



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:10 AM UTC

PDB ID : 4C30 / pdb_00004c30
Title : Crystal structure of Deinococcus radiodurans UvrD in complex with DNA, form 2
Authors : Stelter, M.; Acajjaoui, S.; McSweeney, S.; Timmins, J.
Deposited on : 2013-08-21
Resolution : 3.00 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 types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

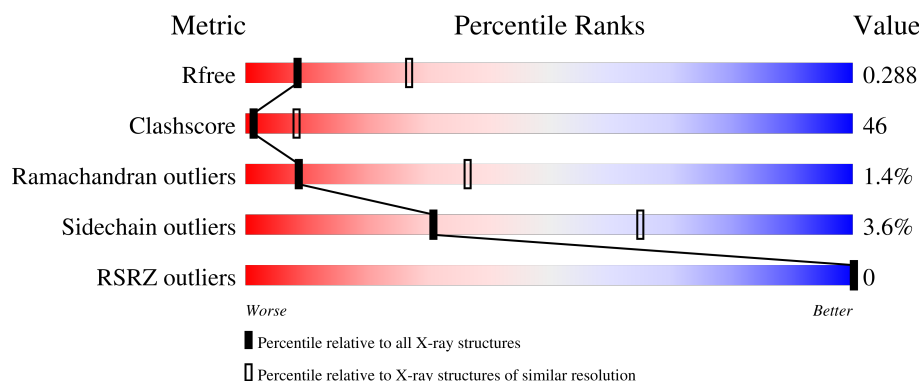
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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.



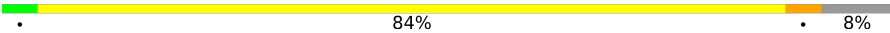
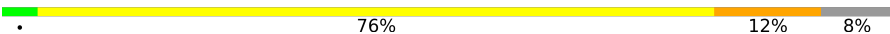
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	665	
1	D	665	
1	F	665	
1	I	665	
2	K	25	

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Mol	Chain	Length	Quality of chain
2	X	25	 84% 8%
3	L	25	 76% 12% 8%
3	Y	25	 84% 8% 8%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ANP	F	1663	-	-	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22073 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 HELICASE II.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	631	Total	C	N	O	S	0	0	0
			4970	3112	898	945	15			
1	D	642	Total	C	N	O	S	0	2	0
			5059	3168	916	961	14			
1	F	632	Total	C	N	O	S	0	0	0
			4978	3118	899	946	15			
1	I	638	Total	C	N	O	S	0	1	0
			5025	3145	909	957	14			

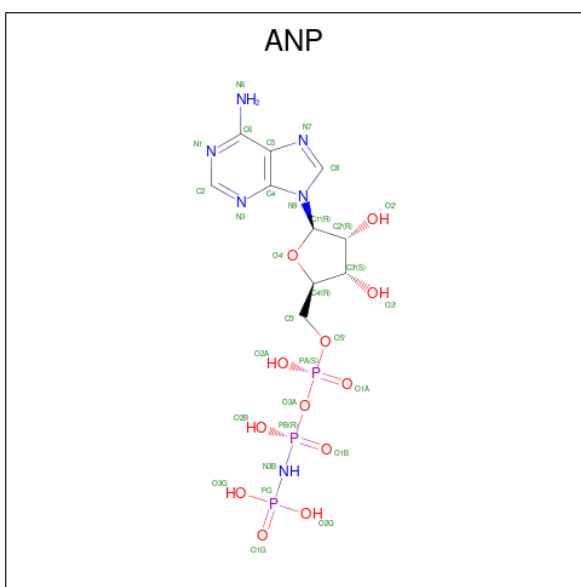
- Molecule 2 is a DNA chain called DNA STRAND FOR25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	K	23	Total	C	N	O	P	0	0	0
			471	225	78	145	23			
2	X	23	Total	C	N	O	P	0	0	0
			471	225	78	145	23			

- Molecule 3 is a DNA chain called DNA STRAND REV25.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	23	Total	C	N	O	P	0	0	0
			467	223	80	141	23			
3	Y	23	Total	C	N	O	P	0	0	0
			467	223	80	141	23			

- Molecule 4 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (CCD ID: ANP) (formula: C₁₀H₁₇N₆O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 6	O 12	P 3	0	0
4	F	1	Total 31	C 10	N 6	O 12	P 3	0	0

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	2	Total Mg 2 2	0	0
5	D	1	Total Mg 1 1	0	0
5	F	2	Total Mg 2 2	0	0
5	I	1	Total Mg 1 1	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	6	Total O 6 6	0	0
6	D	28	Total O 28 28	0	0
6	F	26	Total O 26 26	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	I	36	Total 36	O 36	0	0
6	Y	1	Total 1	O 1	0	0

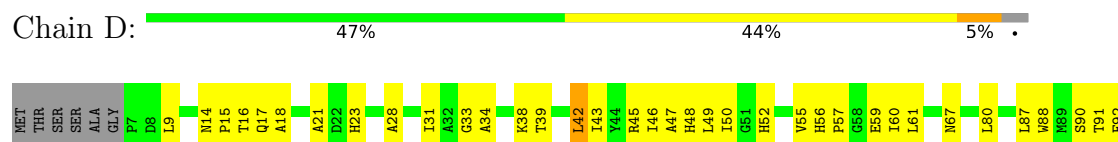
3 Residue-property plots

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

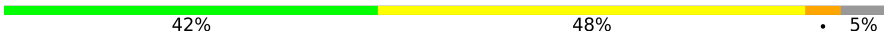


• Molecule 1: DNA HELICASE II

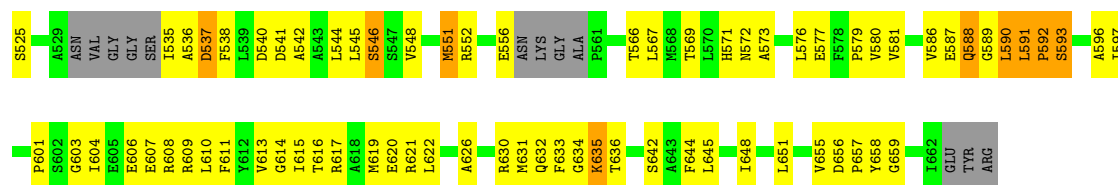


F644	L645	E646	D647	E648	E649	G650	L651	F652	D653	T654	V655	D656	F657	Y658	G659	Q660	P661	I662	GLU	TYR	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																							
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• Molecule 1: DNA HELICASE II

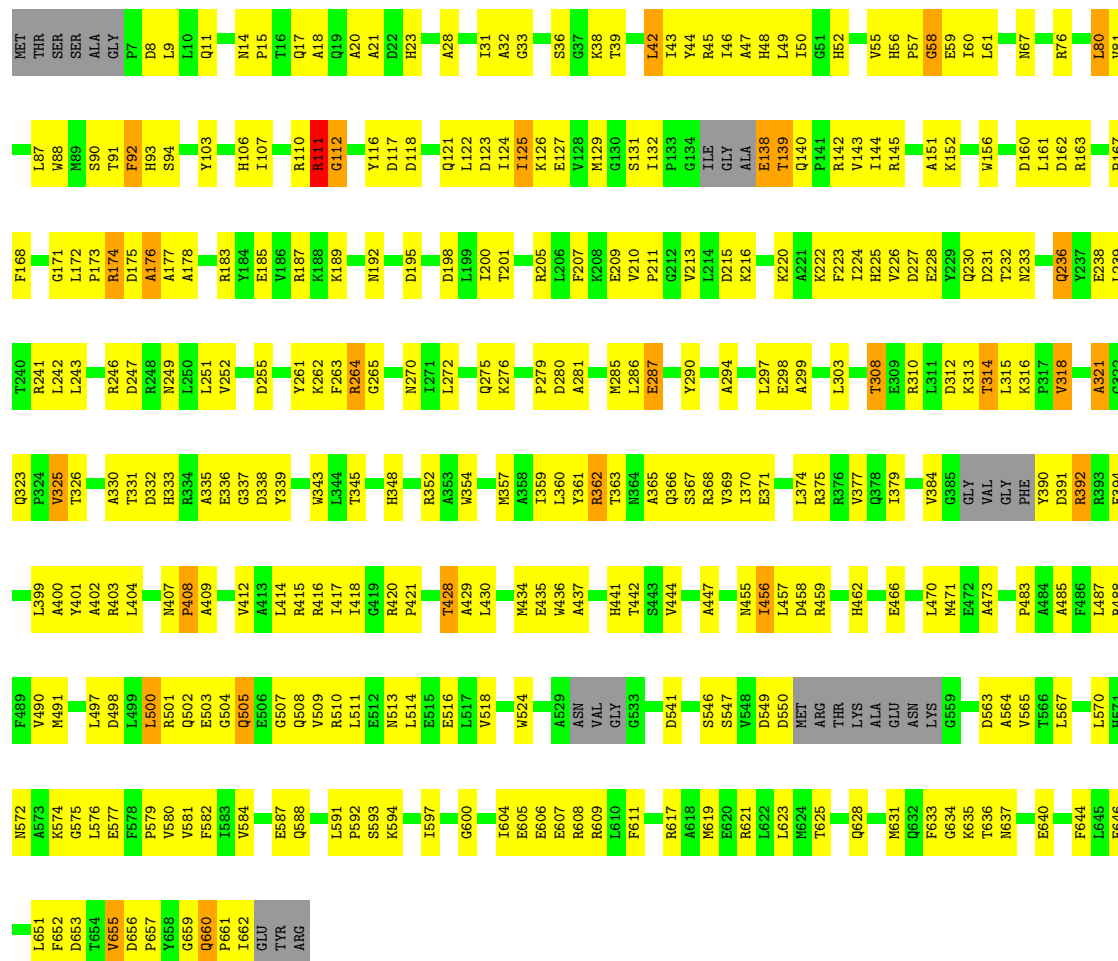
Chain F:  42% 48% 5%

V384	K302	V226	L155	E72	MET
G385	L303	D227	W156	M73	THR
G386	I304	E228	T157	SER	
V387	E305	R76		R76	SER
G388	N306	Q230	D160		ALA
F389	N307	D231	L161	H79	GLY
Y390	T308		D162		P7
D391	E309	A235		D86	
R392	R310	Q236	R165	L87	L13
R393	L311	Y237	E166	W88	
E394	D312	E238	P167	M89	Q17
I395	K313	L239	PHE	S90	
R396	L314	T240	ILE	T91	A20
D397	L315	R241	SER	F92	
			GLY		H23
I398	V318	S245	LEU	A95	F24
L399	K319		P173	G96	T25
A400	E320	R248	R174	V97	G26
Y401	A321	N249	D175	R98	P27
A402		L250	A176	I99	A28
R403		L251		L100	L29
L404	P324	V252	R183	R101	V30
		V253		T102	I31
N407	F327	G254	V186		G33
P408	H328	D255	R187	H106	
A409	R329	P256	K188	I107	G35
D410		D257	K189	G108	
D411	D332	Q258	G190	S36	
F486	H333	S259	G191	F113	G37
L487	R334	L260	N192	V114	K38
R488		V261	A193	I115	
F489	L414	K262	Y116		
V490	R415	F263	D195	D117	L42
M491	I417		F196		
	W343				I43
G495	I418				Y44
Y496	G419	I271	G197	D120	R45
L497	R420	L272	D198	Q121	I46
D498	P421	D273	L199	L122	A47
L499	G349	F274	I200	D123	H48
R422		Q275	T201	I124	L49
L500	R423		E202	I125	I50
R501	R352		T203	K126	G51
		P279			
		D280	V204	E127	H52
G504	R362	A281	R205	V128	Y53
Q505	T363	R282	L206	M129	
E506	N364	K282	F207		H56
G507	A365	V283	K208	I132	P57
Q508	Q431	Y284	E209		G58
V509	L433	S367	M285	I135	E59
R510	M434	R368	L286	T139	
	E435	V369	E287	P211	I60
L511	E436	I370	H288	G212	L61
N512	A437	E371	N289	V213	A62
N513	R438		Y290	L214	V63
L514	T439		R291	P141	
E515		L374		D215	T64
E516		R375			F65
L517	V444	V376	A294	Q218	G66
V518	L445	V377	L297	I147	T66
		Q378	E298	N67	
E522	C448	I379	L299	K222	K68
E523	A449		E299	A151	A69
E524	N450	T383		K152	A70
					F74



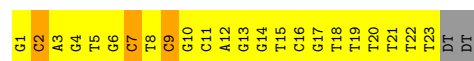
• Molecule 1: DNA HELICASE II

Chain I: 48% 44%



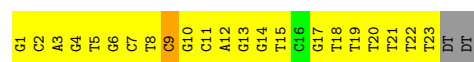
• Molecule 2: DNA STRAND FOR25

Chain K: 80% 12% 8%

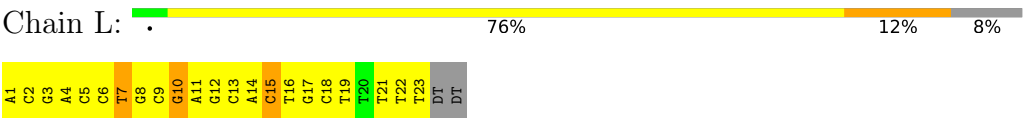


• Molecule 2: DNA STRAND FOR25

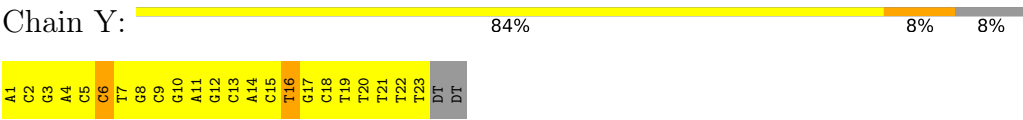
Chain X: 84% 8%



● Molecule 3: DNA STRAND REV25



● Molecule 3: DNA STRAND REV25



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	68.49Å 89.78Å 293.80Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	66.18 – 3.00 66.18 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.2 (66.18-3.00) 87.2 (66.18-3.00)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0085	Depositor
R, R_{free}	0.228 , 0.288 0.231 , 0.288	Depositor DCC
R_{free} test set	3128 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	71.2	Xtriage
Anisotropy	0.942	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 87.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.439 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	22073	wwPDB-VP
Average B, all atoms (Å ²)	104.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% 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

5.1 Standard geometry

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

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	0.71	3/5059 (0.1%)	1.09	14/6838 (0.2%)
1	D	0.80	3/5156 (0.1%)	1.10	19/6972 (0.3%)
1	F	0.68	1/5067 (0.0%)	1.06	14/6849 (0.2%)
1	I	0.82	3/5117 (0.1%)	1.15	19/6919 (0.3%)
2	K	0.81	1/525 (0.2%)	1.20	6/809 (0.7%)
2	X	0.56	0/525	1.09	1/809 (0.1%)
3	L	0.61	0/521	1.13	3/801 (0.4%)
3	Y	0.69	1/521 (0.2%)	1.10	1/801 (0.1%)
All	All	0.75	12/22491 (0.1%)	1.10	77/30798 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	2
1	F	0	1
1	I	0	2
All	All	0	5

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	2	DC	O3'-P	-12.78	1.42	1.61
1	I	111	ARG	C-N	12.23	1.41	1.33
3	Y	16	DT	O3'-P	-6.28	1.51	1.61
1	D	111	ARG	C-N	5.82	1.41	1.33
1	A	271	ILE	CA-C	5.82	1.59	1.52
1	I	581	VAL	CA-CB	-5.43	1.47	1.54
1	F	37	GLY	C-N	-5.27	1.27	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	353	ALA	CA-CB	-5.19	1.45	1.53
1	D	615	ILE	CA-CB	-5.17	1.48	1.54
1	D	661	PRO	N-CD	-5.10	1.40	1.47
1	A	133	PRO	N-CD	-5.08	1.40	1.47
1	I	112	GLY	N-CA	5.02	1.52	1.45

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ILE	N-CA-C	17.03	128.24	110.36
1	F	590	LEU	N-CA-C	14.41	128.98	111.40
1	A	272	LEU	N-CA-C	12.39	124.78	111.28
1	I	111	ARG	CA-C-N	-10.32	111.71	121.62
1	I	111	ARG	C-N-CA	-10.32	111.71	121.62
1	I	501	ARG	N-CA-C	-9.13	98.89	112.04
1	I	392	ARG	N-CA-C	8.54	120.20	111.07
1	D	111	ARG	N-CA-C	8.39	122.77	107.99
1	I	20	ALA	N-CA-C	-8.09	102.55	111.36
1	D	112	GLY	N-CA-C	-7.63	91.19	113.30
1	I	655	VAL	N-CA-C	7.55	121.05	108.81
1	I	92	PHE	N-CA-C	-7.52	103.03	111.07
1	I	500	LEU	CB-CA-C	-7.42	97.98	110.81
1	D	591	LEU	N-CA-C	-7.41	97.86	109.87
1	A	194	ILE	N-CA-C	7.39	119.96	107.18
1	F	591	LEU	CB-CA-C	-7.26	95.87	110.17
3	L	15	DC	O3'-P-O5'	-7.17	93.25	104.00
2	K	2	DC	C5'-C4'-O4'	-7.10	98.75	109.40
1	A	69	ALA	N-CA-C	-7.09	103.49	111.07
1	D	111	ARG	CB-CA-C	-7.02	99.36	111.30
1	F	245	SER	N-CA-C	6.94	121.37	112.34
1	F	69	ALA	N-CA-C	-6.89	102.61	111.02
1	A	131	SER	N-CA-C	6.72	118.61	111.28
3	Y	6	DC	P-O3'-C3'	6.69	130.24	120.20
2	K	9	DC	C1'-O4'-C4'	-6.69	99.67	109.70
1	D	658	TYR	N-CA-C	-6.56	102.07	110.53
1	A	389	PHE	N-CA-C	-6.44	104.26	111.28
1	F	101	ARG	N-CA-C	6.37	117.89	111.07
1	A	660	GLN	N-CA-C	6.35	123.84	109.81
1	I	314	THR	N-CA-C	6.33	116.59	108.24
1	I	408	PRO	CA-C-N	-6.29	116.99	126.86
1	I	408	PRO	C-N-CA	-6.29	116.99	126.86
1	D	655	VAL	N-CA-C	6.26	117.37	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	505	GLN	N-CA-C	-6.20	105.75	113.38
1	F	389	PHE	N-CA-C	-6.18	104.54	111.28
1	I	408	PRO	N-CA-C	-6.16	102.52	111.33
2	K	2	DC	P-O3'-C3'	6.11	129.36	120.20
1	D	392	ARG	N-CA-C	6.05	117.95	111.36
1	F	204	VAL	CB-CA-C	-5.93	104.40	111.81
1	A	39	THR	O-C-N	5.81	128.77	122.15
1	I	281	ALA	N-CA-C	-5.81	102.31	110.50
1	A	271	ILE	N-CA-CB	-5.77	104.10	110.51
1	F	591	LEU	C-N-CD	-5.67	101.77	125.00
1	D	139	THR	N-CA-C	5.62	116.86	108.31
1	I	139	THR	N-CA-C	5.62	116.85	108.31
1	I	176	ALA	N-CA-C	-5.62	105.16	111.28
1	F	379	ILE	CB-CA-C	-5.58	104.86	110.89
1	A	536	ALA	N-CA-C	-5.53	105.34	111.36
1	F	318	VAL	N-CA-C	-5.52	107.06	111.81
1	I	402	ALA	N-CA-C	-5.49	105.37	111.36
1	D	402	ALA	N-CA-C	-5.45	105.23	111.07
2	K	7	DC	C1'-O4'-C4'	-5.45	101.53	109.70
1	A	38	LYS	O-C-N	-5.44	115.86	122.11
1	D	432	LYS	N-CA-C	-5.40	105.31	111.14
1	A	135	ILE	N-CA-C	5.34	118.60	111.44
1	F	379	ILE	N-CA-C	5.30	114.15	108.95
2	K	7	DC	O3'-P-O5'	-5.30	96.05	104.00
2	X	9	DC	C1'-O4'-C4'	-5.29	101.76	109.70
1	D	660	GLN	CA-C-N	5.26	125.32	119.32
1	D	660	GLN	C-N-CA	5.26	125.32	119.32
1	D	314	THR	N-CA-C	5.22	115.94	108.74
1	F	588	GLN	N-CA-C	5.19	117.35	111.02
2	K	9	DC	O4'-C1'-C2'	-5.19	98.61	106.40
1	D	446	THR	N-CA-C	-5.18	105.81	111.82
1	A	210	VAL	CA-C-N	5.15	124.81	119.56
1	A	210	VAL	C-N-CA	5.15	124.81	119.56
1	F	139	THR	N-CA-C	-5.14	105.68	111.28
3	L	10	DG	C1'-O4'-C4'	-5.11	102.04	109.70
1	D	423	ARG	N-CA-C	-5.10	106.75	113.17
1	D	292	SER	N-CA-C	5.09	118.32	110.42
1	D	382	ARG	N-CA-C	-5.08	100.62	108.90
3	L	7	DT	C1'-O4'-C4'	-5.06	102.11	109.70
1	D	311	LEU	N-CA-C	5.04	117.66	110.24
1	I	58	GLY	N-CA-C	-5.04	107.70	114.25
1	D	139	THR	CB-CA-C	-5.03	110.75	116.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	343	TRP	N-CA-C	5.03	116.84	111.36
1	I	139	THR	CB-CA-C	-5.01	110.77	116.54

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	111	ARG	Peptide
1	D	420	ARG	Peptide
1	F	396	ARG	Sidechain
1	I	111	ARG	Peptide
1	I	362	ARG	Sidechain

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	4970	0	4901	465	0
1	D	5059	0	4993	383	0
1	F	4978	0	4912	450	0
1	I	5025	0	4955	362	0
2	K	471	0	263	121	0
2	X	471	0	263	88	0
3	L	467	0	261	98	0
3	Y	467	0	261	86	0
4	A	31	0	13	5	0
4	F	31	0	13	11	0
5	A	2	0	0	0	0
5	D	1	0	0	0	0
5	F	2	0	0	0	0
5	I	1	0	0	0	0
6	A	6	0	0	0	0
6	D	28	0	0	7	0
6	F	26	0	0	3	0
6	I	36	0	0	3	0
6	Y	1	0	0	0	0
All	All	22073	0	20835	1950	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 46.

