



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:02 am GMT

PDB ID : 3KLG  
Title : Crystal structure of AZT-resistant HIV-1 Reverse Transcriptase crosslinked to pre-translocation AZTMP-Terminated DNA (COMPLEX N)  
Authors : Tu, X.; Sarafianos, S.G.; Arnold, E.  
Deposited on : 2009-11-07  
Resolution : 3.65 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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

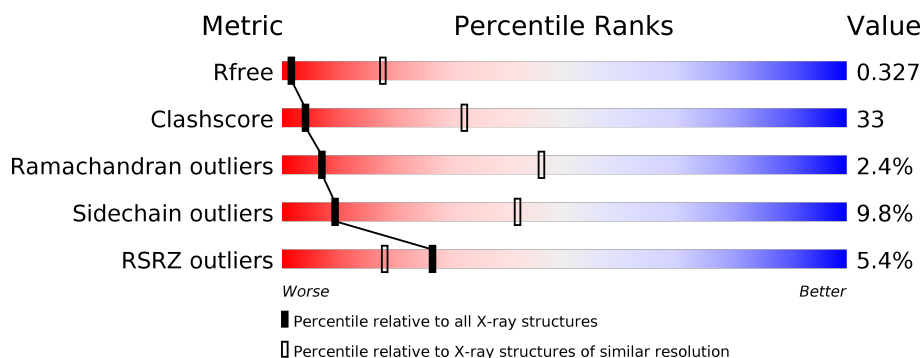
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.65 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.




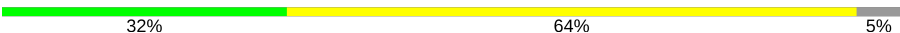
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	100719	1134 (3.82-3.50)
Clashscore	112137	1267 (3.82-3.50)
Ramachandran outliers	110173	1219 (3.82-3.50)
Sidechain outliers	110143	1218 (3.82-3.50)
RSRZ outliers	101464	1160 (3.82-3.50)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	562	<div> <div>46%</div> <div>47%</div> <div>6%</div> </div>
1	E	562	<div>11%</div> <div>51%</div> <div>41%</div> <div>7%</div>

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Mol	Chain	Length	Quality of chain
4	D	22	
4	H	22	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ATM	H	823	-	-	X	-

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17640 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Reverse transcriptase/ribonuclease H.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	554	Total	C	N	O	S	0	0	0
			4513	2922	752	832	7			
1	E	554	Total	C	N	O	S	0	0	0
			4513	2922	752	832	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	MET	-	EXPRESSION TAG	UNP P03366
A	0	VAL	-	EXPRESSION TAG	UNP P03366
A	41	LEU	MET	ENGINEERED	UNP P03366
A	67	ASN	ASP	ENGINEERED	UNP P03366
A	70	ARG	LYS	ENGINEERED	UNP P03366
A	215	TYR	THR	ENGINEERED	UNP P03366
A	219	GLN	LYS	ENGINEERED	UNP P03366
A	258	CYS	GLN	ENGINEERED	UNP P03366
A	280	SER	CYS	ENGINEERED	UNP P03366
A	559	VAL	ILE	SEE REMARK 999	UNP P03366
E	-1	MET	-	EXPRESSION TAG	UNP P03366
E	0	VAL	-	EXPRESSION TAG	UNP P03366
E	41	LEU	MET	ENGINEERED	UNP P03366
E	67	ASN	ASP	ENGINEERED	UNP P03366
E	70	ARG	LYS	ENGINEERED	UNP P03366
E	215	TYR	THR	ENGINEERED	UNP P03366
E	219	GLN	LYS	ENGINEERED	UNP P03366
E	258	CYS	GLN	ENGINEERED	UNP P03366
E	280	SER	CYS	ENGINEERED	UNP P03366
E	559	VAL	ILE	SEE REMARK 999	UNP P03366

- Molecule 2 is a protein called p51 RT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	413	Total	C	N	O	S	0	0	0
			3405	2215	564	620	6			
2	F	413	Total	C	N	O	S	0	0	0
			3405	2215	564	620	6			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	280	SER	CYS	ENGINEERED	UNP P03366
B	429	GLY	-	EXPRESSION TAG	UNP P03366
B	430	GLY	-	EXPRESSION TAG	UNP P03366
B	431	HIS	-	EXPRESSION TAG	UNP P03366
B	432	HIS	-	EXPRESSION TAG	UNP P03366
B	433	HIS	-	EXPRESSION TAG	UNP P03366
B	434	HIS	-	EXPRESSION TAG	UNP P03366
B	435	HIS	-	EXPRESSION TAG	UNP P03366
B	436	HIS	-	EXPRESSION TAG	UNP P03366
B	437	HIS	-	EXPRESSION TAG	UNP P03366
F	280	SER	CYS	ENGINEERED	UNP P03366
F	429	GLY	-	EXPRESSION TAG	UNP P03366
F	430	GLY	-	EXPRESSION TAG	UNP P03366
F	431	HIS	-	EXPRESSION TAG	UNP P03366
F	432	HIS	-	EXPRESSION TAG	UNP P03366
F	433	HIS	-	EXPRESSION TAG	UNP P03366
F	434	HIS	-	EXPRESSION TAG	UNP P03366
F	435	HIS	-	EXPRESSION TAG	UNP P03366
F	436	HIS	-	EXPRESSION TAG	UNP P03366
F	437	HIS	-	EXPRESSION TAG	UNP P03366

- Molecule 3 is a DNA chain called DNA (5'-D(\*AP\*T\*GP\*CP\*AP\*TP\*GP\*GP\*CP\*GP\*C  
P\*CP\*CP\*GP\*AP\*AP\*CP\*AP\*GP\*GP\*GP\*AP\*CP\*TP\*GP\*TP\*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	23	Total	C	N	O	P	0	0	0
			473	223	95	133	22			
3	G	23	Total	C	N	O	P	0	0	0
			473	223	95	133	22			

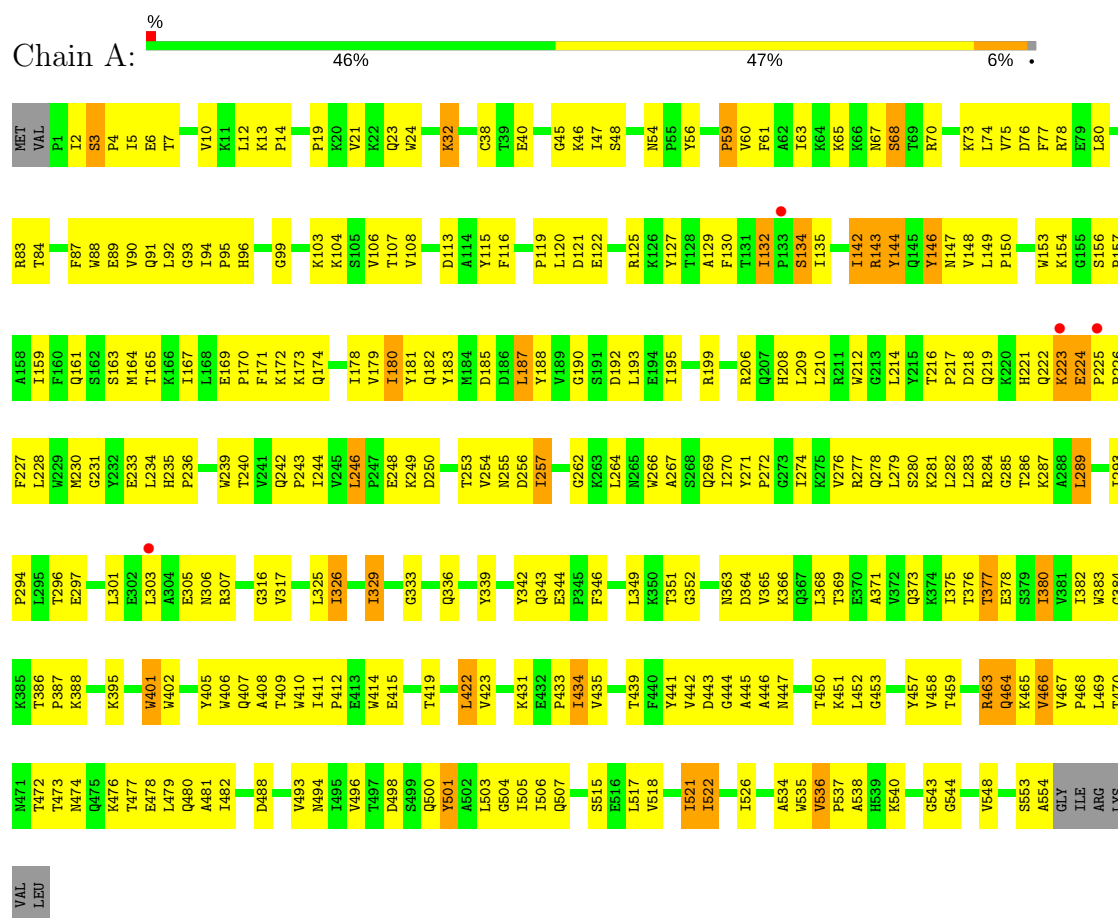
- Molecule 4 is a DNA chain called DNA (5'-D(\*A\*CP\*AP\*GP\*TP\*CP\*CP\*CP\*TP\*GP\*T  
P\*TP\*CP\*GP\*GP\*(MRG)P\*CP\*GP\*CP\*CP\*AP\*(ATM))-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	21	Total 429	C 205	N 77	O 126	P 20	S 1	0	0	0
4	H	21	Total 429	C 205	N 77	O 126	P 20	S 1	0	0	0

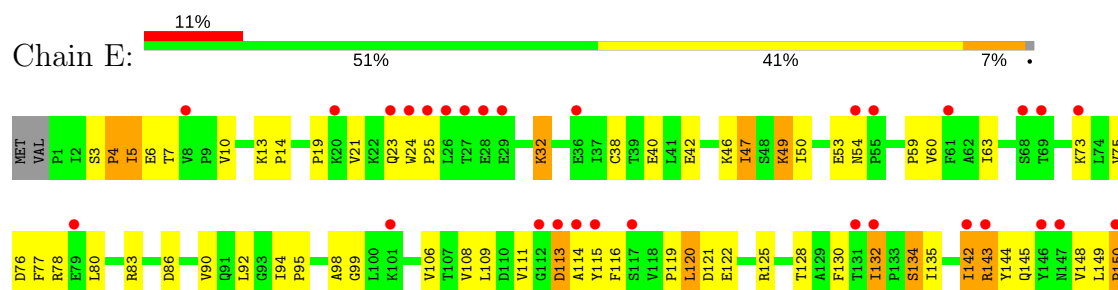
### 3 Residue-property plots

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: Reverse transcriptase/ribonuclease H

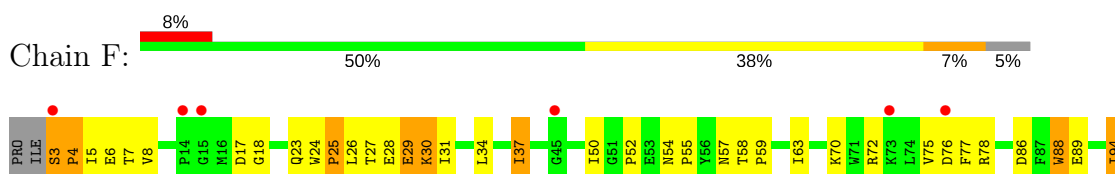


#### • Molecule 1: Reverse transcriptase/ribonuclease H



- Molecule 2: p51 RT

- Molecule 2: p51 RT







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	79.12Å 154.40Å 277.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.97 – 3.65 39.97 – 3.65	Depositor EDS
% Data completeness (in resolution range)	85.0 (39.97-3.65) 83.4 (39.97-3.65)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 3.66Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.312 , 0.350 0.301 , 0.327	Depositor DCC
$R_{free}$ test set	652 reflections (2.02%)	DCC
Wilson B-factor (Å <sup>2</sup> )	120.0	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 78.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	17640	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	120.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z  > 5$	RMSZ	# $ Z  > 5$
1	A	0.54	0/4632	0.68	0/6295
1	E	0.43	1/4632 (0.0%)	0.64	2/6295 (0.0%)
2	B	0.62	1/3502 (0.0%)	0.76	4/4760 (0.1%)
2	F	0.41	0/3502	0.63	1/4760 (0.0%)
3	C	0.83	0/532	0.92	0/820
3	G	0.61	0/532	0.86	0/820
4	D	0.75	0/424	0.88	0/649
4	H	0.64	0/424	0.89	0/649
All	All	0.53	2/18180 (0.0%)	0.70	7/25048 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	478	GLU	CD-OE2	5.98	1.32	1.25
2	B	79	GLU	CG-CD	5.07	1.59	1.51

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	34	LEU	CB-CA-C	-5.98	98.84	110.20
2	F	353	LYS	N-CA-CB	-5.98	99.84	110.60
2	B	213	GLY	N-CA-C	5.57	127.03	113.10
1	E	539	HIS	N-CA-C	-5.54	96.05	111.00
2	B	315	HIS	CB-CA-C	5.48	121.37	110.40
1	E	341	ILE	CB-CA-C	-5.36	100.88	111.60
2	B	93	GLY	N-CA-C	5.35	126.48	113.10

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4513	0	4568	350	0
1	E	4513	0	4568	293	0
2	B	3405	0	3437	244	0
2	F	3405	0	3437	207	0
3	C	473	0	257	37	0
3	G	473	0	257	32	0
4	D	429	0	243	36	0
4	H	429	0	243	35	0
All	All	17640	0	17010	1127	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 33.

