



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 09:12 am BST

PDB ID : 1VFG  
Title : Crystal structure of tRNA nucleotidyltransferase complexed with a primer tRNA and an incoming ATP analog  
Authors : Tomita, K.; Fukai, S.; Ishitani, R.; Ueda, T.; Takeuchi, N.; Vassilyev, D.G.; Nureki, O.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2004-04-13  
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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

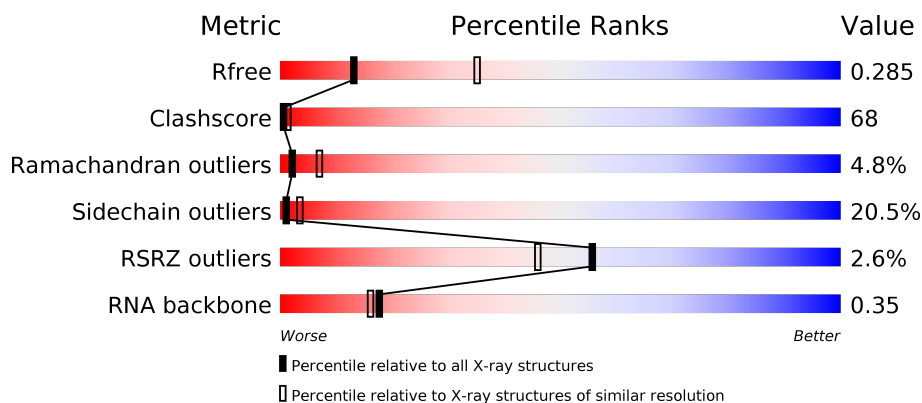
# 1 Overall quality at a glance

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))
$R_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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 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	C	75	
1	D	75	
2	A	390	
2	B	390	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 7319 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a RNA chain called RNA (75-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	31	Total	C	N	O	P	0	0	0
			661	293	116	221	31			
1	D	34	Total	C	N	O	P	0	0	0
			723	321	127	241	34			

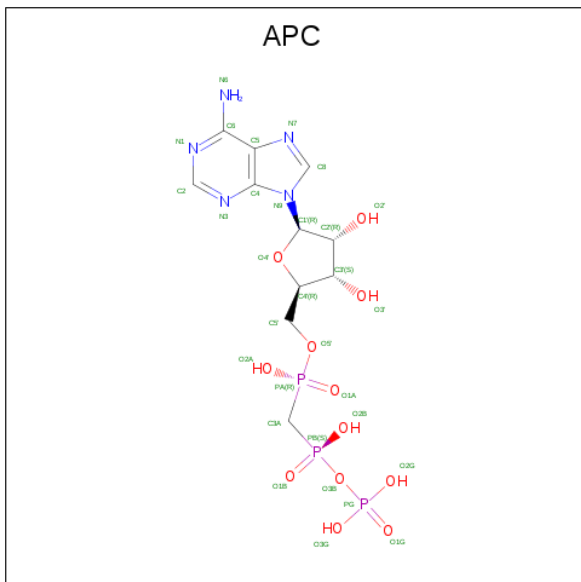
- Molecule 2 is a protein called poly A polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	342	Total	C	N	O	S	0	0	0
			2833	1846	489	492	6			
2	B	358	Total	C	N	O	S	0	0	0
			2961	1928	512	514	7			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	INITIATING METHIONINE	UNP O66728
A	384	LYS	-	CLONING ARTIFACT	UNP O66728
A	385	LEU	-	CLONING ARTIFACT	UNP O66728
A	386	ALA	-	CLONING ARTIFACT	UNP O66728
A	387	ALA	-	CLONING ARTIFACT	UNP O66728
A	388	ALA	-	CLONING ARTIFACT	UNP O66728
A	389	LEU	-	CLONING ARTIFACT	UNP O66728
A	390	GLU	-	CLONING ARTIFACT	UNP O66728
B	1	MET	-	INITIATING METHIONINE	UNP O66728
B	384	LYS	-	CLONING ARTIFACT	UNP O66728
B	385	LEU	-	CLONING ARTIFACT	UNP O66728
B	386	ALA	-	CLONING ARTIFACT	UNP O66728
B	387	ALA	-	CLONING ARTIFACT	UNP O66728
B	388	ALA	-	CLONING ARTIFACT	UNP O66728
B	389	LEU	-	CLONING ARTIFACT	UNP O66728
B	390	GLU	-	CLONING ARTIFACT	UNP O66728

- Molecule 3 is DIPHOSPHOMETHYLPHOSPHONIC ACID ADENOSYL ESTER (three-letter code: APC) (formula:  $C_{11}H_{18}N_5O_{12}P_3$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
3	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- Molecule 4 is water.

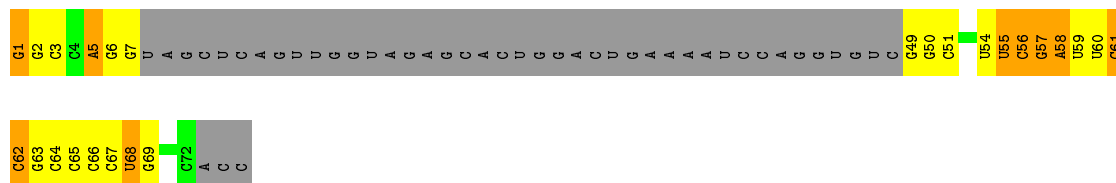
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	2	Total	O	0	0
			2	2		
4	D	8	Total	O	0	0
			8	8		
4	A	31	Total	O	0	0
			31	31		
4	B	38	Total	O	0	0
			38	38		

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

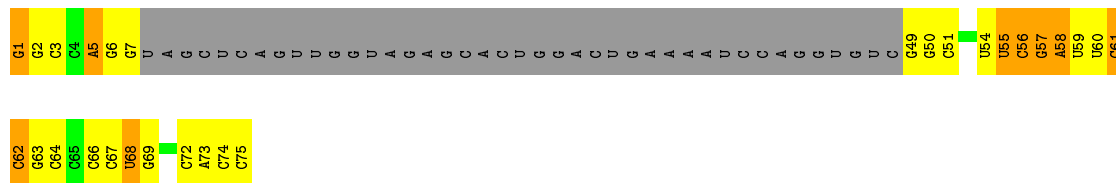
- Molecule 1: RNA (75-MER)

Chain C: 



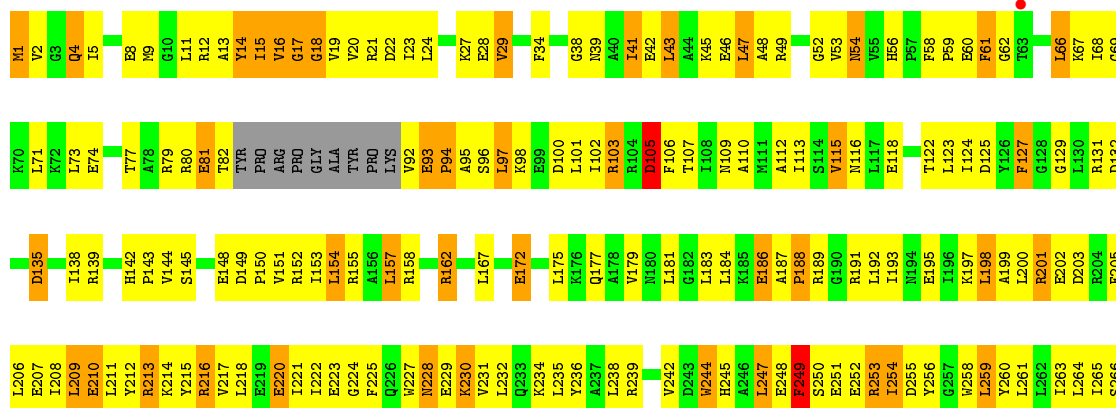
- Molecule 1: RNA (75-MER)

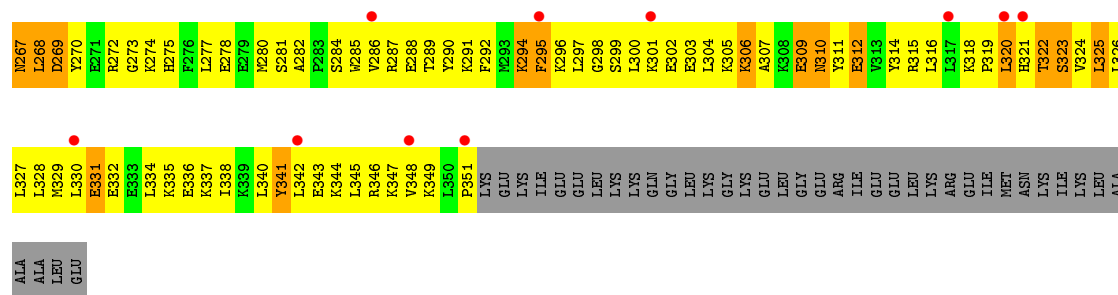
Chain D: 



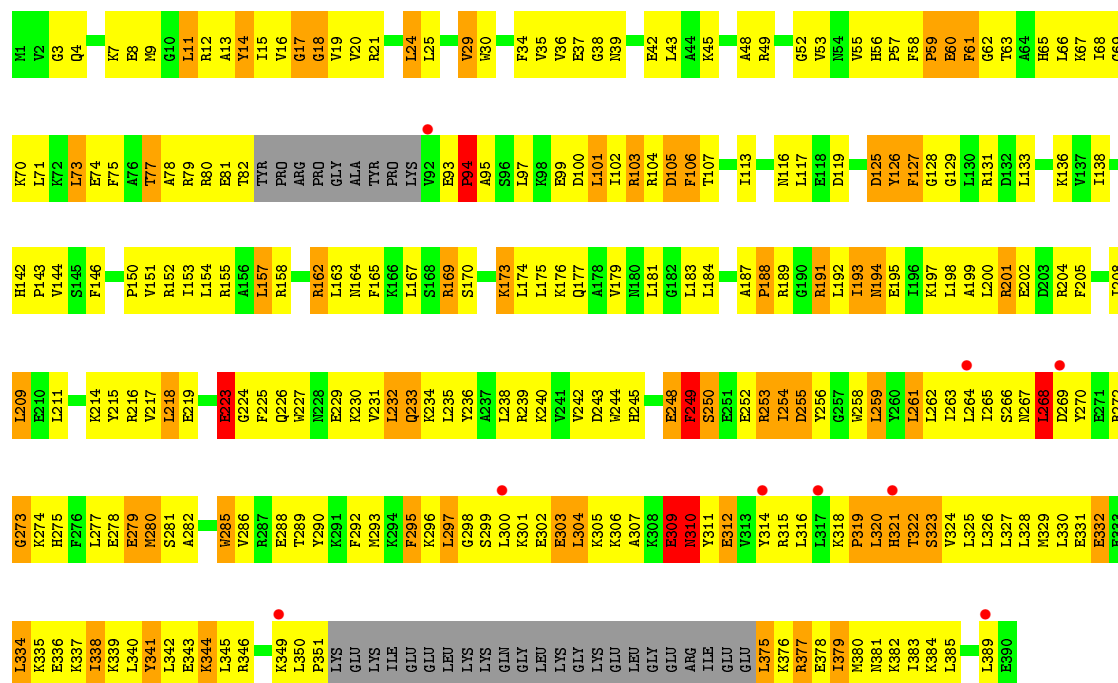
- Molecule 2: poly A polymerase

Chain A: 





- Molecule 2: poly A polymerase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	109.48 Å   125.90 Å   58.92 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	40.00 – 2.80 39.19 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-2.80) 99.1 (39.19-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.92 (at 2.81 Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.230 , 0.286 0.228 , 0.285	Depositor DCC
$R_{free}$ test set	1945 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.5	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 82.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.499 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7319	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	C	0.62	1/735 (0.1%)	0.93	0/1140
1	D	0.64	1/804 (0.1%)	0.93	0/1247
2	A	0.61	1/2885 (0.0%)	0.78	3/3876 (0.1%)
2	B	0.63	0/3012	0.79	2/4041 (0.0%)
All	All	0.62	3/7436 (0.0%)	0.82	5/10304 (0.0%)

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	C	0	1
1	D	0	1
All	All	0	2

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1	G	OP3-P	-7.11	1.52	1.61
1	D	1	G	OP3-P	-7.07	1.52	1.61
2	A	1	MET	CG-SD	5.60	1.95	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1	MET	CB-CG-SD	5.53	128.99	112.40
2	B	307	ALA	N-CA-C	5.49	125.83	111.00
2	A	81	GLU	N-CA-C	5.46	125.73	111.00
2	A	307	ALA	N-CA-C	5.40	125.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	259	LEU	CA-CB-CG	5.14	127.13	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	59	U	Sidechain
1	D	59	U	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	C	661	0	338	37	0
1	D	723	0	371	57	0
2	A	2833	0	2976	399	0
2	B	2961	0	3124	468	0
3	A	31	0	14	5	0
3	B	31	0	14	5	0
4	A	31	0	0	9	0
4	B	38	0	0	24	0
4	C	2	0	0	0	0
4	D	8	0	0	1	0
All	All	7319	0	6837	952	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 68.

