	I350	G283	R221	I154	N88
LYS	V953	E874	R806	T740	R654	E584	Q426	F351	G283	R221	I154	E89
ALA	K954	V875	Q807	V741	R655	E505	E427	F352	Q284	L222	Y156	M90
THR	V955	V876	R808	K742	R655	K506	E428	K356	Q285	E223	L156	A91
A1034	T957	R877	E809	K742	S863	L508	E428	N357	Y286	N224	A157	K92
K1035	L958	K878	R810	D745	R664	P509	Y430	G358	A287	L225	L158	K92
Y1036		L811	L811	E746	K665	H510	P431	G358	L226	L226	L158	V93
F1037		Y812	L813	L747	K666	H511	F432	Y359	L227	A227	H160	D94
F1038		L813	L813	V748	L666	L514	L433	G361	F290	Q228	M161	F97
Y1039		Y814	L814	K749	R671	L597	K434	Y362	L291	L229	I162	F98
S1040		L815	L815	V750	D672	I600		I363	A292	P230	K163	H99
M1041		Q817	S675	M751	S675	I601		D364	N295	G231	F164	A100
I1042		N818	I679	H754	I679	I601		A367	S297	K234	G166	E102
M1043		L886	K688	K755	P756	K604		S368	D298	F168	G167	E103
H1044		N888	R820	P756		D605		Q369	I300	L169	S104	S104
F1045		A889	D821			V527			A299		F105	F105
Y1051		K890	M822	V760	F682	K528		F372	G239		L106	L106
L1052		L891	Y823	I761	F606	Y529		Y373	L301		E171	V107
T1053		T892	Y824	E762	L607	V530		K374	G172		E108	E108
A1053		T893	D825	M763	D686	T531		F375	L243		K111	K111
M1054		Q894	Q826	A764		E613		I376	L243		K112	K112
G1055		R895	E827	R765		D614		L380	L305		H113	H113
E1056		R896	L828	ASN	I615	M534		D384	L306		E114	E114
R1060		F897	L828	GLN	I615	R535		M383	R307		E115	E115
P1061		T901	I830	THR	D618	P537		G385	L246		P117	P117
L1062		K902	M694	THR	I619	K536		T386	L248		I118	I118
T1063		G907	Q895	GLN	V620	L538			L249		F119	F119
E1064		L908	L696	LYS	L621	K545		A315	P250		N121	N121
T1065		S909	H898	GLY	T622	K546		P316	F252		G120	G120
V1073		E910	D835	GLN	T624	K546		L390	K253		V122	V122
K1076		L911	Y836	LYS	L625	V549		L317	L317		D124	D124
F1080		D912	D839	LYS	F626	K550		S320	F256		E125	E125
F1080		K913	A840	THR	E627	L551		M321	D257		V126	V126
F1080		K918	T841	THR	L702	L552		I322	A259		A127	A127
R1084		L921	V842	GLN	T703	F553		K401	E260		Y128	Y128
L1087		E923	P843	GLY	F704	K554		R403	D261		H129	H129
S1088		T924	Q844	GLY	K705	T555		T404	A262		P200	P200
M1089		R925	S845	GLY	E630	K556		F405	LYS		I132	I132
P1090		R925	K848	GLY	M631	R557		D406	LEU		P133	P133
Q1091		E1007	F846	GLY	I632	K558		N407	GLN		T134	T134
F1092		F1008	K848	GLY	E633	V559		G408	LEU		I135	I135
N1093		N1093	D853	GLY	E634	T560		S267	VAL		H137	H137
I1094		S937	K789	GLY	R635	L636		I410	D269		L138	L138
V1095		R938	E790	GLY	R635	K562		P411	A208		K139	K139
K1096			L791	GLY	G717	Q563		H412	Z270		A209	A209
			L720	GLY	L642	L564		V481	T271		K140	K140
			Q794	GLY	L642	E566		D483	D272		A210	A210



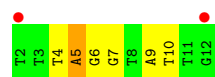
- Molecule 3: DNA (5'-D(\*CP\*AP\*AP\*TP\*AP\*CP\*CP\*TP\*TP\*TP\*TP\*AP\*TP\*CP\*CP\*AP\*TP\*AP\*AP\*AP\*TP\*TP\*CP\*G)-3')



- Molecule 3: DNA (5'-D(\*CP\*AP\*AP\*TP\*AP\*CP\*CP\*TP\*TP\*TP\*TP\*AP\*TP\*CP\*CP\*AP\*TP\*AP\*AP\*AP\*TP\*TP\*CP\*G)-3')



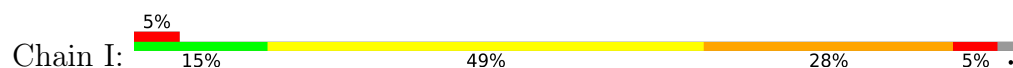
- Molecule 4: DNA (5'-D(\*TP\*TP\*TP\*AP\*GP\*GP\*TP\*AP\*TP\*TP\*G)-3')

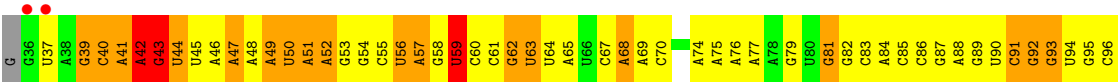


- Molecule 4: DNA (5'-D(\*TP\*TP\*TP\*AP\*GP\*GP\*TP\*AP\*TP\*TP\*G)-3')

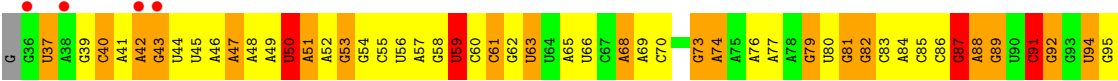
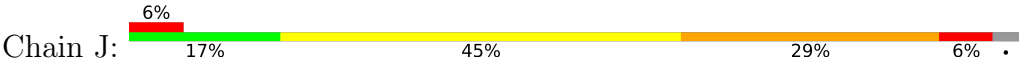


- Molecule 5: RNA (65-MER)





• Molecule 5: RNA (65-MER)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	144.74Å 131.10Å 146.63Å 90.00° 103.68° 90.00°	Depositor
Resolution (Å)	48.03 – 3.42 48.03 – 3.42	Depositor EDS
% Data completeness (in resolution range)	69.1 (48.03-3.42) 79.6 (48.03-3.42)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.38 (at 3.40Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, $R_{free}$	0.237 , 0.246 0.237 , 0.243	Depositor DCC
$R_{free}$ test set	70163 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 46.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.034 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	26963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	1.15	4/811 (0.5%)	1.97	39/1261 (3.1%)
1	E	0.83	0/742	1.61	14/1154 (1.2%)
2	B	0.59	3/10954 (0.0%)	0.79	8/14725 (0.1%)
2	F	0.59	0/10882	0.78	9/14639 (0.1%)
3	C	1.52	8/537 (1.5%)	1.53	8/825 (1.0%)
3	G	1.30	2/537 (0.4%)	1.36	6/825 (0.7%)
4	D	1.51	1/251 (0.4%)	1.36	2/387 (0.5%)
4	H	1.37	1/251 (0.4%)	1.33	0/387
5	I	1.06	7/1509 (0.5%)	1.84	63/2350 (2.7%)
5	J	0.97	1/1509 (0.1%)	1.77	46/2350 (2.0%)
All	All	0.74	27/27983 (0.1%)	1.09	195/38903 (0.5%)

All (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1103	GLY	C-O	9.66	1.39	1.23
1	A	26	A	N9-C4	-9.26	1.32	1.37
4	H	5	DA	C3'-O3'	-7.84	1.33	1.44
4	D	5	DA	C3'-O3'	-7.05	1.34	1.44
3	C	11	DT	C1'-N1	6.10	1.57	1.49
1	A	18	A	N3-C4	-5.99	1.31	1.34
3	C	8	DT	C3'-O3'	-5.97	1.36	1.44
5	I	47	A	N9-C4	-5.94	1.34	1.37
3	C	9	DT	N1-C6	-5.91	1.34	1.38
2	B	627	GLU	CB-CG	5.80	1.63	1.52
2	B	627	GLU	CG-CD	5.72	1.60	1.51
3	G	19	DA	C3'-O3'	-5.70	1.36	1.44
3	C	9	DT	C1'-N1	-5.57	1.39	1.47
5	I	47	A	C6-N1	-5.49	1.31	1.35
3	C	19	DA	C3'-O3'	-5.42	1.36	1.44
5	I	65	A	N7-C5	-5.40	1.36	1.39
5	I	46	A	N7-C5	-5.37	1.36	1.39
1	A	18	A	C6-N1	-5.35	1.31	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	12	DA	C5'-C4'	5.22	1.57	1.51
5	I	43	G	N9-C4	5.19	1.42	1.38
5	I	47	A	C6-N6	-5.16	1.29	1.33
3	C	9	DT	N3-C4	-5.10	1.34	1.38
5	I	47	A	P-O5'	-5.08	1.54	1.59
3	G	18	DA	N3-C4	-5.07	1.31	1.34
1	A	18	A	N7-C5	-5.03	1.36	1.39
3	C	10	DT	C4-C5	-5.02	1.40	1.45
5	J	88	A	C5-C6	-5.01	1.36	1.41

All (195) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	C	C6-N1-C2	-11.04	115.89	120.30
5	J	79	G	C8-N9-C4	9.88	110.35	106.40
5	J	61	C	C6-N1-C2	-9.65	116.44	120.30
5	J	89	G	N1-C6-O6	9.63	125.68	119.90
5	I	52	A	N1-C6-N6	-9.50	112.90	118.60
3	C	14	DC	O4'-C4'-C3'	-9.30	100.42	106.00
5	J	91	C	N3-C2-O2	9.29	128.40	121.90
5	J	89	G	C5-C6-O6	-8.99	123.20	128.60
5	I	52	A	N9-C4-C5	8.91	109.36	105.80
1	A	18	A	C4-C5-C6	8.83	121.42	117.00
5	I	59	U	O5'-P-OP2	-8.81	97.77	105.70
1	A	27	G	C5-C6-O6	-8.72	123.37	128.60
1	E	15	G	C8-N9-C4	8.68	109.87	106.40
1	A	18	A	N1-C2-N3	8.39	133.50	129.30
5	I	43	G	N3-C4-C5	-8.36	124.42	128.60
1	A	13	U	N1-C2-O2	-8.23	117.04	122.80
5	J	81	G	C5-C6-O6	-8.18	123.69	128.60
2	F	246	LEU	CA-CB-CG	8.13	133.99	115.30
1	A	22	U	C6-N1-C2	-8.11	116.13	121.00
5	I	49	A	C8-N9-C4	-8.10	102.56	105.80
1	A	26	A	N3-C4-C5	8.09	132.47	126.80
5	I	53	G	C5-C6-N1	-8.08	107.46	111.50
5	J	89	G	C6-C5-N7	-7.98	125.61	130.40
2	B	343	LEU	CA-CB-CG	7.91	133.49	115.30
5	I	63	U	C5-C4-O4	-7.89	121.17	125.90
5	I	52	A	C8-N9-C4	-7.86	102.66	105.80
1	A	26	A	C2-N3-C4	-7.64	106.78	110.60
5	I	41	A	C2-N3-C4	-7.63	106.79	110.60
1	E	16	A	C8-N9-C4	7.59	108.84	105.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	43	G	C2-N3-C4	7.56	115.68	111.90
1	A	13	U	N3-C2-O2	7.37	127.36	122.20
1	A	29	G	N1-C6-O6	7.16	124.20	119.90
1	A	24	U	N3-C4-O4	7.12	124.38	119.40
2	B	305	ILE	CG1-CB-CG2	-7.10	95.79	111.40
3	G	14	DC	O4'-C4'-C3'	-7.09	101.66	104.50
5	I	49	A	C5-N7-C8	-7.05	100.37	103.90
1	A	27	G	C4-C5-N7	6.93	113.57	110.80
1	A	5	C	C5-C6-N1	6.92	124.46	121.00
1	A	13	U	N3-C4-O4	6.89	124.23	119.40
5	J	73	G	C8-N9-C4	-6.89	103.64	106.40
5	I	57	A	O5'-P-OP1	-6.85	99.54	105.70
2	F	1043	MET	CB-CG-SD	-6.81	91.97	112.40
1	A	21	G	C8-N9-C4	-6.77	103.69	106.40
2	F	1319	GLY	C-N-CA	-6.77	104.78	121.70
5	I	56	U	O5'-P-OP1	-6.77	99.61	105.70
5	J	59	U	C6-N1-C2	6.75	125.05	121.00
5	J	47	A	N1-C6-N6	6.74	122.64	118.60
5	J	91	C	C6-N1-C2	6.69	122.98	120.30
1	A	7	A	N1-C6-N6	-6.67	114.60	118.60
5	I	41	A	N1-C6-N6	6.67	122.60	118.60
5	I	57	A	N9-C4-C5	6.59	108.44	105.80
3	C	11	DT	O4'-C1'-N1	6.56	112.59	108.00
1	A	19	A	OP1-P-OP2	-6.55	109.77	119.60
5	J	88	A	C2-N3-C4	-6.54	107.33	110.60
1	A	18	A	OP2-P-O3'	6.54	119.58	105.20
1	E	11	U	N3-C2-O2	-6.51	117.64	122.20
1	E	21	G	N3-C2-N2	6.51	124.46	119.90
3	G	12	DA	O4'-C1'-N9	6.51	112.56	108.00
3	C	13	DT	O4'-C4'-C3'	-6.50	101.90	104.50
1	A	21	G	C2-N3-C4	6.46	115.13	111.90
1	E	22	U	O4'-C1'-N1	6.42	113.33	108.20
5	J	87	G	C5-C6-O6	6.41	132.45	128.60
5	I	76	A	C8-N9-C4	6.41	108.36	105.80
1	A	22	U	N3-C4-C5	-6.40	110.76	114.60
3	C	8	DT	O5'-P-OP2	-6.40	99.94	105.70
3	C	13	DT	O5'-P-OP1	-6.40	99.94	105.70
5	J	81	G	N3-C4-C5	-6.39	125.40	128.60
5	I	93	G	C8-N9-C4	-6.39	103.84	106.40
5	I	63	U	O5'-P-OP2	-6.32	100.02	105.70
1	A	23	U	C5-C4-O4	-6.30	122.12	125.90
1	E	15	G	N7-C8-N9	-6.25	109.97	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	66	U	N1-C2-O2	-6.24	118.43	122.80
5	J	81	G	N1-C6-O6	6.24	123.64	119.90
4	D	6	DG	C1'-O4'-C4'	-6.20	103.90	110.10
5	J	81	G	C6-C5-N7	-6.18	126.69	130.40
5	I	41	A	O5'-P-OP1	6.15	118.08	110.70
1	A	26	A	C8-N9-C4	6.12	108.25	105.80
1	A	22	U	C5-C6-N1	6.09	125.74	122.70
1	A	26	A	C4-C5-N7	6.09	113.74	110.70
5	J	94	U	C5-C4-O4	-6.05	122.27	125.90
1	E	11	U	C5-C4-O4	6.01	129.51	125.90
5	J	79	G	N7-C8-N9	-6.01	110.09	113.10
5	J	91	C	C4-C5-C6	-6.01	114.40	117.40
5	I	64	U	N3-C4-C5	-6.00	111.00	114.60
5	I	46	A	OP2-P-O3'	5.96	118.32	105.20
3	G	6	DC	O4'-C1'-N1	5.95	112.17	108.00
5	I	43	G	C8-N9-C4	-5.95	104.02	106.40
5	J	53	G	C8-N9-C4	-5.95	104.02	106.40
2	F	30	LYS	CD-CE-NZ	5.94	125.37	111.70
5	J	81	G	C8-N9-C4	-5.93	104.03	106.40
5	I	52	A	C6-N1-C2	-5.92	115.05	118.60
5	J	82	G	N1-C6-O6	5.91	123.44	119.90
5	I	96	C	C6-N1-C2	-5.90	117.94	120.30
5	J	61	C	C5-C6-N1	5.90	123.95	121.00
5	J	82	G	C4-C5-N7	5.88	113.15	110.80
2	F	625	LEU	CA-CB-CG	5.87	128.79	115.30
5	I	46	A	C6-N1-C2	-5.86	115.08	118.60
1	A	17	U	C5-C4-O4	-5.82	122.41	125.90
5	I	45	U	OP1-P-OP2	-5.82	110.88	119.60
1	A	21	G	N3-C4-C5	-5.81	125.69	128.60
5	I	67	C	C6-N1-C2	5.81	122.62	120.30
5	I	42	A	C8-N9-C4	-5.80	103.48	105.80
1	A	20	A	O5'-P-OP1	5.71	117.56	110.70
5	I	64	U	C6-N1-C2	-5.68	117.59	121.00
2	B	1319	GLY	C-N-CA	-5.66	107.55	121.70
1	A	12	A	C4-C5-N7	5.65	113.53	110.70
5	I	58	G	N3-C4-C5	-5.65	125.78	128.60
5	J	81	G	C6-N1-C2	-5.63	121.72	125.10
5	J	61	C	N3-C4-C5	-5.62	119.65	121.90
1	A	26	A	C5-N7-C8	-5.62	101.09	103.90
5	I	51	A	C4-C5-C6	5.61	119.81	117.00
1	A	22	U	C2-N3-C4	5.60	130.36	127.00
1	E	21	G	N1-C6-O6	-5.60	116.54	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	J	91	C	C5-C4-N4	-5.60	116.28	120.20
1	A	13	U	C5-C4-O4	-5.58	122.55	125.90
3	C	1	DC	O4'-C1'-N1	5.56	111.89	108.00
2	F	74	ARG	NE-CZ-NH1	-5.56	117.52	120.30
5	I	41	A	C8-N9-C4	5.55	108.02	105.80
5	I	62	G	N3-C2-N2	5.54	123.78	119.90
5	I	46	A	C5-C6-N1	5.53	120.46	117.70
5	J	82	G	C6-C5-N7	-5.52	127.09	130.40
5	I	75	A	C8-N9-C4	5.51	108.00	105.80
5	I	63	U	C2-N3-C4	-5.51	123.69	127.00
3	G	10	DT	O4'-C1'-N1	5.50	111.85	108.00
5	I	43	G	C4-C5-N7	-5.50	108.60	110.80
1	A	24	U	C5-C4-O4	-5.49	122.61	125.90
2	B	115	ARG	NE-CZ-NH2	-5.49	117.56	120.30
1	E	16	A	N7-C8-N9	-5.48	111.06	113.80
1	E	11	U	N1-C2-O2	5.47	126.63	122.80
5	I	53	G	C4-C5-C6	5.45	122.07	118.80
5	J	66	U	N3-C4-C5	-5.45	111.33	114.60
1	A	7	A	N9-C4-C5	5.41	107.96	105.80
5	I	96	C	N3-C4-N4	5.40	121.78	118.00
1	E	22	U	C5-C4-O4	5.38	129.13	125.90
5	J	66	U	N3-C4-O4	5.37	123.16	119.40
5	J	91	C	N1-C2-N3	-5.37	115.44	119.20
5	I	44	U	OP2-P-O3'	5.36	116.99	105.20
5	J	94	U	OP2-P-O3'	5.34	116.95	105.20
5	I	47	A	C5-N7-C8	-5.34	101.23	103.90
5	I	54	G	C6-C5-N7	-5.33	127.20	130.40
1	E	22	U	N3-C2-O2	-5.33	118.47	122.20
5	I	49	A	C4-C5-N7	5.31	113.36	110.70
5	I	43	G	N9-C4-C5	5.30	107.52	105.40
5	I	49	A	N7-C8-N9	5.30	116.45	113.80
5	I	52	A	C2-N3-C4	5.29	113.24	110.60
5	J	50	U	C6-N1-C2	5.28	124.17	121.00
2	F	21	ILE	CG1-CB-CG2	-5.27	99.80	111.40
2	B	289	LEU	CA-CB-CG	5.26	127.41	115.30
1	A	12	A	C5-N7-C8	-5.26	101.27	103.90
1	A	16	A	N1-C6-N6	-5.25	115.45	118.60
5	I	52	A	C4-C5-N7	-5.24	108.08	110.70
5	J	79	G	N9-C4-C5	-5.23	103.31	105.40
5	J	88	A	N1-C6-N6	5.23	121.74	118.60
1	A	18	A	N9-C4-C5	5.22	107.89	105.80
1	A	20	A	O5'-P-OP2	-5.22	101.00	105.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	514	LEU	CA-CB-CG	5.22	127.31	115.30
5	I	62	G	OP2-P-O3'	5.22	116.68	105.20
5	J	53	G	N9-C4-C5	5.22	107.49	105.40
4	D	7	DG	OP1-P-OP2	5.20	127.40	119.60
3	G	10	DT	N3-C4-O4	5.19	123.02	119.90
5	J	70	C	O5'-P-OP1	5.18	116.92	110.70
5	J	59	U	C5-C6-N1	-5.18	120.11	122.70
5	J	73	G	C6-C5-N7	-5.18	127.29	130.40
5	I	42	A	C2'-C3'-O3'	5.18	121.98	113.70
5	J	61	C	N3-C2-O2	-5.18	118.28	121.90
1	A	5	C	N3-C4-C5	-5.17	119.83	121.90
5	J	73	G	N7-C8-N9	5.16	115.68	113.10
5	I	57	A	C4-C5-N7	-5.15	108.12	110.70
5	J	50	U	C5-C6-N1	-5.14	120.13	122.70
5	I	79	G	C5-C6-O6	-5.14	125.52	128.60
1	E	27	G	P-O3'-C3'	5.13	125.86	119.70
5	I	55	C	C5-C4-N4	-5.12	116.61	120.20
2	F	289	LEU	CA-CB-CG	5.12	127.07	115.30
5	J	89	G	C4-C5-C6	5.11	121.87	118.80
5	I	90	U	C2-N3-C4	5.11	130.07	127.00
5	J	88	A	C6-C5-N7	-5.10	128.73	132.30
5	I	76	A	N9-C4-C5	-5.09	103.76	105.80
5	I	65	A	C4-C5-C6	5.09	119.54	117.00
1	A	13	U	O5'-P-OP2	-5.08	101.13	105.70
5	I	45	U	C5-C6-N1	5.08	125.24	122.70
5	I	51	A	N1-C2-N3	5.08	131.84	129.30
5	I	64	U	OP2-P-O3'	5.06	116.33	105.20
5	I	81	G	C5-C6-N1	5.06	114.03	111.50
2	B	169	LEU	CB-CG-CD1	-5.05	102.41	111.00
2	F	380	LEU	CA-CB-CG	5.05	126.93	115.30
3	G	9	DT	N3-C4-O4	5.05	122.93	119.90
5	I	53	G	C2-N3-C4	-5.04	109.38	111.90
5	J	65	A	C4-C5-N7	5.04	113.22	110.70
3	C	1	DC	C1'-O4'-C4'	-5.03	105.07	110.10
2	B	169	LEU	CA-CB-CG	-5.02	103.75	115.30
3	C	10	DT	N3-C4-O4	5.02	122.91	119.90
5	I	45	U	C6-N1-C2	-5.02	117.99	121.00
5	I	57	A	C4-C5-C6	5.02	119.51	117.00
5	I	50	U	N3-C4-O4	5.01	122.91	119.40
1	E	15	G	C5-C6-O6	-5.00	125.60	128.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	725	0	362	21	0
1	E	663	0	331	26	0
2	B	10769	0	10864	508	0
2	F	10698	0	10745	605	0
3	C	481	0	275	11	0
3	G	481	0	275	10	0
4	D	225	0	129	3	0
4	H	225	0	129	7	0
5	I	1348	0	678	43	0
5	J	1348	0	678	68	0
All	All	26963	0	24466	1217	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 24.