All (1127) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:ILE:H	1:E:142:ILE:HD13	1.01	1.16
1:A:24:TRP:HA	3:C:703:DG:H21	1.09	1.10
2:B:5:ILE:HG22	2:B:6:GLU:N	1.53	1.10
2:B:5:ILE:HG22	2:B:6:GLU:H	0.94	1.08
1:E:540:LYS:O	1:E:542:ILE:HD12	1.53	1.08
1:E:49:LYS:HB3	1:E:144:TYR:HE1	1.15	1.08
1:A:142:ILE:HB	1:A:144:TYR:CE2	1.90	1.07
1:E:49:LYS:HB3	1:E:144:TYR:CE1	1.90	1.07
1:A:458:VAL:HA	1:A:463:ARG:O	1.52	1.06
1:E:24:TRP:HA	3:G:703:DG:N2	1.70	1.05
1:A:142:ILE:HD12	1:A:142:ILE:H	1.20	1.04
2:B:402:TRP:HH2	2:B:411:ILE:HD13	1.19	1.03
1:E:406:TRP:CE2	2:F:420:PRO:HB3	1.93	1.03
1:A:142:ILE:HG21	1:A:144:TYR:CZ	1.93	1.03
2:B:34:LEU:O	2:B:37:ILE:HG22	1.57	1.03
1:E:24:TRP:HA	3:G:703:DG:H21	0.91	1.03
2:B:54:ASN:HB3	2:B:143:ARG:NH2	1.75	1.02
1:E:443:ASP:O	1:E:481:ALA:HB2	1.60	1.02
2:B:109:LEU:HB2	2:B:187:LEU:HB3	1.38	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:34:LEU:O	2:F:37:ILE:HG22	1.60	1.00
1:E:172:LYS:HE2	1:E:180:ILE:HG21	1.02	1.00
1:E:24:TRP:CA	3:G:703:DG:H21	1.75	0.99
1:A:441:TYR:CE2	1:A:544:GLY:HA3	1.97	0.98
2:B:5:ILE:CG2	2:B:6:GLU:N	2.26	0.98
2:B:5:ILE:CG2	2:B:6:GLU:H	1.74	0.98
1:A:67:ASN:O	1:A:68:SER:HB2	1.59	0.97
1:A:153:TRP:CD1	1:A:154:LYS:N	2.32	0.97
1:A:60:VAL:HG12	1:A:75:VAL:HG13	1.46	0.96
1:A:143:ARG:O	1:A:143:ARG:HG2	1.63	0.96
2:B:295:LEU:HD23	2:B:300:GLU:HG2	1.48	0.96
1:E:172:LYS:CE	1:E:180:ILE:HG21	1.96	0.95
2:F:54:ASN:HB3	2:F:143:ARG:NH2	1.82	0.95
1:A:144:TYR:HD2	1:A:144:TYR:H	1.14	0.94
1:E:142:ILE:CD1	1:E:142:ILE:H	1.78	0.94
2:B:402:TRP:CH2	2:B:411:ILE:HD13	2.01	0.93
1:A:142:ILE:CG2	1:A:144:TYR:CZ	2.51	0.93
2:B:357:MET:O	2:B:358:ARG:HB2	1.64	0.93
1:A:144:TYR:CD2	1:A:144:TYR:N	2.34	0.92
1:A:24:TRP:HA	3:C:703:DG:N2	1.83	0.92
1:A:199:ARG:HH22	1:A:223:LYS:CE	1.83	0.92
1:E:172:LYS:HE2	1:E:180:ILE:CG2	1.97	0.91
1:A:142:ILE:HB	1:A:144:TYR:HE2	1.28	0.90
1:A:23:GLN:HE21	1:A:60:VAL:H	1.18	0.90
1:A:209:LEU:HD22	1:A:214:LEU:HD22	1.51	0.90
2:B:122:GLU:HA	2:B:125:ARG:HD2	1.51	0.90
2:B:125:ARG:HH12	2:B:147:ASN:HD22	1.17	0.90
2:F:163:SER:O	2:F:167:ILE:HG13	1.72	0.89
1:E:143:ARG:HG2	1:E:143:ARG:O	1.70	0.89
1:E:49:LYS:HA	1:E:144:TYR:HD1	1.35	0.89
1:E:142:ILE:N	1:E:142:ILE:HD13	1.87	0.89
1:A:453:GLY:O	1:A:469:LEU:HB2	1.72	0.89
1:A:384:GLY:HA3	2:B:28:GLU:H	1.38	0.89
2:F:378:GLU:O	2:F:382:ILE:HG13	1.73	0.89
2:F:122:GLU:HA	2:F:125:ARG:HD2	1.53	0.89
1:A:342:TYR:HD2	1:A:344:GLU:O	1.56	0.87
2:F:380:ILE:HA	2:F:384:GLY:HA2	1.56	0.86
1:A:75:VAL:HG21	1:A:146:TYR:HE1	1.38	0.86
1:E:384:GLY:O	2:F:27:THR:HB	1.76	0.86
2:F:295:LEU:HD23	2:F:300:GLU:HG2	1.56	0.85
1:A:144:TYR:HD2	1:A:144:TYR:N	1.70	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:ARG:HH22	1:A:223:LYS:HE2	1.42	0.85
2:B:88:TRP:O	2:B:88:TRP:HE3	1.59	0.85
1:E:371:ALA:O	1:E:375:ILE:HD12	1.75	0.84
1:A:75:VAL:HG21	1:A:146:TYR:CE1	2.13	0.84
1:E:49:LYS:CA	1:E:144:TYR:HD1	1.90	0.84
2:B:125:ARG:HH12	2:B:147:ASN:ND2	1.76	0.83
2:B:398:TRP:HZ3	2:B:414:TRP:CZ2	1.96	0.83
2:B:210:LEU:HD13	2:B:215:THR:HG23	1.61	0.83
2:F:163:SER:O	2:F:167:ILE:CG1	2.26	0.83
1:A:91:GLN:HB2	1:A:161:GLN:OE1	1.77	0.83
2:B:103:LYS:HG3	2:B:191:SER:O	1.78	0.83
1:A:255:ASN:HB2	1:A:289:LEU:HB2	1.59	0.83
1:A:142:ILE:CB	1:A:144:TYR:CE2	2.63	0.82
2:F:382:ILE:HG22	2:F:383:TRP:CE2	2.14	0.82
2:F:97:PRO:HG2	2:F:100:LEU:HB2	1.61	0.82
1:E:5:ILE:HG12	1:E:167:ILE:HD11	1.60	0.82
1:A:443:ASP:OD1	1:A:444:GLY:N	2.13	0.82
1:E:10:VAL:HG21	1:E:153:TRP:HH2	1.45	0.81
1:A:254:VAL:O	1:A:257:ILE:HG22	1.79	0.81
1:E:23:GLN:HE21	1:E:60:VAL:H	1.26	0.81
1:A:76:ASP:OD1	3:C:705:DA:H4'	1.81	0.81
1:E:373:GLN:OE1	2:F:397:THR:HG22	1.81	0.81
1:E:163:SER:O	1:E:167:ILE:HD12	1.81	0.80
1:A:469:LEU:HD13	1:A:472:THR:HG21	1.64	0.80
2:B:378:GLU:O	2:B:382:ILE:HG13	1.82	0.80
2:F:183:TYR:CE2	2:F:380:ILE:HD12	2.17	0.80
1:A:24:TRP:CA	3:C:703:DG:H21	1.92	0.80
1:E:540:LYS:O	1:E:542:ILE:CD1	2.30	0.79
1:E:443:ASP:OD1	1:E:444:GLY:N	2.15	0.79
2:F:180:ILE:CG2	2:F:187:LEU:HD11	2.12	0.79
1:A:406:TRP:CE2	2:B:420:PRO:HB3	2.17	0.79
1:A:469:LEU:CD1	1:A:472:THR:HG21	2.12	0.79
2:F:378:GLU:O	2:F:382:ILE:CG1	2.31	0.78
1:E:439:THR:HG22	1:E:441:TYR:HE1	1.48	0.78
2:B:402:TRP:HH2	2:B:411:ILE:CD1	1.96	0.78
1:A:464:GLN:HB2	1:E:466:VAL:HG13	1.64	0.78
1:E:255:ASN:HB2	1:E:289:LEU:HB2	1.66	0.78
2:B:185:ASP:OD1	2:B:185:ASP:N	2.17	0.78
2:F:421:PRO:CB	2:F:425:LEU:HD13	2.13	0.78
3:G:705:DA:C2'	3:G:706:DT:H5'	2.13	0.78
1:A:142:ILE:CG2	1:A:144:TYR:CE2	2.67	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:125:ARG:HH12	2:F:147:ASN:HD22	1.32	0.78
2:F:421:PRO:HB3	2:F:425:LEU:HD13	1.65	0.77
1:A:406:TRP:HD1	1:A:407:GLN:HE21	1.31	0.77
2:B:329:ILE:N	2:B:329:ILE:HD12	1.98	0.77
1:E:49:LYS:HA	1:E:144:TYR:CD1	2.18	0.77
2:F:180:ILE:HG21	2:F:187:LEU:HD11	1.67	0.77
2:F:382:ILE:CG2	2:F:383:TRP:CE2	2.67	0.77
2:B:262:GLY:HA3	2:B:423:VAL:HG11	1.67	0.76
2:B:75:VAL:HG11	2:B:77:PHE:CE2	2.20	0.76
2:F:8:VAL:HG21	2:F:159:ILE:HD13	1.65	0.76
3:C:705:DA:H2''	3:C:706:DT:H5''	1.68	0.76
1:A:10:VAL:HG21	1:A:153:TRP:HH2	1.50	0.76
1:A:277:ARG:HB2	1:A:336:GLN:HE21	1.51	0.76
2:F:402:TRP:HH2	2:F:411:ILE:CD1	1.98	0.76
2:B:270:ILE:HG22	2:B:314:VAL:HG21	1.68	0.76
1:E:254:VAL:O	1:E:257:ILE:HG22	1.84	0.76
1:E:92:LEU:CD1	2:F:133:PRO:HB3	2.15	0.76
2:F:329:ILE:N	2:F:329:ILE:HD12	1.99	0.76
1:A:264:LEU:HD21	1:A:306:ASN:HD22	1.49	0.75
2:B:270:ILE:HG22	2:B:314:VAL:CG2	2.15	0.75
3:G:705:DA:H2''	3:G:706:DT:C5'	2.17	0.75
1:A:2:ILE:HD11	1:A:46:LYS:HA	1.68	0.75
2:F:421:PRO:HB3	2:F:425:LEU:CD1	2.16	0.75
1:A:142:ILE:HD12	1:A:142:ILE:N	2.01	0.75
1:A:373:GLN:OE1	2:B:397:THR:HG22	1.86	0.75
1:A:2:ILE:O	1:A:3:SER:OG	2.05	0.75
1:A:246:LEU:HD11	1:A:307:ARG:HG3	1.68	0.75
1:E:439:THR:CG2	1:E:441:TYR:HE1	2.00	0.75
1:E:466:VAL:HG22	1:E:466:VAL:O	1.87	0.75
3:G:705:DA:H2'	3:G:706:DT:H5'	1.69	0.75
1:A:87:PHE:HZ	1:A:153:TRP:CZ2	2.05	0.75
1:A:115:TYR:CE2	4:D:823:ATM:H1'	2.21	0.75
2:B:132:ILE:HG13	2:B:132:ILE:O	1.87	0.74
2:B:332:GLN:OE1	2:B:425:LEU:HD13	1.87	0.74
2:B:54:ASN:HB3	2:B:143:ARG:HH22	1.48	0.74
1:E:145:GLN:HG3	1:E:145:GLN:O	1.87	0.74
1:A:142:ILE:HG21	1:A:144:TYR:OH	1.88	0.74
1:E:439:THR:HG22	1:E:441:TYR:CE1	2.22	0.74
1:E:49:LYS:CA	1:E:144:TYR:CD1	2.71	0.74
1:A:5:ILE:HG12	1:A:167:ILE:HD11	1.70	0.74
1:A:76:ASP:OD1	1:A:78:ARG:HD3	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:705:DA:H2''	3:C:706:DT:C5'	2.16	0.74
2:B:97:PRO:HG2	2:B:100:LEU:HB2	1.69	0.73
1:E:293:ILE:HD12	1:E:294:PRO:HD2	1.70	0.73
1:E:148:VAL:HG22	1:E:149:LEU:H	1.54	0.73
2:F:183:TYR:CE2	2:F:380:ILE:CD1	2.71	0.73
3:C:705:DA:C2'	3:C:706:DT:H5'	2.18	0.73
1:A:384:GLY:O	2:B:27:THR:HG22	1.88	0.73
3:C:707:DG:H2''	3:C:708:DG:H5'	1.71	0.73
3:G:709:DC:H2''	3:G:710:DG:H5'	1.69	0.73
1:A:224:GLU:HB3	1:A:226:PRO:HD2	1.70	0.73
1:E:38:CYS:SG	1:E:132:ILE:HD12	2.29	0.73
1:A:115:TYR:CD2	4:D:823:ATM:H2'	2.23	0.72
1:E:156:SER:OG	1:E:157:PRO:HD3	1.90	0.72
2:F:380:ILE:CA	2:F:384:GLY:HA2	2.20	0.72
1:E:406:TRP:CD2	2:F:420:PRO:HB3	2.24	0.72
1:A:441:TYR:CD2	1:A:544:GLY:HA3	2.24	0.72
2:F:125:ARG:HH12	2:F:147:ASN:ND2	1.87	0.72
1:E:406:TRP:HD1	1:E:407:GLN:HE21	1.35	0.72
2:B:180:ILE:O	2:B:180:ILE:HD12	1.90	0.72
3:C:709:DC:H2''	3:C:710:DG:H5'	1.71	0.72
1:A:326:ILE:N	1:A:326:ILE:HD13	2.05	0.71
1:E:76:ASP:OD1	3:G:705:DA:H4'	1.90	0.71
2:B:377:THR:O	2:B:381:VAL:HG23	1.90	0.71
1:E:458:VAL:HA	1:E:463:ARG:O	1.91	0.71
1:A:464:GLN:CB	1:E:466:VAL:HG13	2.20	0.71
1:A:106:VAL:HG12	1:A:190:GLY:HA3	1.71	0.71
2:B:23:GLN:HE21	2:B:26:LEU:HD11	1.55	0.71
1:E:443:ASP:O	1:E:481:ALA:CB	2.37	0.71
1:A:153:TRP:CG	1:A:154:LYS:N	2.58	0.71
1:A:384:GLY:HA3	2:B:28:GLU:N	2.05	0.71
3:C:706:DT:H2''	3:C:707:DG:H5'	1.73	0.70
3:C:705:DA:H2'	3:C:706:DT:H5'	1.73	0.70
1:E:505:ILE:HD12	1:E:505:ILE:H	1.56	0.70
1:A:371:ALA:O	1:A:375:ILE:HD12	1.90	0.70
1:E:225:PRO:HB2	1:E:226:PRO:HD3	1.73	0.70
1:E:406:TRP:CD1	1:E:407:GLN:HG2	2.27	0.70
2:F:54:ASN:HB3	2:F:143:ARG:HH22	1.51	0.70
2:B:185:ASP:C	2:B:186:ASP:OD1	2.30	0.70
1:E:76:ASP:OD1	1:E:78:ARG:HD3	1.92	0.70
1:A:84:THR:HG21	1:A:153:TRP:CZ2	2.26	0.70
1:A:293:ILE:HD12	1:A:294:PRO:HD2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:92:LEU:HB2	2:F:137:ASN:OD1	1.92	0.69
2:F:380:ILE:HA	2:F:384:GLY:CA	2.21	0.69