All (952) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ARG:HH11	2:B:253:ARG:HB3	1.04	1.15
2:B:302:GLU:HA	2:B:305:LYS:HE3	1.26	1.13
2:A:15:ILE:HD11	2:A:113:ILE:HB	1.22	1.10
2:A:5:ILE:HD12	2:A:47:LEU:HD22	1.32	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:39:ASN:HD21	2:A:41:ILE:HG12	1.12	1.06
2:A:97:LEU:HD11	2:A:101:LEU:HD22	1.34	1.05
1:C:57:G:H2'	1:C:58:A:H5'	1.41	1.03
2:B:268:LEU:HD13	2:B:272:ARG:H	1.24	1.02
2:B:334:LEU:HD23	2:B:334:LEU:H	1.24	1.01
2:B:274:LYS:HA	2:B:277:LEU:HD13	1.43	1.00
2:B:128:GLY:HA2	2:B:131:ARG:HH21	1.25	1.00
2:A:268:LEU:HD13	2:A:272:ARG:H	1.27	1.00
2:A:300:LEU:HA	2:A:315:ARG:HH12	1.23	0.99
2:A:253:ARG:NH1	2:A:253:ARG:HB3	1.77	0.98
1:D:75:C:H41	2:B:191:ARG:HH22	1.07	0.97
2:B:15:ILE:HG22	2:B:34:PHE:HE2	1.24	0.97
1:D:57:G:H2'	1:D:58:A:H5'	1.46	0.97
2:B:79:ARG:HG3	2:B:103:ARG:NH1	1.79	0.97
2:B:79:ARG:HG3	2:B:103:ARG:HH12	1.26	0.97
2:B:253:ARG:HB3	2:B:253:ARG:NH1	1.81	0.96
2:A:304:LEU:O	2:A:304:LEU:HD23	1.66	0.96
2:A:19:VAL:HG23	2:A:29:VAL:HG21	1.48	0.95
2:B:223:GLU:HG3	2:B:224:GLY:H	1.31	0.95
2:B:380:MET:HA	2:B:383:ILE:CD1	1.96	0.95
2:B:67:LYS:HD3	2:B:67:LYS:O	1.66	0.95
2:B:233:GLN:HE21	2:B:234:LYS:N	1.64	0.95
2:A:15:ILE:HD11	2:A:113:ILE:CB	1.97	0.94
2:B:67:LYS:HE2	2:B:69:GLY:N	1.82	0.94
2:B:193:ILE:HG23	2:B:197:LYS:HE3	1.50	0.93
2:B:277:LEU:HD12	2:B:277:LEU:H	1.33	0.93
2:B:7:LYS:NZ	2:B:117:LEU:H	1.66	0.92
2:B:189:ARG:NH1	2:B:279:GLU:HG2	1.84	0.92
1:C:54:U:H3'	1:C:55:U:H5''	1.52	0.92
2:B:342:LEU:O	2:B:346:ARG:HG3	1.69	0.92
2:A:183:LEU:HA	2:A:186:GLU:HG3	1.52	0.91
2:B:245:HIS:CE1	2:B:249:PHE:HB3	2.05	0.91
2:A:342:LEU:O	2:A:346:ARG:HG3	1.70	0.91
2:A:39:ASN:ND2	2:A:41:ILE:HG12	1.84	0.91
2:B:344:LYS:NZ	2:B:345:LEU:HG	1.85	0.90
1:D:75:C:H41	2:B:191:ARG:NH2	1.70	0.90
2:A:300:LEU:HA	2:A:315:ARG:NH1	1.86	0.90
2:B:7:LYS:HZ1	2:B:117:LEU:H	0.94	0.90
2:B:15:ILE:HG22	2:B:34:PHE:CE2	2.05	0.90
2:A:316:LEU:C	2:A:319:PRO:HD2	1.92	0.90
2:B:268:LEU:HD22	2:B:272:ARG:HA	1.53	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:54:U:H3'	1:D:55:U:H5''	1.52	0.89
2:A:213:ARG:HH11	2:A:213:ARG:HB3	1.37	0.89
2:A:15:ILE:CD1	2:A:113:ILE:HB	2.02	0.89
2:A:183:LEU:HA	2:A:186:GLU:CG	2.01	0.89
2:A:200:LEU:HD22	2:A:201:ARG:HH21	1.36	0.89
1:D:50:G:H2'	1:D:51:C:C6	2.08	0.88
1:C:50:G:H2'	1:C:51:C:C6	2.08	0.88
2:B:345:LEU:HD12	4:B:1511:HOH:O	1.74	0.88
2:A:41:ILE:HG22	2:A:45:LYS:HE3	1.55	0.88
2:B:297:LEU:HA	4:B:1519:HOH:O	1.74	0.87
2:A:197:LYS:HG2	2:A:201:ARG:HH22	1.38	0.87
2:A:261:LEU:O	2:A:265:ILE:HG12	1.75	0.87
2:A:253:ARG:HB3	2:A:253:ARG:CZ	2.05	0.86
2:A:41:ILE:CG2	2:A:45:LYS:HE3	2.06	0.86
2:B:384:LYS:HG3	2:B:385:LEU:HD23	1.57	0.85
2:B:7:LYS:NZ	2:B:117:LEU:HG	1.91	0.85
1:C:68:U:H2'	1:C:69:G:C8	2.11	0.85
2:A:206:LEU:HD23	2:A:239:ARG:HD2	1.54	0.85
2:A:19:VAL:O	2:A:23:ILE:HD12	1.75	0.85
1:D:54:U:C3'	1:D:55:U:H5''	2.07	0.85
2:A:149:ASP:OD1	2:A:151:VAL:HG12	1.77	0.84
2:B:268:LEU:HD13	2:B:272:ARG:N	1.91	0.84
1:C:54:U:C3'	1:C:55:U:H5''	2.06	0.84
2:A:39:ASN:HD21	2:A:41:ILE:CG1	1.90	0.84
2:B:256:TYR:HA	2:B:259:LEU:HD13	1.57	0.84
1:D:68:U:H2'	1:D:69:G:C8	2.12	0.84
2:B:12:ARG:HA	2:B:116:ASN:HD21	1.40	0.84
2:A:343:GLU:HB3	2:A:347:LYS:HZ2	1.42	0.84
2:B:19:VAL:HG23	2:B:29:VAL:HG21	1.58	0.84
2:B:309:GLU:O	2:B:311:TYR:N	2.11	0.84
2:B:322:THR:HG22	2:B:326:LEU:HD21	1.58	0.83
2:A:222:ILE:CG2	2:A:225:PHE:HB2	2.09	0.83
2:A:43:LEU:HD12	2:A:47:LEU:HD23	1.59	0.83
2:B:285:TRP:HE1	2:B:323:SER:HB3	1.41	0.83
2:B:297:LEU:HD23	2:B:298:GLY:N	1.94	0.83
2:A:80:ARG:HE	2:A:95:ALA:HB2	1.43	0.83
1:C:67:C:H2'	1:C:68:U:C5	2.14	0.82
2:A:193:ILE:HG23	2:A:280:MET:HE1	1.58	0.82
2:B:343:GLU:HA	2:B:346:ARG:HD2	1.61	0.82
2:A:131:ARG:HH22	2:A:139:ARG:HH12	1.27	0.82
1:D:74:C:H4'	4:D:76:HOH:O	1.78	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:261:LEU:HA	2:B:264:LEU:HD12	1.61	0.82
2:B:224:GLY:HA3	2:B:269:ASP:HB2	1.62	0.81
2:A:144:VAL:O	2:A:148:GLU:HG3	1.80	0.81
2:B:227:TRP:CZ3	2:B:232:LEU:HD12	2.16	0.81
2:A:59:PRO:O	2:A:61:PHE:HD1	1.63	0.81
1:D:67:C:H2'	1:D:68:U:C5	2.16	0.80
2:A:309:GLU:O	2:A:311:TYR:N	2.13	0.80
2:A:304:LEU:HA	2:A:315:ARG:HH21	1.47	0.80
2:A:316:LEU:O	2:A:319:PRO:HD2	1.82	0.80
2:B:3:GLY:O	2:B:7:LYS:HG2	1.81	0.80
2:A:97:LEU:O	2:A:97:LEU:HD12	1.83	0.79
2:B:376:LYS:HD2	2:B:379:ILE:HD11	1.63	0.79
2:A:268:LEU:HD13	2:A:272:ARG:N	1.98	0.79
2:B:253:ARG:CB	2:B:253:ARG:HH11	1.92	0.79
2:A:205:PHE:HA	2:A:208:ILE:HD12	1.64	0.79
2:B:268:LEU:HD22	2:B:272:ARG:CA	2.12	0.79
2:A:222:ILE:HG22	2:A:225:PHE:HB2	1.63	0.79
2:A:216:ARG:NH1	2:A:216:ARG:HB2	1.98	0.79
2:B:245:HIS:CD2	2:B:326:LEU:HD11	2.18	0.79
2:A:13:ALA:H	2:A:116:ASN:HD21	1.28	0.78
2:A:242:VAL:HG13	2:A:256:TYR:CD2	2.17	0.78
2:B:316:LEU:C	2:B:319:PRO:HD2	2.03	0.78
2:A:258:TRP:HH2	2:A:280:MET:HB3	1.48	0.78
2:A:154:LEU:H	2:A:154:LEU:CD2	1.97	0.78
2:B:62:GLY:O	2:B:77:THR:HG22	1.83	0.78
2:B:30:TRP:CZ3	2:B:71:LEU:HG	2.19	0.77
2:A:268:LEU:HD22	2:A:272:ARG:HA	1.64	0.77
2:B:341:TYR:HD2	2:B:342:LEU:N	1.81	0.77
2:A:205:PHE:CE2	2:A:209:LEU:HD21	2.20	0.77
2:B:67:LYS:HE2	2:B:69:GLY:H	1.47	0.77
2:B:272:ARG:HG2	2:B:272:ARG:HH11	1.49	0.76
2:B:322:THR:HG22	2:B:326:LEU:CD2	2.14	0.76
2:B:377:ARG:HD2	2:B:378:GLU:H	1.47	0.76
2:A:297:LEU:O	2:A:301:LYS:HD2	1.85	0.76
2:A:343:GLU:O	2:A:347:LYS:HD2	1.86	0.76
2:B:335:LYS:HE2	2:B:339:LYS:HE3	1.67	0.76
2:A:15:ILE:HD12	2:A:20:VAL:HG22	1.66	0.75
2:A:38:GLY:O	2:A:77:THR:HG23	1.86	0.75
2:A:154:LEU:H	2:A:154:LEU:HD22	1.52	0.75
2:A:205:PHE:O	2:A:209:LEU:HD22	1.87	0.75
2:B:245:HIS:HD2	2:B:326:LEU:HD11	1.48	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:LYS:HZ1	2:B:117:LEU:HG	1.49	0.75
2:B:174:LEU:HA	2:B:177:GLN:HG3	1.69	0.75
2:B:164:ASN:HB2	2:B:204:ARG:NH2	2.01	0.75
2:A:295:PHE:N	2:A:295:PHE:CD2	2.54	0.75
2:B:11:LEU:HD23	2:B:12:ARG:H	1.51	0.75
2:B:268:LEU:CD1	2:B:272:ARG:H	1.98	0.75
2:A:206:LEU:HA	2:A:209:LEU:HD23	1.69	0.74
2:B:229:GLU:H	2:B:229:GLU:CD	1.90	0.74
2:B:380:MET:HA	2:B:383:ILE:HD12	1.69	0.74
2:B:302:GLU:HA	2:B:305:LYS:CE	2.12	0.74
2:B:344:LYS:HD2	2:B:345:LEU:N	2.02	0.74
2:A:285:TRP:HB3	2:A:321:HIS:NE2	2.02	0.74
2:B:344:LYS:HZ1	2:B:345:LEU:HG	1.48	0.74
1:C:57:G:C2'	1:C:58:A:H5'	2.16	0.73
2:B:7:LYS:HZ1	2:B:117:LEU:N	1.80	0.73
1:C:67:C:H2'	1:C:68:U:C6	2.24	0.73
2:A:149:ASP:OD2	2:A:191:ARG:NH2	2.21	0.73
2:A:193:ILE:HG23	2:A:280:MET:CE	2.18	0.73
2:A:213:ARG:NH1	2:A:213:ARG:HB3	2.04	0.73
2:B:242:VAL:HG13	2:B:256:TYR:CD1	2.23	0.72
2:A:216:ARG:HB2	2:A:216:ARG:CZ	2.19	0.72
2:A:5:ILE:HD12	2:A:47:LEU:CD2	2.17	0.72
2:A:197:LYS:HG2	2:A:201:ARG:NH2	2.04	0.72
2:A:189:ARG:O	2:A:193:ILE:HG12	1.90	0.72
2:B:214:LYS:HE3	4:B:1531:HOH:O	1.88	0.72
2:A:59:PRO:O	2:A:61:PHE:CD1	2.42	0.72
2:B:341:TYR:CE2	2:B:345:LEU:HD12	2.24	0.72
2:B:293:MET:O	2:B:297:LEU:HB3	1.90	0.72
1:D:72:C:H2'	1:D:73:A:C8	2.25	0.72
2:A:304:LEU:CA	2:A:315:ARG:HH21	2.02	0.71
2:A:54:ASN:H	2:A:54:ASN:ND2	1.88	0.71
2:B:382:LYS:HA	2:B:385:LEU:CD1	2.21	0.71
1:D:67:C:H2'	1:D:68:U:C6	2.25	0.71
2:B:226:GLN:HA	4:B:1512:HOH:O	1.89	0.71
2:B:334:LEU:CD2	2:B:334:LEU:H	2.03	0.71
2:B:341:TYR:C	2:B:341:TYR:CD2	2.64	0.71
2:A:144:VAL:HG23	4:A:530:HOH:O	1.89	0.71
2:A:228:ASN:ND2	2:A:231:VAL:HG23	2.05	0.71
2:A:242:VAL:HG22	2:A:256:TYR:HD2	1.56	0.70
2:B:326:LEU:N	2:B:326:LEU:HD22	2.06	0.70
2:A:258:TRP:CH2	2:A:280:MET:HB3	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:LEU:HD12	2:B:277:LEU:N	2.05	0.70
2:A:42:GLU:HA	2:A:45:LYS:HD2	1.73	0.70
2:B:312:GLU:OE2	2:B:344:LYS:HE3	1.92	0.70
2:A:167:LEU:HD12	2:A:172:GLU:HG2	1.74	0.70
2:B:344:LYS:HD2	2:B:344:LYS:C	2.12	0.70
2:A:19:VAL:HG22	2:A:23:ILE:HD11	1.73	0.69
2:B:334:LEU:HA	2:B:337:LYS:HG3	1.73	0.69
2:A:209:LEU:HA	2:A:212:TYR:HD2	1.57	0.69
2:B:381:ASN:O	2:B:384:LYS:HG2	1.92	0.69
2:A:260:TYR:O	2:A:264:LEU:HD12	1.92	0.69
2:B:193:ILE:HG22	2:B:194:ASN:N	2.06	0.69
2:A:345:LEU:HA	2:A:348:VAL:HG23	1.74	0.69
2:B:194:ASN:O	2:B:198:LEU:HD23	1.92	0.69
2:A:343:GLU:HB3	2:A:347:LYS:NZ	2.07	0.69
2:B:233:GLN:HE21	2:B:233:GLN:C	1.96	0.69
2:B:296:LYS:HD3	2:B:299:SER:HB2	1.74	0.69
1:D:57:G:C2'	1:D:58:A:H5'	2.21	0.69
2:A:127:PHE:N	2:A:127:PHE:CD1	2.61	0.69
2:B:326:LEU:HA	2:B:329:MET:CE	2.23	0.69
2:A:239:ARG:HA	2:A:260:TYR:OH	1.93	0.68
2:B:223:GLU:HG3	2:B:224:GLY:N	2.05	0.68
