



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:18 PM GMT

PDB ID : 1EYG  
Title : Crystal structure of chymotryptic fragment of E. coli ssb bound to two 35-mer single strand DNAs  
Authors : Raghunathan, S.; Waksman, G.  
Deposited on : 2000-05-06  
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

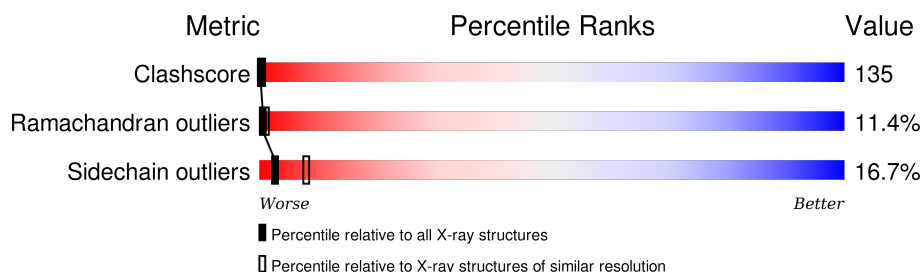
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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))
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	Q	35	
1	R	35	
2	A	116	
2	B	116	
2	C	116	
2	D	116	

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 4244 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 DNA chain called SINGLE STRANDED 28-MER OF D(C).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	28	Total	C	N	O	P	0	0	0
			529	252	84	166	27			
1	R	23	Total	C	N	O	P	0	0	0
			431	207	69	134	21			

- Molecule 2 is a protein called SINGLE-STRAND DNA-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	112	Total	C	N	O	S	0	0	0
			833	523	147	159	4			
2	B	104	Total	C	N	O	S	0	0	0
			765	479	134	149	3			
2	C	112	Total	C	N	O	S	0	0	0
			819	511	143	161	4			
2	D	112	Total	C	N	O	S	0	0	0
			828	517	148	160	3			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	O	0	0
			4	4		
3	B	2	Total	O	0	0
			2	2		
3	C	6	Total	O	0	0
			6	6		
3	D	7	Total	O	0	0
			7	7		
3	Q	12	Total	O	0	0
			12	12		
3	R	8	Total	O	0	0
			8	8		

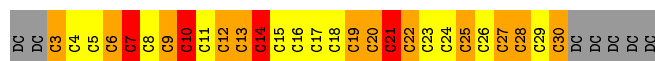
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

Note EDS was not executed.

- Molecule 1: SINGLE STRANDED 28-MER OF D(C)

Chain Q: 



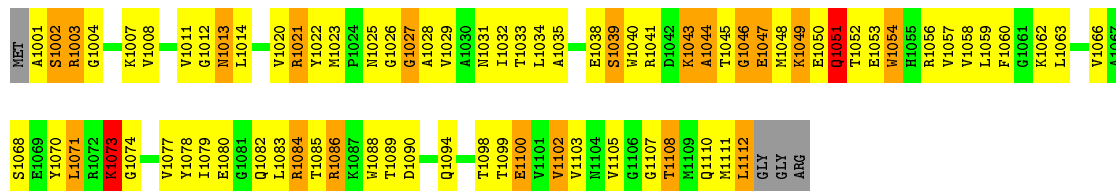
- Molecule 1: SINGLE STRANDED 28-MER OF D(C)

Chain R: 



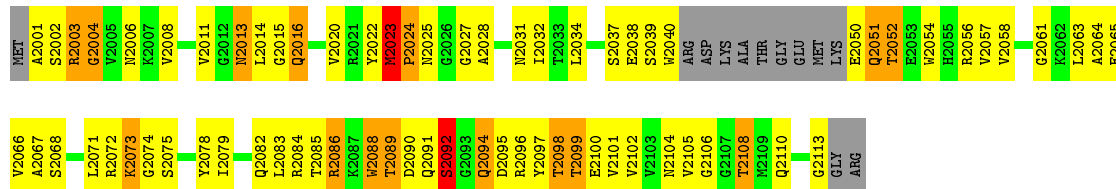
- Molecule 2: SINGLE-STRAND DNA-BINDING PROTEIN

Chain A: 



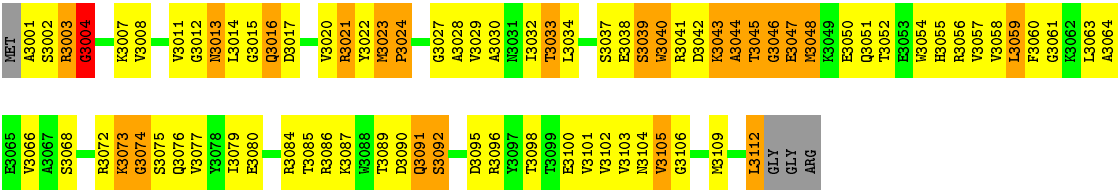
- Molecule 2: SINGLE-STRAND DNA-BINDING PROTEIN

Chain B: 

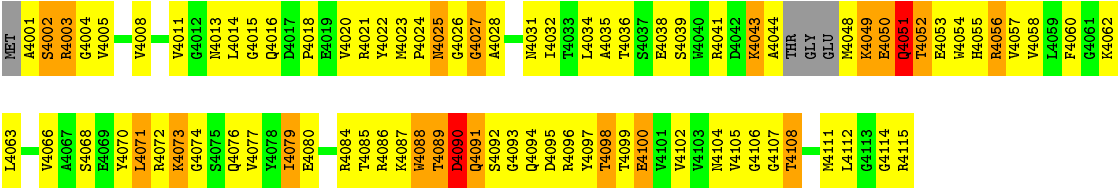
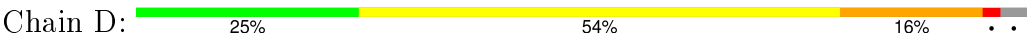


- Molecule 2: SINGLE-STRAND DNA-BINDING PROTEIN

Chain C: 



• Molecule 2: SINGLE-STRAND DNA-BINDING PROTEIN



## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be incomplete.

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.69 Å   71.08 Å   79.16 Å 90.00°   91.93°   90.00°	Depositor
Resolution (Å)	30.00 – 2.80	Depositor
% Data completeness (in resolution range)	91.3 (30.00-2.80)	Depositor
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
Refinement program	CNS	Depositor
R, $R_{free}$	0.256 , 0.298	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4244	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	51.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	Q	1.01	2/584 (0.3%)	1.68	21/888 (2.4%)
1	R	1.10	4/475 (0.8%)	2.16	16/720 (2.2%)
2	A	0.83	2/846 (0.2%)	1.04	6/1146 (0.5%)
2	B	0.80	0/776	0.96	0/1054
2	C	0.77	0/831	0.97	1/1129 (0.1%)
2	D	1.42	2/840 (0.2%)	1.11	3/1137 (0.3%)
All	All	1.01	10/4352 (0.2%)	1.32	47/6074 (0.8%)

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	Q	1	5
2	D	0	1
All	All	1	6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	4091	GLN	N-CA	32.42	2.11	1.46
2	D	4089	THR	C-O	-11.59	1.01	1.23
2	A	1089	THR	C-O	-10.43	1.03	1.23
1	R	111	DC	C5'-C4'	7.79	1.59	1.51
1	Q	21	DC	O3'-P	6.11	1.68	1.61
1	R	110	DC	C3'-O3'	5.69	1.51	1.44
1	R	111	DC	P-O5'	5.63	1.65	1.59
1	R	110	DC	O3'-P	5.31	1.67	1.61
2	A	1054	TRP	CB-CG	-5.28	1.40	1.50
1	Q	22	DC	C3'-O3'	-5.13	1.37	1.44

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	R	104	DC	O5'-P-OP1	-27.93	77.19	110.70
1	R	103	DC	OP1-P-O3'	-19.76	61.73	105.20
1	R	104	DC	O5'-P-OP2	-14.09	93.02	105.70
1	R	103	DC	OP2-P-O3'	-12.18	78.40	105.20
1	Q	21	DC	O4'-C1'-N1	10.84	115.59	108.00
1	Q	14	DC	O4'-C4'-C3'	-10.69	99.58	106.00
2	D	4091	GLN	N-CA-C	-9.82	84.49	111.00
1	R	126	DC	O4'-C4'-C3'	-9.28	100.43	106.00
1	R	107	DC	O4'-C1'-N1	8.99	114.29	108.00
2	A	1084	ARG	NE-CZ-NH1	-8.69	115.95	120.30
1	R	120	DC	O4'-C4'-C3'	-8.36	100.98	106.00
1	Q	28	DC	O4'-C1'-N1	8.01	113.61	108.00
1	Q	21	DC	O4'-C4'-C3'	-7.98	101.21	106.00
2	A	1034	LEU	CA-CB-CG	7.94	133.56	115.30
1	R	110	DC	O4'-C4'-C3'	7.90	110.74	106.00
1	Q	30	DC	O4'-C4'-C3'	-7.49	101.51	104.50
2	D	4089	THR	CA-C-N	7.34	133.36	117.20
1	R	103	DC	O3'-P-O5'	7.02	117.33	104.00
1	Q	12	DC	O4'-C4'-C3'	-6.87	101.75	104.50
1	Q	27	DC	O4'-C4'-C3'	6.81	110.08	106.00
1	R	111	DC	C5'-C4'-C3'	6.48	125.77	114.10
2	D	4089	THR	O-C-N	-6.42	112.43	122.70
1	Q	22	DC	C4'-C3'-C2'	6.41	108.87	103.10
2	A	1044	ALA	N-CA-C	6.27	127.92	111.00
1	Q	3	DC	N1-C1'-C2'	6.25	124.47	112.60
1	R	110	DC	N1-C1'-C2'	6.07	124.12	112.60
1	Q	13	DC	O4'-C4'-C3'	5.95	109.57	106.00
1	R	126	DC	C5'-C4'-C3'	5.94	124.80	114.10
2	A	1089	THR	O-C-N	-5.92	113.22	122.70
1	Q	14	DC	O4'-C1'-N1	5.81	112.07	108.00
1	R	126	DC	C4'-C3'-O3'	5.80	124.20	109.70
2	A	1089	THR	CA-C-N	5.80	129.96	117.20
1	Q	10	DC	N1-C1'-C2'	5.77	123.56	112.60
1	Q	21	DC	O3'-P-O5'	5.75	114.92	104.00
1	Q	13	DC	N1-C1'-C2'	5.72	123.47	112.60
1	R	120	DC	N1-C1'-C2'	-5.56	102.03	112.60
1	Q	20	DC	O4'-C1'-C2'	5.41	110.23	105.90
1	Q	20	DC	N1-C1'-C2'	5.38	122.81	112.60
2	A	1084	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	Q	9	DC	N1-C1'-C2'	5.29	122.65	112.60
1	Q	7	DC	O4'-C4'-C3'	-5.27	102.39	104.50
1	R	110	DC	O3'-P-O5'	5.27	114.01	104.00
1	R	113	DC	O4'-C1'-C2'	5.27	110.11	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	Q	25	DC	O4'-C1'-N1	5.19	111.63	108.00
2	C	3004	GLY	N-CA-C	5.18	126.05	113.10
1	Q	6	DC	O4'-C1'-C2'	5.12	110.00	105.90
1	Q	22	DC	C4'-C3'-O3'	5.11	122.52	112.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	Q	22	DC	C3'

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	4090	ASP	Peptide
1	Q	10	DC	Sidechain
1	Q	14	DC	Sidechain
1	Q	19	DC	Sidechain
1	Q	21	DC	Sidechain
1	Q	7	DC	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	Q	529	0	310	369	0
1	R	431	0	257	318	0
2	A	833	0	802	185	0
2	B	765	0	726	206	1
2	C	819	0	770	258	1
2	D	828	0	784	254	0
3	A	4	0	0	2	0
3	B	2	0	0	0	0
3	C	6	0	0	2	0
3	D	7	0	0	2	0
3	Q	12	0	0	4	0
3	R	8	0	0	4	0
All	All	4244	0	3649	1062	1

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 135.