All (1217) 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)
2:B:243:ALA:CA	2:B:246:LEU:HD23	1.44	1.38
2:B:243:ALA:HA	2:B:246:LEU:CD2	1.64	1.28
2:B:980:ASN:HB2	2:B:1225:GLU:OE2	1.39	1.21
2:F:1207:GLU:OE2	2:F:1210:ARG:NH1	1.79	1.14
2:B:243:ALA:CA	2:B:246:LEU:CD2	2.22	1.13
2:B:525:THR:HG23	2:B:690:ASN:HB3	1.12	1.12
2:F:525:THR:HG23	2:F:690:ASN:HB2	1.22	1.11
2:F:249:THR:HG1	2:F:267:SER:N	1.48	1.11
2:B:525:THR:CG2	2:B:690:ASN:HB3	1.89	1.02
2:B:1224:ASN:HB2	2:B:1280:VAL:HG11	1.38	1.02
2:B:270:THR:OG1	2:B:274:ASP:OD2	1.78	1.00
2:F:1060:ARG:HH11	2:F:1060:ARG:HB3	1.23	0.98
2:B:539:PHE:HB3	2:B:690:ASN:ND2	1.80	0.97
2:F:545:LYS:HZ2	2:F:690:ASN:HD22	1.11	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1123:LYS:HD2	5:J:53:G:OP1	1.66	0.95
2:B:1120:ILE:HD11	2:B:1137:PRO:HG3	1.49	0.95
2:F:1045:PHE:HB2	2:F:1064:GLU:HG2	1.46	0.95
2:F:226:ILE:HG13	2:F:232:GLU:HG2	1.49	0.94
2:B:539:PHE:HB3	2:B:690:ASN:HD22	1.32	0.94
2:F:63:ARG:HA	2:F:66:ARG:HG3	1.49	0.94
2:F:380:LEU:HD11	2:F:390:LEU:HG	1.51	0.93
2:F:1210:ARG:NH2	2:F:1341:GLU:OE1	2.01	0.93
2:F:425:ARG:HG3	2:F:426:GLN:HG2	1.51	0.93
2:F:485:GLY:HA3	2:F:631:MET:HG3	1.49	0.91
1:A:2:U:H3	1:A:4:A:H3'	1.37	0.89
2:F:978:ILE:HD12	2:F:1228:LEU:HD23	1.52	0.89
2:B:1308:ASN:HD22	2:B:1327:PHE:H	1.19	0.89
2:F:525:THR:CG2	2:F:690:ASN:HB2	2.02	0.88
2:B:980:ASN:CB	2:B:1225:GLU:OE2	2.20	0.88
2:F:70:ARG:NE	5:J:61:C:OP2	2.07	0.87
2:F:545:LYS:HZ2	2:F:690:ASN:ND2	1.72	0.87
2:F:184:LEU:HD13	2:F:295:ASN:HB3	1.54	0.87
2:F:142:LEU:HD22	2:F:422:ILE:HG23	1.57	0.87
2:F:1294:TYR:HE1	2:F:1305:GLN:HE21	1.21	0.87
2:F:978:ILE:HD13	2:F:1233:VAL:HG22	1.59	0.85
2:F:1060:ARG:HH11	2:F:1060:ARG:CB	1.89	0.84
2:F:221:ARG:HA	2:F:224:ASN:HB2	1.58	0.84
2:B:46:ASN:ND2	2:B:1091:GLN:OE1	2.10	0.84
1:E:15:G:OP1	2:F:66:ARG:NH2	2.10	0.83
2:B:530:VAL:HG22	2:B:537:PRO:HB3	1.60	0.83
2:B:246:LEU:H	2:B:246:LEU:HD22	1.44	0.83
2:B:548:ILE:HG23	2:B:552:LEU:HD12	1.60	0.82
5:J:46:A:H2'	5:J:47:A:C8	2.15	0.82
2:F:525:THR:OG1	2:F:545:LYS:NZ	2.13	0.82
2:F:1212:ARG:NH2	2:F:1280:VAL:O	2.13	0.81
2:F:70:ARG:NH2	5:J:61:C:OP1	2.13	0.81
2:F:451:TYR:O	2:F:464:TRP:NE1	2.14	0.80
2:B:725:ALA:O	2:B:734:LYS:NZ	2.14	0.80
2:F:1045:PHE:O	2:F:1076:LYS:NZ	2.14	0.80
2:F:777:SER:HA	2:F:807:GLN:HE21	1.46	0.79
2:F:545:LYS:NZ	2:F:690:ASN:HD22	1.81	0.79
2:B:137:HIS:HA	2:B:322:ILE:HD11	1.64	0.79
2:F:826:GLN:OE1	2:F:859:ARG:NH1	2.15	0.79
2:F:829:ASP:OD1	2:F:832:ARG:N	2.10	0.79
2:B:1207:GLU:CD	2:B:1210:ARG:HH11	1.85	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1210:ARG:NH2	2:B:1341:GLU:OE1	2.17	0.78
2:B:1211:LYS:O	2:B:1223:GLY:HA3	1.83	0.78
2:F:525:THR:HG23	2:F:690:ASN:CB	2.09	0.78
2:F:1091:GLN:HG3	5:J:91:C:H5''	1.66	0.78
2:B:9:LEU:HD12	2:B:761:ILE:HG22	1.64	0.78
2:B:220:ARG:O	2:B:224:ASN:ND2	2.14	0.77
2:B:539:PHE:CD2	2:B:689:ALA:HA	2.18	0.77
2:B:823:TYR:HA	2:B:875:VAL:HG11	1.66	0.77
2:F:249:THR:OG1	2:F:267:SER:N	2.18	0.77
1:E:27:G:N2	5:J:44:U:OP2	2.17	0.77
1:A:27:G:H5'	1:A:28:A:H5''	1.67	0.77
2:F:1266:LEU:HD12	2:F:1309:ILE:HD12	1.67	0.77
2:B:902:LYS:HA	2:B:905:ARG:HE	1.50	0.76
2:F:1051:THR:HG22	2:F:1053:ALA:H	1.50	0.76
2:F:467:ARG:HA	2:F:482:VAL:HG22	1.67	0.76
2:B:270:THR:O	2:B:274:ASP:OD2	2.03	0.76
2:F:672:ASP:OD1	2:F:703:THR:HG22	1.85	0.76
2:F:886:LEU:HA	2:F:891:LEU:HD21	1.68	0.76
2:F:522:ASN:OD1	2:F:692:ASN:ND2	2.19	0.76
2:F:253:LYS:HB2	2:F:262:ALA:H	1.49	0.76
2:B:243:ALA:C	2:B:246:LEU:HD23	2.05	0.75
2:F:94:ASP:HB3	2:F:97:PHE:HB2	1.67	0.75
2:B:342:GLN:HE22	2:B:383:MET:HA	1.51	0.75
2:F:844:GLN:HG3	2:F:848:LYS:HD2	1.67	0.75
2:B:114:GLU:HG3	2:B:116:HIS:H	1.50	0.75
2:F:878:LYS:HB3	2:F:879:MET:SD	2.26	0.75
2:B:1147:ALA:HB2	2:B:1190:VAL:HA	1.67	0.75
2:B:727:LEU:HD12	2:B:927:ILE:HD12	1.69	0.75
2:F:918:LYS:HZ2	2:F:1018:VAL:HG11	1.52	0.75
1:E:32:A:N6	5:J:37:U:O4	2.20	0.74
2:F:527:VAL:HA	2:F:582:GLY:HA3	1.67	0.74
2:B:1135:ASP:OD1	2:B:1136:SER:N	2.20	0.74
2:F:918:LYS:HZ2	2:F:1018:VAL:CG1	2.00	0.74
2:B:400:ARG:NH2	2:B:406:ASP:OD2	2.20	0.74
2:F:89:GLU:OE2	2:F:92:LYS:NZ	2.21	0.74
2:B:1110:ILE:HD12	2:B:1122:ARG:HD2	1.69	0.73
2:F:145:SER:O	2:F:425:ARG:NH1	2.21	0.73
2:B:540:LEU:O	2:B:690:ASN:ND2	2.20	0.73
2:B:909:SER:O	2:B:913:LYS:N	2.21	0.73
2:B:913:LYS:HA	2:B:916:PHE:HD2	1.54	0.73
2:F:143:VAL:O	2:F:425:ARG:CZ	2.37	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:262:ALA:HB1	2:F:278:LEU:HG	1.70	0.72
2:F:892:ILE:HB	2:F:896:LYS:HE2	1.71	0.72
2:B:601:ILE:HD11	2:B:607:LEU:HD21	1.70	0.72
2:F:178:ASN:ND2	2:F:295:ASN:OD1	2.22	0.72
2:B:1357:GLU:OE1	2:B:1359:ARG:NH1	2.22	0.72
2:F:846:PHE:O	2:F:1040:SER:OG	2.08	0.72
2:F:1041:ASN:O	2:F:1043:MET:N	2.17	0.72
2:B:1037:PHE:CE1	2:B:1039:TYR:CD2	2.78	0.72
2:F:841:ILE:HD12	2:F:854:ASN:HA	1.72	0.72
2:B:763:MET:SD	2:B:928:THR:HG22	2.30	0.71
2:F:1124:LYS:N	5:J:53:G:OP1	2.16	0.71
2:B:229:LEU:HB2	2:B:230:PRO:HD2	1.71	0.71
2:F:1108:GLU:HB2	3:G:9:DT:H5''	1.72	0.71
2:F:646:LYS:O	2:F:650:GLN:NE2	2.17	0.71
2:B:243:ALA:HA	2:B:246:LEU:HD23	0.74	0.71
2:F:180:ASP:HB2	2:F:184:LEU:HG	1.73	0.71
2:B:644:ASP:HB3	2:B:647:VAL:HG23	1.71	0.70
2:F:90:MET:HA	2:F:151:LEU:HD21	1.71	0.70
2:F:121:ASN:HB2	2:F:123:VAL:HG12	1.72	0.70
2:B:249:THR:HG22	2:B:265:GLN:HB2	1.73	0.70
2:B:860:SER:OG	2:B:863:ASN:OD1	2.08	0.70
2:B:1037:PHE:HE1	2:B:1039:TYR:CD2	2.10	0.70
2:B:1241:HIS:CE1	2:B:1244:LYS:HA	2.26	0.70
2:F:893:THR:HG23	2:F:896:LYS:H	1.57	0.70
1:E:23:U:H5''	2:F:1112:PRO:HG3	1.72	0.70
2:F:165:ARG:HD2	2:F:168:PHE:HE1	1.56	0.70
2:F:913:LYS:HG3	2:F:1040:SER:HB3	1.74	0.70
2:F:531:THR:HG21	2:F:575:PHE:CE1	2.26	0.70
2:F:545:LYS:HD2	2:F:690:ASN:ND2	2.07	0.69
2:F:1060:ARG:HB3	2:F:1060:ARG:NH1	2.04	0.69
2:B:1333:ARG:NH1	2:B:1335:ARG:HD2	2.07	0.69
2:F:918:LYS:NZ	2:F:1018:VAL:CG1	2.55	0.69
2:F:978:ILE:CD1	2:F:1233:VAL:HG22	2.22	0.69
1:A:14:G:OP2	2:B:63:ARG:NH1	2.25	0.69
2:B:1041:ASN:HB2	2:B:1044:ASN:HD21	1.57	0.69
2:B:558:LYS:HE3	2:B:590:SER:HB3	1.75	0.69
2:F:675:SER:CB	2:F:682:PHE:HZ	2.06	0.69
2:F:174:LEU:HD11	2:F:302:LEU:HD21	1.73	0.68
2:B:45:LYS:NZ	2:B:1357:GLU:OE2	2.22	0.68
2:B:1207:GLU:OE2	2:B:1210:ARG:NH1	2.26	0.68
1:E:15:G:P	2:F:66:ARG:HH22	2.17	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:776:ASN:O	2:F:780:ARG:HG2	1.92	0.68
2:F:1236:LEU:HD11	2:F:1269:ILE:HD13	1.76	0.68
2:F:818:ASN:ND2	2:F:818:ASN:O	2.26	0.68
2:F:1312:LEU:HD21	2:F:1326:TYR:HD1	1.59	0.68
2:B:22:THR:HG22	2:B:23:ASP:H	1.59	0.68
2:B:242:ILE:HG22	2:B:246:LEU:HD21	1.75	0.68
2:F:649:LYS:O	2:F:653:ARG:NE	2.27	0.68
2:B:516:GLU:O	2:B:519:THR:HG22	1.94	0.67
5:J:44:U:O2'	5:J:45:U:H5'	1.94	0.67
2:B:94:ASP:OD2	2:B:100:ARG:NH2	2.27	0.67
2:B:1258:PHE:HE1	2:B:1262:HIS:CD2	2.13	0.67
3:C:22:DT:H2''	3:C:23:DC:O5'	1.94	0.67
2:F:137:HIS:HA	2:F:322:ILE:HD11	1.76	0.67
2:B:526:LYS:HE2	2:B:692:ASN:HB2	1.76	0.67
2:F:967:ARG:NH1	2:F:974:LYS:HE3	2.10	0.67
2:B:982:HIS:HA	2:B:985:HIS:HB2	1.77	0.67
1:E:18:A:N7	2:F:71:ARG:NH2	2.43	0.67
2:F:737:ILE:O	2:F:740:THR:HG22	1.95	0.67
5:J:73:G:H5'	5:J:74:A:OP2	1.95	0.67
2:F:1215:ALA:HB2	2:F:1221:GLN:HG3	1.77	0.67
2:B:1179:ILE:HD11	2:B:1192:LYS:HD2	1.77	0.67
2:F:999:LYS:HB3	2:F:1073:VAL:HG12	1.77	0.66
2:F:413:GLN:O	2:F:417:GLY:N	2.22	0.66
2:F:821:ASP:HB2	2:F:828:LEU:HD21	1.77	0.66
2:B:1037:PHE:HD1	2:B:1039:TYR:H	1.43	0.66
2:F:1097:LYS:HD3	2:F:1099:GLU:OE2	1.95	0.66
1:A:1:U:H5	2:B:661:ARG:HH12	1.43	0.66
2:B:746:GLU:OE2	2:B:1353:THR:OG1	2.09	0.66
2:F:46:ASN:ND2	2:F:1089:MET:SD	2.69	0.66
2:F:302:LEU:HD22	2:F:306:LEU:HD22	1.78	0.66
2:B:662:LEU:HD23	2:B:666:LEU:HD22	1.78	0.66
2:B:1109:SER:OG	3:C:9:DT:OP2	2.09	0.66
2:B:679:ILE:O	2:B:683:LEU:HD13	1.96	0.66
2:B:1236:LEU:HD11	2:B:1269:ILE:HD13	1.77	0.66
1:E:25:U:H5'	2:F:107:VAL:HG12	1.77	0.65
2:F:545:LYS:HD2	2:F:690:ASN:HD21	1.61	0.65
2:B:1333:ARG:CZ	2:B:1335:ARG:HD2	2.26	0.65
2:F:998:ILE:HG22	2:F:1008:PHE:HE1	1.59	0.65
2:F:936:ASP:OD1	2:F:940:ASN:ND2	2.29	0.65
2:B:594:TYR:OH	2:B:608:ASP:OD1	2.15	0.65
2:B:70:ARG:NH2	5:I:61:C:OP1	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:545:LYS:NZ	2:F:683:LEU:O	2.29	0.65
2:B:70:ARG:HH21	5:I:61:C:P	2.19	0.65
2:B:226:ILE:HA	2:B:229:LEU:HG	1.78	0.65
2:B:787:GLY:HA3	2:B:891:LEU:HD21	1.78	0.65
2:B:824:VAL:HG11	2:B:859:ARG:HH12	1.61	0.65
2:B:1207:GLU:CD	2:B:1210:ARG:NH1	2.51	0.64
2:B:69:ARG:HD3	5:I:62:G:N7	2.12	0.64
2:B:1226:LEU:HB2	2:B:1276:PHE:CE2	2.32	0.64
5:J:94:U:H2'	5:J:95:G:C8	2.32	0.64
2:F:139:ARG:NH2	2:F:418:GLU:OE1	2.25	0.64
2:F:1206:LEU:HD11	2:F:1210:ARG:NH2	2.12	0.64
2:B:823:TYR:HD2	2:B:858:THR:HG21	1.62	0.64
2:B:1356:TYR:HB3	5:I:81:G:C6	2.33	0.64
2:F:332:LEU:HD11	2:F:336:LYS:HE3	1.79	0.64
2:B:317:LEU:HB2	2:B:414:ILE:HD12	1.80	0.64
2:F:44:LYS:HD3	5:J:92:G:N7	2.13	0.64
2:B:967:ARG:HE	2:B:974:LYS:HB2	1.63	0.64
2:F:63:ARG:HG3	2:F:66:ARG:NH1	2.11	0.64
2:F:760:VAL:HG22	2:F:956:ILE:HD12	1.80	0.64
2:F:328:HIS:NE2	2:F:359:TYR:OH	2.30	0.64
2:F:666:LEU:HD21	2:F:693:PHE:CZ	2.33	0.64
1:A:22:U:O2'	2:B:1110:ILE:HB	1.97	0.63
2:F:505:GLU:HG3	2:F:665:LYS:HB2	1.80	0.63
2:F:530:VAL:HG22	2:F:537:PRO:HB3	1.80	0.63
2:F:1203:LEU:HD23	2:F:1348:ILE:HB	1.80	0.63
2:B:1271:GLU:O	2:B:1274:SER:OG	2.16	0.63
2:F:189:VAL:HG13	2:F:201:ILE:HG22	1.79	0.63
2:F:226:ILE:CG1	2:F:232:GLU:HG2	2.25	0.63
2:B:116:HIS:CE1	2:B:122:ILE:HG12	2.33	0.63
2:B:818:ASN:O	2:B:818:ASN:ND2	2.32	0.63
2:F:309:ASN:OD1	2:F:312:ILE:HG23	1.99	0.63
2:F:234:LYS:H	2:F:234:LYS:HD3	1.62	0.63
2:F:972:PHE:CE1	2:F:1084:ARG:HG2	2.34	0.63
1:E:14:G:OP2	2:F:63:ARG:HD3	1.99	0.63
2:F:601:ILE:HD11	2:F:607:LEU:HD11	1.81	0.63
2:B:183:LYS:NZ	2:B:311:GLU:OE2	2.31	0.63
2:F:1216:SER:OG	4:H:7:DG:OP1	2.16	0.63
2:F:138:LEU:HD21	2:F:153:LEU:HD21	1.81	0.62
2:F:272:ASP:HA	2:F:275:LEU:HB3	1.80	0.62
2:B:781:MET:HG3	2:B:803:ASN:ND2	2.14	0.62
2:F:158:LEU:HA	2:F:161:MET:SD	2.40	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1224:ASN:CB	2:B:1280:VAL:HG11	2.22	0.62
2:F:70:ARG:HH21	5:J:61:C:P	2.22	0.62
2:F:745:ASP:OD2	2:F:938:ARG:NH2	2.33	0.62
2:F:1241:HIS:CE1	2:F:1244:LYS:HA	2.35	0.62
2:B:5:TYR:CE2	2:B:756:PRO:HB3	2.35	0.62
2:B:930:HIS:O	2:B:934:ILE:HG13	1.98	0.62
2:B:745:ASP:OD2	2:B:938:ARG:NH2	2.33	0.61
2:B:1147:ALA:HB1	2:B:1188:LYS:O	2.00	0.61
2:F:626:PHE:CE1	2:F:635:ARG:NH1	2.68	0.61
2:B:281:GLN:OE1	2:B:281:GLN:N	2.27	0.61
2:B:1000:LYS:HB3	2:B:1001:TYR:CE2	2.36	0.61
2:F:35:LEU:HB2	2:F:1358:THR:HG22	1.80	0.61
2:F:918:LYS:HE3	2:F:1018:VAL:HG11	1.81	0.61
2:F:1207:GLU:CD	2:F:1210:ARG:NH1	2.54	0.61
2:F:635:ARG:HG3	2:F:635:ARG:HH11	1.64	0.61
2:F:671:ARG:H	2:F:671:ARG:HD3	1.65	0.61
2:F:918:LYS:HZ3	2:F:1007:GLU:CD	2.03	0.61
2:F:163:LYS:HG2	2:F:164:PHE:CE1	2.36	0.61
2:F:380:LEU:HD11	2:F:390:LEU:CG	2.29	0.61
2:F:918:LYS:NZ	2:F:1018:VAL:HG11	2.14	0.61