2:A:296:LYS:HB3	2:A:300:LEU:HD13	1.75	0.68
2:A:316:LEU:O	2:A:316:LEU:HD23	1.93	0.68
2:B:316:LEU:HG	2:B:341:TYR:OH	1.94	0.68
2:B:169:ARG:HH21	2:B:173:LYS:HZ2	1.38	0.68
2:A:202:GLU:HG3	2:A:208:ILE:HD11	1.75	0.67
2:A:216:ARG:CB	2:A:216:ARG:NH1	2.57	0.67
2:B:381:ASN:O	2:B:385:LEU:HG	1.94	0.67
2:A:304:LEU:HD13	2:A:334:LEU:HD22	1.75	0.67
2:B:197:LYS:O	2:B:201:ARG:HG2	1.93	0.67
2:A:295:PHE:N	2:A:295:PHE:HD2	1.92	0.67
2:A:304:LEU:N	2:A:315:ARG:NH2	2.43	0.67
2:B:170:SER:O	2:B:174:LEU:HG	1.94	0.67
2:B:254:ILE:HG12	2:B:285:TRP:CH2	2.30	0.67
2:A:5:ILE:HG21	2:A:43:LEU:HD13	1.76	0.67
2:A:238:LEU:HD21	2:A:259:LEU:HB3	1.77	0.67
2:B:344:LYS:HZ3	2:B:345:LEU:H	1.40	0.67
2:A:318:LYS:HE2	4:A:531:HOH:O	1.93	0.66
2:B:285:TRP:HB2	2:B:321:HIS:CE1	2.30	0.66
2:A:183:LEU:HA	2:A:186:GLU:HG2	1.76	0.66
1:C:1:G:H2'	1:C:1:G:N3	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:210:GLU:HA	2:A:210:GLU:OE1	1.94	0.66
2:A:213:ARG:HA	4:A:522:HOH:O	1.95	0.66
2:A:324:VAL:O	2:A:328:LEU:HG	1.96	0.66
2:B:195:GLU:O	2:B:198:LEU:HB2	1.95	0.66
2:B:199:ALA:HA	2:B:202:GLU:HG2	1.77	0.66
2:B:380:MET:HA	2:B:383:ILE:HD11	1.77	0.66
2:A:162:ARG:HH11	2:A:162:ARG:HG3	1.60	0.66
2:B:311:TYR:O	2:B:315:ARG:HG2	1.96	0.66
2:B:316:LEU:O	2:B:316:LEU:HD23	1.96	0.66
2:B:375:LEU:HA	2:B:377:ARG:NE	2.10	0.66
2:A:289:THR:HG23	2:A:324:VAL:HG22	1.77	0.66
2:A:200:LEU:HD22	2:A:201:ARG:NH2	2.10	0.65
1:D:75:C:N4	2:B:191:ARG:NH2	2.42	0.65
2:A:272:ARG:O	2:A:274:LYS:N	2.29	0.65
2:A:343:GLU:O	2:A:346:ARG:HB2	1.96	0.65
1:D:1:G:N3	1:D:1:G:H2'	2.11	0.65
2:B:272:ARG:O	2:B:274:LYS:N	2.28	0.65
2:B:342:LEU:HB3	2:B:346:ARG:HH21	1.62	0.65
2:B:66:LEU:O	2:B:73:LEU:HD23	1.96	0.65
2:B:259:LEU:HA	2:B:262:LEU:HD12	1.79	0.65
2:B:128:GLY:HA2	2:B:131:ARG:NH2	2.04	0.65
2:B:150:PRO:HG2	2:B:187:ALA:HB2	1.77	0.65
2:A:183:LEU:HD23	2:A:186:GLU:HG3	1.79	0.65
2:A:131:ARG:HG2	2:A:135:ASP:OD2	1.97	0.64
2:A:238:LEU:HD22	2:A:263:ILE:HD11	1.78	0.64
2:B:30:TRP:HZ3	2:B:71:LEU:HG	1.61	0.64
2:A:224:GLY:HA3	2:A:269:ASP:HB3	1.78	0.64
2:A:315:ARG:O	2:A:319:PRO:HD3	1.97	0.64
2:A:97:LEU:HD12	2:A:97:LEU:C	2.16	0.64
2:B:11:LEU:HD21	2:B:37:GLU:C	2.17	0.64
2:B:79:ARG:CG	2:B:103:ARG:HH12	2.05	0.64
2:B:126:TYR:HB2	2:B:127:PHE:CD2	2.32	0.64
2:A:294:LYS:HZ2	2:A:295:PHE:HE2	1.44	0.64
2:B:66:LEU:HD11	2:B:68:ILE:HD11	1.79	0.64
2:A:157:LEU:CD1	2:A:157:LEU:N	2.61	0.64
2:B:377:ARG:O	2:B:381:ASN:N	2.22	0.64
2:A:287:ARG:HG3	2:A:287:ARG:HH11	1.63	0.64
1:D:73:A:O2'	1:D:74:C:H5'	1.99	0.63
2:B:12:ARG:HA	2:B:116:ASN:ND2	2.12	0.63
2:B:300:LEU:O	2:B:304:LEU:HD12	1.98	0.63
2:B:341:TYR:CD2	2:B:342:LEU:N	2.66	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:189:ARG:CZ	2:B:279:GLU:HG2	2.27	0.63
2:B:193:ILE:CG2	2:B:197:LYS:HE3	2.27	0.63
2:A:300:LEU:O	2:A:304:LEU:HB2	1.97	0.63
2:A:334:LEU:O	2:A:338:ILE:HD13	1.99	0.63
2:B:285:TRP:HB2	2:B:321:HIS:CG	2.34	0.63
2:A:228:ASN:HD22	2:A:231:VAL:HG23	1.60	0.63
2:A:297:LEU:HA	2:A:301:LYS:HZ3	1.63	0.63
2:A:304:LEU:HD21	2:A:337:LYS:HD3	1.79	0.63
2:B:285:TRP:NE1	2:B:323:SER:HB3	2.13	0.63
2:B:66:LEU:CD1	2:B:68:ILE:HD11	2.27	0.63
2:A:115:VAL:HG23	2:A:115:VAL:O	1.98	0.63
2:A:316:LEU:HD12	2:A:345:LEU:HD21	1.81	0.63
2:B:248:GLU:CD	2:B:248:GLU:N	2.52	0.63
2:B:99:GLU:O	2:B:102:ILE:HG22	1.97	0.63
2:A:105:ASP:N	3:A:500:APC:H2	2.14	0.62
2:B:285:TRP:HB2	2:B:321:HIS:ND1	2.14	0.62
2:A:254:ILE:HG12	2:A:255:ASP:N	2.15	0.62
2:B:236:TYR:O	2:B:239:ARG:HB3	1.99	0.62
2:B:244:TRP:O	2:B:248:GLU:OE2	2.16	0.62
2:A:259:LEU:CD1	2:A:327:LEU:HD21	2.28	0.62
2:A:43:LEU:CD1	2:A:47:LEU:HD23	2.28	0.62
2:B:169:ARG:NH2	2:B:173:LYS:HZ2	1.97	0.62
2:B:277:LEU:H	2:B:277:LEU:CD1	2.06	0.62
2:B:274:LYS:HG3	2:B:290:TYR:CD2	2.35	0.62
2:B:342:LEU:HA	4:B:1511:HOH:O	1.99	0.62
1:D:73:A:H2'	1:D:74:C:O4'	1.99	0.62
2:A:61:PHE:N	2:A:61:PHE:CD1	2.65	0.62
2:B:193:ILE:CG2	2:B:194:ASN:N	2.62	0.61
2:A:285:TRP:HB2	2:A:321:HIS:CG	2.35	0.61
2:B:223:GLU:CG	2:B:224:GLY:H	2.10	0.61
1:C:5:A:C2	1:C:69:G:C6	2.88	0.61
2:B:325:LEU:HA	2:B:328:LEU:HD12	1.83	0.61
2:B:339:LYS:HD2	4:B:1534:HOH:O	1.99	0.61
1:D:5:A:C2	1:D:69:G:C6	2.89	0.61
2:B:66:LEU:CD1	2:B:73:LEU:HD21	2.30	0.61
2:A:154:LEU:N	2:A:154:LEU:HD22	2.15	0.61
2:A:59:PRO:O	2:A:60:GLU:HB3	2.00	0.61
2:B:343:GLU:O	2:B:346:ARG:HB2	2.01	0.61
2:A:205:PHE:O	2:A:208:ILE:HB	2.01	0.61
2:A:131:ARG:NH2	2:A:139:ARG:HH12	1.96	0.61
2:A:259:LEU:HD11	2:A:327:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:384:LYS:HG3	2:B:385:LEU:CD2	2.29	0.61
2:A:13:ALA:C	2:A:14:TYR:CD1	2.74	0.60
2:A:285:TRP:CB	2:A:321:HIS:CE1	2.83	0.60
2:A:53:VAL:HG11	2:A:67:LYS:O	2.02	0.60
2:B:184:LEU:HD11	2:B:217:VAL:HG13	1.83	0.60
2:B:256:TYR:HA	2:B:259:LEU:CD1	2.29	0.60
2:B:30:TRP:CE3	2:B:71:LEU:HG	2.36	0.60
2:A:232:LEU:O	2:A:235:LEU:HB2	2.01	0.60
2:A:322:THR:HG23	2:A:325:LEU:HD22	1.82	0.60
2:B:15:ILE:HG12	2:B:113:ILE:HB	1.84	0.60
2:B:292:PHE:CE1	2:B:296:LYS:HB2	2.37	0.60
1:D:73:A:O5'	1:D:73:A:H8	1.84	0.60
2:A:15:ILE:HD12	2:A:20:VAL:CG2	2.31	0.60
2:B:175:LEU:C	2:B:175:LEU:HD23	2.22	0.60
2:B:336:GLU:OE2	2:B:339:LYS:HD2	2.01	0.60
2:A:205:PHE:CZ	2:A:209:LEU:HD21	2.36	0.60
2:B:229:GLU:O	2:B:233:GLN:HG3	2.01	0.60
1:D:74:C:OP1	2:B:191:ARG:NH2	2.35	0.60
2:A:242:VAL:HG22	2:A:256:TYR:CD2	2.37	0.60
2:A:48:ALA:HB1	2:A:53:VAL:O	2.01	0.60
2:A:312:GLU:OE2	2:A:345:LEU:HD11	2.02	0.60
2:B:97:LEU:HG	2:B:101:LEU:HD22	1.83	0.60
2:B:15:ILE:HD11	2:B:113:ILE:HD12	1.83	0.60
2:B:169:ARG:NH2	2:B:173:LYS:NZ	2.50	0.60
2:B:105:ASP:HB3	2:B:106:PHE:CD1	2.37	0.59
2:A:304:LEU:CA	2:A:315:ARG:NH2	2.64	0.59
2:B:335:LYS:NZ	2:B:339:LYS:NZ	2.50	0.59
2:B:280:MET:O	2:B:282:ALA:N	2.34	0.59
2:B:11:LEU:HD21	2:B:38:GLY:N	2.18	0.59
2:B:20:VAL:HG13	2:B:113:ILE:HD11	1.84	0.59
2:B:335:LYS:HG2	4:B:1534:HOH:O	2.02	0.59
1:D:5:A:H2'	1:D:6:G:C8	2.36	0.59
2:A:15:ILE:CD1	2:A:20:VAL:HG22	2.32	0.59
2:B:341:TYR:HD2	2:B:341:TYR:C	2.04	0.59
2:B:303:GLU:HA	2:B:306:LYS:NZ	2.18	0.59
2:B:173:LYS:O	2:B:177:GLN:HG2	2.02	0.59
2:B:324:VAL:O	2:B:328:LEU:HG	2.02	0.59
2:A:285:TRP:HB3	2:A:321:HIS:CD2	2.38	0.58
1:C:5:A:H2'	1:C:6:G:C8	2.37	0.58
2:A:345:LEU:O	2:A:349:LYS:HD3	2.03	0.58
2:B:230:LYS:O	2:B:233:GLN:NE2	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ARG:NH1	2:B:81:GLU:C	2.56	0.58
2:A:153:ILE:HD12	2:A:184:LEU:HD21	1.86	0.58
2:A:197:LYS:O	2:A:201:ARG:NE	2.36	0.58
2:A:41:ILE:O	2:A:45:LYS:HG3	2.03	0.58
2:B:342:LEU:HB3	2:B:346:ARG:NH2	2.17	0.58
2:A:216:ARG:CB	2:A:216:ARG:HH11	2.16	0.58
2:B:376:LYS:O	2:B:379:ILE:HG13	2.04	0.58
2:B:39:ASN:OD1	2:B:42:GLU:HB2	2.03	0.58
1:C:5:A:O2'	1:C:69:G:N2	2.35	0.58
2:A:110:ALA:O	2:A:127:PHE:CE1	2.57	0.58
2:A:131:ARG:HH11	2:A:131:ARG:HB3	1.68	0.58
2:B:268:LEU:HD12	2:B:268:LEU:C	2.23	0.58
2:B:7:LYS:CE	2:B:117:LEU:H	2.17	0.58
2:B:173:LYS:O	2:B:177:GLN:CG	2.51	0.58
2:B:230:LYS:O	2:B:234:LYS:HB2	2.03	0.58
2:B:138:ILE:HB	2:B:167:LEU:HD23	1.84	0.58
2:A:122:THR:HG22	2:A:124:ILE:HD12	1.86	0.58
2:A:199:ALA:O	2:A:202:GLU:HB2	2.03	0.58
2:B:227:TRP:CE3	2:B:232:LEU:HD12	2.38	0.58
1:D:5:A:O2'	1:D:69:G:N2	2.37	0.58
2:A:19:VAL:HG22	2:A:23:ILE:CD1	2.34	0.57
2:B:164:ASN:N	2:B:204:ARG:HH21	2.01	0.57
2:A:67:LYS:HE3	2:A:69:GLY:O	2.03	0.57
2:B:170:SER:HA	2:B:173:LYS:CE	2.34	0.57
2:B:377:ARG:HD2	2:B:378:GLU:N	2.18	0.57
1:D:58:A:N1	1:D:60:U:O4	2.38	0.57
2:A:153:ILE:HD12	2:A:184:LEU:CD2	2.34	0.57
2:B:377:ARG:O	2:B:381:ASN:CG	2.42	0.57
2:B:379:ILE:O	2:B:383:ILE:HG13	2.04	0.57
2:B:316:LEU:HG	2:B:341:TYR:CZ	2.39	0.57
2:B:66:LEU:HG	2:B:73:LEU:HD21	1.85	0.57
2:A:15:ILE:HD11	2:A:113:ILE:CG1	2.33	0.57
2:A:214:LYS:HE3	2:A:215:TYR:HH	1.69	0.57
1:D:73:A:C2'	1:D:74:C:H5'	2.35	0.57
2:A:230:LYS:O	2:A:234:LYS:HB2	2.03	0.57
2:B:298:GLY:O	2:B:302:GLU:HG3	2.05	0.57
2:B:310:ASN:ND2	2:B:379:ILE:HG22	2.20	0.57
2:B:315:ARG:O	2:B:319:PRO:HD3	2.05	0.57
2:A:230:LYS:HE2	2:A:234:LYS:CE	2.34	0.57
2:A:19:VAL:C	2:A:23:ILE:HD12	2.25	0.57
1:D:75:C:N4	2:B:191:ARG:HH22	1.89	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:63:G:H2'	1:D:64:C:O4'	2.05	0.57
1:D:66:C:N4	1:D:67:C:N4	2.52	0.57
2:A:175:LEU:O	2:A:179:VAL:HG23	2.05	0.57
2:A:261:LEU:HD11	2:A:265:ILE:HD11	1.87	0.57
2:B:381:ASN:O	2:B:385:LEU:CG	2.52	0.57
2:B:59:PRO:O	2:B:60:GLU:HB2	2.05	0.57
2:A:239:ARG:CA	2:A:260:TYR:OH	2.52	0.56