All (1062) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4111:MET:CE	2:D:4111:MET:SD	2.02	1.47
1:R:109:DC:H2'	1:R:110:DC:C6	1.51	1.46
1:R:111:DC:C5'	2:B:2102:VAL:HG11	1.55	1.36
1:R:125:DC:H5'	2:A:1056:ARG:NH2	1.42	1.34
1:R:121:DC:O5'	2:A:1054:TRP:HZ2	1.08	1.28
1:R:127:DC:H4'	2:A:1084:ARG:NH1	1.47	1.27
1:Q:10:DC:OP1	2:C:3098:THR:HB	1.30	1.26
1:R:111:DC:H5''	2:B:2102:VAL:CG1	1.66	1.25
1:R:127:DC:C4'	2:A:1084:ARG:HH12	1.50	1.25
1:R:113:DC:H2''	2:B:2001:ALA:N	1.56	1.21
1:R:126:DC:H4'	2:A:1021:ARG:NH2	1.55	1.21
1:R:125:DC:H5'	2:A:1056:ARG:CZ	1.69	1.19
1:R:110:DC:H3'	2:B:2086:ARG:CD	1.72	1.18
1:R:111:DC:H5'	2:B:2084:ARG:CZ	1.71	1.18
1:Q:4:DC:H2'	2:C:3054:TRP:HH2	1.10	1.17
1:Q:4:DC:C2'	2:C:3054:TRP:HH2	1.55	1.17
1:Q:10:DC:C1'	2:C:3100:GLU:HB3	1.75	1.16
1:Q:22:DC:H1'	2:D:4054:TRP:CD1	1.82	1.15
1:Q:9:DC:H2'	2:C:3086:ARG:NH2	1.62	1.14
1:Q:25:DC:H2''	2:D:4031:ASN:HD21	1.03	1.14
1:R:111:DC:C3'	2:B:2084:ARG:HD3	1.75	1.14
1:R:110:DC:H4'	2:B:2100:GLU:OE1	1.45	1.13
1:R:114:DC:OP1	2:B:2001:ALA:N	1.80	1.13
1:R:116:DC:H1'	2:D:4070:TYR:CE1	1.83	1.13
1:R:121:DC:O5'	2:A:1054:TRP:CZ2	2.00	1.13
2:D:4091:GLN:CA	2:D:4091:GLN:N	2.11	1.13
2:C:3020:VAL:HG21	2:C:3068:SER:HB2	1.28	1.13
1:Q:6:DC:H2''	1:Q:7:DC:H3'	1.31	1.12
1:Q:28:DC:H2''	1:Q:29:DC:OP1	1.48	1.12
1:R:113:DC:H1'	2:B:2001:ALA:CB	1.79	1.12
2:C:3039:SER:HG	2:D:4001:ALA:N	1.46	1.12
1:Q:10:DC:H5''	2:C:3086:ARG:HG2	1.26	1.12
2:D:4084:ARG:HH21	2:D:4086:ARG:HG3	1.13	1.11
2:A:1056:ARG:NH1	2:A:1100:GLU:HG2	1.65	1.11
1:Q:21:DC:H41	2:D:4052:THR:HG23	1.13	1.11
1:Q:29:DC:H2''	1:Q:30:DC:H5'	1.11	1.11
2:A:1056:ARG:HH11	2:A:1100:GLU:HG2	0.95	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:111:DC:O4'	2:B:2102:VAL:HG21	1.48	1.10
1:Q:24:DC:H2''	2:D:4056:ARG:CD	1.82	1.10
1:R:111:DC:O5'	2:B:2084:ARG:NE	1.84	1.09
1:R:110:DC:C3'	2:B:2086:ARG:HD3	1.81	1.09
1:R:111:DC:H3'	2:B:2084:ARG:HD3	1.30	1.09
1:Q:22:DC:H5''	1:Q:23:DC:OP2	1.52	1.09
1:R:106:DC:H2''	1:R:107:DC:H3'	1.29	1.08
1:Q:10:DC:OP2	2:C:3086:ARG:CZ	2.01	1.08
1:R:109:DC:H5'	2:B:2088:TRP:CH2	1.89	1.08
2:C:3001:ALA:HA	2:D:4038:GLU:HA	1.35	1.08
1:Q:24:DC:C2'	2:D:4056:ARG:HD2	1.82	1.08
1:R:104:DC:H2'	2:B:2054:TRP:HH2	1.19	1.07
1:Q:26:DC:H4'	2:D:4058:VAL:HG11	1.34	1.07
1:R:113:DC:H1'	2:B:2001:ALA:HB2	1.11	1.07
1:Q:11:DC:H2'	1:Q:12:DC:O4'	1.52	1.06
1:R:113:DC:H2''	1:R:114:DC:H5'	1.11	1.06
2:C:3056:ARG:O	2:C:3100:GLU:HG3	1.54	1.06
1:Q:29:DC:H5'	2:C:3040:TRP:HB3	1.37	1.05
2:A:1045:THR:O	2:A:1047:GLU:N	1.88	1.05
2:D:4056:ARG:HH12	2:D:4098:THR:HB	0.99	1.05
1:Q:28:DC:H3'	2:C:3051:GLN:HE22	1.14	1.05
1:Q:15:DC:H2''	2:A:1066:VAL:HG21	1.37	1.05
1:Q:7:DC:H41	2:C:3033:THR:CB	1.68	1.04
1:R:113:DC:C2'	1:R:114:DC:H5'	1.87	1.04
1:Q:7:DC:H41	2:C:3033:THR:HB	1.19	1.04
1:Q:10:DC:O4'	2:C:3100:GLU:HB3	1.58	1.03
1:R:111:DC:C5'	2:B:2084:ARG:CZ	2.35	1.03
1:Q:10:DC:O3'	2:C:3084:ARG:NE	1.92	1.03
1:R:113:DC:C2'	2:B:2001:ALA:N	2.22	1.02
1:Q:4:DC:C2'	2:C:3054:TRP:CH2	2.42	1.02
1:R:104:DC:C2'	2:B:2054:TRP:HH2	1.73	1.01
1:R:104:DC:H4'	1:R:105:DC:OP1	1.57	1.01
1:R:127:DC:H4'	2:A:1084:ARG:HH12	0.92	1.01
2:A:1011:VAL:O	2:B:2004:GLY:HA3	1.60	1.01
1:Q:25:DC:H2''	2:D:4031:ASN:ND2	1.75	1.01
2:C:3015:GLY:HA2	3:C:123:HOH:O	1.59	1.00
2:D:4003:ARG:HH11	2:D:4003:ARG:HB3	1.23	1.00
1:R:107:DC:H41	2:B:2056:ARG:N	1.58	1.00
1:R:126:DC:C4'	2:A:1021:ARG:CZ	2.38	1.00
2:A:1001:ALA:HA	2:B:2038:GLU:HA	1.41	1.00
1:R:125:DC:H5''	2:A:1086:ARG:HH22	1.19	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:28:DC:H3'	2:C:3051:GLN:NE2	1.77	1.00
1:R:104:DC:H2'	2:B:2054:TRP:CH2	1.95	1.00
1:R:104:DC:H3'	2:B:2015:GLY:HA2	1.41	0.99
1:Q:24:DC:H2''	2:D:4056:ARG:NE	1.77	0.99
1:R:120:DC:H2'	1:R:121:DC:H5''	1.42	0.99
1:Q:26:DC:P	2:D:4100:GLU:HG2	2.02	0.98
1:Q:13:DC:O3'	2:C:3001:ALA:N	1.96	0.98
1:Q:10:DC:C5'	2:C:3086:ARG:HG2	1.92	0.98
1:R:126:DC:H4'	2:A:1021:ARG:CZ	1.94	0.98
1:R:109:DC:C2'	1:R:110:DC:C6	2.47	0.98
1:Q:23:DC:H2''	1:Q:24:DC:H5'	1.46	0.97
2:D:4084:ARG:NH2	2:D:4086:ARG:HG3	1.78	0.97
1:Q:6:DC:C2'	1:Q:7:DC:H3'	1.94	0.97
1:R:125:DC:C5'	2:A:1056:ARG:NH2	2.27	0.97
1:Q:24:DC:H2''	2:D:4056:ARG:HD2	1.42	0.97
1:Q:30:DC:H5''	2:D:4001:ALA:C	1.85	0.97
1:Q:6:DC:N4	2:C:3016:GLN:HG2	1.80	0.97
2:C:3038:GLU:HA	2:D:4001:ALA:CB	1.94	0.96
1:R:110:DC:C6	2:B:2086:ARG:NH2	2.33	0.95
1:R:106:DC:H4'	1:R:107:DC:O5'	1.64	0.95
2:C:3084:ARG:HH22	2:C:3102:VAL:HB	1.30	0.95
2:B:2057:VAL:HG11	2:B:2079:ILE:HD13	1.48	0.95
1:Q:12:DC:H5'	2:D:4038:GLU:OE1	1.67	0.95
2:A:1057:VAL:HG11	2:A:1079:ILE:HD13	1.46	0.95
1:Q:27:DC:OP1	2:D:4102:VAL:HG21	1.67	0.95
1:Q:4:DC:H2'	2:C:3054:TRP:CH2	2.02	0.94
1:Q:10:DC:OP1	2:C:3098:THR:CB	2.14	0.94
1:R:107:DC:N4	2:B:2056:ARG:H	1.65	0.94
1:R:126:DC:C4'	2:A:1021:ARG:NH2	2.30	0.94
1:Q:10:DC:H5''	2:C:3086:ARG:CG	1.97	0.94
1:Q:3:DC:C2	2:D:4003:ARG:HD2	2.02	0.94
2:A:1038:GLU:HA	2:B:2001:ALA:HA	1.49	0.94
1:Q:29:DC:H2''	1:Q:30:DC:C5'	1.97	0.94
1:Q:7:DC:N4	2:C:3033:THR:HB	1.83	0.93
2:C:3001:ALA:CA	2:D:4038:GLU:HA	1.97	0.93
2:C:3021:ARG:CZ	2:C:3023:MET:HA	1.98	0.93
1:R:126:DC:OP1	2:A:1031:ASN:OD1	1.87	0.93
2:C:3084:ARG:HH12	2:C:3102:VAL:HG11	1.31	0.93
1:Q:7:DC:H2''	1:Q:8:DC:O5'	1.67	0.93
1:Q:27:DC:H3'	1:Q:28:DC:H5''	1.48	0.93
2:D:4014:LEU:HB2	2:D:4073:LYS:O	1.68	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:9:DC:H2''	1:Q:10:DC:N3	1.84	0.93
1:R:109:DC:C2'	1:R:110:DC:H6	1.81	0.92
2:D:4056:ARG:NH1	2:D:4098:THR:HB	1.83	0.92
1:R:110:DC:H6	2:B:2086:ARG:HH12	1.17	0.92
1:R:111:DC:H3'	2:B:2084:ARG:HH11	1.32	0.92
1:R:113:DC:O4'	2:A:1038:GLU:HG3	1.70	0.92
1:R:106:DC:H2''	1:R:107:DC:C3'	1.99	0.91
2:D:4088:TRP:HE1	2:D:4090:ASP:HB3	1.34	0.91
1:R:110:DC:H5''	2:B:2086:ARG:HH11	1.33	0.91
1:Q:3:DC:O2	2:D:4003:ARG:HD2	1.70	0.91
1:R:107:DC:H2'	3:R:143:HOH:O	1.70	0.91
1:R:110:DC:C6	2:B:2086:ARG:NH1	2.39	0.90
1:Q:10:DC:H1'	2:C:3100:GLU:OE1	1.70	0.90
1:Q:30:DC:H5'	2:D:4001:ALA:HB3	1.52	0.90
2:D:4087:LYS:HG3	2:D:4097:TYR:CE2	2.06	0.90
1:R:116:DC:H1'	2:D:4070:TYR:HE1	1.36	0.90
2:D:4003:ARG:NH1	2:D:4003:ARG:HB3	1.86	0.90
1:Q:26:DC:H5''	2:D:4100:GLU:OE2	1.72	0.90
1:Q:13:DC:C1'	2:C:3001:ALA:HB3	2.01	0.90
2:C:3040:TRP:HD1	2:C:3042:ASP:HB2	1.36	0.90
1:R:110:DC:H4'	2:B:2100:GLU:CD	1.92	0.89
1:R:111:DC:C4'	2:B:2102:VAL:HG21	2.03	0.89
1:Q:28:DC:C3'	2:C:3051:GLN:HE22	1.85	0.89
2:C:3021:ARG:NH2	2:C:3023:MET:HA	1.88	0.88
1:R:111:DC:OP1	2:B:2100:GLU:HB2	1.71	0.88
1:R:110:DC:O3'	2:B:2084:ARG:NH2	2.07	0.88
1:Q:11:DC:H1'	2:C:3104:ASN:CB	2.03	0.88
1:R:110:DC:C4'	2:B:2100:GLU:OE1	2.21	0.88
1:R:107:DC:H2''	1:R:108:DC:O5'	1.74	0.88
1:R:121:DC:H2''	1:R:122:DC:O5'	1.73	0.88
2:C:3001:ALA:HB2	2:D:4038:GLU:HG3	1.54	0.88
1:Q:29:DC:C2'	1:Q:30:DC:H5'	2.00	0.88
2:D:4084:ARG:HH21	2:D:4086:ARG:CG	1.86	0.88
1:Q:23:DC:C2'	1:Q:24:DC:H5'	2.02	0.88
1:R:125:DC:H5''	2:A:1086:ARG:NH2	1.88	0.88
1:Q:26:DC:C5'	2:D:4058:VAL:HG21	2.04	0.88
1:Q:6:DC:H42	2:C:3016:GLN:NE2	1.72	0.88
1:Q:9:DC:H2'	2:C:3086:ARG:HH22	1.39	0.88
1:R:103:DC:H2''	1:R:104:DC:OP1	1.73	0.87
1:Q:25:DC:C5'	2:D:4056:ARG:HH21	1.87	0.87
1:Q:24:DC:C2'	2:D:4056:ARG:CD	2.48	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:120:DC:H2'	1:R:121:DC:C5'	2.04	0.87
1:R:114:DC:P	2:B:2001:ALA:N	2.48	0.87
1:Q:26:DC:OP1	2:D:4100:GLU:HG2	1.75	0.87
1:R:104:DC:C3'	2:B:2015:GLY:HA2	2.05	0.86
2:A:1014:LEU:HB2	2:A:1073:LYS:O	1.74	0.86
1:Q:24:DC:N4	2:D:4054:TRP:HB2	1.89	0.86
1:Q:10:DC:H1'	2:C:3100:GLU:CG	2.06	0.86
1:Q:4:DC:H2''	2:C:3054:TRP:CH2	2.08	0.86
1:Q:4:DC:H4'	1:Q:5:DC:OP1	1.74	0.86
1:R:120:DC:H2''	1:R:121:DC:OP1	1.75	0.85
2:C:3084:ARG:CZ	2:C:3084:ARG:HB3	2.05	0.85
2:A:1040:TRP:O	2:A:1049:LYS:HB2	1.76	0.85
1:R:124:DC:H2''	1:R:125:DC:O5'	1.76	0.85
1:Q:29:DC:C2'	2:D:4001:ALA:HB3	2.06	0.85
2:C:3022:TYR:HB3	2:C:3027:GLY:HA3	1.59	0.85
1:R:113:DC:H2''	1:R:114:DC:C5'	2.04	0.84
1:Q:27:DC:H3'	1:Q:28:DC:C5'	2.07	0.84
1:R:112:DC:H2''	1:R:113:DC:OP1	1.78	0.84
1:Q:15:DC:H2''	2:A:1066:VAL:CG2	2.06	0.84
1:Q:11:DC:H4'	2:C:3084:ARG:NH1	1.93	0.84
1:R:107:DC:O2	2:A:1085:THR:HG21	1.77	0.84
1:R:121:DC:P	2:A:1054:TRP:HZ2	2.01	0.84
1:R:110:DC:H3'	2:B:2086:ARG:HD3	0.88	0.84
1:Q:20:DC:H2'	2:D:4015:GLY:HA2	1.57	0.83
1:R:105:DC:H2''	1:R:106:DC:O5'	1.75	0.83
1:R:127:DC:C4'	2:A:1084:ARG:NH1	2.23	0.83
2:A:1073:LYS:HE2	2:A:1074:GLY:HA2	1.60	0.83
1:R:111:DC:H5''	2:B:2102:VAL:HG11	0.83	0.83
1:R:123:DC:H2''	1:R:124:DC:O5'	1.77	0.83
2:B:2006:ASN:HD21	2:B:2082:GLN:HB3	1.44	0.83
1:Q:22:DC:H1'	2:D:4054:TRP:CG	2.14	0.83
1:Q:18:DC:O2	1:Q:18:DC:H3'	1.79	0.83
1:R:113:DC:H4'	2:A:1039:SER:H	1.44	0.83
1:R:109:DC:C5'	2:B:2088:TRP:CH2	2.61	0.82
1:Q:10:DC:C6	2:C:3100:GLU:HB2	2.14	0.82
1:Q:21:DC:N4	2:D:4052:THR:HG23	1.93	0.82
1:Q:10:DC:H5'	2:C:3098:THR:O	1.79	0.82
1:Q:10:DC:P	2:C:3098:THR:HB	2.18	0.82
1:Q:26:DC:O5'	2:D:4058:VAL:HG21	1.78	0.82
1:Q:28:DC:H5'	2:C:3051:GLN:CD	2.00	0.82
1:R:121:DC:P	2:A:1054:TRP:CZ2	2.72	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:11:DC:O5'	2:C:3084:ARG:CZ	2.29	0.81
1:Q:5:DC:H2''	1:Q:6:DC:O5'	1.79	0.81
1:R:111:DC:H5'	2:B:2084:ARG:NH1	1.96	0.81
2:C:3012:GLY:C	2:C:3013:ASN:HD22	1.84	0.81
1:R:111:DC:H2'	1:R:112:DC:O4'	1.81	0.81
1:R:115:DC:H2''	2:D:4066:VAL:HG11	1.62	0.81
1:Q:10:DC:H2''	2:C:3084:ARG:HH21	1.46	0.81
1:R:110:DC:H5''	2:B:2086:ARG:NH1	1.94	0.81
1:R:115:DC:H4'	3:R:138:HOH:O	1.79	0.81