2:B:163:SER:O	2:B:167:ILE:HG13	1.91	0.69
1:A:163:SER:O	1:A:167:ILE:HD12	1.92	0.69
1:A:67:ASN:O	1:A:68:SER:CB	2.36	0.69
2:F:398:TRP:HZ3	2:F:414:TRP:CZ2	2.10	0.69
3:G:707:DG:H2''	3:G:708:DG:H5'	1.73	0.69
2:F:115:TYR:O	2:F:149:LEU:HB2	1.92	0.69
3:G:705:DA:H2''	3:G:706:DT:H5''	1.73	0.69
1:E:326:ILE:N	1:E:326:ILE:HD13	2.08	0.69
1:A:181:TYR:CE2	2:B:138:GLU:HA	2.27	0.69
4:D:818:DC:H2''	4:D:819:DG:H5'	1.74	0.69
2:B:363:ASN:HD22	2:B:366:LYS:HB2	1.57	0.69
2:F:382:ILE:HG21	2:F:383:TRP:CZ2	2.28	0.69
1:A:172:LYS:HE2	1:A:180:ILE:HG21	1.73	0.69
1:A:459:THR:HG23	1:A:463:ARG:HB3	1.75	0.68
2:B:169:GLU:HB3	2:B:170:PRO:HD3	1.74	0.68
1:A:464:GLN:HB2	1:E:466:VAL:CG1	2.22	0.68
1:E:544:GLY:H	1:E:547:GLN:HE22	1.40	0.68
1:E:506:ILE:HD13	1:E:506:ILE:N	2.08	0.68
1:E:99:GLY:HA2	1:E:383:TRP:HE1	1.58	0.68
2:F:132:ILE:O	2:F:132:ILE:HG13	1.92	0.68
2:F:75:VAL:HG11	2:F:77:PHE:CE2	2.29	0.68
1:A:384:GLY:C	2:B:27:THR:HG22	2.13	0.68
1:E:90:VAL:HG12	2:F:140:PRO:HB2	1.76	0.68
2:F:169:GLU:HB3	2:F:170:PRO:HD3	1.75	0.68
1:E:108:VAL:HG13	1:E:187:LEU:O	1.94	0.68
1:E:106:VAL:HG12	1:E:190:GLY:HA3	1.75	0.67
1:A:12:LEU:HD11	1:A:127:TYR:CZ	2.29	0.67
1:A:108:VAL:HG13	1:A:187:LEU:O	1.95	0.67
1:A:284:ARG:HA	3:C:714:DG:OP1	1.94	0.67
2:F:402:TRP:CH2	2:F:411:ILE:HD13	2.29	0.67
2:F:7:THR:HB	2:F:121:ASP:HA	1.75	0.67
4:H:818:DC:H2''	4:H:819:DG:H5'	1.75	0.67
2:B:88:TRP:CE3	2:B:88:TRP:O	2.47	0.67
1:E:246:LEU:HD11	1:E:307:ARG:HG3	1.76	0.67
2:F:359:GLY:O	2:F:360:ALA:HB3	1.94	0.67
2:F:402:TRP:HH2	2:F:411:ILE:HD13	1.59	0.67
2:F:423:VAL:CG2	2:F:426:TRP:HD1	2.06	0.67
1:A:199:ARG:HH22	1:A:223:LYS:NZ	1.93	0.67
1:A:61:PHE:CE1	1:A:74:LEU:HB2	2.28	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:388:LYS:HA	2:F:413:GLU:O	1.95	0.66
2:F:205:LEU:O	2:F:205:LEU:HD23	1.95	0.66
1:A:199:ARG:NH2	1:A:223:LYS:CE	2.56	0.66
2:F:171:PHE:HZ	2:F:204:GLU:HG2	1.61	0.66
2:B:150:PRO:HG2	2:B:153:TRP:HB3	1.78	0.66
1:E:115:TYR:HD2	4:H:823:ATM:H2'	1.60	0.66
2:B:185:ASP:O	2:B:186:ASP:CG	2.34	0.66
2:B:23:GLN:HG2	2:B:133:PRO:HG3	1.78	0.66
1:A:505:ILE:HD12	1:A:505:ILE:H	1.60	0.66
2:F:363:ASN:HD22	2:F:366:LYS:HB2	1.61	0.66
1:A:199:ARG:NH2	1:A:223:LYS:HE2	2.09	0.65
2:B:27:THR:OG1	2:B:30:LYS:HE2	1.96	0.65
3:C:705:DA:C2'	3:C:706:DT:C5'	2.75	0.65
1:A:464:GLN:CB	1:E:466:VAL:CG1	2.75	0.65
1:E:369:THR:HA	1:E:411:ILE:HD11	1.77	0.65
1:A:442:VAL:HB	1:A:481:ALA:HB1	1.78	0.65
1:E:199:ARG:HH22	1:E:223:LYS:HD3	1.62	0.65
2:B:171:PHE:HZ	2:B:204:GLU:HG2	1.62	0.65
2:B:61:PHE:HZ	2:B:411:ILE:HD11	1.60	0.65
1:E:108:VAL:HB	1:E:221:HIS:CD2	2.32	0.65
1:A:326:ILE:H	1:A:326:ILE:HD13	1.62	0.65
1:A:408:ALA:HB1	2:B:364:ASP:HB3	1.77	0.65
2:F:94:ILE:HD13	2:F:94:ILE:N	2.12	0.65
1:A:103:LYS:HE3	1:A:179:VAL:HG21	1.78	0.65
1:A:180:ILE:HG23	1:A:180:ILE:O	1.96	0.65
1:E:181:TYR:HB2	1:E:188:TYR:HB3	1.77	0.65
1:A:88:TRP:CE3	1:A:89:GLU:O	2.50	0.64
1:E:272:PRO:HB3	1:E:351:THR:HG21	1.79	0.64
3:G:706:DT:H2''	3:G:707:DG:H5'	1.79	0.64
1:A:339:TYR:CZ	1:A:352:GLY:HA3	2.32	0.64
1:A:371:ALA:O	1:A:375:ILE:CD1	2.45	0.64
1:E:537:PRO:HB2	1:E:540:LYS:HB2	1.79	0.64
2:F:121:ASP:O	2:F:125:ARG:HG3	1.98	0.64
2:F:422:LEU:HB2	2:F:426:TRP:HE1	1.62	0.64
3:G:705:DA:C2'	3:G:706:DT:C5'	2.75	0.64
1:A:87:PHE:CZ	1:A:153:TRP:CZ2	2.85	0.64
2:B:84:THR:O	2:B:84:THR:HG22	1.98	0.64
2:F:72:ARG:NH2	2:F:151:GLN:NE2	2.45	0.64
1:A:142:ILE:CD1	1:A:142:ILE:H	2.00	0.63
2:F:203:GLU:O	2:F:207:GLN:HG2	1.97	0.63
1:A:363:ASN:OD1	1:A:364:ASP:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HA	2:B:136:ASN:OD1	1.98	0.63
2:B:54:ASN:HB3	2:B:143:ARG:HH21	1.63	0.63
2:B:359:GLY:O	2:B:360:ALA:HB3	1.97	0.63
2:B:376:THR:HG23	2:B:386:THR:HG23	1.80	0.63
1:A:537:PRO:HB2	1:A:540:LYS:HB2	1.81	0.63
1:E:339:TYR:CZ	1:E:352:GLY:HA3	2.34	0.63
1:A:122:GLU:O	1:A:125:ARG:HD2	1.98	0.63
2:B:205:LEU:O	2:B:205:LEU:HD23	1.99	0.63
1:A:87:PHE:HZ	1:A:153:TRP:CH2	2.16	0.63
2:B:261:VAL:HG13	2:B:276:VAL:HG21	1.80	0.63
2:B:325:LEU:HD12	2:B:343:GLN:HE21	1.64	0.63
2:B:181:TYR:O	2:B:188:TYR:HB2	1.99	0.63
2:F:109:LEU:HB2	2:F:187:LEU:HB3	1.80	0.63
2:F:120:LEU:HD11	2:F:150:PRO:HD3	1.80	0.63
1:A:142:ILE:HG12	1:A:144:TYR:OH	1.98	0.63
2:B:212:TRP:CD1	2:B:212:TRP:N	2.67	0.63
1:A:142:ILE:CB	1:A:144:TYR:CZ	2.82	0.62
2:B:109:LEU:O	2:B:187:LEU:N	2.28	0.62
2:B:388:LYS:HA	2:B:413:GLU:O	1.98	0.62
1:A:246:LEU:H	1:A:246:LEU:HD23	1.64	0.62
1:A:99:GLY:HA2	1:A:383:TRP:HE1	1.62	0.62
1:E:60:VAL:HG12	1:E:75:VAL:HG13	1.79	0.62
1:A:346:PHE:O	1:A:346:PHE:CD1	2.53	0.62
2:B:191:SER:OG	2:B:198:HIS:ND1	2.29	0.62
2:B:75:VAL:CG1	2:B:77:PHE:CE2	2.83	0.62
2:F:156:SER:N	2:F:157:PRO:HD2	2.15	0.62
4:H:808:DC:H1'	4:H:809:DC:H5'	1.82	0.62
1:A:103:LYS:HE3	1:A:179:VAL:CG2	2.30	0.62
1:A:506:ILE:N	1:A:506:ILE:HD13	2.14	0.62
1:A:435:VAL:HG22	2:B:290:THR:HG21	1.81	0.62
1:E:217:PRO:C	1:E:219:GLN:H	2.02	0.62
1:E:344:GLU:HB2	1:E:347:LYS:HB2	1.81	0.62
1:E:134:SER:O	1:E:135:ILE:HD13	2.00	0.61
1:E:505:ILE:HD12	1:E:505:ILE:N	2.15	0.61
1:E:49:LYS:CB	1:E:144:TYR:CE1	2.76	0.61
1:E:384:GLY:HA3	2:F:28:GLU:N	2.15	0.61
1:E:151:GLN:NE2	4:H:823:ATM:H2''	2.15	0.61
2:F:191:SER:HG	2:F:198:HIS:CE1	2.18	0.61
2:F:393:ILE:HG12	2:F:397:THR:OG1	2.00	0.61
1:A:518:VAL:HA	1:A:521:ILE:HG13	1.82	0.61
1:E:153:TRP:CD1	1:E:154:LYS:N	2.64	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HB	1:A:144:TYR:CZ	2.35	0.61
1:A:225:PRO:HB2	1:A:226:PRO:HD3	1.82	0.61
1:E:344:GLU:O	1:E:345:PRO:C	2.37	0.61
1:E:494:ASN:HB3	2:F:289:LEU:HD22	1.83	0.61
1:A:369:THR:HA	1:A:411:ILE:HD11	1.83	0.61
2:B:8:VAL:HG11	2:B:159:ILE:HD13	1.82	0.61
1:A:445:ALA:O	1:A:477:THR:HG21	2.00	0.61
1:A:93:GLY:O	2:B:137:ASN:CG	2.39	0.60
1:E:340:GLN:HB3	1:E:351:THR:HG22	1.83	0.60
1:E:180:ILE:O	1:E:180:ILE:HG23	2.01	0.60
1:E:246:LEU:HD23	1:E:246:LEU:H	1.66	0.60
2:B:84:THR:HG21	2:B:153:TRP:HZ2	1.66	0.60
2:F:163:SER:O	2:F:167:ILE:HG12	2.01	0.60
1:A:90:VAL:HG12	2:B:140:PRO:HB2	1.84	0.60
2:B:402:TRP:NE1	2:B:403:THR:HG23	2.16	0.60
1:E:326:ILE:H	1:E:326:ILE:HD13	1.65	0.60
1:A:181:TYR:HB2	1:A:188:TYR:HB3	1.83	0.60
2:B:125:ARG:HB3	2:B:145:GLN:HE21	1.66	0.60
2:B:88:TRP:C	2:B:88:TRP:CE3	2.75	0.60
1:E:7:THR:HB	1:E:121:ASP:HA	1.82	0.60
2:F:23:GLN:HE21	2:F:26:LEU:HD11	1.67	0.60
2:F:382:ILE:HG21	2:F:383:TRP:CE2	2.37	0.60
1:A:169:GLU:HB3	1:A:170:PRO:HD3	1.82	0.60
2:B:121:ASP:O	2:B:125:ARG:HG3	2.01	0.60
1:E:120:LEU:HD12	1:E:125:ARG:HG3	1.83	0.60
1:A:199:ARG:HH12	1:A:223:LYS:HZ2	1.48	0.60
1:A:267:ALA:O	1:A:271:TYR:HB2	2.01	0.60
1:E:182:GLN:HG3	1:E:182:GLN:O	2.01	0.60
1:E:406:TRP:HD1	1:E:407:GLN:HG2	1.66	0.60
1:A:434:ILE:N	1:A:434:ILE:HD13	2.17	0.59
1:E:47:ILE:HG22	1:E:144:TYR:HB3	1.82	0.59
1:A:153:TRP:HB3	1:A:156:SER:OG	2.02	0.59
2:B:125:ARG:NH1	2:B:147:ASN:ND2	2.50	0.59
2:F:406:TRP:HZ2	2:F:410:TRP:O	1.85	0.59
3:G:709:DC:H2'	3:G:710:DG:H8	1.66	0.59
1:A:23:GLN:HG2	1:A:59:PRO:HA	1.85	0.59
1:A:505:ILE:HD12	1:A:505:ILE:N	2.18	0.59
4:D:822:DA:H2''	4:D:823:ATM:H5'	1.83	0.59
1:E:49:LYS:HA	1:E:143:ARG:O	2.02	0.59
2:F:94:ILE:HD11	2:F:158:ALA:HA	1.85	0.59
1:E:264:LEU:HD21	1:E:306:ASN:HD22	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:168:LEU:HD21	2:B:209:LEU:HD21	1.83	0.59
2:B:23:GLN:NE2	2:B:26:LEU:HD11	2.18	0.59
3:C:707:DG:H2''	3:C:708:DG:C5'	2.33	0.59
4:D:808:DC:H1'	4:D:809:DC:H5'	1.83	0.59
1:E:47:ILE:CG2	1:E:144:TYR:HB3	2.32	0.59
1:E:5:ILE:HG22	1:E:6:GLU:H	1.67	0.59
3:G:710:DG:H2''	3:G:711:DC:H5'	1.85	0.59
4:H:805:DG:H2''	4:H:806:DT:OP2	2.03	0.59
1:A:553:SER:O	1:A:554:ALA:HB3	2.03	0.58
3:C:710:DG:H2''	3:C:711:DC:H5'	1.84	0.58
1:E:537:PRO:HB2	1:E:540:LYS:CB	2.34	0.58
1:E:439:THR:O	1:E:439:THR:HG22	2.04	0.58
2:F:382:ILE:HG22	2:F:383:TRP:CD2	2.37	0.58
2:F:262:GLY:HA3	2:F:423:VAL:HG11	1.85	0.58
4:H:822:DA:H2''	4:H:823:ATM:H5'	1.85	0.58
1:A:264:LEU:HD23	1:A:276:VAL:HG12	1.85	0.58
2:F:115:TYR:CD1	2:F:156:SER:HB3	2.39	0.58
2:F:174:GLN:HG3	2:F:175:ASN:OD1	2.03	0.58
1:A:38:CYS:O	1:A:47:ILE:HD11	2.03	0.58
1:A:224:GLU:HG2	1:A:225:PRO:HD2	1.86	0.58
1:E:125:ARG:O	1:E:128:THR:HG22	2.04	0.58
2:F:72:ARG:CZ	2:F:151:GLN:NE2	2.66	0.58
2:B:325:LEU:O	2:B:387:PRO:HA	2.04	0.58
2:B:185:ASP:C	2:B:186:ASP:CG	2.61	0.58
1:A:115:TYR:OH	1:A:157:PRO:HG3	2.03	0.58