2:A:81:GLU:O	2:A:82:THR:C	2.43	0.56
2:B:151:VAL:HG22	2:B:192:LEU:HD23	1.87	0.56
2:B:268:LEU:HD12	2:B:269:ASP:N	2.20	0.56
2:A:79:ARG:CZ	2:A:103:ARG:HH12	2.18	0.56
2:A:20:VAL:HG13	2:A:113:ILE:HD11	1.86	0.56
2:B:66:LEU:HG	2:B:73:LEU:CD2	2.34	0.56
1:C:58:A:N1	1:C:60:U:O4	2.38	0.56
2:B:126:TYR:HB2	2:B:127:PHE:CE2	2.40	0.56
2:B:248:GLU:C	2:B:250:SER:H	2.08	0.56
2:B:339:LYS:CD	4:B:1534:HOH:O	2.52	0.56
2:A:318:LYS:HG2	4:A:531:HOH:O	2.05	0.56
2:A:184:LEU:HB2	2:A:220:GLU:OE1	2.05	0.56
2:B:253:ARG:NH1	2:B:256:TYR:CZ	2.74	0.56
2:B:334:LEU:N	2:B:334:LEU:HD23	2.07	0.56
2:A:100:ASP:O	2:A:103:ARG:HG3	2.06	0.56
2:A:263:ILE:O	2:A:266:SER:HB3	2.04	0.56
2:B:67:LYS:C	2:B:67:LYS:HD3	2.25	0.56
2:B:7:LYS:NZ	2:B:117:LEU:N	2.47	0.56
2:B:155:ARG:HG2	4:B:1504:HOH:O	2.05	0.56
2:B:16:VAL:HG11	2:B:35:VAL:CG2	2.35	0.56
2:B:312:GLU:CD	2:B:344:LYS:HE3	2.26	0.56
2:A:225:PHE:HE2	2:A:227:TRP:CD1	2.23	0.56
2:B:274:LYS:HG3	2:B:290:TYR:CE2	2.40	0.56
2:A:149:ASP:CG	2:A:151:VAL:HG12	2.27	0.56
2:A:214:LYS:HE3	2:A:215:TYR:CE2	2.41	0.56
2:A:20:VAL:O	2:A:24:LEU:HD22	2.05	0.56
2:B:146:PHE:CE2	2:B:153:ILE:HA	2.40	0.56
2:A:341:TYR:C	2:A:341:TYR:CD1	2.79	0.55
2:B:382:LYS:HA	2:B:385:LEU:HD12	1.87	0.55
2:A:144:VAL:HG12	2:A:144:VAL:O	2.07	0.55
1:D:56:C:H2'	1:D:57:G:O4'	2.06	0.55
1:D:61:C:H2'	1:D:62:C:C6	2.41	0.55
2:B:231:VAL:O	2:B:235:LEU:HG	2.05	0.55
2:B:285:TRP:HE1	2:B:323:SER:CB	2.14	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:335:LYS:HZ3	2:B:339:LYS:HZ2	1.55	0.55
2:A:244:TRP:HA	2:A:247:LEU:HG	1.88	0.55
2:B:20:VAL:O	2:B:24:LEU:HD22	2.06	0.55
2:B:81:GLU:O	2:B:82:THR:C	2.45	0.55
2:A:214:LYS:HG2	2:A:215:TYR:CE2	2.41	0.55
2:A:316:LEU:HD23	2:A:316:LEU:C	2.27	0.55
2:A:248:GLU:C	2:A:250:SER:H	2.10	0.55
2:B:316:LEU:O	2:B:319:PRO:HD2	2.05	0.55
1:C:63:G:H2'	1:C:64:C:O4'	2.06	0.55
2:A:316:LEU:HG	2:A:341:TYR:OH	2.07	0.55
2:B:7:LYS:HG3	2:B:117:LEU:HD12	1.87	0.54
2:B:274:LYS:CA	2:B:277:LEU:HD13	2.28	0.54
2:B:382:LYS:HA	2:B:385:LEU:HG	1.88	0.54
2:B:94:PRO:O	2:B:95:ALA:HB3	2.07	0.54
2:A:253:ARG:HB3	2:A:253:ARG:HH11	1.64	0.54
2:A:285:TRP:CB	2:A:321:HIS:CD2	2.91	0.54
2:A:61:PHE:N	2:A:61:PHE:HD1	2.05	0.54
2:A:94:PRO:O	2:A:95:ALA:HB3	2.07	0.54
2:B:21:ARG:NH2	2:B:162:ARG:NH2	2.55	0.54
2:B:375:LEU:C	2:B:377:ARG:H	2.10	0.54
2:A:316:LEU:CG	2:A:341:TYR:OH	2.55	0.54
2:A:9:MET:O	2:A:11:LEU:HG	2.06	0.54
2:B:261:LEU:O	2:B:265:ILE:HG12	2.06	0.54
2:B:7:LYS:HZ2	2:B:116:ASN:HA	1.72	0.54
2:A:59:PRO:C	2:A:61:PHE:H	2.11	0.54
2:B:341:TYR:CE2	4:B:1511:HOH:O	2.54	0.54
2:A:122:THR:HG22	2:A:124:ILE:CD1	2.37	0.54
2:A:14:TYR:N	2:A:14:TYR:CD1	2.76	0.54
2:A:205:PHE:CZ	2:A:209:LEU:HD11	2.42	0.54
2:A:261:LEU:CD1	2:A:265:ILE:HD11	2.38	0.54
2:A:41:ILE:HD11	2:A:62:GLY:HA2	1.89	0.54
2:B:170:SER:HA	2:B:173:LYS:HE2	1.90	0.54
2:A:197:LYS:HE2	2:A:280:MET:HA	1.89	0.54
2:A:296:LYS:HD3	2:A:299:SER:HB2	1.88	0.54
2:B:328:LEU:HB2	2:B:338:ILE:CD1	2.38	0.54
2:A:107:THR:HB	2:A:129:GLY:HA2	1.89	0.54
2:A:299:SER:O	2:A:303:GLU:HG3	2.08	0.54
1:D:73:A:H4'	2:B:191:ARG:HA	1.90	0.54
2:A:153:ILE:HB	2:A:154:LEU:HD22	1.90	0.54
2:B:181:LEU:HG	2:B:183:LEU:HD11	1.89	0.54
2:B:223:GLU:CD	2:B:270:TYR:HB2	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:79:ARG:HH12	2:B:81:GLU:C	2.11	0.54
1:C:66:C:N4	1:C:67:C:N4	2.56	0.54
2:A:296:LYS:O	2:A:300:LEU:HB2	2.08	0.54
2:B:7:LYS:CE	2:B:117:LEU:N	2.71	0.54
2:A:298:GLY:O	2:A:302:GLU:OE1	2.26	0.53
2:B:15:ILE:HD11	2:B:20:VAL:HG22	1.90	0.53
2:A:268:LEU:HD22	2:A:272:ARG:CA	2.36	0.53
2:B:245:HIS:NE2	2:B:249:PHE:HD2	2.06	0.53
2:B:310:ASN:ND2	2:B:383:ILE:HD11	2.24	0.53
2:A:162:ARG:HD2	2:A:202:GLU:OE2	2.07	0.53
2:A:138:ILE:HB	2:A:167:LEU:HD23	1.91	0.53
2:A:322:THR:HG22	2:A:326:LEU:CD1	2.39	0.53
2:B:240:LYS:HA	2:B:240:LYS:HE2	1.90	0.53
2:B:349:LYS:O	2:B:350:LEU:HD23	2.08	0.53
2:B:310:ASN:OD1	2:B:383:ILE:HD13	2.07	0.53
2:B:48:ALA:HB1	2:B:53:VAL:O	2.08	0.53
2:A:131:ARG:NH1	2:A:131:ARG:HB3	2.22	0.53
2:A:222:ILE:HG21	2:A:225:PHE:HB2	1.89	0.53
2:B:344:LYS:HZ3	2:B:345:LEU:N	2.05	0.53
3:A:500:APC:H3'	3:A:500:APC:O1B	2.09	0.53
2:B:101:LEU:O	2:B:104:ARG:HG2	2.08	0.53
2:A:338:ILE:HD12	2:A:338:ILE:N	2.23	0.53
1:C:61:C:H2'	1:C:62:C:C6	2.43	0.53
2:A:15:ILE:HD11	2:A:113:ILE:HD12	1.90	0.53
2:A:177:GLN:O	2:A:181:LEU:HB2	2.09	0.53
2:A:187:ALA:HB3	2:A:192:LEU:HD11	1.91	0.53
2:A:5:ILE:HA	2:A:8:GLU:HG3	1.91	0.53
2:B:11:LEU:CD2	2:B:12:ARG:H	2.19	0.53
2:B:239:ARG:O	2:B:243:ASP:CG	2.48	0.53
2:B:326:LEU:HD13	2:B:329:MET:HE1	1.91	0.53
2:B:377:ARG:HB2	2:B:381:ASN:HD21	1.73	0.53
2:A:125:ASP:OD2	2:A:129:GLY:N	2.42	0.53
2:A:280:MET:O	2:A:282:ALA:N	2.34	0.52
2:B:268:LEU:HD22	2:B:272:ARG:CB	2.39	0.52
1:D:61:C:C4'	2:B:320:LEU:HD22	2.38	0.52
2:B:375:LEU:O	2:B:377:ARG:HD2	2.09	0.52
2:A:157:LEU:HD11	2:A:175:LEU:HD11	1.91	0.52
2:B:73:LEU:HD23	2:B:73:LEU:H	1.73	0.52
2:A:275:HIS:HA	2:A:278:GLU:HG3	1.91	0.52
2:A:344:LYS:HG2	2:A:345:LEU:HD12	1.91	0.52
2:A:343:GLU:C	2:A:347:LYS:HZ2	2.13	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:ARG:HA	2:B:208:ILE:CD1	2.39	0.52
2:B:343:GLU:HA	2:B:346:ARG:CD	2.34	0.52
1:C:56:C:H2'	1:C:57:G:O4'	2.09	0.52
1:D:74:C:O5'	1:D:74:C:C6	2.62	0.52
2:A:216:ARG:HH11	2:A:216:ARG:HB3	1.75	0.52
2:A:329:MET:HE1	2:A:335:LYS:O	2.08	0.52
2:B:183:LEU:HD12	2:B:183:LEU:N	2.25	0.52
2:B:292:PHE:CZ	2:B:296:LYS:HB2	2.44	0.52
2:A:46:GLU:CD	2:A:49:ARG:NH2	2.63	0.52
2:B:125:ASP:OD2	2:B:131:ARG:NH2	2.43	0.52
2:B:242:VAL:HG13	2:B:256:TYR:CE1	2.44	0.52
2:B:68:ILE:HD12	2:B:68:ILE:N	2.24	0.52
2:A:329:MET:SD	2:A:338:ILE:HB	2.49	0.52
3:B:1500:APC:H3'	3:B:1500:APC:H3A1	1.92	0.52
2:B:232:LEU:O	2:B:235:LEU:HB2	2.08	0.52
2:B:335:LYS:CG	4:B:1534:HOH:O	2.58	0.52
2:B:59:PRO:C	2:B:61:PHE:H	2.14	0.52
2:A:34:PHE:HD1	2:A:74:GLU:O	1.93	0.52
2:B:199:ALA:O	2:B:202:GLU:HG2	2.09	0.52
2:A:285:TRP:HB3	2:A:321:HIS:CE1	2.45	0.52
2:B:263:ILE:O	2:B:266:SER:OG	2.17	0.52
2:B:375:LEU:HA	2:B:377:ARG:CZ	2.40	0.52
2:B:80:ARG:HA	2:B:103:ARG:HD2	1.91	0.52
2:B:81:GLU:H	2:B:103:ARG:CZ	2.23	0.51
2:A:155:ARG:NH1	4:A:501:HOH:O	2.31	0.51
2:B:310:ASN:HD22	2:B:379:ILE:CG2	2.22	0.51
2:B:304:LEU:HD13	2:B:334:LEU:CD1	2.40	0.51
2:B:336:GLU:HA	2:B:339:LYS:HB2	1.90	0.51
2:A:150:PRO:HG2	2:A:187:ALA:HB2	1.91	0.51
2:A:303:GLU:HA	2:A:306:LYS:HE3	1.91	0.51
2:A:5:ILE:HG21	2:A:43:LEU:CD1	2.40	0.51
2:A:228:ASN:HD21	2:A:230:LYS:HB3	1.76	0.51
2:A:319:PRO:C	2:A:321:HIS:N	2.63	0.51
2:B:162:ARG:HG3	2:B:163:LEU:HD23	1.93	0.51
2:B:7:LYS:HE2	2:B:117:LEU:HB2	1.93	0.51
2:B:187:ALA:HB3	2:B:192:LEU:HD11	1.93	0.51
2:B:136:LYS:HA	2:B:165:PHE:CE2	2.46	0.51
1:C:49:G:O2'	1:C:50:G:H5'	2.11	0.51
1:C:54:U:C2'	1:C:55:U:H5''	2.41	0.51
2:A:79:ARG:NH1	2:A:103:ARG:NH1	2.59	0.51
1:D:54:U:C2'	1:D:55:U:H5''	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:GLU:O	2:B:382:LYS:HG3	2.10	0.51
2:A:294:LYS:HB2	2:A:295:PHE:CD2	2.46	0.51
2:B:100:ASP:O	2:B:103:ARG:HG3	2.11	0.51
2:B:304:LEU:HD13	2:B:334:LEU:HD12	1.92	0.51
2:A:4:GLN:NE2	4:A:502:HOH:O	2.44	0.50
2:B:181:LEU:HB3	2:B:183:LEU:HD13	1.93	0.50
2:A:336:GLU:O	2:A:340:LEU:HG	2.12	0.50
2:B:175:LEU:O	2:B:179:VAL:HG23	2.12	0.50
2:B:326:LEU:N	2:B:326:LEU:CD2	2.74	0.50
2:B:144:VAL:HG12	2:B:144:VAL:O	2.10	0.50
2:A:131:ARG:HH22	2:A:139:ARG:NH1	2.03	0.50
2:A:268:LEU:HD13	2:A:272:ARG:CA	2.42	0.50
2:B:151:VAL:HG21	2:B:191:ARG:HB3	1.93	0.50
2:B:344:LYS:HZ3	2:B:345:LEU:HG	1.75	0.50
2:A:304:LEU:CD2	2:A:337:LYS:HD3	2.41	0.50
2:A:102:ILE:HG12	2:A:102:ILE:O	2.11	0.50
2:A:294:LYS:NZ	2:A:294:LYS:CB	2.74	0.50
1:D:74:C:OP2	1:D:74:C:C5	2.65	0.50
2:A:301:LYS:HA	2:A:334:LEU:HD21	1.93	0.50
2:A:344:LYS:HG2	2:A:345:LEU:N	2.26	0.50
2:B:244:TRP:CE2	2:B:248:GLU:HG3	2.46	0.50
2:B:197:LYS:HE2	2:B:281:SER:H	1.77	0.50
2:A:142:HIS:HB2	2:A:143:PRO:CD	2.42	0.50
2:A:235:LEU:HD22	2:A:260:TYR:HD2	1.77	0.50
2:B:253:ARG:NH2	2:B:256:TYR:CE1	2.80	0.50
2:B:319:PRO:C	2:B:321:HIS:N	2.65	0.50
2:A:292:PHE:CZ	2:A:296:LYS:HB2	2.47	0.49
2:B:193:ILE:HG22	2:B:194:ASN:H	1.77	0.49
2:B:292:PHE:HZ	2:B:300:LEU:HD22	1.78	0.49
1:D:5:A:C6	1:D:6:G:C6	3.00	0.49
2:A:294:LYS:HZ2	2:A:294:LYS:HB2	1.77	0.49
2:A:34:PHE:N	2:A:34:PHE:CD1	2.80	0.49
2:B:322:THR:CG2	2:B:326:LEU:HD21	2.36	0.49
2:A:66:LEU:HD23	2:A:66:LEU:N	2.28	0.49
2:B:316:LEU:HG	2:B:341:TYR:CE1	2.47	0.49