1:R:120:DC:N4	2:A:1050:GLU:OE2	2.14	0.81
2:A:1021:ARG:HH22	2:A:1023:MET:HG3	1.44	0.81
2:C:3013:ASN:N	2:C:3013:ASN:HD22	1.78	0.81
1:Q:29:DC:H2''	2:D:4001:ALA:HB3	1.60	0.81
2:C:3058:VAL:HB	2:C:3100:GLU:OE1	1.80	0.81
1:Q:29:DC:H5'	2:C:3039:SER:O	1.81	0.81
2:B:2092:SER:HB3	2:B:2094:GLN:HG3	1.63	0.81
2:C:3061:GLY:O	2:C:3064:ALA:HB3	1.81	0.80
1:R:115:DC:C2'	2:D:4066:VAL:HG11	2.11	0.80
2:B:2020:VAL:HG21	2:B:2068:SER:HB2	1.62	0.80
1:R:108:DC:N3	2:B:2056:ARG:CB	2.44	0.80
1:R:110:DC:C5'	2:B:2100:GLU:CD	2.49	0.80
2:C:3039:SER:N	2:D:4001:ALA:HB2	1.96	0.80
1:Q:10:DC:H3'	2:C:3086:ARG:HE	1.46	0.80
1:Q:13:DC:H4'	2:C:3001:ALA:N	1.96	0.80
1:R:111:DC:H6	2:B:2084:ARG:NH1	1.79	0.80
1:Q:23:DC:H2'	1:Q:24:DC:C6	2.17	0.80
1:Q:9:DC:H2''	1:Q:10:DC:C2	2.17	0.79
1:Q:10:DC:C6	2:C:3100:GLU:CB	2.64	0.79
2:D:4084:ARG:NH1	2:D:4100:GLU:OE1	2.16	0.79
1:R:121:DC:H5	2:A:1051:GLN:NE2	1.79	0.79
1:Q:10:DC:C1'	2:C:3100:GLU:CB	2.58	0.79
2:A:1013:ASN:HD22	2:A:1013:ASN:N	1.81	0.79
2:C:3023:MET:HB2	2:C:3024:PRO:HD2	1.64	0.79
2:B:2006:ASN:ND2	2:B:2082:GLN:HB3	1.97	0.79
1:Q:5:DC:N3	2:C:3052:THR:HG21	1.98	0.79
1:R:120:DC:C2'	1:R:121:DC:OP1	2.31	0.79
1:Q:27:DC:OP1	2:D:4084:ARG:NH1	2.16	0.79
2:D:4023:MET:H	2:D:4027:GLY:HA2	1.48	0.79
1:R:110:DC:C6	2:B:2086:ARG:CZ	2.65	0.78
1:R:127:DC:H4'	2:A:1084:ARG:CZ	2.12	0.78
1:R:111:DC:H6	2:B:2084:ARG:HH12	1.31	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3039:SER:H	2:D:4001:ALA:HB2	1.47	0.78
1:Q:10:DC:H1'	2:C:3100:GLU:CD	2.03	0.78
2:A:1057:VAL:HG11	2:A:1079:ILE:CD1	2.12	0.78
2:A:1001:ALA:N	2:B:2039:SER:H	1.81	0.78
1:Q:14:DC:H5'	2:C:3001:ALA:C	2.03	0.78
2:A:1001:ALA:HA	2:B:2038:GLU:CA	2.12	0.78
2:C:3038:GLU:HG2	2:D:4001:ALA:HB1	1.65	0.78
2:D:4084:ARG:NH2	2:D:4100:GLU:OE2	2.15	0.78
1:Q:10:DC:H1'	2:C:3100:GLU:HB3	1.63	0.77
2:A:1090:ASP:OD2	2:A:1094:GLN:HB2	1.85	0.77
1:R:111:DC:P	2:B:2084:ARG:HE	2.07	0.77
1:Q:29:DC:H4'	2:D:4001:ALA:HB2	1.65	0.77
1:R:109:DC:H5'	2:B:2088:TRP:CZ3	2.18	0.77
1:R:126:DC:H4'	2:A:1021:ARG:HH21	1.49	0.77
2:A:1043:LYS:H	2:A:1049:LYS:NZ	1.83	0.77
1:R:123:DC:H41	2:A:1054:TRP:HB2	1.50	0.76
1:Q:27:DC:OP1	2:D:4084:ARG:HD3	1.86	0.76
2:D:4091:GLN:N	2:D:4092:SER:N	2.33	0.76
2:C:3038:GLU:HA	2:D:4001:ALA:HB1	1.66	0.76
1:Q:13:DC:H1'	2:C:3001:ALA:HB3	1.66	0.76
1:R:104:DC:C2'	2:B:2054:TRP:CH2	2.62	0.76
2:C:3084:ARG:CZ	2:C:3084:ARG:CB	2.64	0.76
2:D:4085:THR:OG1	2:D:4099:THR:HG22	1.86	0.76
1:Q:7:DC:C2'	1:Q:8:DC:O4'	2.34	0.76
1:R:116:DC:H1'	2:D:4070:TYR:CZ	2.22	0.75
1:Q:11:DC:H3'	3:Q:130:HOH:O	1.86	0.75
1:Q:9:DC:C2'	2:C:3086:ARG:NH2	2.44	0.75
1:Q:11:DC:C4'	2:C:3102:VAL:HG21	2.16	0.75
2:D:4089:THR:O	2:D:4094:GLN:O	2.03	0.75
1:Q:7:DC:N4	2:C:3033:THR:CB	2.44	0.75
2:B:2023:MET:HG3	2:B:2024:PRO:HD2	1.69	0.75
1:R:125:DC:C2'	1:R:126:DC:H5'	2.17	0.74
1:Q:27:DC:O4'	2:D:4102:VAL:HG11	1.87	0.74
1:R:105:DC:OP1	2:B:2073:LYS:NZ	2.19	0.74
2:A:1023:MET:HG3	2:A:1029:VAL:HG21	1.68	0.74
1:Q:20:DC:H3'	2:D:4015:GLY:O	1.87	0.74
1:Q:30:DC:C4	2:B:2108:THR:HG21	2.23	0.74
2:B:2090:ASP:CB	2:B:2094:GLN:HE22	2.01	0.74
1:R:108:DC:H2'	2:B:2098:THR:CG2	2.17	0.74
1:R:109:DC:H4'	1:R:110:DC:OP1	1.88	0.73
1:R:127:DC:O3'	2:A:1084:ARG:NH1	2.21	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4084:ARG:HH11	2:D:4084:ARG:HB3	1.52	0.73
1:Q:26:DC:C5	2:D:4086:ARG:NH1	2.56	0.73
1:R:114:DC:H2"	3:R:138:HOH:O	1.89	0.73
1:R:119:DC:H3'	1:R:120:DC:C5	2.23	0.73
1:Q:11:DC:O4'	2:C:3102:VAL:HG21	1.87	0.73
2:D:4111:MET:CE	2:D:4111:MET:HB3	2.17	0.73
1:Q:26:DC:OP2	2:D:4100:GLU:OE2	2.05	0.73
1:R:121:DC:H5	2:A:1051:GLN:HE22	1.33	0.73
2:A:1056:ARG:NH1	2:A:1100:GLU:CG	2.48	0.73
1:Q:27:DC:P	2:D:4084:ARG:CZ	2.76	0.73
1:R:126:DC:P	2:A:1056:ARG:HH22	2.11	0.73
2:C:3096:ARG:HG2	2:D:4096:ARG:HH12	1.52	0.73
1:Q:10:DC:H1'	2:C:3100:GLU:CB	2.17	0.73
1:R:110:DC:N1	2:B:2086:ARG:NH2	2.35	0.73
2:C:3040:TRP:CD1	2:C:3042:ASP:HB2	2.24	0.72
2:C:3004:GLY:HA3	2:D:4011:VAL:O	1.89	0.72
1:R:119:DC:H3'	1:R:120:DC:C6	2.24	0.72
1:Q:22:DC:C1'	2:D:4054:TRP:CD1	2.70	0.72
1:Q:25:DC:H2'	1:Q:26:DC:O4'	1.89	0.72
2:A:1021:ARG:NH2	2:A:1023:MET:HG3	2.04	0.72
1:Q:10:DC:H2'	1:Q:10:DC:O2	1.88	0.72
1:Q:14:DC:H5"	2:C:3002:SER:HA	1.70	0.72
2:C:3001:ALA:CB	2:D:4038:GLU:HA	2.20	0.72
1:R:110:DC:C4'	2:B:2100:GLU:CD	2.57	0.72
1:R:121:DC:H2"	1:R:122:DC:H4'	1.69	0.72
1:Q:27:DC:OP2	2:D:4084:ARG:NE	2.22	0.72
2:C:3001:ALA:HA	2:D:4038:GLU:CA	2.17	0.72
1:Q:10:DC:C1'	2:C:3100:GLU:OE1	2.36	0.72
2:C:3038:GLU:CA	2:D:4001:ALA:CB	2.68	0.72
1:Q:6:DC:H2'	1:Q:6:DC:O2	1.90	0.72
1:R:116:DC:C1'	2:D:4070:TYR:CE1	2.68	0.72
1:R:126:DC:P	2:A:1056:ARG:NH2	2.62	0.72
2:A:1023:MET:H	2:A:1027:GLY:HA2	1.54	0.72
2:C:3001:ALA:HB2	2:D:4038:GLU:CG	2.20	0.72
1:R:103:DC:N4	2:B:2050:GLU:OE2	2.23	0.72
1:R:111:DC:C5'	2:B:2084:ARG:NE	2.51	0.71
1:Q:28:DC:H5'	2:C:3051:GLN:NE2	2.05	0.71
1:Q:7:DC:H41	2:C:3033:THR:CG2	2.03	0.71
1:Q:18:DC:OP1	1:Q:18:DC:O4'	2.08	0.71
2:A:1046:GLY:C	2:A:1048:MET:H	1.93	0.71
1:Q:18:DC:O2	1:Q:18:DC:H5"	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:111:DC:H5'	2:B:2084:ARG:NH2	2.05	0.71
1:R:111:DC:O5'	2:B:2084:ARG:HB3	1.90	0.71
1:R:109:DC:O3'	2:B:2098:THR:CB	2.38	0.71
2:C:3038:GLU:HA	2:D:4001:ALA:CA	2.21	0.71
1:R:127:DC:C3'	2:A:1084:ARG:NH1	2.53	0.71
2:C:3084:ARG:NH1	2:C:3084:ARG:HB2	2.05	0.71
1:Q:26:DC:H5'	2:D:4058:VAL:HG21	1.70	0.71
1:R:107:DC:H41	2:B:2056:ARG:H	0.80	0.70
1:Q:22:DC:O2	1:Q:24:DC:H5	1.72	0.70
1:Q:9:DC:O2	1:Q:9:DC:H2'	1.91	0.70
2:B:2020:VAL:HG21	2:B:2068:SER:CB	2.20	0.70
2:A:1073:LYS:CE	2:A:1074:GLY:HA2	2.21	0.70
1:Q:7:DC:N3	2:C:3056:ARG:N	2.40	0.70
2:C:3084:ARG:HH22	2:C:3102:VAL:CB	2.03	0.70
1:Q:21:DC:C2'	1:Q:22:DC:O5'	2.40	0.70
1:Q:11:DC:P	2:C:3084:ARG:HE	2.14	0.70
1:Q:7:DC:C2'	1:Q:8:DC:O5'	2.39	0.70
1:Q:8:DC:H2'	1:Q:9:DC:H4'	1.74	0.70
2:D:4041:ARG:HA	3:D:134:HOH:O	1.92	0.70
1:R:110:DC:H5'	2:B:2100:GLU:CD	2.13	0.69
1:Q:11:DC:P	2:C:3084:ARG:NE	2.65	0.69
2:C:3039:SER:H	2:D:4001:ALA:CA	2.05	0.69
1:Q:10:DC:OP2	2:C:3086:ARG:NH1	2.25	0.69
1:Q:10:DC:C2	2:C:3100:GLU:OE1	2.45	0.69
1:R:111:DC:H3'	2:B:2084:ARG:NH1	2.07	0.69
1:Q:7:DC:H1'	3:Q:138:HOH:O	1.91	0.69
2:D:4062:LYS:HG3	2:D:4063:LEU:H	1.57	0.69
1:R:105:DC:C2'	1:R:106:DC:O5'	2.40	0.69
1:R:111:DC:P	2:B:2084:ARG:NE	2.65	0.69
2:C:3039:SER:O	2:C:3040:TRP:HB3	1.90	0.69
2:D:4063:LEU:HA	2:D:4066:VAL:HG22	1.74	0.69
1:R:109:DC:H2'	1:R:110:DC:C5	2.21	0.69
1:Q:30:DC:H5''	2:D:4002:SER:N	2.07	0.69
1:R:113:DC:C4'	2:A:1038:GLU:HG3	2.22	0.69
1:Q:20:DC:C2'	2:D:4015:GLY:HA2	2.22	0.69
1:R:121:DC:C2'	1:R:122:DC:H4'	2.22	0.69
2:C:3034:LEU:HD21	2:C:3077:VAL:HG22	1.72	0.69
1:R:108:DC:C2'	2:B:2098:THR:CG2	2.71	0.69
1:R:127:DC:C3'	2:A:1084:ARG:HH12	2.05	0.69
1:R:127:DC:C5'	2:A:1084:ARG:HH12	2.06	0.68
1:Q:27:DC:OP1	2:D:4084:ARG:CZ	2.42	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:127:DC:OP2	2:A:1023:MET:CE	2.41	0.68
1:Q:9:DC:OP1	2:C:3098:THR:OG1	2.11	0.68
2:B:2014:LEU:HB2	2:B:2073:LYS:O	1.93	0.68
1:R:103:DC:C2'	1:R:104:DC:OP1	2.32	0.68
2:D:4088:TRP:CE2	2:D:4096:ARG:HB2	2.28	0.68
1:R:113:DC:C1'	2:B:2001:ALA:HB2	2.06	0.68
1:R:113:DC:H41	2:B:2106:GLY:CA	2.07	0.68
1:Q:25:DC:H5'	2:D:4056:ARG:HH21	1.57	0.68
2:C:3013:ASN:N	2:C:3013:ASN:ND2	2.42	0.68
2:C:3084:ARG:CB	2:C:3084:ARG:NH1	2.56	0.68
1:Q:22:DC:H2'	1:Q:22:DC:O2	1.94	0.68
1:R:113:DC:H41	2:B:2106:GLY:HA3	1.59	0.67
1:R:112:DC:C2'	1:R:113:DC:OP1	2.42	0.67
1:Q:6:DC:H2''	1:Q:7:DC:C3'	2.19	0.67
2:A:1001:ALA:CA	2:B:2039:SER:H	2.07	0.67
1:R:111:DC:O3'	2:B:2084:ARG:HD3	1.94	0.67
1:R:113:DC:H41	2:B:2106:GLY:H	1.41	0.67
1:Q:15:DC:H2'	1:Q:16:DC:C6	2.30	0.67
2:B:2090:ASP:HB3	2:B:2094:GLN:HE22	1.59	0.67
2:B:2090:ASP:HB3	2:B:2094:GLN:NE2	2.09	0.67
1:R:126:DC:H5''	2:A:1021:ARG:NE	2.09	0.67
2:D:4091:GLN:C	2:D:4091:GLN:N	2.47	0.67
2:D:4023:MET:N	2:D:4027:GLY:HA2	2.09	0.67
1:R:109:DC:O3'	2:B:2098:THR:HB	1.95	0.67
2:C:3039:SER:H	2:D:4001:ALA:CB	2.07	0.67
1:Q:13:DC:H41	2:C:3106:GLY:CA	2.08	0.67
2:C:3011:VAL:HG12	2:D:4004:GLY:HA2	1.77	0.67
1:R:113:DC:H5'	2:A:1039:SER:O	1.94	0.66
1:R:114:DC:H5'	2:B:2001:ALA:N	2.10	0.66
1:Q:16:DC:H2''	2:A:1070:TYR:CZ	2.30	0.66
2:C:3032:ILE:HG13	2:C:3057:VAL:HB	1.77	0.66
1:Q:10:DC:C6	2:C:3100:GLU:HB3	2.29	0.66
1:Q:9:DC:H2''	1:Q:10:DC:C4	2.31	0.66
1:R:113:DC:H41	2:B:2106:GLY:N	1.93	0.66
1:R:120:DC:C6	1:R:120:DC:OP2	2.49	0.66
1:R:121:DC:C5	2:A:1051:GLN:NE2	2.63	0.66
2:D:4088:TRP:CD1	2:D:4088:TRP:C	2.68	0.66
1:R:120:DC:C2	1:R:121:DC:H5''	2.30	0.66
1:Q:11:DC:H2'	1:Q:12:DC:C1'	2.25	0.66
1:Q:12:DC:C2'	1:Q:13:DC:OP1	2.44	0.66
1:Q:28:DC:H5'	2:C:3051:GLN:OE1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:12:DC:H2''	1:Q:13:DC:OP1	1.95	0.65
1:R:126:DC:O4'	2:A:1021:ARG:CZ	2.44	0.65
2:D:4060:PHE:HE1	2:D:4102:VAL:HG13	1.62	0.65
2:C:3050:GLU:HG2	2:C:3051:GLN:H	1.62	0.65
2:D:4085:THR:CB	2:D:4099:THR:HG22	2.27	0.65
1:Q:21:DC:H2''	1:Q:22:DC:O5'	1.77	0.65
1:R:121:DC:H2''	1:R:122:DC:C4'	2.26	0.65
1:Q:13:DC:H41	2:C:3106:GLY:HA3	1.60	0.65
1:Q:7:DC:N4	2:C:3033:THR:HA	2.12	0.65
1:R:104:DC:O2	1:R:105:DC:C5	2.50	0.65
1:Q:24:DC:C1'	2:D:4056:ARG:HD2	2.27	0.65
1:Q:20:DC:H4'	1:Q:21:DC:OP1	1.93	0.65
1:Q:20:DC:C3'	2:D:4015:GLY:O	2.44	0.65
1:Q:30:DC:H5''	2:D:4001:ALA:CA	2.27	0.65
2:D:4020:VAL:HG21	2:D:4068:SER:OG	1.97	0.65
2:A:1050:GLU:HG2	2:A:1051:GLN:N	2.12	0.64
2:D:4043:LYS:O	2:D:4044:ALA:HB2	1.98	0.64