5:I:88:A:N6	5:I:91:C:H42	1.99	0.61
2:F:258:LEU:HD22	2:F:260:GLU:H	1.65	0.61
2:F:671:ARG:HD3	2:F:671:ARG:N	2.16	0.61
2:B:472:THR:HG23	5:I:59:U:OP2	2.01	0.61
2:B:926:GLN:HG2	3:C:20:DA:P	2.40	0.61
2:F:867:SER:HB2	2:F:1054:ASN:N	2.16	0.61
2:B:340:ARG:HH21	5:I:41:A:P	2.24	0.61
2:B:1308:ASN:HD22	2:B:1327:PHE:N	1.96	0.61
2:F:139:ARG:HG3	2:F:139:ARG:HH11	1.65	0.60
2:F:1167:THR:HG23	2:F:1170:GLU:H	1.66	0.60
2:F:1326:TYR:HE2	2:F:1327:PHE:HD2	1.47	0.60
2:B:448:ILE:HD13	2:B:455:LEU:HD13	1.83	0.60
2:F:824:VAL:HG12	2:F:825:ASP:H	1.65	0.60
2:F:841:ILE:HD11	2:F:896:LYS:HG3	1.82	0.60
2:B:243:ALA:C	2:B:246:LEU:CD2	2.69	0.60
2:B:554:LYS:HG2	2:B:594:TYR:CE2	2.35	0.60
2:F:918:LYS:NZ	2:F:1018:VAL:HG12	2.15	0.60
2:B:893:THR:HG23	2:B:896:LYS:H	1.65	0.60
2:B:1002:PRO:HD2	2:B:1036:TYR:OH	2.01	0.60
2:B:539:PHE:HD2	2:B:689:ALA:HA	1.67	0.60
2:F:985:HIS:CD2	2:F:1087:LEU:HD22	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:514:LEU:HD21	2:F:664:ARG:HH21	1.66	0.60
2:F:1206:LEU:HD11	2:F:1210:ARG:HH22	1.66	0.60
2:B:694:MET:HG3	2:B:698:HIS:CD2	2.37	0.60
2:B:813:LEU:HD11	2:B:855:LYS:HB3	1.84	0.60
2:B:1286:ASN:ND2	2:B:1332:ASP:O	2.34	0.60
2:F:690:ASN:OD1	2:F:690:ASN:N	2.35	0.60
5:I:52:A:OP2	5:I:62:G:N2	2.34	0.60
2:B:879:MET:HG3	2:B:882:TYR:HB3	1.81	0.60
2:F:489:GLN:HG3	2:F:625:LEU:HD21	1.83	0.60
2:F:853:ASP:OD1	2:F:893:THR:HG21	2.01	0.60
2:F:632:ILE:O	2:F:636:LEU:HD13	2.01	0.59
5:J:88:A:C2	5:J:91:C:N3	2.70	0.59
2:B:620:VAL:HG13	2:B:656:TYR:HD2	1.67	0.59
2:B:881:ASN:OD1	2:B:885:GLN:NE2	2.27	0.59
2:B:1236:LEU:HA	2:B:1239:ALA:HB3	1.83	0.59
2:F:165:ARG:HD2	2:F:168:PHE:CE1	2.36	0.59
2:F:180:ASP:HB3	2:F:183:LYS:HD2	1.85	0.59
2:F:958:LEU:HD22	2:F:962:LEU:HD12	1.84	0.59
2:F:1061:PRO:O	2:F:1076:LYS:HE2	2.02	0.59
2:B:386:THR:O	2:B:386:THR:HG22	2.01	0.59
2:B:427:GLU:HB2	2:B:434:LYS:HB2	1.83	0.59
2:F:1347:LEU:N	2:F:1360:ILE:O	2.34	0.59
2:B:794:GLN:HG2	2:B:798:GLU:HG3	1.84	0.59
2:B:1037:PHE:CE1	2:B:1039:TYR:CG	2.90	0.59
2:B:1207:GLU:HG3	2:B:1208:ASN:H	1.67	0.59
2:B:21:ILE:HD11	2:B:995:THR:HG21	1.83	0.59
2:B:1108:GLU:N	3:C:9:DT:OP1	2.31	0.59
2:F:40:ARG:NE	2:F:43:ILE:HD11	2.18	0.59
2:B:212:LEU:O	2:B:221:ARG:HD2	2.02	0.59
2:B:1356:TYR:HB3	5:I:81:G:N1	2.17	0.59
2:F:923:GLU:HG2	2:F:928:THR:HG21	1.85	0.59
2:F:1110:ILE:HD13	2:F:1122:ARG:CZ	2.32	0.59
2:F:1120:ILE:HD11	2:F:1137:PRO:HD3	1.84	0.59
2:F:1236:LEU:O	2:F:1240:SER:OG	2.14	0.59
5:J:40:C:H2'	5:J:41:A:C8	2.38	0.59
2:B:380:LEU:O	2:B:386:THR:HG21	2.02	0.59
2:F:149:ALA:H	2:F:426:GLN:HE22	1.51	0.58
2:F:1224:ASN:HB2	2:F:1280:VAL:HG11	1.85	0.58
2:F:1290:VAL:HG22	2:F:1331:ILE:HD13	1.85	0.58
2:B:107:VAL:HG22	2:B:1131:TYR:OH	2.02	0.58
2:B:979:ASN:OD1	2:B:980:ASN:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:LEU:HD22	2:B:414:ILE:HD11	1.84	0.58
2:B:1120:ILE:HB	2:B:1134:PHE:HB2	1.84	0.58
2:F:189:VAL:HG13	2:F:201:ILE:CG2	2.32	0.58
2:B:1011:GLY:O	2:B:1014:LYS:N	2.36	0.58
2:F:14:ASN:OD1	2:F:55:SER:OG	2.19	0.58
1:A:2:U:N3	1:A:4:A:H3'	2.13	0.58
2:B:48:ILE:O	2:B:1093:ASN:ND2	2.33	0.58
2:F:207:ASP:O	2:F:211:ILE:HG12	2.03	0.58
2:F:1219:GLU:OE1	2:F:1335:ARG:NH2	2.28	0.58
2:B:5:TYR:OH	2:B:754:HIS:O	2.21	0.58
2:F:967:ARG:NH1	2:F:986:ASP:OD1	2.36	0.58
5:J:40:C:H2'	5:J:41:A:H8	1.68	0.58
2:B:1123:LYS:NZ	5:I:52:A:OP1	2.37	0.58
2:B:1206:LEU:HB3	2:B:1345:ALA:HB2	1.84	0.58
2:F:821:ASP:HA	2:F:828:LEU:HD11	1.86	0.58
2:B:621:LEU:O	2:B:625:LEU:HB2	2.03	0.58
2:F:25:TYR:O	2:F:988:TYR:OH	2.21	0.58
2:F:860:SER:OG	2:F:863:ASN:OD1	2.20	0.58
2:B:181:VAL:O	2:B:185:PHE:N	2.31	0.58
2:B:305:ILE:HG13	2:B:306:LEU:N	2.19	0.57
2:B:343:LEU:HD21	2:B:346:LYS:HG3	1.85	0.57
2:B:620:VAL:HG13	2:B:656:TYR:CD2	2.39	0.57
2:F:954:LYS:NZ	2:F:998:ILE:HD13	2.19	0.57
2:B:118:ILE:O	2:B:152:ARG:HD2	2.04	0.57
2:B:1251:ASP:HB3	2:B:1255:LYS:HE2	1.85	0.57
2:B:1256:GLN:O	2:B:1256:GLN:NE2	2.38	0.57
2:F:178:ASN:HB3	2:F:184:LEU:HD11	1.87	0.57
2:F:220:ARG:O	2:F:224:ASN:N	2.32	0.57
2:B:233:LYS:HG2	2:B:235:ASN:H	1.69	0.57
2:F:48:ILE:HG12	2:F:984:ALA:HB1	1.86	0.57
2:F:258:LEU:HD12	2:F:281:GLN:HE22	1.68	0.57
1:A:27:G:H5'	1:A:28:A:C5'	2.33	0.57
2:B:640:ALA:HA	2:B:648:MET:HE2	1.86	0.57
2:B:1235:PHE:O	2:B:1239:ALA:N	2.32	0.57
2:F:63:ARG:HG3	2:F:66:ARG:HH12	1.69	0.57
2:F:697:ILE:HD11	2:F:708:ILE:HG13	1.86	0.57
1:A:12:A:H61	3:C:17:DT:H3	1.51	0.57
2:F:843:PRO:HG3	2:F:864:ARG:HH22	1.68	0.57
5:J:91:C:O2'	5:J:92:G:P	2.63	0.57
2:B:143:VAL:HG13	2:B:421:ALA:CB	2.33	0.57
2:B:699:ASP:HB3	2:B:702:LEU:HD12	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:823:TYR:HA	2:B:875:VAL:CG1	2.31	0.57
2:B:184:LEU:HD12	2:B:299:ALA:HB2	1.86	0.57
2:B:525:THR:CG2	2:B:690:ASN:CB	2.75	0.57
2:B:1140:ALA:HB2	2:B:1168:ILE:HG12	1.85	0.57
2:F:867:SER:HB2	2:F:1053:ALA:C	2.25	0.57
2:F:1096:LYS:HG2	2:F:1201:TYR:CD2	2.40	0.57
2:B:373:TYR:OH	2:B:398:LEU:N	2.31	0.57
2:F:979:ASN:OD1	2:F:981:TYR:N	2.31	0.57
2:B:686:ASP:HB3	2:B:690:ASN:HA	1.86	0.57
2:B:353:ASP:CG	2:B:356:LYS:HG2	2.25	0.57
2:B:465:MET:HE2	2:B:467:ARG:HG2	1.87	0.57
2:B:1074:TRP:HZ2	2:B:1080:PHE:CE2	2.23	0.57
2:F:165:ARG:O	2:F:415:HIS:HD2	1.87	0.57
2:B:977:GLU:N	2:B:977:GLU:OE1	2.38	0.56
2:F:312:ILE:HG13	2:F:313:THR:N	2.19	0.56
2:F:646:LYS:HG3	2:F:650:GLN:NE2	2.20	0.56
2:F:918:LYS:CE	2:F:1018:VAL:HG11	2.35	0.56
2:B:1315:LEU:HB2	2:B:1324:PHE:CE1	2.40	0.56
2:F:1060:ARG:HH11	2:F:1060:ARG:CG	2.16	0.56
2:B:978:ILE:HD12	2:B:1233:VAL:HG22	1.85	0.56
2:B:1200:LYS:HG2	2:B:1201:TYR:CD1	2.40	0.56
2:F:737:ILE:HA	2:F:740:THR:HG22	1.87	0.56
2:F:750:VAL:HG21	2:F:1355:LEU:HD12	1.87	0.56
2:B:634:GLU:OE2	2:B:637:LYS:NZ	2.38	0.56
2:F:199:ASN:O	2:F:201:ILE:CD1	2.53	0.56
2:F:1108:GLU:N	3:G:9:DT:OP1	2.30	0.56
3:G:3:DA:N6	4:H:9:DA:H61	2.04	0.56
2:B:985:HIS:ND1	2:B:1087:LEU:HD13	2.20	0.56
2:B:1314:THR:HG21	2:B:1324:PHE:HB3	1.87	0.56
2:F:643:PHE:HD1	2:F:647:VAL:HG11	1.71	0.56
2:F:886:LEU:HD22	2:F:891:LEU:HD11	1.88	0.56
2:B:465:MET:CE	2:B:467:ARG:HG2	2.35	0.56
2:F:446:PHE:HE2	2:F:448:ILE:HD13	1.70	0.56
2:B:672:ASP:HA	2:B:703:THR:HG22	1.88	0.56
2:B:864:ARG:HB2	2:B:871:PRO:HA	1.88	0.56
2:B:1116:SER:OG	2:B:1117:ASP:N	2.38	0.56
2:B:1228:LEU:HD12	2:B:1229:PRO:HD2	1.88	0.56
2:F:841:ILE:CD1	2:F:896:LYS:HG3	2.36	0.56
2:F:1095:VAL:HG13	2:F:1350:GLN:OE1	2.06	0.56
2:F:1326:TYR:HE2	2:F:1327:PHE:CD2	2.23	0.56
2:F:621:LEU:O	2:F:625:LEU:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:644:ASP:HB3	2:F:647:VAL:HG23	1.88	0.56
2:B:358:GLY:O	2:B:362:TYR:N	2.34	0.56
2:B:1177:ASN:ND2	2:B:1180:ASP:OD2	2.38	0.56
2:B:45:LYS:NZ	2:B:1354:GLY:O	2.36	0.55
2:B:315:ALA:HB1	2:B:418:GLU:OE2	2.06	0.55
2:F:535:ARG:HD2	2:F:535:ARG:H	1.71	0.55
2:F:633:GLU:O	2:F:637:LYS:N	2.38	0.55
2:B:427:GLU:OE1	2:B:437:ARG:NH1	2.38	0.55
2:F:1349:HIS:CE1	5:J:69:A:H5'	2.40	0.55
2:B:1211:LYS:C	2:B:1223:GLY:HA3	2.27	0.55
2:F:139:ARG:HG3	2:F:139:ARG:NH1	2.21	0.55
2:F:839:ASP:OD2	2:F:864:ARG:HD2	2.06	0.55
2:B:565:LYS:HE2	2:B:580:ILE:HG12	1.88	0.55
2:F:448:ILE:HD12	2:F:455:LEU:HD11	1.88	0.55
2:F:468:LYS:HE3	2:F:483:ASP:HB3	1.88	0.55
2:B:30:LYS:HD3	5:I:83:C:P	2.46	0.55
2:B:302:LEU:HA	2:B:305:ILE:HG12	1.88	0.55
2:F:939:MET:HG3	2:F:953:VAL:HG11	1.89	0.55
2:F:1264:HIS:O	2:F:1268:GLU:HG3	2.07	0.55
5:J:88:A:C6	5:J:91:C:N4	2.72	0.55
2:F:1207:GLU:CD	2:F:1210:ARG:HH11	2.08	0.55
2:F:1270:ILE:HG13	2:F:1294:TYR:CD2	2.42	0.55
2:B:672:ASP:HA	2:B:703:THR:CG2	2.37	0.55
2:B:489:GLN:HG3	2:B:625:LEU:HD21	1.87	0.55
2:F:369:GLN:HG2	2:F:373:TYR:HE2	1.71	0.55
2:F:977:GLU:HG3	2:F:1310:ILE:CG2	2.37	0.55
2:F:675:SER:HB2	2:F:682:PHE:HZ	1.71	0.55
3:G:6:DC:H2''	3:G:7:DC:O5'	2.06	0.55
2:F:887:LEU:HD21	2:F:894:GLN:HG2	1.88	0.55
2:B:833:LEU:HD22	2:B:857:LEU:HD21	1.89	0.54
2:F:199:ASN:O	2:F:201:ILE:HD11	2.06	0.54
2:F:972:PHE:HE1	2:F:1084:ARG:HG2	1.71	0.54
5:J:83:C:H2'	5:J:84:A:H8	1.72	0.54
2:F:755:LYS:HD3	2:F:939:MET:HE3	1.89	0.54
2:B:139:ARG:NH2	2:B:161:MET:HG2	2.22	0.54
2:B:1060:ARG:NH1	2:B:1064:GLU:OE2	2.40	0.54
2:B:1222:LYS:NZ	2:B:1315:LEU:O	2.34	0.54
2:F:794:GLN:H	2:F:794:GLN:CD	2.10	0.54
2:F:943:TYR:CE2	2:F:949:LEU:HD13	2.42	0.54
2:F:1135:ASP:OD1	2:F:1136:SER:N	2.40	0.54
2:F:1347:LEU:HB3	2:F:1360:ILE:HB	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:978:ILE:CD1	2:B:1233:VAL:HG22	2.37	0.54
2:F:618:ASP:HB3	2:F:639:TYR:OH	2.08	0.54
2:B:218:LYS:H	2:B:218:LYS:HD2	1.73	0.54
2:B:345:GLU:N	2:B:345:GLU:OE1	2.39	0.54
2:F:350:ILE:O	2:F:359:TYR:N	2.40	0.54
2:B:531:THR:HG21	2:B:575:PHE:CE2	2.43	0.54
2:B:814:TYR:CE2	2:B:819:GLY:HA2	2.43	0.54
2:B:116:HIS:HE1	2:B:122:ILE:HG12	1.70	0.54
1:E:6:G:H1	3:G:23:DC:H42	1.55	0.54
2:F:672:ASP:HB3	2:F:675:SER:HB2	1.88	0.54
2:F:962:LEU:HB3	2:F:1043:MET:CE	2.38	0.54
2:F:1147:ALA:HB2	2:F:1190:VAL:HA	1.89	0.54
2:B:1062:LEU:HD23	2:B:1062:LEU:H	1.72	0.54
2:F:140:LYS:HE3	2:F:313:THR:OG1	2.07	0.54
2:B:118:ILE:HG12	2:B:156:LEU:HD11	1.90	0.54
2:B:853:ASP:CG	2:B:893:THR:HG21	2.28	0.54
2:B:1105:PHE:CG	2:B:1169:MET:HG3	2.43	0.54
2:F:90:MET:SD	2:F:151:LEU:HD23	2.47	0.54
2:F:324:ARG:O	2:F:327:GLU:HB2	2.08	0.54
2:F:868:ASP:O	2:F:869:ASN:HB2	2.08	0.54
2:F:1207:GLU:HG3	2:F:1208:ASN:H	1.72	0.54
2:F:1347:LEU:HD23	2:F:1348:ILE:N	2.23	0.54
1:A:8:A:H2'	1:A:9:U:C6	2.43	0.53
2:F:1019:ARG:O	2:F:1021:MET:N	2.35	0.53
2:B:233:LYS:HB3	2:B:236:GLY:H	1.74	0.53
2:B:240:ASN:HB3	2:B:252:PHE:CE2	2.44	0.53
2:F:1106:SER:HA	2:F:1137:PRO:HA	1.91	0.53
2:B:38:THR:HG22	2:B:40:ARG:H	1.73	0.53
2:B:165:ARG:NH2	2:B:446:PHE:O	2.40	0.53
2:B:305:ILE:HD11	2:B:414:ILE:HG21	1.91	0.53
2:B:597:LEU:O	2:B:601:ILE:HG12	2.07	0.53
2:F:971:GLN:HG2	2:F:973:TYR:CE2	2.43	0.53
2:B:1206:LEU:HD11	2:B:1210:ARG:NH2	2.24	0.53
2:F:351:PHE:HD1	5:J:43:G:O6	1.91	0.53
2:F:923:GLU:OE2	2:F:925:ARG:NH1	2.41	0.53
2:F:1205:GLU:OE1	2:F:1359:ARG:NH2	2.36	0.53
2:B:526:LYS:NZ	2:B:690:ASN:O	2.28	0.53
2:B:951:ARG:NH2	2:B:1011:GLY:HA2	2.23	0.53
2:F:1123:LYS:HD2	5:J:53:G:P	2.49	0.53
2:B:279:LEU:HD11	2:B:284:ASP:HA	1.91	0.53
2:F:174:LEU:CD1	2:F:302:LEU:HD21	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:165:ARG:O	2:B:415:HIS:HD2	1.91	0.53
2:F:167:HIS:CD2	2:F:169:LEU:HB2	2.43	0.53
2:F:323:LYS:HE3	2:F:327:GLU:OE2	2.08	0.53
5:J:94:U:H2'	5:J:95:G:H8	1.73	0.53
2:B:455:LEU:HD23	2:B:473:ILE:HD12	1.91	0.53
2:B:1236:LEU:O	2:B:1240:SER:OG	2.23	0.53
2:B:1266:LEU:O	2:B:1270:ILE:HG12	2.09	0.53
2:F:154:ILE:HG23	2:F:158:LEU:HG	1.89	0.53
2:F:554:LYS:HB3	2:F:594:TYR:CE2	2.44	0.53
2:F:1286:ASN:O	2:F:1290:VAL:HG23	2.08	0.53
2:B:143:VAL:HG13	2:B:421:ALA:HB1	1.90	0.53
2:B:273:ASP:N	2:B:273:ASP:OD1	2.37	0.53
2:F:167:HIS:HD2	2:F:169:LEU:H	1.57	0.53
2:F:563:GLN:O	2:F:567:ASP:HB2	2.08	0.53
2:F:1326:TYR:CE2	2:F:1327:PHE:HD2	2.26	0.53
2:F:794:GLN:HE21	2:F:798:GLU:CD	2.13	0.53
2:F:911:LEU:HD12	2:F:911:LEU:H	1.74	0.53