2:B:67:LYS:C	2:B:67:LYS:CD	2.80	0.49
2:B:127:PHE:N	2:B:127:PHE:CD2	2.76	0.49
2:B:377:ARG:C	2:B:381:ASN:ND2	2.65	0.49
2:B:66:LEU:CG	2:B:73:LEU:HD21	2.43	0.49
2:A:209:LEU:HA	2:A:212:TYR:CD2	2.44	0.49
2:A:300:LEU:O	2:A:315:ARG:NH2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:191:ARG:HB3	2:B:191:ARG:HH11	1.78	0.49
2:A:179:VAL:HG13	2:A:184:LEU:HD12	1.95	0.49
2:B:238:LEU:HD11	2:B:259:LEU:HD22	1.94	0.49
2:B:280:MET:SD	4:B:1530:HOH:O	2.60	0.49
2:B:310:ASN:OD1	2:B:383:ILE:CD1	2.60	0.49
1:C:5:A:N3	1:C:69:G:N1	2.61	0.49
1:D:66:C:H2'	1:D:67:C:C6	2.48	0.49
2:B:384:LYS:HE3	2:B:385:LEU:HD21	1.94	0.49
2:A:292:PHE:CE2	2:A:300:LEU:HD22	2.47	0.49
2:A:318:LYS:N	2:A:319:PRO:CD	2.76	0.49
2:B:223:GLU:CG	2:B:224:GLY:N	2.71	0.49
2:B:273:GLY:O	2:B:277:LEU:CD1	2.60	0.49
2:A:304:LEU:C	2:A:304:LEU:HD23	2.30	0.48
2:A:58:PHE:O	2:A:61:PHE:HB2	2.13	0.48
2:B:377:ARG:HB2	2:B:381:ASN:OD1	2.12	0.48
1:C:5:A:C6	1:C:6:G:C6	3.01	0.48
2:B:311:TYR:CE2	2:B:314:TYR:HB3	2.48	0.48
2:B:375:LEU:C	2:B:377:ARG:N	2.65	0.48
1:D:5:A:N3	1:D:69:G:N1	2.61	0.48
2:B:199:ALA:HA	2:B:202:GLU:CG	2.44	0.48
2:B:253:ARG:CZ	2:B:256:TYR:CZ	2.95	0.48
2:A:184:LEU:HB2	2:A:220:GLU:CD	2.34	0.48
2:A:301:LYS:HD3	2:A:331:GLU:CD	2.34	0.48
2:B:7:LYS:NZ	2:B:116:ASN:HA	2.29	0.48
2:B:255:ASP:HB3	2:B:258:TRP:CD1	2.49	0.48
2:B:344:LYS:CE	2:B:345:LEU:HG	2.43	0.48
2:A:285:TRP:HB2	2:A:321:HIS:ND1	2.29	0.48
2:B:211:LEU:HD21	4:B:1537:HOH:O	2.13	0.48
2:B:231:VAL:HG13	2:B:263:ILE:HG22	1.94	0.48
1:D:66:C:C4	1:D:67:C:N4	2.81	0.48
2:B:285:TRP:CB	2:B:321:HIS:CE1	2.97	0.48
2:B:73:LEU:CD2	2:B:73:LEU:H	2.27	0.48
2:A:322:THR:O	2:A:325:LEU:N	2.44	0.48
2:B:301:LYS:O	2:B:304:LEU:HB2	2.13	0.48
2:B:375:LEU:HD13	2:B:375:LEU:C	2.34	0.48
2:A:206:LEU:HD22	2:A:260:TYR:CE2	2.47	0.48
2:A:274:LYS:HA	2:A:277:LEU:HD13	1.96	0.48
1:D:61:C:H4'	2:B:320:LEU:HD22	1.95	0.48
1:D:49:G:O2'	1:D:50:G:H5'	2.13	0.48
2:A:19:VAL:CG2	2:A:29:VAL:HG21	2.32	0.48
2:A:68:ILE:O	2:A:71:LEU:HB2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1500:APC:H3A2	3:B:1500:APC:O2G	2.14	0.48
2:B:176:LYS:NZ	2:B:215:TYR:HE2	2.12	0.48
2:B:326:LEU:O	2:B:330:LEU:HD23	2.14	0.48
2:B:107:THR:HB	2:B:129:GLY:HA2	1.95	0.47
2:B:316:LEU:HD11	2:B:345:LEU:HD11	1.96	0.47
2:A:345:LEU:HD23	2:A:349:LYS:HZ3	1.78	0.47
2:B:68:ILE:O	2:B:71:LEU:HB2	2.14	0.47
1:C:66:C:H2'	1:C:67:C:C6	2.48	0.47
2:B:267:ASN:O	2:B:268:LEU:O	2.32	0.47
2:B:65:HIS:NE2	2:B:74:GLU:HG3	2.29	0.47
1:D:68:U:O5'	1:D:68:U:H6	1.97	0.47
2:A:12:ARG:HB3	2:A:14:TYR:OH	2.14	0.47
2:A:157:LEU:HD13	2:A:157:LEU:N	2.27	0.47
2:A:238:LEU:HA	2:A:330:LEU:HD21	1.95	0.47
2:A:93:GLU:HB3	2:A:94:PRO:CD	2.43	0.47
2:B:336:GLU:N	4:B:1534:HOH:O	2.46	0.47
2:B:335:LYS:NZ	2:B:339:LYS:HZ2	2.12	0.47
2:A:15:ILE:CG1	2:A:113:ILE:HB	2.44	0.47
2:A:154:LEU:HB2	2:A:195:GLU:HG2	1.96	0.47
2:A:21:ARG:NH1	2:A:109:ASN:OD1	2.47	0.47
2:A:152:ARG:NE	3:A:500:APC:N1	2.58	0.47
2:B:184:LEU:CD1	2:B:217:VAL:HG13	2.43	0.47
1:C:6:G:C6	1:C:7:G:N7	2.83	0.47
2:B:286:VAL:C	2:B:288:GLU:N	2.68	0.47
2:A:20:VAL:O	2:A:24:LEU:CD2	2.62	0.47
2:B:11:LEU:CD2	2:B:36:VAL:HG12	2.45	0.47
2:B:152:ARG:HA	2:B:155:ARG:HB2	1.96	0.47
2:B:155:ARG:CG	4:B:1504:HOH:O	2.61	0.47
2:B:154:LEU:HB2	2:B:195:GLU:HG2	1.96	0.47
2:B:25:LEU:HD21	2:B:133:LEU:HD11	1.97	0.47
2:B:376:LYS:HB3	2:B:379:ILE:HD12	1.95	0.47
2:A:183:LEU:CA	2:A:186:GLU:HG2	2.43	0.47
2:B:377:ARG:O	2:B:378:GLU:C	2.52	0.47
1:C:5:A:C2	1:C:69:G:N1	2.83	0.47
1:D:50:G:C2	1:D:51:C:N3	2.83	0.47
2:A:286:VAL:C	2:A:288:GLU:N	2.68	0.47
2:B:102:ILE:HG13	2:B:102:ILE:O	2.15	0.47
2:B:191:ARG:HD2	4:B:1522:HOH:O	2.13	0.47
2:B:316:LEU:O	2:B:316:LEU:CD2	2.63	0.47
2:B:14:TYR:CD1	2:B:14:TYR:N	2.83	0.47
2:B:245:HIS:HE2	2:B:249:PHE:HD2	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:381:ASN:HA	2:B:384:LYS:HE2	1.97	0.47
2:B:381:ASN:O	2:B:385:LEU:CD2	2.63	0.46
2:B:381:ASN:O	2:B:385:LEU:HD21	2.15	0.46
2:B:382:LYS:HA	2:B:385:LEU:CG	2.44	0.46
1:C:68:U:O5'	1:C:68:U:H6	1.98	0.46
2:B:146:PHE:HE2	2:B:153:ILE:HA	1.79	0.46
1:C:66:C:C4	1:C:67:C:N4	2.84	0.46
2:A:15:ILE:HG13	2:A:113:ILE:O	2.16	0.46
2:A:267:ASN:O	2:A:268:LEU:O	2.34	0.46
2:B:218:LEU:HD12	2:B:218:LEU:HA	1.75	0.46
2:B:79:ARG:NH1	2:B:82:THR:N	2.63	0.46
2:A:157:LEU:H	2:A:157:LEU:HD13	1.81	0.46
2:A:205:PHE:CD2	2:A:209:LEU:HD21	2.49	0.46
2:A:318:LYS:CE	4:A:531:HOH:O	2.59	0.46
2:A:319:PRO:O	2:A:321:HIS:N	2.48	0.46
2:A:222:ILE:HG22	2:A:225:PHE:CB	2.39	0.46
2:B:125:ASP:C	2:B:125:ASP:OD1	2.54	0.46
2:B:12:ARG:HG3	4:B:1538:HOH:O	2.15	0.46
2:B:238:LEU:HA	2:B:330:LEU:HD11	1.96	0.46
2:A:155:ARG:NH2	3:A:500:APC:H2'	2.31	0.46
1:C:50:G:C2	1:C:51:C:N3	2.83	0.46
2:A:142:HIS:HB2	2:A:143:PRO:HD2	1.98	0.46
2:A:323:SER:O	2:A:326:LEU:HB2	2.16	0.46
2:B:199:ALA:CA	2:B:202:GLU:HG2	2.44	0.46
2:B:295:PHE:N	2:B:295:PHE:CD1	2.84	0.46
2:B:300:LEU:C	2:B:304:LEU:HD12	2.36	0.46
1:D:2:G:H5'	2:B:201:ARG:HH21	1.81	0.46
2:A:225:PHE:HE2	2:A:227:TRP:NE1	2.14	0.46
2:B:269:ASP:CG	2:B:270:TYR:H	2.19	0.46
2:B:303:GLU:HA	2:B:306:LYS:HZ2	1.79	0.46
1:D:61:C:H4'	2:B:320:LEU:HD13	1.97	0.46
2:B:326:LEU:CD1	2:B:329:MET:HE1	2.46	0.46
2:A:15:ILE:H	2:A:15:ILE:HG13	1.49	0.46
2:A:15:ILE:HD11	2:A:113:ILE:CD1	2.46	0.46
2:A:197:LYS:NZ	2:A:281:SER:H	2.13	0.46
2:B:335:LYS:HZ3	2:B:339:LYS:NZ	2.13	0.46
1:D:5:A:C2	1:D:69:G:N1	2.84	0.46
2:A:301:LYS:HE2	2:A:331:GLU:OE1	2.16	0.46
2:A:345:LEU:HA	2:A:348:VAL:CG2	2.44	0.46
2:A:46:GLU:OE1	2:A:49:ARG:NH2	2.49	0.45
2:B:322:THR:O	2:B:325:LEU:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:377:ARG:HB2	2:B:381:ASN:ND2	2.32	0.45
2:B:376:LYS:CD	2:B:379:ILE:HD11	2.39	0.45
2:B:389:LEU:C	2:B:389:LEU:HD23	2.37	0.45
2:A:214:LYS:HE3	2:A:215:TYR:OH	2.15	0.45
2:A:221:ILE:HD12	2:A:221:ILE:N	2.31	0.45
2:A:255:ASP:HB2	2:A:285:TRP:HZ2	1.81	0.45
2:B:105:ASP:OD2	2:B:155:ARG:NH2	2.48	0.45
2:B:67:LYS:CE	2:B:69:GLY:H	2.23	0.45
1:C:2:G:H2'	1:C:3:C:O4'	2.16	0.45
2:A:154:LEU:CD2	2:A:154:LEU:N	2.70	0.45
2:A:230:LYS:HE2	2:A:234:LYS:NZ	2.31	0.45
2:A:213:ARG:CG	2:A:227:TRP:CD2	3.00	0.45
2:A:54:ASN:H	2:A:54:ASN:HD22	1.59	0.45
2:B:181:LEU:HG	2:B:183:LEU:CD1	2.46	0.45
2:B:268:LEU:CD2	2:B:272:ARG:HA	2.35	0.45
2:B:3:GLY:O	2:B:7:LYS:NZ	2.35	0.45
2:B:158:ARG:HE	2:B:195:GLU:CD	2.20	0.45
2:B:70:LYS:N	2:B:70:LYS:HD2	2.30	0.45
1:D:73:A:H3'	1:D:74:C:C6	2.52	0.45
2:A:344:LYS:HA	2:A:347:LYS:HD3	1.98	0.45
2:B:216:ARG:N	2:B:216:ARG:HD2	2.31	0.45
2:B:304:LEU:HA	2:B:315:ARG:NH2	2.31	0.45
2:B:318:LYS:N	2:B:319:PRO:CD	2.80	0.45
2:B:322:THR:O	2:B:323:SER:C	2.54	0.45
1:D:58:A:C2	1:D:60:U:O4	2.70	0.45
1:D:6:G:C6	1:D:7:G:N7	2.85	0.45
2:A:210:GLU:OE2	2:A:213:ARG:NH2	2.49	0.45
2:A:231:VAL:HG13	2:A:263:ILE:HG22	1.98	0.45
2:A:341:TYR:C	2:A:341:TYR:HD1	2.20	0.45
2:A:67:LYS:HE2	2:A:67:LYS:HB3	1.83	0.45
2:B:153:ILE:O	2:B:157:LEU:HD22	2.17	0.45
2:B:218:LEU:HB3	2:B:225:PHE:CE2	2.52	0.45
2:B:277:LEU:HD22	2:B:290:TYR:CD2	2.51	0.45
2:B:292:PHE:CZ	2:B:296:LYS:CB	3.00	0.45
2:B:248:GLU:CD	2:B:248:GLU:H	2.18	0.45
2:A:142:HIS:HD2	4:A:530:HOH:O	2.00	0.45
2:A:304:LEU:HD23	2:A:337:LYS:NZ	2.32	0.45
2:B:155:ARG:HH22	3:B:1500:APC:C3A	2.30	0.45
2:B:183:LEU:CD1	2:B:183:LEU:H	2.30	0.45
2:B:20:VAL:HG12	2:B:24:LEU:CD2	2.48	0.45
2:B:272:ARG:HG2	2:B:272:ARG:NH1	2.22	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:167:LEU:HB2	2:A:172:GLU:HG2	1.99	0.44
2:B:154:LEU:HD21	2:B:217:VAL:HG11	1.99	0.44
2:B:268:LEU:HD13	2:B:272:ARG:CA	2.46	0.44
2:A:131:ARG:NH2	2:A:139:ARG:NH1	2.64	0.44
2:A:316:LEU:HD12	2:A:341:TYR:OH	2.17	0.44
2:B:341:TYR:HE2	4:B:1511:HOH:O	1.95	0.44
1:D:2:G:H2'	1:D:3:C:O4'	2.18	0.44
2:A:106:PHE:N	2:A:106:PHE:CD1	2.84	0.44
2:A:297:LEU:O	2:A:301:LYS:CD	2.60	0.44
2:A:322:THR:O	2:A:324:VAL:N	2.51	0.44
2:A:341:TYR:HD1	2:A:342:LEU:N	2.15	0.44
2:B:223:GLU:OE1	2:B:270:TYR:CD1	2.69	0.44
2:B:289:THR:HG23	2:B:324:VAL:HG22	1.98	0.44
2:B:319:PRO:O	2:B:321:HIS:N	2.50	0.44
1:C:58:A:C2	1:C:60:U:O4	2.70	0.44
2:A:223:GLU:O	2:A:223:GLU:OE2	2.36	0.44
2:A:304:LEU:HD23	2:A:337:LYS:HZ3	1.82	0.44
2:A:345:LEU:HB3	2:A:349:LYS:NZ	2.33	0.44
2:A:48:ALA:O	2:A:52:GLY:N	2.51	0.44
2:A:97:LEU:HG	2:A:98:LYS:N	2.32	0.44
2:B:163:LEU:C	2:B:204:ARG:NH2	2.70	0.44
2:B:8:GLU:C	2:B:9:MET:SD	2.96	0.44
1:D:73:A:H2'	1:D:74:C:C5'	2.47	0.44
