



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:30 PM BST

PDB ID : 4Y7N
Title : The Structure Insight into 5-Carboxycytosine Recognition by RNA Polymerase II during Transcription Elongation.
Authors : Wang, L.; Chong, J.; Wang, D.
Deposited on : 2015-02-15
Resolution : 3.30 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

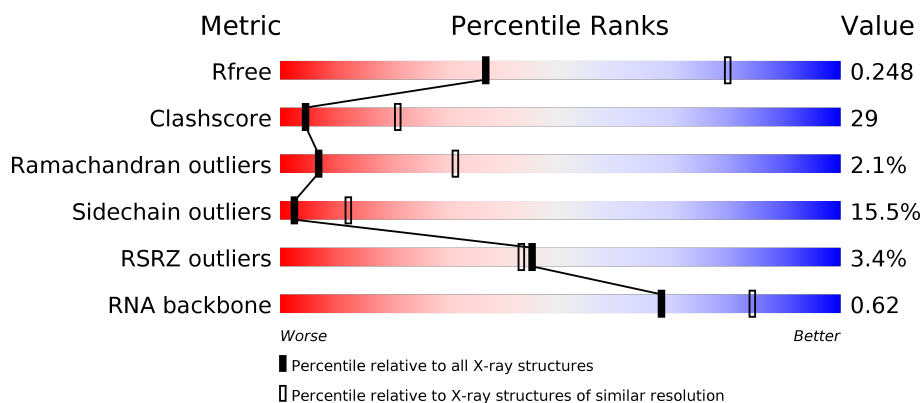
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1733	<div> <div>3%</div> <div> <div>43%</div> <div>30%</div> <div>7%</div> <div>20%</div> </div> </div>
2	B	1224	<div> <div>2%</div> <div> <div>48%</div> <div>35%</div> <div>6%</div> <div>10%</div> </div> </div>
3	C	318	<div> <div>44%</div> <div>34%</div> <div>6%</div> <div>16%</div> </div>
4	E	215	<div> <div>5%</div> <div> <div>59%</div> <div>35%</div> <div>6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
5	F	155	<div><div></div><div>27%21%6%46%</div></div>
6	H	146	<div><div>8%</div><div>38%40%12%9%</div></div>
7	I	122	<div><div>%</div><div>54%37%7%</div></div>
8	J	70	<div><div></div><div>33%49%11%7%</div></div>
9	K	120	<div><div></div><div>64%28%5%</div></div>
10	L	70	<div><div>4%</div><div>20%31%10%37%</div></div>
11	T	29	<div><div>38%</div><div>14%76%10%</div></div>
12	N	14	<div><div>57%</div><div>100%</div></div>
13	R	9	<div><div></div><div>44%33%22%</div></div>

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29193 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 protein called DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1393	Total	C	N	O	S	0	0	0
			10953	6908	1921	2063	61			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2,DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1103	Total	C	N	O	S	0	0	0
			8762	5549	1532	1626	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	266	Total	C	N	O	S	0	0	0
			2095	1317	348	417	13			

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	133	Total	C	N	O	S	0	0	0
			1068	673	180	211	4			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	K	114	Total	C	N	O	S	0	0	0
			919	590	156	171	2			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	L	44	Total	C	N	O	S	0	0	0
			351	217	70	60	4			

- Molecule 11 is a DNA chain called DNA (29-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	T	29	Total	C	N	O	P	0	0	0
			587	280	108	171	28			

- Molecule 12 is a DNA chain called DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

- Molecule 13 is a RNA chain called RNA (5'-D(*AP*UP*GP*GP*AP*GP*AP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	R	9	Total	C	N	O	P	0	0	0
			198	89	42	59	8			

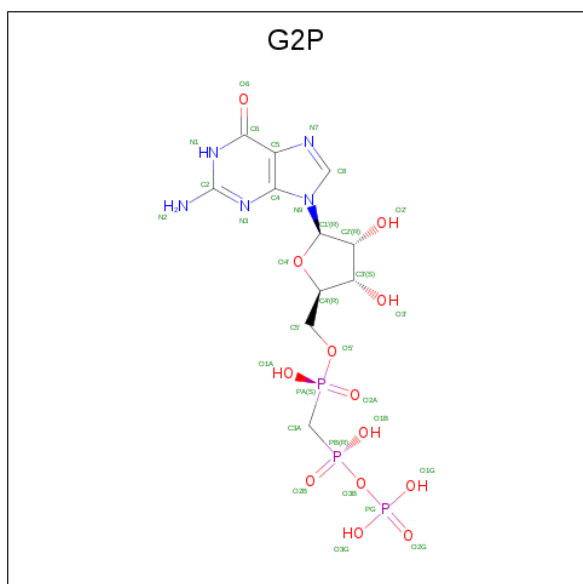
- Molecule 14 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	J	1	Total	Zn	0	0
			1	1		
14	B	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	C	1	Total	Zn	0	0
			1	1		
14	A	2	Total	Zn	0	0
			2	2		
14	L	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is PHOSPHOMETHYLPHOSPHONIC ACID GUANYLATE ESTER (three-letter code: G2P) (formula: C₁₁H₁₈N₅O₁₃P₃).

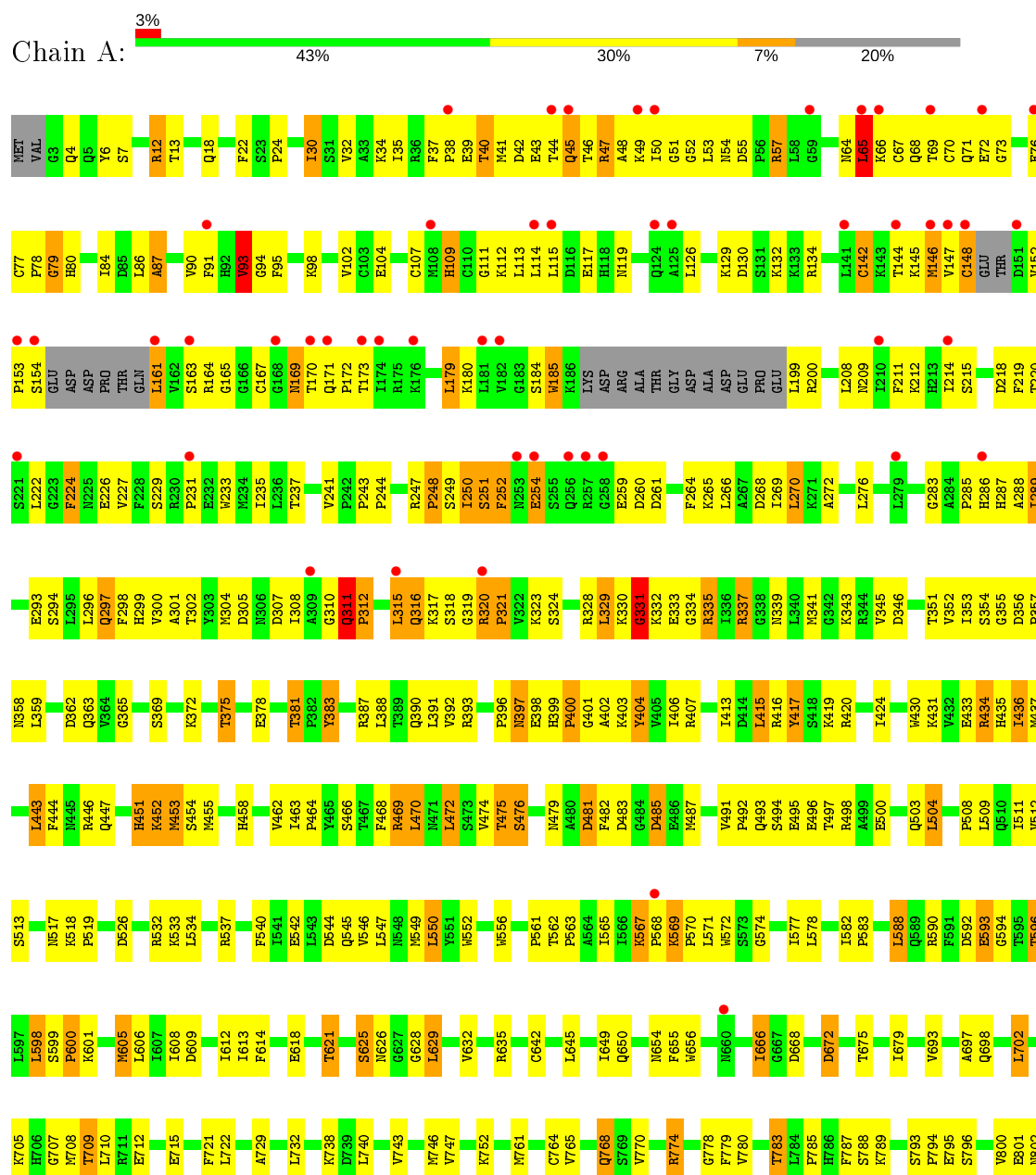


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
16	T	1	Total	C	N	O	P	0	0
			32	11	5	13	3		

3 Residue-property plots

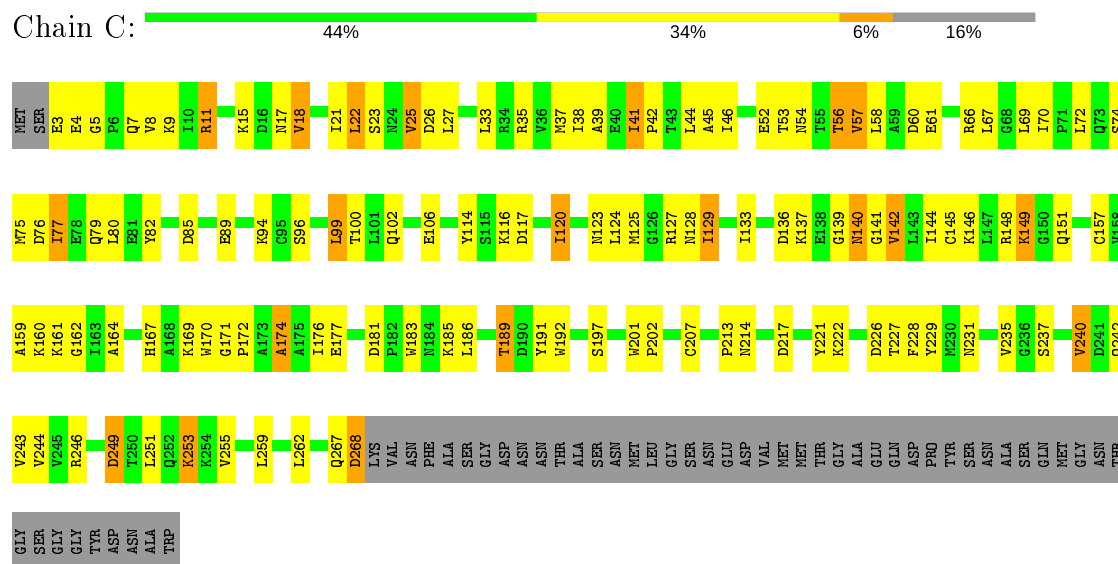
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: DNA-directed RNA polymerase II subunit RPB1

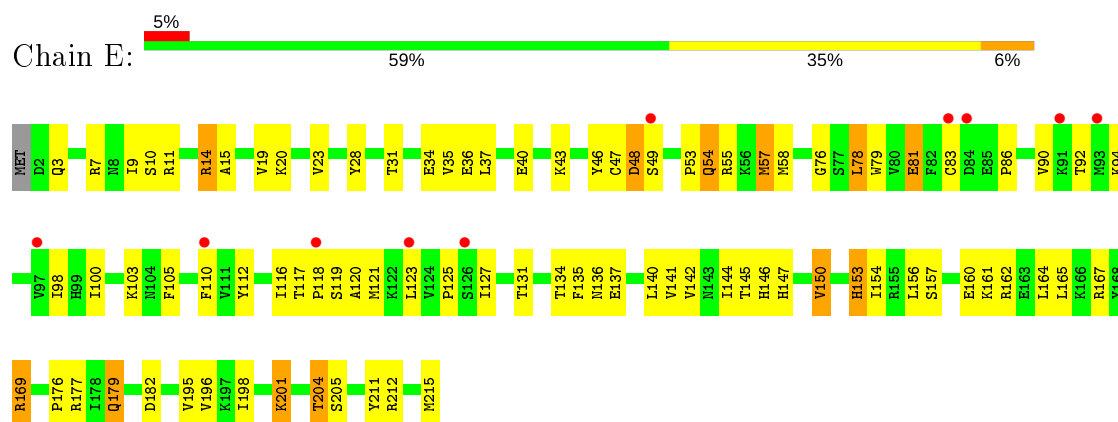


Q1205	R1122	A1044	T880	Y798	GLU	V640	M542	G464	L378	I301	R217	ARG
E1206	S1123	S1045	R881	F799	GLU	E641	T549	N465	M381	M313	I222	GLU
L1207	R1124	F1047	T882	Q800	ASN	D643	D550	G467	I382	L314		LEU
		T1048	R884	R801	LEU	D643	M551	Q468	L385	K315	V225	LYS
I1212	F1130	D1049	D896	T806	D722	H648	M552	Q469	L386	P316	F226	TYR
R1220	E1134	T1050	R897	R807	Y793	K649	M553	K470	L387	C317	K227	GLY
S1221	R1135	T1052	T899	A808	D724	E650	I554	K471		G317	K228	LEU
ASP	D1136	V1053	A900	E810	K727	M652	I555	A472		E319	A229	ILE
PHE		G1054	P901	Y811		G653	T556	M473	K393	G320	A230	ALA
	I1139	I1055	G902	L812	R730	R654	I558	S474	D394	G321		GLU
					R731	K655		S475				S91
					R732		M563	R476	Q395			F92
	G1142	L1059	S906	P818	S732	I658		A477		T324	I240	GLU
		R1060			H733				R398	Q325	R241	ASP
	E1149	T990	T911	N822	H734		L566	G478		D326	S242	ASP
	R1150	G991	I912	A823	A735	L661		V479	G402	R327	A243	ASP
L1151	S1066	I992	I912	R824	T736		Y569	Q480	E328	E245	K246	GLU
M1152		T993	I918	Y625	T737	T664	V570	V482	D407	T329	K247	SER
E1153	F1069	Y994	S919	A826		E665		L483	L408			K99
A1154		R995	PRU	I827	I743	Y666	Q573		A409	D332	S248	GLY
	M1072	R996	GLU	Y830	H744	D667	D576	Y486		F333	R249	M101
	Y1073	D998	GLU	S831	S746	D668		Y488	L416	I334	F250	V102
	T1077	M999	GLU	G832	M747		V580	S489	F417	G335	I167	N103
	G1078	P1000	LEU	Y833		GLY	F581	S490	K418		G168	E104
C1163	K1079	F1001	GLY	R834	V751	GLY	V582	L491		ARG	R169	D106
G1164	T1080	T1002	GLN	R835		PHE		T492	K423	THR	V256	G107
I1165	L1081	A1003	ARG	Q835	S754	GLU	V585		L424	ALA	K257	V108
	M1082	E1004	THR		I755	ASP		T500	T425	GLY	L258	T109
	Q1083	G1005	ALA		I756	VAL	V589	P501	K426	ILE	R261	L112
	Q1084	I1006	TYR	R840	I757	GLU	H590	I502	D427	LYS	R262	L113
	I1085	V1007	ILS	R841	F758	E678	P593	GLY	I428	K345	G263	F114
A1173	F1086	P1008	S933	N842	Y679	T660		ARG	F429	E346	G264	L181
L1175	G1088	D1009	R934	Q843	M762		L596	ASP	R430	S265	S265	S182
M1176	P1089	L1010	R935	S844	Q763		L597	GLY	Y431	A266	A266	E183
	T1090		D936	S845	S764	L684	M597	LYS	M432	R267		L119
	Y1091	M1013		L846	P765		E598	LEU	Q433	T268	D188	R120
Q1179	Y1092	R1014	L941	D847	Q770	I683	T599	A509	R434	T269	L189	I121
F1180	E1181	H1015	R942	R848		D694	L600	K510	T435	L356	Y190	L122
C1182	C1182	Q1093	S943	G849	Q776	A695		P511	V436	K357	K191	T123
K1183	L1095	I1017	L850	L850	A777	E696	L603	R512	E437	E194	K193	Y124
C1184	R1096	P1018	I946	F851	M778			Q513	GLU	K277	E194	S125
C1185	H1097	R1020			G779		M609		ALA	K358	C195	L128
	H1098	M1021			Y780		M610	N516	HIS	E359	P196	F129
	V1099	V1023	L963	F856	T781	L702	M615	T517	ASP	L361		V130
			V954	R857	L782	I703	I616	W519	PHE	H363	P203	K133
			T955	S858	T783	A704	B617	W519	ASN	I364	I205	K134
			T956	Y859	T784	M705			MET	T365	G207	ARG
					M784	Q706	R620	V522	LYS	Q366	E207	THR
					Y785	P707			L446	L367	S208	TYR
					M786	E708	I626	T527	A447	E368	E209	GLU
					V787	D709	F627	Q531	I448	G369	K210	ILE
					R788	L710		A532		P293	V211	ASP
					M789	E711	R635		T454	F370	L212	ILE
						P712	P636			R373	I213	ASP
					M792	A713	P637	V536	A460		E296	PRU
						E714	L637	K537	L461	F376	A214	VAL
					L796	A715	F638	L541	T463		E216	GLY
					Y797	ASN	I639			F377		

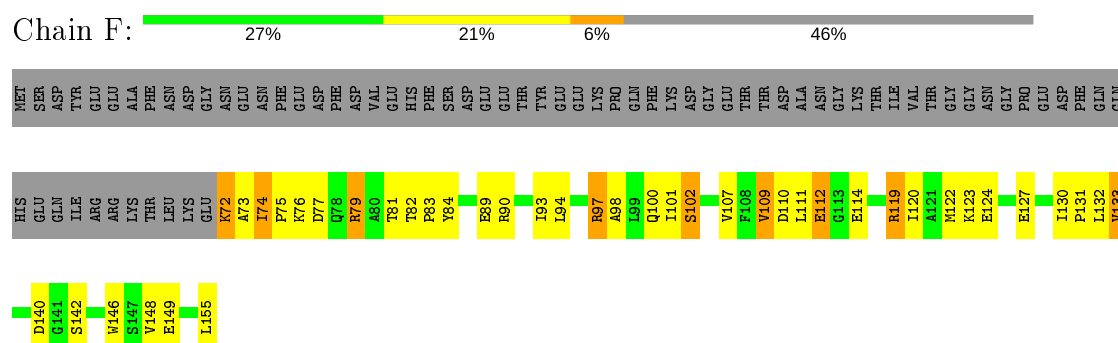
- Molecule 3: DNA-directed RNA polymerase II subunit RPB3



- Molecule 4: DNA-directed RNA polymerases I, II, and III subunit RPABC1

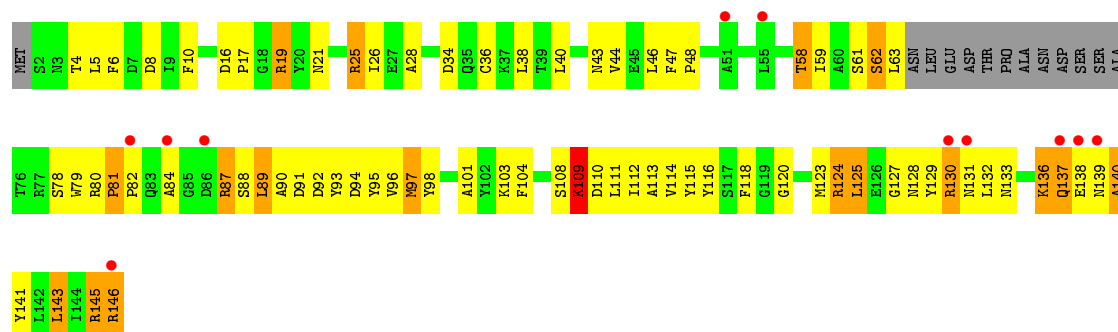


- Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC2



- Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC3





- Molecule 7: DNA-directed RNA polymerase II subunit RPB9



- Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC5



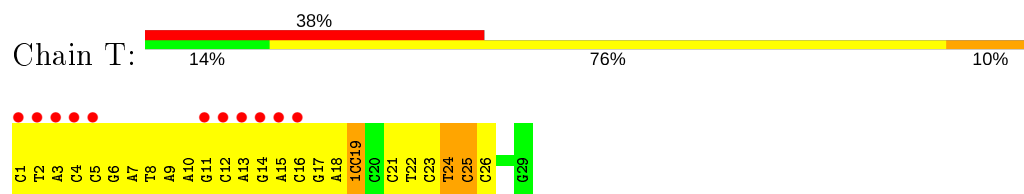
- Molecule 9: DNA-directed RNA polymerase II subunit RPB11



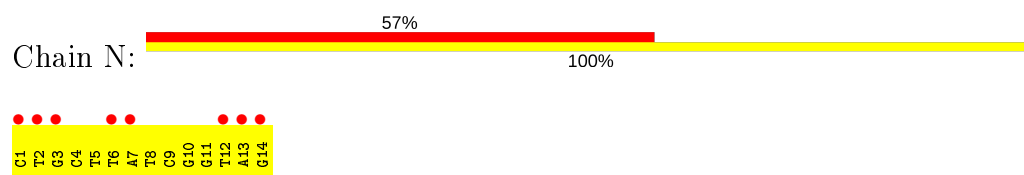
- Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC4



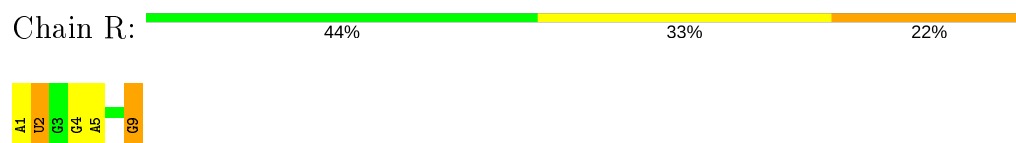
- Molecule 11: DNA (29-MER)



- Molecule 12: DNA (5'-D(*CP*TP*GP*CP*TP*TP*AP*TP*CP*GP*GP*TP*AP*G)-3')



- Molecule 13: RNA (5'-D(*AP*UP*GP*GP*AP*GP*AP*GP*G)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.18Å 222.61Å 192.83Å 90.00° 101.59° 90.00°	Depositor
Resolution (Å)	48.88 – 3.30 48.88 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.88-3.30) 98.1 (48.88-3.26)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.64 (at 3.25Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.207 , 0.250 0.205 , 0.248	Depositor DCC
R_{free} test set	5268 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 52.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	29193	wwPDB-VP
Average B, all atoms (Å ²)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.70% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 1CC, ZN, MG, G2P

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.43	1/11146 (0.0%)	0.65	5/15066 (0.0%)
2	B	0.47	1/8932 (0.0%)	0.67	3/12045 (0.0%)
3	C	0.47	0/2133	0.71	1/2891 (0.0%)
4	E	0.38	0/1788	0.55	0/2406
5	F	0.40	0/691	0.61	0/933
6	H	0.38	0/1086	0.56	0/1470
7	I	0.40	0/989	0.64	1/1331 (0.1%)
8	J	0.49	0/541	0.69	0/727
9	K	0.46	0/937	0.61	0/1265
10	L	0.32	0/353	0.63	0/468
11	T	0.61	0/632	1.17	7/969 (0.7%)
12	N	0.18	0/317	0.56	0/488
13	R	0.56	0/223	1.01	0/348
All	All	0.44	2/29768 (0.0%)	0.67	17/40407 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	707	PRO	N-CD	5.28	1.55	1.47
1	A	400	PRO	N-CD	5.19	1.55	1.47

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	331	GLY	N-CA-C	7.95	132.97	113.10
11	T	24	DT	N3-C4-O4	7.17	124.20	119.90
11	T	24	DT	P-O5'-C5'	-6.69	110.20	120.90
1	A	919	ILE	CB-CA-C	-6.33	98.94	111.60
11	T	25	DC	O4'-C4'-C3'	-6.09	102.06	104.50
1	A	311	GLN	C-N-CD	6.05	141.10	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	174	ALA	N-CA-C	-5.96	94.90	111.00
11	T	22	DT	P-O5'-C5'	-5.95	111.38	120.90
2	B	248	SER	N-CA-C	-5.78	95.40	111.00
11	T	26	DC	O4'-C1'-N1	5.76	112.03	108.00
1	A	598	LEU	N-CA-C	-5.71	95.58	111.00
1	A	77	CYS	N-CA-C	-5.52	96.10	111.00
11	T	23	DC	C4'-C3'-C2'	-5.38	98.25	103.10
2	B	712	PRO	CA-N-CD	-5.31	104.07	111.50
11	T	24	DT	C5-C4-O4	-5.28	121.20	124.90
7	I	75	CYS	C-N-CD	-5.15	109.27	120.60
2	B	780	VAL	CB-CA-C	-5.09	101.73	111.40

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	10953	0	11053	681	0
2	B	8762	0	8797	459	0
3	C	2095	0	2051	104	0
4	E	1752	0	1776	60	0
5	F	679	0	701	31	0
6	H	1068	0	1040	88	0
7	I	971	0	927	36	0
8	J	532	0	542	66	0
9	K	919	0	929	29	0
10	L	351	0	374	65	0
11	T	587	0	326	123	0
12	N	284	0	161	49	0
13	R	198	0	99	9	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	T	32	0	14	2	0
All	All	29193	0	28790	1651	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 29.