1:Q:30:DC:C5'	2:D:4001:ALA:C	2.63	0.64
1:R:113:DC:C5'	2:A:1039:SER:O	2.45	0.64
2:A:1041:ARG:HA	2:A:1049:LYS:HD2	1.80	0.64
2:D:4088:TRP:HZ3	2:D:4098:THR:CG2	2.11	0.64
2:A:1032:ILE:HG13	2:A:1057:VAL:HB	1.79	0.64
2:B:2037:SER:HB3	2:B:2052:THR:HB	1.78	0.64
1:Q:29:DC:H2'	1:Q:30:DC:H3'	1.79	0.64
2:D:4056:ARG:HH12	2:D:4098:THR:CB	1.92	0.64
2:A:1073:LYS:HE2	2:A:1074:GLY:CA	2.25	0.64
2:A:1086:ARG:HH11	2:A:1086:ARG:CG	2.11	0.64
2:C:3038:GLU:HA	2:D:4001:ALA:HA	1.80	0.64
1:Q:13:DC:C4	1:Q:14:DC:N4	2.66	0.64
2:C:3050:GLU:HG2	2:C:3051:GLN:N	2.13	0.64
2:C:3058:VAL:CB	2:C:3100:GLU:OE1	2.46	0.64
1:Q:26:DC:OP2	2:D:4100:GLU:HG2	1.97	0.64
1:R:123:DC:N4	2:A:1054:TRP:HB2	2.12	0.63
2:D:4034:LEU:HD11	2:D:4079:ILE:HD13	1.80	0.63
1:Q:4:DC:C4'	1:Q:5:DC:OP1	2.45	0.63
2:C:3021:ARG:CZ	2:C:3023:MET:CA	2.74	0.63
2:D:4020:VAL:HG21	2:D:4068:SER:CB	2.28	0.63
1:Q:29:DC:H4'	2:D:4001:ALA:CB	2.28	0.63
1:Q:18:DC:O2	1:Q:18:DC:C3'	2.46	0.63
1:Q:4:DC:H42	2:D:4003:ARG:NH1	1.96	0.63
1:Q:8:DC:O2	1:Q:10:DC:N4	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3100:GLU:CG	2:C:3101:VAL:N	2.61	0.63
1:R:111:DC:O4'	2:B:2102:VAL:CG2	2.38	0.63
1:R:111:DC:H3'	2:B:2084:ARG:CD	2.20	0.63
1:R:111:DC:O5'	2:B:2084:ARG:CZ	2.41	0.62
1:R:108:DC:H2'	2:B:2098:THR:HG21	1.82	0.62
2:C:3058:VAL:CG1	2:C:3100:GLU:OE1	2.47	0.62
1:Q:11:DC:C2	1:Q:12:DC:H1'	2.35	0.62
1:Q:13:DC:H2'	1:Q:14:DC:C6	2.35	0.62
1:Q:7:DC:H2'	1:Q:8:DC:O4'	1.98	0.62
2:A:1021:ARG:HH22	2:A:1023:MET:CG	2.12	0.62
1:R:110:DC:H2'	2:B:2086:ARG:CZ	2.30	0.62
1:R:110:DC:OP2	2:B:2098:THR:CG2	2.48	0.62
2:A:1107:GLY:O	2:A:1108:THR:HB	1.99	0.62
1:Q:6:DC:H42	2:C:3016:GLN:HE21	1.47	0.62
1:Q:7:DC:N3	2:C:3055:HIS:C	2.53	0.62
1:R:121:DC:H3'	2:A:1054:TRP:NE1	2.15	0.61
2:D:4022:TYR:HB3	2:D:4027:GLY:HA3	1.80	0.61
1:Q:19:DC:O2	1:Q:19:DC:O4'	2.17	0.61
1:R:110:DC:C2'	2:B:2086:ARG:CZ	2.78	0.61
2:A:1062:LYS:HG3	2:A:1063:LEU:H	1.65	0.61
1:Q:13:DC:C2'	2:C:3001:ALA:HB3	2.30	0.61
1:R:113:DC:N4	2:B:2106:GLY:H	1.97	0.61
2:A:1021:ARG:HH21	2:A:1029:VAL:HG11	1.66	0.61
1:Q:16:DC:H2''	2:A:1070:TYR:OH	2.00	0.61
1:Q:11:DC:H4'	2:C:3084:ARG:CZ	2.31	0.61
2:B:2022:TYR:HB3	2:B:2027:GLY:HA3	1.80	0.61
1:Q:14:DC:H5''	2:C:3002:SER:CA	2.29	0.61
2:D:4091:GLN:N	2:D:4092:SER:H	1.97	0.61
1:Q:25:DC:H5'	2:D:4056:ARG:NH2	2.16	0.61
1:R:110:DC:C3'	2:B:2084:ARG:HH21	2.14	0.61
1:Q:22:DC:H1'	2:D:4054:TRP:NE1	2.14	0.61
1:Q:11:DC:O5'	2:C:3084:ARG:NE	2.34	0.61
1:Q:30:DC:C5'	2:D:4001:ALA:N	2.63	0.61
1:Q:6:DC:N4	2:C:3016:GLN:CG	2.60	0.61
1:Q:10:DC:C2'	2:C:3084:ARG:HH21	2.12	0.61
1:Q:27:DC:P	2:D:4084:ARG:NE	2.74	0.61
2:A:1023:MET:N	2:A:1027:GLY:HA2	2.16	0.60
2:C:3016:GLN:OE1	2:C:3033:THR:HG23	2.01	0.60
1:R:112:DC:H3'	2:A:1040:TRP:NE1	2.15	0.60
1:R:114:DC:C5'	2:B:2001:ALA:N	2.63	0.60
1:Q:5:DC:H4'	1:Q:6:DC:OP1	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:110:DC:H2'	2:B:2086:ARG:NE	2.17	0.60
1:R:127:DC:O4'	2:A:1060:PHE:CZ	2.54	0.60
1:Q:26:DC:H5''	2:D:4084:ARG:HH22	1.66	0.60
2:D:4111:MET:HE3	2:D:4111:MET:HB3	1.82	0.60
1:Q:6:DC:H4'	1:Q:7:DC:OP1	1.99	0.60
2:B:2061:GLY:O	2:B:2064:ALA:HB3	2.02	0.60
1:R:125:DC:C5'	2:A:1056:ARG:CZ	2.63	0.60
1:R:111:DC:O5'	2:B:2084:ARG:CD	2.50	0.60
1:Q:14:DC:C2'	2:A:1108:THR:OG1	2.50	0.60
2:C:3090:ASP:O	2:C:3092:SER:N	2.35	0.60
1:R:115:DC:N3	1:R:116:DC:C4	2.70	0.60
2:A:1071:LEU:HD11	2:A:1111:MET:HG2	1.84	0.60
1:R:120:DC:N4	2:A:1052:THR:OG1	2.35	0.60
2:A:1086:ARG:NH1	2:A:1098:THR:HB	2.16	0.60
1:R:120:DC:H6	1:R:120:DC:OP2	1.84	0.60
2:C:3039:SER:OG	2:D:4001:ALA:N	2.27	0.60
1:Q:10:DC:O3'	2:C:3084:ARG:CZ	2.49	0.60
2:A:1062:LYS:HG3	2:A:1063:LEU:HG	1.84	0.59
1:Q:13:DC:C6	1:Q:14:DC:C5	2.90	0.59
1:R:121:DC:H3'	2:A:1054:TRP:HE1	1.67	0.59
1:Q:22:DC:C6	1:Q:22:DC:O5'	2.55	0.59
1:R:125:DC:O3'	2:A:1056:ARG:NH2	2.34	0.59
2:A:1080:GLU:HB3	2:A:1108:THR:HG22	1.84	0.59
1:Q:11:DC:O2	1:Q:12:DC:H1'	2.02	0.59
1:Q:7:DC:H42	2:C:3056:ARG:HA	1.66	0.59
2:A:1001:ALA:HA	2:B:2039:SER:H	1.67	0.59
1:Q:10:DC:P	2:C:3086:ARG:HG2	2.43	0.59
1:Q:4:DC:H5	2:C:3013:ASN:HB2	1.67	0.59
2:B:2086:ARG:HG3	2:B:2086:ARG:NH1	2.17	0.59
1:Q:30:DC:H5''	2:D:4001:ALA:N	2.18	0.59
1:R:113:DC:O2	2:B:2001:ALA:HB2	2.01	0.59
1:Q:29:DC:C5'	2:C:3039:SER:O	2.51	0.59
2:C:3058:VAL:O	2:C:3058:VAL:HG13	2.02	0.59
2:B:2063:LEU:O	2:B:2066:VAL:HG12	2.03	0.59
1:R:119:DC:H2'	1:R:120:DC:C6	2.38	0.59
1:R:122:DC:H2''	1:R:123:DC:C6	2.38	0.58
1:Q:9:DC:O3'	2:C:3098:THR:HG21	2.03	0.58
1:R:121:DC:OP2	2:A:1054:TRP:CZ2	2.55	0.58
1:Q:11:DC:H2'	1:Q:12:DC:C4'	2.33	0.58
2:A:1013:ASN:N	2:A:1013:ASN:ND2	2.52	0.58
2:A:1048:MET:HG2	2:A:1049:LYS:N	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3001:ALA:N	2:D:4039:SER:H	2.01	0.58
2:B:2088:TRP:HZ3	2:B:2098:THR:HG1	1.50	0.58
2:D:4084:ARG:NH1	2:D:4084:ARG:HB3	2.17	0.58
1:Q:14:DC:P	2:C:3001:ALA:N	2.77	0.58
1:Q:15:DC:H2'	1:Q:16:DC:H6	1.68	0.58
2:B:2090:ASP:O	2:B:2092:SER:N	2.35	0.58
1:R:110:DC:P	2:B:2098:THR:HG21	2.43	0.58
1:R:124:DC:N4	2:A:1033:THR:OG1	2.37	0.58
2:A:1062:LYS:HG3	2:A:1063:LEU:N	2.19	0.58
1:Q:10:DC:H3'	2:C:3086:ARG:NE	2.16	0.58
2:C:3038:GLU:CA	2:D:4001:ALA:HB2	2.34	0.58
1:Q:26:DC:H3'	2:D:4084:ARG:NH2	2.18	0.58
1:R:109:DC:H2'	1:R:110:DC:H6	0.89	0.58
1:Q:9:DC:C2'	1:Q:10:DC:C4	2.87	0.58
1:R:114:DC:OP2	2:A:1039:SER:HB3	2.04	0.57
1:Q:29:DC:C3'	2:D:4001:ALA:HB3	2.33	0.57
1:R:113:DC:C3'	2:B:2001:ALA:N	2.66	0.57
1:R:115:DC:N3	1:R:116:DC:N4	2.53	0.57
1:Q:29:DC:H41	2:D:4106:GLY:H	1.50	0.57
1:Q:14:DC:H5'	2:C:3001:ALA:O	2.04	0.57
1:Q:29:DC:O4'	2:C:3038:GLU:OE2	2.21	0.57
2:D:4095:ASP:C	2:D:4096:ARG:HG2	2.25	0.57
1:Q:27:DC:OP2	2:D:4084:ARG:CZ	2.53	0.57
1:Q:29:DC:H4'	2:C:3039:SER:O	2.04	0.57
1:R:110:DC:P	2:B:2098:THR:HB	2.45	0.57
2:C:3040:TRP:CD1	2:C:3040:TRP:O	2.58	0.57
1:Q:3:DC:O2	2:D:4003:ARG:CD	2.48	0.57
2:A:1043:LYS:N	2:A:1049:LYS:NZ	2.50	0.57
1:Q:7:DC:H2'	1:Q:8:DC:C6	2.39	0.57
2:B:2090:ASP:HB2	2:B:2094:GLN:HE22	1.70	0.57
2:A:1046:GLY:O	2:A:1048:MET:N	2.36	0.56
2:B:2088:TRP:CZ3	2:B:2098:THR:OG1	2.57	0.56
1:R:116:DC:O2	2:D:4070:TYR:HE1	1.88	0.56
1:R:111:DC:H5''	2:B:2102:VAL:CB	2.32	0.56
1:R:125:DC:C4'	2:A:1056:ARG:NH2	2.67	0.56
1:R:121:DC:H4'	1:R:122:DC:OP1	2.03	0.56
2:D:4002:SER:O	2:D:4003:ARG:C	2.43	0.56
1:Q:6:DC:H42	2:C:3016:GLN:CD	2.08	0.56
2:B:2032:ILE:CG1	2:B:2057:VAL:HB	2.36	0.56
2:C:3034:LEU:HD21	2:C:3077:VAL:CG2	2.33	0.56
2:A:1020:VAL:HG11	2:A:1068:SER:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:1056:ARG:NH1	2:A:1100:GLU:OE2	2.35	0.56
2:B:2051:GLN:O	2:B:2051:GLN:HG3	2.04	0.56
2:A:1050:GLU:HG2	2:A:1051:GLN:H	1.70	0.56
1:R:121:DC:C2'	1:R:122:DC:C4'	2.83	0.56
1:Q:28:DC:C5'	2:C:3051:GLN:NE2	2.67	0.56
1:R:109:DC:C2	1:R:110:DC:C5	2.93	0.56
1:R:109:DC:N1	1:R:110:DC:C5	2.74	0.56
2:C:3040:TRP:O	2:C:3041:ARG:C	2.44	0.56
2:A:1012:GLY:C	2:A:1013:ASN:HD22	2.08	0.56
1:R:110:DC:O5'	2:B:2100:GLU:OE2	2.24	0.56
2:D:4111:MET:CE	2:D:4111:MET:CB	2.83	0.56
1:R:126:DC:C5'	2:A:1021:ARG:NE	2.69	0.56
1:Q:4:DC:OP2	2:C:3074:GLY:HA2	2.05	0.55
1:Q:9:DC:C2'	1:Q:10:DC:N3	2.65	0.55
1:Q:25:DC:C5'	2:D:4056:ARG:NH2	2.64	0.55
1:R:111:DC:OP2	2:B:2086:ARG:HD3	2.05	0.55
1:Q:7:DC:C4	2:C:3033:THR:HB	2.42	0.55
2:A:1058:VAL:HG13	2:A:1102:VAL:HA	1.88	0.55
2:C:3002:SER:O	2:C:3003:ARG:O	2.24	0.55
1:Q:4:DC:H2''	2:C:3054:TRP:CZ2	2.42	0.55
1:Q:9:DC:H2'	2:C:3086:ARG:HH21	1.63	0.55
2:A:1073:LYS:HE2	2:A:1074:GLY:N	2.21	0.55
1:R:113:DC:C4	1:R:114:DC:N4	2.74	0.55
2:A:1027:GLY:O	2:A:1028:ALA:HB3	2.07	0.55
1:R:122:DC:H2''	1:R:123:DC:C5	2.41	0.55
2:D:4060:PHE:CE1	2:D:4102:VAL:HG13	2.41	0.55
2:A:1048:MET:O	2:A:1049:LYS:HG3	2.07	0.55
1:R:110:DC:H5'	2:B:2100:GLU:CG	2.37	0.55
2:C:3047:GLU:OE2	2:C:3047:GLU:HA	2.06	0.55
2:D:4085:THR:OG1	2:D:4099:THR:CG2	2.54	0.55
1:R:110:DC:H5'	2:B:2100:GLU:HG3	1.88	0.55
1:Q:30:DC:C5'	2:D:4001:ALA:CA	2.85	0.55
1:Q:11:DC:O2	2:C:3104:ASN:CB	2.55	0.55
1:R:125:DC:O4'	1:R:125:DC:OP2	2.25	0.54
1:Q:20:DC:N3	2:D:4013:ASN:HB2	2.22	0.54
2:B:2034:LEU:HD22	2:B:2079:ILE:HD12	1.89	0.54
1:R:110:DC:C3'	2:B:2086:ARG:CD	2.62	0.54
1:R:113:DC:H4'	2:A:1039:SER:N	2.20	0.54
2:D:4090:ASP:O	2:D:4093:GLY:N	2.40	0.54
1:R:115:DC:H1'	2:D:4062:LYS:HB2	1.88	0.54
1:Q:24:DC:H2'	2:D:4056:ARG:HG3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:13:DC:OP2	1:Q:13:DC:C6	2.61	0.54
1:R:115:DC:C1'	2:D:4062:LYS:HB2	2.38	0.54
2:B:2088:TRP:CH2	2:B:2096:ARG:CB	2.90	0.54
1:R:111:DC:O2	2:B:2104:ASN:CB	2.56	0.54
1:R:110:DC:C2	2:B:2086:ARG:NH2	2.76	0.54
2:A:1058:VAL:HG22	2:A:1060:PHE:CE1	2.43	0.54
2:A:1086:ARG:CG	2:A:1086:ARG:NH1	2.68	0.54
2:B:2090:ASP:HB3	2:B:2094:GLN:OE1	2.07	0.54
1:R:113:DC:O5'	2:A:1038:GLU:HG2	2.08	0.54
3:A:104:HOH:O	2:B:2094:GLN:HB3	2.06	0.54
1:R:125:DC:H2'	1:R:126:DC:H5'	1.90	0.54
2:C:3001:ALA:HB2	2:D:4038:GLU:HA	1.90	0.54
2:D:4020:VAL:HG21	2:D:4068:SER:HB2	1.90	0.54
2:C:3011:VAL:O	2:D:4004:GLY:HA3	2.08	0.54
2:C:3023:MET:O	2:C:3024:PRO:O	2.25	0.54
1:R:105:DC:H3'	1:R:106:DC:C5	2.43	0.54
2:C:3041:ARG:HA	2:C:3047:GLU:HA	1.90	0.54
2:D:4084:ARG:HH21	2:D:4086:ARG:CD	2.21	0.54
1:R:125:DC:H6	2:A:1086:ARG:NH2	2.05	0.53
1:Q:7:DC:N4	2:C:3033:THR:CA	2.71	0.53
2:B:2020:VAL:CG2	2:B:2068:SER:HB2	2.34	0.53
1:R:126:DC:O4'	2:A:1021:ARG:NH1	2.40	0.53
1:Q:14:DC:C5'	2:C:3001:ALA:C	2.76	0.53
1:Q:27:DC:C4'	2:D:4102:VAL:HG11	2.37	0.53
1:Q:27:DC:H2''	2:D:4104:ASN:CB	2.39	0.53
1:Q:13:DC:H2''	1:Q:14:DC:O4'	2.09	0.53