2:A:2:VAL:HG11	2:A:115:VAL:HG21	2.00	0.44
2:A:322:THR:O	2:A:323:SER:C	2.55	0.44
1:C:55:U:OP1	2:A:349:LYS:HG2	2.18	0.44
2:B:80:ARG:NH2	2:B:99:GLU:OE1	2.51	0.44
2:A:206:LEU:HD11	2:A:235:LEU:HB3	2.00	0.44
2:A:304:LEU:CD2	2:A:337:LYS:NZ	2.80	0.44
2:B:11:LEU:HD22	2:B:36:VAL:CG1	2.48	0.44
2:B:328:LEU:C	2:B:330:LEU:N	2.71	0.44
1:C:55:U:OP1	2:A:349:LYS:CG	2.66	0.44
2:A:285:TRP:HB2	2:A:321:HIS:CE1	2.52	0.44
2:A:183:LEU:C	2:A:186:GLU:HG2	2.38	0.44
2:A:294:LYS:HB2	2:A:295:PHE:HD2	1.83	0.44
2:A:316:LEU:CD1	2:A:345:LEU:HD21	2.47	0.44
2:B:334:LEU:N	2:B:334:LEU:CD2	2.76	0.44
1:C:67:C:H2'	1:C:68:U:H5	1.78	0.44
2:A:20:VAL:HA	2:A:23:ILE:HD12	2.00	0.44
2:A:245:HIS:CE1	2:A:249:PHE:HB3	2.53	0.44
2:A:284:SER:O	2:A:288:GLU:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:67:LYS:C	2:A:68:ILE:HD12	2.38	0.44
2:B:245:HIS:ND1	2:B:245:HIS:C	2.71	0.44
2:B:318:LYS:C	2:B:320:LEU:H	2.21	0.44
2:B:330:LEU:N	2:B:330:LEU:HD22	2.33	0.44
1:D:54:U:H2'	1:D:55:U:H5''	2.00	0.44
2:A:183:LEU:CD2	2:A:186:GLU:HG3	2.44	0.43
2:A:303:GLU:HA	2:A:306:LYS:CE	2.47	0.43
2:B:323:SER:O	2:B:326:LEU:HB2	2.18	0.43
2:A:214:LYS:HE3	2:A:215:TYR:CZ	2.53	0.43
2:A:255:ASP:HB2	2:A:285:TRP:CZ2	2.53	0.43
2:A:292:PHE:CZ	2:A:318:LYS:HD2	2.54	0.43
2:A:349:LYS:C	2:A:351:PRO:HD3	2.38	0.43
2:A:79:ARG:CZ	2:A:103:ARG:NH1	2.82	0.43
2:B:376:LYS:HB2	2:B:380:MET:CE	2.48	0.43
2:A:105:ASP:HB3	2:A:106:PHE:H	1.40	0.43
2:B:345:LEU:HB2	4:B:1511:HOH:O	2.19	0.43
2:A:105:ASP:HB3	2:A:106:PHE:CD1	2.54	0.43
2:A:152:ARG:HA	2:A:155:ARG:HG3	2.01	0.43
2:A:158:ARG:CZ	2:A:198:LEU:HD22	2.48	0.43
2:A:231:VAL:O	2:A:235:LEU:HG	2.18	0.43
2:B:310:ASN:HD21	2:B:383:ILE:HD11	1.82	0.43
2:B:376:LYS:HB2	2:B:380:MET:HE1	2.00	0.43
2:A:217:VAL:O	2:A:221:ILE:HD13	2.18	0.43
2:A:22:ASP:HB3	2:A:27:LYS:HB3	2.01	0.43
2:A:325:LEU:HD23	2:A:326:LEU:HD12	1.99	0.43
2:A:343:GLU:CB	2:A:347:LYS:HZ2	2.21	0.43
2:B:142:HIS:NE2	2:B:144:VAL:HB	2.33	0.43
2:B:183:LEU:H	2:B:183:LEU:HD12	1.81	0.43
2:B:344:LYS:CD	2:B:345:LEU:N	2.78	0.43
2:A:206:LEU:O	2:A:209:LEU:HB2	2.18	0.43
2:A:211:LEU:HD23	2:A:214:LYS:HD3	1.99	0.43
2:A:200:LEU:HD12	2:A:261:LEU:HD22	2.00	0.43
2:A:288:GLU:C	2:A:290:TYR:N	2.72	0.43
2:B:13:ALA:C	2:B:14:TYR:CD1	2.91	0.43
1:D:61:C:O4'	2:B:320:LEU:HD22	2.17	0.43
2:A:323:SER:O	2:A:326:LEU:N	2.47	0.43
2:B:101:LEU:HD12	2:B:101:LEU:HA	1.80	0.43
2:B:219:GLU:OE1	2:B:227:TRP:HD1	2.02	0.43
2:B:261:LEU:CA	2:B:264:LEU:HD12	2.41	0.43
2:A:272:ARG:HH12	2:A:291:LYS:HE3	1.84	0.43
2:A:318:LYS:C	2:A:320:LEU:H	2.23	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:155:ARG:HH22	3:B:1500:APC:H3A1	1.84	0.43
2:B:225:PHE:CG	2:B:226:GLN:N	2.87	0.43
2:B:318:LYS:HA	2:B:318:LYS:HD3	1.71	0.43
2:A:184:LEU:HD22	2:A:221:ILE:HD11	2.01	0.43
2:A:213:ARG:HG3	2:A:227:TRP:CD2	2.54	0.43
2:A:329:MET:C	2:A:331:GLU:H	2.23	0.43
2:B:238:LEU:HD12	2:B:238:LEU:O	2.19	0.43
2:B:20:VAL:O	2:B:24:LEU:CD2	2.67	0.43
2:B:289:THR:HG23	2:B:324:VAL:CG2	2.49	0.43
2:B:301:LYS:CE	4:B:1536:HOH:O	2.67	0.43
2:B:301:LYS:HE3	4:B:1536:HOH:O	2.19	0.43
1:D:54:U:H2'	1:D:55:U:O4'	2.19	0.43
2:A:93:GLU:HB3	2:A:94:PRO:HD2	2.00	0.42
2:B:322:THR:O	2:B:324:VAL:N	2.52	0.42
2:B:325:LEU:O	2:B:325:LEU:HD23	2.18	0.42
2:A:123:LEU:C	2:A:124:ILE:HD12	2.40	0.42
2:A:280:MET:C	2:A:282:ALA:N	2.72	0.42
2:A:41:ILE:CB	2:A:45:LYS:HE3	2.49	0.42
2:B:303:GLU:C	2:B:315:ARG:HH22	2.22	0.42
2:B:48:ALA:CB	2:B:55:VAL:HG22	2.49	0.42
2:A:181:LEU:HD12	2:A:181:LEU:HA	1.79	0.42
2:B:164:ASN:N	2:B:204:ARG:NH2	2.68	0.42
2:B:295:PHE:N	2:B:295:PHE:HD1	2.17	0.42
2:B:335:LYS:CE	2:B:339:LYS:HE3	2.44	0.42
1:C:67:C:C4	1:C:68:U:O4	2.72	0.42
2:A:153:ILE:O	2:A:157:LEU:HD13	2.19	0.42
2:A:175:LEU:O	2:A:175:LEU:HD23	2.19	0.42
2:B:43:LEU:HD12	2:B:43:LEU:O	2.19	0.42
2:B:57:PRO:O	2:B:58:PHE:CD1	2.73	0.42
2:A:162:ARG:HB2	2:A:202:GLU:CD	2.39	0.42
2:A:303:GLU:C	2:A:315:ARG:NH2	2.73	0.42
2:A:298:GLY:O	2:A:302:GLU:HB2	2.20	0.42
2:B:131:ARG:HG3	2:B:131:ARG:HH11	1.82	0.42
2:B:205:PHE:O	2:B:208:ILE:HB	2.19	0.42
2:B:240:LYS:HA	2:B:240:LYS:CE	2.48	0.42
2:A:328:LEU:C	2:A:330:LEU:N	2.72	0.42
2:B:188:PRO:O	2:B:189:ARG:C	2.57	0.42
2:B:233:GLN:NE2	2:B:234:LYS:N	2.48	0.42
2:B:329:MET:C	2:B:331:GLU:H	2.23	0.42
2:A:97:LEU:HD12	2:A:101:LEU:HB2	2.02	0.42
2:A:162:ARG:HG3	2:A:162:ARG:NH1	2.30	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:320:LEU:HD23	2:A:320:LEU:HA	1.92	0.42
2:A:301:LYS:HD3	2:A:331:GLU:OE2	2.19	0.42
2:A:5:ILE:HD13	2:A:46:GLU:HG2	2.02	0.42
2:B:250:SER:HA	2:B:253:ARG:HD3	2.02	0.42
2:B:349:LYS:C	2:B:351:PRO:HD3	2.40	0.42
2:B:310:ASN:ND2	2:B:379:ILE:CG2	2.81	0.42
1:C:54:U:H2'	1:C:55:U:H5''	2.01	0.42
2:A:188:PRO:O	2:A:189:ARG:C	2.57	0.42
2:A:234:LYS:HA	2:A:234:LYS:HD3	1.90	0.42
2:A:297:LEU:C	2:A:297:LEU:HD23	2.40	0.42
2:A:46:GLU:OE2	2:A:49:ARG:NH2	2.51	0.42
3:A:500:APC:PB	3:A:500:APC:H5'1	2.60	0.42
2:B:12:ARG:NH2	2:B:116:ASN:HB2	2.34	0.42
2:A:13:ALA:N	2:A:116:ASN:HD21	2.07	0.42
2:A:225:PHE:CE2	2:A:227:TRP:CD1	3.07	0.42
2:A:229:GLU:OE1	2:A:232:LEU:HD23	2.20	0.42
2:B:327:LEU:N	2:B:327:LEU:HD23	2.35	0.42
2:B:151:VAL:HG22	2:B:192:LEU:CD2	2.48	0.41
2:B:274:LYS:HG3	2:B:290:TYR:HD2	1.80	0.41
1:D:66:C:N4	1:D:67:C:H41	2.18	0.41
2:A:274:LYS:CE	4:A:524:HOH:O	2.67	0.41
2:A:274:LYS:O	2:A:278:GLU:HG2	2.20	0.41
2:B:11:LEU:HD23	2:B:12:ARG:N	2.29	0.41
2:B:173:LYS:O	2:B:177:GLN:HG3	2.18	0.41
2:B:275:HIS:HA	2:B:278:GLU:CD	2.40	0.41
2:B:335:LYS:HZ1	2:B:339:LYS:HZ1	1.68	0.41
2:B:380:MET:HA	2:B:383:ILE:CG1	2.48	0.41
2:B:15:ILE:CD1	2:B:20:VAL:HG22	2.50	0.41
2:B:7:LYS:HE2	2:B:117:LEU:CB	2.50	0.41
1:D:56:C:N4	1:D:57:G:C6	2.89	0.41
2:A:16:VAL:HG23	2:A:112:ALA:HB2	2.02	0.41
2:A:17:GLY:O	2:A:18:GLY:C	2.58	0.41
2:A:341:TYR:CE1	2:A:345:LEU:HD22	2.54	0.41
2:B:7:LYS:HZ3	2:B:117:LEU:HG	1.81	0.41
2:B:16:VAL:HG11	2:B:35:VAL:HG21	2.02	0.41
2:B:341:TYR:O	2:B:344:LYS:HB3	2.20	0.41
2:B:16:VAL:HG21	2:B:35:VAL:HG23	2.02	0.41
2:B:66:LEU:HD12	2:B:68:ILE:HD11	2.00	0.41
2:A:236:TYR:O	2:A:239:ARG:HB3	2.20	0.41
2:A:319:PRO:C	2:A:321:HIS:H	2.24	0.41
2:B:173:LYS:HG2	2:B:174:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:253:ARG:CZ	2:B:256:TYR:CE1	3.03	0.41
2:A:20:VAL:HG12	2:A:24:LEU:CD2	2.51	0.41
2:A:268:LEU:HD22	2:A:272:ARG:CB	2.49	0.41
2:A:285:TRP:CD1	2:A:285:TRP:C	2.94	0.41
2:B:200:LEU:C	2:B:200:LEU:HD23	2.41	0.41
2:B:211:LEU:CD2	4:B:1537:HOH:O	2.68	0.41
2:A:259:LEU:HD12	2:A:259:LEU:HA	1.57	0.41
2:A:341:TYR:O	2:A:344:LYS:HB3	2.20	0.41
2:B:248:GLU:C	2:B:250:SER:N	2.74	0.41
2:B:336:GLU:HA	4:B:1534:HOH:O	2.20	0.41
2:B:48:ALA:O	2:B:52:GLY:N	2.54	0.41
2:A:15:ILE:CD1	2:A:113:ILE:HD12	2.50	0.41
2:A:184:LEU:HD13	2:A:221:ILE:CD1	2.51	0.41
2:A:309:GLU:HB3	2:A:310:ASN:H	1.71	0.41
2:A:292:PHE:HE1	2:A:318:LYS:HZ2	1.67	0.41
2:B:341:TYR:HD2	2:B:342:LEU:CA	2.31	0.41
2:A:61:PHE:H	2:A:61:PHE:HD1	1.69	0.41
2:B:233:GLN:HG3	2:B:233:GLN:H	1.70	0.41
2:A:294:LYS:H	2:A:294:LYS:HG3	1.57	0.41
2:B:16:VAL:HB	2:B:104:ARG:HH21	1.85	0.41
2:B:255:ASP:HB3	2:B:258:TRP:HD1	1.85	0.41
2:B:326:LEU:HA	2:B:329:MET:HE1	2.00	0.41
2:B:302:GLU:O	2:B:305:LYS:HG3	2.21	0.40
2:B:376:LYS:CB	2:B:380:MET:HE1	2.50	0.40
2:B:78:ALA:HA	2:B:100:ASP:OD2	2.21	0.40
2:B:292:PHE:CE1	2:B:318:LYS:HD2	2.55	0.40
2:B:34:PHE:CD1	2:B:75:PHE:CZ	3.09	0.40
2:A:184:LEU:CD1	2:A:217:VAL:HG13	2.51	0.40
2:B:17:GLY:O	2:B:18:GLY:C	2.60	0.40
2:B:176:LYS:HZ1	2:B:215:TYR:HE2	1.68	0.40
2:B:200:LEU:HD11	2:B:258:TRP:CE3	2.57	0.40
2:B:262:LEU:O	2:B:266:SER:N	2.54	0.40
2:B:304:LEU:HD22	4:B:1525:HOH:O	2.21	0.40
2:B:11:LEU:HD22	2:B:36:VAL:HG12	2.04	0.40
2:A:224:GLY:HA3	2:A:269:ASP:CB	2.48	0.40
2:B:254:ILE:HG22	2:B:256:TYR:HD2	1.84	0.40
2:B:280:MET:C	2:B:282:ALA:N	2.73	0.40
1:C:2:G:H8	1:C:2:G:O5'	2.03	0.40
1:C:65:C:N4	1:C:66:C:N4	2.69	0.40
1:D:58:A:C4	1:D:60:U:H5	2.39	0.40
1:D:5:A:C2	1:D:6:G:C5	3.10	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:286:VAL:C	2:A:288:GLU:H	2.24	0.40
2:A:325:LEU:CD2	2:A:326:LEU:HD12	2.51	0.40
2:B:209:LEU:HA	2:B:209:LEU:HD12	1.69	0.40
1:C:58:A:C4	1:C:60:U:H5	2.38	0.40
1:D:75:C:H3'	3:B:1500:APC:O4'	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	338/390 (87%)	274 (81%)	48 (14%)	16 (5%)	2	7
2	B	352/390 (90%)	285 (81%)	50 (14%)	17 (5%)	2	7
All	All	690/780 (88%)	559 (81%)	98 (14%)	33 (5%)	2	7