All (1651) 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)
1:A:317:LYS:CG	1:A:318:SER:HB2	1.25	1.56
2:B:714:GLU:HA	2:B:715:ALA:CB	1.40	1.45
1:A:317:LYS:HG3	1:A:318:SER:CB	1.46	1.42
1:A:317:LYS:CG	1:A:318:SER:CB	1.98	1.42
10:L:38:LEU:HD12	10:L:40:LEU:CG	1.52	1.36
11:T:5:DC:C2'	11:T:6:DG:H5'	1.56	1.34
2:B:711:GLU:HB2	2:B:712:PRO:CA	1.57	1.33
1:A:317:LYS:CB	1:A:318:SER:HB2	1.62	1.30
1:A:43:GLU:HB2	1:A:50:ILE:CD1	1.61	1.30
1:A:43:GLU:CB	1:A:50:ILE:HD12	1.63	1.28
2:B:714:GLU:CA	2:B:715:ALA:HB2	1.62	1.28
1:A:1175:SER:HA	1:A:1176:LEU:C	1.37	1.27
1:A:57:ARG:HB3	1:A:68:GLN:CG	1.65	1.26
11:T:17:DG:H2''	11:T:18:DA:C5'	1.63	1.25
2:B:711:GLU:CB	2:B:712:PRO:HA	1.65	1.21
1:A:316:GLN:CB	1:A:318:SER:HA	1.72	1.18
1:A:403:LYS:HB3	1:A:404:TYR:CD1	1.80	1.17
3:C:41:ILE:HG13	3:C:172:PRO:HG3	1.26	1.16
1:A:38:PRO:HB3	1:A:270:LEU:HB3	1.19	1.15
1:A:57:ARG:HB3	1:A:68:GLN:CB	1.78	1.12
11:T:5:DC:H2''	11:T:6:DG:C5'	1.80	1.12
1:A:912:LEU:CD2	1:A:1036:ARG:HH21	1.62	1.11
6:H:137:GLN:HB2	6:H:138:GLU:HA	1.18	1.11
1:A:57:ARG:HB3	1:A:68:GLN:HG2	1.15	1.10
1:A:251:SER:HB2	1:A:252:PHE:HB3	1.33	1.09
6:H:137:GLN:CB	6:H:138:GLU:HA	1.81	1.08
6:H:62:SER:O	6:H:63:LEU:CD1	2.02	1.08
12:N:6:DT:H2''	12:N:7:DA:OP2	1.50	1.08
11:T:18:DA:H2''	11:T:19:1CC:OP2	1.49	1.07
11:T:12:DC:H1'	11:T:13:DA:N9	1.68	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1175:SER:CA	1:A:1176:LEU:C	2.23	1.07
1:A:316:GLN:HB3	1:A:318:SER:HA	1.10	1.07
12:N:3:DG:H2''	12:N:4:DC:H5'	1.35	1.06
1:A:316:GLN:CB	1:A:317:LYS:HA	1.79	1.06
1:A:38:PRO:HB3	1:A:270:LEU:CB	1.85	1.06
1:A:57:ARG:CB	1:A:68:GLN:HG2	1.85	1.06
1:A:249:SER:HB2	1:A:250:ILE:HB	1.32	1.05
1:A:316:GLN:HB2	1:A:317:LYS:HA	1.08	1.05
5:F:74:ILE:HG13	5:F:75:PRO:HD2	1.39	1.04
1:A:399:HIS:CD2	1:A:400:PRO:HA	1.91	1.04
11:T:16:DC:H2''	11:T:17:DG:H5''	1.37	1.04
1:A:57:ARG:HB3	1:A:68:GLN:HB3	1.37	1.04
2:B:714:GLU:CA	2:B:715:ALA:CB	2.22	1.03
1:A:39:GLU:HA	1:A:40:THR:HB	1.37	1.03
10:L:46:VAL:HB	10:L:47:ARG:HA	1.36	1.03
11:T:8:DT:H1'	11:T:9:DA:C8	1.93	1.03
2:B:711:GLU:HB3	2:B:713:ALA:HA	1.41	1.02
10:L:47:ARG:HB3	10:L:54:ARG:HB3	1.41	1.02
1:A:38:PRO:HG2	1:A:39:GLU:OE1	1.58	1.02
10:L:38:LEU:HD12	10:L:40:LEU:HG	1.06	1.01
10:L:38:LEU:CD1	10:L:40:LEU:HD21	1.91	1.01
1:A:265:LYS:HE3	1:A:302:THR:HG23	1.40	1.01
2:B:710:LEU:O	2:B:711:GLU:HG2	1.59	1.00
11:T:17:DG:H2''	11:T:18:DA:H5'	1.43	1.00
1:A:912:LEU:HD23	1:A:1036:ARG:HH21	1.22	1.00
6:H:62:SER:O	6:H:63:LEU:HD13	1.61	1.00
1:A:570:PRO:HB2	1:A:572:TRP:CZ3	1.98	0.99
2:B:711:GLU:CB	2:B:713:ALA:HA	1.92	0.99
1:A:885:THR:CG2	1:A:943:LEU:HD12	1.90	0.99
1:A:317:LYS:HG3	1:A:318:SER:HB3	1.40	0.99
1:A:316:GLN:HB3	1:A:319:GLY:HA2	1.43	0.98
12:N:3:DG:C2'	12:N:4:DC:H5'	1.93	0.98
1:A:403:LYS:HB3	1:A:404:TYR:HD1	1.24	0.98
1:A:399:HIS:HD2	1:A:400:PRO:HA	1.29	0.97
10:L:38:LEU:HD12	10:L:40:LEU:CD2	1.95	0.97
11:T:13:DA:H5'	11:T:14:DG:OP2	1.65	0.97
1:A:46:THR:HG22	1:A:47:ARG:H	1.30	0.96
11:T:9:DA:N6	12:N:6:DT:H3	1.63	0.96
2:B:1187:ASN:HD21	2:B:1190:ASP:HB2	1.27	0.96
1:A:317:LYS:HG3	1:A:318:SER:HB2	1.09	0.95
1:A:406:ILE:HB	1:A:431:LYS:HB2	1.45	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:68:GLN:NE2	1:A:80:HIS:HD2	1.64	0.95
2:B:1187:ASN:HD21	2:B:1190:ASP:CB	1.80	0.95
1:A:317:LYS:HG2	1:A:318:SER:CB	1.94	0.95
13:R:1:A:H2'	13:R:2:U:H5''	1.46	0.95
1:A:563:PRO:HB3	1:A:572:TRP:CE2	2.01	0.94
10:L:38:LEU:HD11	10:L:49:LYS:CD	1.98	0.94
1:A:249:SER:CB	1:A:250:ILE:HB	1.97	0.94
11:T:12:DC:H1'	11:T:13:DA:C1'	1.98	0.94
10:L:38:LEU:CD1	10:L:40:LEU:CG	2.46	0.94
10:L:38:LEU:CD1	10:L:40:LEU:CD2	2.46	0.93
2:B:25:ILE:HD11	2:B:653:VAL:HB	1.48	0.93
1:A:38:PRO:CB	1:A:270:LEU:HB3	1.96	0.93
1:A:316:GLN:CB	1:A:319:GLY:HA2	1.98	0.93
10:L:46:VAL:CB	10:L:47:ARG:HA	1.95	0.93
2:B:708:GLU:O	2:B:712:PRO:HB3	1.70	0.92
11:T:6:DG:H1'	11:T:7:DA:C8	2.05	0.92
8:J:6:ARG:HG3	8:J:13:VAL:HA	1.52	0.92
13:R:1:A:H8	13:R:1:A:HO5'	0.98	0.92
1:A:563:PRO:HB3	1:A:572:TRP:CZ2	2.04	0.92
1:A:828:ALA:O	1:A:831:THR:HG22	1.69	0.92
1:A:317:LYS:CA	1:A:318:SER:HB2	2.00	0.92
1:A:392:VAL:HG13	1:A:415:LEU:HD11	1.50	0.91
1:A:1435:PRO:HA	1:A:1439:GLY:O	1.70	0.91
10:L:47:ARG:HG2	10:L:48:CYS:H	1.34	0.90
2:B:706:GLN:O	2:B:709:ASP:HB2	1.71	0.90
2:B:784:ASN:ND2	2:B:788:ARG:HD2	1.87	0.90
11:T:5:DC:H2''	11:T:6:DG:H5'	0.91	0.90
1:A:1435:PRO:C	1:A:1436:ILE:HD12	1.92	0.90
1:A:592:ASP:O	1:A:593:GLU:HB2	1.71	0.90
10:L:38:LEU:CD1	10:L:40:LEU:HG	2.00	0.90
2:B:884:ARG:HG3	2:B:935:ARG:HG2	1.53	0.90
2:B:1002:THR:HG23	2:B:1004:GLU:H	1.37	0.89
10:L:38:LEU:HD21	10:L:49:LYS:HB2	1.50	0.89
2:B:855:PHE:HZ	2:B:857:ARG:NH1	1.70	0.89
11:T:7:DA:H2'	11:T:8:DT:C6	2.08	0.89
1:A:912:LEU:HD23	1:A:1036:ARG:NH2	1.86	0.89
1:A:316:GLN:HB2	1:A:317:LYS:CA	2.01	0.89
11:T:5:DC:C1'	11:T:6:DG:H5'	2.02	0.89
1:A:323:LYS:HE2	1:A:328:ARG:HE	1.37	0.89
2:B:711:GLU:HB3	2:B:713:ALA:CA	2.03	0.89
1:A:317:LYS:HG2	1:A:318:SER:HB2	1.48	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:VAL:HB	1:A:929:LEU:HD13	1.56	0.88
1:A:57:ARG:CB	1:A:68:GLN:HB3	2.04	0.88
2:B:911:ILE:HD11	2:B:941:LEU:HD23	1.56	0.88
6:H:62:SER:O	6:H:63:LEU:HD12	1.71	0.88
1:A:316:GLN:HB3	1:A:319:GLY:CA	2.04	0.88
1:A:50:ILE:HG23	1:A:51:GLY:H	1.39	0.88
3:C:70:ILE:HD11	3:C:144:ILE:HD11	1.53	0.87
1:A:317:LYS:CG	1:A:318:SER:HB3	1.99	0.87
2:B:711:GLU:HB2	2:B:712:PRO:HA	0.87	0.87
6:H:137:GLN:HB2	6:H:138:GLU:CA	2.04	0.87
1:A:316:GLN:HG2	1:A:319:GLY:O	1.75	0.87
1:A:981:LEU:HD23	1:A:981:LEU:N	1.90	0.87
1:A:42:ASP:HB2	1:A:48:ALA:O	1.74	0.86
12:N:1:DC:H4'	12:N:2:DT:OP1	1.73	0.86
1:A:1161:THR:HG22	1:A:1163:ILE:H	1.38	0.86
1:A:1116:LEU:H	1:A:1308:THR:HB	1.40	0.86
6:H:130:ARG:HH11	6:H:130:ARG:HG2	1.40	0.86
11:T:10:DA:H2''	11:T:11:DG:OP2	1.76	0.86
11:T:7:DA:H2''	11:T:8:DT:H5'	1.56	0.86
11:T:6:DG:H1'	11:T:7:DA:N7	1.90	0.86
1:A:399:HIS:CD2	1:A:400:PRO:CA	2.58	0.85
1:A:407:ARG:HD2	1:A:413:ILE:HD11	1.57	0.85
1:A:35:ILE:HG23	1:A:52:GLY:O	1.75	0.85
2:B:648:HIS:CD2	2:B:711:GLU:HG3	2.10	0.85
1:A:403:LYS:HB3	1:A:404:TYR:CE1	2.10	0.85
1:A:979:SER:HB2	1:A:981:LEU:HD21	1.56	0.85
5:F:111:LEU:O	5:F:112:GLU:HG3	1.75	0.85
5:F:74:ILE:HG13	5:F:75:PRO:CD	2.07	0.85
1:A:250:ILE:HG23	1:A:251:SER:O	1.77	0.85
1:A:68:GLN:NE2	1:A:80:HIS:CD2	2.45	0.84
1:A:709:THR:HG23	1:A:712:GLU:HB2	1.60	0.84
12:N:2:DT:O2	12:N:3:DG:C6	2.30	0.84
1:A:981:LEU:HD12	1:A:986:ILE:HD11	1.57	0.84
1:A:251:SER:HB2	1:A:252:PHE:CB	2.06	0.83
2:B:29:ASP:HB3	2:B:658:ILE:HG12	1.61	0.83
12:N:9:DC:O2	12:N:10:DG:C6	2.31	0.83
2:B:855:PHE:HZ	2:B:857:ARG:HH12	1.24	0.83
1:A:46:THR:HG22	1:A:47:ARG:N	1.93	0.83
7:I:109:ILE:CG2	7:I:120:GLN:HG3	2.09	0.83
1:A:40:THR:HG23	1:A:41:MET:HG3	1.59	0.82
2:B:416:LEU:HD12	2:B:466:TRP:CZ2	2.14	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:710:LEU:O	2:B:712:PRO:HA	1.79	0.82
1:A:1132:LYS:HG3	1:A:1135:ARG:HH12	1.44	0.82
1:A:407:ARG:CD	1:A:413:ILE:HD11	2.08	0.82
1:A:67:CYS:HB3	1:A:70:CYS:SG	2.19	0.82
10:L:30:ILE:HA	10:L:36:SER:O	1.79	0.82
1:A:316:GLN:HB3	1:A:318:SER:CA	2.04	0.81
1:A:372:LYS:HA	1:A:435:HIS:ND1	1.94	0.81
2:B:108:VAL:HG12	2:B:109:THR:H	1.45	0.81
1:A:84:ILE:HD11	1:A:270:LEU:HG	1.63	0.81
1:A:912:LEU:CD2	1:A:1036:ARG:NH2	2.43	0.81
12:N:3:DG:C1'	12:N:4:DC:H5'	2.09	0.81
12:N:2:DT:H2''	12:N:3:DG:N7	1.96	0.81
1:A:1224:LEU:HD21	1:A:1240:CYS:HB3	1.62	0.80
6:H:137:GLN:CB	6:H:138:GLU:CA	2.60	0.80
1:A:67:CYS:SG	1:A:68:GLN:OE1	2.40	0.80
3:C:66:ARG:HA	8:J:5:VAL:HG21	1.62	0.80
2:B:635:ARG:HG3	2:B:637:LEU:HD21	1.64	0.80
2:B:843:GLN:HB2	2:B:993:THR:HB	1.61	0.80
11:T:12:DC:H1'	11:T:13:DA:C8	2.16	0.80
11:T:17:DG:H2''	11:T:18:DA:H5''	1.63	0.80
1:A:1063:MET:SD	1:A:1436:ILE:HG23	2.21	0.80
2:B:711:GLU:CB	2:B:712:PRO:CA	2.38	0.80
2:B:710:LEU:O	2:B:711:GLU:CG	2.30	0.80
10:L:31:CYS:HB3	10:L:34:CYS:SG	2.22	0.79
1:A:53:LEU:HD23	1:A:54:ASN:HB2	1.65	0.79
2:B:464:GLY:HA2	2:B:480:SER:OG	1.82	0.79
1:A:249:SER:CA	1:A:250:ILE:HB	2.13	0.79
1:A:1063:MET:CE	1:A:1436:ILE:HG13	2.12	0.79
1:A:323:LYS:CE	1:A:328:ARG:HE	1.95	0.79
6:H:111:LEU:O	6:H:112:ILE:HD13	1.83	0.79
12:N:3:DG:H1'	12:N:4:DC:H5'	1.62	0.79
1:A:316:GLN:CG	1:A:319:GLY:HA2	2.13	0.79
1:A:839:ARG:HG2	1:A:839:ARG:HH11	1.45	0.79
2:B:169:ARG:H	2:B:454:THR:HG23	1.48	0.78
12:N:3:DG:H1'	12:N:4:DC:C5'	2.13	0.78
1:A:316:GLN:HE21	1:A:319:GLY:HA2	1.47	0.78
2:B:436:VAL:O	2:B:437:GLU:HG3	1.82	0.78
1:A:147:VAL:HG12	1:A:170:THR:HA	1.65	0.78
1:A:666:ILE:HD11	2:B:1030:LEU:HD13	1.64	0.78
11:T:7:DA:H8	11:T:7:DA:P	2.06	0.78
1:A:444:PHE:HE2	1:A:470:LEU:HD23	1.47	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:THR:HG23	1:A:943:LEU:HD12	1.65	0.78
1:A:304:MET:O	1:A:324:SER:HB2	1.83	0.78
1:A:43:GLU:HB2	1:A:50:ILE:HD12	0.80	0.78
7:I:78:CYS:SG	7:I:80:SER:HB3	2.24	0.78
10:L:38:LEU:HD12	10:L:40:LEU:CD1	2.13	0.78
2:B:642:ASP:HB3	2:B:649:LYS:HG3	1.64	0.77
3:C:56:THR:HG23	3:C:58:LEU:H	1.48	0.77
2:B:711:GLU:HB2	2:B:712:PRO:C	2.04	0.77
2:B:195:CYS:HB2	2:B:784:ASN:OD1	1.85	0.77
6:H:136:LYS:O	6:H:137:GLN:HG2	1.85	0.77
2:B:1173:ALA:HA	2:B:1180:PHE:HD1	1.49	0.76
13:R:1:A:H2'	13:R:2:U:C5'	2.15	0.76
11:T:15:DA:C8	11:T:16:DC:C5	2.74	0.76
1:A:1176:LEU:H	1:A:1176:LEU:HD12	1.48	0.76
1:A:316:GLN:HB2	1:A:318:SER:HA	1.68	0.76
12:N:2:DT:C2	12:N:3:DG:O6	2.39	0.76
1:A:849:MET:HB3	1:A:1063:MET:CE	2.16	0.76
1:A:399:HIS:CE1	1:A:462:VAL:HG21	2.20	0.76
10:L:29:TYR:HE1	10:L:58:LYS:HD2	1.52	0.75
1:A:1063:MET:HE2	1:A:1436:ILE:HG13	1.67	0.75
1:A:705:LYS:HD2	1:A:708:MET:HE1	1.69	0.75
2:B:1072:MET:HG3	2:B:1085:ILE:HB	1.67	0.75
10:L:38:LEU:HD11	10:L:49:LYS:HD3	1.66	0.75
1:A:1435:PRO:O	1:A:1436:ILE:HD12	1.86	0.75
11:T:2:DT:O4	12:N:13:DA:N6	2.20	0.75
2:B:864:LYS:HD2	2:B:866:TYR:H	1.52	0.75
1:A:68:GLN:HE22	1:A:80:HIS:CD2	2.05	0.75
2:B:955:THR:HG23	2:B:956:THR:O	1.86	0.75
1:A:249:SER:HB2	1:A:250:ILE:CB	2.15	0.74
1:A:871:ASP:HB3	4:E:204:THR:HG23	1.68	0.74
2:B:1077:THR:HG23	2:B:1079:LYS:H	1.51	0.74
2:B:257:LYS:NZ	2:B:279:ASP:OD2	2.20	0.74
10:L:38:LEU:HD11	10:L:40:LEU:HD21	1.67	0.74
10:L:38:LEU:HD11	10:L:49:LYS:HD2	1.69	0.74
1:A:346:ASP:HB3	2:B:1107:ALA:O	1.87	0.74
3:C:41:ILE:HG13	3:C:172:PRO:CG	2.13	0.74
10:L:31:CYS:HB3	10:L:34:CYS:O	1.86	0.74
11:T:10:DA:H1'	11:T:11:DG:C8	2.22	0.74
2:B:1187:ASN:ND2	2:B:1190:ASP:HB2	2.03	0.74
2:B:640:VAL:HG22	2:B:651:LEU:HD23	1.68	0.74
1:A:821:ARG:O	1:A:825:ILE:HG12	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:702:LEU:HD23	2:B:737:THR:O	1.87	0.74
10:L:46:VAL:HB	10:L:47:ARG:CA	2.16	0.74
1:A:1035:TYR:O	1:A:1036:ARG:HB2	1.87	0.74
2:B:778:MET:HE1	2:B:1094:ARG:HD2	1.68	0.74
11:T:5:DC:C2'	11:T:6:DG:C5'	2.51	0.74
1:A:570:PRO:HB2	1:A:572:TRP:HZ3	1.53	0.73
2:B:883:LEU:O	2:B:884:ARG:HB2	1.86	0.73
6:H:80:ARG:HG2	9:K:57:LEU:HD22	1.69	0.73
8:J:8:PHE:CD1	8:J:49:MET:SD	2.82	0.73
11:T:6:DG:H1'	11:T:7:DA:C5	2.24	0.73
2:B:25:ILE:HG23	2:B:29:ASP:HB2	1.70	0.73
1:A:567:LYS:HB2	6:H:96:VAL:HB	1.69	0.73
1:A:1162:VAL:HG11	7:I:41:PRO:HG3	1.71	0.73
1:A:1420:ASP:HB3	1:A:1422:ARG:HG2	1.71	0.73
1:A:254:GLU:OE2	2:B:918:ILE:HD12	1.89	0.73
12:N:6:DT:C2'	12:N:7:DA:OP2	2.31	0.73
2:B:470:LYS:HB3	2:B:471:LYS:HA	1.71	0.72
1:A:1063:MET:SD	1:A:1436:ILE:HG13	2.28	0.72
2:B:714:GLU:CG	2:B:715:ALA:HB3	2.19	0.72
1:A:399:HIS:CD2	1:A:400:PRO:HB3	2.24	0.72
1:A:901:LEU:HD22	1:A:919:ILE:HG23	1.68	0.72
2:B:789:MET:HE2	2:B:965:LYS:HB3	1.72	0.72
1:A:164:ARG:HG2	1:A:165:GLY:H	1.54	0.72
2:B:801:LYS:O	8:J:52:THR:HG23	1.89	0.72
1:A:963:ILE:HD12	1:A:1049:ILE:HG13	1.71	0.72
1:A:469:ARG:NH2	2:B:991:GLY:O	2.23	0.72
11:T:5:DC:H1'	11:T:6:DG:C5'	2.20	0.72
1:A:849:MET:HB3	1:A:1063:MET:HE3	1.71	0.72
1:A:403:LYS:CB	1:A:404:TYR:HD1	2.01	0.71
2:B:213:ILE:O	2:B:215:GLN:NE2	2.23	0.71
2:B:244:LEU:HD12	2:B:244:LEU:H	1.55	0.71
4:E:169:ARG:HG2	4:E:169:ARG:HH11	1.55	0.71
1:A:606:LEU:HD23	1:A:614:PHE:CE2	2.25	0.71
1:A:330:LYS:O	1:A:334:GLY:HA3	1.90	0.71
1:A:853:ASP:OD1	1:A:855:THR:HB	1.90	0.71
4:E:169:ARG:HG2	4:E:169:ARG:NH1	2.04	0.71
2:B:460:ALA:HB1	2:B:466:TRP:CE3	2.25	0.71
2:B:642:ASP:HA	2:B:649:LYS:HA	1.73	0.71
2:B:1117:GLN:NE2	2:B:1199:ALA:HB2	2.06	0.71
2:B:899:ILE:HG21	2:B:949:VAL:HG21	1.72	0.71
2:B:487:THR:HG22	2:B:490:SER:H	1.55	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:38:LEU:HD12	6:H:125:LEU:HD21	1.72	0.71
10:L:47:ARG:HB3	10:L:54:ARG:CB	2.21	0.71
1:A:316:GLN:HE21	1:A:319:GLY:CA	2.03	0.70
1:A:317:LYS:CA	1:A:318:SER:CB	2.66	0.70
2:B:711:GLU:C	2:B:713:ALA:HA	2.12	0.70
1:A:152:VAL:CG1	1:A:153:PRO:HD2	2.22	0.70
1:A:316:GLN:CB	1:A:317:LYS:CA	2.66	0.70
1:A:981:LEU:HD23	1:A:981:LEU:H	1.55	0.70
11:T:5:DC:C5	11:T:6:DG:C5	2.80	0.70
1:A:57:ARG:CG	1:A:68:GLN:HB3	2.21	0.70
2:B:980:PHE:CE2	2:B:1094:ARG:HG3	2.26	0.70
3:C:45:ALA:HB3	3:C:170:TRP:NE1	2.07	0.70
1:A:84:ILE:CD1	1:A:270:LEU:HG	2.21	0.70
4:E:79:TRP:HB2	4:E:105:PHE:HD2	1.54	0.70
1:A:1329:THR:HB	1:A:1331:SER:H	1.56	0.69
1:A:114:LEU:HD13	1:A:145:LYS:CB	2.22	0.69
11:T:3:DA:N6	12:N:11:DG:C6	2.60	0.69
2:B:269:ILE:HD11	2:B:386:LEU:HD21	1.74	0.69
6:H:5:LEU:HB2	6:H:59:ILE:O	1.92	0.69
1:A:310:GLY:C	1:A:312:PRO:HD3	2.11	0.69
1:A:57:ARG:HG2	1:A:68:GLN:HB3	1.72	0.69
3:C:45:ALA:HB3	3:C:170:TRP:CD1	2.26	0.69
11:T:15:DA:C5	11:T:16:DC:C4	2.81	0.69
1:A:50:ILE:HG23	1:A:51:GLY:N	2.07	0.69
1:A:249:SER:HA	1:A:250:ILE:HB	1.72	0.69
1:A:875:ALA:HB2	1:A:1366:ARG:HD2	1.74	0.69
1:A:885:THR:CG2	1:A:943:LEU:CD1	2.68	0.69
11:T:10:DA:C2	11:T:11:DG:C2	2.81	0.69
1:A:1356:ILE:HG22	1:A:1361:SER:HB2	1.74	0.69
1:A:668:ASP:HB3	1:A:743:VAL:HG23	1.75	0.69
1:A:1111:MET:HG3	1:A:1114:PRO:HG3	1.74	0.69
2:B:378:LEU:O	2:B:382:ILE:HG12	1.92	0.69
12:N:7:DA:H2''	12:N:8:DT:H71	1.72	0.69
11:T:17:DG:H2''	11:T:18:DA:O5'	1.93	0.69
11:T:2:DT:H2''	11:T:3:DA:OP2	1.92	0.69
1:A:1277:GLU:O	1:A:1278:ASN:HB2	1.93	0.69
1:A:30:ILE:HG12	2:B:1170:THR:HG21	1.75	0.69
8:J:8:PHE:CE1	8:J:49:MET:SD	2.86	0.69
11:T:10:DA:H2''	11:T:11:DG:C8	2.28	0.69
11:T:10:DA:H1'	11:T:11:DG:N9	2.08	0.69
2:B:287:ARG:NH1	2:B:324:ILE:O	2.26	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:111:THR:HG22	7:I:113:ASP:H	1.56	0.68
1:A:919:ILE:CG2	1:A:920:LEU:N	2.56	0.68
11:T:5:DC:H1'	11:T:6:DG:H5'	1.75	0.68
8:J:3:VAL:HG21	8:J:18:TRP:HB2	1.75	0.68
1:A:112:LYS:HG2	1:A:113:LEU:N	2.06	0.68
1:A:399:HIS:CD2	1:A:400:PRO:CB	2.77	0.68
1:A:57:ARG:CA	1:A:68:GLN:HG2	2.23	0.68
1:A:779:PHE:CE2	1:A:785:PRO:HD3	2.29	0.68
1:A:901:LEU:HB2	1:A:926:GLN:HG2	1.75	0.68
1:A:343:LYS:HD2	2:B:1151:LEU:HA	1.76	0.68
2:B:824:ILE:HG12	8:J:48:ARG:HH22	1.59	0.68
11:T:6:DG:H2''	11:T:7:DA:N7	2.08	0.68
1:A:1345:ARG:HD2	1:A:1373:ASP:OD1	1.93	0.68
2:B:855:PHE:CZ	2:B:857:ARG:NH1	2.60	0.68
10:L:31:CYS:CB	10:L:34:CYS:SG	2.81	0.68
2:B:784:ASN:HD21	2:B:788:ARG:HD2	1.57	0.68
9:K:41:THR:HG22	9:K:42:LEU:N	2.07	0.68
2:B:475:SER:O	2:B:476:ARG:HB2	1.94	0.68
1:A:780:VAL:HG23	1:A:789:LYS:HE2	1.76	0.68
2:B:710:LEU:O	2:B:711:GLU:CB	2.41	0.68
12:N:2:DT:C2	12:N:3:DG:C6	2.81	0.68
2:B:1084:GLN:HE22	3:C:191:TYR:HA	1.58	0.67
2:B:1031:LEU:HD13	2:B:1055:ILE:HD13	1.76	0.67
3:C:69:LEU:HB2	8:J:5:VAL:HG11	1.76	0.67
11:T:10:DA:C2	11:T:11:DG:N3	2.62	0.67
1:A:129:LYS:HA	1:A:134:ARG:HH21	1.59	0.67
2:B:428:ILE:HD11	2:B:448:ILE:HA	1.76	0.67
2:B:33:VAL:HG21	2:B:638:PHE:CZ	2.30	0.67
3:C:66:ARG:NH2	8:J:3:VAL:O	2.27	0.67
1:A:550:LEU:HG	1:A:556:TRP:CE2	2.30	0.67
2:B:955:THR:OG1	10:L:55:ILE:HA	1.93	0.67
11:T:3:DA:C2	12:N:13:DA:N1	2.63	0.67
1:A:1134:ILE:O	1:A:1138:ILE:HG12	1.95	0.67
3:C:38:ILE:HG13	3:C:176:ILE:HD12	1.76	0.67
11:T:16:DC:C2'	11:T:17:DG:H5''	2.21	0.67
1:A:38:PRO:HD3	1:A:270:LEU:HD22	1.77	0.67
3:C:11:ARG:HH21	3:C:229:TYR:HD2	1.43	0.67
6:H:93:TYR:CG	6:H:145:ARG:HD3	2.30	0.67
1:A:351:THR:HG21	1:A:466:SER:O	1.95	0.67
2:B:356:LEU:HA	2:B:360:PHE:HB3	1.76	0.66
8:J:48:ARG:HD2	8:J:48:ARG:C	2.15	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:PHE:CE2	1:A:317:LYS:HD3	2.30	0.66
1:A:899:VAL:CB	1:A:929:LEU:HD13	2.25	0.66
2:B:648:HIS:CD2	2:B:711:GLU:CG	2.78	0.66
4:E:135:PHE:HD2	4:E:140:LEU:HD21	1.60	0.66
6:H:116:TYR:HB2	6:H:123:MET:HB3	1.77	0.66
11:T:6:DG:C1'	11:T:7:DA:N7	2.57	0.66
1:A:693:VAL:HG21	1:A:721:PHE:HE2	1.61	0.66
1:A:981:LEU:HD12	1:A:986:ILE:CD1	2.23	0.66
1:A:38:PRO:HG2	1:A:39:GLU:CD	2.15	0.66
2:B:1181:GLU:HG2	2:B:1188:LYS:HG3	1.78	0.66
3:C:142:VAL:H	8:J:16:ASP:HB3	1.60	0.66
10:L:47:ARG:H	10:L:47:ARG:CD	2.07	0.66
1:A:71:GLN:O	1:A:72:GLU:HB2	1.95	0.66
6:H:136:LYS:O	6:H:137:GLN:CG	2.44	0.66
1:A:343:LYS:O	1:A:345:VAL:HG13	1.96	0.65
7:I:78:CYS:O	7:I:79:HIS:HB2	1.97	0.65
1:A:215:SER:HB3	1:A:218:ASP:HB2	1.78	0.65
1:A:67:CYS:O	1:A:70:CYS:SG	2.54	0.65
2:B:784:ASN:ND2	2:B:788:ARG:CD	2.60	0.65
2:B:1084:GLN:HE22	3:C:192:TRP:H	1.41	0.65
3:C:57:VAL:HG12	3:C:58:LEU:HD23	1.79	0.65
1:A:378:GLU:OE1	1:A:434:ARG:HD3	1.96	0.65
1:A:392:VAL:CG1	1:A:415:LEU:HD11	2.25	0.65
2:B:976:ILE:O	2:B:1099:VAL:HG21	1.97	0.65
2:B:465:ASN:HD22	2:B:465:ASN:N	1.94	0.65
1:A:1174:PHE:O	1:A:1176:LEU:HB2	1.96	0.65
2:B:806:THR:HG22	2:B:808:ALA:H	1.61	0.65
1:A:563:PRO:CB	1:A:572:TRP:CZ2	2.79	0.64
11:T:15:DA:H2''	11:T:16:DC:H5'	1.79	0.64
2:B:460:ALA:HB1	2:B:466:TRP:CZ3	2.32	0.64
1:A:114:LEU:HD13	1:A:145:LYS:HB3	1.80	0.64
1:A:67:CYS:SG	1:A:68:GLN:CD	2.76	0.64
4:E:117:THR:O	4:E:120:ALA:N	2.31	0.64
7:I:34:TYR:HE1	7:I:36:GLU:HB3	1.63	0.64
8:J:6:ARG:HG2	8:J:11:GLY:O	1.96	0.64
12:N:9:DC:C2	12:N:10:DG:C6	2.85	0.64
12:N:13:DA:H2''	12:N:14:DG:C8	2.32	0.64
2:B:711:GLU:CB	2:B:713:ALA:CA	2.68	0.64
2:B:969:ARG:NH1	3:C:61:GLU:OE1	2.31	0.64
1:A:572:TRP:HH2	6:H:79:TRP:CZ3	2.15	0.64
6:H:93:TYR:CD2	6:H:145:ARG:HD3	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:42:LYS:HG3	8:J:43:ARG:H	1.63	0.64
1:A:145:LYS:HG3	1:A:146:MET:H	1.63	0.64
1:A:888:GLY:O	1:A:940:ARG:NH2	2.31	0.64
2:B:797:TYR:HB3	2:B:798:TYR:CD1	2.32	0.64
2:B:857:ARG:HD3	2:B:859:TYR:CZ	2.32	0.64
1:A:783:THR:HG21	1:A:796:SER:O	1.97	0.64
2:B:711:GLU:HB3	2:B:713:ALA:CB	2.28	0.64
11:T:6:DG:C1'	11:T:7:DA:C8	2.80	0.64
2:B:955:THR:HG23	2:B:956:THR:N	2.13	0.64
1:A:44:THR:O	1:A:45:GLN:HG3	1.98	0.64
6:H:91:ASP:O	6:H:93:TYR:CD1	2.51	0.64
10:L:38:LEU:HD21	10:L:49:LYS:HD2	1.80	0.64
11:T:12:DC:OP2	11:T:12:DC:H3'	1.97	0.64
5:F:110:ASP:O	5:F:111:LEU:HB2	1.97	0.63
1:A:761:MET:HG3	2:B:1021:MET:HG2	1.80	0.63
2:B:62:ILE:HG23	2:B:418:LYS:HG2	1.80	0.63
2:B:784:ASN:HD21	2:B:788:ARG:CD	2.11	0.63
7:I:74:GLU:HB3	7:I:81:ARG:NE	2.13	0.63
11:T:6:DG:O3'	11:T:7:DA:C8	2.51	0.63
2:B:301:ILE:HG21	2:B:314:LEU:HD11	1.81	0.63
1:A:134:ARG:NH1	1:A:220:THR:O	2.31	0.63
1:A:316:GLN:NE2	1:A:319:GLY:HA2	2.14	0.63
2:B:884:ARG:HB2	2:B:936:ASP:H	1.62	0.63
10:L:47:ARG:H	10:L:47:ARG:HD2	1.64	0.63
11:T:3:DA:H2''	11:T:4:DC:H5'	1.80	0.63
11:T:7:DA:C2'	11:T:8:DT:C6	2.80	0.63
1:A:341:MET:HE1	1:A:1425:SER:HB3	1.81	0.63
1:A:41:MET:O	1:A:42:ASP:HB3	1.99	0.63
1:A:629:LEU:HD13	1:A:645:LEU:HD21	1.78	0.63
1:A:977:LYS:HG3	1:A:978:PRO:HD2	1.81	0.63
2:B:33:VAL:HG21	2:B:638:PHE:HZ	1.64	0.63
4:E:79:TRP:HB2	4:E:105:PHE:CD2	2.32	0.63
6:H:137:GLN:CG	6:H:138:GLU:HA	2.29	0.63
1:A:420:ARG:O	1:A:424:ILE:HG13	1.99	0.63
2:B:1051:THR:HG22	2:B:1053:GLU:H	1.62	0.63
2:B:708:GLU:O	2:B:712:PRO:CB	2.45	0.63
8:J:3:VAL:HG21	8:J:18:TRP:CB	2.28	0.63
10:L:27:LEU:O	10:L:39:SER:HA	1.98	0.63
4:E:54:GLN:HG2	4:E:57:MET:HE3	1.81	0.63
7:I:109:ILE:HG21	7:I:120:GLN:HG3	1.79	0.63
10:L:40:LEU:HD11	10:L:49:LYS:HE3	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1176:LEU:N	1:A:1176:LEU:HD12	2.13	0.63
11:T:1:DC:H2'	11:T:2:DT:C6	2.34	0.63
11:T:9:DA:H61	12:N:6:DT:H3	0.79	0.63
1:A:269:ILE:HD11	1:A:300:VAL:HA	1.80	0.63
2:B:1032:SER:HB3	2:B:1089:PRO:HB2	1.81	0.63
8:J:49:MET:HA	8:J:49:MET:HE2	1.81	0.63
11:T:7:DA:C2'	11:T:8:DT:H5'	2.28	0.63
1:A:42:ASP:HA	1:A:50:ILE:HB	1.81	0.62
1:A:563:PRO:CB	1:A:572:TRP:CE2	2.81	0.62
1:A:600:PRO:HA	6:H:25:ARG:NH1	2.13	0.62
2:B:710:LEU:C	2:B:711:GLU:HG2	2.18	0.62
1:A:79:GLY:O	1:A:243:PRO:HG3	1.99	0.62
1:A:472:LEU:O	1:A:475:THR:HB	1.99	0.62
2:B:416:LEU:HD12	2:B:466:TRP:CE2	2.33	0.62
6:H:38:LEU:HD23	6:H:38:LEU:C	2.19	0.62
1:A:42:ASP:OD1	1:A:43:GLU:N	2.31	0.62
1:A:870:GLU:HB2	4:E:204:THR:HG21	1.81	0.62
2:B:714:GLU:HA	2:B:715:ALA:HB2	0.65	0.62
4:E:20:LYS:NZ	4:E:34:GLU:O	2.32	0.62
6:H:91:ASP:O	6:H:93:TYR:HD1	1.83	0.62
10:L:29:TYR:HD1	10:L:58:LYS:HA	1.65	0.62
3:C:167:HIS:HD2	3:C:169:LYS:H	1.46	0.62
6:H:47:PHE:HB3	6:H:95:TYR:CD2	2.35	0.62
1:A:354:SER:HA	1:A:482:PHE:CD1	2.35	0.62
2:B:977:GLY:HA3	2:B:1099:VAL:CG2	2.30	0.62
1:A:1400:CYS:O	1:A:1405:THR:HG22	2.00	0.61
1:A:57:ARG:CB	1:A:68:GLN:CG	2.55	0.61
8:J:28:ASP:N	8:J:28:ASP:OD1	2.32	0.61
2:B:987:LYS:NZ	13:R:9:G:OP1	2.27	0.61
11:T:6:DG:N3	11:T:7:DA:C6	2.68	0.61
1:A:283:GLY:O	1:A:285:PRO:HD3	2.00	0.61
1:A:316:GLN:CB	1:A:318:SER:CA	2.65	0.61
11:T:6:DG:O3'	11:T:7:DA:H8	1.83	0.61
2:B:1048:THR:OG1	2:B:1050:ILE:HD12	1.99	0.61
5:F:97:ARG:NH1	5:F:100:GLN:OE1	2.33	0.61
1:A:317:LYS:HA	1:A:318:SER:CB	2.31	0.61
1:A:650:GLN:O	1:A:654:ASN:HB2	2.00	0.61
1:A:244:PRO:O	1:A:247:ARG:N	2.29	0.61
3:C:114:TYR:CG	3:C:140:ASN:HB2	2.35	0.61
1:A:981:LEU:CD1	1:A:986:ILE:HD11	2.28	0.61
2:B:1163:CYS:HA	2:B:1191:ILE:HD12	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:CYS:HA	2:B:1174:LYS:HD3	1.83	0.61
4:E:169:ARG:HH11	4:E:169:ARG:CG	2.14	0.61
10:L:55:ILE:HG23	10:L:55:ILE:O	2.01	0.61
11:T:6:DG:C2'	11:T:7:DA:C8	2.84	0.61
1:A:381:THR:HG23	1:A:383:TYR:H	1.66	0.61
1:A:466:SER:HB2	2:B:1099:VAL:HG11	1.82	0.61
1:A:981:LEU:HD12	1:A:986:ILE:CG1	2.30	0.61
2:B:114:PRO:HG2	2:B:181:LEU:HD11	1.81	0.60
1:A:563:PRO:HB3	1:A:572:TRP:CH2	2.36	0.60
2:B:435:THR:O	2:B:435:THR:HG22	2.00	0.60
1:A:479:ASN:ND2	16:T:101:G2P:O3'	2.34	0.60
1:A:114:LEU:HD12	1:A:142:CYS:SG	2.41	0.60
5:F:119:ARG:HG3	5:F:119:ARG:HH11	1.67	0.60
7:I:34:TYR:CE1	7:I:36:GLU:HB3	2.36	0.60
10:L:28:LYS:HA	10:L:39:SER:HA	1.82	0.60
1:A:147:VAL:O	1:A:148:CYS:C	2.39	0.60
2:B:724:ASP:HB3	2:B:727:LYS:HG3	1.84	0.60
1:A:912:LEU:HD22	1:A:1036:ARG:HH21	1.61	0.60
1:A:38:PRO:CG	1:A:39:GLU:OE1	2.44	0.60
1:A:901:LEU:HD22	1:A:919:ILE:CG2	2.32	0.60
2:B:470:LYS:CB	2:B:471:LYS:HA	2.29	0.60
11:T:6:DG:N2	11:T:7:DA:C2	2.70	0.60
6:H:47:PHE:HZ	6:H:146:ARG:HG3	1.65	0.60
1:A:869:GLY:O	4:E:204:THR:HG21	2.02	0.60
1:A:980:ASP:H	1:A:981:LEU:HD23	1.65	0.60
10:L:47:ARG:HB2	10:L:54:ARG:HA	1.83	0.60
11:T:18:DA:C2'	11:T:19:1CC:OP2	2.37	0.60
1:A:768:GLN:HG2	1:A:816:HIS:HA	1.82	0.60
1:A:963:ILE:HD13	1:A:1048:ASN:HB3	1.83	0.60
2:B:470:LYS:HB3	2:B:471:LYS:CA	2.32	0.60
2:B:884:ARG:O	2:B:936:ASP:HB3	2.02	0.60
6:H:91:ASP:OD1	6:H:92:ASP:N	2.35	0.60
11:T:6:DG:H2''	11:T:7:DA:C8	2.37	0.60
2:B:244:LEU:HD12	2:B:244:LEU:N	2.17	0.59
2:B:911:ILE:CD1	2:B:941:LEU:HD23	2.31	0.59
1:A:406:ILE:HD13	1:A:431:LYS:CB	2.32	0.59
1:A:470:LEU:HD21	1:A:487:MET:HE3	1.84	0.59
2:B:284:ILE:HG21	2:B:333:PHE:HD2	1.66	0.59
2:B:487:THR:O	2:B:490:SER:HB3	2.02	0.59
2:B:65:GLU:HG3	2:B:246:LYS:NZ	2.17	0.59
9:K:41:THR:CG2	9:K:42:LEU:N	2.65	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:ILE:CD1	1:A:431:LYS:HB2	2.32	0.59
2:B:1164:GLY:HA3	2:B:1190:ASP:HB3	1.83	0.59
1:A:265:LYS:CE	1:A:302:THR:HG23	2.23	0.59
1:A:355:GLY:CA	1:A:482:PHE:CZ	2.85	0.59
1:A:185:TRP:HZ3	1:A:200:ARG:HG2	1.68	0.59
6:H:130:ARG:HG2	6:H:130:ARG:NH1	2.15	0.59
11:T:10:DA:N3	11:T:11:DG:N3	2.51	0.59
1:A:920:LEU:HD23	1:A:921:GLY:H	1.66	0.59
1:A:977:LYS:HE3	1:A:977:LYS:HA	1.84	0.59
2:B:1220:ARG:O	2:B:1221:SER:HB2	2.01	0.59
5:F:119:ARG:CG	5:F:119:ARG:HH11	2.16	0.59
2:B:1162:ILE:HG22	2:B:1163:CYS:H	1.67	0.59
1:A:1155:ASP:O	1:A:1241:ARG:NH1	2.35	0.59
1:A:606:LEU:HG	1:A:613:ILE:HB	1.84	0.59
2:B:977:GLY:HA3	2:B:1099:VAL:HG21	1.84	0.59
2:B:977:GLY:C	2:B:1099:VAL:HG23	2.23	0.59
2:B:287:ARG:HG2	2:B:292:ILE:HA	1.84	0.59
1:A:247:ARG:N	1:A:248:PRO:HD3	2.18	0.59
2:B:714:GLU:CA	2:B:715:ALA:HB3	2.25	0.59
2:B:30:SER:OG	2:B:743:ILE:O	2.21	0.59
12:N:11:DG:H2"	12:N:12:DT:C7	2.33	0.59
2:B:1084:GLN:NE2	3:C:191:TYR:HA	2.17	0.59
2:B:737:THR:HG23	2:B:737:THR:O	2.03	0.59
3:C:45:ALA:HA	3:C:72:LEU:HD12	1.84	0.59
1:A:565:ILE:O	1:A:570:PRO:HA	2.03	0.58
1:A:979:SER:HB2	1:A:981:LEU:CD2	2.30	0.58
2:B:696:GLU:O	2:B:699:GLU:HB2	2.03	0.58
2:B:778:MET:HE1	2:B:1094:ARG:CD	2.33	0.58
1:A:251:SER:CB	1:A:252:PHE:HB3	2.22	0.58