1:Q:26:DC:C5	2:D:4086:ARG:CZ	2.91	0.53
2:D:4048:MET:O	2:D:4049:LYS:CB	2.55	0.53
1:R:113:DC:C1'	2:B:2001:ALA:N	2.71	0.53
1:R:107:DC:H6	3:R:143:HOH:O	1.91	0.53
2:A:1086:ARG:HH12	2:A:1098:THR:HB	1.74	0.53
2:A:1062:LYS:O	2:A:1066:VAL:HG23	2.08	0.53
2:C:3029:VAL:HG12	2:C:3029:VAL:O	2.08	0.53
1:R:111:DC:H4'	2:B:2084:ARG:HB2	1.90	0.53
2:C:3039:SER:O	2:C:3040:TRP:HE3	1.91	0.53
1:Q:10:DC:O3'	2:C:3084:ARG:NH2	2.42	0.53
2:A:1043:LYS:N	2:A:1049:LYS:HZ1	2.05	0.53
1:Q:10:DC:H2''	2:C:3084:ARG:NH2	2.20	0.53
1:Q:30:DC:O2	2:B:2110:GLN:OE1	2.25	0.53
1:R:110:DC:OP2	2:B:2098:THR:HB	2.09	0.53
1:R:125:DC:N4	1:R:126:DC:N4	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4085:THR:HA	2:D:4099:THR:HG22	1.90	0.53
1:Q:9:DC:O3'	2:C:3098:THR:CG2	2.56	0.53
1:Q:6:DC:N4	2:C:3016:GLN:HE21	2.07	0.53
1:R:116:DC:O4'	2:D:4066:VAL:HG12	2.08	0.53
1:R:110:DC:P	2:B:2098:THR:CG2	2.96	0.53
2:C:3039:SER:H	2:D:4001:ALA:N	2.07	0.53
1:Q:20:DC:C2'	2:D:4054:TRP:HH2	2.22	0.53
1:R:119:DC:C3'	1:R:120:DC:C6	2.91	0.53
2:C:3020:VAL:CG2	2:C:3068:SER:HB2	2.20	0.53
2:B:2086:ARG:HG3	2:B:2086:ARG:HH11	1.74	0.52
2:C:3039:SER:O	2:C:3040:TRP:CB	2.57	0.52
1:Q:29:DC:C4'	2:D:4001:ALA:CB	2.87	0.52
2:D:4084:ARG:CZ	2:D:4100:GLU:OE1	2.58	0.52
1:Q:28:DC:OP2	2:D:4084:ARG:HG3	2.08	0.52
2:D:4022:TYR:CD1	2:D:4022:TYR:N	2.77	0.52
1:R:109:DC:H2''	1:R:110:DC:O5'	2.09	0.52
1:Q:25:DC:C6	2:D:4021:ARG:NH1	2.78	0.52
2:D:4076:GLN:HG2	2:D:4112:LEU:HD12	1.90	0.52
1:Q:17:DC:C2'	1:Q:18:DC:OP1	2.56	0.52
1:R:108:DC:H2''	2:B:2098:THR:CG2	2.38	0.52
2:A:1050:GLU:CG	2:A:1051:GLN:H	2.22	0.52
2:D:4084:ARG:NH1	2:D:4102:VAL:CG2	2.72	0.52
2:B:2023:MET:HG3	2:B:2024:PRO:CD	2.37	0.52
2:C:3001:ALA:C	2:C:3002:SER:O	2.44	0.52
2:A:1050:GLU:CG	2:A:1051:GLN:N	2.73	0.52
1:R:125:DC:C3'	1:R:126:DC:H5'	2.39	0.52
1:Q:24:DC:H4'	1:Q:25:DC:OP1	2.08	0.52
2:B:2089:THR:HG23	2:B:2095:ASP:OD1	2.10	0.52
1:Q:6:DC:C4'	1:Q:7:DC:OP1	2.57	0.52
1:Q:6:DC:H41	2:C:3016:GLN:HG2	1.68	0.52
1:Q:14:DC:H5	3:A:124:HOH:O	1.92	0.52
2:A:1073:LYS:HE2	2:A:1073:LYS:C	2.30	0.52
2:C:3059:LEU:HD12	2:C:3103:VAL:HB	1.91	0.52
1:R:107:DC:N4	2:B:2056:ARG:N	2.39	0.52
2:A:1086:ARG:NH1	2:A:1086:ARG:HG3	2.24	0.52
1:Q:7:DC:N3	2:C:3056:ARG:CA	2.73	0.52
1:Q:3:DC:O2	2:D:4003:ARG:NH1	2.43	0.52
2:D:4090:ASP:OD2	2:D:4091:GLN:N	2.40	0.52
2:A:1004:GLY:HA3	2:B:2011:VAL:O	2.10	0.52
1:R:106:DC:C2'	1:R:107:DC:H3'	2.20	0.51
2:C:3038:GLU:O	2:C:3050:GLU:HA	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:113:DC:OP2	2:A:1038:GLU:OE2	2.27	0.51
2:C:3060:PHE:HE2	2:C:3102:VAL:CG2	2.23	0.51
2:D:4087:LYS:HD2	2:D:4087:LYS:N	2.25	0.51
1:R:125:DC:C3'	2:A:1056:ARG:NH2	2.73	0.51
2:A:1007:LYS:HE3	2:C:3080:GLU:OE1	2.11	0.51
1:R:110:DC:H3'	2:B:2086:ARG:NE	2.24	0.51
2:A:1022:TYR:HA	2:A:1027:GLY:HA3	1.92	0.51
1:Q:10:DC:N1	2:C:3100:GLU:HB3	2.25	0.51
2:A:1073:LYS:HD3	2:A:1074:GLY:N	2.25	0.51
1:Q:27:DC:OP1	2:D:4084:ARG:CD	2.56	0.51
2:B:2031:ASN:ND2	2:B:2058:VAL:HG12	2.26	0.51
1:R:110:DC:N1	2:B:2086:ARG:CZ	2.72	0.51
1:Q:11:DC:P	2:C:3084:ARG:CZ	2.99	0.51
1:Q:11:DC:H4'	2:C:3084:ARG:HH12	1.71	0.51
2:A:1002:SER:O	2:A:1003:ARG:C	2.49	0.51
2:C:3100:GLU:HG3	2:C:3101:VAL:H	1.76	0.51
2:D:4022:TYR:HA	2:D:4027:GLY:HA3	1.92	0.51
2:B:2066:VAL:HG13	2:B:2067:ALA:N	2.25	0.51
1:Q:15:DC:H5''	2:A:1062:LYS:NZ	2.26	0.51
1:Q:14:DC:H2'	2:A:1108:THR:OG1	2.12	0.50
1:Q:26:DC:H2'	1:Q:26:DC:O2	2.10	0.50
1:Q:4:DC:H3'	3:C:123:HOH:O	2.11	0.50
1:Q:7:DC:H2'	1:Q:8:DC:H6	1.75	0.50
2:A:1048:MET:O	2:A:1049:LYS:CG	2.59	0.50
1:R:115:DC:H2'	2:D:4066:VAL:HG11	1.89	0.50
1:R:126:DC:H5''	2:A:1021:ARG:CD	2.41	0.50
1:Q:10:DC:OP2	2:C:3086:ARG:NE	2.44	0.50
1:Q:17:DC:N3	1:Q:18:DC:C5	2.80	0.50
2:D:4027:GLY:O	2:D:4028:ALA:HB3	2.12	0.50
1:R:110:DC:C5'	2:B:2086:ARG:NH1	2.72	0.50
2:A:1014:LEU:O	2:A:1073:LYS:HE3	2.11	0.50
2:A:1051:GLN:HE21	2:A:1051:GLN:CA	2.25	0.50
1:R:125:DC:H6	2:A:1086:ARG:HH21	1.58	0.50
2:B:2088:TRP:CH2	2:B:2096:ARG:HB3	2.46	0.50
2:A:1051:GLN:HA	2:A:1051:GLN:HE21	1.77	0.50
2:B:2090:ASP:HB3	2:B:2094:GLN:CD	2.31	0.50
2:D:4076:GLN:HG2	2:D:4112:LEU:HB2	1.94	0.50
1:R:115:DC:C2'	2:D:4066:VAL:CG1	2.88	0.50
2:C:3023:MET:CB	2:C:3024:PRO:HD2	2.39	0.50
2:B:2113:GLY:N	2:C:3076:GLN:HE22	2.09	0.50
1:Q:20:DC:O3'	2:D:4015:GLY:O	2.30	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4043:LYS:O	2:D:4044:ALA:CB	2.60	0.50
1:R:116:DC:H5'	2:D:4066:VAL:HG11	1.95	0.49
1:R:121:DC:H2''	1:R:122:DC:C5'	2.42	0.49
2:B:2110:GLN:HE22	2:D:4004:GLY:N	2.10	0.49
1:Q:11:DC:H4'	2:C:3102:VAL:HG11	1.93	0.49
1:Q:17:DC:C2	1:Q:18:DC:C4	3.00	0.49
2:B:2089:THR:CG2	2:B:2095:ASP:OD1	2.59	0.49
2:D:4090:ASP:CG	2:D:4091:GLN:N	2.66	0.49
1:R:127:DC:OP2	2:A:1023:MET:HE3	2.12	0.49
2:D:4085:THR:CA	2:D:4099:THR:HG22	2.42	0.49
1:Q:25:DC:C6	1:Q:26:DC:C5	3.01	0.49
2:B:2065:GLU:HA	2:B:2065:GLU:OE2	2.11	0.49
2:A:1048:MET:HG2	2:A:1049:LYS:H	1.76	0.49
1:R:120:DC:H2'	1:R:121:DC:O5'	2.09	0.49
2:C:3038:GLU:CG	2:D:4001:ALA:HB1	2.39	0.49
1:R:121:DC:H5'	2:A:1052:THR:HG21	1.95	0.49
2:D:4088:TRP:HD1	2:D:4089:THR:N	2.09	0.49
1:Q:10:DC:O5'	2:C:3086:ARG:NE	2.46	0.49
1:Q:17:DC:O2	1:Q:18:DC:C4	2.66	0.49
1:Q:17:DC:C2	1:Q:18:DC:C5	3.00	0.49
1:R:111:DC:OP1	2:B:2100:GLU:OE1	2.31	0.49
1:Q:24:DC:H42	2:D:4054:TRP:HB2	1.71	0.49
1:Q:30:DC:H5'	2:D:4001:ALA:CB	2.34	0.49
2:C:3020:VAL:HG22	2:C:3030:ALA:HB2	1.93	0.49
2:C:3021:ARG:HG2	2:C:3022:TYR:N	2.28	0.49
1:Q:17:DC:H2'	1:Q:18:DC:OP1	2.13	0.49
2:B:2088:TRP:CZ3	2:B:2096:ARG:HB2	2.47	0.49
2:D:4051:GLN:HA	2:D:4051:GLN:HE21	1.76	0.49
1:R:115:DC:N4	1:R:116:DC:H41	2.10	0.49
1:R:126:DC:C4'	2:A:1021:ARG:NE	2.76	0.49
1:Q:7:DC:H2''	1:Q:8:DC:C5'	2.43	0.49
1:Q:7:DC:H41	2:C:3033:THR:HG22	1.77	0.49
1:R:106:DC:C4'	1:R:107:DC:O5'	2.51	0.49
1:Q:26:DC:O5'	2:D:4058:VAL:CG2	2.57	0.49
2:B:2072:ARG:O	2:B:2073:LYS:C	2.50	0.49
1:R:111:DC:O5'	2:B:2102:VAL:HG11	2.11	0.49
2:A:1057:VAL:CG1	2:A:1079:ILE:HD13	2.31	0.49
2:C:3102:VAL:O	2:C:3102:VAL:HG13	2.13	0.48
1:Q:20:DC:H4'	1:Q:21:DC:O5'	2.05	0.48
1:Q:3:DC:H2'	1:Q:4:DC:C4	2.47	0.48
1:R:110:DC:H4'	2:B:2100:GLU:OE2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:115:DC:H42	1:R:116:DC:H41	1.61	0.48
1:Q:9:DC:O4'	1:Q:10:DC:N4	2.46	0.48
1:Q:12:DC:H3'	2:D:4038:GLU:HG2	1.95	0.48
1:Q:20:DC:OP2	1:Q:20:DC:O2	2.31	0.48
2:C:3079:ILE:HD13	2:C:3109:MET:HG2	1.94	0.48
1:R:104:DC:O3'	2:B:2015:GLY:HA2	2.13	0.48
1:Q:13:DC:OP1	2:C:3105:VAL:CB	2.60	0.48
2:A:1073:LYS:CD	2:A:1074:GLY:N	2.77	0.48
2:D:4084:ARG:HH11	2:D:4102:VAL:HG21	1.78	0.48
1:Q:15:DC:C5'	2:A:1062:LYS:NZ	2.76	0.48
2:C:3037:SER:OG	2:D:4003:ARG:HB2	2.14	0.48
2:C:3084:ARG:NH2	2:C:3102:VAL:HB	2.12	0.48
2:C:3063:LEU:HA	2:C:3066:VAL:CG1	2.44	0.48
1:Q:25:DC:C3'	2:D:4056:ARG:HH21	2.25	0.48
2:D:4022:TYR:CB	2:D:4027:GLY:HA3	2.44	0.48
2:B:2023:MET:O	2:B:2024:PRO:O	2.31	0.48
2:D:4032:ILE:HG13	2:D:4057:VAL:HB	1.94	0.48
1:R:110:DC:C1'	2:B:2086:ARG:CZ	2.92	0.48
1:Q:11:DC:P	2:C:3084:ARG:NH2	2.87	0.48
1:Q:11:DC:C2'	1:Q:12:DC:O4'	2.44	0.48
1:R:111:DC:H2''	1:R:112:DC:OP1	2.13	0.48
1:Q:29:DC:C4'	2:C:3039:SER:O	2.61	0.48
2:D:4063:LEU:O	2:D:4066:VAL:HG22	2.14	0.48
2:D:4099:THR:C	2:D:4100:GLU:HG3	2.34	0.48
1:Q:28:DC:C2'	1:Q:29:DC:OP1	2.40	0.48
1:R:111:DC:O5'	2:B:2084:ARG:CB	2.60	0.47
2:A:1038:GLU:HA	2:B:2001:ALA:CA	2.33	0.47
1:R:108:DC:C2'	2:B:2098:THR:HG22	2.41	0.47
1:R:126:DC:C6	1:R:126:DC:C3'	2.97	0.47
1:R:126:DC:H2'	1:R:127:DC:OP1	2.14	0.47
1:Q:9:DC:H4'	1:Q:10:DC:C5	2.50	0.47
2:D:4114:GLY:O	2:D:4115:ARG:O	2.32	0.47
1:R:126:DC:H2''	2:A:1021:ARG:HH22	1.79	0.47
1:Q:20:DC:OP2	2:D:4074:GLY:HA2	2.14	0.47
1:Q:22:DC:H5''	1:Q:23:DC:P	2.53	0.47
1:Q:9:DC:C1'	1:Q:10:DC:C4	2.98	0.47
2:C:3043:LYS:O	2:C:3044:ALA:CB	2.62	0.47
1:R:126:DC:H5''	2:A:1021:ARG:HD3	1.96	0.47
1:R:120:DC:P	1:R:120:DC:H6	2.37	0.47
1:Q:29:DC:C2'	1:Q:30:DC:H3'	2.44	0.47
1:Q:5:DC:C4	2:C:3052:THR:HG21	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:3056:ARG:O	2:C:3100:GLU:CG	2.43	0.47
1:Q:10:DC:P	2:C:3086:ARG:CG	3.02	0.47
1:Q:15:DC:C4	1:Q:16:DC:C4	3.02	0.47
1:Q:15:DC:H5''	2:A:1062:LYS:HZ2	1.79	0.47
2:C:3072:ARG:O	2:C:3073:LYS:C	2.52	0.47
2:B:2088:TRP:HZ3	2:B:2098:THR:OG1	1.94	0.47
1:R:120:DC:N4	2:A:1052:THR:HG1	2.13	0.47
1:Q:15:DC:C5'	2:A:1062:LYS:HZ1	2.28	0.47
1:Q:10:DC:OP1	2:C:3098:THR:O	2.33	0.47
1:Q:22:DC:C1'	2:D:4054:TRP:NE1	2.77	0.47
1:Q:24:DC:H2'	2:D:4056:ARG:HD2	1.88	0.47
1:Q:11:DC:C2'	1:Q:12:DC:C4'	2.92	0.47
2:A:1046:GLY:C	2:A:1048:MET:N	2.63	0.47
2:C:3079:ILE:CD1	2:C:3109:MET:HG2	2.44	0.47
1:Q:6:DC:N4	2:C:3016:GLN:NE2	2.52	0.47
2:C:3040:TRP:O	2:C:3042:ASP:N	2.48	0.47
1:Q:20:DC:C3'	2:D:4015:GLY:HA2	2.44	0.47
2:D:4035:ALA:HB2	2:D:4054:TRP:CZ3	2.50	0.47
1:R:109:DC:C4	1:R:110:DC:N4	2.83	0.47
1:R:111:DC:C2'	1:R:112:DC:O5'	2.62	0.47
2:C:3063:LEU:HA	2:C:3066:VAL:HG12	1.97	0.47
2:A:1043:LYS:H	2:A:1049:LYS:HZ2	1.60	0.46
1:R:121:DC:C3'	2:A:1054:TRP:HE1	2.27	0.46
1:R:111:DC:C2'	1:R:112:DC:O4'	2.60	0.46
1:Q:6:DC:H42	2:C:3016:GLN:CG	2.26	0.46
1:R:123:DC:O4'	2:B:2097:TYR:OH	2.27	0.46
2:D:4088:TRP:HZ3	2:D:4098:THR:HG23	1.79	0.46
1:Q:8:DC:H3'	1:Q:9:DC:H5''	1.98	0.46
2:C:3090:ASP:OD1	2:C:3096:ARG:HD2	2.16	0.46
2:D:4084:ARG:NH1	2:D:4102:VAL:HG21	2.30	0.46
1:Q:11:DC:H6	1:Q:11:DC:H5'	1.80	0.46
2:A:1001:ALA:HA	2:B:2039:SER:N	2.31	0.46
1:Q:28:DC:H3'	2:C:3051:GLN:CD	2.36	0.46
1:R:110:DC:OP2	2:B:2098:THR:HG22	2.14	0.46