2:B:395:LYS:NZ	4:D:813:DT:OP2	2.34	0.58
2:F:88:TRP:CE3	2:F:89:GLU:HB2	2.39	0.57
1:A:142:ILE:CB	1:A:144:TYR:OH	2.52	0.57
1:A:406:TRP:CD1	1:A:407:GLN:HG2	2.38	0.57
2:B:180:ILE:HG22	2:B:189:VAL:HG22	1.86	0.57
1:E:115:TYR:HE2	4:H:823:ATM:H1'	1.69	0.57
3:G:707:DG:H2''	3:G:708:DG:C5'	2.34	0.57
1:A:5:ILE:HG22	1:A:6:GLU:H	1.68	0.57
1:E:384:GLY:HA3	2:F:28:GLU:H	1.67	0.57
1:E:457:TYR:CE2	1:E:465:LYS:HB3	2.39	0.57
1:E:505:ILE:H	1:E:505:ILE:CD1	2.17	0.57
2:F:23:GLN:HG2	2:F:133:PRO:HG3	1.85	0.57
3:C:720:DG:H2''	3:C:721:DG:OP2	2.04	0.57
3:G:707:DG:H2'	3:G:708:DG:C8	2.40	0.57
2:B:328:GLU:C	2:B:329:ILE:HD12	2.24	0.57
1:E:115:TYR:OH	1:E:157:PRO:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:27:THR:H	2:F:30:LYS:HE2	1.70	0.57
1:A:277:ARG:HB2	1:A:336:GLN:NE2	2.20	0.57
1:E:342:TYR:HA	1:E:349:LEU:HD23	1.87	0.57
1:A:87:PHE:CZ	1:A:153:TRP:CH2	2.92	0.57
1:A:264:LEU:HD23	1:A:276:VAL:CG1	2.35	0.57
1:E:115:TYR:HD1	1:E:149:LEU:HD23	1.68	0.57
1:E:408:ALA:HB1	2:F:364:ASP:HB3	1.87	0.57
2:F:214:LEU:HD12	2:F:214:LEU:N	2.19	0.57
1:A:446:ALA:HB2	1:A:477:THR:HG21	1.87	0.57
2:B:10:VAL:HG11	2:B:124:PHE:CE1	2.39	0.57
1:E:374:LYS:HD3	1:E:374:LYS:O	2.04	0.57
1:E:115:TYR:CD2	4:H:823:ATM:H4'	2.39	0.57
2:B:254:VAL:HG23	2:B:291:GLU:O	2.05	0.56
2:B:70:LYS:HA	2:B:70:LYS:HE2	1.87	0.56
1:E:115:TYR:CE2	4:H:823:ATM:H1'	2.40	0.56
2:F:114:ALA:HB2	2:F:214:LEU:CD2	2.35	0.56
1:A:65:LYS:HD2	1:A:70:ARG:HB2	1.86	0.56
1:A:70:ARG:HH11	1:A:70:ARG:HG2	1.70	0.56
2:B:23:GLN:HG2	2:B:133:PRO:CG	2.35	0.56
2:B:266:TRP:CD1	2:B:426:TRP:CD1	2.92	0.56
1:E:169:GLU:HB3	1:E:170:PRO:HD3	1.87	0.56
3:G:720:DG:H2''	3:G:721:DG:OP2	2.04	0.56
2:F:261:VAL:HG13	2:F:276:VAL:HG21	1.88	0.56
2:B:210:LEU:CD1	2:B:215:THR:HG23	2.34	0.56
1:E:544:GLY:HA2	2:F:286:THR:HG22	1.86	0.56
2:F:183:TYR:CD2	2:F:380:ILE:HD12	2.40	0.56
1:A:505:ILE:CD1	1:A:505:ILE:H	2.18	0.56
2:B:331:LYS:HG2	2:B:332:GLN:N	2.20	0.56
2:B:423:VAL:CG2	2:B:426:TRP:HD1	2.19	0.56
2:B:109:LEU:CB	2:B:187:LEU:HB3	2.25	0.56
1:E:108:VAL:HG22	1:E:188:TYR:HA	1.88	0.56
1:A:376:THR:C	1:A:378:GLU:H	2.10	0.56
2:B:174:GLN:HG3	2:B:175:ASN:OD1	2.05	0.56
2:B:387:PRO:HG2	2:B:389:PHE:CE1	2.40	0.56
1:A:209:LEU:O	1:A:212:TRP:N	2.38	0.56
1:A:441:TYR:HE2	1:A:543:GLY:O	1.89	0.56
1:A:5:ILE:HG22	1:A:6:GLU:N	2.20	0.56
4:D:806:DT:H1'	4:D:807:DC:H5'	1.87	0.56
1:E:23:GLN:HG2	1:E:59:PRO:HA	1.88	0.56
1:A:165:THR:HA	1:A:182:GLN:HE22	1.71	0.55
1:A:342:TYR:CD2	1:A:344:GLU:O	2.48	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ASN:HB3	1:A:366:LYS:HB2	1.87	0.55
1:A:439:THR:O	1:A:439:THR:HG22	2.06	0.55
1:A:465:LYS:HD3	1:A:488:ASP:OD2	2.06	0.55
1:A:92:LEU:HB2	2:B:137:ASN:OD1	2.06	0.55
2:B:406:TRP:HZ2	2:B:410:TRP:O	1.87	0.55
2:B:94:ILE:N	2:B:94:ILE:HD13	2.21	0.55
3:C:713:DC:H2''	3:C:714:DG:C8	2.41	0.55
2:B:134:SER:OG	2:B:138:GLU:HB3	2.05	0.55
4:D:808:DC:H2''	4:D:809:DC:H5'	1.87	0.55
2:F:402:TRP:NE1	2:F:403:THR:HG23	2.21	0.55
1:E:32:LYS:HZ1	1:E:135:ILE:HD11	1.71	0.55
1:A:233:GLU:HB3	1:A:240:THR:HG23	1.88	0.55
2:B:214:LEU:HD12	2:B:214:LEU:N	2.22	0.55
2:B:23:GLN:OE1	2:B:59:PRO:HA	2.07	0.55
4:D:805:DG:H2''	4:D:806:DT:OP2	2.05	0.55
1:E:109:LEU:HD13	1:E:216:THR:HG21	1.89	0.55
2:F:423:VAL:CG2	2:F:426:TRP:CD1	2.88	0.55
1:A:346:PHE:C	1:A:346:PHE:CD1	2.80	0.55
2:B:58:THR:HG23	2:B:59:PRO:HD2	1.88	0.55
2:B:369:THR:O	2:B:373:GLN:HG3	2.06	0.55
4:D:808:DC:H6	4:D:808:DC:H5'	1.70	0.55
1:E:165:THR:HA	1:E:182:GLN:HE22	1.72	0.55
1:E:267:ALA:O	1:E:271:TYR:HB2	2.07	0.55
1:A:225:PRO:HB3	1:A:235:HIS:CD2	2.42	0.55
1:A:80:LEU:O	1:A:83:ARG:N	2.25	0.55
1:A:535:TRP:C	1:A:536:VAL:HG22	2.28	0.55
2:B:234:LEU:O	2:B:234:LEU:HD12	2.07	0.55
2:B:266:TRP:HZ2	2:B:422:LEU:HD12	1.72	0.55
2:B:76:ASP:OD1	2:B:78:ARG:HB2	2.06	0.55
2:F:325:LEU:HD12	2:F:343:GLN:HE21	1.72	0.55
1:A:134:SER:O	1:A:135:ILE:HD13	2.06	0.54
1:A:280:SER:HA	1:A:283:LEU:HD23	1.89	0.54
1:A:395:LYS:HA	1:A:414:TRP:HH2	1.72	0.54
2:B:103:LYS:CG	2:B:191:SER:O	2.53	0.54
2:B:88:TRP:C	2:B:88:TRP:HE3	2.10	0.54
1:E:21:VAL:HG13	1:E:59:PRO:HD3	1.88	0.54
1:A:142:ILE:CG2	1:A:144:TYR:OH	2.54	0.54
2:B:363:ASN:HD21	2:B:365:VAL:HG23	1.71	0.54
2:B:403:THR:O	2:B:405:TYR:N	2.40	0.54
3:C:707:DG:H2'	3:C:708:DG:C8	2.42	0.54
2:F:254:VAL:O	2:F:258:GLN:HG2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLN:O	1:A:182:GLN:HG3	2.07	0.54
1:E:346:PHE:O	1:E:347:LYS:C	2.45	0.54
2:F:23:GLN:OE1	2:F:59:PRO:HA	2.07	0.54
3:G:707:DG:H2'	3:G:708:DG:H8	1.71	0.54
1:A:442:VAL:HG12	1:A:457:TYR:HB3	1.89	0.54
2:B:72:ARG:NH2	2:B:151:GLN:HG2	2.23	0.54
3:C:709:DC:H2'	3:C:710:DG:H8	1.72	0.54
1:A:21:VAL:HG13	1:A:59:PRO:HD3	1.90	0.54
2:B:357:MET:O	2:B:358:ARG:CB	2.45	0.54
3:C:717:DC:H1'	3:C:718:DA:H5'	1.88	0.54
4:D:818:DC:H2'	4:D:819:DG:H8	1.73	0.54
2:F:8:VAL:CG2	2:F:159:ILE:HD13	2.37	0.54
2:F:215:THR:O	2:F:216:THR:C	2.46	0.54
1:A:178:ILE:O	1:A:178:ILE:HD12	2.08	0.54
1:E:340:GLN:CB	1:E:351:THR:HG22	2.37	0.54
1:E:478:GLU:OE2	1:E:498:ASP:OD1	2.26	0.54
1:A:225:PRO:N	1:A:226:PRO:CD	2.69	0.54
1:E:217:PRO:O	1:E:219:GLN:N	2.40	0.54
2:F:180:ILE:CG2	2:F:187:LEU:CD1	2.84	0.54
2:F:340:GLN:O	2:F:341:ILE:HG12	2.07	0.54
1:A:439:THR:HA	1:A:494:ASN:HB2	1.89	0.54
1:E:80:LEU:O	1:E:83:ARG:N	2.32	0.54
3:G:722:DA:H2''	3:G:723:DC:OP2	2.07	0.54
1:E:151:GLN:HE21	4:H:823:ATM:H2''	1.72	0.54
2:F:325:LEU:O	2:F:387:PRO:HA	2.08	0.54
1:A:2:ILE:HD13	1:A:148:VAL:HG12	1.90	0.54
2:F:50:ILE:CD1	2:F:143:ARG:HB3	2.38	0.54
2:B:375:ILE:HD13	2:B:375:ILE:N	2.22	0.53
1:E:181:TYR:CE2	2:F:138:GLU:HA	2.43	0.53
2:F:379:SER:HB3	2:F:385:LYS:O	2.08	0.53
1:A:84:THR:HG21	1:A:153:TRP:CE2	2.42	0.53
1:A:553:SER:OG	1:A:554:ALA:N	2.41	0.53
1:A:181:TYR:CD2	2:B:138:GLU:HA	2.43	0.53
3:C:722:DA:H2''	3:C:723:DC:OP2	2.09	0.53
2:F:213:GLY:C	2:F:214:LEU:HD12	2.28	0.53
1:A:199:ARG:HH12	1:A:223:LYS:NZ	2.05	0.53
1:A:84:THR:HG21	1:A:153:TRP:NE1	2.24	0.53
2:B:371:ALA:O	2:B:375:ILE:HG12	2.08	0.53
1:E:536:VAL:HG12	1:E:537:PRO:HD2	1.91	0.53
2:F:125:ARG:HB3	2:F:145:GLN:HE21	1.73	0.53
2:F:320:ASP:OD2	2:F:322:SER:HB3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:54:ASN:HB3	2:F:143:ARG:HH21	1.71	0.53
1:E:384:GLY:HA2	2:F:27:THR:HA	1.90	0.53
2:F:421:PRO:HB2	2:F:425:LEU:HD13	1.91	0.53
1:A:130:PHE:CD1	1:A:130:PHE:N	2.77	0.53
1:A:142:ILE:HG22	1:A:144:TYR:CE2	2.44	0.53
1:A:501:TYR:C	1:A:501:TYR:CD1	2.82	0.53
1:E:283:LEU:HD22	1:E:283:LEU:H	1.73	0.53
2:F:375:ILE:N	2:F:375:ILE:HD13	2.24	0.53
1:A:96:HIS:H	2:B:136:ASN:ND2	2.07	0.53
1:E:32:LYS:NZ	1:E:135:ILE:HD11	2.24	0.53
1:E:442:VAL:HB	1:E:481:ALA:HB1	1.89	0.53
4:H:808:DC:H5'	4:H:808:DC:H6	1.74	0.53
1:A:274:ILE:HG22	1:A:274:ILE:O	2.09	0.53
1:E:501:TYR:C	1:E:501:TYR:CD1	2.83	0.53
3:G:713:DC:H2''	3:G:714:DG:C8	2.44	0.53
1:A:267:ALA:HB1	1:A:271:TYR:HD2	1.73	0.52
1:A:458:VAL:CA	1:A:463:ARG:O	2.41	0.52
2:B:50:ILE:CD1	2:B:143:ARG:HB3	2.39	0.52
1:A:159:ILE:HD13	2:B:52:PRO:HG2	1.92	0.52
2:F:94:ILE:HD12	2:F:161:GLN:OE1	2.08	0.52
1:A:48:SER:C	1:A:144:TYR:HB3	2.28	0.52
1:A:199:ARG:HH22	1:A:223:LYS:HZ3	1.57	0.52
1:E:363:ASN:OD1	1:E:364:ASP:N	2.41	0.52
1:E:406:TRP:NE1	2:F:420:PRO:HB3	2.23	0.52
1:A:419:THR:O	1:A:419:THR:HG23	2.10	0.52
1:A:458:VAL:HG12	1:A:548:VAL:CG2	2.39	0.52
1:A:3:SER:H	1:A:119:PRO:HG3	1.74	0.52
1:A:376:THR:O	1:A:378:GLU:N	2.42	0.52
2:B:76:ASP:C	2:B:78:ARG:H	2.13	0.52
1:E:395:LYS:HA	1:E:414:TRP:HH2	1.75	0.52
2:F:75:VAL:CG1	2:F:77:PHE:CE2	2.93	0.52
1:A:296:THR:HG22	1:A:297:GLU:N	2.24	0.52
2:B:363:ASN:ND2	2:B:365:VAL:HG23	2.24	0.52
1:E:284:ARG:HA	3:G:714:DG:OP1	2.10	0.52
2:F:328:GLU:C	2:F:329:ILE:HD12	2.29	0.52
1:A:142:ILE:CG1	1:A:144:TYR:OH	2.57	0.52
1:A:23:GLN:NE2	1:A:60:VAL:H	1.99	0.52
1:A:95:PRO:HG3	2:B:137:ASN:O	2.09	0.52
2:B:84:THR:HG22	2:B:87:PHE:HB3	1.92	0.52
2:F:234:LEU:HD12	2:F:234:LEU:O	2.09	0.52
4:D:808:DC:H2''	4:D:809:DC:C5'	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:818:DC:H2''	4:D:819:DG:C5'	2.40	0.52
1:A:221:HIS:HE1	1:A:228:LEU:H	1.57	0.52
1:A:284:ARG:CA	3:C:714:DG:OP1	2.57	0.52
2:B:393:ILE:HG12	2:B:397:THR:OG1	2.10	0.52
1:A:266:TRP:CE2	4:D:820:DC:H4'	2.45	0.52
1:E:122:GLU:O	1:E:125:ARG:HD2	2.10	0.52
3:C:722:DA:C4	3:C:723:DC:C5	2.98	0.52
1:E:38:CYS:SG	1:E:132:ILE:CD1	2.98	0.52