2:B:108:VAL:HG12	2:B:109:THR:N	2.16	0.58
12:N:11:DG:H2"	12:N:12:DT:C5	2.38	0.58
1:A:1011:GLN:NE2	1:A:1015:VAL:HG21	2.17	0.58
9:K:49:GLU:HG3	9:K:94:ILE:HG12	1.84	0.58
1:A:244:PRO:O	1:A:248:PRO:HD3	2.03	0.58
1:A:316:GLN:CG	1:A:319:GLY:O	2.51	0.58
2:B:570:VAL:HB	2:B:573:GLN:HG2	1.84	0.58
10:L:47:ARG:HG2	10:L:48:CYS:N	2.12	0.58
1:A:323:LYS:HE2	1:A:328:ARG:NE	2.12	0.58
8:J:49:MET:HA	8:J:49:MET:CE	2.33	0.58
10:L:32:ALA:HB2	10:L:55:ILE:HG23	1.85	0.58
1:A:259:GLU:HB3	1:A:264:PHE:CZ	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:H:139:ASN:O	6:H:140:ALA:HB2	2.03	0.58
6:H:4:THR:HG22	6:H:5:LEU:N	2.18	0.58
7:I:113:ASP:OD2	7:I:116:ASN:ND2	2.37	0.58
1:A:316:GLN:HG2	1:A:319:GLY:CA	2.34	0.58
1:A:920:LEU:HD23	1:A:921:GLY:N	2.18	0.58
2:B:778:MET:HE1	2:B:1094:ARG:HH11	1.68	0.58
3:C:183:TRP:CZ2	3:C:207:CYS:HB3	2.39	0.58
1:A:316:GLN:HB3	1:A:319:GLY:C	2.24	0.58
1:A:45:GLN:O	1:A:45:GLN:HG3	2.02	0.58
1:A:946:VAL:HG22	4:E:201:LYS:HD3	1.86	0.58
11:T:3:DA:N6	12:N:11:DG:C5	2.72	0.58
1:A:606:LEU:HD23	1:A:614:PHE:HE2	1.68	0.58
1:A:709:THR:HG23	1:A:712:GLU:CB	2.33	0.58
2:B:1187:ASN:ND2	2:B:1190:ASP:CB	2.61	0.58
1:A:1444:MET:HB2	5:F:133:VAL:HG12	1.84	0.58
1:A:164:ARG:CG	1:A:165:GLY:H	2.16	0.57
9:K:42:LEU:CD1	9:K:46:ILE:HG13	2.34	0.57
11:T:1:DC:H2''	11:T:2:DT:O4'	2.04	0.57
8:J:48:ARG:HE	8:J:49:MET:HG2	1.69	0.57
2:B:824:ILE:HG12	8:J:48:ARG:NH2	2.19	0.57
1:A:588:LEU:HD23	1:A:632:VAL:HG21	1.86	0.57
2:B:106:ASP:OD1	2:B:107:GLY:N	2.36	0.57
3:C:66:ARG:HB3	8:J:5:VAL:CG2	2.34	0.57
10:L:30:ILE:HG22	10:L:36:SER:O	2.04	0.57
1:A:44:THR:O	1:A:45:GLN:C	2.42	0.57
2:B:1051:THR:HG22	2:B:1053:GLU:N	2.19	0.57
3:C:162:GLY:HA3	3:C:170:TRP:CD2	2.39	0.57
12:N:3:DG:H1'	12:N:4:DC:H5''	1.86	0.57
2:B:857:ARG:HB2	2:B:857:ARG:HH11	1.69	0.57
2:B:864:LYS:HB3	2:B:872:GLU:H	1.69	0.57
4:E:9:ILE:HD11	4:E:53:PRO:HD3	1.87	0.57
8:J:2:ILE:O	8:J:3:VAL:O	2.23	0.57
1:A:316:GLN:CG	1:A:319:GLY:CA	2.82	0.57
2:B:475:SER:O	2:B:476:ARG:CB	2.52	0.57
2:B:58:THR:O	2:B:62:ILE:HG12	2.04	0.57
3:C:77:ILE:HD12	3:C:161:LYS:HG3	1.86	0.57
1:A:251:SER:HB2	1:A:252:PHE:CA	2.35	0.57
2:B:280:ILE:HB	2:B:285:ILE:HD11	1.87	0.57
3:C:69:LEU:CB	8:J:5:VAL:HG11	2.35	0.57
1:A:152:VAL:HG12	1:A:153:PRO:HD2	1.86	0.57
1:A:173:THR:HB	1:A:184:SER:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:ASP:O	1:A:299:HIS:ND1	2.34	0.57
2:B:712:PRO:N	2:B:713:ALA:HA	2.16	0.57
3:C:148:ARG:HG2	3:C:149:LYS:H	1.70	0.57
6:H:130:ARG:HH11	6:H:130:ARG:CG	2.14	0.57
1:A:378:GLU:HG2	1:A:388:LEU:HD11	1.86	0.57
1:A:981:LEU:HD22	1:A:1038:THR:C	2.25	0.57
1:A:353:ILE:HD13	1:A:487:MET:HE3	1.87	0.56
2:B:31:TRP:HA	2:B:34:ILE:HD12	1.87	0.56
2:B:799:PRO:HB2	2:B:818:PRO:HG2	1.87	0.56
11:T:5:DC:N4	12:N:10:DG:H1	2.03	0.56
11:T:6:DG:C2	11:T:7:DA:N1	2.74	0.56
1:A:840:ARG:HG2	1:A:1402:PHE:HZ	1.70	0.56
6:H:103:LYS:HB3	6:H:115:TYR:HD2	1.69	0.56
10:L:47:ARG:CB	10:L:54:ARG:HB3	2.26	0.56
11:T:10:DA:C4	11:T:11:DG:C4	2.93	0.56
1:A:1038:THR:O	1:A:1042:PHE:HB3	2.05	0.56
1:A:1441:PHE:CZ	5:F:89:GLU:HA	2.40	0.56
2:B:102:VAL:HG22	2:B:112:LEU:HD22	1.87	0.56
2:B:711:GLU:CA	2:B:713:ALA:HA	2.35	0.56
2:B:205:ILE:HG13	2:B:461:LEU:HB3	1.87	0.56
2:B:258:LEU:HB2	2:B:385:LEU:HD21	1.86	0.56
4:E:157:SER:N	4:E:160:GLU:OE1	2.30	0.56
10:L:32:ALA:CB	10:L:55:ILE:HG23	2.35	0.56
11:T:3:DA:H2'	11:T:4:DC:O4'	2.05	0.56
1:A:1209:MET:SD	1:A:1236:LEU:HB3	2.45	0.56
1:A:152:VAL:HG13	1:A:153:PRO:HD2	1.87	0.56
11:T:8:DT:OP2	11:T:8:DT:H3'	2.05	0.56
1:A:32:VAL:HG21	1:A:57:ARG:O	2.06	0.56
1:A:980:ASP:N	1:A:981:LEU:HD23	2.21	0.56
2:B:373:ARG:HA	2:B:566:LEU:HD23	1.86	0.56
2:B:370:PHE:HD2	2:B:373:ARG:HG3	1.71	0.56
2:B:847:ASP:OD2	9:K:6:ARG:NH2	2.35	0.56
3:C:177:GLU:HB2	3:C:231:ASN:HB3	1.87	0.56
11:T:10:DA:C1'	11:T:11:DG:C8	2.87	0.56
1:A:563:PRO:HB3	1:A:572:TRP:CD2	2.38	0.56
2:B:762:ASN:ND2	2:B:1022:THR:HA	2.20	0.56
2:B:246:LYS:HG3	2:B:246:LYS:O	2.05	0.56
11:T:8:DT:C1'	11:T:9:DA:C8	2.80	0.56
1:A:1312:ASN:O	1:A:1316:VAL:HG23	2.06	0.56
1:A:302:THR:HA	1:A:305:ASP:O	2.06	0.56
11:T:12:DC:C1'	11:T:13:DA:C1'	2.81	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:679:ILE:HG23	1:A:729:ALA:HB1	1.88	0.55
2:B:844:SER:HB2	2:B:996:ARG:H	1.69	0.55
2:B:979:LYS:HE3	2:B:987:LYS:HG3	1.86	0.55
1:A:546:VAL:HG13	1:A:577:ILE:HG21	1.87	0.55
1:A:885:THR:HG21	1:A:943:LEU:HD12	1.84	0.55
11:T:5:DC:H42	12:N:10:DG:H1	1.55	0.55
11:T:6:DG:C2'	11:T:7:DA:N7	2.68	0.55
2:B:95:ILE:HD12	2:B:130:VAL:HG22	1.87	0.55
3:C:251:LEU:O	3:C:255:VAL:HG23	2.05	0.55
3:C:66:ARG:CA	8:J:5:VAL:HG21	2.33	0.55
1:A:795:GLU:HG2	1:A:796:SER:N	2.21	0.55
2:B:129:PHE:CE1	2:B:166:PHE:HB2	2.42	0.55
2:B:883:LEU:HD22	2:B:884:ARG:H	1.72	0.55
6:H:40:LEU:HD13	6:H:123:MET:HG3	1.89	0.55
7:I:47:GLU:HG2	7:I:50:THR:HG23	1.87	0.55
2:B:640:VAL:HG22	2:B:651:LEU:CD2	2.37	0.55
4:E:46:TYR:CD1	4:E:58:MET:HG3	2.42	0.55
1:A:1118:VAL:HB	1:A:1306:LEU:HB2	1.87	0.55
1:A:406:ILE:CD1	1:A:431:LYS:CB	2.85	0.55
1:A:497:THR:HG21	2:B:1149:GLU:OE2	2.07	0.55
2:B:1162:ILE:O	2:B:1191:ILE:HG13	2.06	0.55
2:B:469:GLN:HG3	2:B:469:GLN:O	2.05	0.55
6:H:38:LEU:CD1	6:H:125:LEU:HD21	2.37	0.55
11:T:13:DA:C5'	11:T:14:DG:OP2	2.48	0.55
2:B:486:TYR:CZ	2:B:1096:ARG:HB3	2.42	0.55
2:B:363:HIS:O	2:B:364:ILE:HB	2.07	0.55
2:B:756:ILE:HG12	2:B:770:GLN:HG2	1.89	0.55
1:A:447:GLN:NE2	11:T:21:DC:H4'	2.21	0.55
1:A:1161:THR:HG22	1:A:1163:ILE:N	2.15	0.55
1:A:1323:ASP:OD1	1:A:1325:THR:HG22	2.07	0.55
2:B:62:ILE:HD12	2:B:418:LYS:HG3	1.89	0.55
1:A:241:VAL:HG13	1:A:266:LEU:HD13	1.89	0.55
1:A:53:LEU:HD23	1:A:53:LEU:C	2.27	0.55
1:A:981:LEU:CD2	1:A:1038:THR:HA	2.37	0.55
5:F:123:LYS:NZ	5:F:127:GLU:OE2	2.39	0.55
1:A:949:ASP:N	1:A:949:ASP:OD1	2.40	0.55
3:C:7:GLN:HB2	3:C:23:SER:HB2	1.89	0.55
5:F:97:ARG:HE	5:F:124:GLU:CD	2.10	0.55
1:A:783:THR:HG22	1:A:787:PHE:CD2	2.43	0.54
9:K:45:LEU:HG	9:K:94:ILE:HD13	1.88	0.54
10:L:48:CYS:SG	10:L:49:LYS:N	2.80	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:GLN:HG2	1:A:549:MET:HE3	1.89	0.54
2:B:977:GLY:C	2:B:1099:VAL:CG2	2.76	0.54
11:T:3:DA:C2'	11:T:4:DC:O4'	2.56	0.54
1:A:1116:LEU:HD22	1:A:1311:VAL:HG22	1.88	0.54
1:A:899:VAL:CG1	1:A:929:LEU:HD13	2.37	0.54
2:B:345:LYS:HG2	2:B:348:ARG:HH12	1.73	0.54
3:C:22:LEU:HD22	3:C:25:VAL:HG21	1.88	0.54
1:A:436:ILE:HD11	1:A:491:VAL:HG11	1.88	0.54
2:B:955:THR:CG2	2:B:956:THR:O	2.55	0.54
11:T:5:DC:N4	12:N:10:DG:N1	2.56	0.54
1:A:145:LYS:HG3	1:A:146:MET:N	2.22	0.54
2:B:1002:THR:HG22	2:B:1006:ILE:N	2.22	0.54
4:E:179:GLN:O	4:E:182:ASP:HB2	2.08	0.54
2:B:714:GLU:CB	2:B:715:ALA:HB3	2.37	0.54
6:H:89:LEU:HD23	6:H:92:ASP:H	1.72	0.54
8:J:8:PHE:HD1	8:J:49:MET:SD	2.28	0.54
2:B:792:MET:HE1	11:T:25:DC:P	2.48	0.54
1:A:167:CYS:SG	1:A:169:ASN:OD1	2.66	0.54
2:B:1002:THR:HG23	2:B:1004:GLU:N	2.16	0.54
2:B:1084:GLN:NE2	3:C:192:TRP:H	2.04	0.54
2:B:590:HIS:HD2	2:B:596:LEU:HD22	1.72	0.54
1:A:1342:GLU:HG3	4:E:198:ILE:HD13	1.89	0.54
2:B:519:TRP:CZ2	2:B:705:MET:HE1	2.43	0.54
3:C:60:ASP:HB3	10:L:67:PHE:CE2	2.43	0.54
2:B:1095:LEU:C	2:B:1097:HIS:H	2.12	0.54
2:B:325:GLN:OE1	7:I:12:ASN:ND2	2.39	0.54
2:B:549:THR:HG21	2:B:610:ASN:HD22	1.73	0.54
3:C:120:ILE:HG21	3:C:124:LEU:HD21	1.90	0.54
6:H:44:VAL:HG13	6:H:48:PRO:HA	1.90	0.54
6:H:36:CYS:SG	6:H:130:ARG:NH2	2.82	0.53
11:T:12:DC:N4	12:N:3:DG:O6	2.41	0.53
11:T:9:DA:H2'	11:T:10:DA:C8	2.43	0.53
1:A:765:VAL:HG22	1:A:800:VAL:HB	1.88	0.53
1:A:981:LEU:N	1:A:981:LEU:CD2	2.64	0.53
5:F:111:LEU:O	5:F:112:GLU:CG	2.51	0.53
1:A:401:GLY:C	1:A:435:HIS:CD2	2.82	0.53
1:A:492:PRO:HB2	1:A:497:THR:HG23	1.89	0.53
1:A:90:VAL:HB	1:A:297:GLN:NE2	2.24	0.53
10:L:47:ARG:HD2	10:L:47:ARG:N	2.24	0.53
1:A:1376:THR:HG23	4:E:212:ARG:HH22	1.71	0.53
4:E:15:ALA:O	4:E:19:VAL:HG23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:38:LEU:CD1	10:L:40:LEU:CD1	2.85	0.53
1:A:404:TYR:CD1	1:A:404:TYR:N	2.76	0.53
1:A:839:ARG:HH11	1:A:839:ARG:CG	2.14	0.53
2:B:247:GLY:HA3	2:B:418:LYS:HE3	1.90	0.53
6:H:58:THR:HG21	6:H:93:TYR:CZ	2.44	0.53
6:H:81:PRO:HB2	6:H:82:PRO:HD2	1.90	0.53
1:A:45:GLN:O	1:A:45:GLN:CG	2.52	0.53
10:L:38:LEU:CD1	10:L:40:LEU:HD11	2.38	0.53
11:T:11:DG:OP2	11:T:11:DG:H8	1.90	0.53
1:A:1349:TYR:HB2	1:A:1372:VAL:HG21	1.91	0.53
1:A:599:SER:O	1:A:601:LYS:N	2.41	0.53
2:B:714:GLU:HG3	2:B:715:ALA:HB3	1.91	0.53
11:T:15:DA:N7	11:T:16:DC:C5	2.77	0.53
1:A:1142:THR:O	1:A:1145:SER:OG	2.26	0.53
1:A:114:LEU:HB3	1:A:145:LYS:HG2	1.91	0.53
1:A:335:ARG:NH1	2:B:1206:GLU:OE1	2.41	0.53
1:A:463:ILE:HB	1:A:464:PRO:HD2	1.91	0.53
2:B:983:ARG:NH1	2:B:1091:TYR:HB3	2.24	0.53
2:B:778:MET:CE	2:B:1094:ARG:HD2	2.38	0.53
3:C:75:MET:O	3:C:246:ARG:NH2	2.42	0.53
7:I:117:LYS:HE2	7:I:117:LYS:O	2.08	0.53
8:J:30:LEU:HD22	8:J:34:THR:HG21	1.91	0.53
11:T:11:DG:C2	11:T:12:DC:N4	2.77	0.53
1:A:526:ASP:HB2	2:B:835:GLN:CD	2.30	0.53
2:B:1095:LEU:O	2:B:1097:HIS:N	2.41	0.53
2:B:541:LEU:HB2	2:B:747:MET:HE3	1.90	0.53
2:B:998:ASP:OD1	3:C:35:ARG:NH2	2.41	0.53
1:A:1038:THR:O	1:A:1042:PHE:CB	2.57	0.53
1:A:252:PHE:CD1	1:A:252:PHE:N	2.76	0.53
2:B:468:GLU:C	2:B:470:LYS:H	2.13	0.53
3:C:164:ALA:HB2	3:C:171:GLY:HA2	1.90	0.53
1:A:903:ASN:HD22	1:A:904:THR:H	1.57	0.52
2:B:842:ASN:ND2	2:B:845:SER:OG	2.42	0.52
7:I:103:CYS:HB3	7:I:108:HIS:H	1.73	0.52
1:A:1015:VAL:HG12	1:A:1019:CYS:SG	2.49	0.52
1:A:311:GLN:N	1:A:312:PRO:HD3	2.23	0.52
1:A:317:LYS:CB	1:A:318:SER:CB	2.58	0.52
1:A:39:GLU:HA	1:A:40:THR:CB	2.14	0.52
1:A:1324:PRO:HB2	4:E:142:VAL:HG11	1.90	0.52
6:H:58:THR:CG2	6:H:93:TYR:CE2	2.92	0.52
1:A:353:ILE:HG22	1:A:468:PHE:HB2	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:503:GLN:OE1	5:F:90:ARG:NH2	2.42	0.52
1:A:351:THR:HG23	2:B:1103:ILE:HG12	1.90	0.52
2:B:1179:GLN:O	2:B:1180:PHE:CD1	2.62	0.52
2:B:465:ASN:CG	2:B:477:ALA:HB2	2.29	0.52
3:C:76:ASP:OD2	3:C:128:ASN:N	2.35	0.52
4:E:100:ILE:HG23	4:E:105:PHE:HB2	1.90	0.52
4:E:55:ARG:HD2	4:E:83:CYS:O	2.10	0.52
7:I:116:ASN:OD1	7:I:116:ASN:N	2.41	0.52
1:A:594:GLY:O	1:A:596:THR:CG2	2.58	0.52
2:B:1081:LEU:O	3:C:189:THR:HG23	2.09	0.52
1:A:569:LYS:HG2	1:A:570:PRO:HD2	1.92	0.52
1:A:24:PRO:HD2	1:A:233:TRP:CD1	2.45	0.52
2:B:714:GLU:CB	2:B:715:ALA:CB	2.87	0.52
6:H:115:TYR:CE1	6:H:124:ARG:HG3	2.45	0.52
11:T:5:DC:H1'	11:T:6:DG:H5''	1.89	0.52
1:A:466:SER:HB2	2:B:1099:VAL:CG1	2.40	0.52
1:A:540:PHE:HB3	1:A:571:LEU:HB3	1.92	0.52
2:B:1002:THR:HG22	2:B:1006:ILE:H	1.74	0.52
4:E:156:LEU:HD11	4:E:195:VAL:HB	1.91	0.52
1:A:1130:GLN:O	1:A:1134:ILE:HD12	2.10	0.52
1:A:351:THR:HG22	1:A:352:VAL:N	2.25	0.52
2:B:710:LEU:C	2:B:711:GLU:CG	2.76	0.52
3:C:114:TYR:CD2	3:C:140:ASN:HB2	2.45	0.52
10:L:54:ARG:O	10:L:55:ILE:HB	2.10	0.52
1:A:1206:ASP:O	1:A:1274:ARG:NH1	2.43	0.52
1:A:1224:LEU:CD2	1:A:1240:CYS:HB3	2.37	0.52
1:A:114:LEU:HD11	1:A:171:GLN:OE1	2.10	0.52
2:B:1165:ILE:HB	2:B:1185:CYS:SG	2.50	0.52
2:B:293:PRO:HG2	2:B:296:GLU:HB3	1.92	0.52
12:N:9:DC:C2	12:N:10:DG:O6	2.63	0.52
12:N:3:DG:H2''	12:N:4:DC:C5'	2.24	0.52
2:B:661:LEU:HD11	2:B:684:LEU:HD11	1.91	0.52
1:A:1132:LYS:HG3	1:A:1135:ARG:NH1	2.21	0.51
1:A:1176:LEU:N	1:A:1176:LEU:CD1	2.73	0.51
1:A:250:ILE:CG1	1:A:251:SER:N	2.73	0.51
1:A:534:LEU:O	1:A:574:GLY:HA3	2.10	0.51
1:A:919:ILE:HG22	1:A:920:LEU:N	2.26	0.51
2:B:345:LYS:HG2	2:B:348:ARG:NH1	2.24	0.51
2:B:712:PRO:N	2:B:713:ALA:CA	2.73	0.51
6:H:129:TYR:CE1	6:H:130:ARG:NH1	2.77	0.51
6:H:47:PHE:HB3	6:H:95:TYR:HD2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:HD2	1:A:400:PRO:CA	2.07	0.51
1:A:50:ILE:HG23	1:A:52:GLY:H	1.74	0.51
2:B:487:THR:H	2:B:490:SER:HB3	1.75	0.51
2:B:487:THR:HG22	2:B:490:SER:N	2.22	0.51
5:F:77:ASP:N	5:F:77:ASP:OD1	2.43	0.51
6:H:93:TYR:HA	6:H:145:ARG:HG3	1.91	0.51
11:T:3:DA:H2''	11:T:4:DC:C5'	2.39	0.51
1:A:1004:ASN:ND2	4:E:167:ARG:HD2	2.26	0.51
1:A:65:LEU:HA	1:A:73:GLY:HA2	1.93	0.51
1:A:185:TRP:HE3	1:A:199:LEU:HB2	1.74	0.51
1:A:219:PHE:HB3	1:A:224:PHE:HB2	1.93	0.51
1:A:500:GLU:O	1:A:504:LEU:HB2	2.11	0.51
1:A:50:ILE:CG2	1:A:51:GLY:H	2.18	0.51
1:A:828:ALA:O	1:A:831:THR:CG2	2.51	0.51
2:B:1002:THR:CG2	2:B:1006:ILE:HB	2.41	0.51
2:B:1162:ILE:HG22	2:B:1163:CYS:N	2.24	0.51
1:A:35:ILE:CG2	1:A:52:GLY:O	2.52	0.51
6:H:97:MET:HB2	6:H:118:PHE:CD2	2.46	0.51
7:I:32:CYS:SG	7:I:33:SER:N	2.78	0.51
1:A:482:PHE:HB2	2:B:838:SER:HB3	1.91	0.51
1:A:966:ASN:O	1:A:970:THR:HG22	2.10	0.51
3:C:17:ASN:HD22	3:C:231:ASN:HD21	1.58	0.51
11:T:10:DA:N3	11:T:11:DG:C4	2.79	0.51
1:A:1383:SER:O	1:A:1388:GLY:HA3	2.10	0.51
1:A:785:PRO:HB2	2:B:703:ILE:HD12	1.93	0.51
2:B:1159:ARG:HE	2:B:1193:GLN:NE2	2.08	0.51
2:B:48:LEU:HD23	2:B:173:MET:SD	2.50	0.51
2:B:840:ILE:HG12	2:B:992:ILE:HG22	1.93	0.51
2:B:104:GLU:CD	10:L:54:ARG:NH1	2.64	0.51
11:T:7:DA:H8	11:T:7:DA:OP2	1.93	0.51
1:A:871:ASP:OD1	1:A:1366:ARG:NH2	2.43	0.51
1:A:51:GLY:HA2	1:A:55:ASP:HB2	1.93	0.51
2:B:637:LEU:HD12	2:B:693:ILE:HG13	1.93	0.51
2:B:955:THR:HG22	2:B:963:PHE:HE1	1.75	0.51
3:C:3:GLU:HB3	9:K:104:ASN:OD1	2.11	0.51
11:T:7:DA:OP2	11:T:8:DT:H73	2.09	0.51
1:A:1345:ARG:HG2	1:A:1372:VAL:CG1	2.40	0.51
2:B:1135:ARG:NH2	2:B:1136:ASP:OD1	2.44	0.51
2:B:247:GLY:CA	2:B:418:LYS:HE3	2.39	0.51
2:B:651:LEU:HG	2:B:710:LEU:HD12	1.93	0.51
8:J:64:ASN:N	8:J:65:PRO:HD2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:CB	6:H:96:VAL:HB	2.39	0.51
1:A:697:ALA:HA	1:A:702:LEU:HB2	1.93	0.51
1:A:1409:LEU:HD13	2:B:1207:LEU:HD21	1.92	0.51
6:H:103:LYS:HB3	6:H:115:TYR:CD2	2.46	0.51
1:A:1072:ILE:HD11	1:A:1368:MET:HA	1.92	0.50
1:A:746:MET:SD	2:B:1015:HIS:HD2	2.33	0.50
2:B:117:ALA:HA	2:B:122:LEU:HB2	1.93	0.50
2:B:784:ASN:O	2:B:784:ASN:ND2	2.44	0.50
6:H:127:GLY:HA3	6:H:130:ARG:CZ	2.41	0.50
6:H:36:CYS:HB2	6:H:130:ARG:NH2	2.25	0.50
9:K:91:CYS:O	9:K:95:ILE:HG13	2.11	0.50
12:N:4:DC:H2"	12:N:5:DT:H72	1.93	0.50
1:A:145:LYS:CG	1:A:146:MET:H	2.24	0.50
1:A:78:PRO:O	2:B:1205:GLN:NE2	2.43	0.50
2:B:100:PRO:HD2	2:B:180:TYR:CE2	2.46	0.50
2:B:912:ILE:HD11	2:B:966:VAL:HG23	1.93	0.50
6:H:128:ASN:OD1	6:H:129:TYR:N	2.44	0.50
1:A:407:ARG:HG2	1:A:430:TRP:CZ2	2.47	0.50
1:A:67:CYS:CB	1:A:70:CYS:SG	2.92	0.50
1:A:1223:ASP:O	1:A:1224:LEU:HB2	2.12	0.50
1:A:114:LEU:HB2	1:A:142:CYS:SG	2.52	0.50
1:A:494:SER:H	1:A:497:THR:CG2	2.24	0.50
2:B:550:ASP:OD1	2:B:551:PRO:HD2	2.12	0.50
3:C:44:LEU:HD12	3:C:160:LYS:C	2.32	0.50
6:H:130:ARG:CG	6:H:130:ARG:NH1	2.73	0.50
1:A:896:ARG:HD2	1:A:897:TYR:CE2	2.46	0.50
2:B:977:GLY:CA	2:B:1099:VAL:CG2	2.90	0.50
2:B:859:TYR:OH	2:B:941:LEU:HD22	2.11	0.50
10:L:47:ARG:NH1	10:L:54:ARG:HE	2.10	0.50
1:A:251:SER:CB	1:A:252:PHE:CA	2.89	0.50
2:B:361:LEU:HD21	2:B:377:PHE:CD2	2.47	0.50
1:A:778:GLY:HA3	2:B:516:ASN:HB2	1.92	0.50
3:C:69:LEU:CB	8:J:5:VAL:CG1	2.89	0.50
6:H:58:THR:HG23	6:H:143:LEU:HB2	1.92	0.50
3:C:145:CYS:SG	3:C:146:LYS:N	2.85	0.50
6:H:84:ALA:HA	6:H:87:ARG:HB2	1.92	0.50
2:B:637:LEU:HA	2:B:743:ILE:HG12	1.93	0.50
6:H:104:PHE:CE2	6:H:114:VAL:HG23	2.47	0.50
3:C:235:VAL:HG21	8:J:6:ARG:HH21	1.77	0.50
1:A:49:LYS:HD2	1:A:49:LYS:N	2.27	0.50
1:A:839:ARG:NH1	1:A:839:ARG:CG	2.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:899:ILE:HG13	2:B:911:ILE:HG23	1.94	0.50
3:C:185:LYS:HG2	3:C:213:PRO:HG3	1.94	0.50
7:I:73:ARG:O	7:I:83:ASN:ND2	2.44	0.50
8:J:13:VAL:HG13	8:J:13:VAL:O	2.12	0.50
10:L:29:TYR:CD1	10:L:58:LYS:HA	2.46	0.50
1:A:185:TRP:HB2	1:A:199:LEU:HD13	1.93	0.49
1:A:249:SER:HA	1:A:250:ILE:CB	2.36	0.49
1:A:746:MET:SD	2:B:1015:HIS:CD2	3.05	0.49
1:A:899:VAL:CG1	1:A:929:LEU:CD1	2.90	0.49
2:B:532:ALA:HB1	2:B:536:VAL:HG23	1.93	0.49
2:B:796:LEU:O	2:B:799:PRO:HD3	2.12	0.49
3:C:181:ASP:CG	3:C:186:LEU:HD13	2.32	0.49
3:C:46:ILE:HA	3:C:159:ALA:HA	1.94	0.49
1:A:38:PRO:HA	1:A:270:LEU:HD13	1.94	0.49
1:A:645:LEU:HD11	1:A:649:ILE:HD11	1.94	0.49
2:B:834:ASN:HB3	2:B:840:ILE:HG13	1.94	0.49
4:E:55:ARG:HH11	4:E:55:ARG:HG3	1.77	0.49
1:A:1169:ILE:HD12	1:A:1169:ILE:H	1.76	0.49
1:A:40:THR:HG23	1:A:41:MET:N	2.27	0.49
1:A:594:GLY:O	1:A:596:THR:HG23	2.12	0.49
1:A:605:MET:HG3	1:A:606:LEU:N	2.26	0.49
1:A:508:PRO:O	1:A:511:ILE:HG13	2.13	0.49
1:A:855:THR:CG2	1:A:857:ARG:HE	2.26	0.49
2:B:710:LEU:O	2:B:711:GLU:HB2	2.13	0.49
3:C:15:LYS:O	3:C:240:VAL:HG22	2.12	0.49
7:I:74:GLU:O	7:I:74:GLU:HG3	2.12	0.49
12:N:12:DT:H2"	12:N:13:DA:OP2	2.12	0.49
11:T:10:DA:H1'	11:T:11:DG:C1'	2.43	0.49
1:A:316:GLN:HG2	1:A:319:GLY:C	2.30	0.49
2:B:65:GLU:HG3	2:B:246:LYS:HZ3	1.78	0.49
2:B:251:ILE:O	2:B:251:ILE:HG23	2.12	0.49
2:B:651:LEU:HG	2:B:710:LEU:CD1	2.43	0.49
6:H:58:THR:HG21	6:H:93:TYR:CE2	2.47	0.49
1:A:606:LEU:HD11	1:A:608:ILE:HG12	1.95	0.49
1:A:64:ASN:O	1:A:66:LYS:N	2.38	0.49
1:A:339:ASN:HB3	2:B:1117:GLN:HE22	1.77	0.49
1:A:842:VAL:HG11	2:B:1136:ASP:OD2	2.12	0.49
2:B:732:SER:HB2	2:B:734:HIS:CE1	2.47	0.49
6:H:80:ARG:HG2	9:K:57:LEU:CD2	2.40	0.49
1:A:1017:LEU:HB2	4:E:205:SER:C	2.33	0.49
1:A:32:VAL:CG2	1:A:57:ARG:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:LEU:HD11	2:B:460:ALA:CB	2.42	0.49
2:B:64:CYS:O	2:B:65:GLU:HB3	2.13	0.49
2:B:899:ILE:HG22	2:B:900:ALA:N	2.28	0.49
4:E:161:LYS:HD2	4:E:195:VAL:HG23	1.95	0.49
11:T:5:DC:C5	11:T:6:DG:C6	3.00	0.49
2:B:169:ARG:N	2:B:454:THR:HG23	2.24	0.49
2:B:65:GLU:HG3	2:B:246:LYS:CE	2.43	0.49
2:B:776:GLN:HG2	2:B:1096:ARG:HD3	1.95	0.49
1:A:357:PRO:HD2	2:B:833:TYR:CZ	2.47	0.49
1:A:1438:THR:HG23	2:B:1142:GLY:O	2.13	0.49
1:A:372:LYS:HA	1:A:435:HIS:CE1	2.47	0.49
1:A:912:LEU:HD11	1:A:1033:GLN:HG3	1.95	0.49
2:B:287:ARG:NH1	2:B:321:GLY:O	2.46	0.49
2:B:275:TYR:HE1	2:B:355:ILE:HG12	1.78	0.49
3:C:167:HIS:HD2	3:C:169:LYS:N	2.10	0.49
1:A:1325:THR:OG1	4:E:146:HIS:O	2.31	0.49
6:H:26:ILE:HG22	6:H:40:LEU:HB3	1.93	0.49
7:I:109:ILE:HG22	7:I:120:GLN:HG3	1.92	0.49
11:T:5:DC:N4	12:N:10:DG:C6	2.81	0.49
12:N:12:DT:HI'	12:N:13:DA:C8	2.48	0.49
1:A:1116:LEU:HD13	1:A:1329:THR:HG23	1.95	0.49
1:A:57:ARG:CB	1:A:68:GLN:CB	2.67	0.49
1:A:770:VAL:HA	1:A:822:GLU:OE2	2.13	0.49
2:B:247:GLY:HA3	2:B:418:LYS:CE	2.42	0.49
2:B:358:LYS:HA	2:B:366:GLN:HG2	1.94	0.49
2:B:882:THR:O	2:B:882:THR:HG22	2.13	0.49
2:B:884:ARG:HG3	2:B:935:ARG:CG	2.32	0.49
2:B:896:ASP:OD2	10:L:29:TYR:OH	2.29	0.49
2:B:859:TYR:N	2:B:966:VAL:O	2.39	0.49
3:C:46:ILE:HG23	3:C:157:CYS:HB3	1.95	0.49
8:J:48:ARG:O	8:J:52:THR:HB	2.12	0.49
4:E:46:TYR:CE1	4:E:58:MET:HG2	2.47	0.48
5:F:83:PRO:HA	5:F:146:TRP:CZ3	2.47	0.48
1:A:261:ASP:HB2	1:A:323:LYS:NZ	2.28	0.48
2:B:955:THR:HG22	2:B:963:PHE:CE1	2.48	0.48
3:C:69:LEU:HB2	8:J:5:VAL:CG1	2.43	0.48
4:E:198:ILE:HD11	4:E:212:ARG:HG3	1.95	0.48
7:I:5:ARG:HH21	7:I:36:GLU:CD	2.16	0.48
9:K:42:LEU:HD13	9:K:46:ILE:HG13	1.95	0.48
9:K:7:PHE:HB2	9:K:11:LEU:HD22	1.95	0.48
1:A:1155:ASP:OD1	1:A:1162:VAL:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1215:ARG:HG2	1:A:1273:LEU:HA	1.95	0.48
1:A:169:ASN:ND2	1:A:169:ASN:O	2.46	0.48
1:A:46:THR:CG2	1:A:47:ARG:H	2.00	0.48
1:A:552:TRP:NE1	1:A:655:PHE:CD2	2.81	0.48
1:A:86:LEU:HD13	1:A:90:VAL:HG22	1.94	0.48
2:B:849:GLY:C	8:J:8:PHE:HE2	2.16	0.48
2:B:708:GLU:O	2:B:712:PRO:HG3	2.13	0.48
3:C:133:ILE:HD11	3:C:237:SER:HA	1.94	0.48
3:C:52:GLU:HA	10:L:64:LEU:HD11	1.95	0.48
4:E:136:ASN:OD1	4:E:137:GLU:N	2.46	0.48
11:T:10:DA:C2'	11:T:11:DG:C8	2.94	0.48
1:A:268:ASP:HB3	1:A:299:HIS:CE1	2.49	0.48
1:A:53:LEU:CD2	1:A:54:ASN:HB2	2.41	0.48
1:A:962:ARG:O	1:A:966:ASN:HB2	2.13	0.48
2:B:582:VAL:HG22	2:B:626:ILE:HB	1.94	0.48
2:B:995:ARG:NH1	2:B:997:GLU:OE2	2.46	0.48
1:A:115:LEU:HD22	1:A:119:ASN:HB2	1.94	0.48
1:A:1402:PHE:CG	1:A:1403:GLU:HG2	2.47	0.48
1:A:260:ASP:OD1	1:A:261:ASP:N	2.47	0.48
1:A:310:GLY:CA	1:A:312:PRO:HD3	2.43	0.48
1:A:315:LEU:HA	1:A:320:ARG:HG2	1.95	0.48
11:T:6:DG:N2	12:N:10:DG:H1	2.11	0.48
1:A:406:ILE:CB	1:A:431:LYS:HB2	2.33	0.48
1:A:542:GLU:O	1:A:546:VAL:HG23	2.13	0.48
1:A:715:GLU:OE2	1:A:774:ARG:NH1	2.47	0.48
2:B:1174:LYS:HB3	2:B:1179:GLN:HB2	1.95	0.48
2:B:376:PHE:CE1	2:B:569:TYR:HD2	2.32	0.48
1:A:472:LEU:HD21	2:B:835:GLN:HB2	1.95	0.48
2:B:792:MET:HG3	2:B:855:PHE:HE1	1.79	0.48
11:T:7:DA:H2'	11:T:8:DT:C5	2.45	0.48
2:B:711:GLU:HB3	2:B:713:ALA:HB2	1.96	0.48
4:E:147:HIS:HB3	4:E:150:VAL:HG23	1.95	0.48
4:E:28:TYR:CE2	4:E:78:LEU:HD13	2.49	0.48
5:F:83:PRO:HG2	5:F:84:TYR:HD1	1.78	0.48
10:L:29:TYR:HE1	10:L:58:LYS:CD	2.22	0.48
1:A:1364:ASN:OD1	1:A:1366:ARG:HG2	2.14	0.48
1:A:24:PRO:HB3	1:A:237:THR:HB	1.96	0.48
8:J:8:PHE:HE1	8:J:49:MET:CE	2.27	0.48
9:K:39:ASP:N	9:K:39:ASP:OD1	2.45	0.48
11:T:3:DA:C2	12:N:13:DA:C2	3.01	0.48
1:A:161:LEU:CD2	1:A:161:LEU:N	2.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:HIS:HB3	1:A:167:CYS:SG	2.53	0.48
2:B:1065:GLN:HE21	2:B:1069:PHE:HD2	1.62	0.48
2:B:226:PHE:HA	2:B:395:GLN:HG3	1.95	0.48
6:H:131:ASN:OD1	6:H:132:LEU:HG	2.14	0.48
9:K:33:ILE:HD13	9:K:87:LEU:HD22	1.95	0.48
1:A:1392:SER:O	1:A:1394:THR:N	2.47	0.47
1:A:908:LEU:CD1	1:A:983:ILE:HD11	2.44	0.47
2:B:1173:ALA:HA	2:B:1180:PHE:CD1	2.40	0.47
3:C:136:ASP:OD1	3:C:139:GLY:N	2.47	0.47
1:A:672:ASP:HB3	1:A:675:THR:H	1.79	0.47
2:B:1117:GLN:HE21	2:B:1199:ALA:HB2	1.77	0.47
2:B:203:PHE:HE2	2:B:212:LEU:HD12	1.79	0.47
2:B:364:ILE:HD13	2:B:585:VAL:HG13	1.95	0.47
2:B:65:GLU:OE2	2:B:246:LYS:HE3	2.14	0.47
1:A:1095:THR:HG21	1:A:1112:LYS:HE2	1.96	0.47
1:A:1189:SER:OG	1:A:1190:PRO:HD2	2.14	0.47
1:A:565:ILE:HG22	1:A:569:LYS:O	2.14	0.47
1:A:628:GLY:O	1:A:632:VAL:HG23	2.13	0.47
3:C:214:ASN:HB2	3:C:217:ASP:OD2	2.14	0.47
11:T:15:DA:C8	11:T:16:DC:H5	2.31	0.47
11:T:15:DA:C5	11:T:16:DC:N4	2.83	0.47
1:A:37:PHE:HB2	1:A:52:GLY:HA3	1.96	0.47
2:B:394:ASP:OD1	2:B:394:ASP:N	2.35	0.47
2:B:476:ARG:O	2:B:477:ALA:C	2.51	0.47
2:B:492:LEU:HA	2:B:492:LEU:HD23	1.74	0.47
1:A:845:LEU:CD2	1:A:1374:VAL:HG11	2.45	0.47
2:B:209:GLU:OE1	2:B:788:ARG:NH2	2.47	0.47
2:B:598:GLU:HG3	2:B:598:GLU:O	2.13	0.47
11:T:16:DC:H1'	11:T:17:DG:O4'	2.15	0.47
1:A:1011:GLN:HE22	1:A:1015:VAL:HG21	1.78	0.47
1:A:705:LYS:HB2	1:A:708:MET:HE2	1.96	0.47
2:B:1187:ASN:OD1	2:B:1188:LYS:N	2.47	0.47
2:B:314:LEU:O	2:B:317:CYS:HB2	2.13	0.47
4:E:23:VAL:HG12	4:E:28:TYR:HB2	1.97	0.47
2:B:620:ARG:NH1	7:I:68:LEU:HD21	2.29	0.47
9:K:44:ASN:HA	9:K:47:ARG:HG2	1.97	0.47
1:A:152:VAL:HG12	1:A:153:PRO:CD	2.44	0.47
2:B:408:LEU:HB3	2:B:409:ALA:H	1.58	0.47
2:B:43:LEU:HD11	2:B:811:TYR:O	2.14	0.47
2:B:830:TYR:CE2	2:B:1000:PRO:HD3	2.50	0.47
7:I:32:CYS:O	7:I:33:SER:OG	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:J:8:PHE:HE1	8:J:49:MET:SD	2.38	0.47
1:A:39:GLU:CA	1:A:40:THR:HB	2.27	0.47
1:A:415:LEU:CD2	1:A:415:LEU:N	2.77	0.47
1:A:495:GLU:O	1:A:498:ARG:HG3	2.14	0.47
2:B:195:CYS:HB3	2:B:782:LEU:HD22	1.96	0.47
9:K:12:LEU:HD12	9:K:12:LEU:H	1.79	0.47
13:R:1:A:C2'	13:R:2:U:C5'	2.91	0.47
11:T:10:DA:H1'	11:T:11:DG:O4'	2.15	0.47
1:A:605:MET:SD	1:A:621:THR:HG21	2.55	0.47
3:C:99:LEU:HD23	3:C:99:LEU:N	2.30	0.47
7:I:10:CYS:SG	7:I:32:CYS:HB3	2.55	0.47
2:B:783:THR:HG23	8:J:60:PHE:CD1	2.50	0.47
1:A:1138:ILE:HG22	1:A:1279:ILE:HG21	1.97	0.47
1:A:1397:LEU:HB2	1:A:1426:GLU:OE2	2.15	0.47
2:B:702:LEU:HD21	2:B:735:ALA:HB1	1.97	0.47
5:F:107:VAL:HG11	5:F:111:LEU:HD11	1.96	0.47
1:A:1037:LEU:HD21	1:A:1045:VAL:HG21	1.96	0.47
1:A:399:HIS:NE2	1:A:400:PRO:HB3	2.29	0.47
1:A:492:PRO:CB	1:A:497:THR:HG23	2.44	0.47
2:B:465:ASN:ND2	2:B:465:ASN:N	2.61	0.47
2:B:468:GLU:CG	2:B:469:GLN:H	2.28	0.47
2:B:789:MET:CE	2:B:965:LYS:HB3	2.44	0.47
4:E:153:HIS:O	4:E:154:ILE:HD13	2.15	0.47
1:A:378:GLU:OE2	1:A:387:ARG:NH2	2.44	0.46
1:A:494:SER:O	1:A:497:THR:HG22	2.15	0.46
1:A:569:LYS:HZ1	3:C:221:TYR:HB2	1.80	0.46
1:A:569:LYS:NZ	3:C:221:TYR:HB2	2.30	0.46
1:A:351:THR:CG2	2:B:1103:ILE:HG12	2.45	0.46
2:B:211:VAL:O	2:B:480:SER:HA	2.14	0.46
10:L:31:CYS:SG	10:L:32:ALA:N	2.88	0.46
10:L:37:LYS:O	10:L:39:SER:N	2.47	0.46
11:T:12:DC:O2	11:T:13:DA:H1'	2.15	0.46
1:A:1402:PHE:CD1	1:A:1403:GLU:HG2	2.51	0.46
1:A:596:THR:O	1:A:596:THR:OG1	2.34	0.46
1:A:1431:GLY:HA3	2:B:1197:PRO:HD3	1.98	0.46
2:B:176:SER:O	2:B:182:SER:HB3	2.15	0.46
2:B:808:ALA:O	2:B:812:LEU:HG	2.16	0.46
4:E:19:VAL:O	4:E:23:VAL:HG23	2.15	0.46
1:A:1224:LEU:HD21	1:A:1240:CYS:CB	2.40	0.46
1:A:68:GLN:O	1:A:69:THR:HB	2.16	0.46
1:A:7:SER:HB3	2:B:1193:GLN:OE1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:41:ILE:HD11	3:C:243:VAL:HG13	1.97	0.46
3:C:54:ASN:OD1	3:C:56:THR:HG22	2.15	0.46
7:I:50:THR:HG22	7:I:52:ILE:HG22	1.97	0.46
1:A:250:ILE:CG1	1:A:251:SER:H	2.29	0.46
1:A:285:PRO:HB2	1:A:288:ALA:HB3	1.97	0.46