1:Q:28:DC:C5'	2:C:3051:GLN:HE22	2.28	0.46
2:B:2002:SER:O	2:B:2003:ARG:O	2.34	0.46
1:Q:3:DC:N3	2:D:4003:ARG:HD2	2.31	0.46
1:Q:27:DC:H3'	1:Q:28:DC:C4'	2.46	0.46
1:R:120:DC:H2'	1:R:121:DC:OP1	2.14	0.46
1:Q:14:DC:OP1	2:C:3001:ALA:N	2.49	0.46
1:Q:7:DC:C5	2:C:3033:THR:HB	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:111:DC:C4'	2:B:2084:ARG:HD3	2.44	0.46
2:D:4056:ARG:HH22	2:D:4086:ARG:HH21	1.64	0.46
1:Q:25:DC:C6	1:Q:26:DC:C6	3.04	0.46
2:A:1001:ALA:CB	2:B:2038:GLU:HB2	2.45	0.46
2:A:1073:LYS:NZ	2:A:1074:GLY:HA2	2.31	0.46
2:D:4034:LEU:HD21	2:D:4077:VAL:HG22	1.97	0.46
2:B:2102:VAL:O	2:B:2102:VAL:HG23	2.16	0.45
2:D:4063:LEU:HD12	3:D:128:HOH:O	2.16	0.45
2:D:4056:ARG:NH2	2:D:4086:ARG:HH21	2.13	0.45
1:Q:26:DC:OP2	2:D:4100:GLU:CG	2.63	0.45
2:B:2024:PRO:O	2:B:2025:ASN:C	2.55	0.45
1:Q:9:DC:C1'	1:Q:10:DC:N4	2.79	0.45
1:Q:6:DC:H2'	1:Q:7:DC:H3'	1.91	0.45
2:D:4072:ARG:O	2:D:4073:LYS:C	2.55	0.45
2:D:4088:TRP:CD1	2:D:4089:THR:N	2.83	0.45
2:D:4026:GLY:O	2:D:4027:GLY:O	2.34	0.45
1:R:111:DC:C2	1:R:112:DC:H1'	2.51	0.45
1:R:127:DC:OP2	2:A:1023:MET:SD	2.74	0.45
1:Q:27:DC:OP1	1:Q:27:DC:H4'	2.17	0.45
1:Q:4:DC:C5	2:C:3013:ASN:HB2	2.49	0.45
2:B:2063:LEU:O	2:B:2066:VAL:CG1	2.64	0.45
2:D:4084:ARG:HH11	2:D:4102:VAL:CG2	2.29	0.45
2:B:2022:TYR:O	2:B:2023:MET:O	2.35	0.45
1:Q:20:DC:OP1	2:D:4074:GLY:HA3	2.17	0.45
1:Q:7:DC:H2''	1:Q:8:DC:C4'	2.46	0.45
1:R:104:DC:C2	1:R:105:DC:C5	3.04	0.45
2:A:1033:THR:O	2:A:1033:THR:HG23	2.17	0.45
1:R:125:DC:C5'	2:A:1086:ARG:HH22	2.09	0.45
1:Q:10:DC:C3'	2:C:3084:ARG:HH21	2.29	0.45
2:C:3090:ASP:OD2	2:C:3092:SER:HB2	2.17	0.45
2:C:3076:GLN:HE21	2:C:3112:LEU:HB3	1.82	0.45
2:C:3021:ARG:NH1	2:C:3023:MET:HB3	2.31	0.45
1:R:111:DC:P	2:B:2084:ARG:HH21	2.36	0.45
2:B:2088:TRP:CH2	2:B:2096:ARG:HB2	2.52	0.45
1:R:111:DC:N3	1:R:112:DC:C2	2.85	0.45
1:R:115:DC:N3	1:R:116:DC:C5	2.85	0.45
1:R:121:DC:H6	2:A:1052:THR:HB	1.82	0.45
1:Q:3:DC:H5''	2:C:3074:GLY:O	2.17	0.45
1:Q:24:DC:C4'	1:Q:25:DC:OP1	2.64	0.45
2:D:4050:GLU:O	2:D:4051:GLN:CB	2.65	0.45
1:Q:15:DC:C2'	2:A:1066:VAL:HG21	2.27	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:21:DC:H41	2:D:4052:THR:CG2	2.03	0.44
2:C:3014:LEU:HB2	2:C:3073:LYS:O	2.17	0.44
1:R:109:DC:O5'	2:B:2098:THR:HG21	2.17	0.44
1:Q:24:DC:H1'	2:D:4056:ARG:HD2	1.99	0.44
2:D:4056:ARG:O	2:D:4100:GLU:HB3	2.17	0.44
2:D:4084:ARG:CZ	2:D:4086:ARG:HG3	2.43	0.44
1:R:127:DC:C1'	2:A:1060:PHE:CZ	3.00	0.44
2:A:1032:ILE:CG1	2:A:1057:VAL:HB	2.46	0.44
2:B:2001:ALA:C	2:B:2002:SER:O	2.52	0.44
1:Q:29:DC:C1'	2:D:4001:ALA:HB3	2.47	0.44
1:Q:9:DC:C2'	2:C:3086:ARG:HH21	2.22	0.44
1:R:103:DC:O2	1:R:104:DC:C2	2.71	0.44
1:R:110:DC:OP2	2:B:2098:THR:CB	2.65	0.44
1:Q:10:DC:H5''	2:C:3086:ARG:CD	2.46	0.44
2:C:3087:LYS:HE2	2:C:3095:ASP:OD2	2.18	0.44
1:Q:27:DC:C2'	2:D:4104:ASN:CB	2.96	0.44
1:Q:3:DC:O2	2:D:4003:ARG:CZ	2.65	0.44
2:D:4062:LYS:HG3	2:D:4063:LEU:N	2.30	0.44
1:R:110:DC:P	2:B:2098:THR:CB	3.05	0.44
2:A:1023:MET:CG	2:A:1029:VAL:HG21	2.42	0.44
1:Q:25:DC:H3'	2:D:4086:ARG:NH2	2.32	0.44
1:Q:14:DC:P	1:Q:15:DC:OP1	2.76	0.44
1:Q:17:DC:N3	1:Q:18:DC:N4	2.66	0.44
1:R:107:DC:C2'	1:R:108:DC:O5'	2.56	0.44
2:C:3100:GLU:HG3	2:C:3101:VAL:N	2.28	0.44
2:B:2078:TYR:CE2	2:D:4005:VAL:HG21	2.53	0.44
2:A:1043:LYS:H	2:A:1049:LYS:HZ1	1.59	0.43
1:R:111:DC:OP2	2:B:2086:ARG:CD	2.66	0.43
1:R:116:DC:H5'	2:D:4066:VAL:CG1	2.48	0.43
2:C:3084:ARG:HH11	2:C:3084:ARG:HB2	1.77	0.43
1:Q:10:DC:C2'	2:C:3100:GLU:OE1	2.66	0.43
1:R:104:DC:H2''	2:B:2054:TRP:HH2	1.74	0.43
2:C:3041:ARG:CB	2:C:3047:GLU:OE2	2.66	0.43
2:D:4088:TRP:CZ3	2:D:4098:THR:HG23	2.52	0.43
1:Q:9:DC:P	2:C:3098:THR:OG1	2.76	0.43
2:A:1077:VAL:HG22	2:A:1078:TYR:N	2.33	0.43
2:B:2008:VAL:CG1	2:B:2101:VAL:HG13	2.48	0.43
2:B:2084:ARG:NE	2:B:2086:ARG:HD2	2.33	0.43
1:R:106:DC:O3'	1:R:107:DC:O3'	2.35	0.43
1:Q:13:DC:O4'	2:C:3001:ALA:HB3	2.17	0.43
1:Q:23:DC:N4	3:Q:120:HOH:O	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4024:PRO:O	2:D:4025:ASN:CB	2.66	0.43
2:C:3038:GLU:CA	2:D:4001:ALA:HB1	2.38	0.43
2:D:4094:GLN:HG2	2:D:4095:ASP:N	2.33	0.43
2:B:2113:GLY:H	2:C:3076:GLN:HE22	1.67	0.43
1:Q:14:DC:OP2	1:Q:15:DC:OP1	2.36	0.43
2:B:2084:ARG:HE	2:B:2086:ARG:HD2	1.83	0.43
1:R:115:DC:C2'	1:R:116:DC:O5'	2.66	0.43
1:Q:9:DC:H1'	1:Q:10:DC:N3	2.34	0.43
2:B:2063:LEU:H	2:B:2063:LEU:HD22	1.84	0.43
2:B:2013:ASN:HA	2:B:2075:SER:O	2.17	0.43
2:B:2084:ARG:O	2:B:2099:THR:HA	2.18	0.43
1:R:105:DC:H2''	1:R:106:DC:OP1	2.12	0.43
1:R:111:DC:H4'	2:B:2084:ARG:CB	2.48	0.43
1:R:116:DC:H1'	2:D:4070:TYR:OH	2.18	0.43
1:R:127:DC:O4'	2:A:1060:PHE:CE2	2.72	0.43
1:Q:17:DC:O2	1:Q:18:DC:N4	2.51	0.43
2:B:2002:SER:O	2:B:2003:ARG:C	2.56	0.43
2:D:4063:LEU:CA	2:D:4066:VAL:HG22	2.47	0.43
1:R:115:DC:C4	1:R:116:DC:C5	3.06	0.43
2:C:3011:VAL:O	2:D:4004:GLY:CA	2.66	0.43
1:Q:27:DC:H5'	2:D:4084:ARG:CD	2.49	0.43
1:Q:29:DC:C1'	2:C:3038:GLU:OE2	2.67	0.43
1:R:113:DC:C4'	2:A:1039:SER:O	2.67	0.42
2:D:4063:LEU:HA	2:D:4066:VAL:CG2	2.47	0.42
2:C:3033:THR:HA	2:C:3055:HIS:O	2.19	0.42
2:D:4071:LEU:HD21	2:D:4077:VAL:HG11	2.02	0.42
1:R:104:DC:O3'	2:B:2015:GLY:CA	2.67	0.42
1:R:119:DC:C2'	1:R:120:DC:C6	3.02	0.42
1:R:126:DC:H6	1:R:126:DC:C3'	2.32	0.42
2:D:4016:GLN:HA	2:D:4073:LYS:HG3	2.01	0.42
1:Q:29:DC:H2''	1:Q:30:DC:C4'	2.48	0.42
2:A:1004:GLY:CA	2:B:2011:VAL:O	2.67	0.42
2:C:3039:SER:O	2:C:3040:TRP:CE3	2.72	0.42
1:Q:26:DC:O2	1:Q:26:DC:C2'	2.67	0.42
1:R:109:DC:H2'	2:B:2086:ARG:HH12	1.84	0.42
2:A:1026:GLY:O	2:A:1027:GLY:O	2.36	0.42
1:R:119:DC:H2'	1:R:120:DC:O4'	2.20	0.42
2:C:3085:THR:HA	2:C:3098:THR:O	2.19	0.42
2:C:3100:GLU:HG2	2:C:3101:VAL:N	2.34	0.42
2:D:4084:ARG:HH22	2:D:4100:GLU:CD	2.16	0.42
1:Q:20:DC:C4'	1:Q:21:DC:O5'	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:29:DC:N3	1:Q:30:DC:C5	2.87	0.42
2:A:1083:LEU:HD21	2:B:2083:LEU:HD21	2.01	0.42
1:R:121:DC:C5	2:A:1052:THR:O	2.72	0.42
1:Q:18:DC:OP2	2:A:1112:LEU:O	2.37	0.42
1:R:116:DC:C1'	2:D:4070:TYR:HE1	2.16	0.42
1:R:109:DC:C2	1:R:110:DC:C4	3.08	0.42
1:R:125:DC:C5'	2:A:1086:ARG:NH2	2.72	0.42
1:Q:29:DC:C2	2:C:3038:GLU:OE2	2.73	0.42
1:Q:10:DC:N1	2:C:3100:GLU:OE1	2.52	0.42
1:Q:22:DC:O2	1:Q:24:DC:C5	2.61	0.42
1:R:111:DC:P	2:B:2084:ARG:NH2	2.92	0.42
1:R:113:DC:O5'	2:A:1038:GLU:CG	2.67	0.42
2:C:3084:ARG:HH12	2:C:3102:VAL:CG1	2.17	0.42
1:Q:20:DC:H5''	2:D:4073:LYS:HG2	2.01	0.42
1:R:121:DC:H2'	1:R:122:DC:H4'	2.00	0.42
1:Q:13:DC:C4'	2:C:3001:ALA:HB3	2.50	0.42
2:D:4087:LYS:HG3	2:D:4097:TYR:HE2	1.76	0.42
1:R:106:DC:H2''	1:R:107:DC:O3'	2.19	0.42
1:Q:10:DC:P	2:C:3086:ARG:NE	2.93	0.42
2:A:1035:ALA:HA	2:A:1053:GLU:O	2.19	0.42
1:R:122:DC:H2''	1:R:123:DC:H6	1.85	0.41
2:D:4053:GLU:HG3	2:D:4054:TRP:N	2.35	0.41
1:Q:29:DC:H41	2:D:4106:GLY:N	2.17	0.41
2:C:3016:GLN:OE1	2:C:3033:THR:CG2	2.68	0.41
1:Q:7:DC:C2	1:Q:8:DC:H1'	2.55	0.41
1:Q:8:DC:H5''	1:Q:8:DC:H6	1.84	0.41
1:Q:10:DC:P	2:C:3086:ARG:CZ	3.05	0.41
2:D:4080:GLU:HB3	2:D:4108:THR:CG2	2.50	0.41
2:A:1080:GLU:OE2	2:C:3007:LYS:HE2	2.20	0.41
1:Q:18:DC:C5'	1:Q:18:DC:O2	2.64	0.41
1:R:111:DC:C5'	2:B:2084:ARG:NH1	2.69	0.41
1:R:126:DC:H6	1:R:126:DC:H3'	1.85	0.41
1:Q:24:DC:H2'	2:D:4056:ARG:CG	2.50	0.41
2:A:1099:THR:HB	2:B:2099:THR:HG21	2.02	0.41
1:R:110:DC:C2'	2:B:2086:ARG:NE	2.82	0.41
1:Q:29:DC:OP2	2:C:3038:GLU:OE2	2.38	0.41
1:Q:3:DC:N4	3:Q:113:HOH:O	2.53	0.41
2:D:4050:GLU:O	2:D:4051:GLN:HB2	2.21	0.41
1:Q:22:DC:C2'	1:Q:22:DC:O2	2.65	0.41
1:Q:9:DC:C4'	1:Q:10:DC:C4	3.04	0.41
2:C:3021:ARG:HG2	2:C:3022:TYR:H	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:4036:THR:HG23	2:D:4055:HIS:CE1	2.56	0.41
2:C:3045:THR:O	2:C:3046:GLY:C	2.59	0.41
1:R:113:DC:H4'	2:A:1039:SER:O	2.21	0.41
1:R:109:DC:C6	1:R:110:DC:C5	3.08	0.41
1:R:126:DC:OP1	2:A:1056:ARG:NH2	2.53	0.41
1:Q:24:DC:H2'	2:D:4056:ARG:CD	2.45	0.41
2:C:3022:TYR:CB	2:C:3027:GLY:HA3	2.41	0.41
2:D:4071:LEU:HA	2:D:4071:LEU:HD12	1.82	0.41
2:D:4107:GLY:O	2:D:4108:THR:HB	2.21	0.41
2:B:2085:THR:HA	2:B:2098:THR:O	2.21	0.41
1:R:106:DC:H42	2:B:2016:GLN:HB2	1.86	0.41
2:B:2083:LEU:HA	2:B:2083:LEU:HD12	1.79	0.41
1:R:105:DC:H3'	1:R:106:DC:H5	1.84	0.40
1:Q:7:DC:H2''	1:Q:8:DC:O4'	2.20	0.40
2:D:4018:PRO:HD2	2:D:4071:LEU:O	2.21	0.40
2:B:2063:LEU:CD2	2:B:2063:LEU:H	2.34	0.40
2:A:1088:TRP:CD1	2:A:1088:TRP:N	2.89	0.40
1:Q:9:DC:P	2:C:3098:THR:HG1	2.42	0.40
2:C:3058:VAL:HG12	2:C:3100:GLU:OE1	2.20	0.40
2:D:4088:TRP:CE2	2:D:4096:ARG:CB	3.02	0.40
1:Q:13:DC:C1'	2:C:3001:ALA:CB	2.88	0.40
2:B:2090:ASP:CB	2:B:2094:GLN:NE2	2.72	0.40
2:C:3001:ALA:N	2:D:4039:SER:N	2.68	0.40
2:C:3038:GLU:C	2:D:4001:ALA:HB2	2.40	0.40
1:Q:14:DC:OP2	1:Q:15:DC:P	2.80	0.40
1:Q:8:DC:H5''	1:Q:8:DC:C6	2.57	0.40
2:D:4022:TYR:CA	2:D:4027:GLY:HA3	2.51	0.40
2:D:4049:LYS:O	2:D:4050:GLU:O	2.38	0.40
2:B:2085:THR:OG1	2:B:2099:THR:HG22	2.21	0.40
1:R:107:DC:O3'	1:R:107:DC:P	2.80	0.40
1:R:111:DC:OP1	2:B:2102:VAL:CG1	2.69	0.40
1:R:115:DC:H2'	2:D:4066:VAL:CG1	2.52	0.40
1:R:121:DC:O3'	1:R:121:DC:OP1	2.40	0.40
2:A:1103:VAL:CG1	2:A:1108:THR:H	2.35	0.40
2:C:3039:SER:N	2:D:4001:ALA:CB	2.73	0.40
1:Q:11:DC:O3'	2:C:3084:ARG:NH1	2.55	0.40
1:Q:13:DC:O4'	1:Q:13:DC:OP2	2.39	0.40
2:C:3020:VAL:HG22	2:C:3030:ALA:CB	2.52	0.40
2:A:1080:GLU:CD	2:C:3007:LYS:HE2	2.42	0.40
1:Q:25:DC:O5'	2:D:4056:ARG:NH2	2.55	0.40
2:A:1073:LYS:CE	2:A:1074:GLY:CA	2.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2086:ARG:NH2	2:C:3089:THR:O[3_445]	2.17	0.03