1:E:329:ILE:HG23	1:E:339:TYR:HB3	1.92	0.52
2:F:210:LEU:HG	2:F:210:LEU:O	2.09	0.52
2:F:329:ILE:N	2:F:329:ILE:CD1	2.71	0.52
1:A:10:VAL:HG21	1:A:153:TRP:CH2	2.37	0.51
1:A:223:LYS:HA	1:A:227:PHE:CZ	2.45	0.51
2:B:106:VAL:HA	2:B:190:GLY:HA2	1.91	0.51
2:B:320:ASP:OD2	2:B:322:SER:HB3	2.11	0.51
2:B:423:VAL:CG2	2:B:426:TRP:CD1	2.93	0.51
1:E:5:ILE:HG22	1:E:6:GLU:N	2.25	0.51
2:F:254:VAL:HG23	2:F:291:GLU:O	2.08	0.51
2:F:3:SER:N	2:F:4:PRO:HD3	2.26	0.51
2:F:5:ILE:O	2:F:6:GLU:HG3	2.10	0.51
1:A:384:GLY:O	2:B:27:THR:CG2	2.58	0.51
2:B:61:PHE:CZ	2:B:411:ILE:HD11	2.44	0.51
3:C:723:DC:C2'	3:C:724:DT:H71	2.40	0.51
1:E:209:LEU:O	1:E:212:TRP:N	2.43	0.51
2:B:427:TYR:O	2:B:428:GLN:C	2.48	0.51
1:E:115:TYR:HE2	4:H:823:ATM:C1'	2.23	0.51
1:E:342:TYR:HB2	1:E:347:LYS:O	2.11	0.51
1:E:439:THR:HA	1:E:494:ASN:HB2	1.93	0.51
2:F:382:ILE:HG22	2:F:383:TRP:NE1	2.25	0.51
2:F:402:TRP:CH2	2:F:411:ILE:CD1	2.85	0.51
4:H:818:DC:H2'	4:H:819:DG:H8	1.76	0.51
2:B:125:ARG:NH1	2:B:147:ASN:HD22	1.98	0.51
2:B:115:TYR:O	2:B:149:LEU:HB2	2.10	0.51
2:B:170:PRO:O	2:B:174:GLN:HG2	2.10	0.51
1:E:246:LEU:HD22	1:E:310:LEU:HD12	1.91	0.51
1:E:92:LEU:HD11	2:F:133:PRO:HB3	1.91	0.51
2:F:331:LYS:HG2	2:F:332:GLN:N	2.26	0.51
1:E:242:GLN:O	1:E:244:ILE:N	2.44	0.51
1:E:466:VAL:O	1:E:466:VAL:CG2	2.58	0.51
2:F:27:THR:O	2:F:31:ILE:CG1	2.58	0.51
2:F:70:LYS:HE2	2:F:70:LYS:HA	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:378:GLU:O	2:B:382:ILE:CG1	2.57	0.51
2:B:92:LEU:CB	2:B:158:ALA:HB1	2.41	0.51
2:B:109:LEU:O	2:B:186:ASP:HA	2.11	0.51
1:E:49:LYS:N	1:E:144:TYR:HD1	2.08	0.51
1:A:473:THR:OG1	1:A:476:LYS:HG3	2.11	0.51
1:A:96:HIS:H	2:B:136:ASN:HD21	1.58	0.51
2:B:120:LEU:HB2	2:B:147:ASN:O	2.10	0.51
1:E:3:SER:HA	1:E:119:PRO:HG3	1.91	0.51
1:A:501:TYR:C	1:A:501:TYR:HD1	2.15	0.51
2:F:72:ARG:NH2	2:F:151:GLN:HE21	2.08	0.51
1:A:156:SER:HB2	1:A:157:PRO:HD3	1.93	0.51
1:A:515:SER:O	1:A:517:LEU:N	2.41	0.51
1:A:458:VAL:HG12	1:A:548:VAL:HG21	1.93	0.51
2:B:8:VAL:HB	2:B:159:ILE:HD12	1.92	0.51
1:E:115:TYR:CE2	4:H:823:ATM:C1'	2.94	0.50
1:A:171:PHE:HD1	1:A:208:HIS:CD2	2.30	0.50
1:A:61:PHE:CE1	1:A:74:LEU:CB	2.93	0.50
1:E:180:ILE:O	1:E:180:ILE:CG2	2.59	0.50
1:A:326:ILE:HD11	1:A:343:GLN:HA	1.93	0.50
1:A:223:LYS:HA	1:A:227:PHE:HZ	1.76	0.50
1:A:469:LEU:HD12	1:A:472:THR:HG21	1.89	0.50
1:A:284:ARG:HB3	3:C:714:DG:OP1	2.11	0.50
1:E:10:VAL:HG21	1:E:153:TRP:CH2	2.35	0.50
1:A:142:ILE:CD1	1:A:142:ILE:N	2.70	0.50
1:A:467:VAL:HB	1:A:468:PRO:HD2	1.93	0.50
1:A:61:PHE:CD1	1:A:74:LEU:HB2	2.47	0.50
2:B:213:GLY:C	2:B:214:LEU:HD12	2.31	0.50
1:E:156:SER:N	1:E:157:PRO:CD	2.74	0.50
1:E:496:VAL:HG12	1:E:534:ALA:HB3	1.94	0.50
1:A:7:THR:HB	1:A:121:ASP:HA	1.93	0.50
1:A:209:LEU:HD22	1:A:214:LEU:CD2	2.34	0.50
2:B:119:PRO:HA	2:B:148:VAL:HA	1.94	0.50
1:A:95:PRO:HA	2:B:136:ASN:O	2.11	0.50
2:B:260:LEU:O	2:B:260:LEU:HD23	2.11	0.50
2:B:94:ILE:CD1	2:B:94:ILE:N	2.73	0.50
1:E:115:TYR:HD2	4:H:823:ATM:C2'	2.22	0.50
1:E:264:LEU:HD23	1:E:276:VAL:HG12	1.94	0.50
1:E:3:SER:N	1:E:4:PRO:HD3	2.27	0.50
1:E:501:TYR:C	1:E:501:TYR:HD1	2.15	0.50
2:F:423:VAL:HG22	2:F:426:TRP:HD1	1.75	0.50
3:G:717:DC:H1'	3:G:718:DA:H5'	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:73:LYS:NZ	2:B:146:TYR:OH	2.37	0.50
1:E:276:VAL:O	1:E:276:VAL:HG23	2.11	0.50
4:H:818:DC:H2''	4:H:819:DG:C5'	2.39	0.50
1:E:266:TRP:CE2	4:H:820:DC:H4'	2.46	0.50
1:A:84:THR:HG21	1:A:153:TRP:HZ2	1.74	0.50
2:B:58:THR:CG2	2:B:59:PRO:HD2	2.42	0.50
4:D:819:DG:H2'	4:D:820:DC:C6	2.47	0.50
1:E:522:ILE:O	1:E:526:ILE:HG13	2.12	0.50
1:A:325:LEU:HD23	1:A:387:PRO:HB3	1.94	0.49
3:C:707:DG:H2'	3:C:708:DG:H8	1.77	0.49
1:A:115:TYR:HD2	4:D:823:ATM:H2'	1.75	0.49
1:A:465:LYS:HA	1:E:464:GLN:O	2.12	0.49
1:A:180:ILE:CG2	1:A:180:ILE:O	2.59	0.49
1:A:301:LEU:O	1:A:305:GLU:HG2	2.12	0.49
1:A:329:ILE:HG23	1:A:339:TYR:HB3	1.93	0.49
1:A:446:ALA:HB2	1:A:477:THR:CG2	2.42	0.49
1:A:65:LYS:HD2	1:A:70:ARG:CB	2.42	0.49
2:B:312:GLU:O	2:B:313:PRO:O	2.30	0.49
2:F:134:SER:OG	2:F:138:GLU:HB3	2.12	0.49
1:A:231:GLY:HA3	4:D:821:DC:H5''	1.93	0.49
2:B:335:GLY:HA3	2:B:356:ARG:HD2	1.93	0.49
1:E:434:ILE:CD1	1:E:434:ILE:N	2.75	0.49
2:F:356:ARG:HG2	2:F:357:MET:N	2.28	0.49
1:A:326:ILE:HG22	1:A:388:LYS:HB2	1.94	0.49
1:E:364:ASP:HB3	1:E:423:VAL:HG13	1.94	0.49
1:A:469:LEU:HD13	1:A:472:THR:CG2	2.39	0.49
1:A:115:TYR:HE2	4:D:823:ATM:H1'	1.70	0.49
1:A:401:TRP:CZ3	1:A:405:TYR:CG	3.00	0.49
2:B:398:TRP:HZ3	2:B:414:TRP:CH2	2.29	0.49
1:A:464:GLN:HB3	1:E:466:VAL:CG1	2.40	0.49
1:E:501:TYR:O	1:E:501:TYR:HD1	1.96	0.49
2:F:339:TYR:CZ	2:F:375:ILE:HD12	2.47	0.49
1:A:38:CYS:SG	1:A:132:ILE:HD12	2.52	0.49
2:B:254:VAL:O	2:B:258:GLN:HG2	2.12	0.49
4:D:807:DC:C2	4:D:808:DC:C5	3.00	0.49
2:F:148:VAL:O	2:F:149:LEU:C	2.51	0.49
2:F:369:THR:O	2:F:373:GLN:HG3	2.13	0.49
2:F:423:VAL:HG23	2:F:426:TRP:CD1	2.48	0.49
2:B:125:ARG:NH1	2:B:147:ASN:HA	2.28	0.49
2:B:92:LEU:HB3	2:B:158:ALA:HB1	1.93	0.49
2:B:194:GLU:HG3	2:B:195:ILE:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:108:VAL:HB	1:E:221:HIS:HD2	1.76	0.49
2:F:424:LYS:O	2:F:425:LEU:O	2.30	0.49
1:E:108:VAL:H	1:E:221:HIS:HB2	1.78	0.49
1:E:142:ILE:CD1	1:E:142:ILE:N	2.57	0.49
1:E:248:GLU:HA	1:E:252:TRP:HH2	1.77	0.49
2:F:156:SER:HB2	2:F:157:PRO:HD3	1.93	0.49
1:A:10:VAL:HG11	1:A:153:TRP:CZ2	2.48	0.49
2:B:266:TRP:CZ2	2:B:422:LEU:HD12	2.48	0.49
2:B:87:PHE:CE1	2:B:92:LEU:HD23	2.47	0.49
2:F:8:VAL:HG11	2:F:159:ILE:HD13	1.95	0.49
2:B:180:ILE:C	2:B:180:ILE:HD12	2.33	0.48
4:D:818:DC:H2'	4:D:819:DG:C8	2.48	0.48
1:E:111:VAL:HB	1:E:185:ASP:HB2	1.95	0.48
2:F:50:ILE:HD12	2:F:143:ARG:HB3	1.95	0.48
1:E:50:ILE:H	1:E:143:ARG:HG2	1.78	0.48
1:E:178:ILE:HD12	1:E:178:ILE:O	2.13	0.48
1:E:371:ALA:O	1:E:375:ILE:CD1	2.54	0.48
2:F:183:TYR:CG	2:F:380:ILE:HG21	2.48	0.48
2:F:371:ALA:O	2:F:375:ILE:HG12	2.13	0.48
2:F:94:ILE:N	2:F:94:ILE:CD1	2.76	0.48
1:A:108:VAL:HG22	1:A:188:TYR:HA	1.95	0.48
1:A:2:ILE:HD12	1:A:45:GLY:O	2.14	0.48
2:B:24:TRP:CH2	2:B:403:THR:HG21	2.48	0.48
2:B:270:ILE:CG2	2:B:314:VAL:HG21	2.39	0.48
1:E:465:LYS:HD3	1:E:488:ASP:OD2	2.13	0.48
1:A:84:THR:HG21	1:A:153:TRP:HE1	1.79	0.48
2:B:260:LEU:O	2:B:264:LEU:HB2	2.14	0.48
1:E:224:GLU:HB3	1:E:225:PRO:HD2	1.95	0.48
1:A:115:TYR:O	1:A:149:LEU:HB3	2.14	0.48
1:A:3:SER:N	1:A:4:PRO:HD3	2.29	0.48
2:F:23:GLN:NE2	2:F:26:LEU:HD11	2.27	0.48
4:H:809:DC:H1'	4:H:810:DT:H5'	1.95	0.48
1:A:282:LEU:HD11	1:A:296:THR:OG1	2.13	0.48
3:C:710:DG:C6	3:C:711:DC:N4	2.82	0.48
1:E:170:PRO:O	1:E:174:GLN:HG2	2.13	0.48
1:A:453:GLY:O	1:A:469:LEU:CB	2.54	0.48
1:A:99:GLY:HA2	1:A:383:TRP:NE1	2.29	0.48
4:D:809:DC:H1'	4:D:810:DT:C5'	2.44	0.48
1:E:49:LYS:N	1:E:144:TYR:CD1	2.82	0.48
2:F:120:LEU:HB2	2:F:147:ASN:O	2.14	0.48
1:A:108:VAL:H	1:A:221:HIS:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:HIS:N	2:B:136:ASN:OD1	2.46	0.48
2:B:84:THR:CG2	2:B:87:PHE:HB3	2.43	0.48
1:E:342:TYR:HD2	1:E:344:GLU:O	1.96	0.48
2:B:156:SER:HB2	2:B:157:PRO:HD3	1.96	0.47
2:B:363:ASN:ND2	2:B:366:LYS:HB2	2.29	0.47
1:E:156:SER:CB	1:E:157:PRO:HD3	2.44	0.47
2:F:260:LEU:O	2:F:260:LEU:HD23	2.14	0.47
2:F:389:PHE:O	2:F:391:LEU:HG	2.13	0.47
4:H:808:DC:H2''	4:H:809:DC:H5'	1.95	0.47
1:A:73:LYS:NZ	1:A:130:PHE:CE2	2.67	0.47
1:A:264:LEU:HD21	1:A:306:ASN:ND2	2.23	0.47
2:B:148:VAL:O	2:B:149:LEU:C	2.53	0.47
2:B:423:VAL:HG23	2:B:426:TRP:CD1	2.49	0.47
1:E:73:LYS:NZ	1:E:130:PHE:CE2	2.75	0.47
1:E:540:LYS:HB3	1:E:542:ILE:HD11	1.95	0.47
2:B:94:ILE:HD12	2:B:161:GLN:OE1	2.15	0.47
1:E:326:ILE:HG22	1:E:388:LYS:HB2	1.96	0.47
1:A:282:LEU:N	1:A:282:LEU:HD22	2.30	0.47
1:A:380:ILE:HD11	1:A:386:THR:HG22	1.95	0.47
2:B:328:GLU:HB3	2:B:340:GLN:HG3	1.95	0.47
1:E:225:PRO:HB2	1:E:226:PRO:CD	2.44	0.47
1:E:280:SER:HA	1:E:283:LEU:HD23	1.97	0.47
1:E:363:ASN:HB3	1:E:366:LYS:HB2	1.96	0.47
1:E:86:ASP:O	2:F:55:PRO:HB3	2.14	0.47
1:A:206:ARG:HG3	1:A:216:THR:OG1	2.15	0.47
1:A:500:GLN:O	1:A:501:TYR:C	2.51	0.47
1:A:553:SER:O	1:A:554:ALA:CB	2.63	0.47
1:A:90:VAL:HG12	1:A:90:VAL:O	2.13	0.47
2:B:329:ILE:N	2:B:329:ILE:CD1	2.70	0.47
1:E:419:THR:HG23	1:E:419:THR:O	2.14	0.47
1:A:172:LYS:NZ	2:B:139:THR:HG21	2.29	0.47
2:B:114:ALA:HB2	2:B:214:LEU:CD2	2.45	0.47
4:D:808:DC:H2''	4:D:809:DC:O5'	2.15	0.47
1:E:153:TRP:CG	1:E:154:LYS:N	2.82	0.47