1:A:938:LYS:HE3	1:A:938:LYS:HB2	1.78	0.46
2:B:834:ASN:O	2:B:1013:ASN:HB2	2.15	0.46
2:B:797:TYR:HB3	2:B:798:TYR:HD1	1.80	0.46
6:H:109:LYS:HA	6:H:109:LYS:HE3	1.98	0.46
11:T:8:DT:O2	11:T:9:DA:C5	2.69	0.46
1:A:402:ALA:CB	1:A:434:ARG:HA	2.46	0.46
1:A:35:ILE:HG23	1:A:53:LEU:HA	1.96	0.46
1:A:845:LEU:HD21	1:A:1374:VAL:HG11	1.97	0.46
2:B:315:LYS:N	2:B:316:PRO:HD2	2.31	0.46
1:A:369:SER:HB3	9:K:2:ASN:OD1	2.15	0.46
11:T:12:DC:H1'	11:T:13:DA:C4	2.44	0.46
1:A:577:ILE:HD12	1:A:578:LEU:N	2.29	0.46
2:B:487:THR:O	2:B:490:SER:N	2.47	0.46
2:B:848:ARG:HD2	8:J:7:CYS:O	2.16	0.46
3:C:167:HIS:CD2	3:C:169:LYS:H	2.31	0.46
8:J:36:LEU:HD11	8:J:51:LEU:HB2	1.98	0.46
10:L:33:GLU:OE2	10:L:53:HIS:CG	2.69	0.46
1:A:1022:LEU:HD11	1:A:1026:LEU:HD12	1.97	0.46
1:A:1035:TYR:HB3	1:A:1037:LEU:HD12	1.97	0.46
1:A:311:GLN:N	1:A:312:PRO:CD	2.79	0.46
1:A:642:CYS:O	1:A:645:LEU:HB3	2.15	0.46
1:A:761:MET:HG3	2:B:1021:MET:CG	2.46	0.46
1:A:4:GLN:HB3	1:A:76:GLU:OE1	2.16	0.46
1:A:848:ILE:HD11	1:A:1374:VAL:HG21	1.97	0.46
1:A:882:SER:HA	1:A:953:ASN:HA	1.97	0.46
2:B:576:ASP:N	2:B:576:ASP:OD1	2.48	0.46
3:C:74:SER:O	3:C:77:ILE:HB	2.16	0.46
5:F:76:LYS:O	5:F:79:ARG:HD3	2.15	0.46
1:A:224:PHE:CZ	1:A:231:PRO:HG3	2.51	0.46
1:A:316:GLN:NE2	1:A:318:SER:OG	2.49	0.46
1:A:35:ILE:HA	1:A:52:GLY:O	2.15	0.46
1:A:396:PRO:HD3	1:A:415:LEU:HB3	1.97	0.46
1:A:399:HIS:NE2	1:A:437:MET:HG2	2.31	0.46
2:B:1110:PRO:HB2	2:B:1119:VAL:HG13	1.98	0.46
5:F:132:LEU:O	5:F:148:VAL:HG23	2.16	0.46
1:A:537:ARG:HD3	6:H:120:GLY:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:78:CYS:O	7:I:79:HIS:CB	2.64	0.46
1:A:337:ARG:HB3	1:A:337:ARG:HH11	1.81	0.46
1:A:375:THR:HG21	1:A:433:GLU:OE1	2.15	0.46
1:A:768:GLN:CG	1:A:816:HIS:HA	2.45	0.46
1:A:908:LEU:HD11	1:A:983:ILE:HD11	1.96	0.46
2:B:1077:THR:CG2	2:B:1079:LYS:H	2.26	0.46
2:B:261:ARG:HD3	2:B:261:ARG:HA	1.82	0.46
8:J:1:MET:N	8:J:56:LEU:HD12	2.30	0.46
1:A:117:GLU:H	1:A:117:GLU:CD	2.19	0.46
1:A:164:ARG:CG	1:A:165:GLY:N	2.79	0.46
1:A:406:ILE:HD13	1:A:431:LYS:HB2	1.93	0.46
1:A:399:HIS:HE1	1:A:462:VAL:HG21	1.78	0.46
1:A:494:SER:O	1:A:498:ARG:HG2	2.15	0.46
1:A:592:ASP:O	1:A:593:GLU:CB	2.49	0.46
1:A:599:SER:C	1:A:601:LYS:N	2.66	0.46
1:A:839:ARG:NH1	1:A:839:ARG:HG2	2.21	0.46
2:B:1034:VAL:HG22	2:B:1059:LEU:HB2	1.98	0.46
4:E:79:TRP:HE1	4:E:81:GLU:HG3	1.81	0.46
5:F:119:ARG:CG	5:F:119:ARG:NH1	2.75	0.46
6:H:128:ASN:O	6:H:131:ASN:ND2	2.48	0.46
7:I:55:THR:HG21	7:I:120:GLN:HB3	1.98	0.46
10:L:42:ARG:H	10:L:42:ARG:HG3	1.43	0.46
10:L:47:ARG:CB	10:L:54:ARG:HA	2.44	0.46
11:T:24:DT:H2'	11:T:25:DC:O4'	2.16	0.46
1:A:363:GLN:O	1:A:458:HIS:ND1	2.48	0.45
1:A:550:LEU:HD21	1:A:561:PRO:HD2	1.98	0.45
2:B:434:ARG:O	2:B:434:ARG:HG2	2.16	0.45
2:B:864:LYS:HD2	2:B:866:TYR:N	2.24	0.45
4:E:116:ILE:CG2	4:E:121:MET:HG3	2.46	0.45
1:A:868:TYR:CZ	1:A:1064:VAL:HG21	2.51	0.45
1:A:1410:PHE:HD1	2:B:1212:ILE:HD11	1.81	0.45
1:A:38:PRO:CA	1:A:270:LEU:HD13	2.47	0.45
1:A:406:ILE:HD13	1:A:431:LYS:HB3	1.96	0.45
2:B:1084:GLN:OE1	2:B:1084:GLN:N	2.49	0.45
2:B:711:GLU:C	2:B:714:GLU:H	2.19	0.45
2:B:900:ALA:O	2:B:902:GLY:N	2.47	0.45
3:C:56:THR:HG23	3:C:58:LEU:N	2.25	0.45
4:E:204:THR:HG22	4:E:205:SER:N	2.31	0.45
1:A:868:TYR:CE1	1:A:1064:VAL:HG21	2.51	0.45
1:A:738:LYS:HB3	6:H:19:ARG:HH22	1.81	0.45
1:A:903:ASN:ND2	1:A:904:THR:H	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:256:VAL:HG11	2:B:382:ILE:HD13	1.98	0.45
1:A:810:PRO:HB2	2:B:705:MET:SD	2.55	0.45
6:H:109:LYS:HA	6:H:109:LYS:CE	2.46	0.45
6:H:10:PHE:HB3	6:H:28:ALA:HB1	1.97	0.45
11:T:6:DG:C4	11:T:7:DA:C6	3.05	0.45
1:A:318:SER:HA	1:A:319:GLY:HA2	1.64	0.45
1:A:765:VAL:HG13	1:A:802:ASN:O	2.16	0.45
1:A:833:GLU:O	1:A:837:ILE:HG12	2.17	0.45
2:B:620:ARG:CZ	7:I:68:LEU:HD21	2.47	0.45
2:B:763:GLN:HG2	2:B:765:PRO:HD2	1.99	0.45
8:J:2:ILE:O	8:J:3:VAL:C	2.55	0.45
1:A:209:ASN:HA	1:A:212:LYS:HB2	1.99	0.45
1:A:550:LEU:HG	1:A:556:TRP:NE1	2.32	0.45
2:B:313:MET:HE3	2:B:386:LEU:HD22	1.97	0.45
2:B:31:TRP:CE3	2:B:34:ILE:HD13	2.52	0.45
3:C:38:ILE:HG13	3:C:176:ILE:CD1	2.45	0.45
8:J:6:ARG:CG	8:J:12:LYS:O	2.64	0.45
4:E:164:LEU:HD13	4:E:211:TYR:CE2	2.51	0.45
8:J:25:LEU:HA	8:J:25:LEU:HD23	1.78	0.45
1:A:1295:THR:OG1	1:A:1297:GLU:OE1	2.31	0.45
1:A:91:PHE:HA	1:A:235:ILE:HG22	1.99	0.45
1:A:399:HIS:HA	1:A:400:PRO:HA	1.68	0.45
1:A:606:LEU:CD2	1:A:614:PHE:CE2	2.99	0.45
2:B:240:ILE:HG21	2:B:381:MET:HE1	1.97	0.45
2:B:436:VAL:O	2:B:436:VAL:HG13	2.17	0.45
2:B:554:ILE:HD11	2:B:609:ILE:HG23	1.98	0.45
3:C:67:LEU:HD23	3:C:144:ILE:HD11	1.99	0.45
4:E:117:THR:O	4:E:119:SER:N	2.50	0.45
4:E:48:ASP:O	4:E:49:SER:C	2.55	0.45
3:C:8:VAL:HG11	9:K:105:PHE:CD1	2.51	0.45
1:A:849:MET:SD	1:A:1061:GLY:HA2	2.56	0.45
1:A:39:GLU:OE1	1:A:39:GLU:N	2.50	0.45
1:A:44:THR:O	1:A:46:THR:N	2.49	0.45
1:A:821:ARG:HG3	1:A:825:ILE:HD11	1.99	0.45
1:A:981:LEU:HD22	1:A:1038:THR:HA	1.98	0.45
4:E:112:TYR:CD1	4:E:116:ILE:HD11	2.52	0.45
4:E:55:ARG:C	4:E:57:MET:H	2.18	0.45
5:F:94:LEU:HD13	5:F:122:MET:HG2	1.98	0.45
9:K:41:THR:HG22	9:K:42:LEU:H	1.80	0.45
11:T:12:DC:N4	12:N:3:DG:C6	2.84	0.45
1:A:404:TYR:HD1	1:A:404:TYR:N	2.14	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:567:LYS:HA	1:A:568:PRO:HA	1.59	0.45
1:A:743:VAL:O	1:A:747:VAL:HG23	2.17	0.45
2:B:824:ILE:HG22	2:B:1008:PRO:HA	1.98	0.45
1:A:483:ASP:HA	2:B:988:GLY:HA2	1.98	0.45
3:C:99:LEU:HB3	3:C:120:ILE:HA	1.99	0.45
4:E:28:TYR:HE1	4:E:76:GLY:O	1.99	0.45
10:L:42:ARG:NH2	10:L:43:THR:OG1	2.50	0.45
11:T:18:DA:H2''	11:T:19:1CC:H2	1.75	0.45
11:T:1:DC:H6	11:T:1:DC:H3'	1.80	0.45
1:A:1301:GLU:HA	1:A:1302:PRO:HD3	1.83	0.45
1:A:261:ASP:HB2	1:A:323:LYS:HZ3	1.81	0.45
1:A:960:ILE:HG12	1:A:1049:ILE:HD11	1.99	0.45
2:B:1001:PHE:CZ	2:B:1073:TYR:HB2	2.52	0.45
2:B:778:MET:CE	2:B:1094:ARG:CD	2.94	0.45
2:B:1110:PRO:HB2	2:B:1119:VAL:CG1	2.46	0.45
2:B:1189:ILE:HD12	2:B:1190:ASP:H	1.81	0.45
2:B:387:LEU:HD22	2:B:387:LEU:HA	1.85	0.45
5:F:130:ILE:HA	5:F:131:PRO:HD3	1.77	0.45
8:J:42:LYS:HG3	8:J:43:ARG:N	2.30	0.45
1:A:1138:ILE:HD11	1:A:1319:VAL:HG11	1.97	0.44
1:A:164:ARG:HG2	1:A:165:GLY:N	2.28	0.44
2:B:275:TYR:CE1	2:B:355:ILE:HG12	2.52	0.44
2:B:714:GLU:CD	2:B:715:ALA:HB3	2.38	0.44
2:B:955:THR:CG2	2:B:956:THR:N	2.73	0.44
11:T:15:DA:C2'	11:T:16:DC:H5'	2.44	0.44
2:B:1174:LYS:HB2	2:B:1174:LYS:HE3	1.73	0.44
1:A:12:ARG:HD3	2:B:1192:TYR:CD1	2.52	0.44
1:A:698:GLN:HA	7:I:97:MET:O	2.18	0.44
3:C:146:LYS:HB2	8:J:57:ILE:HD13	2.00	0.44
1:A:898:ARG:O	1:A:1029:ARG:NH1	2.51	0.44
1:A:298:PHE:O	1:A:302:THR:HG22	2.17	0.44
1:A:329:LEU:HA	1:A:335:ARG:H	1.82	0.44
1:A:38:PRO:HB3	1:A:270:LEU:CG	2.45	0.44
1:A:403:LYS:O	1:A:415:LEU:HD23	2.18	0.44
1:A:446:ARG:HB2	1:A:487:MET:SD	2.57	0.44
1:A:588:LEU:CD2	1:A:632:VAL:HG21	2.46	0.44
1:A:840:ARG:HG2	1:A:1402:PHE:CZ	2.51	0.44
2:B:1006:ILE:CG2	2:B:1087:PHE:HE2	2.30	0.44
2:B:637:LEU:CD1	2:B:693:ILE:HG13	2.47	0.44
6:H:38:LEU:HD21	6:H:40:LEU:HB2	1.99	0.44
6:H:4:THR:O	6:H:5:LEU:HD22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:L:38:LEU:CD1	10:L:49:LYS:HD2	2.43	0.44
1:A:1212:VAL:O	1:A:1216:ILE:HG13	2.18	0.44
1:A:323:LYS:HE3	1:A:328:ARG:HE	1.80	0.44
1:A:599:SER:C	1:A:601:LYS:H	2.21	0.44
2:B:1002:THR:HG21	2:B:1006:ILE:HB	1.98	0.44
2:B:1084:GLN:HE22	3:C:192:TRP:N	2.13	0.44
2:B:522:VAL:HG11	2:B:537:LYS:HD2	1.98	0.44
2:B:710:LEU:C	2:B:712:PRO:HA	2.37	0.44
7:I:118:ARG:HH11	7:I:118:ARG:CG	2.31	0.44
7:I:34:TYR:CD1	7:I:34:TYR:C	2.90	0.44
12:N:4:DC:H2"	12:N:5:DT:OP2	2.18	0.44
1:A:1345:ARG:HG2	1:A:1372:VAL:HG12	2.00	0.44
1:A:793:SER:HB2	1:A:794:PRO:HD2	2.00	0.44
3:C:242:GLN:HB3	3:C:246:ARG:HD2	1.99	0.44
5:F:109:VAL:HG11	5:F:123:LYS:HG2	2.00	0.44
1:A:1345:ARG:HG3	1:A:1376:THR:HG21	1.98	0.44
1:A:1389:PHE:O	1:A:1392:SER:OG	2.34	0.44
1:A:1389:PHE:HZ	1:A:1402:PHE:CE2	2.36	0.44
1:A:388:LEU:HD23	1:A:391:LEU:HD12	1.99	0.44
1:A:402:ALA:HA	1:A:435:HIS:HD2	1.83	0.44
1:A:451:HIS:H	1:A:451:HIS:CD2	2.36	0.44
2:B:1036:ALA:O	8:J:47:ARG:HD3	2.18	0.44
12:N:7:DA:C8	12:N:7:DA:OP2	2.70	0.44
11:T:15:DA:C5	11:T:16:DC:C5	3.05	0.44
1:A:98:LYS:O	1:A:102:VAL:HG23	2.18	0.44
1:A:145:LYS:CG	1:A:146:MET:N	2.81	0.44
1:A:563:PRO:HD3	1:A:572:TRP:CZ2	2.52	0.44
2:B:800:GLN:HB3	8:J:52:THR:HG22	1.99	0.44
13:R:1:A:C2'	13:R:2:U:H5"	2.33	0.44
11:T:7:DA:C8	11:T:7:DA:OP2	2.71	0.44
1:A:1155:ASP:OD2	1:A:1161:THR:HG23	2.18	0.44
1:A:54:ASN:OD1	1:A:247:ARG:NH1	2.49	0.44
1:A:57:ARG:C	1:A:68:GLN:HG2	2.37	0.44
1:A:899:VAL:HG22	1:A:1029:ARG:HG2	2.00	0.44
2:B:1002:THR:HG23	2:B:1004:GLU:HG3	1.99	0.44
1:A:810:PRO:HD3	2:B:1047:PHE:CD1	2.53	0.44
2:B:708:GLU:HG3	2:B:712:PRO:CG	2.48	0.44
2:B:973:ILE:HG22	2:B:974:PRO:HD2	2.00	0.44
3:C:94:LYS:HE2	3:C:94:LYS:HB3	1.90	0.44
6:H:139:ASN:O	6:H:140:ALA:CB	2.66	0.44
11:T:12:DC:H4'	11:T:13:DA:OP1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:485:ASP:N	1:A:485:ASP:OD1	2.49	0.44
2:B:1160:VAL:HG11	2:B:1169:MET:SD	2.57	0.44
2:B:600:LEU:HD22	2:B:615:MET:SD	2.58	0.44
3:C:66:ARG:HB3	8:J:5:VAL:HG22	2.00	0.44
2:B:953:LEU:HD11	10:L:55:ILE:HG13	2.00	0.44
1:A:1109:LYS:HB3	1:A:1109:LYS:HE3	1.76	0.43
1:A:247:ARG:N	1:A:248:PRO:CD	2.81	0.43
1:A:415:LEU:HD22	1:A:415:LEU:N	2.33	0.43
1:A:912:LEU:CD1	1:A:1033:GLN:HG3	2.48	0.43
1:A:919:ILE:HG23	1:A:920:LEU:N	2.26	0.43
1:A:925:LEU:O	1:A:928:LEU:N	2.50	0.43
5:F:72:LYS:HE2	5:F:73:ALA:HA	1.99	0.43
8:J:3:VAL:CG2	8:J:18:TRP:HB2	2.45	0.43
1:A:987:VAL:HG23	1:A:1028:THR:OG1	2.17	0.43
1:A:545:GLN:O	1:A:549:MET:HG3	2.17	0.43
1:A:568:PRO:HD3	6:H:94:ASP:O	2.19	0.43
1:A:582:ILE:HA	1:A:583:PRO:HD3	1.86	0.43
1:A:722:LEU:HD11	1:A:794:PRO:HB3	2.01	0.43
2:B:118:ARG:HA	2:B:207:GLY:HA2	2.01	0.43
10:L:28:LYS:O	10:L:29:TYR:CG	2.71	0.43
1:A:365:GLY:O	1:A:468:PHE:HA	2.19	0.43
1:A:847:ASP:OD2	1:A:858:ASN:HB2	2.17	0.43
2:B:1060:ARG:HA	2:B:1060:ARG:HD2	1.72	0.43
2:B:1187:ASN:HD21	2:B:1190:ASP:CA	2.30	0.43
2:B:248:SER:C	2:B:250:PHE:H	2.22	0.43
2:B:365:THR:HG21	2:B:370:PHE:CD1	2.54	0.43
2:B:464:GLY:CA	2:B:480:SER:OG	2.61	0.43
2:B:563:MET:HA	2:B:589:VAL:O	2.18	0.43
2:B:884:ARG:CB	2:B:936:ASP:H	2.27	0.43
8:J:21:TYR:CZ	8:J:25:LEU:HD11	2.53	0.43
11:T:12:DC:H2"	11:T:13:DA:C8	2.54	0.43
1:A:994:GLN:HG2	1:A:1019:CYS:SG	2.58	0.43
1:A:1436:ILE:HD12	1:A:1436:ILE:N	2.33	0.43
1:A:298:PHE:CE1	1:A:312:PRO:O	2.71	0.43
1:A:317:LYS:HG2	1:A:318:SER:N	2.33	0.43
1:A:518:LYS:HB2	1:A:519:PRO:HD2	2.00	0.43
2:B:188:ASP:O	2:B:192:LEU:HD12	2.18	0.43
2:B:216:GLU:OE1	2:B:500:THR:OG1	2.31	0.43
12:N:3:DG:H2"	12:N:4:DC:OP2	2.17	0.43
1:A:224:PHE:HB3	1:A:229:SER:O	2.18	0.43
1:A:289:ILE:O	1:A:293:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:549:MET:HE1	1:A:656:TRP:HD1	1.82	0.43
2:B:1065:GLN:NE2	2:B:1069:PHE:HD2	2.15	0.43
2:B:487:THR:O	2:B:488:TYR:C	2.55	0.43
2:B:707:PRO:C	2:B:709:ASP:N	2.71	0.43
2:B:848:ARG:NH1	8:J:8:PHE:O	2.50	0.43
6:H:141:TYR:N	6:H:141:TYR:CD1	2.86	0.43
16:T:101:G2P:O4'	13:R:9:G:H2'	2.18	0.43
11:T:12:DC:C1'	11:T:13:DA:C8	2.97	0.43
11:T:14:DG:H2''	11:T:15:DA:OP2	2.19	0.43
1:A:1021:LEU:HD11	1:A:1025:ARG:NH1	2.34	0.43
1:A:1389:PHE:CZ	1:A:1402:PHE:CE2	3.06	0.43
1:A:308:ILE:HD12	1:A:308:ILE:H	1.84	0.43
1:A:397:ASN:HA	1:A:398:GLU:HA	1.46	0.43
2:B:1017:ILE:HA	2:B:1017:ILE:HD13	1.79	0.43
2:B:222:ILE:HD11	2:B:627:PHE:CE1	2.54	0.43
2:B:402:GLY:HA2	2:B:695:ALA:HB3	2.00	0.43
2:B:846:ILE:HA	2:B:850:LEU:HB3	2.01	0.43
3:C:268:ASP:N	3:C:268:ASP:OD1	2.52	0.43
8:J:9:SER:OG	8:J:48:ARG:NH1	2.51	0.43
1:A:317:LYS:HG2	1:A:318:SER:HB3	1.83	0.43
1:A:331:GLY:HA2	1:A:337:ARG:HG3	2.01	0.43
1:A:779:PHE:CE1	2:B:517:THR:HG22	2.53	0.43
1:A:831:THR:HG23	1:A:832:ALA:N	2.34	0.43
1:A:346:ASP:H	2:B:1154:ALA:HB1	1.81	0.43
2:B:851:PHE:O	2:B:974:PRO:HD3	2.18	0.43
3:C:116:LYS:HG3	3:C:117:ASP:N	2.33	0.43
3:C:46:ILE:CG2	3:C:157:CYS:HB3	2.49	0.43
4:E:169:ARG:NH1	5:F:140:ASP:OD2	2.52	0.43
6:H:46:LEU:HD23	6:H:46:LEU:HA	1.76	0.43
6:H:89:LEU:HD22	6:H:91:ASP:H	1.84	0.43
8:J:37:SER:OG	8:J:47:ARG:NH2	2.48	0.43
12:N:2:DT:O2	12:N:3:DG:N1	2.51	0.43
1:A:550:LEU:HD23	1:A:556:TRP:CZ2	2.53	0.43
1:A:896:ARG:HB3	1:A:897:TYR:CD2	2.53	0.43
2:B:1152:MET:HE2	2:B:1197:PRO:HD3	2.01	0.43
2:B:332:ASP:C	2:B:334:ILE:H	2.22	0.43
5:F:83:PRO:HG2	5:F:84:TYR:CD1	2.53	0.43
8:J:6:ARG:HG3	8:J:12:LYS:O	2.19	0.43
1:A:272:ALA:O	1:A:296:LEU:HB2	2.19	0.43
1:A:590:ARG:HH22	1:A:592:ASP:HB2	1.83	0.43
1:A:810:PRO:CB	2:B:705:MET:SD	3.07	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:968:GLN:HB3	1:A:973:ILE:HD11	2.01	0.43
2:B:997:GLU:H	2:B:997:GLU:HG3	1.30	0.43
4:E:116:ILE:HG21	4:E:121:MET:HG3	2.00	0.43
8:J:23:ASN:O	8:J:27:GLU:HB3	2.18	0.43
8:J:8:PHE:CE1	8:J:49:MET:CE	3.02	0.43
11:T:11:DG:OP2	11:T:11:DG:C8	2.71	0.43
1:A:1094:VAL:HA	1:A:1113:THR:HG21	2.00	0.43
1:A:1402:PHE:CD2	1:A:1403:GLU:HG2	2.54	0.43
1:A:310:GLY:C	1:A:312:PRO:CD	2.86	0.43
1:A:407:ARG:HG2	1:A:430:TRP:CH2	2.54	0.43
1:A:598:LEU:HG	6:H:25:ARG:NH1	2.34	0.43
2:B:1095:LEU:C	2:B:1097:HIS:N	2.73	0.43
2:B:190:TYR:CZ	2:B:196:PRO:HG3	2.54	0.43
2:B:512:ARG:NH2	2:B:531:GLN:O	2.49	0.43
2:B:120:ARG:HG2	2:B:955:THR:HG21	2.00	0.43
8:J:1:MET:H1	8:J:56:LEU:HD12	1.84	0.43
8:J:36:LEU:HD13	8:J:47:ARG:CG	2.49	0.43
1:A:251:SER:CB	1:A:252:PHE:HA	2.48	0.42
1:A:963:ILE:HD12	1:A:1049:ILE:CG1	2.44	0.42
2:B:90:ILE:HA	2:B:133:LYS:O	2.18	0.42
2:B:664:THR:HG1	2:B:678:GLU:N	2.17	0.42
1:A:780:VAL:HG22	2:B:699:GLU:OE2	2.18	0.42
2:B:722:ASP:N	2:B:722:ASP:OD1	2.52	0.42
4:E:177:ARG:HD3	4:E:215:MET:SD	2.59	0.42
13:R:4:G:H2'	13:R:5:A:C8	2.54	0.42
11:T:15:DA:N7	11:T:16:DC:N4	2.67	0.42
1:A:1115:SER:HB3	1:A:1330:ASN:ND2	2.34	0.42
1:A:172:PRO:HB3	1:A:185:TRP:CE2	2.54	0.42
1:A:562:THR:HG23	1:A:563:PRO:HD2	2.00	0.42
1:A:995:GLU:HA	1:A:995:GLU:OE2	2.19	0.42
2:B:469:GLN:O	2:B:470:LYS:HG3	2.19	0.42
2:B:711:GLU:O	2:B:714:GLU:N	2.50	0.42
2:B:841:MET:HE3	2:B:990:ILE:HD11	2.01	0.42
4:E:176:PRO:O	4:E:212:ARG:HA	2.20	0.42
4:E:43:LYS:O	4:E:47:CYS:HB2	2.20	0.42
4:E:57:MET:HB2	4:E:57:MET:HE3	1.90	0.42
8:J:16:ASP:OD1	8:J:17:LYS:HG2	2.20	0.42
10:L:31:CYS:HA	10:L:56:LEU:HD23	2.01	0.42
1:A:355:GLY:HA3	1:A:482:PHE:CE2	2.54	0.42
1:A:388:LEU:HA	1:A:388:LEU:HD23	1.78	0.42
2:B:62:ILE:HD12	2:B:418:LYS:CG	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:779:GLY:HA2	2:B:796:LEU:HB2	2.01	0.42
3:C:249:ASP:O	3:C:253:LYS:HB2	2.20	0.42
3:C:66:ARG:HB3	8:J:5:VAL:HG21	2.01	0.42
3:C:9:LYS:HE2	3:C:9:LYS:HB2	1.79	0.42
2:B:783:THR:HG21	8:J:59:LYS:HB3	2.01	0.42
9:K:20:LYS:O	9:K:33:ILE:HA	2.19	0.42
9:K:47:ARG:HG3	9:K:48:ALA:N	2.33	0.42
1:A:316:GLN:CB	1:A:319:GLY:CA	2.77	0.42
1:A:577:ILE:HD12	1:A:578:LEU:H	1.85	0.42
1:A:783:THR:O	2:B:516:ASN:ND2	2.43	0.42
1:A:901:LEU:HD21	1:A:919:ILE:HD13	2.00	0.42
2:B:826:ALA:HB2	2:B:1087:PHE:CD1	2.54	0.42
1:A:1342:GLU:HG2	4:E:212:ARG:HH11	1.84	0.42
1:A:179:LEU:HD22	1:A:297:GLN:HG3	2.02	0.42
1:A:315:LEU:HB2	1:A:316:GLN:H	1.63	0.42
1:A:329:LEU:HD12	1:A:1406:VAL:HG23	2.00	0.42
2:B:1023:VAL:O	2:B:1027:ILE:HG13	2.19	0.42
2:B:402:GLY:CA	2:B:695:ALA:HB3	2.50	0.42
2:B:424:LEU:HD11	2:B:448:ILE:HG23	2.02	0.42
3:C:5:GLY:O	3:C:7:GLN:HG2	2.20	0.42
8:J:36:LEU:HD13	8:J:47:ARG:HG2	2.01	0.42
12:N:12:DT:H2''	12:N:13:DA:H8	1.83	0.42
11:T:5:DC:C1'	11:T:6:DG:C5'	2.78	0.42
1:A:1044:TRP:O	1:A:1047:SER:N	2.53	0.42
1:A:129:LYS:HA	1:A:134:ARG:NH2	2.31	0.42
1:A:590:ARG:HG2	1:A:590:ARG:HH21	1.82	0.42
2:B:244:LEU:O	2:B:246:LYS:N	2.50	0.42
2:B:423:LYS:O	2:B:427:ASP:HB2	2.19	0.42
6:H:16:ASP:HA	6:H:17:PRO:HD2	1.95	0.42
12:N:12:DT:C2	12:N:13:DA:C5	3.08	0.42
11:T:3:DA:O5'	11:T:3:DA:H8	2.03	0.42
1:A:42:ASP:HA	1:A:50:ILE:CB	2.48	0.42
1:A:494:SER:H	1:A:497:THR:HG22	1.85	0.42
1:A:598:LEU:O	1:A:599:SER:C	2.58	0.42
1:A:606:LEU:C	1:A:606:LEU:HD12	2.40	0.42
1:A:1424:VAL:HG11	2:B:1139:ILE:HD13	2.02	0.42
2:B:326:ASP:OD1	2:B:329:THR:OG1	2.24	0.42
2:B:654:ARG:HA	2:B:654:ARG:HD3	1.78	0.42
3:C:45:ALA:CB	3:C:170:TRP:CD1	2.97	0.42
4:E:144:ILE:HG13	4:E:145:THR:N	2.34	0.42
8:J:8:PHE:CE1	8:J:49:MET:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:12:DC:H1'	11:T:13:DA:O4'	2.18	0.42
1:A:1424:VAL:HG22	1:A:1436:ILE:HD11	2.01	0.42
1:A:353:ILE:HD13	1:A:487:MET:CE	2.49	0.42
1:A:356:ASP:C	1:A:358:ASN:H	2.23	0.42
1:A:390:GLN:O	1:A:393:ARG:HB3	2.20	0.42
1:A:406:ILE:CD1	1:A:431:LYS:HB3	2.49	0.42
1:A:879:GLU:OE1	1:A:962:ARG:NH2	2.53	0.42
1:A:902:LEU:HG	1:A:926:GLN:HG3	2.01	0.42
2:B:636:PRO:C	2:B:637:LEU:HG	2.40	0.42
2:B:651:LEU:CD2	2:B:710:LEU:HD11	2.50	0.42
2:B:727:LYS:HD3	2:B:1049:ASP:CG	2.40	0.42
2:B:96:TYR:HB2	2:B:129:PHE:HB2	2.01	0.42
3:C:129:ILE:HD12	3:C:129:ILE:HA	1.79	0.42
6:H:113:ALA:HA	6:H:125:LEU:O	2.20	0.42
1:A:152:VAL:HG12	1:A:153:PRO:N	2.35	0.42
1:A:169:ASN:ND2	1:A:169:ASN:C	2.73	0.42
1:A:475:THR:HG22	1:A:476:SER:N	2.35	0.42
1:A:804:TYR:HE2	2:B:1021:MET:HE2	1.85	0.42
1:A:94:GLY:O	1:A:95:PHE:CD1	2.73	0.42
2:B:295:GLY:H	2:B:298:LEU:HG	1.85	0.42
4:E:35:VAL:C	4:E:37:LEU:H	2.23	0.42
6:H:4:THR:CG2	6:H:5:LEU:N	2.82	0.42
9:K:42:LEU:HD13	9:K:46:ILE:CG1	2.50	0.42
12:N:12:DT:H2"	12:N:13:DA:C8	2.55	0.42
11:T:6:DG:N2	12:N:10:DG:N1	2.68	0.42
1:A:1396:ALA:HA	1:A:1399:ARG:NH2	2.35	0.42
1:A:815:PHE:O	1:A:818:MET:N	2.53	0.42
1:A:87:ALA:HB3	1:A:276:LEU:HD23	2.01	0.42
2:B:102:VAL:HG23	2:B:112:LEU:HB2	2.02	0.42
2:B:263:GLY:O	2:B:265:SER:N	2.52	0.42
2:B:431:TYR:CZ	2:B:447:ALA:HB3	2.55	0.42
2:B:558:LEU:HD13	2:B:580:VAL:HG11	2.01	0.42
2:B:708:GLU:O	2:B:712:PRO:CG	2.68	0.42
2:B:839:MET:HE2	2:B:1010:LEU:HD21	2.01	0.42
2:B:906:SER:HB3	2:B:946:ASN:HB2	2.01	0.42
6:H:61:SER:O	6:H:62:SER:HB3	2.20	0.42
7:I:78:CYS:SG	7:I:80:SER:CB	3.01	0.42
1:A:1341:ILE:HD13	1:A:1380:GLY:HA2	2.01	0.41
2:B:1189:ILE:HD12	2:B:1190:ASP:N	2.34	0.41
6:H:137:GLN:HG3	6:H:138:GLU:HA	2.01	0.41
8:J:14:VAL:HG12	8:J:41:LEU:HD21	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ILE:HG22	1:A:270:LEU:HD11	2.01	0.41
2:B:1006:ILE:HG21	2:B:1087:PHE:HE2	1.85	0.41
2:B:980:PHE:CE2	2:B:1094:ARG:CG	2.98	0.41
3:C:39:ALA:HA	3:C:164:ALA:HB3	2.02	0.41
2:B:1084:GLN:HG2	3:C:201:TRP:CH2	2.55	0.41
3:C:201:TRP:HA	3:C:202:PRO:HD3	1.87	0.41
3:C:41:ILE:HA	3:C:42:PRO:HD3	1.94	0.41
3:C:69:LEU:O	8:J:6:ARG:NH1	2.54	0.41
1:A:250:ILE:HG13	1:A:251:SER:H	1.85	0.41
1:A:481:ASP:OD1	1:A:485:ASP:OD1	2.38	0.41
1:A:533:LYS:HA	1:A:533:LYS:HD2	1.84	0.41
1:A:53:LEU:C	1:A:55:ASP:H	2.23	0.41
1:A:852:TYR:O	5:F:81:THR:HG22	2.20	0.41
2:B:762:ASN:HD22	2:B:762:ASN:HA	1.55	0.41
2:B:857:ARG:O	2:B:967:ARG:HA	2.20	0.41
3:C:123:ASN:OD1	3:C:125:MET:HB3	2.20	0.41
4:E:7:ARG:O	4:E:10:SER:N	2.52	0.41
8:J:44:TYR:HA	8:J:47:ARG:HB3	2.02	0.41
11:T:9:DA:H2'	11:T:10:DA:N7	2.34	0.41
1:A:362:ASP:N	1:A:362:ASP:OD1	2.46	0.41
2:B:174:LEU:HD21	2:B:204:ILE:HD11	2.01	0.41
2:B:28:GLU:C	2:B:30:SER:H	2.23	0.41
2:B:367:LEU:HB3	2:B:368:GLU:H	1.55	0.41
2:B:831:SER:HG	2:B:994:TYR:HE2	1.66	0.41
3:C:27:LEU:HA	3:C:228:PHE:CZ	2.55	0.41
6:H:108:SER:C	6:H:110:ASP:N	2.74	0.41
3:C:69:LEU:HB3	8:J:5:VAL:CG1	2.49	0.41
3:C:52:GLU:HA	10:L:64:LEU:CD1	2.51	0.41
1:A:1399:ARG:NH1	1:A:1408:ILE:HD12	2.36	0.41
1:A:180:LYS:HE3	1:A:294:SER:HB3	2.01	0.41
1:A:294:SER:HA	1:A:297:GLN:HB3	2.01	0.41
1:A:416:ARG:C	1:A:417:TYR:CD1	2.94	0.41
2:B:758:PHE:CE1	2:B:1044:ALA:HA	2.55	0.41
2:B:1081:LEU:HA	2:B:1081:LEU:HD23	1.71	0.41
2:B:96:TYR:N	2:B:129:PHE:O	2.52	0.41
2:B:46:GLN:H	2:B:46:GLN:HG3	1.49	0.41
5:F:101:ILE:HG21	5:F:120:ILE:HD12	2.03	0.41
6:H:89:LEU:HB2	6:H:91:ASP:OD2	2.20	0.41
9:K:39:ASP:HB2	9:K:40:HIS:H	1.76	0.41
9:K:87:LEU:O	9:K:90:ALA:HB3	2.20	0.41
11:T:15:DA:N7	11:T:16:DC:C4	2.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:7:DA:H2''	11:T:8:DT:C5'	2.38	0.41
1:A:1098:VAL:N	1:A:1099:PRO:HD2	2.36	0.41
1:A:1154:TYR:CE1	1:A:1156:PRO:HG3	2.55	0.41
1:A:259:GLU:HA	1:A:259:GLU:OE1	2.18	0.41
1:A:407:ARG:HD3	1:A:413:ILE:HD11	1.99	0.41
1:A:606:LEU:HD11	1:A:608:ILE:CD1	2.49	0.41
1:A:954:TRP:HA	1:A:955:PRO:HD2	1.85	0.41
2:B:707:PRO:C	2:B:709:ASP:H	2.23	0.41
3:C:164:ALA:HA	3:C:167:HIS:O	2.21	0.41
4:E:46:TYR:CE1	4:E:58:MET:CG	3.03	0.41
5:F:109:VAL:O	5:F:111:LEU:HD22	2.20	0.41
7:I:111:THR:HG22	7:I:112:SER:N	2.35	0.41
9:K:12:LEU:N	9:K:12:LEU:HD12	2.34	0.41
2:B:1110:PRO:C	2:B:1111:MET:HG2	2.40	0.41
2:B:217:ARG:HD3	2:B:407:ASP:OD2	2.21	0.41
3:C:44:LEU:HD12	3:C:160:LYS:O	2.21	0.41
3:C:142:VAL:N	8:J:16:ASP:HB3	2.33	0.41
12:N:12:DT:C1'	12:N:13:DA:C8	3.04	0.41
2:B:241:ARG:HA	2:B:253:THR:HG22	2.01	0.41
3:C:227:THR:HG22	3:C:229:TYR:CE1	2.56	0.41
3:C:18:VAL:HG22	3:C:240:VAL:HB	2.03	0.41
6:H:8:ASP:HB3	6:H:10:PHE:CE1	2.56	0.41
6:H:61:SER:O	6:H:62:SER:CB	2.69	0.41
10:L:38:LEU:HD21	10:L:49:LYS:CD	2.48	0.41
11:T:8:DT:P	11:T:8:DT:H3'	2.60	0.41
1:A:1209:MET:SD	1:A:1236:LEU:HD13	2.61	0.41
1:A:298:PHE:HE1	1:A:312:PRO:O	2.03	0.41
1:A:93:VAL:HG22	1:A:301:ALA:HA	2.02	0.41
1:A:320:ARG:HA	1:A:321:PRO:HA	1.73	0.41
1:A:355:GLY:N	1:A:482:PHE:CZ	2.89	0.41
1:A:482:PHE:HD2	2:B:835:GLN:O	2.04	0.41
1:A:563:PRO:HD3	1:A:572:TRP:HZ2	1.85	0.41
2:B:830:TYR:CZ	2:B:1000:PRO:HD3	2.55	0.41
2:B:37:PHE:O	2:B:39:ARG:N	2.53	0.41
2:B:500:THR:HA	2:B:501:PRO:HD3	1.84	0.41
1:A:547:LEU:HB3	9:K:58:PHE:CE1	2.56	0.41
1:A:852:TYR:CE1	1:A:1060:PRO:HB2	2.56	0.41
1:A:855:THR:HG22	1:A:857:ARG:HG2	2.03	0.41
1:A:925:LEU:HA	1:A:925:LEU:HD23	1.89	0.41
2:B:707:PRO:O	2:B:709:ASP:N	2.54	0.41
2:B:996:ARG:NH2	3:C:174:ALA:O	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:109:VAL:HG12	5:F:110:ASP:H	1.85	0.41
10:L:37:LYS:HE2	10:L:37:LYS:HB3	1.91	0.41
1:A:1291:VAL:HA	1:A:1292:PRO:HD3	1.94	0.41
1:A:357:PRO:HG3	2:B:832:GLY:O	2.21	0.41
1:A:452:LYS:HG3	1:A:453:MET:N	2.36	0.41
1:A:444:PHE:CE2	1:A:470:LEU:HD23	2.38	0.41
1:A:43:GLU:CB	1:A:50:ILE:CD1	2.51	0.41
1:A:563:PRO:CG	1:A:572:TRP:CZ2	3.04	0.41
1:A:707:GLY:C	1:A:708:MET:HG3	2.41	0.41
3:C:33:LEU:HG	3:C:37:MET:CE	2.51	0.41
6:H:63:LEU:HA	6:H:90:ALA:CB	2.51	0.41
12:N:2:DT:H1'	12:N:3:DG:C5	2.56	0.41
1:A:1349:TYR:C	1:A:1349:TYR:CD1	2.94	0.40
2:B:973:ILE:CG2	2:B:974:PRO:HD2	2.51	0.40
6:H:6:PHE:CZ	6:H:8:ASP:HB2	2.56	0.40
7:I:65:ASP:HA	7:I:66:PRO:HD3	1.90	0.40
11:T:2:DT:H1'	11:T:3:DA:O5'	2.21	0.40
1:A:102:VAL:C	1:A:104:GLU:H	2.25	0.40
1:A:249:SER:HB2	1:A:250:ILE:CG2	2.49	0.40
1:A:259:GLU:HB3	1:A:264:PHE:CE1	2.56	0.40
1:A:455:MET:HE1	2:B:1130:PHE:CE1	2.56	0.40
1:A:625:SER:HB2	1:A:626:ASN:H	1.76	0.40
3:C:141:GLY:O	3:C:142:VAL:HB	2.20	0.40
6:H:137:GLN:HE21	6:H:137:GLN:HB3	1.61	0.40
7:I:15:TYR:N	7:I:15:TYR:CD1	2.89	0.40
1:A:485:ASP:OD2	13:R:9:G:O2'	2.38	0.40
1:A:779:PHE:CZ	2:B:517:THR:HA	2.56	0.40
1:A:873:MET:HB2	1:A:878:ILE:HD11	2.02	0.40
2:B:123:THR:O	2:B:125:SER:N	2.55	0.40
2:B:599:THR:O	2:B:603:LEU:HG	2.22	0.40
2:B:648:HIS:HB2	2:B:711:GLU:CD	2.42	0.40
1:A:357:PRO:HD2	2:B:833:TYR:CE2	2.55	0.40
2:B:843:GLN:NE2	2:B:843:GLN:O	2.54	0.40
4:E:54:GLN:HB3	4:E:57:MET:HB3	2.03	0.40
5:F:98:ALA:O	5:F:102:SER:HB3	2.22	0.40
6:H:101:ALA:HB2	6:H:116:TYR:CE1	2.57	0.40
7:I:75:CYS:SG	7:I:103:CYS:HB2	2.61	0.40
9:K:61:TYR:HA	9:K:72:LYS:O	2.21	0.40
10:L:47:ARG:CB	10:L:54:ARG:CA	2.99	0.40
12:N:7:DA:H8	12:N:7:DA:OP2	2.04	0.40
11:T:7:DA:O5'	11:T:8:DT:H71	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:T:9:DA:C2'	11:T:10:DA:C8	3.04	0.40
1:A:1153:TYR:CE2	1:A:1163:ILE:HD11	2.56	0.40
1:A:455:MET:HE3	2:B:1134:GLU:HG3	2.03	0.40
1:A:68:GLN:CD	1:A:80:HIS:CD2	2.94	0.40
2:B:745:PRO:HB2	2:B:1047:PHE:CD2	2.57	0.40
2:B:228:LYS:HB3	2:B:228:LYS:HE2	1.90	0.40
3:C:11:ARG:HE	3:C:21:ILE:HD11	1.87	0.40
4:E:14:ARG:NH1	4:E:141:VAL:HG12	2.37	0.40
4:E:20:LYS:HD2	4:E:34:GLU:HG2	2.02	0.40
6:H:91:ASP:C	6:H:93:TYR:HD1	2.24	0.40
6:H:98:TYR:C	6:H:98:TYR:CD1	2.94	0.40
3:C:262:LEU:HD11	9:K:87:LEU:HD23	2.03	0.40
1:A:1143:LEU:O	1:A:1146:VAL:HG23	2.22	0.40
1:A:443:LEU:HD23	1:A:443:LEU:HA	1.84	0.40
1:A:981:LEU:HD22	1:A:1038:THR:CA	2.51	0.40
2:B:426:LYS:HE2	2:B:430:ARG:HH12	1.86	0.40
2:B:213:ILE:N	2:B:479:VAL:O	2.49	0.40
3:C:127:ARG:HB2	3:C:127:ARG:HE	1.73	0.40
3:C:82:TYR:O	3:C:85:ASP:HB2	2.20	0.40
6:H:108:SER:O	6:H:110:ASP:N	2.55	0.40
7:I:75:CYS:HA	7:I:76:PRO:HD3	1.75	0.40
9:K:22:ASP:HA	9:K:23:PRO:HD3	1.87	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	
1	A	1379/1733 (80%)	1169 (85%)	177 (13%)	33 (2%)	6	28
2	B	1085/1224 (89%)	927 (85%)	135 (12%)	23 (2%)	7	31
3	C	264/318 (83%)	228 (86%)	35 (13%)	1 (0%)	34	66