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	110/116 (95%)	87 (79%)	11 (10%)	12 (11%)	0	1
2	B	100/116 (86%)	82 (82%)	8 (8%)	10 (10%)	1	1
2	C	110/116 (95%)	82 (74%)	11 (10%)	17 (16%)	0	0
2	D	108/116 (93%)	85 (79%)	13 (12%)	10 (9%)	1	1
All	All	428/464 (92%)	336 (78%)	43 (10%)	49 (11%)	0	1

All (49) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	1027	GLY
2	A	1046	GLY
2	A	1047	GLU
2	A	1105	VAL
2	B	2004	GLY
2	B	2024	PRO
2	B	2073	LYS
2	B	2105	VAL
2	C	3003	ARG
2	C	3024	PRO
2	C	3040	TRP
2	C	3044	ALA
2	C	3045	THR
2	C	3073	LYS
2	C	3105	VAL

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Mol	Chain	Res	Type
2	D	4027	GLY
2	D	4049	LYS
2	D	4050	GLU
2	D	4051	GLN
2	D	4105	VAL
2	A	1073	LYS
2	A	1108	THR
2	B	2074	GLY
2	B	2091	GLN
2	C	3004	GLY
2	C	3023	MET
2	C	3046	GLY
2	D	4073	LYS
2	D	4108	THR
2	A	1044	ALA
2	A	1051	GLN
2	B	2003	ARG
2	B	2023	MET
2	B	2092	SER
2	C	3043	LYS
2	C	3048	MET
2	C	3091	GLN
2	C	3092	SER
2	D	4025	ASN
2	A	1049	LYS
2	C	3047	GLU
2	C	3074	GLY
2	D	4002	SER
2	A	1002	SER
2	A	1003	ARG
2	B	2028	ALA
2	C	3028	ALA
2	D	4043	LYS
2	A	1025	ASN