1:E:544:GLY:H	1:E:547:GLN:NE2	2.10	0.47
4:H:808:DC:H2''	4:H:809:DC:C5'	2.45	0.47
1:A:106:VAL:HG23	1:A:227:PHE:HE1	1.79	0.47
1:A:32:LYS:HZ1	1:A:135:ILE:HD11	1.79	0.47
1:A:223:LYS:HE3	1:A:223:LYS:HB2	1.49	0.47
2:B:357:MET:HE3	2:B:357:MET:HB3	1.85	0.47
2:B:409:THR:O	2:B:409:THR:OG1	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:THR:HG21	2:B:153:TRP:CZ2	2.49	0.47
1:E:225:PRO:CB	1:E:226:PRO:HD3	2.43	0.47
2:F:27:THR:OG1	2:F:30:LYS:HG2	2.15	0.47
2:F:357:MET:O	2:F:358:ARG:C	2.52	0.47
2:F:402:TRP:HH2	2:F:411:ILE:HD12	1.79	0.47
1:E:32:LYS:NZ	1:E:135:ILE:CD1	2.78	0.47
2:F:27:THR:H	2:F:30:LYS:CE	2.28	0.47
1:A:414:TRP:HE3	1:A:415:GLU:O	1.98	0.47
1:A:501:TYR:O	1:A:501:TYR:HD1	1.98	0.47
1:E:340:GLN:HA	1:E:351:THR:HA	1.97	0.47
1:E:437:ALA:HB2	1:E:492:GLU:HB3	1.96	0.47
2:F:8:VAL:HB	2:F:159:ILE:CD1	2.45	0.47
2:F:359:GLY:O	2:F:360:ALA:CB	2.63	0.47
3:C:714:DG:C4	3:C:715:DA:N7	2.83	0.47
1:E:277:ARG:HB2	1:E:336:GLN:HE21	1.80	0.47
1:A:522:ILE:O	1:A:526:ILE:HG13	2.14	0.46
2:B:184:MET:HB3	2:B:185:ASP:OD1	2.15	0.46
4:D:809:DC:H1'	4:D:810:DT:H5'	1.96	0.46
1:E:19:PRO:HD3	1:E:80:LEU:HD13	1.97	0.46
4:H:809:DC:H1'	4:H:810:DT:C5'	2.45	0.46
4:H:818:DC:H2'	4:H:819:DG:C8	2.50	0.46
1:A:280:SER:C	1:A:282:LEU:H	2.19	0.46
2:B:252:TRP:CE3	2:B:252:TRP:HA	2.50	0.46
2:B:85:GLN:HA	2:B:88:TRP:CE2	2.49	0.46
1:A:233:GLU:HB3	1:A:240:THR:CG2	2.46	0.46
1:E:341:ILE:O	1:E:349:LEU:HB2	2.15	0.46
1:A:56:TYR:O	1:A:129:ALA:HB3	2.15	0.46
2:B:8:VAL:HG21	2:B:159:ILE:HG23	1.97	0.46
2:B:92:LEU:N	2:B:92:LEU:HD22	2.31	0.46
1:E:317:VAL:HG12	1:E:348:ASN:O	2.15	0.46
1:E:376:THR:C	1:E:378:GLU:H	2.19	0.46
1:E:90:VAL:CG1	2:F:140:PRO:HB2	2.45	0.46
1:A:384:GLY:HA2	2:B:27:THR:HA	1.98	0.46
2:B:180:ILE:HG22	2:B:189:VAL:HA	1.96	0.46
1:E:380:ILE:HD11	1:E:386:THR:HG22	1.98	0.46
1:E:77:PHE:HB3	1:E:80:LEU:HB3	1.97	0.46
1:A:254:VAL:HG21	1:A:287:LYS:HB3	1.97	0.46
1:E:114:ALA:HB1	1:E:160:PHE:CZ	2.51	0.46
2:F:423:VAL:HG22	2:F:426:TRP:CD1	2.51	0.46
1:A:170:PRO:O	1:A:174:GLN:HG2	2.16	0.46
2:B:3:SER:OG	2:B:4:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:LYS:O	1:A:147:ASN:HB3	2.16	0.46
1:E:113:ASP:HA	4:H:823:ATM:N5'	2.30	0.46
1:E:98:ALA:O	1:E:319:TYR:HB2	2.15	0.46
1:E:517:LEU:O	1:E:521:ILE:HG13	2.15	0.46
2:F:358:ARG:HB3	2:F:359:GLY:H	1.57	0.46
1:A:234:LEU:HD12	1:A:234:LEU:N	2.31	0.46
1:A:496:VAL:HG12	1:A:534:ALA:HB3	1.97	0.46
2:B:326:ILE:HD12	2:B:326:ILE:N	2.31	0.46
1:E:329:ILE:CD1	1:E:375:ILE:HD13	2.45	0.46
2:F:23:GLN:HG2	2:F:133:PRO:CG	2.46	0.46
2:F:376:THR:O	2:F:379:SER:HB2	2.15	0.46
1:A:4:PRO:HG2	1:A:5:ILE:HD12	1.98	0.46
1:E:264:LEU:HD23	1:E:276:VAL:CG1	2.46	0.46
1:E:407:GLN:OE1	2:F:418:ASN:HA	2.16	0.46
1:E:409:THR:O	1:E:410:TRP:HB2	2.16	0.46
4:H:808:DC:H2''	4:H:809:DC:O5'	2.17	0.46
1:A:239:TRP:NE1	1:A:316:GLY:HA3	2.32	0.45
1:A:61:PHE:HE2	1:A:76:ASP:HB2	1.81	0.45
1:E:217:PRO:C	1:E:219:GLN:N	2.68	0.45
1:A:266:TRP:CD2	4:D:820:DC:H4'	2.51	0.45
2:B:180:ILE:HA	2:B:188:TYR:O	2.16	0.45
2:B:37:ILE:CG2	2:B:38:CYS:N	2.79	0.45
2:F:76:ASP:C	2:F:78:ARG:H	2.18	0.45
1:A:75:VAL:CG2	1:A:146:TYR:HE1	2.18	0.45
1:A:409:THR:O	1:A:410:TRP:HB2	2.16	0.45
1:A:466:VAL:HG13	1:E:464:GLN:HB2	1.99	0.45
2:B:46:LYS:HE3	2:B:116:PHE:HB3	1.97	0.45
3:C:718:DA:C2	4:D:811:DG:C2	3.04	0.45
4:D:820:DC:H2'	4:D:821:DC:C6	2.52	0.45
1:E:343:GLN:HG2	1:E:349:LEU:HD21	1.98	0.45
2:F:97:PRO:CG	2:F:100:LEU:HB2	2.39	0.45
1:A:506:ILE:O	1:A:507:GLN:C	2.54	0.45
1:E:333:GLY:H	1:E:336:GLN:HB2	1.82	0.45
2:F:58:THR:HG23	2:F:59:PRO:HD2	1.97	0.45
1:A:19:PRO:HD3	1:A:80:LEU:HD13	1.99	0.45
2:B:206:ARG:HB2	2:B:206:ARG:NH1	2.31	0.45
1:E:215:TYR:CZ	1:E:217:PRO:HA	2.52	0.45
2:F:160:PHE:CD2	2:F:160:PHE:O	2.70	0.45
3:G:722:DA:C4	3:G:723:DC:C5	3.03	0.45
1:A:235:HIS:HB3	1:A:236:PRO:HD2	1.98	0.45
2:F:76:ASP:OD1	2:F:78:ARG:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:49:LYS:CB	1:E:144:TYR:CD1	2.99	0.45
1:E:381:VAL:HG22	2:F:25:PRO:HG2	1.97	0.45
2:F:194:GLU:HG3	2:F:195:ILE:N	2.31	0.45
1:A:217:PRO:C	1:A:219:GLN:H	2.19	0.45
1:A:269:GLN:O	1:A:351:THR:N	2.48	0.45
1:A:458:VAL:CG1	1:A:548:VAL:CG2	2.95	0.45
2:B:88:TRP:CZ3	2:B:89:GLU:HB2	2.52	0.45
1:A:380:ILE:HD11	1:A:386:THR:CG2	2.47	0.45
2:B:110:ASP:HB3	2:B:216:THR:CG2	2.46	0.45
1:E:221:HIS:CE1	1:E:228:LEU:N	2.85	0.45
2:F:109:LEU:O	2:F:186:ASP:HA	2.17	0.45
1:A:537:PRO:HB2	1:A:540:LYS:CB	2.45	0.45
2:B:150:PRO:HG2	2:B:153:TRP:CB	2.47	0.45
2:B:317:VAL:HG13	2:B:317:VAL:O	2.17	0.45
4:D:815:DG:C6	4:D:816:DG:O6	2.70	0.45
1:E:159:ILE:HD13	2:F:52:PRO:HG2	1.99	0.45
2:F:260:LEU:O	2:F:264:LEU:HB2	2.18	0.45
4:H:820:DC:H2''	4:H:821:DC:H5'	1.98	0.45
1:A:2:ILE:CD1	1:A:148:VAL:CG1	2.96	0.44
1:E:414:TRP:HE3	1:E:415:GLU:O	2.01	0.44
2:F:125:ARG:NH1	2:F:147:ASN:HA	2.31	0.44
1:A:406:TRP:HD1	1:A:407:GLN:HG2	1.81	0.44
2:B:24:TRP:HH2	2:B:403:THR:HG21	1.82	0.44
1:E:283:LEU:HD22	1:E:283:LEU:N	2.31	0.44
2:F:156:SER:N	2:F:157:PRO:CD	2.79	0.44
1:E:434:ILE:HD13	1:E:434:ILE:N	2.31	0.44
2:F:24:TRP:HA	2:F:25:PRO:HD3	1.89	0.44
2:F:281:LYS:HE2	2:F:284:ARG:HD2	1.99	0.44
1:A:282:LEU:N	1:A:282:LEU:CD2	2.81	0.44
1:A:333:GLY:H	1:A:336:GLN:HB2	1.83	0.44
1:E:171:PHE:HD1	1:E:208:HIS:CD2	2.35	0.44
1:E:90:VAL:HG12	1:E:90:VAL:O	2.16	0.44
1:A:2:ILE:HD13	1:A:148:VAL:CG1	2.47	0.44
1:A:401:TRP:CZ3	1:A:405:TYR:HB2	2.52	0.44
2:B:206:ARG:HB2	2:B:206:ARG:HH11	1.83	0.44
2:B:57:ASN:O	2:B:58:THR:OG1	2.33	0.44
1:E:233:GLU:HB3	1:E:240:THR:HG23	2.00	0.44
2:F:29:GLU:HG2	2:F:29:GLU:H	1.46	0.44
4:H:806:DT:H1'	4:H:807:DC:H5'	1.98	0.44
1:A:121:ASP:O	1:A:125:ARG:HD2	2.17	0.44
1:A:178:ILE:C	1:A:178:ILE:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:PRO:CB	1:A:226:PRO:HD3	2.46	0.44
1:A:221:HIS:HE1	1:A:228:LEU:N	2.16	0.44
1:A:422:LEU:HD23	1:A:422:LEU:H	1.81	0.44
1:A:536:VAL:HG12	1:A:537:PRO:HD2	1.99	0.44
2:B:110:ASP:HB3	2:B:216:THR:HG22	1.99	0.44
2:B:333:GLY:C	2:B:335:GLY:H	2.20	0.44
4:D:810:DT:H2'	4:D:810:DT:H6	1.54	0.44
1:E:401:TRP:O	1:E:401:TRP:HE3	2.01	0.44
1:E:94:ILE:HA	1:E:95:PRO:HD3	1.85	0.44
2:F:125:ARG:NH1	2:F:147:ASN:ND2	2.60	0.44
2:F:382:ILE:HG22	2:F:383:TRP:CD1	2.53	0.44
1:A:246:LEU:CD1	1:A:307:ARG:HG3	2.41	0.44
1:E:296:THR:HG22	1:E:297:GLU:N	2.33	0.44
2:F:106:VAL:HA	2:F:190:GLY:HA2	2.00	0.44
2:F:183:TYR:CZ	2:F:380:ILE:HD13	2.53	0.44
1:A:107:THR:CG2	1:A:223:LYS:HG2	2.47	0.44
1:A:493:VAL:HG12	1:A:494:ASN:N	2.33	0.44
2:B:179:VAL:HG12	2:B:180:ILE:N	2.33	0.44
2:B:351:THR:OG1	2:B:351:THR:O	2.30	0.44
1:E:248:GLU:HA	1:E:252:TRP:CH2	2.52	0.44
2:F:161:GLN:O	2:F:165:THR:HG23	2.18	0.44
2:F:336:GLN:C	2:F:337:TRP:CD1	2.91	0.44
2:F:340:GLN:HG2	2:F:341:ILE:N	2.32	0.44
1:A:32:LYS:NZ	1:A:135:ILE:HD11	2.33	0.44
1:A:401:TRP:O	1:A:401:TRP:HE3	2.01	0.44
2:B:142:ILE:HG12	2:B:142:ILE:H	1.50	0.44
2:B:210:LEU:CD1	2:B:215:THR:OG1	2.66	0.44
2:B:104:LYS:O	2:B:235:HIS:HB3	2.18	0.44
2:B:398:TRP:C	2:B:400:THR:H	2.21	0.44
3:C:712:DC:O2	4:D:817:MRG:H211	2.17	0.44
1:E:453:GLY:O	1:E:469:LEU:HB2	2.17	0.44
1:E:99:GLY:HA2	1:E:383:TRP:NE1	2.30	0.44
1:A:280:SER:C	1:A:282:LEU:N	2.71	0.43
1:A:457:TYR:OH	1:A:488:ASP:OD2	2.29	0.43
2:B:29:GLU:H	2:B:29:GLU:HG2	1.43	0.43
1:A:77:PHE:HB3	1:A:80:LEU:HB3	1.99	0.43
2:B:281:LYS:HE2	2:B:284:ARG:HD2	2.00	0.43
2:B:38:CYS:O	2:B:42:GLU:N	2.51	0.43
1:E:380:ILE:HD11	1:E:386:THR:CG2	2.48	0.43
1:E:384:GLY:CA	2:F:27:THR:HA	2.48	0.43
1:A:364:ASP:HB3	1:A:423:VAL:HG13	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LYS:HG2	1:A:414:TRP:CH2	2.53	0.43
2:B:360:ALA:O	2:B:361:HIS:CD2	2.72	0.43
2:B:26:LEU:HD21	2:B:60:VAL:O	2.18	0.43
1:E:225:PRO:HB3	1:E:235:HIS:CD2	2.53	0.43
1:E:326:ILE:HG12	1:E:342:TYR:O	2.17	0.43
1:E:422:LEU:H	1:E:422:LEU:HD23	1.83	0.43
1:E:506:ILE:CD1	1:E:506:ILE:N	2.81	0.43
3:G:714:DG:C4	3:G:715:DA:N7	2.86	0.43
1:A:183:TYR:CD2	1:A:230:MET:SD	3.11	0.43
1:A:368:LEU:O	1:A:368:LEU:HD23	2.17	0.43
1:A:498:ASP:HB2	1:A:538:ALA:HA	2.00	0.43
2:B:391:LEU:HA	2:B:392:PRO:HD2	1.84	0.43
2:B:398:TRP:C	2:B:400:THR:N	2.70	0.43
1:A:262:GLY:C	4:D:819:DG:H4'	2.39	0.43
1:E:262:GLY:C	4:H:819:DG:H4'	2.38	0.43
1:A:120:LEU:HD23	1:A:125:ARG:HG3	2.01	0.43
1:A:278:GLN:O	1:A:281:LYS:N	2.50	0.43
1:A:92:LEU:O	1:A:93:GLY:C	2.56	0.43
2:B:389:PHE:O	2:B:391:LEU:HG	2.17	0.43