All (1950) 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:D:576:LEU:O	1:D:617:ARG:HD2	1.30	1.30
1:I:171:GLY:O	1:I:172:LEU:HG	1.29	1.26
1:A:401:TYR:OH	1:A:421:PRO:HG2	1.36	1.26
1:D:592:PRO:HD3	1:D:644:PHE:CE2	1.69	1.25
1:A:194:ILE:HD11	1:A:198:ASP:CB	1.65	1.25
1:I:67:ASN:ND2	3:L:23:DT:H5'	1.53	1.23
2:X:2:DC:H2''	2:X:3:DA:C5'	1.68	1.22
1:I:661:PRO:O	1:I:662:ILE:HG13	1.07	1.21
1:F:394:GLU:HB3	1:F:514:LEU:HD11	1.21	1.19
1:A:14:ASN:ND2	1:A:15:PRO:HD2	1.58	1.18
2:X:2:DC:H2''	2:X:3:DA:H5'	1.24	1.17
1:F:401:TYR:OH	1:F:421:PRO:HG2	1.41	1.16
1:F:61:LEU:HD21	1:F:63:VAL:HG13	1.21	1.16
1:A:200:ILE:HG23	1:A:239:LEU:CD1	1.74	1.15
1:I:67:ASN:HD21	3:L:23:DT:H5'	1.00	1.15
3:Y:21:DT:H4'	3:Y:22:DT:OP1	1.43	1.15
3:L:3:DG:H2''	3:L:4:DA:OP2	1.38	1.13
1:A:188:LYS:HD3	1:A:193:ALA:O	1.50	1.12
1:A:194:ILE:HD11	1:A:198:ASP:CG	1.74	1.12
1:I:661:PRO:O	1:I:662:ILE:CG1	1.97	1.12
3:Y:5:DC:H2''	3:Y:6:DC:O5'	1.25	1.12
1:F:61:LEU:HD21	1:F:63:VAL:CG1	1.77	1.12
1:A:194:ILE:CD1	1:A:198:ASP:HB3	1.80	1.11
1:F:257:ASP:OD2	1:F:313:LYS:HE3	1.50	1.11
3:L:5:DC:H2''	3:L:6:DC:O5'	1.33	1.11
1:A:194:ILE:HD11	1:A:198:ASP:HB3	1.15	1.11
1:F:569:THR:HG21	2:K:22:DT:OP1	1.51	1.11
1:I:174:ARG:HG3	1:I:175:ASP:N	1.63	1.11
1:I:574:LYS:HA	1:I:617:ARG:HH21	1.15	1.10
1:A:34:ALA:CB	1:A:616:THR:HG21	1.79	1.10
2:X:1:DG:H2''	2:X:2:DC:O5'	1.41	1.10
1:A:34:ALA:HB3	1:A:616:THR:HG21	1.26	1.10
1:A:194:ILE:CD1	1:A:198:ASP:CB	2.29	1.10
1:A:194:ILE:CG1	1:A:198:ASP:CB	2.30	1.09
1:I:174:ARG:CG	1:I:175:ASP:H	1.62	1.09
1:D:67:ASN:OD1	3:Y:23:DT:H5'	1.52	1.09
1:F:552:ARG:O	1:F:556:GLU:HG3	1.52	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:12:DA:H2''	2:X:13:DG:O5'	1.49	1.09
1:F:34:ALA:CB	1:F:616:THR:HG21	1.83	1.08
2:K:12:DA:H2''	2:K:13:DG:O5'	1.53	1.08
2:X:18:DT:H2''	2:X:19:DT:OP1	1.52	1.08
1:D:591:LEU:CG	1:D:592:PRO:HD2	1.84	1.07
3:L:17:DG:H4'	3:L:18:DC:OP1	1.47	1.07
1:D:210:VAL:HG12	1:D:213:VAL:HG23	1.31	1.07
3:L:6:DC:H2''	3:L:7:DT:O5'	1.55	1.07
1:F:61:LEU:CD2	1:F:63:VAL:HG13	1.85	1.07
1:D:591:LEU:HG	1:D:592:PRO:HD2	1.10	1.06
3:Y:17:DG:H4'	3:Y:18:DC:OP1	1.52	1.06
1:A:132:ILE:HD11	1:A:183:ARG:HH21	1.20	1.05
1:F:394:GLU:HB3	1:F:514:LEU:CD1	1.84	1.05
3:Y:3:DG:H2''	3:Y:4:DA:OP2	1.55	1.05
1:A:198:ASP:HA	1:A:201:THR:OG1	1.57	1.04
1:D:504:GLY:O	1:D:508:GLN:HG3	1.57	1.04
1:D:634:GLY:O	1:D:635:LYS:HG2	1.56	1.04
3:Y:16:DT:H4'	3:Y:17:DG:OP1	1.52	1.04
1:F:426:GLY:HA3	2:K:8:DT:OP1	1.56	1.04
1:D:592:PRO:HD3	1:D:644:PHE:HE2	0.91	1.04
1:A:194:ILE:CD1	1:A:198:ASP:CG	2.30	1.03
1:D:575:GLY:H	1:D:617:ARG:NH2	1.55	1.03
1:F:589:GLY:O	1:F:593:SER:HA	1.58	1.03
1:F:394:GLU:CB	1:F:514:LEU:HD11	1.87	1.03
1:A:167:PRO:HB2	1:A:173:PRO:HD2	1.35	1.03
1:F:632:GLN:HG2	2:K:19:DT:H72	1.36	1.03
1:D:396:ARG:HB3	6:D:2020:HOH:O	1.58	1.02
1:I:172:LEU:HD13	1:I:176:ALA:HB3	1.38	1.02
1:A:132:ILE:HG23	1:A:133:PRO:HD2	1.41	1.02
2:K:1:DG:H2''	2:K:2:DC:O5'	1.53	1.02
1:I:233:ASN:ND2	1:I:236:GLN:HG3	1.75	1.01
1:I:576:LEU:O	1:I:617:ARG:HD2	1.60	1.01
3:L:12:DG:H2''	3:L:13:DC:C6	1.96	1.01
1:F:362:ARG:NH1	1:F:571:HIS:HE1	1.57	1.01
1:A:200:ILE:HG23	1:A:239:LEU:HD11	1.05	1.00
1:I:39:THR:O	1:I:43:ILE:HD12	1.60	1.00
3:Y:5:DC:C2'	3:Y:6:DC:O5'	2.09	1.00
3:L:21:DT:H4'	3:L:22:DT:OP1	1.56	1.00
1:A:545:LEU:HD21	1:A:551:MET:HG3	1.41	0.99
3:L:5:DC:C2'	3:L:6:DC:O5'	2.09	0.99
1:A:194:ILE:CG1	1:A:198:ASP:HB2	1.90	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:232:THR:HG23	1:D:270:ASN:HD22	1.26	0.99
1:I:67:ASN:ND2	3:L:23:DT:C5'	2.24	0.99
1:I:174:ARG:HG3	1:I:175:ASP:H	0.83	0.99
1:D:592:PRO:CD	1:D:644:PHE:CE2	2.45	0.99
1:F:65:PHE:O	1:F:66:THR:HG23	1.63	0.99
1:D:591:LEU:HG	1:D:592:PRO:CD	1.93	0.99
1:I:487:LEU:O	1:I:491:MET:HG3	1.63	0.99
1:F:362:ARG:HH12	1:F:571:HIS:CE1	1.81	0.99
1:F:586:VAL:CG1	1:F:591:LEU:HD22	1.92	0.99
2:K:14:DG:H2''	2:K:15:DT:H5''	1.43	0.99
1:I:67:ASN:HD21	3:L:23:DT:C5'	1.76	0.98
2:K:6:DG:H2''	2:K:7:DC:O5'	1.63	0.98
1:F:592:PRO:O	1:F:607:GLU:HG3	1.62	0.98
1:F:591:LEU:HB3	1:F:592:PRO:HD3	1.45	0.98
1:F:655:VAL:HG13	1:F:659:GLY:HA2	1.44	0.98
2:K:14:DG:H2''	2:K:15:DT:C5'	1.94	0.98
2:K:17:DG:H4'	2:K:18:DT:OP1	1.62	0.98
2:X:14:DG:H2''	2:X:15:DT:H5''	1.44	0.98
2:X:11:DC:H42	3:Y:8:DG:H1	1.08	0.98
1:A:14:ASN:HD22	1:A:15:PRO:HD2	1.26	0.97
1:A:200:ILE:O	1:A:203:THR:HB	1.63	0.97
2:K:1:DG:H1	3:L:18:DC:N4	1.61	0.97
2:X:6:DG:H2''	2:X:7:DC:O5'	1.61	0.97
2:K:9:DC:OP2	2:K:9:DC:H2'	1.64	0.97
3:L:16:DT:H4'	3:L:17:DG:OP1	1.65	0.96
1:A:268:ILE:O	1:A:271:ILE:HG13	1.65	0.96
1:D:56:HIS:CD2	1:D:57:PRO:HD2	1.99	0.96
1:D:655:VAL:HG12	1:D:656:ASP:O	1.64	0.96
2:K:3:DA:H2''	2:K:4:DG:OP2	1.62	0.96
2:K:19:DT:H4'	2:K:20:DT:H5''	1.44	0.96
1:I:232:THR:HG23	1:I:270:ASN:HD22	1.29	0.95
2:K:18:DT:H2''	2:K:19:DT:OP1	1.60	0.95
1:A:43:ILE:HD11	1:A:73:MET:CG	1.96	0.95
1:F:34:ALA:HB3	1:F:616:THR:HG21	1.45	0.95
2:X:1:DG:H1	3:Y:18:DC:N4	1.64	0.95
1:D:592:PRO:CD	1:D:644:PHE:HE2	1.79	0.95
1:A:267:ASP:HB3	1:A:270:ASN:HB2	1.48	0.94
1:A:552:ARG:O	1:A:556:GLU:HG3	1.67	0.94
1:F:32:ALA:HB2	1:F:286:LEU:HB2	1.49	0.94
1:D:210:VAL:CG1	1:D:213:VAL:HG23	1.96	0.94
1:D:575:GLY:N	1:D:617:ARG:HH21	1.66	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:TYR:CE2	1:A:271:ILE:HA	2.04	0.93
3:Y:14:DA:H2'	3:Y:14:DA:OP2	1.67	0.93
1:F:655:VAL:CG1	1:F:659:GLY:HA2	1.99	0.93
3:L:19:DT:O2	3:L:19:DT:H2'	1.65	0.93
1:F:167:PRO:HB2	1:F:173:PRO:HD2	1.50	0.93
1:A:592:PRO:O	1:A:607:GLU:HG3	1.67	0.93
1:D:332:ASP:HB3	1:D:335:ALA:H	1.33	0.92
1:F:303:LEU:HD13	1:F:611:PHE:CE1	2.04	0.92
1:D:294:ALA:HB3	1:D:321:ALA:HA	1.51	0.92
2:X:11:DC:N4	3:Y:8:DG:H1	1.67	0.92
1:I:487:LEU:HA	1:I:490:VAL:HG22	1.47	0.92
2:X:8:DT:H2'	2:X:9:DC:C6	2.04	0.92
1:I:428:THR:HG23	3:L:8:DG:OP2	1.70	0.92
1:A:32:ALA:HB2	1:A:286:LEU:HB2	1.50	0.92
1:F:401:TYR:HH	1:F:421:PRO:HG2	1.25	0.92
3:L:14:DA:H2'	3:L:14:DA:OP2	1.69	0.92
1:A:257:ASP:OD2	1:A:313:LYS:HE3	1.67	0.92
1:A:591:LEU:HB3	1:A:592:PRO:HD3	1.52	0.91
1:I:127:GLU:HG2	1:I:187:ARG:NH1	1.84	0.91
1:I:592:PRO:HG3	1:I:644:PHE:CE2	2.06	0.91
1:I:462:HIS:O	1:I:466:GLU:HG3	1.70	0.91
1:F:362:ARG:HH12	1:F:571:HIS:HE1	0.92	0.91
2:X:14:DG:H2''	2:X:15:DT:C5'	2.00	0.91
1:F:591:LEU:HD23	1:F:642:SER:CB	2.01	0.91
1:I:31:ILE:HG21	1:I:313:LYS:HD3	1.53	0.91
1:D:487:LEU:HA	1:D:490:VAL:HG22	1.52	0.90
1:F:194:ILE:HG13	1:F:198:ASP:HB3	1.52	0.90
1:A:200:ILE:CG2	1:A:239:LEU:HD11	1.99	0.90
1:A:236:GLN:O	1:A:240:THR:HG23	1.72	0.90
1:D:577:GLU:HB2	1:D:619:MET:HE3	1.53	0.89
1:A:114:VAL:HG21	1:A:403:ARG:HD2	1.53	0.89
1:D:575:GLY:H	1:D:617:ARG:HH21	0.90	0.89
1:I:331:THR:HA	1:I:628:GLN:HG3	1.51	0.89
1:F:97:VAL:HG11	1:F:544:LEU:HD11	1.53	0.89
1:F:545:LEU:HD21	1:F:551:MET:HG3	1.54	0.89
3:L:14:DA:H1'	3:L:15:DC:OP1	1.73	0.89
1:A:230:GLN:HG2	1:A:255:ASP:H	1.34	0.89
3:Y:13:DC:H2''	3:Y:14:DA:C8	2.08	0.89
3:Y:14:DA:H1'	3:Y:15:DC:OP1	1.73	0.89
2:K:11:DC:H42	3:L:8:DG:H1	1.21	0.89
1:D:164:SER:O	1:D:174:ARG:HD3	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ARG:CG	1:A:270:ASN:HD21	1.84	0.88
1:F:579:PRO:HA	1:F:619:MET:HB2	1.55	0.88
1:D:524:TRP:CH2	1:D:541:ASP:OD2	2.25	0.88
1:F:200:ILE:HG23	1:F:239:LEU:CD1	2.02	0.88
1:A:43:ILE:HD11	1:A:73:MET:HG3	1.56	0.88
1:I:593:SER:OG	3:L:19:DT:H73	1.73	0.88
1:A:229:TYR:HE2	1:A:271:ILE:HA	1.37	0.87
1:D:661:PRO:O	1:D:662:ILE:HB	1.71	0.87
1:A:194:ILE:HG13	1:A:198:ASP:HB2	1.53	0.87
1:A:591:LEU:HB3	1:A:592:PRO:CD	2.04	0.87
3:L:3:DG:C2'	3:L:4:DA:OP2	2.22	0.87
1:D:576:LEU:O	1:D:617:ARG:CD	2.22	0.87
1:A:267:ASP:HB3	1:A:270:ASN:CB	2.04	0.87
1:A:234:ARG:HG3	1:A:270:ASN:HD21	1.37	0.87
1:I:171:GLY:O	1:I:172:LEU:CG	2.21	0.87
1:D:524:TRP:HH2	1:D:541:ASP:OD2	1.57	0.87
1:I:56:HIS:ND1	1:I:57:PRO:HD2	1.88	0.87
1:F:586:VAL:HG12	1:F:591:LEU:HD22	1.56	0.87
1:D:114:VAL:HG13	1:D:193:ALA:HB2	1.58	0.86
2:X:6:DG:H2''	2:X:7:DC:C5'	2.05	0.86
1:I:160:ASP:HA	1:I:163:ARG:HG3	1.58	0.86
1:A:421:PRO:HA	1:A:499:LEU:HD11	1.56	0.86
1:I:294:ALA:HB3	1:I:321:ALA:HA	1.57	0.86
1:F:606:GLU:HA	1:F:609:ARG:NH1	1.90	0.86
1:I:14:ASN:OD1	1:I:15:PRO:HD2	1.76	0.86
1:A:229:TYR:HE2	1:A:271:ILE:CA	1.90	0.85
1:F:76:ARG:HA	1:F:79:HIS:NE2	1.91	0.85
3:L:12:DG:H2''	3:L:13:DC:C5	2.12	0.85
1:F:586:VAL:HG13	1:F:591:LEU:HD22	1.59	0.85
2:K:21:DT:H5'	2:K:22:DT:OP2	1.77	0.85
1:I:634:GLY:O	1:I:635:LYS:HG2	1.77	0.84
1:A:132:ILE:CG2	1:A:133:PRO:HD2	2.05	0.84
1:D:459:ARG:O	1:D:462:HIS:CE1	2.30	0.84
3:L:12:DG:C2'	3:L:13:DC:C5	2.60	0.84
1:I:233:ASN:ND2	1:I:236:GLN:CG	2.40	0.84
1:D:126:LYS:HA	1:D:129:MET:HE2	1.60	0.84
1:F:65:PHE:O	1:F:66:THR:CG2	2.25	0.84
1:I:210:VAL:HG12	1:I:213:VAL:HG23	1.60	0.84
1:D:308:THR:HG22	1:D:605:GLU:OE2	1.77	0.83
1:F:422:ARG:HD2	2:K:9:DC:H3'	1.59	0.83
2:K:19:DT:H2''	2:K:20:DT:O5'	1.76	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:420:ARG:HB2	1:F:421:PRO:HD3	1.61	0.83
1:A:660:GLN:HB2	1:A:661:PRO:HD3	1.60	0.83
1:D:487:LEU:O	1:D:491:MET:HG3	1.76	0.83
1:F:655:VAL:HG12	1:F:656:ASP:O	1.78	0.83
1:A:34:ALA:HB3	1:A:616:THR:CG2	2.08	0.83
1:D:46:ILE:O	1:D:50:ILE:HD12	1.78	0.83
1:D:14:ASN:OD1	1:D:15:PRO:HD2	1.76	0.83
1:F:45:ARG:HD2	1:F:251:LEU:HD22	1.61	0.83
1:A:65:PHE:O	1:A:66:THR:CG2	2.27	0.83
1:D:362:ARG:HH12	1:D:593:SER:HB3	1.44	0.83
1:I:173:PRO:O	1:I:174:ARG:O	1.96	0.82
1:F:32:ALA:CB	1:F:286:LEU:HB2	2.09	0.82
2:K:8:DT:H2'	2:K:9:DC:C6	2.15	0.82
1:F:45:ARG:HD3	1:F:225:HIS:HE1	1.44	0.82
1:I:9:LEU:HD23	1:I:18:ALA:O	1.80	0.82
1:F:655:VAL:HG13	1:F:659:GLY:CA	2.10	0.82
2:K:8:DT:C2'	2:K:9:DC:C6	2.62	0.82
1:I:661:PRO:C	1:I:662:ILE:HG13	2.04	0.82
1:A:194:ILE:HG13	1:A:198:ASP:CB	2.10	0.81
1:I:574:LYS:HA	1:I:617:ARG:NH2	1.95	0.81
1:A:577:GLU:CG	1:A:619:MET:HE3	2.09	0.81
2:X:17:DG:H1	3:Y:2:DC:H42	1.27	0.81
1:A:43:ILE:HD11	1:A:73:MET:HG2	1.62	0.81
1:A:229:TYR:CE2	1:A:271:ILE:CA	2.63	0.81
1:A:401:TYR:HH	1:A:421:PRO:HG2	1.43	0.81
3:Y:13:DC:H2''	3:Y:14:DA:H8	1.43	0.81
1:F:303:LEU:HD13	1:F:611:PHE:CD1	2.15	0.81
1:D:331:THR:HA	1:D:628:GLN:HB2	1.63	0.80
1:F:577:GLU:CG	1:F:619:MET:HE3	2.11	0.80
1:F:592:PRO:O	1:F:607:GLU:CG	2.29	0.80
3:L:14:DA:C1'	3:L:15:DC:OP1	2.30	0.80
1:A:24:PHE:CD2	1:A:25:THR:HG23	2.15	0.80
1:A:198:ASP:CA	1:A:201:THR:OG1	2.30	0.80
1:F:200:ILE:HG23	1:F:239:LEU:HD11	1.62	0.80
2:X:12:DA:C2'	2:X:13:DG:O5'	2.30	0.80
3:L:14:DA:C4'	3:L:15:DC:OP1	2.30	0.80
3:L:14:DA:OP2	3:L:14:DA:C2'	2.30	0.80
3:Y:6:DC:H2''	3:Y:7:DT:O5'	1.82	0.80
3:Y:14:DA:C1'	3:Y:15:DC:OP1	2.30	0.80
1:F:194:ILE:CG1	1:F:198:ASP:HB3	2.12	0.80
1:F:611:PHE:CE1	1:F:615:ILE:HD11	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:6:DG:C2'	2:X:7:DC:O5'	2.30	0.79
1:A:65:PHE:O	1:A:66:THR:HG23	1.82	0.79
1:D:363:THR:O	1:D:366:GLN:HG3	1.80	0.79
1:I:39:THR:O	1:I:43:ILE:CD1	2.29	0.79
1:I:655:VAL:HG12	1:I:656:ASP:O	1.83	0.79
1:D:48:HIS:NE2	1:D:52:HIS:ND1	2.29	0.79
1:D:606:GLU:HA	1:D:609:ARG:NH1	1.96	0.79
3:Y:1:DA:H2''	3:Y:2:DC:O5'	1.81	0.79
1:A:615:ILE:HG23	1:A:622:LEU:HD22	1.65	0.79
1:I:362:ARG:NH1	1:I:593:SER:HB3	1.97	0.79
1:D:631:MET:HB2	1:D:635:LYS:O	1.83	0.79
1:I:172:LEU:HD13	1:I:176:ALA:CB	2.12	0.79
3:Y:6:DC:H2''	3:Y:7:DT:C5'	2.12	0.79
3:Y:14:DA:C4'	3:Y:15:DC:OP1	2.30	0.79
3:Y:14:DA:OP2	3:Y:14:DA:C2'	2.30	0.79
1:A:587:GLU:CD	1:A:630:ARG:HH12	1.91	0.79
2:K:2:DC:H2''	2:K:3:DA:H5'	1.64	0.79
1:F:122:LEU:HA	1:F:125:ILE:HD12	1.63	0.78
1:D:560:ALA:HB1	1:D:561:PRO:HD2	1.65	0.78
2:K:9:DC:OP2	2:K:9:DC:C2'	2.30	0.78
1:D:39:THR:O	1:D:43:ILE:CD1	2.31	0.78
1:F:362:ARG:NH1	1:F:571:HIS:CE1	2.45	0.78
1:A:302:LYS:O	1:A:305:GLU:HG2	1.84	0.78
1:A:654:THR:O	1:A:661:PRO:C	2.27	0.78
1:I:357:MET:HG2	1:I:580:VAL:HB	1.64	0.78
1:D:357:MET:HG2	1:D:580:VAL:HB	1.66	0.78
3:Y:3:DG:C2'	3:Y:4:DA:OP2	2.32	0.78
1:A:194:ILE:HG13	1:A:198:ASP:OD2	1.83	0.78
1:D:591:LEU:CB	1:D:592:PRO:HD2	2.14	0.78
2:K:19:DT:C4'	2:K:20:DT:H5''	2.14	0.78
1:A:424:GLY:O	1:A:463:LYS:CD	2.32	0.78
1:F:589:GLY:O	1:F:593:SER:CA	2.32	0.78
1:I:23:HIS:CE1	1:I:28:ALA:HB2	2.18	0.78
3:Y:19:DT:O2	3:Y:19:DT:H2'	1.82	0.78
1:D:389:PHE:HB3	1:D:392:ARG:HB2	1.66	0.77
1:F:569:THR:HG23	1:F:572:ASN:H	1.48	0.77
1:F:488:ARG:HH11	1:F:518:VAL:HG11	1.49	0.77
3:L:11:DA:C4	3:L:12:DG:C8	2.73	0.77
1:A:257:ASP:O	1:A:609:ARG:HG3	1.84	0.77
1:F:577:GLU:CD	1:F:619:MET:HE3	2.10	0.77
1:I:399:LEU:O	1:I:403:ARG:HG2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:X:2:DC:H2''	2:X:3:DA:H5''	1.65	0.77
1:A:655:VAL:HG13	1:A:659:GLY:HA2	1.66	0.77
1:F:248:ARG:HH12	1:F:279:PRO:HD2	1.49	0.77
1:I:577:GLU:CD	1:I:619:MET:HE3	2.09	0.77
1:A:26:GLY:HA2	1:A:248:ARG:O	1.84	0.77
1:D:125:ILE:O	1:D:129:MET:HG3	1.85	0.77
1:D:127:GLU:HG2	1:D:187:ARG:NH1	2.00	0.77
3:L:11:DA:C5	3:L:12:DG:N7	2.52	0.77
1:A:586:VAL:HG13	1:A:591:LEU:HD22	1.67	0.77
1:D:577:GLU:CD	1:D:619:MET:CE	2.58	0.77
1:I:48:HIS:NE2	1:I:52:HIS:ND1	2.31	0.77
1:A:579:PRO:HA	1:A:619:MET:HB2	1.66	0.77
1:A:35:GLY:H	4:A:1662:ANP:HNB1	1.33	0.76
1:A:196:PHE:O	1:A:199:LEU:HB2	1.85	0.76
3:L:11:DA:H2''	3:L:12:DG:H5''	1.67	0.76
1:F:634:GLY:HA2	3:L:1:DA:H5'	1.66	0.76
2:K:8:DT:H2''	2:K:9:DC:O4'	1.85	0.76
3:L:12:DG:C4	3:L:13:DC:C4	2.72	0.76
1:D:291:ARG:HH11	1:D:577:GLU:HB3	1.49	0.76
1:I:428:THR:HG21	3:L:7:DT:H3'	1.66	0.76
1:F:591:LEU:CB	1:F:592:PRO:HD3	2.16	0.76
1:F:500:LEU:HD22	1:F:511:LEU:HB3	1.65	0.76
3:L:11:DA:C6	3:L:12:DG:C5	2.74	0.76
2:X:2:DC:C2'	2:X:3:DA:C5'	2.60	0.76
2:X:8:DT:H2''	2:X:9:DC:O4'	1.86	0.76
1:A:194:ILE:CD1	1:A:198:ASP:OD2	2.34	0.75
1:F:60:ILE:HG12	1:F:223:PHE:HB2	1.66	0.75
1:I:142:ARG:HE	1:I:145:ARG:HH21	1.33	0.75
3:Y:21:DT:C4'	3:Y:22:DT:OP1	2.23	0.75
1:I:279:PRO:O	1:I:280:ASP:CG	2.29	0.75
2:K:1:DG:C2'	2:K:2:DC:O5'	2.34	0.75
1:A:195:ASP:OD1	1:A:198:ASP:CG	2.30	0.75
1:D:437:ALA:HA	1:D:442:THR:HG22	1.68	0.75
1:I:47:ALA:HB2	1:I:80:LEU:CD1	2.15	0.75
1:F:393:ARG:HG3	1:F:397:ASP:OD2	1.87	0.75
1:I:279:PRO:O	1:I:280:ASP:OD1	2.05	0.75
1:D:56:HIS:CD2	1:D:57:PRO:CD	2.69	0.75
1:A:32:ALA:CB	1:A:286:LEU:HB2	2.16	0.75
1:A:195:ASP:CG	1:A:198:ASP:OD2	2.30	0.75
1:I:441:HIS:HD2	6:I:2034:HOH:O	1.70	0.75
1:A:196:PHE:O	1:A:197:GLY:C	2.30	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:457:LEU:O	1:D:458:ASP:CG	2.30	0.75
1:I:428:THR:CG2	3:L:8:DG:OP2	2.34	0.75
3:L:14:DA:H4'	3:L:15:DC:OP1	1.83	0.75
1:D:660:GLN:HE22	1:I:76:ARG:HG2	1.52	0.74
1:F:34:ALA:CB	1:F:616:THR:CG2	2.63	0.74
1:A:101:ARG:HH22	1:A:536:ALA:HB3	1.52	0.74
1:A:500:LEU:HD22	1:A:511:LEU:HB3	1.66	0.74
1:I:391:ASP:HB2	1:I:547:SER:HA	1.70	0.74
3:Y:3:DG:H1'	3:Y:4:DA:H5'	1.69	0.74
1:D:415:ARG:HB3	1:D:416:ARG:HH11	1.53	0.74
1:D:507:GLY:O	1:D:508:GLN:HB2	1.87	0.74
2:K:19:DT:OP1	2:K:19:DT:O2	2.06	0.74
1:D:142:ARG:O	1:D:145:ARG:N	2.19	0.74
1:F:42:LEU:O	1:F:46:ILE:HD12	1.87	0.74
1:F:45:ARG:HD2	1:F:251:LEU:CD2	2.17	0.74
1:I:331:THR:HA	1:I:628:GLN:CG	2.17	0.74
1:I:262:LYS:HB3	1:I:606:GLU:OE1	1.87	0.74
1:A:195:ASP:CG	1:A:198:ASP:CG	2.56	0.74
1:D:362:ARG:NH1	1:D:607:GLU:OE2	2.21	0.73
1:I:408:PRO:O	1:I:409:ALA:HB3	1.87	0.73
1:F:569:THR:CG2	1:F:572:ASN:H	2.00	0.73
1:A:268:ILE:HG23	1:A:269:GLN:N	2.03	0.73
1:I:524:TRP:CH2	1:I:541:ASP:OD2	2.41	0.73
1:I:437:ALA:HA	1:I:442:THR:HG22	1.69	0.73
2:K:14:DG:H2'	2:K:15:DT:H72	1.70	0.73
1:A:357:MET:HG2	1:A:580:VAL:HB	1.70	0.73
3:L:9:DC:H2''	3:L:10:DG:O4'	1.87	0.73
1:I:656:ASP:OD1	1:I:657:PRO:HD2	1.88	0.73
1:A:132:ILE:HD11	1:A:183:ARG:NH2	2.02	0.73
1:I:514:LEU:O	1:I:518:VAL:HG23	1.88	0.73
3:L:12:DG:H2''	3:L:13:DC:H6	1.51	0.73
1:A:26:GLY:H	1:A:249:ASN:HD22	1.36	0.73
1:A:43:ILE:CD1	1:A:73:MET:HG2	2.19	0.73
1:F:422:ARG:NE	2:K:10:DG:OP2	2.22	0.73
2:X:18:DT:C2'	2:X:19:DT:OP1	2.35	0.73
1:I:103:TYR:CD2	1:I:213:VAL:HG13	2.24	0.73
1:A:69:ALA:O	1:A:73:MET:HB2	1.89	0.72
1:A:121:GLN:O	1:A:125:ILE:HD12	1.89	0.72
1:D:264[A]:ARG:HB3	1:D:264[A]:ARG:HH11	1.54	0.72
1:D:362:ARG:NH1	1:D:593:SER:HB3	2.04	0.72
1:F:362:ARG:NH2	1:F:607:GLU:OE2	2.21	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:197:GLY:O	1:A:198:ASP:C	2.30	0.72
1:A:448:CYS:O	1:A:464:ALA:HB1	1.90	0.72
1:F:289:ASN:OD1	1:F:297:LEU:HD13	1.88	0.72
1:F:426:GLY:CA	2:K:8:DT:OP1	2.37	0.72
1:D:460:GLY:O	1:D:463:LYS:N	2.22	0.72
1:D:655:VAL:C	1:D:662:ILE:HD11	2.14	0.72
1:D:294:ALA:O	1:D:298:GLU:HG3	1.90	0.72
1:D:457:LEU:O	1:D:458:ASP:OD1	2.07	0.72
1:F:125:ILE:HD13	1:F:145:ARG:HB3	1.71	0.72
1:F:394:GLU:CB	1:F:514:LEU:CD1	2.57	0.72
1:I:576:LEU:O	1:I:617:ARG:CD	2.34	0.72
2:X:8:DT:C2'	2:X:9:DC:C6	2.73	0.72
1:D:656:ASP:HB2	1:D:657:PRO:HD2	1.69	0.72
1:A:14:ASN:HD22	1:A:15:PRO:CD	2.02	0.72
1:A:57:PRO:HG2	1:A:86:ASP:HB2	1.72	0.72
1:A:188:LYS:CD	1:A:193:ALA:O	2.33	0.72
1:A:34:ALA:CB	1:A:616:THR:CG2	2.65	0.72
1:F:101:ARG:HH22	1:F:536:ALA:HB3	1.55	0.72
1:F:362:ARG:NH2	2:K:21:DT:O2	2.22	0.72
1:F:569:THR:CG2	2:K:22:DT:OP1	2.37	0.72
1:I:9:LEU:HD13	1:I:48:HIS:ND1	2.05	0.72
1:A:569:THR:HG23	1:A:572:ASN:H	1.55	0.71
1:D:462:HIS:O	1:D:466:GLU:HG3	1.90	0.71
1:A:106:HIS:O	1:A:107:ILE:HG22	1.90	0.71
1:A:229:TYR:CD2	1:A:271:ILE:HB	2.25	0.71
1:A:497:LEU:HD21	1:A:501:ARG:CZ	2.20	0.71
1:F:34:ALA:HB3	1:F:616:THR:CG2	2.17	0.71
2:X:2:DC:H42	3:Y:17:DG:H1	1.37	0.71
2:K:17:DG:C4'	2:K:18:DT:OP1	2.38	0.71
1:A:66:THR:HG21	1:A:548:VAL:HG22	1.71	0.71
1:D:291:ARG:NH1	1:D:577:GLU:HB3	2.05	0.71
1:F:411:ASP:HB3	1:F:444:VAL:HG11	1.70	0.71
1:I:226:VAL:HG22	1:I:252:VAL:HG12	1.71	0.71
1:F:45:ARG:HD3	1:F:225:HIS:CE1	2.26	0.71
1:D:132:ILE:HD12	1:D:132:ILE:N	2.06	0.71
1:A:606:GLU:HA	1:A:609:ARG:NH1	2.05	0.71
1:D:142:ARG:HE	1:D:145:ARG:NH2	1.89	0.71
1:F:289:ASN:ND2	1:F:291:ARG:H	1.89	0.71
1:A:421:PRO:CA	1:A:499:LEU:HD11	2.20	0.71
1:A:569:THR:CG2	1:A:572:ASN:H	2.03	0.71
1:F:61:LEU:HD12	1:F:88:TRP:CD2	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:200:ILE:O	1:F:204:VAL:HG23	1.91	0.71
1:F:230:GLN:HG2	1:F:255:ASP:H	1.56	0.71
2:K:2:DC:H2"	2:K:3:DA:C5'	2.19	0.71
1:A:656:ASP:HB3	1:A:661:PRO:HD2	1.71	0.70
1:F:426:GLY:HA3	2:K:8:DT:P	2.31	0.70
1:D:318:VAL:HG12	1:D:318:VAL:O	1.89	0.70
1:F:188:LYS:HD3	1:F:193:ALA:O	1.90	0.70
1:A:194:ILE:CG1	1:A:198:ASP:HB3	2.13	0.70
1:F:107:ILE:CG2	1:F:205:ARG:HH22	2.05	0.70
1:F:194:ILE:HG13	1:F:198:ASP:CB	2.20	0.70
2:K:2:DC:H2"	2:K:3:DA:OP2	1.88	0.70
1:D:9:LEU:HD13	1:D:48:HIS:ND1	2.05	0.70
1:F:592:PRO:O	1:F:607:GLU:CD	2.34	0.70
3:Y:18:DC:H2"	3:Y:19:DT:OP2	1.85	0.70
2:K:15:DT:H6	2:K:15:DT:H5'	1.56	0.70
1:D:39:THR:O	1:D:43:ILE:HD12	1.90	0.70
1:I:239:LEU:O	1:I:243:LEU:HD12	1.91	0.70
1:I:593:SER:OG	3:L:19:DT:C7	2.40	0.70
2:K:11:DC:N4	3:L:8:DG:H1	1.87	0.70
1:A:535:ILE:HG23	1:A:536:ALA:H	1.56	0.70
1:A:591:LEU:CB	1:A:592:PRO:HD3	2.22	0.70
1:D:232:THR:CG2	1:D:270:ASN:HD22	2.02	0.70
1:A:422:ARG:HG3	2:X:10:DG:OP1	1.91	0.70
2:K:8:DT:H2"	2:K:9:DC:C6	2.26	0.70
1:A:393:ARG:NH2	3:Y:4:DA:OP1	2.24	0.70
1:F:61:LEU:HD21	1:F:63:VAL:HG12	1.72	0.70
1:I:574:LYS:CA	1:I:617:ARG:HH21	2.00	0.70
3:Y:11:DA:C6	3:Y:12:DG:C5	2.80	0.70
1:D:460:GLY:O	1:D:461:ALA:C	2.35	0.69
1:F:114:VAL:HG21	1:F:403:ARG:HD3	1.74	0.69
1:D:287:GLU:HG2	1:D:314:THR:H	1.58	0.69
1:F:404:LEU:HD13	1:F:410:ASP:O	1.92	0.69
1:F:436:TRP:HA	1:F:439:THR:HG22	1.73	0.69
1:F:632:GLN:HG2	2:K:19:DT:C7	2.17	0.69
1:F:58:GLY:HA2	1:F:86:ASP:O	1.92	0.69
1:I:9:LEU:CD1	1:I:48:HIS:ND1	2.55	0.69
1:I:31:ILE:CG2	1:I:313:LYS:HD3	2.21	0.69
1:F:591:LEU:HB3	1:F:592:PRO:CD	2.21	0.69
1:I:46:ILE:O	1:I:50:ILE:HD12	1.93	0.69
1:A:422:ARG:NE	2:X:10:DG:OP2	2.26	0.69
1:D:264[A]:ARG:HB3	1:D:264[A]:ARG:NH1	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:MET:HB2	1:A:636:THR:CG2	2.22	0.69
1:D:56:HIS:HB3	1:D:59:GLU:HG3	1.73	0.69
1:D:132:ILE:HG23	1:D:133:PRO:HD2	1.75	0.69
1:D:275:GLN:HE21	1:D:276:LYS:HG3	1.58	0.69
1:D:396:ARG:CB	6:D:2020:HOH:O	2.27	0.69
1:F:608:ARG:HB2	1:F:644:PHE:CE1	2.27	0.69
1:I:210:VAL:CG1	1:I:213:VAL:HG23	2.22	0.69
1:A:194:ILE:HG12	1:A:198:ASP:CB	2.21	0.69
1:A:258:GLN:NE2	4:A:1662:ANP:O2G	2.26	0.69
1:A:417:ILE:O	1:A:421:PRO:HD2	1.92	0.69
1:F:631:MET:HB2	1:F:636:THR:HG22	1.74	0.69
1:I:377:VAL:O	1:I:377:VAL:HG12	1.93	0.69
1:A:231:ASP:HB3	1:A:261:TYR:HB2	1.75	0.69
3:L:11:DA:C6	3:L:12:DG:C6	2.81	0.69
1:A:42:LEU:O	1:A:46:ILE:HD12	1.93	0.68
1:A:229:TYR:CE2	1:A:271:ILE:CB	2.76	0.68
1:F:569:THR:HG22	1:F:572:ASN:HB2	1.75	0.68
1:I:123:ASP:OD2	1:I:415:ARG:NH1	2.26	0.68
1:A:77:ALA:O	1:A:81:VAL:N	2.26	0.68
1:D:142:ARG:HE	1:D:145:ARG:HH21	1.41	0.68
1:A:388:GLY:HA2	1:A:556:GLU:OE2	1.93	0.68
1:A:660:GLN:CB	1:A:661:PRO:HD3	2.24	0.68
1:D:23:HIS:CE1	1:D:28:ALA:HB2	2.28	0.68
1:A:194:ILE:HG12	1:A:198:ASP:HB2	1.72	0.68
1:D:348:HIS:HA	1:D:352:ARG:O	1.94	0.68
1:D:487:LEU:HA	1:D:490:VAL:CG2	2.24	0.68
1:F:631:MET:HB2	1:F:636:THR:CG2	2.23	0.68
1:I:591:LEU:HB3	1:I:592:PRO:HD3	1.76	0.68
3:L:3:DG:H1'	3:L:4:DA:H5'	1.75	0.68
1:I:394:GLU:CD	1:I:510:ARG:HG2	2.19	0.68
3:L:12:DG:C5	3:L:13:DC:N4	2.62	0.68
1:A:229:TYR:CE2	1:A:271:ILE:HB	2.27	0.68
1:A:577:GLU:HG3	1:A:619:MET:HE3	1.75	0.68
1:D:93:HIS:NE2	3:Y:23:DT:O2	2.27	0.68
1:F:418:ILE:HD11	1:F:425:ILE:HG13	1.76	0.68
2:K:3:DA:H5'	2:K:3:DA:C8	2.29	0.68
1:I:48:HIS:CD2	1:I:52:HIS:HB3	2.30	0.67
2:X:8:DT:H2'	2:X:9:DC:H6	1.54	0.67
1:A:187:ARG:NH2	1:A:411:ASP:OD2	2.27	0.67
1:A:215:ASP:HA	1:A:218:GLN:OE1	1.94	0.67