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	105	ASP
2	A	268	LEU
2	A	273	GLY
2	A	310	ASN
2	A	323	SER
2	A	332	GLU
2	B	105	ASP
2	B	268	LEU
2	B	273	GLY
2	B	310	ASN
2	B	323	SER
2	B	332	GLU
2	A	322	THR

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Mol	Chain	Res	Type
2	B	223	GLU
2	B	322	THR
2	A	18	GLY
2	A	93	GLU
2	A	254	ILE
2	B	249	PHE
2	B	254	ILE
2	B	309	GLU
2	A	188	PRO
2	A	249	PHE
2	A	309	GLU
2	A	320	LEU
2	B	18	GLY
2	B	93	GLU
2	B	188	PRO
2	B	320	LEU
2	A	94	PRO
2	B	17	GLY
2	B	94	PRO
2	A	17	GLY

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	303/343 (88%)	241 (80%)	62 (20%)	1	3
2	B	316/343 (92%)	251 (79%)	65 (21%)	1	3
All	All	619/686 (90%)	492 (80%)	127 (20%)	1	3

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	1	MET
2	A	4	GLN
2	A	14	TYR

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Mol	Chain	Res	Type
2	A	15	ILE
2	A	16	VAL
2	A	28	GLU
2	A	29	VAL
2	A	41	ILE
2	A	43	LEU
2	A	47	LEU
2	A	54	ASN
2	A	56	HIS
2	A	61	PHE
2	A	66	LEU
2	A	73	LEU
2	A	92	VAL
2	A	96	SER
2	A	97	LEU
2	A	103	ARG
2	A	105	ASP
2	A	115	VAL
2	A	118	GLU
2	A	127	PHE
2	A	132	ASP
2	A	135	ASP
2	A	145	SER
2	A	154	LEU
2	A	157	LEU
2	A	162	ARG
2	A	172	GLU
2	A	186	GLU
2	A	198	LEU
2	A	201	ARG
2	A	203	ASP
2	A	207	GLU
2	A	209	LEU
2	A	210	GLU
2	A	213	ARG
2	A	216	ARG
2	A	218	LEU
2	A	220	GLU
2	A	228	ASN
2	A	230	LYS
2	A	244	TRP
2	A	247	LEU

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Mol	Chain	Res	Type
2	A	249	PHE
2	A	251	GLU
2	A	252	GLU
2	A	253	ARG
2	A	259	LEU
2	A	267	ASN
2	A	269	ASP
2	A	270	TYR
2	A	294	LYS
2	A	295	PHE
2	A	305	LYS
2	A	306	LYS
2	A	312	GLU
2	A	314	TYR
2	A	325	LEU
2	A	331	GLU
2	A	341	TYR
2	B	4	GLN
2	B	11	LEU
2	B	14	TYR
2	B	24	LEU
2	B	29	VAL
2	B	45	LYS
2	B	49	ARG
2	B	56	HIS
2	B	59	PRO
2	B	60	GLU
2	B	61	PHE
2	B	63	THR
2	B	73	LEU
2	B	77	THR
2	B	94	PRO
2	B	101	LEU
2	B	103	ARG
2	B	106	PHE
2	B	119	ASP
2	B	125	ASP
2	B	126	TYR
2	B	127	PHE
2	B	143	PRO
2	B	157	LEU
2	B	162	ARG

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Mol	Chain	Res	Type
2	B	169	ARG
2	B	173	LYS
2	B	191	ARG
2	B	193	ILE
2	B	194	ASN
2	B	201	ARG
2	B	209	LEU
2	B	218	LEU
2	B	223	GLU
2	B	232	LEU
2	B	233	GLN
2	B	248	GLU
2	B	249	PHE
2	B	250	SER
2	B	252	GLU
2	B	253	ARG
2	B	255	ASP
2	B	261	LEU
2	B	268	LEU
2	B	279	GLU
2	B	280	MET
2	B	285	TRP
2	B	295	PHE
2	B	297	LEU
2	B	303	GLU
2	B	304	LEU
2	B	309	GLU
2	B	310	ASN
2	B	312	GLU
2	B	319	PRO
2	B	321	HIS
2	B	332	GLU
2	B	334	LEU
2	B	338	ILE
2	B	340	LEU
2	B	341	TYR
2	B	344	LYS
2	B	375	LEU
2	B	377	ARG
2	B	379	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	39	ASN
2	A	54	ASN
2	A	116	ASN
2	A	228	ASN
2	B	51	HIS
2	B	116	ASN
2	B	177	GLN
2	B	194	ASN
2	B	226	GLN
2	B	233	GLN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	29/75 (38%)	8 (27%)	0
1	D	32/75 (42%)	8 (25%)	0
All	All	61/150 (40%)	16 (26%)	0

All (16) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	5	A
1	C	55	U
1	C	56	C
1	C	57	G
1	C	58	A
1	C	61	C
1	C	62	C
1	C	68	U
1	D	5	A
1	D	55	U
1	D	56	C
1	D	57	G
1	D	58	A
1	D	61	C
1	D	62	C
1	D	68	U

There are no RNA pucker outliers to report.