2:B:203:ALA:O	2:B:206:VAL:HG22	2.08	0.52
2:B:530:VAL:CG2	2:B:537:PRO:HB3	2.36	0.52
2:B:531:THR:HG21	2:B:575:PHE:HE2	1.73	0.52
2:B:784:ILE:HD13	2:B:815:TYR:HB3	1.91	0.52
2:B:1114:ARG:NH1	4:D:9:DA:OP1	2.42	0.52
2:F:1221:GLN:NE2	2:F:1320:ALA:HB2	2.24	0.52
5:I:83:C:H2'	5:I:84:A:H8	1.74	0.52
2:B:251:ASN:HD21	2:B:253:LYS:HB3	1.74	0.52
2:F:338:LEU:HB3	2:F:383:MET:HE3	1.90	0.52
2:B:94:ASP:HB3	2:B:97:PHE:HB2	1.91	0.52
2:B:925:ARG:HB3	2:B:928:THR:HG23	1.91	0.52
2:F:226:ILE:HD11	2:F:232:GLU:OE1	2.09	0.52
2:F:253:LYS:HG3	2:F:261:ASP:HA	1.91	0.52
2:F:1002:PRO:HD2	2:F:1036:TYR:OH	2.09	0.52
2:F:699:ASP:OD1	2:F:701:SER:OG	2.27	0.52
2:F:1326:TYR:CE2	2:F:1327:PHE:CD2	2.97	0.52
2:F:1167:THR:CG2	2:F:1170:GLU:HG3	2.40	0.52
5:J:96:C:C4	5:J:97:U:C4	2.97	0.52
1:A:25:U:H2'	1:A:26:A:H8	1.74	0.52
2:B:736:GLY:O	2:B:740:THR:N	2.32	0.52
2:F:90:MET:HA	2:F:151:LEU:CD2	2.39	0.52
2:F:795:ILE:HA	2:F:798:GLU:HB2	1.91	0.52
2:B:217:SER:HB2	2:B:220:ARG:HG2	1.92	0.52
2:B:727:LEU:HD12	2:B:927:ILE:CD1	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:737:ILE:O	2:B:740:THR:HG22	2.09	0.52
1:E:11:U:C2	1:E:12:A:C8	2.97	0.52
1:E:18:A:OP2	2:F:71:ARG:HD2	2.09	0.52
2:F:820:ARG:HG3	2:F:826:GLN:O	2.09	0.52
2:B:186:ILE:O	2:B:190:GLN:N	2.37	0.52
2:B:946:ASN:HB3	2:B:948:LYS:HD2	1.92	0.52
2:B:1241:HIS:ND1	2:B:1244:LYS:HA	2.25	0.52
2:F:923:GLU:CG	2:F:928:THR:HG21	2.39	0.52
2:B:180:ASP:HB3	2:B:183:LYS:HB2	1.92	0.52
2:B:369:GLN:HE22	2:B:400:ARG:HD2	1.74	0.52
2:F:1212:ARG:CZ	2:F:1336:TYR:HE2	2.23	0.52
3:G:3:DA:H61	4:H:9:DA:N6	2.07	0.52
2:B:137:HIS:HE1	2:B:325:TYR:CD2	2.28	0.51
2:B:416:LEU:HB2	2:B:444:LEU:HD22	1.92	0.51
2:F:38:THR:HG22	2:F:40:ARG:H	1.75	0.51
2:F:869:ASN:HD21	2:F:907:GLY:HA3	1.75	0.51
2:B:473:ILE:HG12	2:B:481:VAL:HG11	1.92	0.51
2:F:122:ILE:O	2:F:126:VAL:HG23	2.11	0.51
2:F:918:LYS:HE3	2:F:1018:VAL:CG1	2.39	0.51
2:F:1313:PHE:O	2:F:1316:THR:N	2.43	0.51
5:J:85:C:H2'	5:J:86:C:C6	2.45	0.51
5:J:91:C:HO2'	5:J:92:G:P	2.33	0.51
1:E:27:G:H5'	1:E:28:A:C5'	2.41	0.51
2:B:256:PHE:O	2:B:257:ASP:OD1	2.29	0.51
2:F:619:ILE:HD11	2:F:651:LEU:HD11	1.92	0.51
2:F:1205:GLU:HB2	2:F:1348:ILE:HD11	1.91	0.51
3:G:3:DA:H61	4:H:9:DA:H61	1.58	0.51
2:B:1037:PHE:HE2	2:B:1060:ARG:HH21	1.53	0.51
3:C:19:DA:H2'	3:C:20:DA:C8	2.45	0.51
2:F:138:LEU:CD2	2:F:153:LEU:HD11	2.41	0.51
2:F:226:ILE:CG2	2:F:230:PRO:HA	2.41	0.51
2:B:943:TYR:CZ	2:B:949:LEU:HD13	2.46	0.51
2:F:275:LEU:O	2:F:279:LEU:N	2.42	0.51
5:J:79:G:O2'	5:J:80:U:H5'	2.10	0.51
2:F:1207:GLU:HG3	2:F:1208:ASN:N	2.26	0.51
2:F:74:ARG:O	2:F:78:ARG:HG3	2.11	0.51
2:F:137:HIS:HA	2:F:322:ILE:CD1	2.39	0.51
2:F:998:ILE:HG22	2:F:1008:PHE:CE1	2.45	0.51
2:F:1205:GLU:CD	2:F:1359:ARG:HH22	2.14	0.51
1:E:19:A:H4'	2:F:407:ASN:C	2.31	0.51
2:F:666:LEU:HD21	2:F:693:PHE:CE1	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1312:LEU:HD21	2:F:1326:TYR:CD1	2.44	0.51
1:A:16:A:H4'	2:B:448:ILE:O	2.11	0.51
2:B:135:ILE:HG21	2:B:160:HIS:NE2	2.25	0.51
2:B:325:TYR:HD1	5:I:44:U:C2	2.28	0.51
2:B:724:ILE:O	2:B:727:LEU:HB2	2.11	0.51
2:F:511:HIS:O	2:F:593:THR:OG1	2.26	0.51
2:F:671:ARG:H	2:F:671:ARG:CD	2.21	0.51
2:F:853:ASP:CG	2:F:893:THR:HG21	2.31	0.51
2:F:135:ILE:HG21	5:J:46:A:H5'	1.92	0.50
2:F:338:LEU:HD13	2:F:386:THR:HG22	1.93	0.50
2:F:620:VAL:O	2:F:624:THR:N	2.37	0.50
2:F:1347:LEU:HD22	2:F:1349:HIS:CD2	2.46	0.50
2:B:1041:ASN:HB2	2:B:1044:ASN:ND2	2.23	0.50
2:B:1208:ASN:OD1	2:B:1279:ARG:HG3	2.10	0.50
2:F:334:LEU:O	2:F:338:LEU:HG	2.11	0.50
2:F:508:LEU:HD11	2:F:664:ARG:HB2	1.94	0.50
2:F:1357:GLU:O	5:J:81:G:N2	2.38	0.50
2:F:1060:ARG:NH1	2:F:1060:ARG:CG	2.73	0.50
2:F:1135:ASP:OD1	4:H:8:DT:H5''	2.11	0.50
2:B:473:ILE:HD13	2:B:482:VAL:HG23	1.92	0.50
2:F:442:LYS:HB3	2:F:476:TRP:CD1	2.46	0.50
2:F:1241:HIS:ND1	2:F:1244:LYS:HA	2.26	0.50
5:J:91:C:O2'	5:J:92:G:O5'	2.29	0.50
2:B:249:THR:HG22	2:B:265:GLN:CB	2.39	0.50
2:F:108:GLU:HG3	2:F:115:ARG:HD3	1.94	0.50
2:F:138:LEU:HD22	2:F:153:LEU:HD11	1.94	0.50
3:G:7:DC:O2	4:H:7:DG:N2	2.45	0.50
5:I:42:A:H8	5:I:42:A:H5''	1.77	0.50
5:I:83:C:H2'	5:I:84:A:C8	2.47	0.50
5:J:96:C:H2'	5:J:97:U:O4'	2.12	0.50
1:A:31:U:N3	1:A:32:A:N7	2.59	0.50
2:B:331:ASP:OD2	2:B:392:LYS:NZ	2.41	0.50
1:E:27:G:H5'	1:E:28:A:O5'	2.10	0.50
2:F:979:ASN:OD1	2:F:980:ASN:N	2.44	0.50
2:F:853:ASP:HB3	2:F:895:ARG:HD3	1.93	0.50
2:B:661:ARG:HB2	2:B:662:LEU:HD12	1.93	0.50
2:B:939:MET:HG3	2:B:953:VAL:HG11	1.94	0.50
2:F:226:ILE:HG23	2:F:230:PRO:HA	1.93	0.50
2:F:465:MET:SD	2:F:482:VAL:HG21	2.51	0.50
2:F:884:ARG:HG3	2:F:884:ARG:HH11	1.76	0.50
2:F:1198:LEU:HD21	2:F:1347:LEU:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1240:SER:HB2	2:B:1242:TYR:CD1	2.47	0.50
2:F:167:HIS:HD2	2:F:169:LEU:HB2	1.77	0.50
2:F:923:GLU:HA	2:F:923:GLU:OE1	2.12	0.50
2:F:961:LYS:HA	2:F:964:SER:HB3	1.94	0.50
2:B:761:ILE:HG13	2:B:761:ILE:O	2.11	0.49
2:B:874:GLU:HA	2:B:877:LYS:HE3	1.94	0.49
2:F:566:GLU:O	2:F:570:LYS:HB3	2.11	0.49
2:B:198:GLU:HG2	2:B:199:ASN:N	2.27	0.49
2:B:917:ILE:HD11	2:B:1042:ILE:HG22	1.95	0.49
2:B:40:ARG:NE	2:B:43:ILE:HD11	2.27	0.49
2:B:310:THR:OG1	2:B:316:PRO:HB3	2.13	0.49
2:B:943:TYR:CE1	2:B:949:LEU:HD13	2.47	0.49
2:F:271:TYR:O	2:F:275:LEU:N	2.42	0.49
2:B:1037:PHE:HE1	2:B:1039:TYR:CG	2.27	0.49
2:F:180:ASP:HB3	2:F:183:LYS:CD	2.41	0.49
2:F:1333:ARG:CZ	2:F:1335:ARG:HD2	2.41	0.49
2:B:121:ASN:H	2:B:121:ASN:ND2	2.10	0.49
2:B:448:ILE:HD13	2:B:455:LEU:CD1	2.41	0.49
2:B:679:ILE:HD13	2:B:704:PHE:CE2	2.48	0.49
2:B:841:ILE:HD11	2:B:896:LYS:HG3	1.94	0.49
2:F:9:LEU:HD13	2:F:740:THR:OG1	2.12	0.49
2:F:19:ALA:HB2	2:F:48:ILE:HG13	1.93	0.49
2:F:32:PHE:CE1	2:F:1355:LEU:HB3	2.47	0.49
2:F:362:TYR:OH	2:F:401:LYS:HG3	2.13	0.49
2:B:420:HIS:ND1	2:B:441:GLU:OE2	2.46	0.49
2:B:31:LYS:HG2	2:B:42:SER:OG	2.12	0.49
2:B:336:LYS:NZ	5:I:43:G:O6	2.46	0.49
2:B:603:ASP:OD1	2:B:606:PHE:N	2.40	0.49
2:F:925:ARG:HB3	2:F:928:THR:HG22	1.94	0.49
2:F:1216:SER:HB3	2:F:1219:GLU:H	1.77	0.49
2:B:967:ARG:NE	2:B:974:LYS:HB2	2.26	0.49
2:B:1290:VAL:HG22	2:B:1331:ILE:HD13	1.94	0.49
2:B:1305:GLN:O	2:B:1309:ILE:HG13	2.12	0.49
2:F:473:ILE:HG12	2:F:481:VAL:HG11	1.93	0.49
2:F:692:ASN:O	2:F:696:LEU:HG	2.13	0.49
2:B:939:MET:HE2	2:B:953:VAL:HG21	1.94	0.49
2:B:1314:THR:CG2	2:B:1324:PHE:HB3	2.43	0.49
2:F:139:ARG:NH2	2:F:161:MET:HG3	2.27	0.49
2:F:226:ILE:HD11	2:F:232:GLU:CD	2.32	0.49
2:F:628:ASP:O	2:F:632:ILE:HG13	2.13	0.49
2:F:962:LEU:HB3	2:F:1043:MET:HE1	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:182:ASP:O	2:B:186:ILE:HG12	2.12	0.49
2:F:221:ARG:HA	2:F:224:ASN:CB	2.38	0.49
2:F:601:ILE:CD1	2:F:607:LEU:HD21	2.43	0.49
1:A:31:U:C2	1:A:32:A:C8	3.00	0.48
2:F:471:GLU:OE2	2:F:481:VAL:HG22	2.13	0.48
2:F:641:HIS:CD2	2:F:642:LEU:HG	2.48	0.48
2:F:755:LYS:NZ	2:F:939:MET:O	2.35	0.48
2:F:1311:HIS:O	2:F:1314:THR:HG22	2.12	0.48
1:A:20:A:OP2	2:B:403:ARG:NH1	2.46	0.48
2:B:499:ASP:OD2	2:B:663:SER:N	2.39	0.48
2:F:467:ARG:HH21	2:F:473:ILE:HD11	1.79	0.48
2:F:583:VAL:HG22	2:F:584:GLU:N	2.27	0.48
2:F:918:LYS:CE	2:F:1018:VAL:CG1	2.92	0.48
2:B:253:LYS:O	2:B:257:ASP:N	2.43	0.48
2:B:380:LEU:HB3	2:B:386:THR:HG21	1.94	0.48
2:B:645:ASP:O	2:B:649:LYS:HE2	2.14	0.48
2:F:336:LYS:HG2	2:F:351:PHE:CE1	2.49	0.48
5:J:42:A:O2'	5:J:43:G:OP1	2.26	0.48
2:F:629:ARG:HH11	2:F:629:ARG:HG2	1.79	0.48
2:F:1245:LEU:HA	2:F:1245:LEU:HD23	1.59	0.48
2:B:1179:ILE:HD11	2:B:1192:LYS:CD	2.43	0.48
2:F:36:GLY:HA3	2:F:1359:ARG:O	2.13	0.48
2:F:963:VAL:HG21	2:F:990:ASN:OD1	2.13	0.48
5:J:48:A:H2'	5:J:49:A:C8	2.48	0.48
2:B:63:ARG:HG3	2:B:66:ARG:HH21	1.79	0.48
2:B:263:LYS:C	2:B:264:LEU:HD12	2.34	0.48
2:B:971:GLN:O	2:B:971:GLN:HG2	2.13	0.48
1:A:25:U:H2'	1:A:26:A:C8	2.49	0.48
2:B:840:ALA:HA	2:B:854:ASN:O	2.12	0.48
2:B:1207:GLU:HG3	2:B:1208:ASN:N	2.29	0.48
1:E:21:G:H2'	1:E:22:U:O4'	2.14	0.48
2:F:652:LYS:HE3	2:F:652:LYS:HB2	1.62	0.48
2:F:828:LEU:HD22	2:F:836:TYR:CE2	2.49	0.48
2:B:570:LYS:O	2:B:574:CYS:HA	2.14	0.48
2:B:1336:TYR:N	2:B:1336:TYR:CD1	2.81	0.48
2:F:143:VAL:HG22	2:F:422:ILE:HG12	1.95	0.48
2:F:891:LEU:H	2:F:891:LEU:HD23	1.79	0.48
2:F:1284:ASP:OD1	2:F:1284:ASP:N	2.35	0.48
2:B:35:LEU:HB2	2:B:1358:THR:HG22	1.96	0.48
2:B:229:LEU:O	2:B:231:GLY:N	2.47	0.48
2:B:563:GLN:O	2:B:567:ASP:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:25:U:H2'	1:E:26:A:H8	1.79	0.48
2:F:63:ARG:CA	2:F:66:ARG:HG3	2.33	0.48
2:B:275:LEU:O	2:B:279:LEU:N	2.35	0.48
2:B:977:GLU:HG3	2:B:1310:ILE:HG23	1.96	0.48
2:F:545:LYS:CD	2:F:690:ASN:ND2	2.77	0.48
2:B:241:LEU:HD11	2:B:289:LEU:HD21	1.96	0.47
2:F:316:PRO:O	2:F:320:SER:N	2.46	0.47
2:F:359:TYR:CE1	2:F:399:LEU:HD13	2.49	0.47
2:F:746:GLU:HG2	2:F:1353:THR:CG2	2.44	0.47
5:J:53:G:N3	5:J:62:G:C2	2.82	0.47
2:B:1035:LYS:HA	2:B:1035:LYS:HD3	1.71	0.47
2:B:1041:ASN:O	2:B:1044:ASN:ND2	2.47	0.47
2:F:22:THR:HG22	2:F:28:PRO:HG3	1.95	0.47
2:F:180:ASP:HB3	2:F:183:LYS:HB2	1.96	0.47
2:F:691:ARG:HG2	2:F:695:GLN:NE2	2.29	0.47
2:F:882:TYR:CD2	2:F:883:TRP:CD1	3.02	0.47
2:F:164:PHE:CZ	2:F:403:ARG:NH2	2.83	0.47
2:B:199:ASN:N	2:B:200:PRO:HD3	2.29	0.47
2:F:514:LEU:H	2:F:514:LEU:HD12	1.79	0.47
2:B:967:ARG:HB3	2:B:972:PHE:O	2.15	0.47
1:E:18:A:N7	2:F:71:ARG:CZ	2.78	0.47
2:F:114:GLU:HG2	2:F:120:GLY:HA2	1.96	0.47
2:F:410:ILE:HG21	2:F:415:HIS:NE2	2.29	0.47
2:F:943:TYR:HE2	2:F:949:LEU:HD13	1.80	0.47
2:F:954:LYS:HZ3	2:F:998:ILE:HD13	1.78	0.47
2:F:1054:ASN:C	2:F:1056:GLU:H	2.17	0.47
2:B:325:TYR:CD1	5:I:44:U:C2	3.03	0.47
2:B:1349:HIS:HB3	5:I:68:A:N3	2.30	0.47
3:C:1:DC:H2'	3:C:2:DA:C8	2.49	0.47
2:F:5:TYR:CZ	2:F:751:MET:HG3	2.50	0.47
2:F:466:THR:O	2:F:482:VAL:HG13	2.15	0.47
2:F:531:THR:HG22	2:F:534:MET:HG2	1.96	0.47
2:F:1182:LEU:HD13	2:F:1190:VAL:HG11	1.96	0.47
2:B:6:SER:HB3	2:B:758:ASN:HB2	1.97	0.47
2:B:277:ASN:O	2:B:281:GLN:NE2	2.43	0.47
2:B:369:GLN:NE2	2:B:400:ARG:HD2	2.28	0.47
2:B:1050:ILE:HG12	2:B:1059:LYS:N	2.29	0.47
2:F:137:HIS:HA	2:F:322:ILE:CG1	2.45	0.47
2:F:143:VAL:HG22	2:F:422:ILE:CG1	2.44	0.47
2:F:297:SER:HA	2:F:300:ILE:HD12	1.96	0.47
2:F:784:ILE:HD13	2:F:815:TYR:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:824:VAL:HG12	2:F:825:ASP:N	2.30	0.47
2:F:921:LEU:HD21	2:F:1008:PHE:HE2	1.79	0.47
2:F:949:LEU:HD23	2:F:951:ARG:HH22	1.79	0.47
5:J:85:C:C2	5:J:86:C:C5	3.02	0.47
2:B:107:VAL:HG13	2:B:1131:TYR:CE1	2.49	0.47
2:B:208:ALA:O	2:B:212:LEU:HD23	2.15	0.47
2:B:671:ARG:HG3	2:B:678:THR:HG22	1.97	0.47
2:B:917:ILE:O	2:B:921:LEU:HG	2.15	0.47
2:B:1003:LYS:HE3	2:B:1034:ALA:HB1	1.97	0.47
2:B:1251:ASP:O	2:B:1254:GLN:HG3	2.15	0.47
2:F:328:HIS:ND1	5:J:44:U:C2	2.83	0.47
2:F:813:LEU:O	2:F:817:GLN:HG3	2.14	0.47
2:F:1221:GLN:HB3	2:F:1319:GLY:O	2.15	0.47
2:B:22:THR:HG22	2:B:23:ASP:N	2.29	0.47
2:B:249:THR:HG22	2:B:265:GLN:CG	2.45	0.47
2:F:212:LEU:HD13	2:F:300:ILE:HG12	1.97	0.47
2:F:223:GLU:O	2:F:227:ALA:N	2.48	0.47