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	E	212/215 (99%)	183 (86%)	25 (12%)	4 (2%)	8	34
5	F	82/155 (53%)	72 (88%)	10 (12%)	0	100	100
6	H	129/146 (88%)	106 (82%)	16 (12%)	7 (5%)	2	12
7	I	117/122 (96%)	98 (84%)	17 (14%)	2 (2%)	9	35
8	J	63/70 (90%)	56 (89%)	6 (10%)	1 (2%)	9	36
9	K	112/120 (93%)	106 (95%)	6 (5%)	0	100	100
10	L	42/70 (60%)	28 (67%)	11 (26%)	3 (7%)	1	7
All	All	3485/4173 (84%)	2973 (85%)	438 (13%)	74 (2%)	7	31

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	286	HIS
1	A	321	PRO
1	A	593	GLU
1	A	1393	ASN
2	B	230	ALA
2	B	266	ALA
2	B	367	LEU
2	B	711	GLU
2	B	1046	PRO
6	H	62	SER
6	H	140	ALA
7	I	33	SER
10	L	38	LEU
10	L	55	ILE
1	A	40	THR
1	A	65	LEU
1	A	79	GLY
1	A	93	VAL
1	A	142	CYS
1	A	250	ILE
1	A	307	ASP
1	A	311	GLN
1	A	331	GLY
1	A	1234	GLU
2	B	65	GLU
2	B	124	TYR
2	B	275	TYR
2	B	780	VAL