4:D:808:DC:C2'	4:D:809:DC:H5'	2.49	0.43
2:F:114:ALA:HB2	2:F:214:LEU:HD21	2.00	0.43
3:G:723:DC:C2'	3:G:724:DT:H71	2.49	0.43
1:A:13:LYS:HA	1:A:14:PRO:HD2	1.84	0.43
1:A:209:LEU:CD2	1:A:214:LEU:HD22	2.35	0.43
2:B:295:LEU:HG	2:B:299:ALA:HB3	2.00	0.43
1:E:150:PRO:HB2	1:E:153:TRP:HB2	1.99	0.43
1:A:242:GLN:O	1:A:244:ILE:N	2.51	0.43
1:A:433:PRO:HD3	2:B:255:ASN:OD1	2.18	0.43
2:B:101:LYS:O	2:B:236:PRO:HB2	2.18	0.43
2:F:206:ARG:HB2	2:F:206:ARG:HH11	1.84	0.43
1:A:503:LEU:HD11	1:A:507:GLN:HE21	1.84	0.43
3:C:715:DA:C2	3:C:716:DA:C4	3.07	0.43
4:D:806:DT:H5'	4:D:806:DT:H6	1.84	0.43
2:F:363:ASN:HD21	2:F:365:VAL:HG23	1.84	0.43
4:H:820:DC:H2'	4:H:821:DC:C6	2.54	0.43
1:A:406:TRP:HH2	1:A:507:GLN:HB3	1.84	0.43
2:B:46:LYS:HG2	2:B:148:VAL:HG21	2.01	0.43
1:E:46:LYS:C	1:E:47:ILE:HG12	2.39	0.43
1:E:500:GLN:O	1:E:501:TYR:C	2.57	0.43
1:A:317:VAL:HG12	1:A:349:LEU:HD22	2.00	0.43
1:A:377:THR:OG1	2:B:400:THR:HG22	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:434:ILE:HG13	1:E:530:LYS:HE2	2.01	0.43
2:F:8:VAL:CB	2:F:159:ILE:CD1	2.96	0.43
2:F:206:ARG:NH1	2:F:206:ARG:HB2	2.34	0.43
2:F:363:ASN:ND2	2:F:365:VAL:HG23	2.34	0.43
2:F:380:ILE:O	2:F:384:GLY:HA2	2.18	0.43
2:B:156:SER:HB2	2:B:157:PRO:CD	2.48	0.42
3:C:714:DG:C2	3:C:715:DA:C5	3.06	0.42
2:F:295:LEU:HG	2:F:299:ALA:HB3	2.01	0.42
4:H:819:DG:H2'	4:H:820:DC:C6	2.54	0.42
1:A:376:THR:C	1:A:378:GLU:N	2.72	0.42
2:B:332:GLN:HB3	2:B:428:GLN:HE22	1.84	0.42
2:F:88:TRP:CZ3	2:F:89:GLU:HB2	2.53	0.42
3:G:715:DA:C2	3:G:716:DA:C4	3.07	0.42
2:B:65:LYS:HA	2:B:407:GLN:HG2	2.00	0.42
1:E:225:PRO:O	1:E:227:PHE:N	2.52	0.42
1:E:239:TRP:NE1	1:E:316:GLY:HA3	2.34	0.42
1:E:506:ILE:O	1:E:507:GLN:C	2.57	0.42
3:G:724:DT:H2''	3:G:725:DG:N7	2.34	0.42
1:A:363:ASN:HB3	1:A:366:LYS:CB	2.48	0.42
2:B:332:GLN:NE2	2:B:428:GLN:HB2	2.34	0.42
1:E:548:VAL:O	1:E:552:VAL:HG22	2.19	0.42
3:G:712:DC:O2	4:H:817:MRG:H211	2.18	0.42
1:A:253:THR:H	1:A:256:ASP:HB2	1.84	0.42
2:B:186:ASP:N	2:B:186:ASP:OD1	2.52	0.42
2:B:194:GLU:HG3	2:B:196:GLY:H	1.84	0.42
3:C:707:DG:C6	4:D:822:DA:N1	2.88	0.42
1:E:239:TRP:CD1	1:E:316:GLY:C	2.93	0.42
1:E:498:ASP:HB2	1:E:538:ALA:HA	2.02	0.42
2:F:180:ILE:HA	2:F:188:TYR:O	2.19	0.42
1:A:116:PHE:HE1	1:A:146:TYR:HE2	1.68	0.42
1:A:225:PRO:N	1:A:226:PRO:HD2	2.34	0.42
1:A:317:VAL:O	1:A:349:LEU:HD13	2.19	0.42
1:A:450:THR:O	1:A:451:LYS:HB2	2.19	0.42
1:A:47:ILE:HD12	1:A:144:TYR:CD1	2.55	0.42
2:B:107:THR:OG1	2:B:202:ILE:HD11	2.20	0.42
3:C:716:DA:C2	3:C:717:DC:C2	3.07	0.42
1:E:142:ILE:HB	1:E:144:TYR:CE2	2.54	0.42
1:E:373:GLN:HE21	2:F:396:GLU:HG3	1.85	0.42
2:F:252:TRP:CE3	2:F:252:TRP:HA	2.53	0.42
2:F:8:VAL:CB	2:F:159:ILE:HD13	2.50	0.42
1:A:185:ASP:OD2	4:D:823:ATM:OP1	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:372:VAL:HG11	1:E:411:ILE:HG23	2.01	0.42
1:E:429:LEU:HD11	1:E:506:ILE:HG22	2.02	0.42
1:A:115:TYR:CD1	1:A:149:LEU:HD23	2.55	0.42
1:A:2:ILE:HD11	1:A:46:LYS:HD3	2.01	0.42
1:A:474:ASN:O	1:A:477:THR:OG1	2.31	0.42
1:A:96:HIS:O	2:B:136:ASN:ND2	2.48	0.42
2:B:398:TRP:CZ3	2:B:414:TRP:CZ2	2.89	0.42
1:E:244:ILE:HG23	1:E:244:ILE:O	2.18	0.42
1:E:254:VAL:HG21	1:E:287:LYS:HB3	2.02	0.42
1:E:325:LEU:HD23	1:E:387:PRO:HB3	2.01	0.42
1:A:464:GLN:O	1:E:465:LYS:HA	2.20	0.42
2:F:330:GLN:HE21	2:F:330:GLN:HB2	1.60	0.42
2:F:403:THR:O	2:F:405:TYR:N	2.53	0.42
1:A:267:ALA:HB1	1:A:271:TYR:CD2	2.54	0.42
1:A:285:GLY:O	1:A:287:LYS:N	2.53	0.42
1:E:201:LYS:HA	1:E:201:LYS:HD3	1.92	0.42
1:E:206:ARG:HH21	1:E:215:TYR:HE1	1.66	0.42
1:E:283:LEU:H	1:E:283:LEU:CD2	2.32	0.42
1:E:480:GLN:O	1:E:483:TYR:N	2.51	0.42
1:E:501:TYR:O	1:E:505:ILE:HD13	2.20	0.42
2:F:288:ALA:HB3	2:F:291:GLU:HB2	2.02	0.42
4:H:822:DA:H2''	4:H:823:ATM:C5'	2.49	0.42
1:A:2:ILE:CD1	1:A:46:LYS:HA	2.46	0.41
1:A:478:GLU:OE2	1:A:498:ASP:OD1	2.38	0.41
2:B:391:LEU:O	2:B:393:ILE:N	2.50	0.41
2:B:85:GLN:O	2:B:89:GLU:HB3	2.20	0.41
3:C:707:DG:C2'	3:C:708:DG:O5'	2.68	0.41
1:E:116:PHE:C	1:E:148:VAL:HG21	2.40	0.41
1:E:275:LYS:C	1:E:276:VAL:HG13	2.40	0.41
2:F:343:GLN:HG2	2:F:349:LEU:HD11	2.02	0.41
2:F:57:ASN:O	2:F:58:THR:OG1	2.33	0.41
3:G:710:DG:C6	3:G:711:DC:N4	2.88	0.41
1:A:434:ILE:N	1:A:434:ILE:CD1	2.82	0.41
1:A:447:ASN:HB3	1:A:450:THR:OG1	2.20	0.41
2:B:332:GLN:HB3	2:B:428:GLN:NE2	2.35	0.41
1:E:411:ILE:HA	1:E:412:PRO:HD3	1.90	0.41
2:F:306:ASN:HA	2:F:309:ILE:HG22	2.02	0.41
2:B:27:THR:H	2:B:30:LYS:HE2	1.86	0.41
1:E:401:TRP:CZ3	1:E:405:TYR:CG	3.09	0.41
1:E:515:SER:O	1:E:517:LEU:N	2.45	0.41
2:F:142:ILE:HG12	2:F:142:ILE:H	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ARG:HD2	3:C:705:DA:H5''	2.01	0.41
1:E:116:PHE:HA	1:E:148:VAL:HG21	2.03	0.41
1:E:215:TYR:OH	1:E:217:PRO:HA	2.21	0.41
2:F:326:ILE:N	2:F:326:ILE:HD12	2.36	0.41
2:B:13:LYS:HA	2:B:14:PRO:HD3	1.95	0.41
2:B:257:ILE:O	2:B:261:VAL:HG23	2.20	0.41
1:A:108:VAL:HB	1:A:221:HIS:CD2	2.56	0.41
2:B:306:ASN:HA	2:B:309:ILE:HG22	2.02	0.41
4:D:807:DC:H1'	4:D:808:DC:H5''	2.03	0.41
1:E:115:TYR:CD2	4:H:823:ATM:C4'	3.02	0.41
1:E:234:LEU:N	1:E:234:LEU:HD12	2.35	0.41
1:E:303:LEU:HD23	1:E:303:LEU:O	2.20	0.41
2:F:380:ILE:CG2	2:F:384:GLY:HA2	2.51	0.41
1:A:12:LEU:HD11	1:A:127:TYR:CE1	2.55	0.41
1:A:156:SER:CB	1:A:157:PRO:HD3	2.49	0.41
1:A:368:LEU:C	1:A:368:LEU:HD23	2.41	0.41
1:A:407:GLN:OE1	2:B:418:ASN:HA	2.21	0.41
1:A:70:ARG:CG	1:A:70:ARG:HH11	2.29	0.41
2:B:203:GLU:O	2:B:207:GLN:HG2	2.20	0.41
3:C:714:DG:N3	3:C:715:DA:C8	2.88	0.41
4:D:817:MRG:C2	4:D:818:DC:C2	3.03	0.41
1:E:13:LYS:HA	1:E:14:PRO:HD2	1.87	0.41
1:E:277:ARG:HB2	1:E:336:GLN:NE2	2.36	0.41
2:F:333:GLY:C	2:F:335:GLY:H	2.23	0.41
1:A:276:VAL:O	1:A:276:VAL:HG23	2.20	0.41
2:B:325:LEU:CD1	2:B:343:GLN:HE21	2.31	0.41
2:B:94:ILE:HD11	2:B:158:ALA:HA	2.03	0.41
1:E:50:ILE:HG13	1:E:143:ARG:HG3	2.02	0.41
1:E:406:TRP:CE2	2:F:420:PRO:CB	2.85	0.41
1:A:466:VAL:HG13	1:E:464:GLN:CB	2.51	0.41
1:E:517:LEU:CD2	1:E:521:ILE:HD11	2.51	0.41
1:A:84:THR:CG2	1:A:153:TRP:HZ2	2.34	0.41
1:A:104:LYS:HG3	1:A:192:ASP:OD1	2.21	0.41
1:A:380:ILE:HA	1:A:383:TRP:O	2.21	0.41
1:A:517:LEU:HD23	1:A:521:ILE:HD11	2.03	0.41
2:B:336:GLN:C	2:B:337:TRP:CD1	2.94	0.41
1:E:479:LEU:HD12	1:E:517:LEU:HD22	2.03	0.41
1:E:53:GLU:O	1:E:53:GLU:HG2	2.20	0.41
2:F:146:TYR:CE2	2:F:150:PRO:HA	2.56	0.41
1:A:501:TYR:O	1:A:505:ILE:HD13	2.21	0.41
2:B:132:ILE:HA	2:B:133:PRO:HD3	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:816:DG:H2''	4:H:817:MRG:OP2	2.21	0.41
1:E:115:TYR:CD2	4:H:823:ATM:H2'	2.48	0.41
1:A:38:CYS:SG	1:A:132:ILE:CD1	3.09	0.41
1:A:494:ASN:HB3	2:B:289:LEU:HD22	2.03	0.41
2:B:398:TRP:CZ3	2:B:414:TRP:CH2	3.08	0.41
1:E:401:TRP:CZ3	1:E:405:TYR:HB2	2.56	0.41
2:F:207:GLN:O	2:F:211:ARG:HG3	2.21	0.41
2:F:54:ASN:HA	2:F:55:PRO:HD2	2.01	0.41
1:A:384:GLY:CA	2:B:28:GLU:H	2.19	0.40
2:B:376:THR:CG2	2:B:386:THR:HG23	2.49	0.40
2:B:8:VAL:HB	2:B:159:ILE:CD1	2.51	0.40
1:E:130:PHE:CE2	1:E:132:ILE:HD11	2.56	0.40
1:E:456:GLY:HA3	1:E:465:LYS:O	2.20	0.40
2:F:104:LYS:O	2:F:235:HIS:HB3	2.21	0.40
2:F:180:ILE:HG12	2:F:189:VAL:HG22	2.02	0.40
1:A:96:HIS:H	2:B:136:ASN:CG	2.23	0.40
2:B:180:ILE:CG2	2:B:189:VAL:HG22	2.51	0.40
1:E:450:THR:O	1:E:451:LYS:HB2	2.22	0.40
1:E:512:LYS:HA	1:E:512:LYS:HD2	1.80	0.40
1:E:498:ASP:HA	1:E:536:VAL:O	2.21	0.40
3:G:717:DC:H2''	3:G:718:DA:OP2	2.21	0.40
2:B:402:TRP:CD1	2:B:403:THR:HG23	2.57	0.40
2:B:404:GLU:O	2:B:405:TYR:CD1	2.74	0.40
1:E:24:TRP:HB3	3:G:703:DG:N3	2.35	0.40
1:E:275:LYS:O	1:E:276:VAL:CG1	2.69	0.40
1:E:505:ILE:CD1	1:E:505:ILE:N	2.81	0.40
1:A:173:LYS:HZ2	1:A:173:LYS:HB2	1.87	0.40
1:A:365:VAL:CG2	1:A:401:TRP:NE1	2.85	0.40
1:A:90:VAL:HG13	2:B:141:GLY:O	2.22	0.40
1:E:25:PRO:HD2	3:G:703:DG:C2	2.57	0.40
1:E:391:LEU:HA	1:E:392:PRO:HD3	1.95	0.40
2:F:17:ASP:CG	2:F:18:GLY:H	2.25	0.40
2:F:398:TRP:HZ3	2:F:414:TRP:CH2	2.38	0.40
2:F:5:ILE:O	2:F:6:GLU:CG	2.69	0.40
2:F:5:ILE:HG22	2:F:6:GLU:N	2.35	0.40
1:A:70:ARG:CG	1:A:70:ARG:NH1	2.85	0.40
1:E:168:LEU:HB3	1:E:172:LYS:HE3	2.04	0.40
1:E:301:LEU:O	1:E:305:GLU:HG2	2.21	0.40
1:E:32:LYS:HA	1:E:32:LYS:HE3	2.03	0.40
2:F:8:VAL:HG11	2:F:159:ILE:CD1	2.52	0.40
2:F:34:LEU:HD12	2:F:37:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:817:MRG:C2	4:H:818:DC:C2	3.05	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