## 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 carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

2 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
3	APC	B	1500	-	27,33,33	1.40	3 (11%)	31,52,52	1.74	5 (16%)
3	APC	A	500	-	27,33,33	1.75	5 (18%)	31,52,52	1.66	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	APC	B	1500	-	-	5/15/38/38	0/3/3/3
3	APC	A	500	-	-	7/15/38/38	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	APC	PA-O5'	4.92	1.64	1.57
3	B	1500	APC	C2-N3	4.47	1.39	1.32
3	A	500	APC	C2-N3	3.91	1.38	1.32
3	A	500	APC	PB-O3B	2.76	1.61	1.58
3	B	1500	APC	PA-O5'	2.46	1.61	1.57
3	A	500	APC	O4'-C4'	-2.44	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	500	APC	C2-N1	2.32	1.38	1.33
3	B	1500	APC	C2-N1	2.01	1.37	1.33

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500	APC	N3-C2-N1	-5.25	120.47	128.68
3	B	1500	APC	N3-C2-N1	-5.03	120.82	128.68
3	B	1500	APC	C4-C5-N7	-4.09	105.14	109.40
3	B	1500	APC	C5-C6-N6	4.03	126.47	120.35
3	A	500	APC	C4-C5-N7	-3.52	105.73	109.40
3	A	500	APC	C5-C6-N6	3.07	125.01	120.35
3	B	1500	APC	O2G-PG-O3B	2.37	112.57	104.64
3	A	500	APC	C3'-C2'-C1'	2.32	104.47	100.98
3	A	500	APC	O2'-C2'-C3'	2.25	119.08	111.82
3	B	1500	APC	N6-C6-N1	-2.15	114.11	118.57

There are no chirality outliers.

All (12) torsion outliers are listed below:

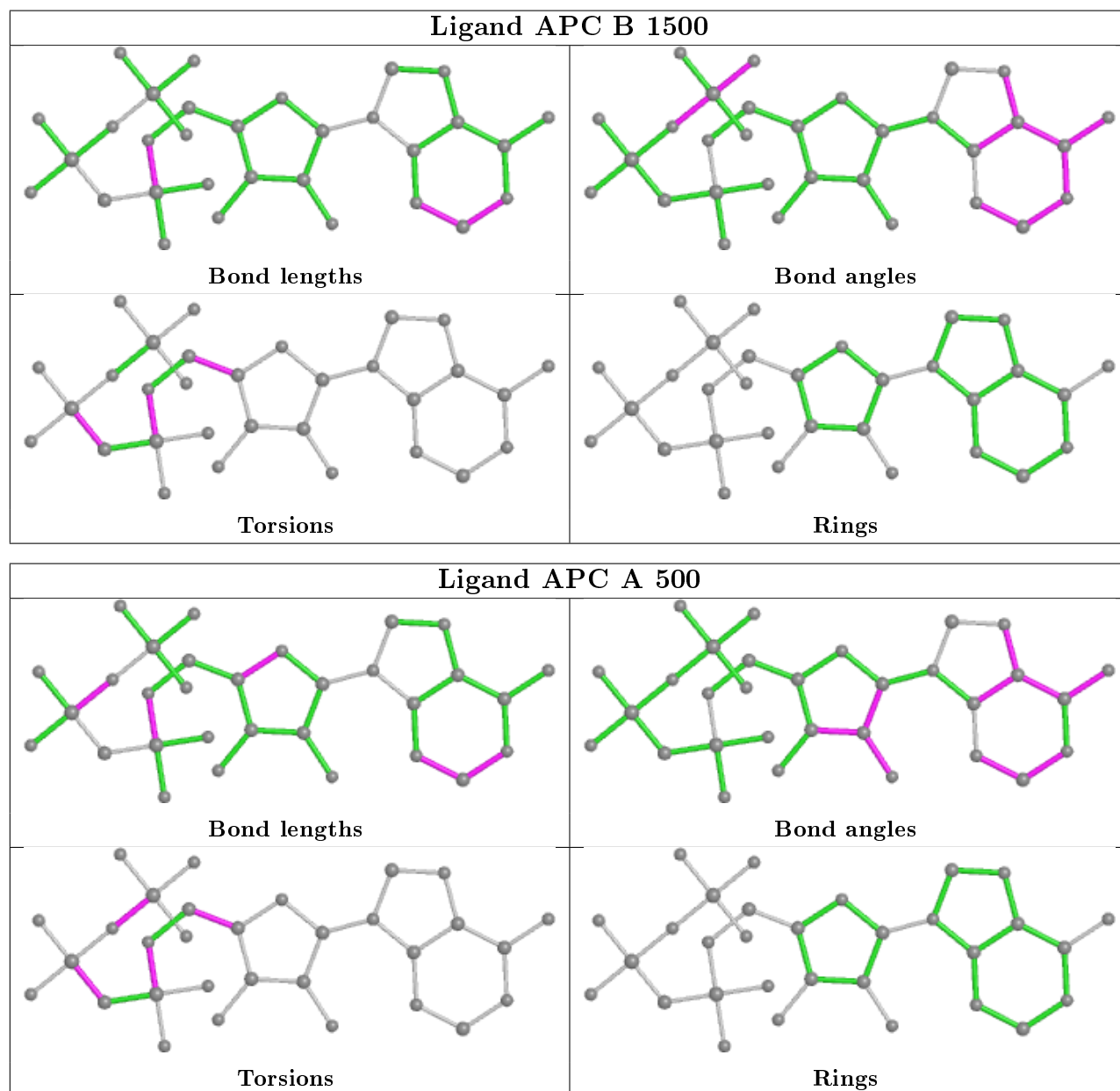
Mol	Chain	Res	Type	Atoms
3	B	1500	APC	PA-C3A-PB-O1B
3	B	1500	APC	PA-C3A-PB-O2B
3	A	500	APC	PB-O3B-PG-O2G
3	A	500	APC	PA-C3A-PB-O1B
3	A	500	APC	PA-C3A-PB-O2B
3	A	500	APC	PA-C3A-PB-O3B
3	A	500	APC	C5'-O5'-PA-C3A
3	A	500	APC	O4'-C4'-C5'-O5'
3	A	500	APC	C3'-C4'-C5'-O5'
3	B	1500	APC	C5'-O5'-PA-O1A
3	B	1500	APC	O4'-C4'-C5'-O5'
3	B	1500	APC	C5'-O5'-PA-O2A

There are no ring outliers.

2 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1500	APC	5	0
3	A	500	APC	5	0

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



## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	C	31/75 (41%)	-0.35	0 100 100	131, 142, 152, 153	0
1	D	34/75 (45%)	-0.40	0 100 100	122, 136, 148, 154	0
2	A	342/390 (87%)	0.07	11 (3%) 47 37	33, 65, 126, 143	0
2	B	358/390 (91%)	-0.00	9 (2%) 57 47	33, 63, 119, 132	0
All	All	765/930 (82%)	-0.00	20 (2%) 56 46	33, 68, 139, 154	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	351	PRO	6.9
2	B	92	VAL	4.5
2	A	348	VAL	4.3
2	B	314	TYR	3.2
2	A	330	LEU	3.0
2	B	321	HIS	3.0
2	A	342	LEU	3.0
2	B	317	LEU	2.9
2	B	389	LEU	2.7
2	A	320	LEU	2.6
2	A	317	LEU	2.6
2	B	269	ASP	2.4
2	B	300	LEU	2.4
2	A	63	THR	2.3
2	B	349	LYS	2.2
2	A	301	LYS	2.2
2	A	286	VAL	2.2
2	A	321	HIS	2.1
2	B	264	LEU	2.1
2	A	295	PHE	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

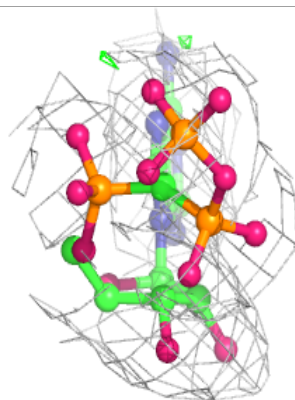
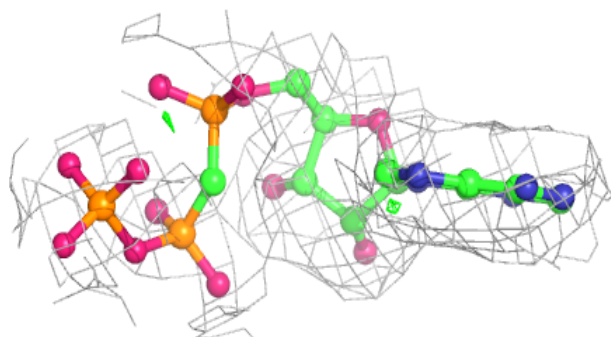
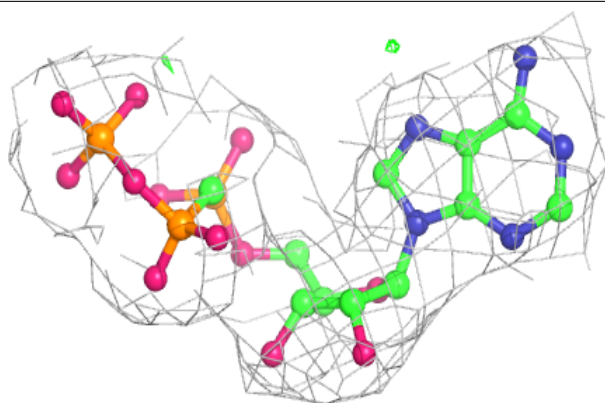
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	APC	B	1500	31/31	0.93	0.17	75,80,89,91	0
3	APC	A	500	31/31	0.93	0.15	65,71,84,84	0

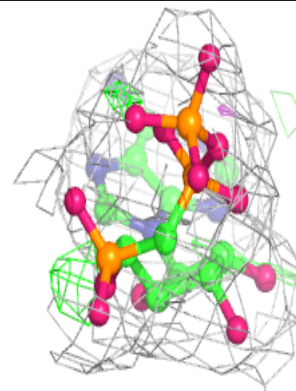
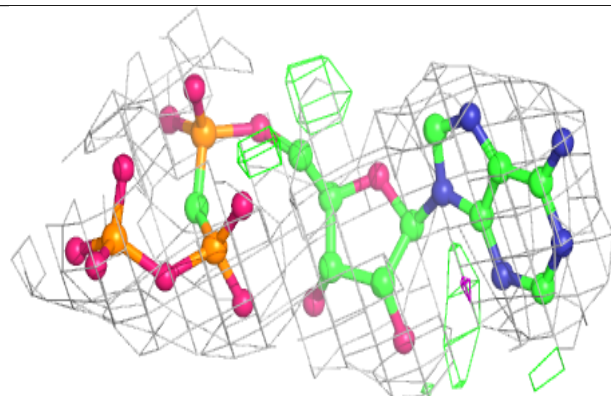
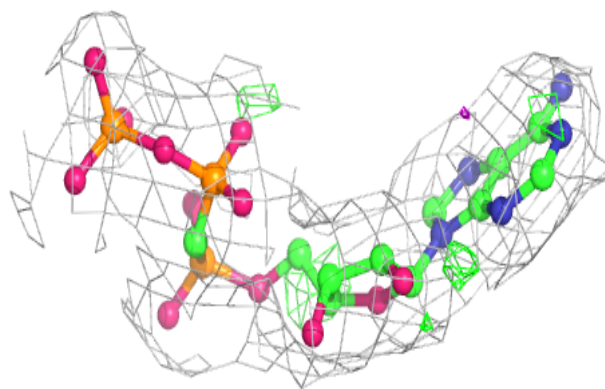
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around APC B 1500:**

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

**Electron density around APC A 500:**

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



## 6.5 Other polymers

There are no such residues in this entry.