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Mol	Chain	Res	Type
2	B	864	LYS
4	E	36	GLU
6	H	87	ARG
7	I	9	ASP
10	L	45	ALA
1	A	87	ALA
1	A	214	ILE
1	A	609	ASP
1	A	1123	GLY
2	B	476	ARG
2	B	865	LYS
3	C	142	VAL
4	E	86	PRO
6	H	133	ASN
1	A	111	GLY
1	A	130	ASP
1	A	248	PRO
1	A	1093	LYS
2	B	466	TRP
2	B	648	HIS
2	B	901	PRO
4	E	125	PRO
8	J	3	VAL
1	A	45	GLN
1	A	224	PHE
1	A	453	MET
1	A	922	ASP
1	A	958	VAL
1	A	1361	SER
1	A	1392	SER
2	B	408	LEU
2	B	469	GLN
1	A	923	LEU
1	A	1156	PRO
2	B	462	ALA
2	B	708	GLU
6	H	43	ASN
6	H	81	PRO
6	H	109	LYS
4	E	118	PRO
2	B	731	VAL
2	B	1103	ILE

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Mol	Chain	Res	Type
1	A	312	PRO
1	A	600	PRO
2	B	167	ILE
2	B	593	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	
1	A	1216/1520 (80%)	1030 (85%)	186 (15%)	2	12
2	B	957/1061 (90%)	813 (85%)	144 (15%)	3	13
3	C	234/274 (85%)	198 (85%)	36 (15%)	2	12
4	E	196/197 (100%)	167 (85%)	29 (15%)	3	13
5	F	74/137 (54%)	59 (80%)	15 (20%)	1	5
6	H	117/128 (91%)	99 (85%)	18 (15%)	2	12
7	I	113/116 (97%)	91 (80%)	22 (20%)	1	5
8	J	60/65 (92%)	50 (83%)	10 (17%)	2	10
9	K	99/102 (97%)	89 (90%)	10 (10%)	7	27
10	L	39/57 (68%)	29 (74%)	10 (26%)	0	2
All	All	3105/3657 (85%)	2625 (84%)	480 (16%)	2	12