1:A:471:MET:SD	1:A:474:MET:HE2	2.34	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:231:ASP:OD2	1:D:574:LYS:NZ	2.28	0.67
1:D:577:GLU:CB	1:D:619:MET:HE3	2.23	0.67
1:I:336:GLU:HB2	1:I:625:THR:HG21	1.75	0.67
1:I:655:VAL:HG11	1:I:659:GLY:HA2	1.76	0.67
1:D:38:LYS:NZ	1:D:227:ASP:OD1	2.25	0.67
1:F:613:VAL:O	1:F:617:ARG:CD	2.42	0.67
2:X:1:DG:C2'	2:X:2:DC:O5'	2.27	0.67
1:D:294:ALA:HB3	1:D:321:ALA:CA	2.23	0.67
1:F:615:ILE:HG23	1:F:622:LEU:HD22	1.76	0.67
1:I:392:ARG:NH1	1:I:546:SER:HB2	2.09	0.67
1:A:200:ILE:CG2	1:A:239:LEU:CD1	2.64	0.67
1:A:414:LEU:HA	1:A:417:ILE:HD11	1.77	0.67
1:D:67:ASN:OD1	3:Y:23:DT:C5'	2.39	0.67
1:D:416:ARG:O	1:D:420:ARG:NH1	2.27	0.67
1:I:152:LYS:NZ	1:I:198:ASP:OD1	2.27	0.67
1:I:348:HIS:HA	1:I:352:ARG:O	1.95	0.67
2:K:11:DC:H2''	2:K:12:DA:O5'	1.95	0.67
2:K:21:DT:H5''	2:K:22:DT:H72	1.75	0.67
3:L:12:DG:C2'	3:L:13:DC:H5	2.07	0.67
1:A:545:LEU:HD21	1:A:551:MET:CG	2.22	0.67
1:D:399:LEU:O	1:D:403:ARG:HG2	1.95	0.67
1:F:448:CYS:O	1:F:464:ALA:HB1	1.95	0.67
1:F:401:TYR:OH	1:F:421:PRO:CG	2.34	0.67
1:I:500:LEU:O	1:I:504:GLY:HA3	1.95	0.67
1:A:232:THR:HG22	1:A:271:ILE:HG22	1.77	0.67
1:A:257:ASP:OD1	1:A:310:ARG:HD2	1.95	0.67
1:D:142:ARG:NE	1:D:145:ARG:NH2	2.43	0.67
1:F:418:ILE:HG12	1:F:425:ILE:HG21	1.77	0.67
1:D:39:THR:O	1:D:43:ILE:HD13	1.95	0.66
1:F:155:LEU:HD23	1:F:201:THR:HG22	1.76	0.66
1:F:224:ILE:HG22	1:F:250:LEU:HD12	1.77	0.66
1:I:631:MET:HB2	1:I:635:LYS:O	1.95	0.66
1:F:291:ARG:NH2	4:F:1663:ANP:HNB1	1.93	0.66
1:F:377:VAL:O	1:F:378:GLN:CG	2.42	0.66
1:F:587:GLU:OE2	1:F:630:ARG:NH2	2.26	0.66
1:F:606:GLU:HA	1:F:609:ARG:HH11	1.57	0.66
1:A:257:ASP:O	1:A:609:ARG:CG	2.44	0.66
1:F:377:VAL:O	1:F:378:GLN:CB	2.43	0.66
1:I:122:LEU:HD21	1:I:145:ARG:HE	1.60	0.66
3:Y:1:DA:C2'	3:Y:2:DC:O5'	2.43	0.66
1:A:72:GLU:O	1:A:76:ARG:HG3	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ILE:HG22	1:A:148:ILE:HD11	1.77	0.66
1:F:36:SER:N	4:F:1663:ANP:O2B	2.22	0.66
3:Y:6:DC:H2"	3:Y:7:DT:H5"	1.77	0.66
1:A:14:ASN:ND2	1:A:15:PRO:CD	2.47	0.66
1:F:107:ILE:HG21	1:F:205:ARG:HH22	1.60	0.66
1:I:47:ALA:CB	1:I:80:LEU:CD1	2.73	0.66
1:I:233:ASN:HD21	1:I:236:GLN:CG	2.08	0.66
1:A:194:ILE:CG1	1:A:198:ASP:OD2	2.43	0.66
1:D:103:TYR:CD2	1:D:213:VAL:HG13	2.31	0.66
2:K:12:DA:C6	2:K:13:DG:C6	2.84	0.66
1:D:577:GLU:CD	1:D:619:MET:HE3	2.21	0.65
1:F:120:ASP:OD1	1:F:396:ARG:NH2	2.29	0.65
1:I:173:PRO:O	1:I:174:ARG:C	2.39	0.65
1:A:23:HIS:CE1	1:A:28:ALA:HB2	2.31	0.65
1:A:587:GLU:OE2	1:A:630:ARG:NH1	2.24	0.65
1:F:132:ILE:HD11	1:F:183:ARG:HE	1.61	0.65
1:F:633:PHE:CE1	2:K:19:DT:C4	2.83	0.65
1:A:631:MET:HB2	1:A:636:THR:HG22	1.79	0.65
1:D:238:GLU:OE2	1:D:241:ARG:NH2	2.26	0.65
2:X:2:DC:N4	3:Y:17:DG:H1	1.95	0.65
1:A:144:ILE:HG22	1:A:148:ILE:CD1	2.27	0.65
1:A:229:TYR:O	1:A:271:ILE:HG21	1.97	0.65
1:F:591:LEU:HD11	1:F:611:PHE:HD2	1.60	0.65
1:F:200:ILE:HG22	1:F:235:ALA:HB1	1.78	0.65
1:F:258:GLN:HE22	4:F:1663:ANP:PG	2.19	0.65
1:A:60:ILE:HG12	1:A:223:PHE:HB2	1.78	0.65
3:L:11:DA:N6	3:L:12:DG:O6	2.30	0.65
1:D:21:ALA:HA	1:D:45:ARG:HB2	1.79	0.65
1:I:549:ASP:O	1:I:550:ASP:HB2	1.96	0.65
1:D:346:ARG:O	1:D:350:GLU:HG2	1.97	0.65
1:F:398:ILE:HD13	1:F:491:MET:HG2	1.78	0.65
1:A:196:PHE:O	1:A:199:LEU:N	2.30	0.64
1:A:198:ASP:O	1:A:200:ILE:N	2.30	0.64
1:A:234:ARG:HG2	1:A:270:ASN:HD21	1.61	0.64
1:F:395:ILE:O	1:F:399:LEU:HG	1.97	0.64
1:F:424:GLY:CA	2:K:9:DC:OP1	2.45	0.64
1:I:577:GLU:CD	1:I:619:MET:CE	2.69	0.64
2:K:9:DC:OP2	2:K:9:DC:C3'	2.45	0.64
1:A:152:LYS:HE3	1:A:195:ASP:OD2	1.96	0.64
1:D:460:GLY:O	1:D:462:HIS:N	2.29	0.64
1:F:334:ARG:NH1	1:F:376:ARG:HH12	1.95	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:632:GLN:CG	2:K:19:DT:H72	2.20	0.64
1:I:142:ARG:HE	1:I:145:ARG:NH2	1.95	0.64
1:I:360:LEU:HD23	1:I:570:LEU:HD23	1.79	0.64
1:I:362:ARG:HH12	1:I:593:SER:HB3	1.59	0.64
1:A:272:LEU:O	1:A:275:GLN:HG3	1.97	0.64
1:D:202:GLU:OE2	1:D:205:ARG:NH1	2.31	0.64
1:D:257:ASP:OD2	1:D:313:LYS:HE2	1.97	0.64
1:I:38:LYS:NZ	1:I:227:ASP:OD1	2.28	0.64
1:F:500:LEU:CD2	1:F:511:LEU:HB3	2.27	0.64
1:A:424:GLY:O	1:A:463:LYS:HD3	1.97	0.64
1:A:591:LEU:HD23	1:A:644:PHE:HD2	1.62	0.64
1:D:459:ARG:O	1:D:462:HIS:ND1	2.29	0.64
2:K:6:DG:C2'	2:K:7:DC:O5'	2.43	0.64
1:A:404:LEU:HD13	1:A:410:ASP:O	1.98	0.64
1:A:606:GLU:HA	1:A:609:ARG:HH11	1.62	0.64
1:D:167:PRO:HA	1:D:174:ARG:HG3	1.79	0.64
1:I:59:GLU:OE1	1:I:222:LYS:HD2	1.97	0.64
1:I:238:GLU:OE2	1:I:241:ARG:NH2	2.31	0.64
1:I:513:ASN:HA	1:I:516:GLU:HB3	1.80	0.64
1:A:59:GLU:HB3	1:A:222:LYS:HB3	1.80	0.63
1:I:462:HIS:O	1:I:466:GLU:CG	2.45	0.63
1:D:232:THR:HG23	1:D:270:ASN:ND2	2.06	0.63
1:F:107:ILE:HG22	1:F:107:ILE:O	1.96	0.63
1:A:32:ALA:O	1:A:38:LYS:HE3	1.98	0.63
3:L:22:DT:H71	3:L:23:DT:H73	1.79	0.63
1:A:33:GLY:O	1:A:38:LYS:NZ	2.22	0.63
1:F:591:LEU:HD23	1:F:642:SER:OG	1.98	0.63
2:K:17:DG:H2''	2:K:18:DT:H71	1.79	0.63
1:A:631:MET:HE3	1:A:636:THR:HG23	1.79	0.63
1:D:336:GLU:O	1:D:340:VAL:HG23	1.99	0.63
1:D:436:TRP:CZ3	1:D:442:THR:HG21	2.33	0.63
2:K:19:DT:H4'	2:K:20:DT:C5'	2.23	0.63
1:A:200:ILE:O	1:A:203:THR:N	2.31	0.63
1:F:26:GLY:HA2	1:F:248:ARG:O	1.98	0.63
1:D:164:SER:O	1:D:174:ARG:CD	2.47	0.63
2:X:21:DT:H5'	2:X:22:DT:OP2	1.99	0.63
1:F:362:ARG:NH1	1:F:610:LEU:HD22	2.14	0.63
1:A:114:VAL:HG13	1:A:193:ALA:HB2	1.79	0.62
1:A:200:ILE:O	1:A:203:THR:CB	2.43	0.62
1:D:613:VAL:O	1:D:617:ARG:HG2	1.99	0.62
1:F:27:PRO:HA	1:F:250:LEU:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:635:LYS:HB3	1:F:635:LYS:NZ	2.14	0.62
1:F:656:ASP:C	1:F:656:ASP:OD1	2.41	0.62
1:A:377:VAL:O	1:A:378:GLN:HB2	1.99	0.62
1:I:90:SER:HB2	1:I:94:SER:HB3	1.82	0.62
3:L:5:DC:H2''	3:L:6:DC:C5'	2.28	0.62
1:A:362:ARG:NH1	1:A:607:GLU:OE1	2.32	0.62
1:F:334:ARG:HH12	1:F:376:ARG:HH12	1.45	0.62
1:I:591:LEU:HD23	1:I:591:LEU:C	2.25	0.62
2:K:1:DG:C2'	2:K:2:DC:C6	2.82	0.62
1:A:195:ASP:OD1	1:A:195:ASP:C	2.42	0.62
1:I:126:LYS:HA	1:I:129:MET:HE2	1.82	0.62
1:I:226:VAL:CG2	1:I:252:VAL:HG12	2.29	0.62
1:F:257:ASP:HB3	1:F:304:ILE:CD1	2.29	0.62
1:A:61:LEU:HA	1:A:88:TRP:O	1.98	0.62
1:D:359:ILE:C	1:D:360:LEU:HD12	2.25	0.62
1:F:117:ASP:OD2	1:F:396:ARG:NH2	2.32	0.62
1:I:67:ASN:CG	3:L:23:DT:H5'	2.22	0.62
1:I:172:LEU:HD12	1:I:173:PRO:O	1.99	0.62
1:I:332:ASP:HB3	1:I:335:ALA:H	1.65	0.62
1:A:200:ILE:HG21	1:A:235:ALA:HB1	1.82	0.62
1:A:395:ILE:HD13	1:A:514:LEU:HD23	1.81	0.62
1:D:173:PRO:HG2	1:D:176:ALA:CB	2.29	0.62
1:I:142:ARG:NE	1:I:145:ARG:HH21	1.98	0.62
1:A:198:ASP:CA	1:A:201:THR:HG1	2.13	0.62
1:A:577:GLU:CD	1:A:619:MET:HE3	2.25	0.62
1:A:655:VAL:HG13	1:A:659:GLY:CA	2.29	0.62
1:F:415:ARG:CZ	1:F:434:MET:HE1	2.29	0.62
2:K:8:DT:H2'	2:K:9:DC:H6	1.65	0.62
1:F:33:GLY:HA2	1:F:313:LYS:HE2	1.80	0.62
1:F:417:ILE:O	1:F:421:PRO:HD2	2.00	0.62
1:I:336:GLU:OE1	1:I:625:THR:CG2	2.48	0.62
1:D:257:ASP:HA	1:D:310[A]:ARG:NH1	2.15	0.61
1:D:287:GLU:HG2	1:D:314:THR:O	2.00	0.61
1:F:57:PRO:HG2	1:F:86:ASP:HB2	1.82	0.61
1:F:91:THR:HG22	1:F:92:PHE:H	1.65	0.61
3:L:3:DG:H1'	3:L:4:DA:C8	2.34	0.61
1:A:26:GLY:H	1:A:249:ASN:ND2	1.97	0.61
1:D:33:GLY:HA2	1:D:255:ASP:OD2	2.00	0.61
1:F:91:THR:HG22	1:F:92:PHE:N	2.15	0.61
3:L:12:DG:C2	3:L:13:DC:N3	2.68	0.61
1:A:195:ASP:OD1	1:A:198:ASP:N	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:595:GLY:HA3	2:X:20:DT:H3	1.65	0.61
1:D:462:HIS:O	1:D:466:GLU:CG	2.48	0.61
1:F:36:SER:H	4:F:1663:ANP:PB	2.23	0.61
1:F:421:PRO:HA	1:F:499:LEU:HD11	1.83	0.61
1:F:424:GLY:HA2	2:K:9:DC:OP1	1.99	0.61
1:F:478:ALA:HA	1:F:486:PHE:CE1	2.36	0.61
1:I:313:LYS:O	1:I:314:THR:HG23	1.99	0.61
1:I:335:ALA:HA	1:I:338:ASP:OD2	2.01	0.61
1:I:336:GLU:OE1	1:I:625:THR:HG22	1.99	0.61
1:A:398:ILE:HD12	1:A:514:LEU:HD22	1.80	0.61
1:D:210:VAL:CG1	1:D:213:VAL:CG2	2.75	0.61
3:L:1:DA:H2''	3:L:2:DC:OP2	2.00	0.61
1:A:191:GLN:HG3	1:A:409:ALA:O	2.01	0.61
1:F:66:THR:HG21	1:F:548:VAL:CG2	2.31	0.61
1:D:357:MET:HG2	1:D:580:VAL:CB	2.30	0.61
1:F:29:LEU:HD21	1:F:31:ILE:HB	1.82	0.61
2:K:2:DC:C2'	2:K:3:DA:OP2	2.48	0.61
1:A:65:PHE:O	1:A:66:THR:HG22	2.00	0.61
1:F:23:HIS:CE1	1:F:28:ALA:HB2	2.35	0.61
2:X:6:DG:H2''	2:X:7:DC:H5'	1.82	0.61
1:A:613:VAL:O	1:A:617:ARG:HD2	2.00	0.61
1:F:200:ILE:CG2	1:F:235:ALA:HB1	2.31	0.61
1:A:326:THR:OG1	1:A:621:ARG:NH2	2.34	0.61
1:I:56:HIS:HB3	1:I:59:GLU:HG3	1.82	0.61
1:I:363:THR:O	1:I:366:GLN:HG3	2.00	0.61
3:L:12:DG:H2'	3:L:13:DC:H5	1.66	0.61
1:D:9:LEU:CD1	1:D:48:HIS:ND1	2.64	0.60
1:D:132:ILE:HD11	1:D:183:ARG:HD2	1.82	0.60
3:L:10:DG:H2''	3:L:11:DA:C8	2.36	0.60
1:D:142:ARG:O	1:D:143:VAL:C	2.44	0.60
1:F:577:GLU:CD	1:F:619:MET:CE	2.73	0.60
3:L:11:DA:C4	3:L:12:DG:N7	2.69	0.60
3:Y:22:DT:H71	3:Y:23:DT:H73	1.83	0.60
1:I:415:ARG:HB3	1:I:416:ARG:HH11	1.66	0.60
1:A:477:ALA:HA	1:A:480:ASN:HD21	1.66	0.60
1:D:48:HIS:CD2	1:D:52:HIS:HB3	2.36	0.60
1:A:230:GLN:HE22	1:A:258:GLN:NE2	2.00	0.60
1:D:114:VAL:HG13	1:D:193:ALA:CB	2.29	0.60
1:D:656:ASP:HB2	1:D:657:PRO:CD	2.30	0.60
1:F:59:GLU:HB3	1:F:222:LYS:HB3	1.83	0.60
3:L:11:DA:N1	3:L:12:DG:C5	2.69	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:171:GLY:O	1:D:172:LEU:CB	2.50	0.60
1:D:233:ASN:HD21	1:D:236:GLN:HG3	1.66	0.60
1:D:365:ALA:O	1:D:368:ARG:HG2	2.01	0.60
1:D:591:LEU:O	1:D:592:PRO:C	2.42	0.60
1:I:491:MET:O	1:I:497:LEU:HD22	2.01	0.60
3:L:3:DG:C1'	3:L:4:DA:H5'	2.31	0.60
1:F:487:LEU:O	1:F:490:VAL:HG22	2.01	0.60
1:I:331:THR:HA	1:I:628:GLN:HB2	1.83	0.60
2:K:12:DA:C2'	2:K:13:DG:O5'	2.41	0.60
1:A:655:VAL:HG12	1:A:656:ASP:O	2.02	0.60
1:I:33:GLY:HA2	1:I:255:ASP:OD2	2.02	0.60
1:A:38:LYS:HE2	1:A:255:ASP:HB2	1.83	0.60
1:A:46:ILE:O	1:A:50:ILE:HD12	2.01	0.60
1:A:411:ASP:O	1:A:415:ARG:HG2	2.02	0.60
1:D:128:VAL:O	1:D:132:ILE:CD1	2.50	0.60
1:D:195:ASP:N	1:D:198:ASP:OD2	2.30	0.60
1:D:257:ASP:OD1	1:D:310[A]:ARG:NH2	2.35	0.60
1:F:229:TYR:HE1	1:F:271:ILE:HA	1.67	0.60
1:F:634:GLY:HA2	3:L:1:DA:C5'	2.31	0.60
1:I:60:ILE:HB	1:I:87:LEU:HD22	1.83	0.60
2:K:12:DA:H2''	2:K:13:DG:C5'	2.31	0.60
1:A:59:GLU:O	1:A:222:LYS:N	2.33	0.60
1:D:285:MET:HE1	1:D:313:LYS:HA	1.84	0.60
1:I:172:LEU:CD1	1:I:176:ALA:HB3	2.25	0.60
1:I:408:PRO:O	1:I:409:ALA:CB	2.50	0.60
1:A:66:THR:HG21	1:A:548:VAL:CG2	2.31	0.59
1:D:442:THR:HG1	1:D:446:THR:HG1	1.47	0.59
1:F:114:VAL:HG13	1:F:193:ALA:HB2	1.84	0.59
1:I:195:ASP:N	1:I:198:ASP:OD2	2.32	0.59
1:I:420:ARG:HB2	1:I:421:PRO:HD3	1.83	0.59
1:A:45:ARG:O	1:A:49:LEU:HD12	2.01	0.59
1:F:394:GLU:HB3	1:F:514:LEU:HD13	1.83	0.59
1:F:426:GLY:CA	2:K:8:DT:P	2.90	0.59
1:I:233:ASN:CG	1:I:236:GLN:HG3	2.27	0.59
1:I:357:MET:HG2	1:I:580:VAL:CB	2.32	0.59
2:X:12:DA:H2'	2:X:13:DG:C8	2.36	0.59
1:A:27:PRO:HD3	1:A:248:ARG:HB3	1.84	0.59
1:A:528:GLU:O	1:A:529:ALA:O	2.20	0.59
1:A:571:HIS:CG	2:X:21:DT:H2''	2.38	0.59
1:D:325:VAL:HG23	1:D:652:PHE:CB	2.32	0.59
1:D:421:PRO:HA	1:D:499:LEU:HD13	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:369:VAL:HG23	6:F:2017:HOH:O	2.01	0.59
1:A:403:ARG:HG2	1:A:539:LEU:HD11	1.83	0.59
1:A:48:HIS:CE1	1:A:52:HIS:CD2	2.90	0.59
1:A:613:VAL:O	1:A:617:ARG:CD	2.50	0.59
1:D:594:LYS:O	1:D:597:ILE:HG22	2.02	0.59
1:A:198:ASP:C	1:A:201:THR:HG1	2.10	0.59
1:A:425:ILE:N	2:X:9:DC:OP1	2.35	0.59
1:I:287:GLU:HB3	1:I:316:LYS:HG2	1.83	0.59
1:A:194:ILE:CG1	1:A:198:ASP:CG	2.70	0.59
1:A:436:TRP:HA	1:A:439:THR:HG22	1.85	0.59
1:D:47:ALA:HB2	1:D:80:LEU:CD1	2.33	0.59
1:F:65:PHE:C	1:F:66:THR:HG23	2.28	0.59
3:L:12:DG:C4	3:L:13:DC:C5	2.91	0.59
3:Y:11:DA:C4	3:Y:12:DG:C8	2.90	0.59
1:D:401:TYR:OH	1:D:420:ARG:O	2.20	0.59
1:D:660:GLN:NE2	1:I:76:ARG:HG2	2.17	0.59
1:I:444:VAL:O	1:I:447:ALA:HB3	2.02	0.59
2:K:1:DG:C8	2:K:2:DC:C5	2.90	0.59
2:X:15:DT:H6	2:X:15:DT:H5'	1.67	0.59
1:D:171:GLY:O	1:D:172:LEU:HG	2.03	0.59
1:D:444:VAL:O	1:D:447:ALA:HB3	2.02	0.59
1:D:500:LEU:O	1:D:504:GLY:N	2.35	0.59
1:F:66:THR:HG21	1:F:548:VAL:HG22	1.85	0.59
1:F:613:VAL:O	1:F:617:ARG:HD2	2.03	0.59
1:I:116:TYR:CE2	1:I:124:ILE:HD11	2.37	0.58
2:X:6:DG:N2	3:Y:13:DC:N3	2.44	0.58
1:F:377:VAL:C	1:F:378:GLN:HG2	2.28	0.58
1:F:421:PRO:CA	1:F:499:LEU:HD11	2.33	0.58
2:K:11:DC:H2''	2:K:12:DA:C5'	2.34	0.58
1:D:361:TYR:OH	1:D:567:LEU:HB3	2.04	0.58
1:F:34:ALA:HB1	1:F:616:THR:HG21	1.78	0.58
1:F:633:PHE:CZ	2:K:19:DT:C5	2.91	0.58
1:I:310:ARG:NH2	1:I:605:GLU:OE1	2.36	0.58
1:D:566:THR:HG21	1:D:568:MET:CE	2.33	0.58
1:D:655:VAL:CA	1:D:662:ILE:HD12	2.33	0.58
1:F:46:ILE:O	1:F:50:ILE:HD12	2.03	0.58
1:I:428:THR:OG1	1:I:429:ALA:N	2.34	0.58
1:A:268:ILE:CG2	1:A:269:GLN:N	2.66	0.58
1:A:576:LEU:H	1:A:617:ARG:HH21	1.50	0.58
1:D:116:TYR:CE2	1:D:124:ILE:HD11	2.38	0.58
1:I:215:ASP:O	1:I:216:LYS:C	2.45	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:414:LEU:HD23	1:I:414:LEU:C	2.29	0.58
1:I:487:LEU:HA	1:I:490:VAL:CG2	2.27	0.58
1:I:549:ASP:O	1:I:550:ASP:CB	2.51	0.58
1:I:656:ASP:OD1	1:I:657:PRO:CD	2.51	0.58
1:A:496:TYR:HA	1:A:499:LEU:HD12	1.85	0.58
1:D:14:ASN:OD1	1:D:15:PRO:CD	2.50	0.58
2:K:12:DA:H2'	2:K:13:DG:C8	2.39	0.58
1:A:268:ILE:HG23	1:A:269:GLN:H	1.67	0.58
1:A:541:ASP:O	1:A:545:LEU:HG	2.03	0.58
1:I:606:GLU:HG3	1:I:609:ARG:NH1	2.18	0.58
2:K:14:DG:H2'	2:K:15:DT:C7	2.33	0.58
1:A:272:LEU:C	1:A:272:LEU:HD23	2.29	0.58
1:F:535:ILE:HG23	1:F:536:ALA:H	1.69	0.58
1:D:34:ALA:HB1	1:D:291:ARG:HH21	1.68	0.58
1:D:483:PRO:O	1:D:487:LEU:HD12	2.04	0.58
1:D:592:PRO:CG	1:D:644:PHE:CE2	2.87	0.58
1:I:56:HIS:ND1	1:I:57:PRO:CD	2.65	0.57
1:I:633:PHE:HB3	2:K:1:DG:C2	2.38	0.57
1:D:331:THR:HA	1:D:628:GLN:HG3	1.87	0.57
1:A:580:VAL:HG22	1:A:621:ARG:HB3	1.86	0.57
1:D:246:ARG:CD	1:D:247:ASP:OD1	2.52	0.57
1:D:392:ARG:NH1	1:D:546:SER:HB2	2.19	0.57
1:F:27:PRO:HD2	1:F:280:ASP:HB2	1.85	0.57
1:F:72:GLU:O	1:F:76:ARG:HG3	2.04	0.57
1:F:632:GLN:CG	2:K:19:DT:C7	2.80	0.57
1:I:231:ASP:OD2	1:I:574:LYS:NZ	2.37	0.57
1:I:503:GLU:O	1:I:507:GLY:N	2.37	0.57
2:K:19:DT:H1'	2:K:20:DT:H5'	1.86	0.57
1:A:614:GLY:O	1:A:617:ARG:HG2	2.03	0.57
1:D:132:ILE:CG2	1:D:133:PRO:HD2	2.35	0.57
3:Y:17:DG:H1'	3:Y:18:DC:C6	2.39	0.57
1:A:194:ILE:HG13	1:A:198:ASP:CG	2.28	0.57
1:A:537:ASP:O	1:A:540:ASP:HB2	2.05	0.57
1:D:56:HIS:HD2	1:D:57:PRO:HD2	1.65	0.57
1:F:577:GLU:HG3	1:F:619:MET:HE3	1.85	0.57
1:I:285:MET:C	1:I:286:LEU:HD12	2.29	0.57
1:I:524:TRP:HH2	1:I:541:ASP:OD2	1.88	0.57
2:K:19:DT:H2''	2:K:20:DT:C5'	2.33	0.57
1:D:128:VAL:O	1:D:132:ILE:HD11	2.05	0.57
1:D:332:ASP:HB3	1:D:335:ALA:N	2.14	0.57
1:F:59:GLU:O	1:F:222:LYS:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:332:ASP:OD1	1:F:334:ARG:HB2	2.05	0.57
1:F:383:ILE:HG22	1:F:384:VAL:N	2.19	0.57
1:I:483:PRO:O	1:I:487:LEU:HD12	2.04	0.57
1:I:656:ASP:HB2	1:I:662:ILE:HD12	1.86	0.57
3:Y:13:DC:C2'	3:Y:14:DA:C8	2.85	0.57
1:F:188:LYS:CD	1:F:193:ALA:O	2.53	0.57
1:F:394:GLU:HG2	1:F:510:ARG:HB3	1.85	0.57
1:F:613:VAL:O	1:F:617:ARG:HD3	2.04	0.57
1:I:287:GLU:HG2	1:I:314:THR:O	2.05	0.57
1:F:362:ARG:HG2	1:F:590:LEU:O	2.05	0.57
1:A:134:GLY:O	1:A:138:GLU:HB2	2.05	0.57
1:A:545:LEU:CD1	1:A:551:MET:HB2	2.35	0.57
1:F:228:GLU:OE1	1:F:230:GLN:CD	2.47	0.57
1:F:385:GLY:HA2	1:F:552:ARG:NH2	2.20	0.57
1:F:396:ARG:HH11	1:F:396:ARG:HG3	1.69	0.57
1:I:275:GLN:H	1:I:275:GLN:CD	2.12	0.57
2:X:13:DG:H2''	2:X:14:DG:C8	2.40	0.57
1:A:327:PHE:CE1	1:A:645:LEU:HD11	2.40	0.57
1:D:408:PRO:HB3	1:D:445:LEU:HD23	1.87	0.57
1:D:640:GLU:HG3	1:D:641:ASP:H	1.68	0.57
1:F:173:PRO:O	1:F:176:ALA:HB3	2.05	0.57
1:F:334:ARG:HH22	1:F:376:ARG:NH1	2.03	0.57
1:F:343:TRP:O	1:F:347:LEU:HD23	2.05	0.57
1:A:289:ASN:ND2	1:A:291:ARG:H	2.03	0.56
1:I:365:ALA:O	1:I:368:ARG:HG2	2.05	0.56
2:K:1:DG:C5	2:K:2:DC:C4	2.93	0.56
1:A:45:ARG:HD2	1:A:251:LEU:HD22	1.87	0.56
1:A:197:GLY:O	1:A:200:ILE:N	2.30	0.56
1:F:299:ALA:HA	1:F:651:LEU:HD13	1.86	0.56
1:F:592:PRO:HA	1:F:607:GLU:HB3	1.87	0.56
1:I:232:THR:HG23	1:I:270:ASN:ND2	2.09	0.56
1:A:117:ASP:C	1:A:117:ASP:OD1	2.46	0.56
1:A:268:ILE:CG2	1:A:269:GLN:H	2.18	0.56
1:A:656:ASP:C	1:A:656:ASP:OD1	2.48	0.56
1:D:106:HIS:HD2	1:D:210:VAL:HG11	1.69	0.56
1:D:140:GLN:HB2	1:D:143:VAL:HG23	1.87	0.56
1:D:504:GLY:O	1:D:508:GLN:CG	2.42	0.56
1:F:196:PHE:O	1:F:199:LEU:HB2	2.05	0.56
1:I:42:LEU:HG	1:I:225:HIS:ND1	2.20	0.56
1:I:92:PHE:HB3	1:I:200:ILE:HD11	1.87	0.56
2:K:15:DT:H5'	2:K:15:DT:C6	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:21:DT:C5'	2:K:22:DT:OP2	2.52	0.56
2:X:2:DC:H1'	2:X:3:DA:H5''	1.87	0.56
2:X:9:DC:C2	2:X:10:DG:C8	2.94	0.56
3:Y:3:DG:H2'	3:Y:3:DG:O5'	2.05	0.56
3:Y:11:DA:N6	3:Y:12:DG:C6	2.74	0.56
1:F:69:ALA:O	1:F:73:MET:HG3	2.06	0.56
2:K:14:DG:H2''	2:K:15:DT:O5'	2.02	0.56
1:A:633:PHE:HE1	2:X:19:DT:C4	2.23	0.56
1:F:200:ILE:HD13	1:F:236:GLN:HG3	1.88	0.56
1:A:267:ASP:O	1:A:268:ILE:C	2.48	0.56
1:D:257:ASP:HA	1:D:310[A]:ARG:HH12	1.69	0.56
1:D:291:ARG:HG2	1:D:619:MET:HG2	1.87	0.56
1:D:656:ASP:N	1:D:662:ILE:HD11	2.20	0.56
1:I:174:ARG:O	1:I:177:ALA:N	2.38	0.56
1:D:504:GLY:O	1:D:508:GLN:N	2.38	0.56
1:D:655:VAL:C	1:D:662:ILE:CD1	2.78	0.56
2:X:14:DG:H2'	2:X:15:DT:H72	1.88	0.56
1:A:37:GLY:O	1:A:38:LYS:C	2.48	0.56
2:K:13:DG:H1	3:L:6:DC:H42	1.52	0.56
3:L:17:DG:C4'	3:L:18:DC:OP1	2.37	0.56
1:A:422:ARG:HD2	2:X:9:DC:H3'	1.87	0.56
1:I:106:HIS:HD2	1:I:210:VAL:HG11	1.70	0.56
1:I:226:VAL:HG23	1:I:226:VAL:O	2.05	0.56
2:K:19:DT:C2'	2:K:20:DT:C5'	2.83	0.56
2:X:17:DG:H1	3:Y:2:DC:N4	2.01	0.56
1:D:656:ASP:OD1	1:D:660:GLN:HB2	2.05	0.56
1:A:167:PRO:HB3	1:A:174:ARG:HB2	1.87	0.55
1:F:187:ARG:NH2	1:F:411:ASP:OD2	2.39	0.55
2:X:14:DG:C2'	2:X:15:DT:H5''	2.28	0.55
1:A:125:ILE:O	1:A:129:MET:HB2	2.06	0.55
1:A:194:ILE:HG23	1:A:194:ILE:O	2.05	0.55
1:A:397:ASP:O	1:A:400:ALA:HB3	2.06	0.55
1:D:161:LEU:HD22	1:D:178:ALA:HB2	1.89	0.55
1:D:173:PRO:HG2	1:D:176:ALA:HB2	1.88	0.55
1:F:393:ARG:O	1:F:397:ASP:OD2	2.23	0.55
1:I:594:LYS:HA	1:I:597:ILE:HD12	1.88	0.55
3:Y:17:DG:C4'	3:Y:18:DC:OP1	2.42	0.55
1:A:577:GLU:CD	1:A:619:MET:CE	2.80	0.55
1:F:61:LEU:HA	1:F:88:TRP:O	2.06	0.55
2:X:18:DT:H3'	2:X:18:DT:OP2	2.06	0.55
1:A:48:HIS:CE1	1:A:52:HIS:HD2	2.24	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:396:ARG:C	6:D:2020:HOH:O	2.50	0.55
1:D:646:GLU:O	1:D:649:GLU:HG2	2.07	0.55
1:I:225:HIS:HA	1:I:251:LEU:O	2.07	0.55
1:I:336:GLU:HB2	1:I:625:THR:CG2	2.37	0.55
1:I:502:GLN:O	1:I:505:GLN:HG2	2.06	0.55
1:I:143:VAL:HG23	1:I:144:ILE:N	2.21	0.55
1:I:420:ARG:CB	1:I:421:PRO:HD3	2.37	0.55
2:K:20:DT:C2	2:K:21:DT:N3	2.74	0.55
3:L:22:DT:C7	3:L:23:DT:H73	2.36	0.55
1:A:424:GLY:C	1:A:463:LYS:CD	2.79	0.55
1:D:307:ASN:HB2	1:D:310[A]:ARG:NH2	2.21	0.55
1:D:506:GLU:C	1:D:506:GLU:CD	2.74	0.55
1:F:422:ARG:HG3	2:K:10:DG:OP1	2.07	0.55
1:F:588:GLN:HE21	1:F:597:ILE:HD11	1.71	0.55
2:X:4:DG:H2''	2:X:5:DT:OP2	2.04	0.55
1:A:395:ILE:O	1:A:399:LEU:HG	2.05	0.55
1:D:162:ASP:HB3	1:D:178:ALA:CB	2.37	0.55
1:I:252:VAL:HG23	1:I:252:VAL:O	2.06	0.55
2:X:19:DT:H4'	2:X:20:DT:H5''	1.87	0.55
1:F:655:VAL:HG11	1:F:659:GLY:HA2	1.87	0.55
1:I:459:ARG:O	1:I:462:HIS:ND1	2.39	0.55
3:Y:21:DT:H2''	3:Y:22:DT:C6	2.42	0.55
1:A:97:VAL:HB	1:A:199:LEU:HD13	1.87	0.55
1:A:576:LEU:N	1:A:617:ARG:HH21	2.05	0.55
1:F:59:GLU:HB3	1:F:222:LYS:CB	2.37	0.55
1:F:167:PRO:HB3	1:F:174:ARG:HB2	1.88	0.55
1:D:325:VAL:CG2	1:D:652:PHE:HB3	2.38	0.54
1:F:99:ILE:HG21	1:F:203:THR:HG23	1.88	0.54
2:K:15:DT:C5'	2:K:15:DT:C6	2.90	0.54
1:D:171:GLY:O	1:D:172:LEU:HB2	2.07	0.54
1:D:655:VAL:HA	1:D:662:ILE:HD12	1.89	0.54
1:I:331:THR:HA	1:I:628:GLN:CB	2.38	0.54
1:I:588:GLN:HB2	1:I:640:GLU:HB2	1.89	0.54
1:A:424:GLY:C	2:X:9:DC:OP1	2.50	0.54
1:D:577:GLU:CG	1:D:619:MET:HE3	2.36	0.54
1:I:275:GLN:HE21	1:I:276:LYS:HG3	1.72	0.54
1:I:436:TRP:CZ3	1:I:442:THR:HG21	2.42	0.54
1:I:588:GLN:HB2	1:I:640:GLU:CB	2.38	0.54
1:A:187:ARG:CZ	1:A:191:GLN:HE22	2.20	0.54
1:A:267:ASP:HB3	1:A:270:ASN:CG	2.33	0.54
3:Y:21:DT:H2''	3:Y:22:DT:OP1	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:HIS:HD2	1:D:57:PRO:CD	2.19	0.54
1:D:330:ALA:O	1:D:628:GLN:N	2.38	0.54
1:D:362:ARG:NH2	3:Y:19:DT:H6	2.05	0.54
1:D:534:SER:O	1:D:537:ASP:HB2	2.08	0.54
1:F:152:LYS:NZ	1:F:198:ASP:CG	2.65	0.54
1:A:398:ILE:HD13	1:A:491:MET:HG2	1.89	0.54
1:D:331:THR:HA	1:D:628:GLN:CB	2.35	0.54
1:D:592:PRO:HG3	1:D:644:PHE:CE2	2.43	0.54
1:I:117:ASP:C	1:I:117:ASP:OD1	2.49	0.54
1:A:408:PRO:HA	1:A:445:LEU:HD12	1.90	0.54
1:I:172:LEU:HD11	1:I:177:ALA:N	2.23	0.54
1:I:487:LEU:CA	1:I:490:VAL:HG22	2.29	0.54
1:I:634:GLY:O	1:I:635:LYS:CG	2.50	0.54
1:A:194:ILE:HD12	1:A:198:ASP:OD2	2.07	0.54
1:A:232:THR:HG22	1:A:271:ILE:CG2	2.38	0.54
1:D:327:PHE:O	1:D:327:PHE:CG	2.60	0.54
1:F:227:ASP:OD1	1:F:228:GLU:N	2.39	0.54
1:I:318:VAL:O	1:I:318:VAL:HG12	2.08	0.54
1:I:497:LEU:HG	1:I:498:ASP:OD1	2.08	0.54
1:I:633:PHE:HB3	2:K:1:DG:N1	2.23	0.54
1:D:132:ILE:HD12	1:D:132:ILE:H	1.73	0.54
3:L:1:DA:H1'	3:L:2:DC:O5'	2.08	0.54
1:D:159:ASP:OD1	1:D:182:ARG:NH2	2.37	0.54
1:D:399:LEU:O	1:D:403:ARG:N	2.34	0.54
1:D:655:VAL:CG1	1:D:656:ASP:N	2.71	0.54
2:K:1:DG:C1'	2:K:2:DC:C6	2.92	0.54
2:X:11:DC:H2''	2:X:12:DA:O5'	2.08	0.54
1:D:582:PHE:CE1	1:D:623:LEU:HD22	2.42	0.53
1:F:183:ARG:HA	1:F:186:VAL:HG22	1.89	0.53
1:F:592:PRO:O	1:F:607:GLU:OE1	2.25	0.53
1:I:313:LYS:O	1:I:314:THR:CG2	2.56	0.53
1:I:591:LEU:HD21	1:I:611:PHE:HB2	1.90	0.53
3:L:12:DG:N3	3:L:13:DC:C4	2.75	0.53
1:A:418:ILE:HD13	1:A:467:PHE:CE2	2.43	0.53
1:A:631:MET:HB2	1:A:636:THR:HG23	1.90	0.53
1:D:395:ILE:HG12	1:D:517:LEU:HD22	1.89	0.53
1:D:507:GLY:O	1:D:508:GLN:CB	2.56	0.53
1:F:152:LYS:HZ3	1:F:198:ASP:CG	2.16	0.53