2:F:307:ARG:HG2	2:F:307:ARG:HH11	1.80	0.47
2:F:427:GLU:OE1	2:F:434:LYS:HA	2.14	0.47
2:F:597:LEU:O	2:F:601:ILE:HG12	2.15	0.47
2:F:1035:LYS:HA	2:F:1035:LYS:HD3	1.71	0.47
5:I:85:C:H42	5:I:93:G:H1	1.62	0.47
2:B:139:ARG:O	2:B:143:VAL:HG23	2.15	0.47
2:B:141:LYS:HD3	2:B:142:LEU:HD23	1.97	0.47
2:B:155:TYR:CE1	2:B:159:ALA:HB2	2.49	0.47
2:B:252:PHE:CE1	2:B:290:PHE:HE2	2.32	0.47
2:B:724:ILE:HA	2:B:727:LEU:HD23	1.98	0.47
2:B:813:LEU:O	2:B:817:GLN:HG3	2.15	0.47
2:B:1270:ILE:HG13	2:B:1294:TYR:CE2	2.50	0.47
2:F:465:MET:SD	2:F:482:VAL:HG11	2.55	0.47
2:F:720:LEU:HD13	2:F:938:ARG:HD2	1.97	0.47
2:B:823:TYR:CD2	2:B:858:THR:HG21	2.46	0.46
2:B:1204:PHE:CG	2:B:1342:VAL:HG13	2.50	0.46
1:E:27:G:H5'	1:E:28:A:H5''	1.96	0.46
2:F:478:PHE:HE2	2:F:482:VAL:HB	1.80	0.46
2:F:679:ILE:HG12	2:F:704:PHE:CE2	2.51	0.46
2:F:889:ALA:HB3	2:F:891:LEU:CD2	2.45	0.46
2:F:1167:THR:OG1	2:F:1168:ILE:N	2.48	0.46
2:F:1270:ILE:HG13	2:F:1294:TYR:CE2	2.50	0.46
2:B:114:GLU:HG2	2:B:120:GLY:O	2.15	0.46
2:B:624:THR:HA	2:B:656:TYR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:69:A:H2'	5:I:70:C:C6	2.51	0.46
2:B:58:THR:HG22	2:B:731:PRO:CG	2.46	0.46
2:B:925:ARG:HG2	2:B:927:ILE:HG22	1.98	0.46
2:F:119:PHE:CD2	2:F:124:ASP:HB3	2.50	0.46
2:F:467:ARG:HD3	2:F:470:GLU:HA	1.97	0.46
2:F:978:ILE:CD1	2:F:1233:VAL:CG2	2.92	0.46
5:J:43:G:O2'	5:J:44:U:H5'	2.14	0.46
2:B:74:ARG:HH21	5:I:60:C:P	2.39	0.46
2:B:525:THR:O	2:B:690:ASN:HB2	2.14	0.46
2:B:1119:LEU:HD12	2:B:1119:LEU:HA	1.75	0.46
2:F:143:VAL:O	2:F:425:ARG:NH1	2.48	0.46
2:F:921:LEU:HG	2:F:1008:PHE:HD2	1.79	0.46
2:F:969:ASP:HB2	2:F:970:PHE:CD2	2.49	0.46
2:F:1286:ASN:ND2	2:F:1332:ASP:O	2.48	0.46
5:J:45:U:C2	5:J:46:A:C8	3.02	0.46
1:A:8:A:H2'	1:A:9:U:H6	1.79	0.46
2:B:976:ARG:HD3	2:B:982:HIS:NE2	2.31	0.46
2:B:1145:VAL:HG11	2:B:1187:TYR:CD2	2.51	0.46
2:B:1357:GLU:O	5:I:81:G:N2	2.40	0.46
3:C:2:DA:H2'	3:C:3:DA:C8	2.51	0.46
3:C:2:DA:H2''	3:C:3:DA:OP1	2.14	0.46
2:F:138:LEU:HD11	2:F:153:LEU:HD21	1.98	0.46
2:F:253:LYS:HA	2:F:256:PHE:HD2	1.80	0.46
2:F:1042:ILE:HD12	2:F:1042:ILE:HA	1.66	0.46
2:F:1094:ILE:HG21	2:F:1225:GLU:OE2	2.16	0.46
5:J:45:U:H2'	5:J:46:A:O4'	2.15	0.46
2:B:516:GLU:HA	2:B:519:THR:HG22	1.97	0.46
2:B:1296:LYS:HA	2:B:1296:LYS:HD3	1.82	0.46
2:F:137:HIS:HE1	2:F:325:TYR:HB3	1.80	0.46
2:F:1314:THR:HG21	2:F:1324:PHE:HB3	1.98	0.46
5:I:47:A:H2'	5:I:48:A:H8	1.81	0.46
2:F:1127:ASP:HB3	2:F:1130:LYS:HE2	1.97	0.46
2:B:332:LEU:HD13	2:B:359:TYR:CE1	2.51	0.46
2:F:243:ALA:O	2:F:246:LEU:HB3	2.16	0.46
2:F:1000:LYS:HB2	2:F:1073:VAL:HG21	1.98	0.46
2:F:1087:LEU:HD23	2:F:1087:LEU:HA	1.57	0.46
5:J:91:C:H6	5:J:91:C:H2'	1.44	0.46
2:B:349:GLU:HG3	2:B:356:LYS:HG3	1.98	0.46
2:B:373:TYR:HH	2:B:398:LEU:H	1.57	0.46
2:B:509:PRO:HB3	2:B:624:THR:HG21	1.98	0.46
2:B:530:VAL:HG22	2:B:537:PRO:CB	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:913:LYS:O	2:B:916:PHE:HB2	2.16	0.46
2:B:1312:LEU:O	2:B:1315:LEU:HB3	2.16	0.46
2:F:855:LYS:NZ	2:F:1246:LYS:O	2.41	0.46
2:F:1291:LEU:HA	2:F:1291:LEU:HD23	1.75	0.46
2:F:1349:HIS:ND1	5:J:69:A:H5'	2.31	0.46
2:F:258:LEU:HB3	2:F:260:GLU:O	2.16	0.46
2:F:373:TYR:O	2:F:376:ILE:HG22	2.15	0.46
2:F:553:PHE:CD2	2:F:559:VAL:HG21	2.51	0.46
2:F:1062:LEU:O	2:F:1062:LEU:HG	2.14	0.46
5:J:96:C:H2'	5:J:97:U:C6	2.51	0.46
2:B:192:TYR:O	2:B:196:PHE:HB2	2.16	0.45
2:B:1111:LEU:HD12	2:B:1135:ASP:HB2	1.98	0.45
2:B:1143:VAL:HG13	2:B:1195:ILE:HG23	1.98	0.45
2:F:40:ARG:HD3	2:F:43:ILE:HD11	1.98	0.45
2:F:167:HIS:CD2	2:F:169:LEU:H	2.34	0.45
2:F:510:LYS:HG2	2:F:511:HIS:CD2	2.51	0.45
2:F:626:PHE:O	2:F:655:ARG:NH1	2.49	0.45
2:F:1219:GLU:O	2:F:1220:LEU:HD23	2.16	0.45
2:B:18:TRP:HZ2	2:B:1353:THR:O	1.99	0.45
2:B:1105:PHE:CD1	2:B:1169:MET:HG3	2.51	0.45
2:F:165:ARG:C	2:F:415:HIS:HD2	2.19	0.45
2:F:167:HIS:HD2	2:F:169:LEU:CB	2.29	0.45
2:F:289:LEU:O	2:F:292:ALA:HB3	2.15	0.45
2:F:802:GLU:HB2	2:F:805:GLN:HG3	1.97	0.45
2:B:340:ARG:NH2	5:I:41:A:P	2.87	0.45
2:B:666:LEU:HD21	2:B:693:PHE:CZ	2.51	0.45
2:B:989:LEU:HD21	2:B:1087:LEU:HD21	1.98	0.45
2:B:1089:MET:HA	2:B:1090:PRO:HD3	1.71	0.45
1:E:10:U:C4	1:E:11:U:C4	3.05	0.45
2:F:111:LYS:HD3	2:F:115:ARG:HA	1.97	0.45
2:F:1205:GLU:CB	2:F:1348:ILE:HD11	2.46	0.45
2:F:1212:ARG:CZ	2:F:1336:TYR:CE2	2.99	0.45
2:B:1254:GLN:HA	2:B:1257:LEU:HB2	1.97	0.45
4:D:4:DT:H2''	4:D:5:DA:C8	2.52	0.45
2:F:549:VAL:HA	2:F:553:PHE:HB2	1.98	0.45
2:F:867:SER:C	2:F:869:ASN:H	2.20	0.45
2:F:897:PHE:CZ	2:F:901:THR:HG21	2.51	0.45
2:B:13:THR:O	2:B:53:PHE:HE1	1.99	0.45
2:B:15:SER:HA	2:B:51:LEU:O	2.16	0.45
2:B:85:ILE:HD12	2:B:440:ILE:HG12	1.98	0.45
2:B:963:VAL:HG21	2:B:990:ASN:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1119:LEU:HD23	2:B:1128:PRO:HB2	1.97	0.45
1:E:25:U:O2'	2:F:111:LYS:NZ	2.50	0.45
2:F:339:VAL:HG12	2:F:347:TYR:HB2	1.99	0.45
2:B:317:LEU:O	2:B:320:SER:HB3	2.17	0.45
2:F:562:LYS:O	2:F:566:GLU:HB2	2.17	0.45
2:F:731:PRO:HA	2:F:734:LYS:HE3	1.99	0.45
2:B:114:GLU:HG3	2:B:116:HIS:N	2.27	0.45
2:B:158:LEU:HD11	2:B:423:LEU:HD21	1.98	0.45
2:B:558:LYS:HD3	2:B:558:LYS:HA	1.76	0.45
2:B:949:LEU:HD12	2:B:950:ILE:H	1.81	0.45
2:F:478:PHE:CE2	2:F:482:VAL:HB	2.52	0.45
2:F:1038:PHE:CD2	2:F:1039:TYR:CE1	3.05	0.45
5:J:53:G:C4	5:J:62:G:N2	2.85	0.45
5:J:85:C:H2'	5:J:86:C:H6	1.81	0.45
1:A:10:U:H2'	1:A:11:U:C6	2.51	0.45
2:B:378:PRO:O	2:B:382:LYS:NZ	2.36	0.45
2:B:1003:LYS:HG2	2:B:1036:TYR:OH	2.16	0.45
2:F:583:VAL:HG22	2:F:584:GLU:H	1.81	0.45
2:B:103:GLU:OE2	2:B:113:HIS:N	2.47	0.45
2:B:864:ARG:NH2	2:B:869:ASN:O	2.50	0.45
2:B:874:GLU:O	2:B:878:LYS:HG3	2.16	0.45
2:F:143:VAL:HG21	2:F:315:ALA:HB2	1.98	0.45
2:F:411:PRO:HB2	2:F:413:GLN:OE1	2.17	0.45
2:F:135:ILE:CG2	5:J:46:A:H5'	2.47	0.45
2:F:615:ILE:HG23	2:F:639:TYR:CE1	2.52	0.45
2:F:823:TYR:CD2	2:F:858:THR:HG21	2.52	0.45
5:I:85:C:H2'	5:I:86:C:C6	2.52	0.45
5:J:95:G:C6	5:J:96:C:N4	2.85	0.45
2:F:51:LEU:HD12	2:F:1095:VAL:HB	2.00	0.44
2:F:803:ASN:OD1	2:F:803:ASN:N	2.50	0.44
2:F:842:VAL:HG23	2:F:908:LEU:HD11	1.99	0.44
5:J:95:G:H2'	5:J:96:C:C6	2.52	0.44
2:B:640:ALA:HA	2:B:648:MET:CE	2.46	0.44
2:B:824:VAL:HG11	2:B:859:ARG:NH1	2.30	0.44
2:B:977:GLU:HG3	2:B:1310:ILE:CG2	2.47	0.44
2:B:1318:LEU:HD23	2:B:1319:GLY:N	2.32	0.44
2:F:11:ILE:HB	2:F:763:MET:HE3	1.98	0.44
2:F:118:ILE:HG21	2:F:128:TYR:HE2	1.82	0.44
2:F:369:GLN:HG2	2:F:373:TYR:CE2	2.51	0.44
2:F:1120:ILE:HB	2:F:1134:PHE:HB2	1.98	0.44
2:B:135:ILE:HG21	2:B:160:HIS:CD2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:887:LEU:HD12	2:B:897:PHE:CG	2.52	0.44
2:B:1232:TYR:HA	2:B:1235:PHE:HB3	1.99	0.44
2:B:1308:ASN:ND2	2:B:1327:PHE:H	2.01	0.44
2:B:1349:HIS:ND1	5:I:69:A:H4'	2.33	0.44
2:F:1167:THR:HG22	2:F:1170:GLU:HG3	1.99	0.44
2:F:1171:ARG:O	2:F:1175:GLU:HG3	2.16	0.44
5:I:92:G:H2'	5:I:93:G:C8	2.52	0.44
5:J:86:C:C4	5:J:87:G:C8	3.04	0.44
2:B:189:VAL:HG22	2:B:238:PHE:HZ	1.83	0.44
2:B:724:ILE:HD13	2:B:934:ILE:HD13	1.99	0.44
2:B:954:LYS:HG2	2:B:1009:VAL:HG21	1.99	0.44
2:B:1146:VAL:HG23	2:B:1161:LYS:HB2	1.98	0.44
2:B:1226:LEU:HD13	2:B:1276:PHE:CG	2.53	0.44
2:F:481:VAL:HG12	2:F:482:VAL:HG23	1.99	0.44
2:F:727:LEU:N	2:F:727:LEU:HD23	2.32	0.44
2:F:844:GLN:CG	2:F:848:LYS:HD2	2.43	0.44
2:F:5:TYR:CE2	2:F:751:MET:HG3	2.52	0.44
2:F:103:GLU:OE2	2:F:113:HIS:N	2.47	0.44
2:F:201:ILE:N	2:F:201:ILE:HD12	2.33	0.44
2:F:256:PHE:CD1	2:F:282:ILE:HD11	2.52	0.44
2:F:398:LEU:CD1	2:F:399:LEU:HG	2.48	0.44
2:F:553:PHE:HZ	2:F:587:PHE:CD2	2.36	0.44
2:F:600:ILE:HD13	2:F:651:LEU:HA	2.00	0.44
2:F:649:LYS:HB3	2:F:653:ARG:HH21	1.83	0.44
2:F:1265:TYR:O	2:F:1268:GLU:N	2.50	0.44
2:B:1201:TYR:CD1	2:B:1201:TYR:N	2.85	0.44
2:F:1200:LYS:HG2	2:F:1201:TYR:CD1	2.51	0.44
2:B:118:ILE:HD13	2:B:128:TYR:CD2	2.53	0.44
2:B:377:LYS:N	2:B:378:PRO:HD2	2.33	0.44
2:B:850:ASP:HB3	2:B:855:LYS:NZ	2.33	0.44
2:B:872:SER:O	2:B:876:VAL:HG23	2.18	0.44
2:B:967:ARG:NH1	2:B:989:LEU:HD12	2.33	0.44
2:B:972:PHE:HE1	2:B:1084:ARG:HB2	1.82	0.44
2:F:83:GLN:O	2:F:87:SER:HB3	2.17	0.44
2:F:112:LYS:O	2:F:113:HIS:ND1	2.39	0.44
2:F:425:ARG:HE	2:F:425:ARG:HB3	1.62	0.44
2:F:962:LEU:HD22	2:F:1043:MET:HE1	1.99	0.44
2:F:1084:ARG:CZ	2:F:1084:ARG:HB3	2.46	0.44
2:F:1114:ARG:O	2:F:1129:LYS:HA	2.18	0.44
2:B:11:ILE:O	2:B:763:MET:HA	2.18	0.44
2:F:174:LEU:HD13	2:F:174:LEU:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:J:58:G:C6	5:J:60:C:C2	3.06	0.44
2:B:875:VAL:HA	2:B:878:LYS:HD2	2.00	0.44
2:F:44:LYS:HG2	5:J:91:C:C5	2.53	0.44
2:F:551:LEU:O	2:F:555:THR:OG1	2.20	0.44
2:F:809:GLU:OE2	2:F:1246:LYS:HG3	2.17	0.44
2:F:958:LEU:HA	2:F:958:LEU:HD23	1.70	0.44
2:F:967:ARG:CZ	2:F:974:LYS:HB2	2.48	0.44
3:G:22:DT:H2''	3:G:23:DC:O5'	2.18	0.44
5:I:39:G:H5'	5:I:40:C:OP2	2.18	0.44
2:B:6:SER:HB2	2:B:21:ILE:CG1	2.48	0.43
2:B:133:PRO:HG2	2:B:137:HIS:ND1	2.33	0.43
2:B:943:TYR:HA	2:B:950:ILE:HG13	2.00	0.43
2:B:1145:VAL:HG11	2:B:1187:TYR:CE2	2.52	0.43
1:E:25:U:O4	1:E:26:A:N6	2.51	0.43
2:F:90:MET:SD	2:F:151:LEU:CD2	3.06	0.43
2:F:154:ILE:CG2	2:F:158:LEU:HG	2.47	0.43
2:F:342:GLN:HB2	2:F:383:MET:HG2	1.99	0.43
2:F:1019:ARG:C	2:F:1021:MET:H	2.21	0.43
2:F:1169:MET:HE3	5:J:52:A:H1'	2.00	0.43
5:I:92:G:H2'	5:I:93:G:H8	1.82	0.43
2:B:165:ARG:O	2:B:412:HIS:HA	2.18	0.43
2:B:276:ASP:HA	2:B:279:LEU:HB3	1.99	0.43
2:B:526:LYS:NZ	2:B:695:GLN:OE1	2.29	0.43
2:B:1202:SER:O	2:B:1213:MET:HA	2.17	0.43
2:F:430:TYR:HB3	2:F:432:PHE:CE2	2.53	0.43
2:F:650:GLN:O	2:F:653:ARG:HG2	2.17	0.43
2:F:742:LYS:NZ	5:J:68:A:OP1	2.51	0.43
2:B:406:ASP:OD1	2:B:406:ASP:N	2.47	0.43
2:B:755:LYS:NZ	2:B:939:MET:O	2.29	0.43
2:B:782:LYS:O	2:B:786:GLU:HG3	2.18	0.43
2:B:917:ILE:HD12	2:B:917:ILE:HA	1.82	0.43
2:B:1047:LYS:HB2	2:B:1050:ILE:HG22	1.99	0.43
5:J:51:A:C2	5:J:62:G:H2'	2.53	0.43
1:A:20:A:P	2:B:403:ARG:NH1	2.92	0.43
2:B:594:TYR:O	2:B:598:LEU:N	2.48	0.43
2:F:514:LEU:CD2	2:F:664:ARG:HH21	2.31	0.43
2:F:1277:SER:O	2:F:1281:ILE:N	2.46	0.43
2:B:497:ASN:OD1	2:B:498:PHE:N	2.51	0.43
2:B:1200:LYS:HG2	2:B:1201:TYR:CE1	2.53	0.43
1:E:25:U:H6	1:E:25:U:O5'	2.00	0.43
1:E:32:A:N6	5:J:37:U:C4	2.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:140:LYS:HB3	2:F:322:ILE:HD12	2.00	0.43
2:F:274:ASP:O	2:F:277:ASN:OD1	2.36	0.43
2:F:475:PRO:HG3	5:J:59:U:O4	2.17	0.43
2:F:647:VAL:O	2:F:651:LEU:HB2	2.18	0.43
2:F:972:PHE:HE1	2:F:1084:ARG:CG	2.31	0.43
5:I:47:A:H2'	5:I:48:A:C8	2.54	0.43
2:B:682:PHE:CB	2:B:696:LEU:HD11	2.49	0.43
2:B:781:MET:O	2:B:785:GLU:HB2	2.18	0.43
2:B:1246:LYS:HB2	2:B:1246:LYS:HE2	1.79	0.43
2:B:1280:VAL:HG12	2:B:1281:ILE:HD13	2.01	0.43
2:F:282:ILE:HG22	2:F:286:TYR:CD1	2.54	0.43
2:F:438:GLU:HA	2:F:441:GLU:OE1	2.19	0.43
2:F:836:TYR:HB2	2:F:857:LEU:HD11	2.01	0.43
2:F:1204:PHE:CG	2:F:1342:VAL:HG13	2.53	0.43
2:B:158:LEU:CD1	2:B:423:LEU:HD21	2.48	0.43
2:B:197:GLU:HA	2:B:200:PRO:HG3	2.01	0.43
2:B:201:ILE:HD12	2:B:238:PHE:CD1	2.53	0.43
2:B:836:TYR:N	2:B:836:TYR:CD1	2.86	0.43