All (480) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	TYR
1	A	12	ARG
1	A	13	THR
1	A	18	GLN
1	A	22	PHE
1	A	30	ILE
1	A	34	LYS
1	A	47	ARG
1	A	57	ARG

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Mol	Chain	Res	Type
1	A	65	LEU
1	A	93	VAL
1	A	107	CYS
1	A	109	HIS
1	A	126	LEU
1	A	132	LYS
1	A	144	THR
1	A	146	MET
1	A	148	CYS
1	A	154	SER
1	A	161	LEU
1	A	163	SER
1	A	169	ASN
1	A	179	LEU
1	A	185	TRP
1	A	208	LEU
1	A	211	PHE
1	A	222	LEU
1	A	226	GLU
1	A	227	VAL
1	A	251	SER
1	A	252	PHE
1	A	254	GLU
1	A	270	LEU
1	A	287	HIS
1	A	289	ILE
1	A	297	GLN
1	A	315	LEU
1	A	316	GLN
1	A	320	ARG
1	A	329	LEU
1	A	332	LYS
1	A	333	GLU
1	A	335	ARG
1	A	337	ARG
1	A	359	LEU
1	A	375	THR
1	A	381	THR
1	A	383	TYR
1	A	397	ASN
1	A	404	TYR
1	A	415	LEU

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Mol	Chain	Res	Type
1	A	417	TYR
1	A	419	LYS
1	A	434	ARG
1	A	436	ILE
1	A	443	LEU
1	A	451	HIS
1	A	452	LYS
1	A	454	SER
1	A	469	ARG
1	A	470	LEU
1	A	472	LEU
1	A	474	VAL
1	A	475	THR
1	A	476	SER
1	A	481	ASP
1	A	485	ASP
1	A	493	GLN
1	A	496	GLU
1	A	504	LEU
1	A	509	LEU
1	A	512	VAL
1	A	513	SER
1	A	517	ASN
1	A	532	ARG
1	A	544	ASP
1	A	550	LEU
1	A	567	LYS
1	A	569	LYS
1	A	588	LEU
1	A	596	THR
1	A	605	MET
1	A	612	ILE
1	A	618	GLU
1	A	621	THR
1	A	625	SER
1	A	629	LEU
1	A	635	ARG
1	A	666	ILE
1	A	672	ASP
1	A	702	LEU
1	A	709	THR
1	A	710	LEU