1:I:152:LYS:HZ1	1:I:198:ASP:CG	2.17	0.53
1:I:261:TYR:O	1:I:264[B]:ARG:HB2	2.08	0.53
1:I:487:LEU:HB3	1:I:491:MET:HE3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:17:DG:C4	3:Y:18:DC:C4	2.95	0.53
1:D:291:ARG:HD2	1:D:292:SER:OG	2.08	0.53
1:D:318:VAL:O	1:D:318:VAL:CG1	2.56	0.53
1:D:332:ASP:CG	1:D:334:ARG:HB3	2.32	0.53
1:F:27:PRO:O	1:F:281:ALA:HA	2.09	0.53
1:F:34:ALA:HB1	1:F:616:THR:CG2	2.35	0.53
1:F:257:ASP:HB3	1:F:304:ILE:HD11	1.89	0.53
2:K:14:DG:C2'	2:K:15:DT:H5''	2.30	0.53
3:L:21:DT:C4'	3:L:22:DT:OP1	2.39	0.53
2:X:14:DG:H2''	2:X:15:DT:O5'	2.06	0.53
3:Y:1:DA:H1'	3:Y:2:DC:O4'	2.09	0.53
1:A:477:ALA:HA	1:A:480:ASN:ND2	2.24	0.53
1:F:27:PRO:HB2	1:F:281:ALA:HB2	1.90	0.53
1:F:591:LEU:CD2	1:F:642:SER:CB	2.84	0.53
1:A:45:ARG:HD2	1:A:251:LEU:CD2	2.38	0.53
1:A:59:GLU:HB3	1:A:222:LYS:CB	2.39	0.53
1:D:264[B]:ARG:NH2	3:Y:22:DT:H1'	2.24	0.53
1:D:455:ASN:O	1:D:456:ILE:HD13	2.08	0.53
1:F:76:ARG:HA	1:F:79:HIS:CE1	2.44	0.53
1:I:582:PHE:CE2	1:I:623:LEU:HD22	2.43	0.53
3:Y:9:DC:H2''	3:Y:10:DG:O4'	2.08	0.53
1:A:16:THR:HG21	1:A:285:MET:O	2.09	0.53
1:A:267:ASP:CB	1:A:270:ASN:HB2	2.29	0.53
1:A:500:LEU:HD21	1:A:507:GLY:O	2.08	0.53
1:A:569:THR:HG22	1:A:572:ASN:HB2	1.90	0.53
1:D:544:LEU:HB3	3:Y:23:DT:H3'	1.91	0.53
1:F:303:LEU:CD1	1:F:611:PHE:CD1	2.91	0.53
1:F:541:ASP:O	1:F:545:LEU:HG	2.09	0.53
2:X:6:DG:H1	3:Y:13:DC:H42	1.55	0.53
1:A:474:MET:SD	1:A:490:VAL:HG12	2.49	0.53
1:A:545:LEU:CD2	1:A:551:MET:HB2	2.38	0.53
1:D:593:SER:OG	3:Y:19:DT:H73	2.08	0.53
1:F:38:LYS:NZ	4:F:1663:ANP:O2G	2.34	0.53
1:F:115:ILE:HD12	1:F:540:ASP:OD1	2.09	0.53
1:F:377:VAL:C	1:F:378:GLN:CG	2.82	0.53
1:F:587:GLU:CD	1:F:630:ARG:HE	2.16	0.53
3:L:18:DC:H2''	3:L:19:DT:OP2	1.98	0.53
1:A:198:ASP:O	1:A:199:LEU:C	2.51	0.53
1:D:460:GLY:C	1:D:462:HIS:N	2.67	0.53
1:F:230:GLN:HB3	1:F:255:ASP:O	2.08	0.53
3:Y:14:DA:H4'	3:Y:15:DC:OP1	1.82	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:ARG:O	1:A:613:VAL:HG23	2.08	0.53
1:I:60:ILE:HB	1:I:87:LEU:CD2	2.39	0.53
1:I:91:THR:H	1:I:94:SER:HB3	1.73	0.53
1:A:468:ALA:O	1:A:472:GLU:HB2	2.09	0.53
1:A:490:VAL:HG23	1:A:491:MET:N	2.24	0.53
1:F:132:ILE:CD1	1:F:183:ARG:HE	2.22	0.53
1:I:333:HIS:O	1:I:336:GLU:HG2	2.09	0.53
1:A:61:LEU:HD22	1:A:88:TRP:CZ3	2.44	0.52
1:A:294:ALA:HB3	1:A:321:ALA:HA	1.90	0.52
1:A:428:THR:OG1	2:X:8:DT:OP2	2.27	0.52
1:F:338:ASP:OD1	1:F:376:ARG:NH2	2.42	0.52
1:F:591:LEU:HD23	1:F:642:SER:HB2	1.86	0.52
2:K:18:DT:C2'	2:K:19:DT:OP1	2.46	0.52
3:Y:21:DT:H2'	3:Y:22:DT:C5	2.44	0.52
1:A:214:LEU:HD12	1:A:215:ASP:N	2.23	0.52
1:A:424:GLY:O	1:A:463:LYS:CE	2.57	0.52
1:A:424:GLY:C	1:A:463:LYS:HD2	2.34	0.52
1:D:159:ASP:O	1:D:163:ARG:HG3	2.09	0.52
1:I:232:THR:CG2	1:I:270:ASN:HD22	2.12	0.52
1:A:424:GLY:O	1:A:463:LYS:HE3	2.10	0.52
1:F:194:ILE:HD11	1:F:202:GLU:HG3	1.90	0.52
1:I:209:GLU:O	1:I:211:PRO:HD3	2.09	0.52
1:I:323:GLN:NE2	1:I:621:ARG:HD2	2.23	0.52
3:L:11:DA:N6	3:L:12:DG:C6	2.77	0.52
1:A:121:GLN:C	1:A:125:ILE:HD12	2.34	0.52
1:A:423:ARG:HE	1:A:470:LEU:HD13	1.74	0.52
1:A:478:ALA:HA	1:A:486:PHE:CE2	2.44	0.52
1:A:591:LEU:CB	1:A:592:PRO:CD	2.72	0.52
1:A:608:ARG:HB2	1:A:644:PHE:CE1	2.44	0.52
1:F:631:MET:HE3	1:F:636:THR:HG23	1.91	0.52
1:A:392:ARG:HB3	1:A:394:GLU:OE1	2.09	0.52
1:A:497:LEU:HD21	1:A:501:ARG:NH1	2.24	0.52
1:D:121:GLN:O	1:D:125:ILE:HD12	2.10	0.52
1:D:123:ASP:OD1	1:D:415:ARG:NH1	2.42	0.52
1:D:285:MET:C	1:D:286:LEU:HD12	2.34	0.52
1:D:414:LEU:HD23	1:D:414:LEU:C	2.35	0.52
1:D:606:GLU:OE1	1:D:609:ARG:NH1	2.42	0.52
1:F:13:LEU:HD23	1:F:17:GLN:OE1	2.09	0.52
1:A:65:PHE:C	1:A:66:THR:HG23	2.34	0.52
1:A:445:LEU:HD21	1:A:467:PHE:HE1	1.73	0.52
1:A:500:LEU:CD2	1:A:511:LEU:HB3	2.36	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:482:GLU:O	1:F:486:PHE:HB2	2.09	0.52
1:I:655:VAL:HG12	1:I:656:ASP:N	2.25	0.52
3:L:13:DC:H2''	3:L:14:DA:C8	2.45	0.52
1:D:55:VAL:HG12	1:D:56:HIS:N	2.25	0.52
1:F:580:VAL:HG22	1:F:621:ARG:HB3	1.91	0.52
1:I:152:LYS:NZ	1:I:198:ASP:CG	2.67	0.52
1:I:470:LEU:O	1:I:473:ALA:HB3	2.09	0.52
3:L:11:DA:C2	3:L:12:DG:C4	2.98	0.52
2:X:2:DC:C2'	2:X:3:DA:H5''	2.33	0.52
1:A:607:GLU:O	1:A:610:LEU:HB3	2.10	0.52
1:F:403:ARG:HD2	1:F:410:ASP:OD2	2.10	0.52
1:I:152:LYS:NZ	1:I:195:ASP:OD2	2.41	0.52
1:I:412:VAL:O	1:I:416:ARG:HG2	2.09	0.52
1:D:61:LEU:HD12	1:D:88:TRP:O	2.10	0.52
1:D:234:ARG:O	1:D:237:TYR:HB3	2.09	0.52
1:F:29:LEU:HD22	1:F:283:VAL:HG23	1.92	0.52
1:F:107:ILE:HG21	1:F:205:ARG:NH2	2.23	0.52
1:F:238:GLU:O	1:F:239:LEU:C	2.53	0.52
1:F:334:ARG:NH2	1:F:376:ARG:HH12	2.07	0.52
1:F:434:MET:O	1:F:438:ARG:HG3	2.10	0.52
1:F:488:ARG:NH1	1:F:518:VAL:HG11	2.20	0.52
1:F:497:LEU:HD21	1:F:501:ARG:CZ	2.39	0.52
3:L:11:DA:C6	3:L:12:DG:N7	2.78	0.52
1:I:392:ARG:HH11	1:I:546:SER:HB2	1.74	0.52
2:K:1:DG:C4	2:K:2:DC:C4	2.99	0.52
1:A:35:GLY:N	4:A:1662:ANP:HNB1	2.04	0.51
1:A:132:ILE:CG1	1:A:183:ARG:HE	2.23	0.51
1:A:259:SER:N	1:A:609:ARG:HD3	2.25	0.51
1:A:473:ALA:O	1:A:477:ALA:N	2.40	0.51
1:D:252:VAL:HG23	1:D:252:VAL:O	2.08	0.51
1:D:500:LEU:O	1:D:504:GLY:CA	2.58	0.51
1:F:210:VAL:HG11	1:F:213:VAL:HG23	1.92	0.51
1:F:263:PHE:C	1:F:263:PHE:CD1	2.88	0.51
1:F:656:ASP:OD1	1:F:658:TYR:N	2.42	0.51
1:I:264[A]:ARG:NH1	1:I:264[A]:ARG:HB3	2.25	0.51
2:K:19:DT:C4'	2:K:20:DT:C5'	2.86	0.51
1:A:199:LEU:O	1:A:203:THR:OG1	2.26	0.51
1:A:421:PRO:HA	1:A:499:LEU:CD1	2.33	0.51
1:F:302:LYS:O	1:F:305:GLU:HG2	2.09	0.51
1:F:506:GLU:O	1:F:509:VAL:HG12	2.10	0.51
1:I:175:ASP:OD1	1:I:176:ALA:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:HG23	1:A:251:LEU:HD11	1.92	0.51
1:A:34:ALA:HB1	1:A:616:THR:HG21	1.83	0.51
1:D:225:HIS:HA	1:D:251:LEU:O	2.10	0.51
1:F:29:LEU:HD23	1:F:29:LEU:C	2.34	0.51
1:F:35:GLY:N	4:F:1663:ANP:N3B	2.55	0.51
2:K:6:DG:H2''	2:K:7:DC:C5'	2.40	0.51
3:Y:11:DA:C6	3:Y:12:DG:C6	2.98	0.51
1:A:229:TYR:O	1:A:230:GLN:C	2.54	0.51
1:A:230:GLN:O	1:A:271:ILE:HG21	2.11	0.51
1:A:232:THR:CG2	1:A:271:ILE:HG22	2.39	0.51
1:D:92:PHE:HB3	1:D:200:ILE:HD11	1.93	0.51
1:D:291:ARG:HG3	1:D:577:GLU:OE1	2.10	0.51
1:F:97:VAL:HB	1:F:199:LEU:HD13	1.91	0.51
1:I:330:ALA:O	1:I:628:GLN:N	2.40	0.51
2:X:19:DT:C2'	2:X:20:DT:OP2	2.58	0.51
1:A:227:ASP:O	1:A:228:GLU:C	2.54	0.51
1:A:415:ARG:CZ	1:A:434:MET:HE1	2.40	0.51
1:D:248:ARG:NH2	1:D:280:ASP:OD1	2.43	0.51
1:F:13:LEU:HD22	1:F:17:GLN:HB3	1.93	0.51
1:F:257:ASP:O	1:F:609:ARG:CG	2.58	0.51
1:D:401:TYR:OH	1:D:423:ARG:NH2	2.44	0.51
2:X:15:DT:C5'	2:X:15:DT:C6	2.93	0.51
1:A:310:ARG:HG3	1:A:311:LEU:O	2.10	0.51
1:F:397:ASP:O	1:F:400:ALA:HB3	2.11	0.51
1:F:592:PRO:O	1:F:596:ALA:HB3	2.11	0.51
1:I:263:PHE:C	1:I:265:GLY:H	2.18	0.51
1:A:63:VAL:HG22	1:A:226:VAL:HG22	1.93	0.51
1:A:338:ASP:CG	1:A:376:ARG:HH22	2.18	0.51
1:F:363:THR:HG22	1:F:365:ALA:HB3	1.93	0.51
1:I:9:LEU:HD11	1:I:48:HIS:ND1	2.26	0.51
1:A:538:PHE:CD1	1:A:538:PHE:C	2.89	0.51
1:F:329:ARG:HA	1:F:626:ALA:O	2.11	0.51
1:A:204:VAL:HG22	1:A:239:LEU:HD12	1.92	0.50
1:A:231:ASP:CB	1:A:261:TYR:HB2	2.39	0.50
1:D:93:HIS:CE1	3:Y:23:DT:O2	2.64	0.50
1:F:510:ARG:O	1:F:514:LEU:HD13	2.10	0.50
1:I:125:ILE:O	1:I:129:MET:HG3	2.10	0.50
1:I:294:ALA:HB3	1:I:321:ALA:CA	2.33	0.50
1:I:458:ASP:C	1:I:458:ASP:OD1	2.54	0.50
2:X:2:DC:N4	3:Y:17:DG:C6	2.79	0.50
1:A:7:PRO:HB3	1:A:80:LEU:HD22	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD12	1:A:88:TRP:O	2.12	0.50
1:A:267:ASP:HB3	1:A:270:ASN:H	1.75	0.50
1:A:588:GLN:OE1	1:A:592:PRO:HG2	2.12	0.50
1:D:16:THR:HG22	6:D:2001:HOH:O	2.12	0.50
1:D:513:ASN:HA	1:D:516:GLU:HB3	1.92	0.50
1:F:100:LEU:HD21	1:F:202:GLU:C	2.35	0.50
1:F:310:ARG:HG3	1:F:311:LEU:O	2.11	0.50
3:Y:11:DA:C5	3:Y:12:DG:N7	2.79	0.50
1:A:228:GLU:OE1	1:A:230:GLN:CD	2.54	0.50
1:A:426:GLY:HA3	2:X:8:DT:P	2.52	0.50
1:D:437:ALA:HA	1:D:442:THR:CG2	2.39	0.50
1:F:545:LEU:CD1	1:F:551:MET:HB2	2.41	0.50
1:D:160:ASP:HA	1:D:163:ARG:HG3	1.94	0.50
1:F:511:LEU:O	1:F:515:GLU:N	2.44	0.50
1:F:587:GLU:HG2	1:F:626:ALA:HB1	1.94	0.50
1:I:91:THR:HG22	1:I:92:PHE:N	2.26	0.50
1:I:430:LEU:O	1:I:434:MET:HG3	2.11	0.50
2:K:19:DT:C3'	2:K:20:DT:H5''	2.37	0.50
1:A:194:ILE:O	1:A:195:ASP:O	2.30	0.50
1:A:507:GLY:O	1:A:510:ARG:HB2	2.12	0.50
1:D:167:PRO:HA	1:D:174:ARG:CG	2.41	0.50
1:D:477:ALA:HB1	1:D:481:TYR:HD2	1.77	0.50
1:A:377:VAL:O	1:A:378:GLN:CB	2.60	0.50
1:D:117:ASP:C	1:D:117:ASP:OD1	2.55	0.50
1:D:325:VAL:HG23	1:D:652:PHE:HB3	1.93	0.50
1:F:73:MET:HB3	1:F:89:MET:HE1	1.94	0.50
1:F:101:ARG:HB2	1:F:113:PHE:HZ	1.75	0.50
1:F:545:LEU:HD21	1:F:551:MET:CG	2.34	0.50
1:I:161:LEU:C	1:I:161:LEU:HD23	2.37	0.50
1:I:655:VAL:CG1	1:I:656:ASP:N	2.74	0.50
2:X:1:DG:C4	2:X:2:DC:C5	2.99	0.50
2:X:4:DG:H2'	2:X:4:DG:O5'	2.11	0.50
1:D:297:LEU:HD22	1:D:315:LEU:HD23	1.93	0.50
1:F:157:THR:O	1:F:160:ASP:OD1	2.29	0.50
1:I:325:VAL:CG2	1:I:652:PHE:HB3	2.42	0.50
1:A:60:ILE:HG23	1:A:223:PHE:O	2.12	0.50
1:A:234:ARG:HG2	1:A:270:ASN:ND2	2.25	0.50
1:D:454:GLN:C	1:D:455:ASN:OD1	2.55	0.50
1:F:231:ASP:HB3	1:F:261:TYR:HB2	1.93	0.50
1:I:455:ASN:O	1:I:456:ILE:HD12	2.12	0.50
3:L:9:DC:H2'	3:L:10:DG:C8	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:90:SER:HB2	1:D:94:SER:HB3	1.94	0.50
2:K:4:DG:O6	3:L:15:DC:N3	2.44	0.50
1:D:514:LEU:O	1:D:518:VAL:HG23	2.12	0.49
1:F:377:VAL:O	1:F:378:GLN:HB2	2.12	0.49
3:Y:14:DA:OP2	3:Y:14:DA:O4'	2.30	0.49
3:Y:19:DT:H2''	3:Y:20:DT:O5'	2.12	0.49
1:A:231:ASP:CG	1:A:261:TYR:HB2	2.37	0.49
1:I:31:ILE:CG2	1:I:313:LYS:CD	2.88	0.49
2:K:15:DT:C5'	2:K:15:DT:H6	2.25	0.49
3:Y:3:DG:C2'	3:Y:3:DG:O5'	2.60	0.49
1:D:485:ALA:HA	1:D:488:ARG:HD2	1.93	0.49
1:F:334:ARG:CZ	1:F:376:ARG:HH12	2.25	0.49
1:F:424:GLY:C	2:K:9:DC:OP1	2.55	0.49
1:I:14:ASN:OD1	1:I:15:PRO:CD	2.53	0.49
2:X:17:DG:H4'	2:X:18:DT:O5'	2.11	0.49
1:A:27:PRO:O	1:A:281:ALA:HA	2.12	0.49
1:D:171:GLY:O	1:D:172:LEU:CG	2.60	0.49
1:F:195:ASP:O	1:F:198:ASP:HB2	2.11	0.49
1:F:388:GLY:HA2	1:F:556:GLU:OE2	2.13	0.49
1:I:50:ILE:HD13	1:I:81:VAL:HG11	1.92	0.49
1:I:336:GLU:O	1:I:339:TYR:HB3	2.12	0.49
1:I:600:GLY:O	1:I:604:ILE:HG12	2.13	0.49
1:I:655:VAL:HG13	1:I:660:GLN:O	2.13	0.49
3:Y:13:DC:H2''	3:Y:14:DA:OP2	2.11	0.49
1:A:198:ASP:C	1:A:200:ILE:N	2.67	0.49
1:D:491:MET:O	1:D:497:LEU:HD22	2.12	0.49
1:F:256:PRO:HG2	1:F:311:LEU:HD22	1.95	0.49
1:I:56:HIS:CE1	1:I:57:PRO:HD2	2.47	0.49
2:X:11:DC:N4	3:Y:8:DG:N1	2.37	0.49
1:A:24:PHE:CD2	1:A:25:THR:CG2	2.90	0.49
1:D:152:LYS:NZ	1:D:195:ASP:OD2	2.45	0.49
1:F:499:LEU:HD22	6:F:2021:HOH:O	2.11	0.49
2:K:19:DT:OP1	2:K:19:DT:O4'	2.30	0.49
1:A:195:ASP:OD2	1:A:198:ASP:OD1	2.30	0.49
1:A:346:ARG:O	1:A:349:GLY:N	2.45	0.49
1:A:482:GLU:O	1:A:486:PHE:CB	2.61	0.49
1:A:576:LEU:O	1:A:617:ARG:NH2	2.45	0.49
1:D:634:GLY:O	1:D:635:LYS:CG	2.45	0.49
1:F:524:TRP:CZ3	1:F:541:ASP:OD2	2.65	0.49
1:F:592:PRO:HA	1:F:607:GLU:CB	2.42	0.49
2:X:17:DG:N2	3:Y:3:DG:N2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:631:MET:HA	1:A:636:THR:HA	1.93	0.49
1:F:383:ILE:CG2	1:F:384:VAL:N	2.75	0.49
3:L:19:DT:O2	3:L:19:DT:C2'	2.43	0.49
1:A:183:ARG:HA	1:A:186:VAL:HG22	1.95	0.49
1:A:232:THR:H	1:A:266:ALA:HB1	1.78	0.49
1:D:339:TYR:O	1:D:343:TRP:HD1	1.95	0.49
1:F:371:GLU:OE2	1:F:383:ILE:HD11	2.13	0.49
1:F:404:LEU:HD23	1:F:471:MET:HE2	1.94	0.49
1:I:121:GLN:O	1:I:125:ILE:HD12	2.12	0.49
1:I:359:ILE:C	1:I:360:LEU:HD12	2.38	0.49
1:I:593:SER:CB	3:L:19:DT:H73	2.43	0.49
2:X:1:DG:H1	3:Y:18:DC:H42	0.80	0.49
1:A:45:ARG:NH1	1:A:251:LEU:HB3	2.28	0.49
1:A:229:TYR:O	1:A:271:ILE:CG2	2.61	0.49
1:A:343:TRP:O	1:A:347:LEU:HD23	2.12	0.49
1:D:47:ALA:CB	1:D:80:LEU:CD1	2.91	0.49
1:F:229:TYR:O	1:F:230:GLN:C	2.56	0.49
1:F:425:ILE:N	2:K:9:DC:OP1	2.46	0.49
1:F:504:GLY:HA2	1:F:507:GLY:HA3	1.95	0.49
1:I:47:ALA:HB2	1:I:80:LEU:HD12	1.92	0.49
1:I:255:ASP:C	1:I:255:ASP:OD1	2.53	0.49
1:A:42:LEU:O	1:A:46:ILE:CD1	2.60	0.48
1:A:151:ALA:C	1:A:153:SER:H	2.21	0.48
1:F:23:HIS:HB2	1:F:284:TYR:OH	2.13	0.48
1:F:92:PHE:O	1:F:96:GLY:N	2.27	0.48
1:I:407:ASN:C	1:I:408:PRO:O	2.53	0.48
2:K:3:DA:OP2	2:K:3:DA:H8	1.96	0.48
2:X:19:DT:H2''	2:X:20:DT:C5'	2.43	0.48
2:K:11:DC:N3	3:L:8:DG:N2	2.52	0.48
3:L:14:DA:OP2	3:L:14:DA:O4'	2.30	0.48
3:Y:21:DT:C2'	3:Y:22:DT:C6	2.96	0.48
1:A:269:GLN:O	1:A:273:ASP:CG	2.57	0.48
1:I:167:PRO:HA	1:I:174:ARG:HB3	1.95	0.48
1:I:174:ARG:CG	1:I:175:ASP:N	2.37	0.48
1:A:66:THR:CG2	1:A:548:VAL:HG22	2.40	0.48
1:A:90:SER:OG	1:A:95:ALA:HB2	2.13	0.48
1:A:195:ASP:N	1:A:198:ASP:OD2	2.46	0.48
1:A:303:LEU:HD11	1:A:611:PHE:HD2	1.78	0.48
1:A:587:GLU:HG2	1:A:626:ALA:HB1	1.96	0.48
1:A:592:PRO:O	1:A:593:SER:CB	2.61	0.48
1:D:325:VAL:HG23	1:D:652:PHE:HB2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:655:VAL:HG13	1:D:660:GLN:H	1.78	0.48
1:F:96:GLY:O	1:F:203:THR:OG1	2.31	0.48
1:A:426:GLY:HA2	2:X:8:DT:O5'	2.13	0.48
1:D:132:ILE:N	1:D:132:ILE:CD1	2.75	0.48
1:D:302:LYS:HD2	1:D:651:LEU:CD1	2.43	0.48
1:D:504:GLY:HA2	1:D:508:GLN:H	1.78	0.48
1:I:513:ASN:HA	1:I:516:GLU:CB	2.44	0.48
2:K:1:DG:H2'	2:K:2:DC:C6	2.49	0.48
1:A:240:THR:O	1:A:241:ARG:C	2.56	0.48
1:A:482:GLU:O	1:A:486:PHE:N	2.46	0.48
1:D:546:SER:O	1:D:547:SER:CB	2.62	0.48
1:F:408:PRO:HA	1:F:445:LEU:HD12	1.96	0.48
1:I:233:ASN:ND2	1:I:236:GLN:CD	2.71	0.48
3:Y:22:DT:OP1	3:Y:22:DT:O4'	2.30	0.48
1:A:33:GLY:HA2	1:A:313:LYS:HE2	1.96	0.48
1:A:343:TRP:O	1:A:347:LEU:CD2	2.62	0.48
1:D:353:ALA:O	1:D:357:MET:HE2	2.14	0.48
1:D:384:VAL:HG12	1:D:572:ASN:ND2	2.29	0.48
1:F:66:THR:CG2	1:F:548:VAL:HG22	2.43	0.48
1:F:302:LYS:HD2	1:F:651:LEU:HD11	1.96	0.48
1:I:91:THR:HB	1:I:94:SER:H	1.78	0.48
1:I:457:LEU:O	1:I:458:ASP:CG	2.57	0.48
3:Y:17:DG:C5	3:Y:18:DC:N4	2.81	0.48
1:A:44:TYR:CE1	1:A:80:LEU:HD21	2.49	0.48
1:D:161:LEU:C	1:D:161:LEU:HD23	2.39	0.48
1:D:400:ALA:CB	1:D:417:ILE:HG23	2.44	0.48
1:I:139:THR:HG23	1:I:140:GLN:H	1.78	0.48
1:I:332:ASP:HB3	1:I:335:ALA:CB	2.43	0.48
2:X:3:DA:H61	3:Y:16:DT:H3	1.62	0.48
1:A:194:ILE:C	1:A:195:ASP:O	2.56	0.48
1:A:230:GLN:CD	1:A:258:GLN:HB3	2.39	0.48
1:D:287:GLU:HB3	1:D:316:LYS:HG2	1.95	0.48
1:F:125:ILE:O	1:F:129:MET:HB2	2.13	0.48
1:F:343:TRP:O	1:F:347:LEU:CD2	2.62	0.48
1:I:505:GLN:C	1:I:508:GLN:OE1	2.57	0.48
3:L:11:DA:N3	3:L:12:DG:C8	2.82	0.48
1:A:27:PRO:HA	1:A:250:LEU:O	2.14	0.48
1:A:607:GLU:OE1	1:A:607:GLU:HA	2.13	0.48
1:D:139:THR:HG23	1:D:140:GLN:H	1.78	0.48
1:D:280:ASP:O	1:D:281:ALA:C	2.57	0.48
1:F:46:ILE:HD12	1:F:46:ILE:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:ASP:HB3	1:F:304:ILE:HD13	1.96	0.48
1:I:21:ALA:HA	1:I:45:ARG:HB2	1.96	0.48
1:A:90:SER:HB2	1:A:94:SER:HB2	1.96	0.47
1:A:195:ASP:OD2	1:A:198:ASP:CG	2.55	0.47
1:A:295:ARG:HG3	1:A:322:GLY:H	1.79	0.47
1:F:297:LEU:HD11	1:F:315:LEU:HD13	1.96	0.47
1:F:334:ARG:HH22	1:F:376:ARG:HH12	1.60	0.47
1:F:566:THR:C	1:F:567:LEU:HD12	2.39	0.47
1:I:238:GLU:OE1	1:I:238:GLU:HA	2.13	0.47
2:X:12:DA:H2''	2:X:13:DG:C5'	2.39	0.47
2:X:19:DT:H4'	2:X:20:DT:C5'	2.44	0.47
1:A:63:VAL:HA	1:A:90:SER:O	2.14	0.47
1:D:117:ASP:O	1:D:121:GLN:HG3	2.13	0.47
1:D:302:LYS:HD2	1:D:651:LEU:HD11	1.96	0.47
1:F:403:ARG:HG3	1:F:404:LEU:N	2.29	0.47
1:I:32:ALA:HB1	1:I:36:SER:OG	2.15	0.47
1:I:50:ILE:HD13	1:I:81:VAL:CG1	2.44	0.47
1:I:504:GLY:HA2	1:I:508:GLN:H	1.79	0.47
1:A:655:VAL:CG1	1:A:659:GLY:HA2	2.40	0.47
1:D:123:ASP:CG	1:D:415:ARG:HH11	2.21	0.47
1:D:307:ASN:HB2	1:D:310[A]:ARG:HH21	1.79	0.47
1:D:421:PRO:HG3	1:D:495:GLY:O	2.13	0.47
1:F:60:ILE:HG23	1:F:223:PHE:O	2.14	0.47
1:I:172:LEU:CD1	1:I:177:ALA:N	2.77	0.47
1:A:104:GLY:C	1:A:106:HIS:H	2.22	0.47
1:D:139:THR:HG23	1:D:140:GLN:N	2.30	0.47
1:D:263:PHE:C	1:D:265:GLY:H	2.21	0.47
1:D:487:LEU:HB3	1:D:491:MET:HE3	1.96	0.47
2:X:19:DT:O2	2:X:19:DT:H2'	2.15	0.47
1:A:257:ASP:OD2	1:A:310:ARG:NH1	2.48	0.47
1:I:222:LYS:O	1:I:249:ASN:HB2	2.14	0.47
1:A:487:LEU:O	1:A:490:VAL:HG22	2.14	0.47
1:D:361:TYR:O	1:D:569:THR:HA	2.15	0.47
1:F:42:LEU:O	1:F:46:ILE:CD1	2.59	0.47
1:F:210:VAL:CG1	1:F:213:VAL:HG23	2.44	0.47
1:F:226:VAL:CG1	1:F:252:VAL:HG12	2.45	0.47
1:F:592:PRO:C	1:F:607:GLU:OE1	2.57	0.47
1:F:631:MET:HA	1:F:636:THR:HA	1.96	0.47
1:I:139:THR:HG23	1:I:140:GLN:N	2.30	0.47
1:A:44:TYR:O	1:A:45:ARG:C	2.58	0.47
1:A:144:ILE:O	1:A:148:ILE:HG13	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:VAL:HG11	1:A:213:VAL:HG23	1.97	0.47
1:A:362:ARG:HH12	1:A:607:GLU:CD	2.23	0.47
1:A:591:LEU:HB3	1:A:592:PRO:HD2	1.93	0.47
1:D:356:GLU:HG2	1:D:579:PRO:HG2	1.96	0.47
1:D:362:ARG:HH22	3:Y:19:DT:H73	1.80	0.47
1:D:441:HIS:N	1:D:441:HIS:CD2	2.82	0.47
1:D:660:GLN:HA	1:D:661:PRO:HD2	1.52	0.47
1:F:70:ALA:HB1	1:F:89:MET:HB3	1.97	0.47
1:F:126:LYS:HA	1:F:129:MET:HE2	1.97	0.47
1:F:362:ARG:CZ	2:K:21:DT:O2	2.62	0.47
1:I:185:GLU:O	1:I:189:LYS:HG3	2.15	0.47
1:I:223:PHE:CE1	1:I:249:ASN:ND2	2.82	0.47
1:I:371:GLU:OE2	1:I:375:ARG:NH2	2.48	0.47
1:I:507:GLY:C	1:I:509:VAL:H	2.22	0.47
1:I:508:GLN:O	1:I:511:LEU:HG	2.15	0.47
1:I:591:LEU:HD23	1:I:591:LEU:O	2.15	0.47
2:K:8:DT:H2''	2:K:9:DC:C1'	2.45	0.47
2:K:19:DT:C3'	2:K:20:DT:C5'	2.92	0.47
1:A:162:ASP:O	1:A:174:ARG:HD2	2.14	0.47
1:F:37:GLY:O	1:F:38:LYS:C	2.54	0.47
1:I:246:ARG:HD2	1:I:247:ASP:OD1	2.14	0.47
1:I:660:GLN:OE1	1:I:660:GLN:HA	2.12	0.47
2:X:19:DT:H2''	2:X:20:DT:H5'	1.96	0.47
1:A:198:ASP:O	1:A:201:THR:N	2.48	0.47
1:A:208:LYS:HG3	1:A:242:LEU:HD21	1.97	0.47
1:A:577:GLU:CB	1:A:619:MET:HE3	2.44	0.47
1:F:393:ARG:NH2	1:F:416:ARG:HB3	2.30	0.47
1:F:576:LEU:N	1:F:617:ARG:HH21	2.12	0.47
1:I:275:GLN:CD	1:I:275:GLN:N	2.72	0.47
1:I:336:GLU:HG3	1:I:337:GLY:N	2.30	0.47
3:L:6:DC:C2'	3:L:7:DT:O5'	2.41	0.47
1:A:411:ASP:HA	1:A:444:VAL:HG11	1.95	0.47
1:D:400:ALA:HB3	1:D:417:ILE:CG2	2.45	0.47
1:D:416:ARG:HB3	6:D:2022:HOH:O	2.14	0.47
1:F:132:ILE:HD11	1:F:183:ARG:NE	2.29	0.47
1:I:107:ILE:HB	1:I:205:ARG:HH22	1.80	0.47
1:I:392:ARG:NH1	1:I:546:SER:CB	2.78	0.47
2:X:12:DA:C6	2:X:13:DG:C6	3.03	0.47
1:A:132:ILE:HG13	1:A:183:ARG:HE	1.80	0.46
1:A:194:ILE:O	1:A:195:ASP:C	2.56	0.46
1:A:240:THR:OG1	1:A:241:ARG:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:THR:HA	1:D:628:GLN:CG	2.45	0.46
1:I:58:GLY:O	1:I:220:LYS:HA	2.15	0.46
1:I:415:ARG:O	1:I:416:ARG:NH1	2.48	0.46
2:K:12:DA:C2'	2:K:13:DG:C8	2.98	0.46
1:A:27:PRO:HG2	1:A:280:ASP:HB2	1.97	0.46
1:A:97:VAL:CG1	1:A:98:ARG:N	2.79	0.46
1:A:356:GLU:HB3	1:A:579:PRO:HG2	1.96	0.46
1:D:132:ILE:HD11	1:D:183:ARG:CD	2.46	0.46
1:F:395:ILE:HD12	1:F:517:LEU:HB2	1.97	0.46
1:F:404:LEU:HD12	1:F:407:ASN:O	2.15	0.46
1:F:586:VAL:HG13	1:F:591:LEU:CD2	2.37	0.46
1:I:294:ALA:O	1:I:298:GLU:HG3	2.15	0.46
1:I:374:LEU:HB3	1:I:379:ILE:HB	1.97	0.46
1:A:577:GLU:HB2	1:A:619:MET:HE3	1.97	0.46
1:F:388:GLY:O	1:F:391:ASP:HB2	2.15	0.46
1:F:545:LEU:CD2	1:F:551:MET:HB2	2.45	0.46
1:F:611:PHE:HE1	1:F:615:ILE:HD11	1.75	0.46
1:I:8:ASP:HB3	1:I:11:GLN:HB2	1.97	0.46
3:L:1:DA:C1'	3:L:2:DC:O5'	2.63	0.46
1:A:97:VAL:HG11	1:A:544:LEU:HD11	1.98	0.46
1:D:477:ALA:HB1	1:D:481:TYR:CD2	2.49	0.46
1:F:200:ILE:HG21	1:F:235:ALA:CB	2.46	0.46
1:F:421:PRO:HA	1:F:499:LEU:CD1	2.44	0.46
1:F:545:LEU:CD2	1:F:551:MET:HG3	2.36	0.46
1:I:111:ARG:HG2	1:I:112:GLY:N	2.30	0.46
1:I:325:VAL:HG23	1:I:652:PHE:CB	2.46	0.46
2:K:12:DA:C5	2:K:13:DG:C6	3.04	0.46
3:Y:22:DT:C7	3:Y:23:DT:H73	2.45	0.46
1:D:114:VAL:HG21	1:D:403:ARG:HH21	1.81	0.46
1:D:173:PRO:HG2	1:D:176:ALA:HB3	1.96	0.46
1:D:215:ASP:O	1:D:216:LYS:C	2.56	0.46
1:D:640:GLU:OE1	1:D:640:GLU:HA	2.14	0.46
1:F:614:GLY:O	1:F:617:ARG:HG2	2.16	0.46
1:A:157:THR:OG1	1:A:158:PRO:HD2	2.15	0.46
1:D:222:LYS:O	1:D:249:ASN:HB2	2.16	0.46
1:I:261:TYR:O	1:I:264[A]:ARG:HB2	2.15	0.46
1:I:354:TRP:HB3	1:I:564:ALA:C	2.41	0.46
3:L:18:DC:H2''	3:L:19:DT:OP1	2.01	0.46
1:D:152:LYS:NZ	1:D:198:ASP:OD1	2.48	0.46
1:D:384:VAL:HG12	1:D:572:ASN:HD21	1.80	0.46
1:I:591:LEU:HB3	1:I:592:PRO:CD	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:THR:O	1:A:69:ALA:HB3	2.15	0.46
1:A:114:VAL:CG2	1:A:115:ILE:N	2.79	0.46
1:A:426:GLY:CA	2:X:8:DT:P	3.04	0.46
1:F:29:LEU:HD12	1:F:274:PHE:HD2	1.81	0.46
1:I:362:ARG:NH1	1:I:607:GLU:OE2	2.47	0.46
3:L:11:DA:C2	3:L:12:DG:C5	3.03	0.46
1:A:229:TYR:HE2	1:A:271:ILE:C	2.24	0.46
1:D:524:TRP:CZ3	1:D:541:ASP:OD2	2.69	0.46
1:I:138:GLU:C	1:I:139:THR:HG22	2.41	0.46
2:K:1:DG:N9	2:K:2:DC:C5	2.84	0.46
1:A:259:SER:H	1:A:609:ARG:HD3	1.81	0.46
1:F:36:SER:HA	1:F:288:HIS:O	2.16	0.46
1:I:280:ASP:OD1	1:I:280:ASP:C	2.58	0.46
1:D:633:PHE:HB3	2:X:1:DG:N1	2.31	0.45
1:D:656:ASP:OD2	1:I:44:TYR:OH	2.28	0.45
1:F:101:ARG:HH22	1:F:536:ALA:CB	2.26	0.45
1:F:415:ARG:NH1	1:F:434:MET:HE1	2.31	0.45
1:F:634:GLY:CA	3:L:1:DA:H5'	2.39	0.45
1:I:287:GLU:HG2	1:I:314:THR:H	1.81	0.45
3:Y:19:DT:O2	3:Y:19:DT:C2'	2.56	0.45
1:A:263:PHE:CD1	1:A:263:PHE:C	2.94	0.45
1:F:56:HIS:O	1:F:59:GLU:HB2	2.16	0.45
1:F:223:PHE:CD2	1:F:249:ASN:HB3	2.51	0.45
1:I:17:GLN:O	1:I:18:ALA:C	2.59	0.45
1:I:286:LEU:N	1:I:286:LEU:CD1	2.79	0.45
3:Y:17:DG:H1'	3:Y:18:DC:C5	2.51	0.45
1:A:207:PHE:O	1:A:214:LEU:HD23	2.16	0.45
1:D:301:ASN:HD21	1:D:315:LEU:HB2	1.80	0.45
1:D:546:SER:O	1:D:547:SER:OG	2.31	0.45
1:F:29:LEU:HD12	1:F:274:PHE:CD2	2.50	0.45
1:F:117:ASP:C	1:F:117:ASP:OD1	2.59	0.45
1:F:191:GLN:HG3	1:F:409:ALA:O	2.17	0.45
1:F:422:ARG:CD	2:K:9:DC:H3'	2.40	0.45
1:F:538:PHE:CD1	1:F:538:PHE:C	2.94	0.45
1:A:46:ILE:HD12	1:A:46:ILE:H	1.81	0.45
1:A:210:VAL:CG1	1:A:213:VAL:HG23	2.46	0.45
1:D:114:VAL:CG1	1:D:193:ALA:HB2	2.40	0.45
1:D:138:GLU:C	1:D:139:THR:HG22	2.41	0.45