2:B:1270:ILE:HG13	2:B:1294:TYR:CD2	2.54	0.43
2:F:8:GLY:O	2:F:987:ALA:HB1	2.19	0.43
2:F:523:GLU:OE1	2:F:589:ALA:N	2.51	0.43
2:F:978:ILE:HD12	2:F:1228:LEU:CD2	2.37	0.43
2:B:351:PHE:C	2:B:360:ALA:HB2	2.39	0.43
2:B:540:LEU:HA	2:B:540:LEU:HD12	1.54	0.43
2:B:861:ASP:O	2:B:864:ARG:HG2	2.18	0.43
2:B:913:LYS:HA	2:B:916:PHE:CD2	2.44	0.43
2:F:275:LEU:HD13	2:F:279:LEU:HG	2.01	0.43
2:F:821:ASP:OD1	2:F:823:TYR:N	2.40	0.43
2:F:1178:PRO:O	2:F:1182:LEU:HG	2.18	0.43
1:A:5:C:H42	3:C:24:DG:H1	1.67	0.43
2:B:7:ILE:HD13	2:B:747:LEU:HD12	2.00	0.43
2:B:37:ASN:OD1	2:B:37:ASN:N	2.52	0.43
2:B:485:GLY:O	2:B:488:ALA:N	2.52	0.43
2:B:644:ASP:HB3	2:B:647:VAL:CG2	2.44	0.43
2:B:1169:MET:HE1	5:I:52:A:H1'	2.00	0.43
2:F:623:LEU:HD11	2:F:654:ARG:O	2.18	0.43
2:F:1154:SER:OG	2:F:1156:LYS:HE2	2.18	0.43
5:J:52:A:N7	5:J:53:G:H1'	2.34	0.43
2:B:246:LEU:CD2	2:B:246:LEU:H	2.19	0.43
2:B:475:PRO:HG3	5:I:59:U:O4	2.19	0.43
2:B:844:GLN:C	2:B:1041:ASN:OD1	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:886:LEU:HD22	2:B:891:LEU:HD12	2.01	0.43
2:B:892:ILE:HB	2:B:896:LYS:HD3	2.01	0.43
2:F:332:LEU:HD13	2:F:359:TYR:CE1	2.54	0.43
2:F:977:GLU:HG3	2:F:1310:ILE:HG22	2.00	0.43
2:B:1111:LEU:HD12	2:B:1135:ASP:CB	2.49	0.42
2:F:531:THR:HG21	2:F:575:PHE:HE1	1.76	0.42
2:F:842:VAL:HG12	2:F:854:ASN:OD1	2.19	0.42
2:F:1147:ALA:HB1	2:F:1188:LYS:O	2.19	0.42
2:F:1156:LYS:HE2	2:F:1156:LYS:HB2	1.78	0.42
2:F:1197:LYS:O	2:F:1199:PRO:HD3	2.19	0.42
2:B:32:PHE:CZ	2:B:1355:LEU:HD13	2.54	0.42
2:B:340:ARG:NH2	5:I:41:A:OP2	2.52	0.42
2:B:1074:TRP:HZ2	2:B:1080:PHE:CD2	2.37	0.42
1:E:27:G:H22	5:J:44:U:P	2.42	0.42
2:F:66:ARG:NH2	2:F:462:PHE:CG	2.87	0.42
2:F:258:LEU:HD23	2:F:259:ALA:H	1.84	0.42
5:J:49:A:H2'	5:J:50:U:O4'	2.19	0.42
2:B:1207:GLU:CG	2:B:1210:ARG:HH11	2.32	0.42
2:B:1219:GLU:HG3	2:B:1220:LEU:N	2.34	0.42
2:F:40:ARG:CD	2:F:43:ILE:HD11	2.49	0.42
2:F:140:LYS:HB3	2:F:322:ILE:CD1	2.49	0.42
2:F:649:LYS:HB2	2:F:650:GLN:NE2	2.33	0.42
2:F:746:GLU:HG2	2:F:1353:THR:HG23	2.01	0.42
1:A:29:G:C4	5:I:41:A:C2	3.07	0.42
2:B:69:ARG:HE	2:B:69:ARG:HB2	1.53	0.42
2:B:395:ARG:NH2	2:B:397:ASP:OD2	2.52	0.42
2:F:237:LEU:HD12	2:F:238:PHE:N	2.35	0.42
2:F:291:LEU:HD12	2:F:291:LEU:HA	1.88	0.42
2:F:561:VAL:HG12	2:F:565:LYS:HD3	2.00	0.42
2:F:1103:GLY:HA2	5:J:63:U:H1'	2.01	0.42
2:B:275:LEU:O	2:B:279:LEU:HB2	2.19	0.42
2:B:876:VAL:O	2:B:880:LYS:N	2.50	0.42
2:B:1143:VAL:HG22	2:B:1197:LYS:HG3	2.01	0.42
2:F:134:THR:O	2:F:137:HIS:HB2	2.19	0.42
2:F:139:ARG:O	2:F:143:VAL:HG23	2.19	0.42
2:F:258:LEU:CD1	2:F:281:GLN:HE22	2.29	0.42
2:F:761:ILE:HG21	2:F:761:ILE:HD13	1.85	0.42
2:F:883:TRP:HB3	2:F:897:PHE:HD1	1.84	0.42
2:F:1060:ARG:HA	2:F:1060:ARG:HD2	1.87	0.42
2:F:909:SER:N	2:F:912:ASP:HB2	2.34	0.42
2:F:958:LEU:CD2	2:F:962:LEU:HD12	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:32:PHE:N	2:B:43:ILE:O	2.38	0.42
2:B:217:SER:HB2	2:B:220:ARG:H	1.84	0.42
2:B:390:LEU:HD23	2:B:390:LEU:HA	1.72	0.42
2:B:507:VAL:HG12	2:B:508:LEU:O	2.20	0.42
2:F:165:ARG:O	2:F:412:HIS:HA	2.20	0.42
2:F:323:LYS:O	2:F:327:GLU:HG2	2.19	0.42
2:F:739:GLN:NE2	2:F:1097:LYS:HE3	2.35	0.42
2:F:980:ASN:HB2	2:F:1225:GLU:OE2	2.19	0.42
2:F:1093:ASN:O	2:F:1094:ILE:HD13	2.19	0.42
1:A:24:U:H2'	1:A:25:U:O4'	2.19	0.42
2:B:643:PHE:HB2	2:B:648:MET:HE2	2.02	0.42
2:B:686:ASP:OD1	2:B:691:ARG:HB2	2.20	0.42
2:B:727:LEU:HD21	2:B:934:ILE:HD11	2.01	0.42
2:B:1000:LYS:O	2:B:1000:LYS:HD3	2.19	0.42
2:B:1212:ARG:CZ	2:B:1336:TYR:CE2	3.03	0.42
2:B:1235:PHE:CE1	2:B:1239:ALA:HB2	2.54	0.42
2:F:93:VAL:HG11	2:F:150:ASP:OD1	2.20	0.42
2:F:168:PHE:CB	2:F:447:ARG:HH11	2.33	0.42
2:F:645:ASP:O	2:F:649:LYS:HG2	2.20	0.42
2:B:51:LEU:HD13	2:B:1095:VAL:HG23	2.02	0.42
2:B:114:GLU:HG3	2:B:115:ARG:N	2.33	0.42
2:B:252:PHE:CD1	2:B:264:LEU:HD13	2.55	0.42
2:B:507:VAL:HG11	2:B:660:GLY:O	2.20	0.42
2:B:1228:LEU:HD12	2:B:1229:PRO:CD	2.50	0.42
2:F:5:TYR:OH	2:F:756:PRO:HG3	2.20	0.42
2:F:20:VAL:HG11	2:F:751:MET:CE	2.50	0.42
2:F:44:LYS:HZ1	5:J:85:C:N4	2.17	0.42
2:F:305:ILE:HG13	2:F:306:LEU:HD13	2.02	0.42
2:F:491:PHE:O	2:F:494:ARG:HG2	2.19	0.42
2:F:922:VAL:HG12	2:F:1007:GLU:HB3	2.01	0.42
2:F:976:ARG:HA	2:F:982:HIS:CD2	2.55	0.42
2:F:1064:GLU:OE1	2:F:1065:THR:N	2.51	0.42
2:F:1101:GLN:O	2:F:1168:ILE:HD11	2.19	0.42
5:J:43:G:H3'	5:J:44:U:H6	1.85	0.42
2:B:30:LYS:HD3	5:I:83:C:OP1	2.19	0.42
2:B:165:ARG:O	2:B:415:HIS:CD2	2.71	0.42
2:B:225:LEU:HD13	2:B:242:ILE:HG21	2.01	0.42
2:B:869:ASN:OD1	2:B:870:VAL:N	2.52	0.42
2:F:44:LYS:NZ	5:J:85:C:H42	2.18	0.42
2:F:47:LEU:HD11	2:F:750:VAL:HG11	2.02	0.42
2:F:939:MET:CE	2:F:953:VAL:HG21	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:THR:HG22	2:B:731:PRO:HG3	2.00	0.41
2:B:526:LYS:NZ	2:B:691:ARG:HA	2.35	0.41
2:B:821:ASP:HB3	2:B:828:LEU:HD11	2.02	0.41
2:B:1212:ARG:HA	2:B:1212:ARG:HD3	1.87	0.41
2:B:1231:LYS:HE3	2:B:1232:TYR:CE2	2.54	0.41
2:F:32:PHE:HD1	2:F:45:LYS:HD3	1.84	0.41
2:F:106:LEU:HD22	2:F:1131:TYR:OH	2.19	0.41
2:F:546:LYS:HE3	2:F:546:LYS:HB3	1.84	0.41
2:B:47:LEU:HD11	2:B:750:VAL:HG11	2.02	0.41
2:B:508:LEU:HD21	2:B:664:ARG:HB2	2.02	0.41
2:B:849:ASP:OD1	2:B:851:SER:OG	2.38	0.41
2:B:1303:ARG:O	2:B:1307:GLU:HG2	2.19	0.41
2:B:1349:HIS:CE1	5:I:69:A:H4'	2.55	0.41
3:C:4:DT:H2''	3:C:5:DA:O5'	2.20	0.41
4:D:10:DT:H6	4:D:10:DT:H2'	1.73	0.41
2:F:258:LEU:HD23	2:F:259:ALA:N	2.35	0.41
2:F:882:TYR:HD2	2:F:883:TRP:CD1	2.38	0.41
2:F:1262:HIS:HB3	2:F:1265:TYR:CD2	2.55	0.41
2:B:70:ARG:HH22	2:B:462:PHE:HD2	1.68	0.41
2:F:18:TRP:CZ2	2:F:49:GLY:HA3	2.55	0.41
2:F:427:GLU:HA	2:F:433:LEU:HB2	2.02	0.41
2:F:795:ILE:O	2:F:795:ILE:HG13	2.20	0.41
5:I:48:A:O2'	5:I:49:A:H5'	2.20	0.41
2:B:151:LEU:HD12	2:B:151:LEU:HA	1.77	0.41
2:B:549:VAL:HA	2:B:553:PHE:HD2	1.85	0.41
2:B:594:TYR:CE1	2:B:607:LEU:HB3	2.55	0.41
2:B:976:ARG:HH11	2:B:982:HIS:HE2	1.68	0.41
2:B:986:ASP:O	2:B:990:ASN:ND2	2.53	0.41
2:B:1096:LYS:HG2	2:B:1201:TYR:CD2	2.55	0.41
2:B:1182:LEU:HD23	2:B:1182:LEU:HA	1.94	0.41
2:F:328:HIS:CG	5:J:44:U:C2	3.08	0.41
2:F:646:LYS:O	2:F:650:GLN:HG2	2.21	0.41
2:F:748:VAL:HG13	2:F:754:HIS:O	2.21	0.41
2:F:971:GLN:HG2	2:F:973:TYR:CZ	2.56	0.41
3:G:19:DA:H2'	3:G:20:DA:C8	2.55	0.41
5:I:94:U:H2'	5:I:95:G:H8	1.86	0.41
2:B:56:GLY:O	2:B:732:ALA:HB2	2.21	0.41
2:B:241:LEU:HA	2:B:241:LEU:HD23	1.81	0.41
2:B:442:LYS:HE3	2:B:476:TRP:HA	2.02	0.41
2:B:921:LEU:HB3	2:B:1008:PHE:HZ	1.84	0.41
2:B:1000:LYS:HB3	2:B:1001:TYR:CD2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1231:LYS:H	2:B:1231:LYS:HG2	1.71	0.41
2:B:1251:ASP:O	2:B:1255:LYS:HG3	2.20	0.41
2:F:140:LYS:HE3	2:F:313:THR:CB	2.50	0.41
2:F:1300:LYS:HG3	2:F:1327:PHE:CZ	2.56	0.41
2:B:326:ASP:O	2:B:330:GLN:HG3	2.20	0.41
2:B:954:LYS:HB2	2:B:954:LYS:HE3	1.71	0.41
2:B:1351:SER:HA	5:I:68:A:N7	2.35	0.41
2:F:499:ASP:OD2	2:F:663:SER:HB3	2.20	0.41
2:F:1105:PHE:CD1	2:F:1169:MET:HG3	2.55	0.41
2:B:86:PHE:O	2:B:87:SER:C	2.59	0.41
2:B:253:LYS:HD3	2:B:261:ASP:HA	2.02	0.41
2:B:642:LEU:HB2	2:B:643:PHE:CD2	2.55	0.41
2:B:1114:ARG:O	2:B:1129:LYS:HA	2.20	0.41
2:F:89:GLU:HG3	2:F:432:PHE:CD2	2.55	0.41
2:F:140:LYS:CB	2:F:322:ILE:HD12	2.50	0.41
2:F:622:THR:HG23	2:F:626:PHE:CD1	2.56	0.41
2:F:1116:SER:HB3	2:F:1119:LEU:HB2	2.02	0.41
2:B:661:ARG:CB	2:B:662:LEU:HD12	2.50	0.41
2:B:1206:LEU:H	2:B:1206:LEU:HD23	1.86	0.41
2:B:1221:GLN:HG2	2:B:1319:GLY:O	2.20	0.41
2:F:308:VAL:HG11	2:F:316:PRO:O	2.21	0.41
2:F:335:LEU:O	2:F:339:VAL:HG23	2.20	0.41
2:F:921:LEU:HG	2:F:1008:PHE:CD2	2.56	0.41
2:F:1266:LEU:O	2:F:1270:ILE:HG12	2.20	0.41
2:B:35:LEU:HD23	2:B:35:LEU:HA	1.80	0.41
2:B:127:ALA:O	2:B:130:GLU:HB2	2.20	0.41
2:B:178:ASN:O	2:B:302:LEU:HD11	2.20	0.41
2:B:424:ARG:NH1	2:B:437:ARG:CZ	2.83	0.41
2:B:478:PHE:CE1	2:B:482:VAL:HG21	2.56	0.41
2:B:820:ARG:HA	2:B:826:GLN:O	2.21	0.41
2:B:824:VAL:HG22	2:B:863:ASN:HD22	1.85	0.41
2:B:1226:LEU:HB2	2:B:1276:PHE:CZ	2.56	0.41
2:B:1252:ASN:HA	2:B:1255:LYS:HD2	2.03	0.41
1:E:25:U:C4	1:E:26:A:N7	2.89	0.41
2:F:32:PHE:O	2:F:42:SER:HA	2.21	0.41
2:F:35:LEU:HB2	2:F:1358:THR:CG2	2.50	0.41
2:F:199:ASN:O	2:F:201:ILE:HD12	2.21	0.41
2:F:429:PHE:N	2:F:429:PHE:CD1	2.87	0.41
2:F:449:PRO:HB2	2:F:452:VAL:HG23	2.03	0.41
2:F:455:LEU:O	5:J:60:C:H5'	2.21	0.41
2:F:510:LYS:HG2	2:F:511:HIS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:684:LYS:C	2:F:685:SER:HG	2.21	0.41
2:F:724:ILE:O	2:F:727:LEU:HG	2.20	0.41
2:F:902:LYS:NZ	2:F:912:ASP:OD2	2.49	0.41
2:F:973:TYR:CG	2:F:1237:TYR:HD1	2.38	0.41
2:F:1163:LEU:HD23	2:F:1163:LEU:HA	1.90	0.41
2:F:1179:ILE:O	2:F:1183:GLU:HG3	2.21	0.41
2:F:1295:ASN:OD1	2:F:1298:ARG:NH1	2.46	0.41
5:I:84:A:C2	5:I:85:C:C2	3.09	0.41
2:B:30:LYS:HD3	5:I:83:C:OP2	2.21	0.41
2:B:529:TYR:CD2	2:B:569:PHE:HE1	2.39	0.41
2:B:666:LEU:HD21	2:B:693:PHE:CE1	2.56	0.41
2:F:939:MET:HE2	2:F:953:VAL:HG21	2.03	0.41
5:J:46:A:C2	5:J:47:A:C5	3.09	0.41
5:J:76:A:C5	5:J:77:A:H1'	2.55	0.41
2:B:222:LEU:HD21	2:B:234:LYS:HG3	2.03	0.40
2:B:298:ASP:O	2:B:302:LEU:HG	2.21	0.40
2:B:513:LEU:HA	2:B:513:LEU:HD23	1.83	0.40
2:B:951:ARG:HH21	2:B:1011:GLY:HA2	1.84	0.40
2:B:1245:LEU:HD12	2:B:1245:LEU:O	2.22	0.40
2:F:97:PHE:HE1	2:F:118:ILE:HA	1.86	0.40
2:B:536:LYS:HG2	2:B:537:PRO:O	2.21	0.40
2:B:1307:GLU:O	2:B:1310:ILE:HB	2.20	0.40
2:F:140:LYS:O	2:F:140:LYS:HE2	2.22	0.40
2:F:223:GLU:HA	2:F:226:ILE:HB	2.03	0.40
2:F:359:TYR:HE1	2:F:399:LEU:HD13	1.86	0.40
2:F:666:LEU:O	2:F:679:ILE:HD12	2.21	0.40
2:F:782:LYS:HA	2:F:785:GLU:HB2	2.03	0.40
2:F:975:VAL:CG1	2:F:978:ILE:CG2	2.98	0.40
2:F:975:VAL:HG11	2:F:978:ILE:HG22	2.03	0.40
5:I:94:U:H2'	5:I:95:G:C8	2.57	0.40
5:J:46:A:C2	5:J:47:A:C6	3.09	0.40
1:E:27:G:H1'	2:F:129:HIS:CD2	2.56	0.40
2:F:136:TYR:CZ	2:F:160:HIS:NE2	2.88	0.40
2:F:998:ILE:CG2	2:F:1008:PHE:HE1	2.30	0.40
4:H:7:DG:H2''	4:H:8:DT:O5'	2.22	0.40
2:B:211:ILE:HD11	2:B:228:GLN:HG3	2.03	0.40
2:F:64:LEU:O	2:F:67:THR:HB	2.21	0.40
2:F:101:LEU:HD12	2:F:117:PRO:HB2	2.04	0.40
2:F:317:LEU:HD21	2:F:410:ILE:HD13	2.04	0.40
2:F:478:PHE:HD2	2:F:478:PHE:O	2.03	0.40
2:F:506:LYS:H	2:F:506:LYS:HG2	1.48	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1110:ILE:HG21	2:F:1122:ARG:NH2	2.37	0.40
2:F:1336:TYR:N	2:F:1336:TYR:CD1	2.89	0.40
5:I:47:A:C5	5:I:48:A:N7	2.89	0.40
2:B:142:LEU:HD23	2:B:142:LEU:HA	1.78	0.40
2:B:433:LEU:HD23	2:B:433:LEU:HA	1.78	0.40
2:B:539:PHE:CB	2:B:690:ASN:ND2	2.68	0.40
2:B:882:TYR:O	2:B:886:LEU:HG	2.21	0.40
2:F:169:LEU:O	2:F:170:ILE:HD12	2.22	0.40
2:F:258:LEU:CD2	2:F:260:GLU:H	2.33	0.40
2:F:275:LEU:CD1	2:F:279:LEU:HG	2.52	0.40
2:F:632:ILE:HG22	2:F:636:LEU:HD22	2.04	0.40
2:F:1200:LYS:HG2	2:F:1201:TYR:CE1	2.57	0.40
2:F:1217:ALA:O	2:F:1339:THR:HG21	2.21	0.40
5:J:54:G:C6	5:J:55:C:N4	2.89	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 X-ray entries followed by that with respect to entries of similar resolution.