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	A	82/95 (86%)	67 (82%)	15 (18%)	2	6
2	B	76/95 (80%)	61 (80%)	15 (20%)	1	5
2	C	80/95 (84%)	68 (85%)	12 (15%)	3	11
2	D	80/95 (84%)	69 (86%)	11 (14%)	4	13
All	All	318/380 (84%)	265 (83%)	53 (17%)	3	8

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1008	VAL
2	A	1013	ASN
2	A	1021	ARG
2	A	1039	SER
2	A	1043	LYS
2	A	1051	GLN
2	A	1059	LEU
2	A	1071	LEU
2	A	1073	LYS
2	A	1082	GLN
2	A	1086	ARG
2	A	1100	GLU
2	A	1102	VAL
2	A	1110	GLN
2	A	1112	LEU
2	B	2013	ASN
2	B	2016	GLN
2	B	2023	MET
2	B	2040	TRP
2	B	2051	GLN
2	B	2052	THR
2	B	2071	LEU
2	B	2086	ARG
2	B	2088	TRP
2	B	2089	THR
2	B	2092	SER
2	B	2094	GLN
2	B	2098	THR
2	B	2099	THR
2	B	2108	THR
2	C	3008	VAL
2	C	3013	ASN
2	C	3016	GLN

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Mol	Chain	Res	Type
2	C	3017	ASP
2	C	3021	ARG
2	C	3033	THR
2	C	3039	SER
2	C	3048	MET
2	C	3059	LEU
2	C	3075	SER
2	C	3091	GLN
2	C	3112	LEU
2	D	4003	ARG
2	D	4008	VAL
2	D	4051	GLN
2	D	4052	THR
2	D	4056	ARG
2	D	4071	LEU
2	D	4079	ILE
2	D	4088	TRP
2	D	4090	ASP
2	D	4098	THR
2	D	4100	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	1013	ASN
2	A	1051	GLN
2	A	1055	HIS
2	B	2016	GLN
2	B	2031	ASN
2	B	2051	GLN
2	B	2055	HIS
2	B	2110	GLN
2	C	3013	ASN
2	C	3016	GLN
2	C	3031	ASN
2	C	3051	GLN
2	C	3076	GLN
2	C	3094	GLN
2	D	4031	ASN
2	D	4051	GLN
2	D	4055	HIS
2	D	4110	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

### 5.7 Other polymers [i](#)

There are no such residues in this entry.

### 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



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

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

EDS was not executed - this section will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

### 6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

### 6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

### 6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.