1:F:215:ASP:HA	1:F:218:GLN:OE1	2.17	0.45
1:F:617:ARG:HD2	1:F:617:ARG:N	2.31	0.45
1:I:92:PHE:CD2	1:I:236:GLN:NE2	2.85	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:441:HIS:CD2	6:I:2034:HOH:O	2.55	0.45
3:Y:14:DA:OP2	3:Y:14:DA:C4'	2.65	0.45
1:A:500:LEU:HD22	1:A:511:LEU:HD23	1.98	0.45
1:D:280:ASP:OD1	1:D:280:ASP:N	2.49	0.45
1:D:591:LEU:CB	1:D:592:PRO:CD	2.92	0.45
1:F:542:ALA:HA	1:F:545:LEU:HG	1.97	0.45
1:F:576:LEU:O	1:F:617:ARG:NH2	2.50	0.45
1:F:635:LYS:HB3	1:F:635:LYS:HZ3	1.82	0.45
1:I:151:ALA:HA	1:I:156:TRP:HE3	1.81	0.45
1:I:252:VAL:O	1:I:252:VAL:CG2	2.64	0.45
1:I:359:ILE:CD1	1:I:565:VAL:HG11	2.46	0.45
3:L:12:DG:C2	3:L:13:DC:C4	3.05	0.45
1:A:249:ASN:HD22	1:A:249:ASN:HA	1.59	0.45
1:A:413:ALA:O	1:A:417:ILE:HG13	2.16	0.45
1:A:488:ARG:HH11	1:A:518:VAL:HG11	1.82	0.45
1:D:9:LEU:HD23	1:D:18:ALA:O	2.16	0.45
1:D:497:LEU:HG	1:D:498:ASP:OD1	2.16	0.45
1:D:500:LEU:O	1:D:504:GLY:HA3	2.17	0.45
1:D:592:PRO:HG3	1:D:644:PHE:CD2	2.51	0.45
1:F:308:THR:O	1:F:309:GLU:HB2	2.16	0.45
1:F:393:ARG:HE	1:F:397:ASP:CG	2.22	0.45
1:F:631:MET:HB2	1:F:636:THR:HG23	1.97	0.45
1:I:129:MET:HA	1:I:132:ILE:HG12	1.98	0.45
1:I:339:TYR:O	1:I:343:TRP:HD1	2.00	0.45
1:I:579:PRO:HA	1:I:619:MET:HB2	1.97	0.45
1:I:584:VAL:HA	1:I:625:THR:HB	1.97	0.45
1:A:151:ALA:HB1	1:A:156:TRP:HB2	1.99	0.45
1:A:198:ASP:O	1:A:200:ILE:C	2.60	0.45
1:F:272:LEU:O	1:F:275:GLN:HG3	2.16	0.45
2:K:13:DG:H1	3:L:6:DC:N4	2.14	0.45
1:A:113:PHE:CD1	1:A:113:PHE:C	2.95	0.45
1:A:115:ILE:HD12	1:A:540:ASP:OD1	2.16	0.45
1:A:325:VAL:HG13	1:A:622:LEU:HD23	1.98	0.45
1:A:483:PRO:HA	1:A:486:PHE:HB3	1.99	0.45
1:A:491:MET:HE3	1:A:514:LEU:HB3	1.98	0.45
1:A:566:THR:C	1:A:567:LEU:HD12	2.41	0.45
1:D:59:GLU:HB3	1:D:222:LYS:HB3	1.99	0.45
1:F:32:ALA:HB3	1:F:38:LYS:HD2	1.99	0.45
1:F:632:GLN:CD	1:F:633:PHE:CE2	2.94	0.45
1:F:633:PHE:CE1	2:K:18:DT:C2	3.04	0.45
1:F:656:ASP:CB	1:F:657:PRO:CD	2.95	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:330:ALA:HB1	1:I:335:ALA:HB3	1.99	0.45
1:A:228:GLU:OE1	1:A:230:GLN:OE1	2.34	0.45
1:D:61:LEU:HD13	1:D:88:TRP:CD2	2.52	0.45
1:D:132:ILE:CD1	1:D:183:ARG:CZ	2.95	0.45
1:F:30:VAL:HB	1:F:253:VAL:HG12	1.98	0.45
1:F:101:ARG:NH2	1:F:537:ASP:OD1	2.49	0.45
1:F:191:GLN:NE2	1:F:411:ASP:OD1	2.50	0.45
1:F:592:PRO:HG3	1:F:644:PHE:CE2	2.52	0.45
2:K:6:DG:H2''	2:K:7:DC:O4'	2.16	0.45
1:D:295:ARG:HG2	1:D:321:ALA:HB1	1.99	0.45
1:D:392:ARG:HH11	1:D:546:SER:HB2	1.82	0.45
1:D:430:LEU:O	1:D:434:MET:HG3	2.17	0.45
1:F:257:ASP:O	1:F:609:ARG:HG2	2.17	0.45
1:I:47:ALA:CB	1:I:80:LEU:HD11	2.46	0.45
1:I:361:TYR:OH	1:I:567:LEU:HB3	2.17	0.45
1:D:138:GLU:O	1:D:139:THR:HG22	2.17	0.44
1:F:35:GLY:H	4:F:1663:ANP:PB	2.41	0.44
1:F:107:ILE:CG2	1:F:107:ILE:O	2.64	0.44
1:F:388:GLY:C	1:F:391:ASP:H	2.24	0.44
1:F:632:GLN:OE1	1:F:633:PHE:HE2	2.00	0.44
1:I:318:VAL:O	1:I:318:VAL:CG1	2.65	0.44
3:L:8:DG:H2''	3:L:9:DC:O4'	2.16	0.44
1:A:45:ARG:HD3	1:A:225:HIS:CE1	2.52	0.44
1:A:301:ASN:HD21	1:A:315:LEU:HB2	1.82	0.44
1:A:411:ASP:OD1	1:A:412:VAL:N	2.50	0.44
1:A:444:VAL:HG13	1:A:445:LEU:N	2.31	0.44
1:A:587:GLU:CD	1:A:630:ARG:NH1	2.69	0.44
1:D:60:ILE:HB	1:D:87:LEU:CD2	2.47	0.44
1:D:114:VAL:CG2	1:D:115:ILE:N	2.80	0.44
1:F:576:LEU:H	1:F:617:ARG:HH21	1.66	0.44
1:I:594:LYS:O	1:I:597:ILE:HB	2.17	0.44
3:Y:11:DA:C2	3:Y:12:DG:C4	3.05	0.44
1:A:45:ARG:HH11	1:A:251:LEU:HB3	1.83	0.44
1:A:303:LEU:HD11	1:A:611:PHE:CD2	2.52	0.44
1:A:383:ILE:HD12	1:A:383:ILE:N	2.33	0.44
1:A:418:ILE:HD13	1:A:467:PHE:CD2	2.52	0.44
1:D:91:THR:HG22	1:D:92:PHE:N	2.33	0.44
1:D:116:TYR:HE2	1:D:124:ILE:HD11	1.80	0.44
1:D:246:ARG:HD3	1:D:247:ASP:OD1	2.17	0.44
1:D:428:THR:HG1	3:Y:8:DG:P	2.37	0.44
1:D:655:VAL:HG12	1:D:656:ASP:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:25:THR:CG2	1:F:26:GLY:N	2.80	0.44
1:F:257:ASP:O	1:F:609:ARG:HG3	2.17	0.44
1:F:291:ARG:HH22	4:F:1663:ANP:HNB1	1.65	0.44
1:I:111:ARG:HA	1:I:112:GLY:HA2	1.64	0.44
1:I:336:GLU:OE1	1:I:625:THR:HG21	2.17	0.44
2:K:9:DC:C2	2:K:10:DG:C8	3.05	0.44
1:A:26:GLY:CA	1:A:248:ARG:O	2.60	0.44
1:D:269:GLN:NE2	1:D:273:ASP:OD2	2.50	0.44
1:D:504:GLY:C	1:D:508:GLN:HG3	2.37	0.44
1:F:124:ILE:O	1:F:128:VAL:HG22	2.17	0.44
1:F:132:ILE:HD11	1:F:183:ARG:HH21	1.83	0.44
1:F:287:GLU:OE2	1:F:288:HIS:CD2	2.70	0.44
1:F:546:SER:HB3	2:K:23:DT:OP1	2.17	0.44
1:F:586:VAL:HG11	1:F:645:LEU:HD21	2.00	0.44
1:I:138:GLU:O	1:I:139:THR:HG22	2.18	0.44
1:I:345:THR:HG23	1:I:379:ILE:HD11	1.98	0.44
2:X:19:DT:C2'	2:X:20:DT:H5'	2.48	0.44
1:F:70:ALA:O	1:F:73:MET:HB2	2.17	0.44
1:F:255:ASP:OD1	1:F:256:PRO:HD2	2.17	0.44
1:F:588:GLN:HE21	1:F:597:ILE:CD1	2.29	0.44
1:I:172:LEU:HD12	1:I:172:LEU:C	2.43	0.44
1:I:299:ALA:HA	1:I:651:LEU:HD13	1.99	0.44
1:I:384:VAL:HG12	1:I:572:ASN:ND2	2.33	0.44
1:A:235:ALA:O	1:A:239:LEU:HD12	2.17	0.44
1:D:566:THR:CG2	1:D:568:MET:CE	2.95	0.44
1:I:49:LEU:O	1:I:55:VAL:HG23	2.17	0.44
2:K:4:DG:H2''	2:K:5:DT:OP2	2.17	0.44
3:Y:14:DA:N3	3:Y:15:DC:C6	2.86	0.44
1:D:566:THR:CG2	1:D:568:MET:HE2	2.48	0.44
1:F:477:ALA:HA	1:F:480:ASN:HD21	1.83	0.44
1:I:61:LEU:HD13	1:I:88:TRP:CD2	2.52	0.44
1:I:117:ASP:O	1:I:121:GLN:HG3	2.18	0.44
1:I:575:GLY:H	1:I:617:ARG:NH2	2.16	0.44
3:L:11:DA:N1	3:L:12:DG:C6	2.86	0.44
1:A:224:ILE:HG22	1:A:250:LEU:CD1	2.48	0.44
1:A:291:ARG:NH2	4:A:1662:ANP:O3G	2.45	0.44
1:F:65:PHE:C	1:F:66:THR:CG2	2.90	0.44
1:F:129:MET:HE1	1:F:141:PRO:HB3	2.00	0.44
1:F:240:THR:O	1:F:241:ARG:C	2.59	0.44
1:F:656:ASP:HB2	1:F:657:PRO:CD	2.48	0.44
1:I:110:ARG:H	1:I:192:ASN:HD21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:198:ASP:HA	1:I:201:THR:OG1	2.18	0.44
1:D:233:ASN:ND2	1:D:236:GLN:HG3	2.32	0.44
1:F:257:ASP:OD1	1:F:310:ARG:HD2	2.18	0.44
1:F:591:LEU:O	1:F:591:LEU:HG	2.17	0.44
1:F:603:GLY:O	1:F:606:GLU:HB3	2.17	0.44
1:I:116:TYR:HE2	1:I:124:ILE:HD11	1.79	0.44
1:I:333:HIS:CD2	1:I:369:VAL:HG21	2.52	0.44
1:I:524:TRP:CZ3	1:I:541:ASP:OD2	2.70	0.44
2:K:1:DG:C2'	2:K:2:DC:H6	2.27	0.44
1:A:118:ASP:HB2	1:A:145:ARG:NH1	2.33	0.43
1:D:57:PRO:O	1:D:87:LEU:HD23	2.18	0.43
1:F:404:LEU:HD23	1:F:417:ILE:HD11	2.00	0.43
2:K:1:DG:H1'	2:K:2:DC:O4'	2.17	0.43
1:D:195:ASP:O	1:D:198:ASP:HB2	2.18	0.43
1:D:303:LEU:HB2	1:D:648:ILE:CG2	2.47	0.43
1:D:394:GLU:CD	1:D:510:ARG:HG2	2.43	0.43
1:F:320:GLU:HG2	6:F:2010:HOH:O	2.17	0.43
1:F:573:ALA:O	1:F:576:LEU:HD12	2.18	0.43
1:F:655:VAL:HG13	1:F:659:GLY:C	2.43	0.43
1:I:143:VAL:CG2	1:I:144:ILE:N	2.80	0.43
1:I:172:LEU:HD11	1:I:177:ALA:CA	2.48	0.43
1:I:308:THR:HG22	1:I:605:GLU:OE2	2.17	0.43
1:I:352:ARG:HD3	1:I:580:VAL:HG21	1.99	0.43
2:K:21:DT:H3'	2:K:22:DT:H72	2.00	0.43
3:L:12:DG:C4	3:L:13:DC:N4	2.85	0.43
1:A:34:ALA:HB1	1:A:616:THR:CG2	2.46	0.43
1:A:62:ALA:HA	1:A:225:HIS:HB2	2.00	0.43
1:A:69:ALA:O	1:A:73:MET:HE3	2.19	0.43
1:A:338:ASP:OD1	1:A:376:ARG:NH2	2.50	0.43
1:A:545:LEU:HD11	1:A:551:MET:HB2	2.00	0.43
1:F:106:HIS:C	1:F:108:GLY:H	2.26	0.43
1:F:260:ILE:HG21	1:F:610:LEU:HD12	2.01	0.43
1:F:606:GLU:HA	1:F:609:ARG:HH12	1.79	0.43
2:X:15:DT:C5'	2:X:15:DT:H6	2.31	0.43
1:A:500:LEU:CD2	1:A:511:LEU:HD23	2.48	0.43
1:D:152:LYS:O	1:D:201:THR:HG21	2.19	0.43
1:D:179:GLU:O	1:D:182:ARG:HB3	2.19	0.43
1:F:66:THR:HG21	1:F:548:VAL:HG21	2.00	0.43
1:F:162:ASP:O	1:F:174:ARG:HD2	2.18	0.43
1:I:167:PRO:O	1:I:174:ARG:N	2.52	0.43
1:I:303:LEU:O	1:I:608:ARG:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:19:DT:C1'	2:K:20:DT:H5'	2.48	0.43
1:A:114:VAL:HG22	1:A:115:ILE:N	2.34	0.43
1:A:232:THR:N	1:A:266:ALA:HB1	2.34	0.43
1:D:31:ILE:HG13	1:D:311:LEU:CD2	2.49	0.43
1:D:275:GLN:CD	1:D:275:GLN:H	2.26	0.43
1:F:97:VAL:HG11	1:F:544:LEU:CD1	2.36	0.43
1:F:424:GLY:HA2	2:K:9:DC:P	2.58	0.43
1:I:38:LYS:CG	1:I:39:THR:N	2.82	0.43
1:I:161:LEU:HD22	1:I:178:ALA:HB2	2.01	0.43
3:L:14:DA:OP2	3:L:14:DA:C4'	2.66	0.43
2:X:22:DT:C2	2:X:23:DT:C4	3.06	0.43
1:A:13:LEU:CD2	1:A:17:GLN:OE1	2.67	0.43
1:A:307:ASN:O	1:A:310:ARG:HG2	2.18	0.43
1:A:472:GLU:OE1	1:A:472:GLU:HA	2.17	0.43
1:A:546:SER:HB3	2:X:23:DT:OP1	2.18	0.43
1:D:61:LEU:O	1:D:224:ILE:HA	2.19	0.43
1:D:91:THR:H	1:D:94:SER:HB3	1.84	0.43
1:D:132:ILE:CD1	1:D:132:ILE:H	2.32	0.43
1:D:252:VAL:O	1:D:252:VAL:CG2	2.66	0.43
1:F:61:LEU:CD2	1:F:63:VAL:CG1	2.62	0.43
1:F:591:LEU:CD2	1:F:642:SER:HB2	2.46	0.43
1:I:354:TRP:HD1	1:I:563:ASP:O	2.01	0.43
1:A:12:ALA:O	1:A:40:ARG:NH1	2.38	0.43
1:D:436:TRP:HZ3	1:D:442:THR:HG21	1.81	0.43
1:F:13:LEU:CD2	1:F:17:GLN:OE1	2.66	0.43
1:F:25:THR:HG22	1:F:26:GLY:N	2.34	0.43
1:F:60:ILE:HG22	1:F:61:LEU:N	2.34	0.43
2:K:1:DG:H1	3:L:18:DC:H42	0.77	0.43
1:A:20:ALA:HA	1:A:284:TYR:CE1	2.54	0.43
1:A:144:ILE:CG2	1:A:148:ILE:HD11	2.45	0.43
1:A:198:ASP:HB3	1:A:202:GLU:HG2	2.00	0.43
1:A:263:PHE:CE1	1:A:264:ARG:HB2	2.54	0.43
1:A:300:ALA:O	1:A:304:ILE:HG22	2.18	0.43
1:A:424:GLY:C	1:A:463:LYS:HD3	2.44	0.43
1:D:210:VAL:HG11	1:D:213:VAL:CG2	2.49	0.43
1:D:470:LEU:O	1:D:474:MET:HG3	2.19	0.43
1:F:224:ILE:HG22	1:F:250:LEU:CD1	2.47	0.43
1:F:228:GLU:OE1	1:F:230:GLN:OE1	2.37	0.43
1:I:264[A]:ARG:HB3	1:I:264[A]:ARG:HH11	1.84	0.43
3:L:14:DA:O4'	3:L:15:DC:OP1	2.35	0.43
1:A:204:VAL:CG2	1:A:239:LEU:HD12	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:PHE:CD1	1:A:214:LEU:HB3	2.53	0.43
1:D:162:ASP:HB3	1:D:178:ALA:HB3	2.00	0.43
1:F:367:SER:HB2	1:F:383:ILE:HD13	2.01	0.43
1:A:401:TYR:OH	1:A:421:PRO:CG	2.31	0.43
1:D:162:ASP:HA	1:D:174:ARG:HB3	2.01	0.43
1:D:272:LEU:O	1:D:275:GLN:NE2	2.47	0.43
1:I:377:VAL:O	1:I:377:VAL:CG1	2.66	0.43
3:L:14:DA:OP2	3:L:14:DA:C1'	2.67	0.43
1:A:65:PHE:HE2	1:A:264:ARG:NH1	2.17	0.42
1:A:118:ASP:O	1:A:121:GLN:HB2	2.19	0.42
1:D:111:ARG:O	1:D:111:ARG:HG2	2.12	0.42
1:F:62:ALA:HA	1:F:225:HIS:O	2.19	0.42
1:F:328:HIS:HD2	1:F:655:VAL:O	2.02	0.42
1:I:312:ASP:C	1:I:312:ASP:OD1	2.62	0.42
1:I:359:ILE:HD11	1:I:565:VAL:HG11	2.01	0.42
3:L:1:DA:H8	3:L:1:DA:OP2	2.02	0.42
1:A:65:PHE:CE2	1:A:264:ARG:NH1	2.85	0.42
1:A:97:VAL:HG13	1:A:98:ARG:N	2.34	0.42
1:A:297:LEU:HD11	1:A:315:LEU:HB3	2.01	0.42
1:A:490:VAL:CG2	1:A:491:MET:N	2.82	0.42
1:A:497:LEU:HD11	1:A:501:ARG:NH2	2.34	0.42
1:D:412:VAL:O	1:D:416:ARG:HG2	2.19	0.42
1:D:587:GLU:HG2	1:D:626:ALA:HB1	2.01	0.42
1:D:623:LEU:N	1:D:623:LEU:HD12	2.33	0.42
1:F:90:SER:OG	1:F:95:ALA:HB2	2.19	0.42
1:F:114:VAL:HG13	1:F:193:ALA:CB	2.48	0.42
1:F:436:TRP:HA	1:F:439:THR:CG2	2.47	0.42
1:I:272:LEU:O	1:I:275:GLN:NE2	2.52	0.42
1:I:326:THR:HA	1:I:653:ASP:O	2.19	0.42
1:A:98:ARG:HG3	1:A:102:THR:HG23	2.00	0.42
1:A:388:GLY:O	1:A:391:ASP:HB2	2.19	0.42
1:F:29:LEU:HD23	1:F:30:VAL:C	2.45	0.42
1:F:199:LEU:HA	1:F:199:LEU:HD23	1.69	0.42
1:F:263:PHE:CD1	2:K:21:DT:H71	2.54	0.42
1:F:327:PHE:CE1	1:F:645:LEU:HD11	2.55	0.42
1:F:482:GLU:O	1:F:486:PHE:CB	2.67	0.42
1:F:542:ALA:HA	1:F:545:LEU:CD1	2.49	0.42
1:I:168:PHE:CD2	1:I:168:PHE:O	2.72	0.42
1:I:500:LEU:HA	1:I:503:GLU:HB2	2.01	0.42
1:A:444:VAL:HG13	1:A:445:LEU:H	1.84	0.42
1:F:44:TYR:O	1:F:45:ARG:C	2.61	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:227:ASP:O	1:F:228:GLU:C	2.62	0.42
1:F:324:PRO:O	1:F:621:ARG:NH1	2.53	0.42
1:F:483:PRO:O	1:F:487:LEU:HG	2.20	0.42
1:F:632:GLN:OE1	1:F:633:PHE:CE2	2.72	0.42
1:I:401:TYR:CZ	1:I:417:ILE:HB	2.54	0.42
1:I:504:GLY:O	1:I:508:GLN:HG3	2.20	0.42
1:A:126:LYS:HA	1:A:129:MET:HE2	2.02	0.42
1:D:327:PHE:O	1:D:327:PHE:CD2	2.73	0.42
1:D:591:LEU:HD12	1:D:591:LEU:HA	1.77	0.42
1:F:291:ARG:HB2	4:F:1663:ANP:H4'	2.00	0.42
1:F:418:ILE:HD12	1:F:423:ARG:HD2	2.02	0.42
1:I:107:ILE:HB	1:I:205:ARG:NH2	2.35	0.42
1:I:290:TYR:CD1	1:I:318:VAL:HG11	2.54	0.42
1:I:399:LEU:O	1:I:403:ARG:N	2.46	0.42
1:I:500:LEU:O	1:I:504:GLY:CA	2.66	0.42
2:X:2:DC:H2''	2:X:3:DA:OP2	2.16	0.42
1:A:91:THR:HG22	1:A:92:PHE:N	2.34	0.42
1:A:200:ILE:CG2	1:A:235:ALA:HB1	2.49	0.42
1:D:111:ARG:HA	1:D:112:GLY:HA2	1.67	0.42
1:F:65:PHE:O	1:F:66:THR:HG22	2.17	0.42
1:F:601:PRO:O	1:F:604:ILE:N	2.53	0.42
1:I:401:TYR:OH	1:I:421:PRO:CD	2.68	0.42
1:I:437:ALA:HA	1:I:442:THR:CG2	2.45	0.42
2:X:23:DT:H6	2:X:23:DT:H2'	1.57	0.42
1:A:424:GLY:CA	2:X:9:DC:OP1	2.68	0.42
1:D:357:MET:CG	1:D:580:VAL:HB	2.44	0.42
1:D:371:GLU:OE2	1:D:375:ARG:NH2	2.53	0.42
1:D:528:GLU:O	1:D:529:ALA:HB3	2.20	0.42
1:I:263:PHE:C	1:I:265:GLY:N	2.78	0.42
2:K:3:DA:C2	3:L:17:DG:N2	2.88	0.42
2:X:15:DT:H5'	2:X:15:DT:C6	2.49	0.42
1:A:70:ALA:O	1:A:73:MET:HB3	2.20	0.42
1:D:332:ASP:HB3	1:D:335:ALA:CB	2.50	0.42
1:D:487:LEU:O	1:D:491:MET:CG	2.58	0.42
1:D:656:ASP:CG	1:D:660:GLN:HB2	2.44	0.42
1:F:209:GLU:O	1:F:211:PRO:HD3	2.20	0.42
1:I:261:TYR:HB3	1:I:264[B]:ARG:HB2	2.01	0.42
1:I:420:ARG:HA	1:I:420:ARG:HD3	1.76	0.42
1:A:29:LEU:HB2	1:A:274:PHE:CE2	2.55	0.42
1:D:110:ARG:H	1:D:192:ASN:HD21	1.68	0.42
1:F:35:GLY:HA2	4:F:1663:ANP:H5'2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:15:DT:H2''	2:K:16:DC:O5'	2.19	0.42
2:X:3:DA:H2''	2:X:4:DG:OP2	2.19	0.42
2:X:17:DG:H4'	2:X:18:DT:OP1	2.18	0.42
2:X:17:DG:H1'	2:X:18:DT:C6	2.54	0.42
1:A:65:PHE:HE2	1:A:264:ARG:HH12	1.66	0.42
1:A:173:PRO:O	1:A:176:ALA:HB3	2.19	0.42
1:A:198:ASP:O	1:A:202:GLU:N	2.39	0.42
1:A:550:ASP:HA	1:A:553:THR:OG1	2.20	0.42
1:D:42:LEU:HD21	1:D:253:VAL:HG11	2.01	0.42
1:D:151:ALA:O	1:D:156:TRP:HB2	2.20	0.42
1:D:374:LEU:HB3	1:D:379:ILE:HB	2.01	0.42
1:F:27:PRO:HD2	1:F:280:ASP:CB	2.50	0.42
1:F:188:LYS:NZ	1:F:189:LYS:HG2	2.34	0.42
1:I:207:PHE:HB2	1:I:242:LEU:HD23	2.02	0.42
1:I:384:VAL:HG12	1:I:572:ASN:HD21	1.85	0.42
1:I:400:ALA:HB3	1:I:417:ILE:CG2	2.49	0.42
1:I:577:GLU:HB2	1:I:619:MET:HE3	2.02	0.42
1:A:343:TRP:CD2	1:A:346:ARG:HD2	2.55	0.41
1:F:256:PRO:HG2	1:F:311:LEU:CD2	2.50	0.41
1:F:522:GLU:HA	1:F:525:SER:HB2	2.02	0.41
1:I:93:HIS:NE2	3:L:23:DT:O2	2.53	0.41
1:I:400:ALA:HA	1:I:403:ARG:HG2	2.00	0.41
1:I:587:GLU:O	1:I:592:PRO:HD2	2.20	0.41
1:A:291:ARG:NH1	4:A:1662:ANP:O3G	2.51	0.41
1:A:424:GLY:HA3	1:A:463:LYS:HD3	2.02	0.41
1:D:194:ILE:HB	1:D:198:ASP:CB	2.50	0.41
1:D:333:HIS:O	1:D:336:GLU:HG2	2.20	0.41
1:D:395:ILE:HD13	1:D:548:VAL:HG22	2.01	0.41
1:D:416:ARG:CB	6:D:2022:HOH:O	2.69	0.41
1:D:416:ARG:N	1:D:416:ARG:HD2	2.35	0.41
1:F:334:ARG:HH12	1:F:376:ARG:NH1	2.15	0.41
1:I:275:GLN:NE2	1:I:276:LYS:HG3	2.35	0.41
1:I:352:ARG:HD3	1:I:580:VAL:CG2	2.50	0.41
1:I:400:ALA:CB	1:I:417:ILE:HG23	2.50	0.41
1:I:404:LEU:HD23	1:I:471:MET:HE2	2.01	0.41
1:A:393:ARG:O	1:A:394:GLU:C	2.62	0.41
1:A:417:ILE:HG13	1:A:417:ILE:H	1.68	0.41
1:D:341:ALA:O	1:D:345:THR:HG23	2.21	0.41
1:D:400:ALA:HB1	1:D:417:ILE:HG23	2.02	0.41
1:D:503:GLU:O	1:D:507:GLY:N	2.53	0.41
1:D:581:VAL:HB	1:D:618:ALA:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:48:HIS:CE1	1:F:52:HIS:CD2	3.07	0.41
1:F:114:VAL:HG22	1:F:115:ILE:N	2.35	0.41
1:I:139:THR:OG1	1:I:140:GLN:N	2.53	0.41
1:I:606:GLU:HG3	1:I:609:ARG:HH11	1.83	0.41
1:I:659:GLY:O	1:I:661:PRO:HD3	2.20	0.41
2:K:4:DG:O6	3:L:15:DC:C4	2.73	0.41
2:X:19:DT:C2'	2:X:19:DT:O2	2.68	0.41
1:A:338:ASP:CG	1:A:376:ARG:NH2	2.78	0.41
1:D:139:THR:OG1	1:D:140:GLN:N	2.53	0.41
1:D:268:ILE:O	1:D:272:LEU:HG	2.20	0.41
1:D:331:THR:CA	1:D:628:GLN:HB2	2.44	0.41
1:D:360:LEU:HD23	1:D:570:LEU:HD23	2.02	0.41
1:D:478:ALA:HB2	1:D:486:PHE:CE1	2.55	0.41
1:F:394:GLU:HB2	1:F:514:LEU:HD11	1.92	0.41
1:F:421:PRO:HA	1:F:499:LEU:HD21	2.02	0.41
1:F:495:GLY:O	1:F:498:ASP:N	2.54	0.41
1:I:428:THR:OG1	3:L:8:DG:OP2	2.38	0.41
1:I:636:THR:C	1:I:637:ASN:OD1	2.64	0.41
2:K:7:DC:H2''	2:K:8:DT:C6	2.55	0.41
3:Y:12:DG:H2'	3:Y:13:DC:C6	2.55	0.41
3:Y:22:DT:C7	3:Y:23:DT:C7	2.98	0.41
1:A:100:LEU:HD21	1:A:202:GLU:C	2.44	0.41
1:A:155:LEU:HD23	1:A:201:THR:HG22	2.03	0.41
1:A:234:ARG:CG	1:A:270:ASN:ND2	2.67	0.41
1:A:587:GLU:OE1	1:A:630:ARG:NH1	2.54	0.41
1:D:17:GLN:O	1:D:18:ALA:C	2.62	0.41
1:D:48:HIS:O	1:D:49:LEU:C	2.61	0.41
1:D:591:LEU:HB3	1:D:592:PRO:HD2	2.00	0.41
1:F:363:THR:HB	1:F:366:GLN:HG3	2.01	0.41
1:F:422:ARG:HD3	1:F:422:ARG:HA	1.78	0.41
1:I:61:LEU:O	1:I:224:ILE:HA	2.21	0.41
1:I:414:LEU:HD23	1:I:415:ARG:N	2.36	0.41
1:I:457:LEU:O	1:I:458:ASP:OD1	2.38	0.41
3:L:1:DA:C2'	3:L:2:DC:O5'	2.67	0.41
1:D:286:LEU:N	1:D:286:LEU:CD1	2.84	0.41
1:D:575:GLY:H	1:D:617:ARG:CZ	2.24	0.41
1:F:38:LYS:NZ	1:F:255:ASP:HB2	2.35	0.41
1:F:200:ILE:CG2	1:F:235:ALA:CB	2.98	0.41
1:F:513:ASN:O	1:F:516:GLU:HB3	2.20	0.41
1:I:286:LEU:HD12	1:I:286:LEU:N	2.34	0.41
1:I:400:ALA:HA	1:I:403:ARG:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:417:ILE:HG13	1:I:418:ILE:N	2.35	0.41
2:K:12:DA:C6	2:K:13:DG:O6	2.74	0.41
3:L:14:DA:H1'	3:L:15:DC:P	2.59	0.41
3:Y:14:DA:O4'	3:Y:15:DC:OP1	2.37	0.41
1:A:124:ILE:O	1:A:128:VAL:HG22	2.21	0.41
1:A:500:LEU:O	1:A:504:GLY:HA3	2.20	0.41
1:A:616:THR:HG22	1:A:616:THR:O	2.21	0.41
1:D:91:THR:O	1:D:92:PHE:C	2.62	0.41
1:D:227:ASP:HA	1:D:253:VAL:HG13	2.03	0.41
1:F:122:LEU:CA	1:F:125:ILE:HD12	2.43	0.41
1:F:632:GLN:HG3	2:K:19:DT:H73	2.02	0.41
1:I:485:ALA:HA	1:I:488:ARG:HD2	2.02	0.41
2:X:11:DC:N4	3:Y:8:DG:C6	2.75	0.41
3:Y:3:DG:C1'	3:Y:4:DA:H5'	2.46	0.41
1:D:577:GLU:OE1	1:D:619:MET:CE	2.69	0.41
1:D:656:ASP:OD1	1:D:658:TYR:O	2.39	0.41
1:F:29:LEU:HB2	1:F:274:PHE:CE2	2.55	0.41
1:F:151:ALA:HB1	1:F:156:TRP:HB2	2.02	0.41
1:I:91:THR:CG2	6:I:2009:HOH:O	2.69	0.41
1:I:325:VAL:HG23	1:I:652:PHE:HB3	2.03	0.41
1:A:76:ARG:HA	1:A:79:HIS:ND1	2.36	0.41
1:A:152:LYS:CE	1:A:195:ASP:OD2	2.68	0.41
1:A:185:GLU:OE1	1:A:188:LYS:HE3	2.21	0.41
1:A:333:HIS:CE1	1:A:631:MET:HB3	2.55	0.41
1:D:114:VAL:HG21	1:D:403:ARG:NH2	2.36	0.41
1:D:407:ASN:O	1:D:407:ASN:OD1	2.39	0.41
1:D:548:VAL:O	1:D:548:VAL:HG12	2.20	0.41
1:F:35:GLY:N	4:F:1663:ANP:PB	2.94	0.41
1:F:66:THR:CG2	1:F:548:VAL:CG2	2.99	0.41
1:F:199:LEU:O	1:F:203:THR:OG1	2.38	0.41
1:F:411:ASP:HB3	1:F:444:VAL:CG1	2.44	0.41
1:F:426:GLY:HA2	2:K:8:DT:P	2.60	0.41
1:F:430:LEU:O	1:F:433:LEU:N	2.54	0.41
1:F:524:TRP:HZ3	1:F:541:ASP:OD2	2.04	0.41
1:F:655:VAL:C	1:F:656:ASP:O	2.63	0.41
1:I:297:LEU:HD22	1:I:315:LEU:HD13	2.01	0.41
1:I:367:SER:O	1:I:370:ILE:HB	2.21	0.41
2:K:8:DT:C2'	2:K:9:DC:H6	2.23	0.41
3:L:12:DG:C2	3:L:13:DC:C2	3.08	0.41
2:X:19:DT:H2''	2:X:20:DT:O5'	2.19	0.41
1:A:97:VAL:HB	1:A:199:LEU:CD1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:GLU:C	1:A:187:ARG:N	2.78	0.41
1:A:545:LEU:HD11	1:A:551:MET:CB	2.51	0.41
1:D:326:THR:HA	1:D:653:ASP:O	2.21	0.41
1:F:63:VAL:HA	1:F:90:SER:O	2.21	0.41
1:F:422:ARG:HG3	2:K:10:DG:P	2.61	0.41
1:F:608:ARG:NE	1:F:644:PHE:CE1	2.89	0.41
1:I:131:SER:HB2	1:I:183:ARG:HH22	1.86	0.41
1:I:228:GLU:OE1	1:I:230:GLN:NE2	2.45	0.41
1:I:390:TYR:O	1:I:391:ASP:HB2	2.21	0.41
2:X:12:DA:H2'	2:X:13:DG:H8	1.82	0.41
3:Y:1:DA:C1'	3:Y:2:DC:O5'	2.69	0.41
1:A:27:PRO:CG	1:A:280:ASP:HB2	2.50	0.40
1:A:60:ILE:HG21	1:A:225:HIS:CD2	2.56	0.40
1:A:60:ILE:HG22	1:A:61:LEU:N	2.36	0.40
1:D:366:GLN:O	1:D:370:ILE:HG12	2.21	0.40
1:D:445:LEU:O	1:D:448:CYS:HB2	2.22	0.40
1:D:566:THR:HG21	1:D:568:MET:HE2	2.02	0.40
1:F:346:ARG:O	1:F:349:GLY:N	2.54	0.40
1:F:487:LEU:O	1:F:491:MET:HG3	2.20	0.40
1:F:537:ASP:O	1:F:540:ASP:HB2	2.21	0.40
1:I:504:GLY:C	1:I:508:GLN:OE1	2.64	0.40
3:Y:21:DT:C2'	3:Y:22:DT:OP1	2.64	0.40
1:D:46:ILE:HG13	1:D:225:HIS:CE1	2.56	0.40
1:D:285:MET:HE1	1:D:313:LYS:CA	2.49	0.40
1:D:307:ASN:CB	1:D:310[A]:ARG:NH2	2.84	0.40
1:D:633:PHE:CD1	1:D:633:PHE:N	2.90	0.40
1:F:113:PHE:CD1	1:F:113:PHE:C	3.00	0.40
1:F:207:PHE:CD1	1:F:214:LEU:HB3	2.56	0.40
1:F:294:ALA:HB3	1:F:321:ALA:HA	2.03	0.40
1:F:400:ALA:HB1	1:F:413:ALA:HB1	2.02	0.40
1:F:592:PRO:O	1:F:593:SER:CB	2.69	0.40
1:I:118:ASP:OD1	1:I:118:ASP:N	2.49	0.40
1:A:120:ASP:OD1	1:A:396:ARG:NH2	2.54	0.40
1:A:200:ILE:O	1:A:201:THR:C	2.64	0.40
1:A:236:GLN:O	1:A:237:TYR:C	2.65	0.40
1:A:388:GLY:C	1:A:391:ASP:H	2.28	0.40
1:A:478:ALA:HA	1:A:486:PHE:HE2	1.87	0.40
1:D:255:ASP:OD1	1:D:255:ASP:C	2.63	0.40
1:I:142:ARG:NE	1:I:145:ARG:NH2	2.63	0.40
1:I:597:ILE:HA	1:I:604:ILE:HD11	2.03	0.40
2:X:2:DC:C2'	2:X:3:DA:OP2	2.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:LEU:HD22	1:A:88:TRP:CE3	2.55	0.40
1:A:332:ASP:C	1:A:332:ASP:OD1	2.63	0.40
1:A:348:HIS:HA	1:A:352:ARG:O	2.21	0.40
1:D:144:ILE:HA	1:D:147:ILE:HD12	2.04	0.40
1:F:98:ARG:NH1	1:F:102:THR:HG21	2.36	0.40
1:F:303:LEU:HD21	1:F:608:ARG:HG3	2.04	0.40
1:F:387:VAL:O	1:F:388:GLY:C	2.64	0.40
1:I:172:LEU:HD11	1:I:177:ALA:HB2	2.03	0.40
1:A:45:ARG:NH1	1:A:251:LEU:CB	2.84	0.40
1:A:303:LEU:CD1	1:A:611:PHE:CD2	3.04	0.40
1:A:385:GLY:HA2	1:A:552:ARG:NH2	2.36	0.40
1:A:592:PRO:O	1:A:596:ALA:HB3	2.22	0.40
1:D:16:THR:CG2	6:D:2001:HOH:O	2.69	0.40
1:D:173:PRO:HD2	1:D:176:ALA:HB3	2.04	0.40
1:D:325:VAL:CG2	1:D:652:PHE:CB	2.96	0.40
1:D:642:SER:HB3	1:D:645:LEU:HD12	2.04	0.40
1:D:657:PRO:HG2	1:I:11:GLN:O	2.21	0.40
1:F:20:ALA:HA	1:F:284:TYR:CE2	2.56	0.40
1:F:307:ASN:OD1	1:F:608:ARG:HD2	2.22	0.40
1:F:394:GLU:O	1:F:398:ILE:HG13	2.22	0.40
1:I:93:HIS:CE1	3:L:23:DT:O2	2.74	0.40
1:I:162:ASP:HB3	1:I:178:ALA:CB	2.52	0.40
1:I:290:TYR:HD1	1:I:318:VAL:HG11	1.87	0.40
1:I:661:PRO:C	1:I:662:ILE:CG1	2.77	0.40
2:K:3:DA:H1'	2:K:4:DG:C8	2.56	0.40
3:L:3:DG:H1'	3:L:4:DA:H8	1.85	0.40
3:Y:14:DA:OP2	3:Y:14:DA:C3'	2.69	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	621/665 (93%)	537 (86%)	71 (11%)	13 (2%)	5	27
1	D	636/665 (96%)	572 (90%)	56 (9%)	8 (1%)	9	38
1	F	622/665 (94%)	553 (89%)	60 (10%)	9 (1%)	9	36
1	I	629/665 (95%)	570 (91%)	54 (9%)	5 (1%)	16	50
All	All	2508/2660 (94%)	2232 (89%)	241 (10%)	35 (1%)	9	36