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	
2	B	1312/1368 (96%)	1275 (97%)	34 (3%)	3 (0%)	44	73
2	F	1313/1368 (96%)	1265 (96%)	40 (3%)	8 (1%)	22	51
All	All	2625/2736 (96%)	2540 (97%)	74 (3%)	11 (0%)	30	61

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	F	1042	ILE
2	F	585	ASP
2	F	869	ASN
2	F	1020	LYS

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Mol	Chain	Res	Type
2	F	1055	GLY
2	F	202	ASN
2	F	117	PRO
2	F	868	ASP
2	B	117	PRO
2	B	250	PRO
2	B	230	PRO

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	
2	B	1173/1225 (96%)	1128 (96%)	45 (4%)	28	53
2	F	1156/1225 (94%)	1097 (95%)	59 (5%)	20	46
All	All	2329/2450 (95%)	2225 (96%)	104 (4%)	23	50

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	40	ARG
2	B	95	ASP
2	B	141	LYS
2	B	145	SER
2	B	218	LYS
2	B	246	LEU
2	B	276	ASP
2	B	291	LEU
2	B	307	ARG
2	B	340	ARG
2	B	383	MET
2	B	425	ARG
2	B	468	LYS
2	B	476	TRP
2	B	494	ARG
2	B	535	ARG

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Mol	Chain	Res	Type
2	B	556	ASN
2	B	557	ARG
2	B	604	LYS
2	B	610	GLU
2	B	627	GLU
2	B	629	ARG
2	B	663	SER
2	B	674	GLN
2	B	685	SER
2	B	751	MET
2	B	763	MET
2	B	765	ARG
2	B	803	ASN
2	B	854	ASN
2	B	879	MET
2	B	884	ARG
2	B	948	LYS
2	B	951	ARG
2	B	1037	PHE
2	B	1062	LEU
2	B	1158	LYS
2	B	1221	GLN
2	B	1225	GLU
2	B	1258	PHE
2	B	1260	GLU
2	B	1262	HIS
2	B	1267	ASP
2	B	1338	SER
2	B	1351	SER
2	F	42	SER
2	F	94	ASP
2	F	116	HIS
2	F	121	ASN
2	F	128	TYR
2	F	140	LYS
2	F	161	MET
2	F	183	LYS
2	F	224	ASN
2	F	229	LEU
2	F	234	LYS
2	F	237	LEU
2	F	241	LEU

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Mol	Chain	Res	Type
2	F	253	LYS
2	F	271	TYR
2	F	279	LEU
2	F	284	ASP
2	F	285	GLN
2	F	383	MET
2	F	384	ASP
2	F	425	ARG
2	F	426	GLN
2	F	467	ARG
2	F	478	PHE
2	F	494	ARG
2	F	510	LYS
2	F	532	GLU
2	F	535	ARG
2	F	567	ASP
2	F	629	ARG
2	F	630	GLU
2	F	631	MET
2	F	635	ARG
2	F	646	LYS
2	F	654	ARG
2	F	671	ARG
2	F	686	ASP
2	F	690	ASN
2	F	803	ASN
2	F	826	GLN
2	F	844	GLN
2	F	891	LEU
2	F	912	ASP
2	F	948	LYS
2	F	977	GLU
2	F	978	ILE
2	F	979	ASN
2	F	1037	PHE
2	F	1060	ARG
2	F	1080	PHE
2	F	1125	ASP
2	F	1202	SER
2	F	1206	LEU
2	F	1210	ARG
2	F	1222	LYS