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

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	552/562 (98%)	469 (85%)	71 (13%)	12 (2%)	8	47
1	E	552/562 (98%)	460 (83%)	78 (14%)	14 (2%)	6	45
2	B	409/437 (94%)	352 (86%)	45 (11%)	12 (3%)	5	42
2	F	409/437 (94%)	348 (85%)	53 (13%)	8 (2%)	9	50
All	All	1922/1998 (96%)	1629 (85%)	247 (13%)	46 (2%)	7	46

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	134	SER
2	B	358	ARG
1	E	134	SER
1	E	345	PRO
1	E	412	PRO
1	E	470	THR
2	F	425	LEU
1	A	68	SER
1	A	377	THR
1	A	412	PRO
1	A	470	THR
2	B	243	PRO
2	B	313	PRO

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Mol	Chain	Res	Type
2	B	404	GLU
1	E	218	ASP
1	E	377	THR
2	F	404	GLU
1	A	218	ASP
1	A	243	PRO
2	B	25	PRO
2	B	425	LEU
1	E	4	PRO
1	E	226	PRO
1	E	243	PRO
2	F	25	PRO
2	F	243	PRO
2	B	5	ILE
1	E	286	THR
2	F	4	PRO
1	A	150	PRO
1	A	286	THR
2	B	194	GLU
2	B	277	ARG
1	E	217	PRO
1	E	276	VAL
2	B	77	PHE
1	E	150	PRO
2	F	194	GLU
2	B	35	VAL
2	F	213	GLY
1	E	462	GLY
1	A	59	PRO
1	A	504	GLY
2	B	111	VAL
2	F	111	VAL

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	495/502 (99%)	445 (90%)	50 (10%)	9	40
1	E	495/502 (99%)	446 (90%)	49 (10%)	9	41
2	B	375/397 (94%)	339 (90%)	36 (10%)	10	43
2	F	375/397 (94%)	340 (91%)	35 (9%)	10	45
All	All	1740/1798 (97%)	1570 (90%)	170 (10%)	9	42

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	40	GLU
1	A	54	ASN
1	A	63	ILE
1	A	94	ILE
1	A	113	ASP
1	A	132	ILE
1	A	142	ILE
1	A	143	ARG
1	A	144	TYR
1	A	146	TYR
1	A	164	MET
1	A	180	ILE
1	A	187	LEU
1	A	193	LEU
1	A	195	ILE
1	A	210	LEU
1	A	222	GLN
1	A	223	LYS
1	A	224	GLU
1	A	246	LEU
1	A	248	GLU
1	A	249	LYS
1	A	250	ASP
1	A	257	ILE
1	A	270	ILE
1	A	272	PRO
1	A	279	LEU
1	A	289	LEU
1	A	303	LEU
1	A	326	ILE
1	A	329	ILE
1	A	380	ILE

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Mol	Chain	Res	Type
1	A	382	ILE
1	A	401	TRP
1	A	402	TRP
1	A	422	LEU
1	A	431	LYS
1	A	434	ILE
1	A	452	LEU
1	A	463	ARG
1	A	464	GLN
1	A	466	VAL
1	A	479	LEU
1	A	480	GLN
1	A	482	ILE
1	A	501	TYR
1	A	521	ILE
1	A	522	ILE
1	A	536	VAL
2	B	27	THR
2	B	29	GLU
2	B	31	ILE
2	B	37	ILE
2	B	63	ILE
2	B	86	ASP
2	B	94	ILE
2	B	135	ILE
2	B	142	ILE
2	B	148	VAL
2	B	151	GLN
2	B	167	ILE
2	B	173	LYS
2	B	177	ASP
2	B	185	ASP
2	B	186	ASP
2	B	206	ARG
2	B	212	TRP
2	B	215	THR
2	B	235	HIS
2	B	257	ILE
2	B	264	LEU
2	B	309	ILE
2	B	318	TYR
2	B	330	GLN

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Mol	Chain	Res	Type
2	B	341	ILE
2	B	357	MET
2	B	365	VAL
2	B	368	LEU
2	B	382	ILE
2	B	400	THR
2	B	401	TRP
2	B	409	THR
2	B	412	PRO
2	B	423	VAL
2	B	426	TRP
1	E	5	ILE
1	E	32	LYS
1	E	40	GLU
1	E	42	GLU
1	E	47	ILE
1	E	49	LYS
1	E	54	ASN
1	E	63	ILE
1	E	113	ASP
1	E	120	LEU
1	E	132	ILE
1	E	142	ILE
1	E	143	ARG
1	E	156	SER
1	E	164	MET
1	E	180	ILE
1	E	187	LEU
1	E	193	LEU
1	E	210	LEU
1	E	246	LEU
1	E	248	GLU
1	E	249	LYS
1	E	250	ASP
1	E	257	ILE
1	E	270	ILE
1	E	272	PRO
1	E	277	ARG
1	E	279	LEU
1	E	326	ILE
1	E	329	ILE
1	E	365	VAL

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Mol	Chain	Res	Type
1	E	382	ILE
1	E	401	TRP
1	E	402	TRP
1	E	411	ILE
1	E	422	LEU
1	E	431	LYS
1	E	434	ILE
1	E	452	LEU
1	E	463	ARG
1	E	464	GLN
1	E	466	VAL
1	E	479	LEU
1	E	482	ILE
1	E	501	TYR
1	E	506	ILE
1	E	522	ILE
1	E	536	VAL
1	E	547	GLN
2	F	3	SER
2	F	29	GLU
2	F	30	LYS
2	F	37	ILE
2	F	63	ILE
2	F	86	ASP
2	F	88	TRP
2	F	94	ILE
2	F	135	ILE
2	F	142	ILE
2	F	161	GLN
2	F	163	SER
2	F	167	ILE
2	F	173	LYS
2	F	177	ASP
2	F	206	ARG
2	F	235	HIS
2	F	257	ILE
2	F	264	LEU
2	F	281	LYS
2	F	300	GLU
2	F	309	ILE
2	F	318	TYR
2	F	330	GLN

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Mol	Chain	Res	Type
2	F	357	MET
2	F	358	ARG
2	F	365	VAL
2	F	368	LEU
2	F	375	ILE
2	F	380	ILE
2	F	401	TRP
2	F	411	ILE
2	F	423	VAL
2	F	425	LEU
2	F	426	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	GLN
1	A	182	GLN
1	A	207	GLN
1	A	221	HIS
1	A	235	HIS
1	A	306	ASN
1	A	336	GLN
1	A	447	ASN
1	A	480	GLN
1	A	509	GLN
1	A	520	GLN
2	B	54	ASN
2	B	145	GLN
2	B	147	ASN
2	B	207	GLN
2	B	330	GLN
2	B	340	GLN
2	B	343	GLN
2	B	361	HIS
2	B	363	ASN
2	B	373	GLN
2	B	407	GLN
2	B	428	GLN
1	E	23	GLN
1	E	182	GLN
1	E	221	HIS
1	E	235	HIS

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Mol	Chain	Res	Type
1	E	278	GLN
1	E	336	GLN
1	E	343	GLN
1	E	447	ASN
1	E	480	GLN
1	E	509	GLN
1	E	520	GLN
1	E	547	GLN
2	F	54	ASN
2	F	145	GLN
2	F	147	ASN
2	F	151	GLN
2	F	207	GLN
2	F	330	GLN
2	F	343	GLN
2	F	363	ASN
2	F	407	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
4	MRG	D	817	3,4	21,28,29	1.65	4 (19%)	24,39,42	3.68	7 (29%)
4	ATM	D	823	3,4	14,23,24	1.23	2 (14%)	18,32,35	3.79	4 (22%)
4	MRG	H	817	3,4	21,28,29	1.52	3 (14%)	24,39,42	3.57	7 (29%)
4	ATM	H	823	3,4	14,23,24	1.36	3 (21%)	18,32,35	4.03	4 (22%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MRG	D	817	3,4	-	0/8/26/27	0/3/3/3
4	ATM	D	823	3,4	-	0/6/24/25	0/2/2/2
4	MRG	H	817	3,4	-	0/8/26/27	0/3/3/3
4	ATM	H	823	3,4	-	0/6/24/25	0/2/2/2

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	817	MRG	C21-N2	-5.15	1.34	1.46
4	H	817	MRG	C21-N2	-5.00	1.34	1.46
4	H	823	ATM	N4'-N3'	-2.64	1.16	1.23
4	D	823	ATM	C6-C5	-2.18	1.34	1.40
4	H	817	MRG	C8-N7	-2.12	1.30	1.34
4	H	823	ATM	C6-C5	-2.07	1.34	1.40
4	D	817	MRG	C8-N7	-2.03	1.30	1.34
4	D	817	MRG	C2-N2	2.08	1.37	1.34
4	D	823	ATM	C4-N3	2.96	1.38	1.33
4	H	823	ATM	C4-N3	3.33	1.39	1.33
4	H	817	MRG	C6-N1	3.62	1.39	1.33
4	D	817	MRG	C6-N1	3.64	1.39	1.33

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	817	MRG	C21-N2-C2	-12.93	100.14	123.68
4	H	817	MRG	C21-N2-C2	-12.47	100.99	123.68
4	H	823	ATM	C5-C4-N3	-9.14	115.16	125.24
4	D	823	ATM	C5-C4-N3	-8.52	115.84	125.24
4	D	817	MRG	C5-C6-N1	-8.47	111.42	123.48
4	H	817	MRG	C5-C6-N1	-8.32	111.64	123.48
4	H	817	MRG	C23-C22-C21	-4.20	99.34	112.67
4	D	817	MRG	C23-C22-C21	-4.18	99.39	112.67
4	D	817	MRG	C2-N3-C4	-3.05	111.63	115.11
4	H	817	MRG	C2-N3-C4	-2.83	111.88	115.11
4	H	817	MRG	C6-C5-C4	-2.06	118.79	120.84
4	H	823	ATM	C5A-C5-C6	2.10	122.87	118.67
4	D	817	MRG	C22-C21-N2	2.17	117.23	111.46
4	D	823	ATM	C5A-C5-C6	2.18	123.03	118.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	817	MRG	C22-C23-S24	2.26	120.19	112.91
4	D	817	MRG	C22-C23-S24	2.30	120.33	112.91
4	H	823	ATM	C2'-C3'-N3'	2.38	115.46	108.81
4	D	823	ATM	C2'-C3'-N3'	2.92	116.96	108.81
4	D	817	MRG	C6-N1-C2	5.63	125.27	115.18
4	H	817	MRG	C6-N1-C2	5.67	125.34	115.18
4	D	823	ATM	C4-N3-C2	12.75	126.31	115.16
4	H	823	ATM	C4-N3-C2	13.74	127.18	115.16

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	817	MRG	2	0
4	D	823	ATM	6	0
4	H	817	MRG	3	0
4	H	823	ATM	14	0

## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	554/562 (98%)	-0.24	4 (0%) 87 79	26, 89, 115, 135	0
1	E	554/562 (98%)	0.61	61 (11%) 6 5	33, 154, 164, 172	0
2	B	413/437 (94%)	-0.16	7 (1%) 70 56	54, 84, 119, 143	0
2	F	413/437 (94%)	0.47	34 (8%) 12 9	127, 153, 165, 171	0
3	C	23/27 (85%)	-0.16	1 (4%) 36 24	65, 90, 125, 141	0
3	G	23/27 (85%)	0.27	1 (4%) 36 24	151, 159, 167, 178	0
4	D	19/22 (86%)	-0.53	0 100 100	75, 100, 127, 136	0
4	H	19/22 (86%)	0.05	0 100 100	149, 159, 170, 171	0
All	All	2018/2096 (96%)	0.16	108 (5%) 26 18	26, 122, 162, 178	0

All (108) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	231	GLY	8.5
1	E	131	THR	6.9
1	E	27	THR	5.0
1	E	327	ALA	4.7
1	E	25	PRO	4.6
1	E	26	LEU	4.6
2	F	45	GLY	4.4
1	E	225	PRO	4.2
2	B	360	ALA	4.1
1	E	224	GLU	4.0
1	E	271	TYR	4.0
1	E	226	PRO	4.0
1	E	272	PRO	3.9
1	E	246	LEU	3.8
2	F	216	THR	3.8
1	A	225	PRO	3.7

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Mol	Chain	Res	Type	RSRZ
1	E	167	ILE	3.7
2	B	3	SER	3.6
1	E	286	THR	3.6
3	C	703	DG	3.5
1	E	114	ALA	3.4
2	F	145	GLN	3.4
2	F	73	LYS	3.3
1	E	113	ASP	3.3
2	F	149	LEU	3.3
1	E	287	LYS	3.3
1	E	423	VAL	3.3
1	E	252	TRP	3.2
1	E	178	ILE	3.1
1	E	274	ILE	3.1
1	E	68	SER	3.1
2	B	4	PRO	3.1
2	F	232	TYR	3.1
1	E	147	ASN	3.1
1	E	325	LEU	3.0
1	E	245	VAL	3.0
2	F	105	SER	3.0
2	F	161	GLN	3.0
2	F	150	PRO	2.9
1	E	101	LYS	2.9
1	E	117	SER	2.9
3	G	703	DG	2.9
2	F	14	PRO	2.8
2	F	202	ILE	2.8
1	E	132	ILE	2.8
1	E	233	GLU	2.8
2	F	343	GLN	2.8
1	E	143	ARG	2.7
2	F	178	ILE	2.7
1	E	146	TYR	2.7
1	E	112	GLY	2.7
2	F	137	ASN	2.7
1	E	55	PRO	2.6
1	E	142	ILE	2.6
1	E	29	GLU	2.6
2	B	423	VAL	2.6
1	E	73	LYS	2.6
2	B	215	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	424	LYS	2.6
2	F	122	GLU	2.6
1	E	270	ILE	2.5
1	E	348	ASN	2.5
1	E	8	VAL	2.5
2	F	95	PRO	2.5
1	E	177	ASP	2.5
1	E	115	TYR	2.4
2	F	358	ARG	2.4
2	F	191	SER	2.4
2	F	205	LEU	2.4
1	E	28	GLU	2.4
1	E	54	ASN	2.4
2	F	123	ASP	2.4
1	E	24	TRP	2.4
2	F	198	HIS	2.3
1	E	20	LYS	2.3
1	E	259	LYS	2.3
1	E	392	PRO	2.3
1	E	288	ALA	2.3
1	E	318	TYR	2.3
2	B	231	GLY	2.2
1	A	133	PRO	2.2
1	E	36	GLU	2.2
1	E	150	PRO	2.2
1	E	23	GLN	2.2
1	E	79	GLU	2.2
2	F	76	ASP	2.2
2	F	195	ILE	2.1
1	E	275	LYS	2.1
2	F	357	MET	2.1
2	F	116	PHE	2.1
2	F	323	LYS	2.1
1	E	290	THR	2.1
1	E	61	PHE	2.1
2	F	127	TYR	2.1
1	E	541	GLY	2.1
1	E	298	GLU	2.1
1	A	303	LEU	2.1
1	E	69	THR	2.1
2	F	15	GLY	2.1
1	E	388	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	223	LYS	2.0
2	F	124	PHE	2.0
1	E	190	GLY	2.0
2	F	197	GLN	2.0
2	F	146	TYR	2.0
2	F	217	PRO	2.0
1	E	217	PRO	2.0
2	F	3	SER	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ATM	H	823	22/23	0.82	0.30	-	155,157,158,158	0
4	MRG	H	817	26/27	0.88	0.25	-	154,157,167,167	0
4	ATM	D	823	22/23	0.95	0.27	-	87,90,92,94	0
4	MRG	D	817	26/27	0.93	0.18	-	89,93,101,108	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

There are no ligands in this entry.

## 6.5 Other polymers [i](#)

There are no such residues in this entry.