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	107	ILE
1	D	143	VAL
1	D	172	LEU
1	D	592	PRO
1	F	107	ILE
1	I	174	ARG
1	A	195	ASP
1	A	197	GLY
1	A	199	LEU
1	A	245	SER
1	D	461	ALA
1	D	647	ASP
1	F	165	ARG
1	F	378	GLN
1	F	592	PRO
1	A	105	GLU
1	A	355	SER
1	A	165	ARG
1	A	196	PHE
1	D	123	ASP
1	F	53	TYR
1	I	264[A]	ARG
1	I	264[B]	ARG
1	I	321	ALA
1	A	378	GLN
1	A	593	SER
1	A	649	GLU
1	D	508	GLN
1	F	593	SER
1	F	279	PRO
1	F	648	ILE
1	F	141	PRO
1	I	318	VAL

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Mol	Chain	Res	Type
1	A	141	PRO
1	D	318	VAL

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	512/536 (96%)	492 (96%)	20 (4%)	28	62
1	D	521/536 (97%)	501 (96%)	20 (4%)	29	63
1	F	513/536 (96%)	491 (96%)	22 (4%)	26	60
1	I	518/536 (97%)	505 (98%)	13 (2%)	42	72
All	All	2064/2144 (96%)	1989 (96%)	75 (4%)	31	65