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Mol	Chain	Res	Type
2	F	1246	LYS
2	F	1256	GLN
2	F	1258	PHE
2	F	1325	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	137	HIS
2	B	342	GLN
2	B	415	HIS
2	B	818	ASN
2	B	1044	ASN
2	B	1066	ASN
2	B	1262	HIS
2	B	1308	ASN
2	B	1350	GLN
2	F	167	HIS
2	F	255	ASN
2	F	281	GLN
2	F	415	HIS
2	F	426	GLN
2	F	690	ASN
2	F	726	ASN
2	F	794	GLN
2	F	807	GLN
2	F	985	HIS
2	F	1252	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	33/34 (97%)	10 (30%)	3 (9%)
1	E	30/34 (88%)	9 (30%)	1 (3%)
5	I	62/65 (95%)	19 (30%)	1 (1%)
5	J	62/65 (95%)	18 (29%)	1 (1%)
All	All	187/198 (94%)	56 (29%)	6 (3%)

All (56) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	2	U
1	A	4	A
1	A	5	C
1	A	6	G
1	A	9	U
1	A	20	A
1	A	28	A
1	A	29	G
1	A	32	A
1	A	33	U
1	E	5	C
1	E	6	G
1	E	9	U
1	E	20	A
1	E	24	U
1	E	28	A
1	E	29	G
1	E	32	A
1	E	33	U
5	I	37	U
5	I	39	G
5	I	40	C
5	I	42	A
5	I	43	G
5	I	50	U
5	I	51	A
5	I	56	U
5	I	57	A
5	I	59	U
5	I	63	U
5	I	68	A
5	I	74	A
5	I	77	A
5	I	82	G
5	I	87	G
5	I	89	G
5	I	91	C
5	I	92	G
5	J	37	U
5	J	39	G
5	J	40	C
5	J	42	A
5	J	43	G

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Mol	Chain	Res	Type
5	J	50	U
5	J	51	A
5	J	56	U
5	J	57	A
5	J	59	U
5	J	63	U
5	J	68	A
5	J	74	A
5	J	82	G
5	J	87	G
5	J	89	G
5	J	91	C
5	J	92	G

All (6) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	8	A
1	A	27	G
1	A	28	A
1	E	27	G
5	I	42	A
5	J	42	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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	34/34 (100%)	0.05	3 (8%) 17 18	7, 28, 140, 153	0
1	E	31/34 (91%)	0.90	3 (9%) 15 16	29, 64, 167, 193	0
2	B	1326/1368 (96%)	0.61	143 (10%) 12 15	4, 56, 173, 204	0
2	F	1327/1368 (97%)	1.02	271 (20%) 3 5	3, 82, 129, 161	0
3	C	24/24 (100%)	0.06	2 (8%) 19 20	16, 28, 79, 123	0
3	G	24/24 (100%)	0.15	1 (4%) 41 36	38, 48, 89, 139	0
4	D	11/11 (100%)	1.02	2 (18%) 4 6	24, 29, 129, 152	0
4	H	11/11 (100%)	0.53	2 (18%) 4 6	29, 48, 101, 160	0
5	I	63/65 (96%)	0.06	3 (4%) 36 32	6, 58, 102, 134	0
5	J	63/65 (96%)	0.28	4 (6%) 27 26	18, 40, 134, 165	0
All	All	2914/3004 (97%)	0.77	434 (14%) 7 9	3, 63, 149, 204	0

All (434) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	1243	GLU	14.3
2	F	305	ILE	10.5
4	D	2	DT	7.8
2	F	301	LEU	7.6
2	F	306	LEU	7.5
2	B	900	LEU	7.1
2	B	841	ILE	6.6
2	F	413	GLN	6.5
2	B	833	LEU	6.4
2	B	813	LEU	6.3
2	B	810	LYS	6.3
2	F	156	LEU	6.3
2	B	881	ASN	6.1

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Mol	Chain	Res	Type	RSRZ
2	B	809	GLU	5.9
2	F	402	GLN	5.7
2	F	400	ARG	5.7
2	F	362	TYR	5.6
2	B	822	MET	5.6
2	F	1246	LYS	5.6
2	F	818	ASN	5.6
2	F	1242	TYR	5.5
2	F	142	LEU	5.5
2	B	842	VAL	5.5
2	B	834	SER	5.4
2	F	181	VAL	5.3
2	B	1052	LEU	5.3
2	B	817	GLN	5.1
2	F	796	LEU	5.1
2	B	812	TYR	5.1
2	F	128	TYR	5.1
2	F	697	ILE	5.1
2	B	858	THR	5.0
2	F	244	LEU	5.0
2	B	883	TRP	4.9
2	F	209	LYS	4.8
2	B	814	TYR	4.6
2	F	82	LEU	4.6
2	F	287	ALA	4.6
2	B	910	GLU	4.6
2	B	857	LEU	4.6
2	B	1045	PHE	4.6
2	B	914	ALA	4.6
2	B	801	VAL	4.5
2	F	246	LEU	4.5
2	B	1243	GLU	4.5
2	F	39	ASP	4.5
2	B	823	TYR	4.5
2	F	830	ILE	4.4
2	B	856	VAL	4.4
2	F	132	TYR	4.4
2	F	312	ILE	4.4
2	F	795	ILE	4.3
2	B	876	VAL	4.3
1	E	34	G	4.3
2	F	473	ILE	4.2

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Mol	Chain	Res	Type	RSRZ
2	F	863	ASN	4.2
2	B	894	GLN	4.2
2	B	852	ILE	4.2
2	F	788	ILE	4.2
2	B	867	SER	4.1
2	F	141	LYS	4.1
2	F	877	LYS	4.1
2	B	1050	ILE	4.1
2	F	314	LYS	4.1
5	J	36	G	4.1
2	B	824	VAL	4.0
2	B	843	PRO	4.0
2	F	252	PHE	4.0
2	F	308	VAL	4.0
2	F	304	ASP	4.0
2	F	267	SER	4.0
2	F	271	TYR	4.0
2	F	815	TYR	4.0
2	F	297	SER	4.0
2	F	114	GLU	4.0
2	F	224	ASN	4.0
2	F	1247	GLY	3.9
2	B	871	PRO	3.9
2	B	816	LEU	3.9
2	B	908	LEU	3.9
2	F	152	ARG	3.9
2	F	703	THR	3.9
2	F	284	ASP	3.8
2	F	679	ILE	3.8
2	F	207	ASP	3.8
2	F	73	THR	3.8
2	B	1073	VAL	3.8
2	F	158	LEU	3.7
2	F	286	TYR	3.7
2	F	702	LEU	3.7
2	F	886	LEU	3.7
2	F	225	LEU	3.7
2	B	243	ALA	3.7
2	F	81	TYR	3.7
2	F	698	HIS	3.7
2	B	830	ILE	3.7
2	F	407	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
2	F	643	PHE	3.6
2	F	257	ASP	3.6
2	B	854	ASN	3.6
2	B	906	GLY	3.6
2	F	174	LEU	3.6
2	F	791	LEU	3.6
2	F	809	GLU	3.6
2	B	903	ALA	3.6
2	F	399	LEU	3.5
2	F	408	GLY	3.5
2	B	1084	ARG	3.5
2	F	307	ARG	3.5
2	F	269	ASP	3.5
2	F	833	LEU	3.4
2	B	1021	MET	3.4
2	B	1051	THR	3.4
2	F	281	GLN	3.4
2	B	901	THR	3.4
2	F	120	GLY	3.4
2	F	784	ILE	3.4
2	F	1123	LYS	3.4
2	B	310	THR	3.4
2	F	359	TYR	3.4
2	F	483	ASP	3.4
2	F	166	GLY	3.4
2	B	885	GLN	3.4
2	B	859	ARG	3.4
5	J	42	A	3.4
2	B	886	LEU	3.3
2	B	902	LYS	3.3
5	J	43	G	3.3
2	B	463	ALA	3.3
2	F	683	LEU	3.3
2	F	145	SER	3.3
2	B	259	ALA	3.3
2	F	243	ALA	3.3
2	F	302	LEU	3.3
2	F	794	GLN	3.3
2	F	1252	ASN	3.3
2	B	268	LYS	3.3
2	F	249	THR	3.3
2	F	133	PRO	3.3

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Mol	Chain	Res	Type	RSRZ
2	F	118	ILE	3.3
2	F	154	ILE	3.3
2	F	799	HIS	3.3
2	F	706	GLU	3.2
2	B	898	ASP	3.2
2	B	912	ASP	3.2
2	F	153	LEU	3.2
2	B	870	VAL	3.2
2	F	811	LEU	3.2
2	F	415	HIS	3.2
2	B	840	ALA	3.2
2	B	855	LYS	3.2
2	F	824	VAL	3.2
2	F	211	ILE	3.2
2	F	443	ILE	3.2
2	B	909	SER	3.1
2	B	808	ASN	3.1
2	F	210	ALA	3.1
2	F	627	GLU	3.1
2	F	423	LEU	3.1
2	F	806	LEU	3.1
2	F	478	PHE	3.1
2	B	836	TYR	3.1
2	F	212	LEU	3.1
2	F	332	LEU	3.1
2	F	891	LEU	3.1
2	F	155	TYR	3.1
2	F	309	ASN	3.1
2	F	694	MET	3.1
2	F	416	LEU	3.1
2	B	861	ASP	3.0
2	F	882	TYR	3.1
2	F	369	GLN	3.0
2	F	440	ILE	3.0
2	B	703	THR	3.0
1	A	1	U	3.0
2	F	873	GLU	3.0
2	F	247	GLY	3.0
2	F	800	PRO	3.0
2	F	421	ALA	3.0
2	F	317	LEU	3.0
2	B	849	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	445	THR	3.0
2	F	135	ILE	3.0
2	F	315	ALA	3.0
2	F	136	TYR	2.9
2	F	119	PHE	2.9
2	B	384	ASP	2.9
2	B	793	SER	2.9
2	F	140	LYS	2.9
2	F	208	ALA	2.9
2	F	705	LYS	2.9
2	F	178	ASN	2.9
2	F	781	MET	2.9
2	F	229	LEU	2.9
2	F	444	LEU	2.9
2	B	462	PHE	2.9
2	F	196	PHE	2.9
2	F	892	ILE	2.9
2	F	357	ASN	2.9
2	B	882	TYR	2.9
2	F	201	ILE	2.9
2	B	803	ASN	2.9
2	F	389	LEU	2.9
2	F	691	ARG	2.9
2	B	1245	LEU	2.8
2	F	117	PRO	2.8
2	F	149	ALA	2.8
2	F	331	ASP	2.8
2	B	673	LYS	2.8
2	B	916	PHE	2.8
2	F	79	ILE	2.8
2	F	351	PHE	2.8
2	F	700	ASP	2.8
2	F	777	SER	2.8
2	B	240	ASN	2.8
2	B	1246	LYS	2.8
2	F	813	LEU	2.8
2	F	482	VAL	2.8
2	B	829	ASP	2.8
2	B	811	LEU	2.8
2	F	485	GLY	2.8
2	F	290	PHE	2.8
2	F	372	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
3	C	1	DC	2.7
4	H	2	DT	2.7
2	B	806	LEU	2.7
2	F	335	LEU	2.7
2	F	398	LEU	2.7
4	D	12	DG	2.7
2	F	693	PHE	2.7
2	F	704	PHE	2.7
2	F	836	TYR	2.7
2	F	874	GLU	2.7
2	B	815	TYR	2.7
2	F	321	MET	2.7
3	C	24	DG	2.7
2	B	784	ILE	2.7
2	F	122	ILE	2.7
2	F	528	LYS	2.7
2	F	651	LEU	2.7
5	I	36	G	2.7
2	F	85	ILE	2.6
2	F	612	ASN	2.6
2	F	157	ALA	2.6
2	B	308	VAL	2.6
2	F	192	TYR	2.6
2	F	701	SER	2.6
2	B	888	ASN	2.6
2	B	1048	THR	2.6
2	F	1126	TRP	2.6
2	F	588	ASN	2.6
2	F	883	TRP	2.6
2	B	1042	ILE	2.6
2	F	950	ILE	2.6
2	B	897	PHE	2.6
2	B	258	LEU	2.6
2	B	904	GLU	2.6
2	B	853	ASP	2.6
2	B	818	ASN	2.6
2	F	881	ASN	2.6
2	F	248	LEU	2.6
2	B	837	ASP	2.6
2	F	298	ASP	2.6
2	B	25	TYR	2.5
2	B	1039	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	E	33	U	2.5
2	B	868	ASP	2.5
1	A	2	U	2.5
2	F	412	HIS	2.5
2	B	304	ASP	2.5
2	F	106	LEU	2.5
2	F	91	ALA	2.5
2	F	163	LYS	2.5
2	B	697	ILE	2.5
2	F	151	LEU	2.5
2	F	804	THR	2.5
2	F	1132	GLY	2.5
2	B	518	PHE	2.5
2	B	1046	PHE	2.5
2	B	1258	PHE	2.5
2	B	1248	SER	2.5
2	F	567	ASP	2.5
2	F	789	LYS	2.5
2	F	878	LYS	2.5
2	B	1034	ALA	2.5
2	F	250	PRO	2.5
2	F	193	ASN	2.4
2	F	202	ASN	2.4
2	F	530	VAL	2.4
2	F	636	LEU	2.4
2	F	98	PHE	2.4
2	F	352	PHE	2.4
2	F	172	GLY	2.4
2	B	838	VAL	2.4
2	F	452	VAL	2.4
2	B	796	LEU	2.4
1	E	28	A	2.4
2	B	721	HIS	2.4
2	B	270	THR	2.4
2	B	1018	VAL	2.4
2	F	143	VAL	2.4
2	B	1040	SER	2.4
2	F	708	ILE	2.4
2	F	887	LEU	2.4
2	F	797	LYS	2.4
2	F	256	PHE	2.4
2	B	799	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
2	F	227	ALA	2.4
2	F	123	VAL	2.4
2	F	347	TYR	2.4
2	F	390	LEU	2.4
2	F	441	GLU	2.4
2	B	687	GLY	2.4
2	F	538	ALA	2.4
2	F	642	LEU	2.3
2	F	268	LYS	2.3
2	F	348	LYS	2.3
2	F	536	LYS	2.3
2	F	240	ASN	2.3
2	F	876	VAL	2.3
2	F	449	PRO	2.3
2	F	1112	PRO	2.3
5	I	98	U	2.3
2	B	860	SER	2.3
2	B	262	ALA	2.3
2	B	911	LEU	2.3
2	F	138	LEU	2.3
2	B	1196	ILE	2.3
2	B	844	GLN	2.3
2	F	581	SER	2.3
2	B	850	ASP	2.3
2	F	150	ASP	2.3
2	F	801	VAL	2.3
2	F	322	ILE	2.3
2	F	709	GLN	2.3
2	F	219	SER	2.3
2	B	260	GLU	2.3
2	B	530	VAL	2.3
2	B	1244	LYS	2.3
2	B	1017	ASP	2.3
2	F	99	HIS	2.3
2	F	162	ILE	2.3
2	F	414	ILE	2.3
2	F	682	PHE	2.3
1	A	34	G	2.3
2	B	832	ARG	2.3
2	B	1020	LYS	2.3
2	F	360	ALA	2.3
2	F	527	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
2	F	604	LYS	2.3
2	F	1244	LYS	2.3
2	B	717	GLY	2.3
2	B	706	GLU	2.3
2	F	802	GLU	2.3
2	B	273	ASP	2.2
5	I	37	U	2.2
2	B	756	PRO	2.2
2	B	807	GLN	2.2
2	F	426	GLN	2.2
2	B	1247	GLY	2.2
2	F	606	PHE	2.2
2	F	685	SER	2.2
2	F	364	ASP	2.2
2	F	853	ASP	2.2
2	B	862	LYS	2.2
2	F	194	GLN	2.2
2	F	169	LEU	2.2
2	F	367	ALA	2.2
2	B	239	GLY	2.2
2	F	105	PHE	2.2
2	F	324	ARG	2.2
2	F	867	SER	2.2
2	B	585	ASP	2.2
2	F	433	LEU	2.2
2	F	363	ILE	2.2
2	F	586	ARG	2.2
2	B	28	PRO	2.2
2	F	230	PRO	2.2
2	F	476	TRP	2.2
2	B	872	SER	2.2
2	B	863	ASN	2.2
2	F	803	ASN	2.2
2	F	397	ASP	2.2
2	F	647	VAL	2.2
2	F	100	ARG	2.1
2	F	356	LYS	2.1
2	F	484	LYS	2.1
2	F	587	PHE	2.1
2	B	527	VAL	2.1
5	J	38	A	2.1
2	F	632	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	783	ARG	2.1
2	B	263	LYS	2.1
2	F	621	LEU	2.1
2	B	777	SER	2.1
2	F	793	SER	2.1
2	F	557	ARG	2.1
3	G	24	DG	2.1
2	F	613	GLU	2.1
2	B	47	LEU	2.1
2	F	1249	PRO	2.1
2	B	1145	VAL	2.1
2	F	350	ILE	2.1
2	F	448	ILE	2.1
2	F	1120	ILE	2.1
2	F	139	ARG	2.1
2	F	885	GLN	2.1
2	F	184	LEU	2.1
2	F	785	GLU	2.1
2	B	1035	LYS	2.1
2	F	442	LYS	2.1
2	F	430	TYR	2.1
2	F	466	THR	2.1
2	F	814	TYR	2.1
2	F	1011	GLY	2.1
2	F	834	SER	2.1
2	F	817	GLN	2.1
2	F	144	ASP	2.1
2	B	922	VAL	2.1
2	B	1036	TYR	2.0
2	F	638	THR	2.0
2	F	805	GLN	2.0
2	F	375	PHE	2.0
2	B	229	LEU	2.0
2	B	839	ASP	2.0
2	B	1236	LEU	2.0
2	F	947	ASP	2.0
2	F	1193	ASP	2.0
2	B	176	PRO	2.0
2	F	798	GLU	2.0
2	F	422	ILE	2.0
2	F	405	PHE	2.0
2	F	571	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
4	H	12	DG	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.