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Mol	Chain	Res	Type
1	A	732	LEU
1	A	740	LEU
1	A	752	LYS
1	A	764	CYS
1	A	768	GLN
1	A	774	ARG
1	A	783	THR
1	A	788	SER
1	A	801	GLU
1	A	821	ARG
1	A	826	ASP
1	A	829	VAL
1	A	838	GLN
1	A	839	ARG
1	A	879	GLU
1	A	881	GLN
1	A	886	ILE
1	A	896	ARG
1	A	903	ASN
1	A	911	SER
1	A	913	LEU
1	A	917	SER
1	A	922	ASP
1	A	926	GLN
1	A	941	LYS
1	A	961	ARG
1	A	970	THR
1	A	976	THR
1	A	977	LYS
1	A	980	ASP
1	A	981	LEU
1	A	995	GLU
1	A	996	ASN
1	A	1000	LEU
1	A	1001	ARG
1	A	1017	LEU
1	A	1025	ARG
1	A	1029	ARG
1	A	1033	GLN
1	A	1036	ARG
1	A	1037	LEU
1	A	1062	GLU

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Mol	Chain	Res	Type
1	A	1063	MET
1	A	1064	VAL
1	A	1067	LEU
1	A	1081	LEU
1	A	1092	LYS
1	A	1093	LYS
1	A	1095	THR
1	A	1128	GLN
1	A	1135	ARG
1	A	1142	THR
1	A	1146	VAL
1	A	1165	GLU
1	A	1172	LEU
1	A	1187	GLN
1	A	1205	LYS
1	A	1206	ASP
1	A	1208	THR
1	A	1223	ASP
1	A	1237	ILE
1	A	1240	CYS
1	A	1257	ASP
1	A	1262	LYS
1	A	1264	GLU
1	A	1267	MET
1	A	1269	GLU
1	A	1288	ASP
1	A	1295	THR
1	A	1297	GLU
1	A	1299	VAL
1	A	1300	LYS
1	A	1322	ILE
1	A	1325	THR
1	A	1333	ILE
1	A	1351	GLU
1	A	1354	ASN
1	A	1359	ASP
1	A	1366	ARG
1	A	1374	VAL
1	A	1376	THR
1	A	1383	SER
1	A	1386	ARG
1	A	1391	ARG

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Mol	Chain	Res	Type
1	A	1405	THR
1	A	1406	VAL
1	A	1407	GLU
1	A	1410	PHE
1	A	1425	SER
1	A	1426	GLU
1	A	1442	ASP
1	A	1443	VAL
1	A	1445	ILE
2	B	20	ASP
2	B	28	GLU
2	B	46	GLN
2	B	63	ILE
2	B	65	GLU
2	B	97	VAL
2	B	98	THR
2	B	103	ASN
2	B	104	GLU
2	B	109	THR
2	B	128	LEU
2	B	134	LYS
2	B	165	VAL
2	B	167	ILE
2	B	175	ARG
2	B	176	SER
2	B	183	GLU
2	B	194	GLU
2	B	217	ARG
2	B	225	VAL
2	B	242	SER
2	B	244	LEU
2	B	248	SER
2	B	249	ARG
2	B	250	PHE
2	B	268	THR
2	B	275	TYR
2	B	277	LYS
2	B	315	LYS
2	B	319	GLU
2	B	328	GLU
2	B	345	LYS
2	B	346	GLU

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Mol	Chain	Res	Type
2	B	351	TYR
2	B	361	LEU
2	B	365	THR
2	B	368	GLU
2	B	387	LEU
2	B	393	LYS
2	B	394	ASP
2	B	398	ARG
2	B	412	LEU
2	B	416	LEU
2	B	425	THR
2	B	426	LYS
2	B	427	ASP
2	B	428	ILE
2	B	432	MET
2	B	437	GLU
2	B	448	ILE
2	B	454	THR
2	B	461	LEU
2	B	465	ASN
2	B	466	TRP
2	B	470	LYS
2	B	473	MET
2	B	475	SER
2	B	481	GLN
2	B	482	VAL
2	B	483	LEU
2	B	487	THR
2	B	510	LYS
2	B	513	GLN
2	B	527	THR
2	B	542	MET
2	B	549	THR
2	B	552	MET
2	B	556	THR
2	B	563	MET
2	B	570	VAL
2	B	598	GLU
2	B	617	ARG
2	B	637	LEU
2	B	653	VAL
2	B	655	LYS

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Mol	Chain	Res	Type
2	B	680	THR
2	B	705	MET
2	B	714	GLU
2	B	730	ARG
2	B	732	SER
2	B	751	VAL
2	B	754	SER
2	B	755	ILE
2	B	762	ASN
2	B	780	VAL
2	B	786	ASN
2	B	788	ARG
2	B	810	GLU
2	B	822	ASN
2	B	827	ILE
2	B	844	SER
2	B	857	ARG
2	B	866	TYR
2	B	878	GLN
2	B	879	ARG
2	B	880	THR
2	B	883	LEU
2	B	933	SER
2	B	935	ARG
2	B	943	SER
2	B	946	ASN
2	B	953	LEU
2	B	955	THR
2	B	957	ASN
2	B	963	PHE
2	B	970	THR
2	B	983	ARG
2	B	987	LYS
2	B	992	ILE
2	B	996	ARG
2	B	997	GLU
2	B	999	MET
2	B	1004	GLU
2	B	1007	VAL
2	B	1019	SER
2	B	1021	MET
2	B	1028	GLU

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Mol	Chain	Res	Type
2	B	1055	ILE
2	B	1065	GLN
2	B	1066	SER
2	B	1072	MET
2	B	1077	THR
2	B	1082	MET
2	B	1092	TYR
2	B	1094	ARG
2	B	1103	ILE
2	B	1113	VAL
2	B	1122	ARG
2	B	1124	ARG
2	B	1150	ARG
2	B	1151	LEU
2	B	1159	ARG
2	B	1160	VAL
2	B	1163	CYS
2	B	1174	LYS
2	B	1176	ASN
2	B	1182	CYS
2	B	1183	LYS
2	B	1185	CYS
2	B	1188	LYS
2	B	1194	ILE
2	B	1202	LEU
2	B	1205	GLN
2	B	1220	ARG
3	C	4	GLU
3	C	11	ARG
3	C	18	VAL
3	C	22	LEU
3	C	25	VAL
3	C	26	ASP
3	C	41	ILE
3	C	53	THR
3	C	56	THR
3	C	57	VAL
3	C	77	ILE
3	C	79	GLN
3	C	80	LEU
3	C	89	GLU
3	C	96	SER

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Mol	Chain	Res	Type
3	C	99	LEU
3	C	100	THR
3	C	102	GLN
3	C	106	GLU
3	C	120	ILE
3	C	129	ILE
3	C	137	LYS
3	C	140	ASN
3	C	149	LYS
3	C	151	GLN
3	C	189	THR
3	C	197	SER
3	C	222	LYS
3	C	226	ASP
3	C	240	VAL
3	C	244	VAL
3	C	249	ASP
3	C	253	LYS
3	C	259	LEU
3	C	267	GLN
3	C	268	ASP
4	E	3	GLN
4	E	11	ARG
4	E	14	ARG
4	E	31	THR
4	E	40	GLU
4	E	48	ASP
4	E	54	GLN
4	E	57	MET
4	E	78	LEU
4	E	81	GLU
4	E	90	VAL
4	E	92	THR
4	E	94	LYS
4	E	98	ILE
4	E	103	LYS
4	E	110	PHE
4	E	123	LEU
4	E	127	ILE
4	E	131	THR
4	E	134	THR
4	E	150	VAL

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Mol	Chain	Res	Type
4	E	153	HIS
4	E	162	ARG
4	E	165	LEU
4	E	169	ARG
4	E	179	GLN
4	E	196	VAL
4	E	201	LYS
4	E	204	THR
5	F	72	LYS
5	F	74	ILE
5	F	79	ARG
5	F	82	THR
5	F	93	ILE
5	F	97	ARG
5	F	102	SER
5	F	109	VAL
5	F	112	GLU
5	F	114	GLU
5	F	119	ARG
5	F	133	VAL
5	F	142	SER
5	F	149	GLU
5	F	155	LEU
6	H	19	ARG
6	H	21	ASN
6	H	25	ARG
6	H	34	ASP
6	H	58	THR
6	H	78	SER
6	H	88	SER
6	H	89	LEU
6	H	97	MET
6	H	109	LYS
6	H	124	ARG
6	H	125	LEU
6	H	130	ARG
6	H	136	LYS
6	H	137	GLN
6	H	143	LEU
6	H	145	ARG
6	H	146	ARG
7	I	2	THR

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Mol	Chain	Res	Type
7	I	3	THR
7	I	7	CYS
7	I	8	ARG
7	I	14	LEU
7	I	15	TYR
7	I	28	GLU
7	I	29	CYS
7	I	50	THR
7	I	55	THR
7	I	60	GLN
7	I	71	SER
7	I	77	LYS
7	I	84	VAL
7	I	89	GLN
7	I	90	GLN
7	I	91	ARG
7	I	95	THR
7	I	107	SER
7	I	116	ASN
7	I	117	LYS
7	I	118	ARG
8	J	6	ARG
8	J	7	CYS
8	J	9	SER
8	J	28	ASP
8	J	29	GLU
8	J	31	ASP
8	J	46	CYS
8	J	48	ARG
8	J	59	LYS
8	J	64	ASN
9	K	1	MET
9	K	6	ARG
9	K	26	LYS
9	K	41	THR
9	K	47	ARG
9	K	77	THR
9	K	101	LEU
9	K	103	THR
9	K	106	GLU
9	K	107	THR
10	L	34	CYS

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Mol	Chain	Res	Type
10	L	38	LEU
10	L	42	ARG
10	L	46	VAL
10	L	47	ARG
10	L	49	LYS
10	L	50	ASP
10	L	51	CYS
10	L	54	ARG
10	L	63	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	80	HIS
1	A	256	GLN
1	A	306	ASN
1	A	316	GLN
1	A	399	HIS
1	A	435	HIS
1	A	479	ASN
1	A	493	GLN
1	A	903	ASN
1	A	1173	HIS
2	B	395	GLN
2	B	465	ASN
2	B	531	GLN
2	B	590	HIS
2	B	734	HIS
2	B	762	ASN
2	B	842	ASN
2	B	843	GLN
2	B	878	GLN
2	B	975	GLN
2	B	1015	HIS
2	B	1025	HIS
2	B	1084	GLN
2	B	1093	GLN
2	B	1193	GLN
3	C	17	ASN
3	C	167	HIS
3	C	195	GLN

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Mol	Chain	Res	Type
3	C	231	ASN
4	E	54	GLN
6	H	134	ASN
6	H	137	GLN
7	I	60	GLN
7	I	108	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
13	R	8/9 (88%)	2 (25%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
13	R	2	U
13	R	9	G

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
11	1CC	T	19	11	15,23,24	1.23	2 (13%)	15,33,36	1.62	3 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	1CC	T	19	11	-	0/4/25/26	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	19	1CC	O5'-C5'	-2.51	1.38	1.44
11	T	19	1CC	C2-N3	-2.26	1.33	1.38

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	19	1CC	C2-N3-C4	4.14	121.02	116.02
11	T	19	1CC	C2'-C1'-N1	-2.86	107.67	114.27
11	T	19	1CC	N4-C4-N3	2.53	120.61	117.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	T	19	1CC	3	0

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
16	G2P	T	101	15	26,34,34	2.81	12 (46%)	30,54,54	1.94	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
16	G2P	T	101	15	-	4/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	T	101	G2P	C4-N9	-8.27	1.36	1.47
16	T	101	G2P	C6-N1	5.12	1.41	1.33
16	T	101	G2P	PB-O2B	4.31	1.61	1.51
16	T	101	G2P	PA-O2A	4.15	1.61	1.51
16	T	101	G2P	C5-C6	-4.14	1.45	1.52
16	T	101	G2P	PG-O2G	3.58	1.62	1.50
16	T	101	G2P	PB-O3B	3.03	1.61	1.58
16	T	101	G2P	PB-O1B	-2.57	1.50	1.56
16	T	101	G2P	C5-C4	-2.37	1.38	1.53
16	T	101	G2P	C8-N9	-2.24	1.37	1.45
16	T	101	G2P	PA-O5'	2.12	1.60	1.57
16	T	101	G2P	O4'-C1'	2.03	1.46	1.42

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	T	101	G2P	C4-C5-N7	6.43	110.99	102.46
16	T	101	G2P	C5-C6-N1	-4.09	113.15	118.19
16	T	101	G2P	O4'-C1'-N9	3.50	114.25	109.04
16	T	101	G2P	O1G-PG-O3B	3.03	114.81	104.64
16	T	101	G2P	O2B-PB-C3A	-2.13	103.44	109.07

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	T	101	G2P	O4'-C4'-C5'-O5'
16	T	101	G2P	C3'-C4'-C5'-O5'

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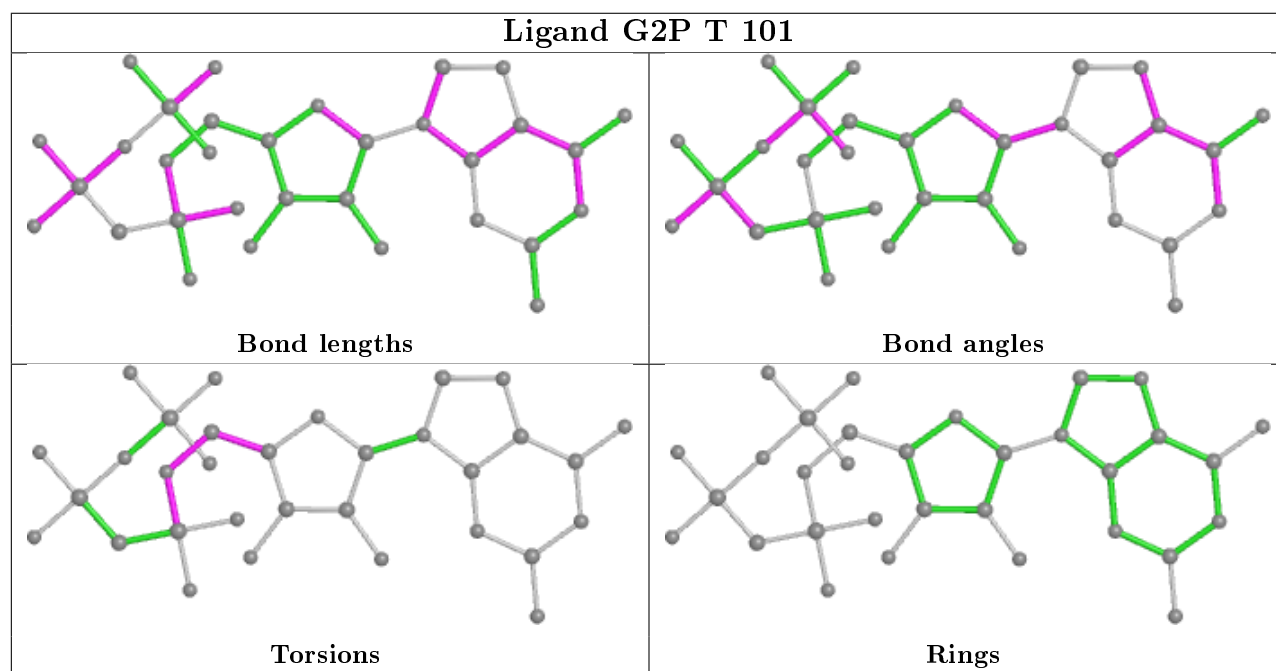
Mol	Chain	Res	Type	Atoms
16	T	101	G2P	C5'-O5'-PA-O1A
16	T	101	G2P	C4'-C5'-O5'-PA

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	T	101	G2P	2	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 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, 95th 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 ²)	Q<0.9
1	A	1393/1733 (80%)	0.05	58 (4%) 36 34	45, 88, 191, 305	0
2	B	1103/1224 (90%)	-0.08	21 (1%) 66 65	42, 79, 153, 277	0
3	C	266/318 (83%)	-0.31	0 100 100	50, 79, 117, 170	0
4	E	214/215 (99%)	0.04	10 (4%) 31 29	63, 114, 201, 236	0
5	F	84/155 (54%)	-0.24	0 100 100	65, 93, 138, 182	0
6	H	133/146 (91%)	0.46	11 (8%) 11 11	75, 116, 207, 288	0
7	I	119/122 (97%)	-0.18	1 (0%) 86 86	58, 97, 139, 186	0
8	J	65/70 (92%)	-0.23	0 100 100	56, 74, 113, 131	0
9	K	114/120 (95%)	-0.13	0 100 100	54, 86, 115, 164	0
10	L	44/70 (62%)	0.69	3 (6%) 17 17	73, 158, 247, 292	0
11	T	28/29 (96%)	1.43	11 (39%) 0 0	60, 289, 368, 372	0
12	N	14/14 (100%)	1.82	8 (57%) 0 0	249, 290, 330, 348	0
13	R	9/9 (100%)	-0.47	0 100 100	54, 66, 111, 116	0
All	All	3586/4225 (84%)	-0.00	123 (3%) 45 43	42, 87, 187, 372	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	257	ARG	6.9
6	H	86	ASP	6.5
2	B	1221	SER	6.1
2	B	250	PHE	5.8
10	L	50	ASP	5.7
11	T	4	DC	5.7
1	A	69	THR	5.3
1	A	253	ASN	5.2
6	H	139	ASN	5.1

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Mol	Chain	Res	Type	RSRZ
1	A	151	ASP	4.8
2	B	249	ARG	4.8
1	A	141	LEU	4.7
1	A	168	GLY	4.6
1	A	146	MET	4.4
11	T	3	DA	4.1
11	T	16	DC	4.0
1	A	320	ARG	4.0
1	A	49	LYS	3.9
4	E	93	MET	3.9
1	A	1176	LEU	3.8
11	T	1	DC	3.7
11	T	15	DA	3.6
1	A	65	LEU	3.5
1	A	173	THR	3.5
4	E	83	CYS	3.5
1	A	254	GLU	3.4
1	A	258	GLY	3.4
2	B	711	GLU	3.4
1	A	72	GLU	3.3
11	T	11	DG	3.3
1	A	125	ALA	3.3
1	A	50	ILE	3.3
1	A	108	MET	3.2
4	E	118	PRO	3.2
4	E	126	SER	3.2
1	A	45	GLN	3.2
1	A	214	ILE	3.2
11	T	2	DT	3.1
2	B	869	SER	3.1
12	N	2	DT	3.1
2	B	865	LYS	3.1
1	A	309	ALA	3.1
6	H	146	ARG	3.0
1	A	147	VAL	3.0
1	A	163	SER	3.0
1	A	174	ILE	2.9
1	A	210	ILE	2.9
2	B	1220	ARG	2.9
12	N	14	DG	2.9
4	E	110	PHE	2.8
1	A	182	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	176	LYS	2.8
2	B	643	ASP	2.8
2	B	715	ALA	2.8
1	A	1040	GLN	2.8
11	T	14	DG	2.8
1	A	38	PRO	2.7
4	E	97	VAL	2.7
1	A	154	SER	2.6
1	A	221	SER	2.6
4	E	123	LEU	2.6
1	A	181	LEU	2.6
1	A	1256	GLU	2.6
10	L	43	THR	2.6
1	A	170	THR	2.5
11	T	12	DC	2.5
12	N	1	DC	2.5
1	A	124	GLN	2.5
2	B	356	LEU	2.5
1	A	91	PHE	2.4
12	N	12	DT	2.4
2	B	69	LEU	2.4
1	A	44	THR	2.4
11	T	13	DA	2.4
1	A	153	PRO	2.4
1	A	148	CYS	2.4
1	A	59	GLY	2.4
1	A	286	HIS	2.4
2	B	92	PHE	2.4
2	B	866	TYR	2.4
2	B	247	GLY	2.3
6	H	82	PRO	2.3
1	A	231	PRO	2.3
6	H	84	ALA	2.3
2	B	437	GLU	2.3
12	N	3	DG	2.3
1	A	1126	ALA	2.3
6	H	131	ASN	2.3
11	T	5	DC	2.3
1	A	66	LYS	2.3
6	H	55	LEU	2.3
1	A	115	LEU	2.3
1	A	1169	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
10	L	29	TYR	2.2
2	B	425	THR	2.2
6	H	51	ALA	2.2
6	H	138	GLU	2.2
1	A	76	GLU	2.2
1	A	315	LEU	2.2
1	A	114	LEU	2.2
2	B	248	SER	2.2
2	B	713	ALA	2.2
7	I	117	LYS	2.2
6	H	137	GLN	2.2
4	E	49	SER	2.1
1	A	1080	THR	2.1
1	A	568	PRO	2.1
1	A	144	THR	2.1
4	E	91	LYS	2.1
1	A	279	LEU	2.1
12	N	13	DA	2.1
1	A	256	GLN	2.1
6	H	130	ARG	2.1
2	B	666	TYR	2.0
1	A	161	LEU	2.0
1	A	1125	ALA	2.0
12	N	6	DT	2.0
2	B	275	TYR	2.0
12	N	7	DA	2.0
2	B	45	SER	2.0
4	E	84	ASP	2.0
1	A	660	ASN	2.0
1	A	171	GLN	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
11	1CC	T	19	22/23	0.95	0.13	71,87,132,144	0

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

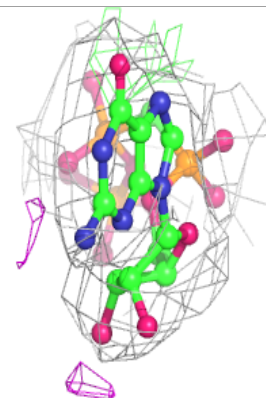
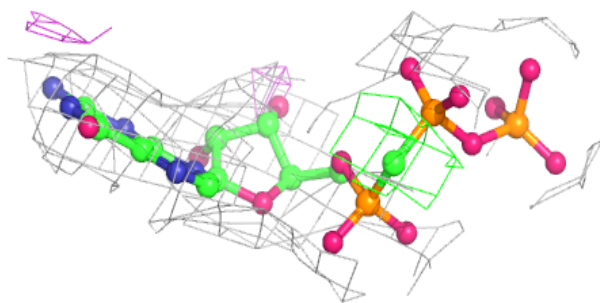
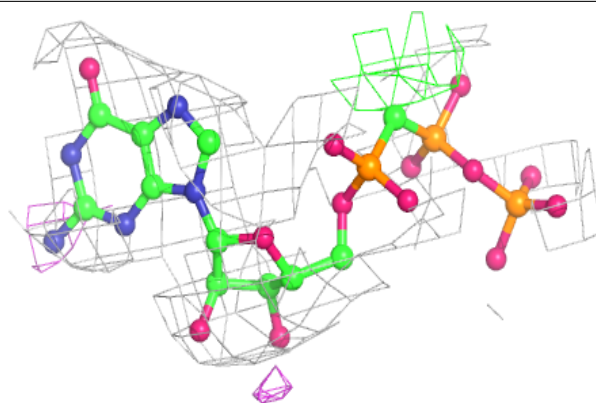
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
14	ZN	A	1801	1/1	0.70	0.08	266,266,266,266	0
15	MG	A	1804	1/1	0.83	0.20	87,87,87,87	0
14	ZN	L	101	1/1	0.87	0.06	172,172,172,172	0
16	G2P	T	101	32/32	0.91	0.18	59,73,127,131	0
14	ZN	A	1802	1/1	0.94	0.08	136,136,136,136	0
14	ZN	B	1301	1/1	0.97	0.12	123,123,123,123	0
14	ZN	J	101	1/1	0.97	0.19	92,92,92,92	0
14	ZN	I	202	1/1	0.97	0.13	93,93,93,93	0
15	MG	A	1803	1/1	0.97	0.17	42,42,42,42	0
14	ZN	I	201	1/1	0.98	0.09	104,104,104,104	0
14	ZN	C	401	1/1	0.99	0.12	107,107,107,107	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around G2P T 101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.