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	THR
1	A	49	LEU
1	A	114	VAL
1	A	199	LEU
1	A	239	LEU
1	A	252	VAL
1	A	258	GLN
1	A	271	ILE
1	A	273	ASP
1	A	275	GLN
1	A	280	ASP
1	A	352	ARG
1	A	374	LEU
1	A	417	ILE
1	A	423	ARG
1	A	425	ILE
1	A	432	LYS
1	A	471	MET
1	A	475	SER

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Mol	Chain	Res	Type
1	A	537	ASP
1	D	42	LEU
1	D	114	VAL
1	D	125	ILE
1	D	132	ILE
1	D	138	GLU
1	D	143	VAL
1	D	264[A]	ARG
1	D	264[B]	ARG
1	D	287	GLU
1	D	309	GLU
1	D	325	VAL
1	D	366	GLN
1	D	435	GLU
1	D	454	GLN
1	D	459	ARG
1	D	487	LEU
1	D	514	LEU
1	D	546	SER
1	D	597	ILE
1	D	633	PHE
1	F	68	LYS
1	F	124	ILE
1	F	132	ILE
1	F	135	ILE
1	F	147	ILE
1	F	226	VAL
1	F	239	LEU
1	F	240	THR
1	F	252	VAL
1	F	289	ASN
1	F	352	ARG
1	F	374	LEU
1	F	383	ILE
1	F	398	ILE
1	F	432	LYS
1	F	475	SER
1	F	537	ASP
1	F	546	SER
1	F	551	MET
1	F	581	VAL
1	F	620	GLU

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Mol	Chain	Res	Type
1	F	635	LYS
1	I	42	LEU
1	I	80	LEU
1	I	125	ILE
1	I	138	GLU
1	I	236	GLN
1	I	287	GLU
1	I	308	THR
1	I	325	VAL
1	I	428	THR
1	I	435	GLU
1	I	456	ILE
1	I	646	GLU
1	I	660	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (67) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	48	HIS
1	A	52	HIS
1	A	191	GLN
1	A	192	ASN
1	A	225	HIS
1	A	249	ASN
1	A	258	GLN
1	A	270	ASN
1	A	288	HIS
1	A	301	ASN
1	A	328	HIS
1	A	348	HIS
1	A	366	GLN
1	A	378	GLN
1	A	407	ASN
1	A	480	ASN
1	A	502	GLN
1	A	513	ASN
1	A	571	HIS
1	D	19	GLN
1	D	56	HIS
1	D	106	HIS
1	D	154	ASN

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Mol	Chain	Res	Type
1	D	192	ASN
1	D	270	ASN
1	D	328	HIS
1	D	441	HIS
1	D	462	HIS
1	D	480	ASN
1	D	572	ASN
1	D	660	GLN
1	F	48	HIS
1	F	52	HIS
1	F	93	HIS
1	F	106	HIS
1	F	191	GLN
1	F	192	ASN
1	F	225	HIS
1	F	258	GLN
1	F	288	HIS
1	F	328	HIS
1	F	366	GLN
1	F	480	ASN
1	F	502	GLN
1	F	505	GLN
1	F	513	ASN
1	F	571	HIS
1	F	588	GLN
1	F	637	ASN
1	I	67	ASN
1	I	106	HIS
1	I	154	ASN
1	I	192	ASN
1	I	269	GLN
1	I	270	ASN
1	I	301	ASN
1	I	323	GLN
1	I	328	HIS
1	I	333	HIS
1	I	364	ASN
1	I	407	ASN
1	I	440	HIS
1	I	450	ASN
1	I	505	GLN
1	I	572	ASN

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Mol	Chain	Res	Type
1	I	632	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
4	ANP	A	1662	5	33,33,33	1.99	12 (36%)	45,52,52	1.96	11 (24%)
4	ANP	F	1663	5	33,33,33	1.92	12 (36%)	45,52,52	2.04	12 (26%)

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
4	ANP	A	1662	5	-	7/18/38/38	0/3/3/3
4	ANP	F	1663	5	-	9/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1663	ANP	PB-N3B	4.50	1.75	1.63
4	A	1662	ANP	PB-N3B	4.35	1.74	1.63
4	F	1663	ANP	C5-C4	4.32	1.46	1.39
4	A	1662	ANP	C5-C4	4.09	1.46	1.39
4	A	1662	ANP	PG-N3B	4.03	1.73	1.63
4	F	1663	ANP	PG-N3B	4.01	1.73	1.63
4	A	1662	ANP	PG-O3G	-3.16	1.48	1.56
4	A	1662	ANP	PA-O3A	2.94	1.62	1.59
4	A	1662	ANP	PG-O2G	-2.94	1.49	1.56
4	F	1663	ANP	PG-O2G	-2.89	1.49	1.56
4	F	1663	ANP	C5-N7	-2.80	1.34	1.39
4	A	1662	ANP	PB-O1B	2.72	1.50	1.46
4	F	1663	ANP	PG-O3G	-2.62	1.49	1.56
4	A	1662	ANP	C5-N7	-2.59	1.34	1.39
4	A	1662	ANP	C5-C6	2.59	1.48	1.41
4	F	1663	ANP	C5-C6	2.53	1.48	1.41
4	A	1662	ANP	C4-N9	-2.42	1.32	1.37
4	F	1663	ANP	C4-N9	-2.38	1.32	1.37
4	A	1662	ANP	PB-O2B	-2.28	1.50	1.56
4	F	1663	ANP	PB-O2B	-2.24	1.50	1.56
4	F	1663	ANP	PB-O1B	2.07	1.49	1.46
4	F	1663	ANP	PG-O1G	2.06	1.49	1.46
4	A	1662	ANP	C8-N9	-2.01	1.34	1.37
4	F	1663	ANP	C8-N9	-2.01	1.34	1.37

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1662	ANP	C5-C4-N3	-5.84	118.68	126.72
4	F	1663	ANP	C5-C4-N3	-5.44	119.23	126.72
4	F	1663	ANP	O1G-PG-N3B	-5.15	104.19	111.77
4	A	1662	ANP	N3-C4-N9	4.84	135.40	127.17
4	F	1663	ANP	N3-C4-N9	4.50	134.82	127.17
4	A	1662	ANP	O2B-PB-O1B	3.81	118.05	109.87
4	F	1663	ANP	O2B-PB-O1B	3.80	118.02	109.87
4	A	1662	ANP	C4-C5-N7	-3.66	106.40	110.58
4	F	1663	ANP	C4-C5-N7	-3.58	106.49	110.58
4	A	1662	ANP	C2-N3-C4	3.51	120.41	111.83
4	A	1662	ANP	C4-N9-C8	3.44	109.35	105.74
4	F	1663	ANP	C2-N3-C4	3.40	120.13	111.83
4	F	1663	ANP	C4-N9-C8	3.15	109.04	105.74
4	F	1663	ANP	N3-C2-N1	-3.12	123.86	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1663	ANP	O1B-PB-N3B	-3.02	107.32	111.77
4	A	1662	ANP	O2G-PG-O3G	2.99	115.62	107.59
4	A	1662	ANP	C5-N7-C8	2.88	107.98	103.45
4	A	1662	ANP	N3-C2-N1	-2.81	124.33	128.58
4	F	1663	ANP	C5-N7-C8	2.79	107.83	103.45
4	A	1662	ANP	N9-C8-N7	-2.54	110.34	113.94
4	F	1663	ANP	N9-C8-N7	-2.29	110.69	113.94
4	F	1663	ANP	C6-C5-N7	2.16	136.25	132.09
4	A	1662	ANP	C6-C5-N7	2.09	136.12	132.09

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1662	ANP	PA-O3A-PB-O2B
4	A	1662	ANP	C5'-O5'-PA-O1A
4	F	1663	ANP	PB-N3B-PG-O1G
4	F	1663	ANP	PG-N3B-PB-O1B
4	F	1663	ANP	PG-N3B-PB-O3A
4	F	1663	ANP	C5'-O5'-PA-O2A
4	F	1663	ANP	C5'-O5'-PA-O3A
4	F	1663	ANP	O4'-C4'-C5'-O5'
4	A	1662	ANP	O4'-C4'-C5'-O5'
4	A	1662	ANP	C3'-C4'-C5'-O5'
4	F	1663	ANP	C3'-C4'-C5'-O5'
4	A	1662	ANP	C5'-O5'-PA-O3A
4	F	1663	ANP	C5'-O5'-PA-O1A
4	F	1663	ANP	PB-O3A-PA-O2A
4	A	1662	ANP	PA-O3A-PB-O1B
4	A	1662	ANP	PG-N3B-PB-O3A

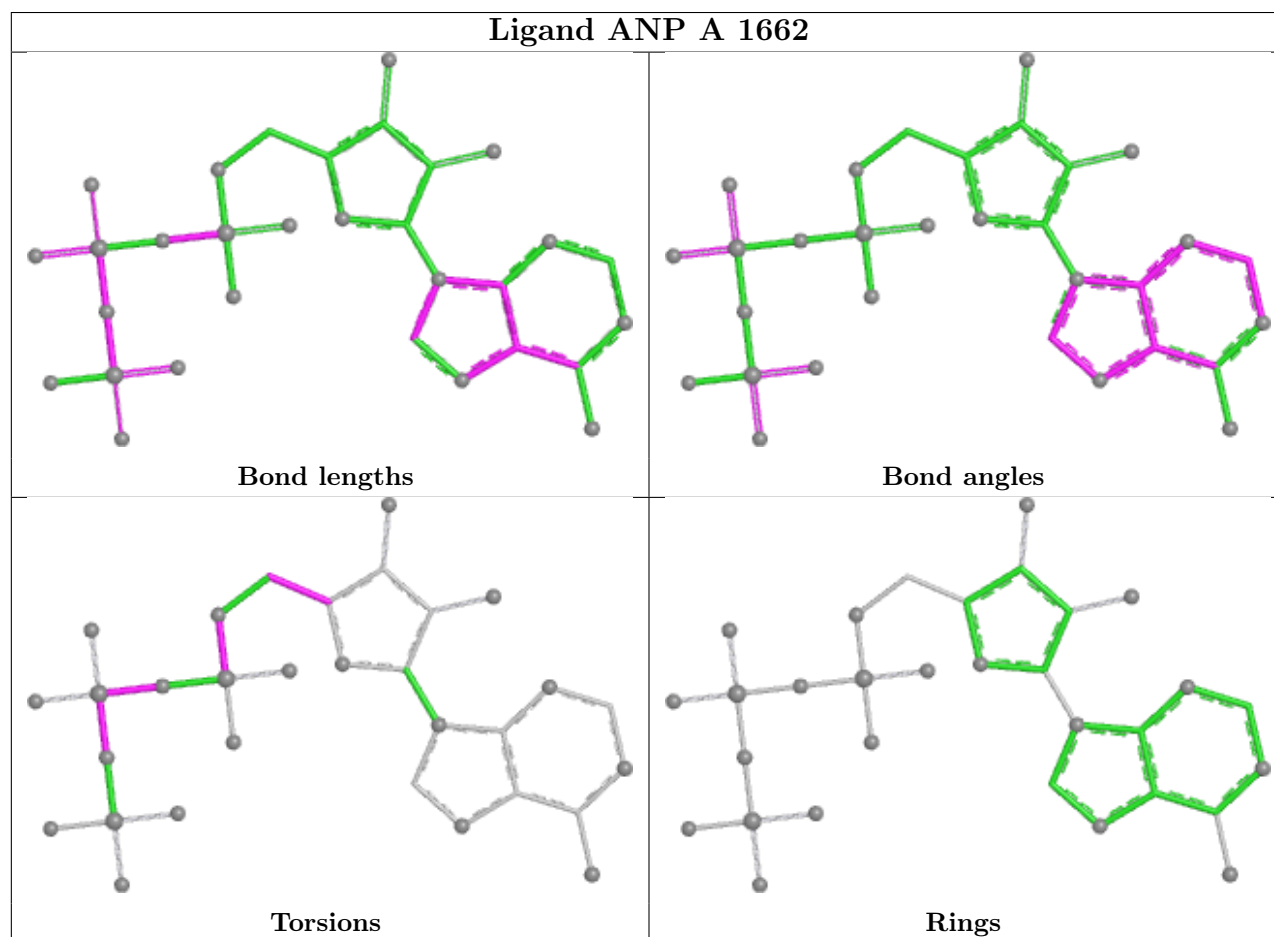
There are no ring outliers.

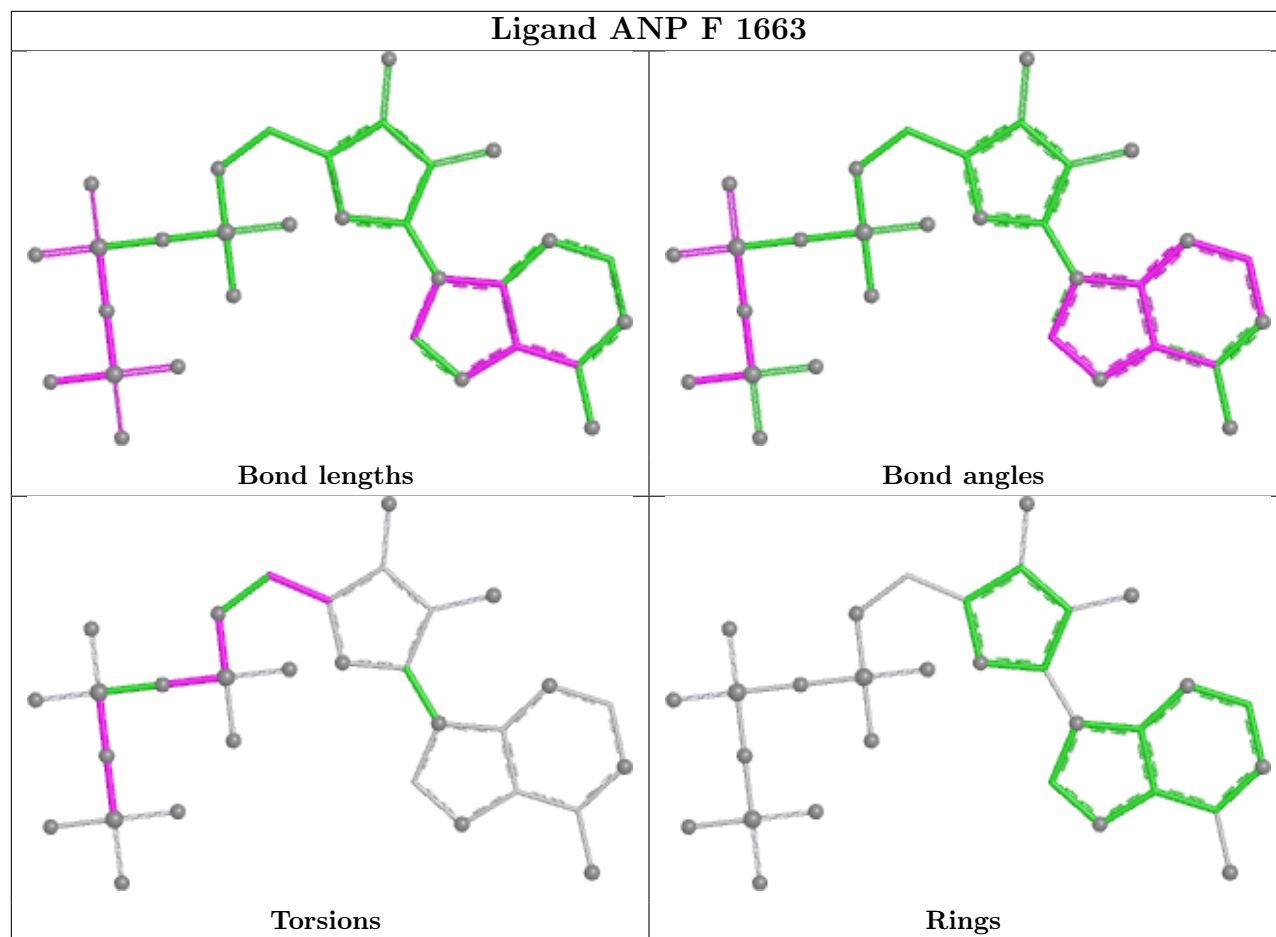
2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1662	ANP	5	0
4	F	1663	ANP	11	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	631/665 (94%)	-0.72	0 100 100	61, 115, 166, 194	0
1	D	642/665 (96%)	-0.99	0 100 100	40, 83, 137, 200	2 (0%)
1	F	632/665 (95%)	-0.71	0 100 100	36, 115, 166, 196	0
1	I	638/665 (95%)	-0.98	0 100 100	42, 83, 137, 199	1 (0%)
2	K	23/25 (92%)	-0.41	0 100 100	117, 131, 152, 202	0
2	X	23/25 (92%)	-0.50	0 100 100	110, 125, 145, 187	0
3	L	23/25 (92%)	-0.48	0 100 100	91, 132, 169, 194	0
3	Y	23/25 (92%)	-0.57	0 100 100	89, 130, 147, 165	0
All	All	2635/2760 (95%)	-0.84	0 100 100	36, 95, 161, 202	3 (0%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

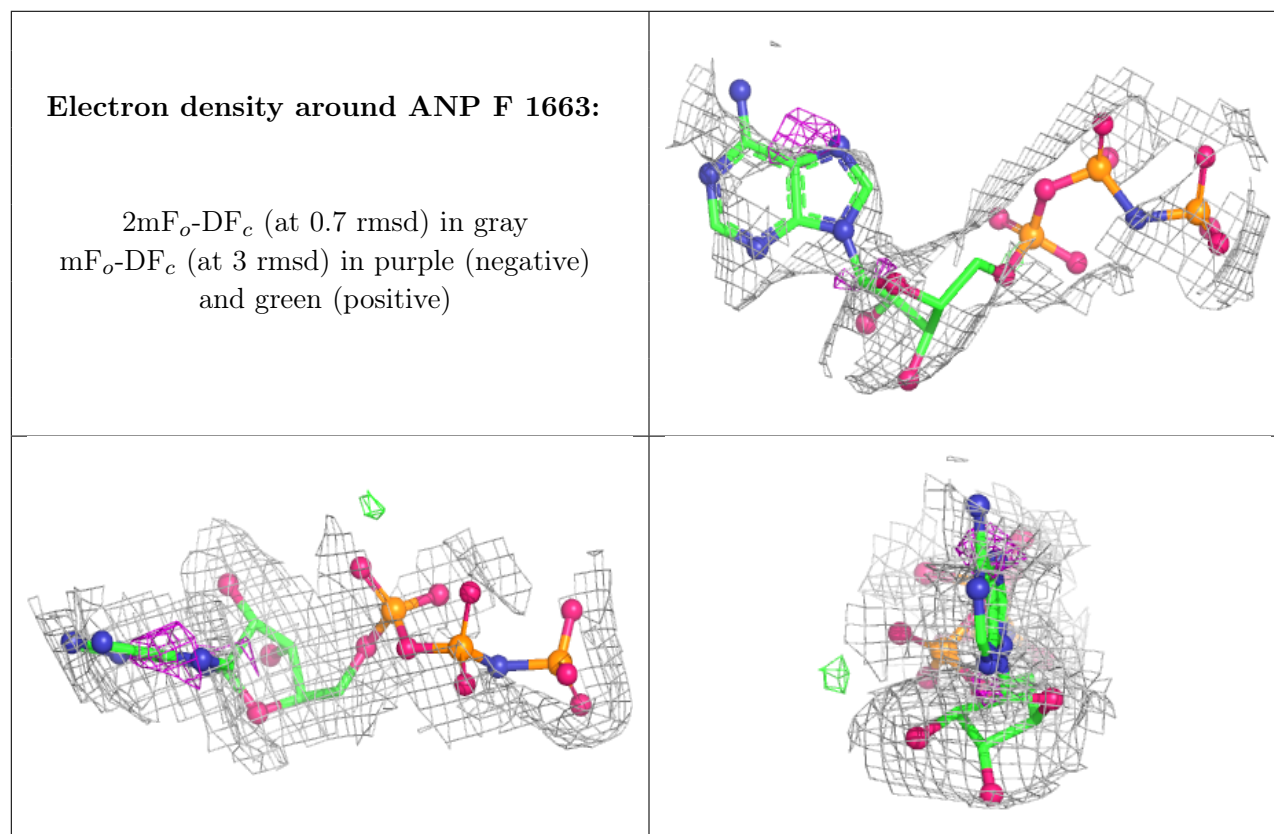
There are no oligosaccharides in this entry.

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.

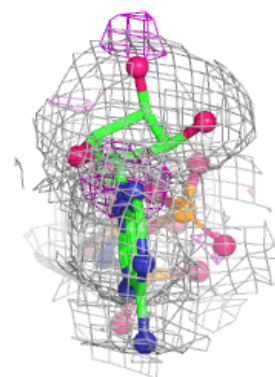
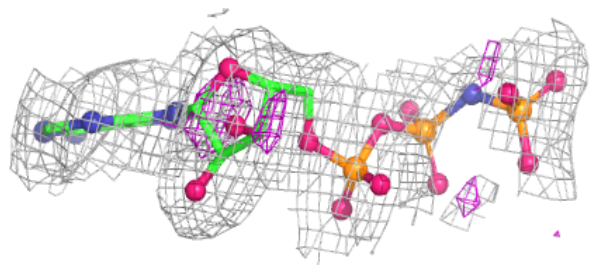
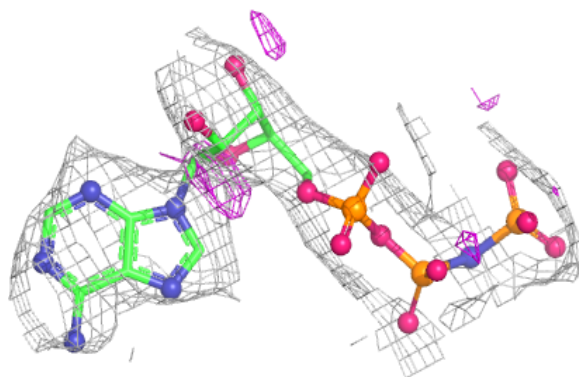
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	MG	A	1664	1/1	0.93	0.07	112,112,112,112	0
5	MG	F	1664	1/1	0.96	0.08	98,98,98,98	0
5	MG	A	1663	1/1	0.98	0.07	190,190,190,190	0
4	ANP	F	1663	31/31	0.99	0.06	72,85,91,95	0
5	MG	D	1663	1/1	0.99	0.04	53,53,53,53	0
4	ANP	A	1662	31/31	0.99	0.05	71,82,92,93	0
5	MG	F	1665	1/1	0.99	0.04	137,137,137,137	0
5	MG	I	1663	1/1	0.99	0.04	45,45,45,45	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 ANP A 1662:

$2mF_o-DF_c$ (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.