



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 03:15 AM UTC

PDB ID : 2D6F / pdb_00002d6f
Title : Crystal structure of Glu-tRNA(Gln) amidotransferase in the complex with tRNA(Gln)
Authors : Nureki, O.
Deposited on : 2005-11-13
Resolution : 3.15 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

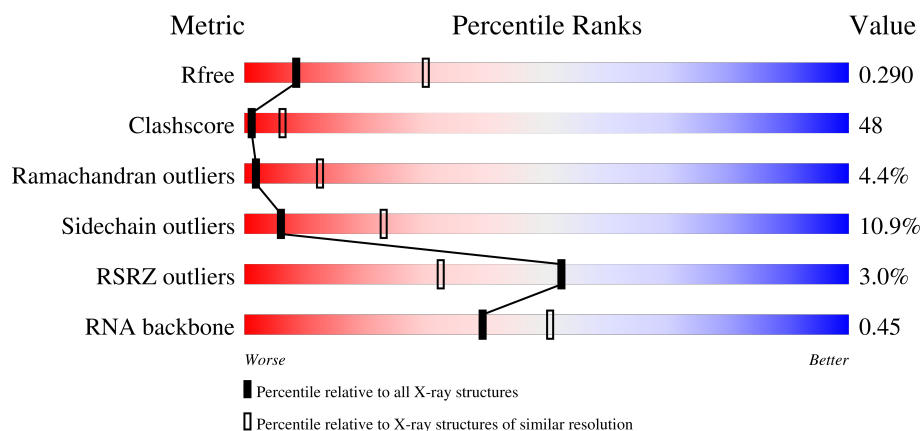
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)
RNA backbone	3983	1113 (3.42-2.90)

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

Mol	Chain	Length	Quality of chain
1	E	74	9% 18% 59% 20% .
1	F	74	4% 27% 49% 23% .
2	A	435	% 35% 48% 13% ..
2	B	435	33% 52% 12% ..

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Mol	Chain	Length	Quality of chain
3	C	619	5% 24%47%7%22%
3	D	619	3% 28%46%10%16%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 17816 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 tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	E	72	Total	C	N	O	P	0	0	0
			1539	684	272	511	72			
1	F	74	Total	C	N	O	P	0	0	0
			1579	702	278	525	74			

- Molecule 2 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit D.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	424	Total	C	N	O	S	0	0	0
			3268	2028	575	641	24			
2	B	424	Total	C	N	O	S	0	0	0
			3274	2032	575	643	24			

- Molecule 3 is a protein called Glutamyl-tRNA(Gln) amidotransferase subunit E.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	485	Total	C	N	O	S	0	0	0
			3847	2390	690	752	15			
3	D	522	Total	C	N	O	S	0	0	0
			4127	2563	741	808	15			

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Zn	0	0
			1	1		
4	D	1	Total	Zn	0	0
			1	1		

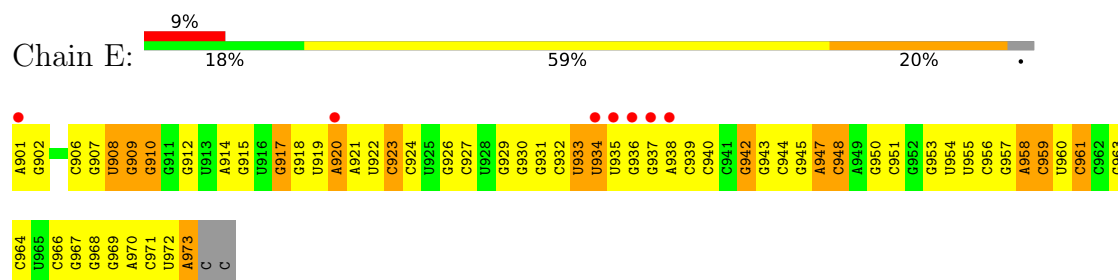
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	E	16	Total 16	O 16	0	0
5	F	24	Total 24	O 24	0	0
5	A	31	Total 31	O 31	0	0
5	B	24	Total 24	O 24	0	0
5	C	36	Total 36	O 36	0	0
5	D	49	Total 49	O 49	0	0

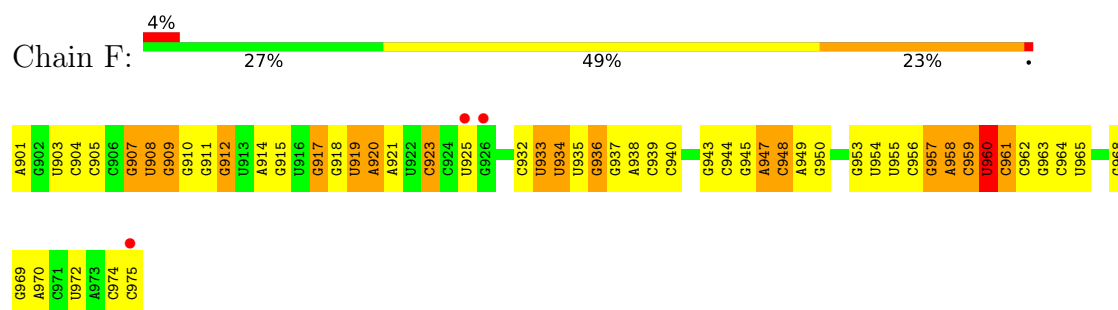
3 Residue-property plots

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

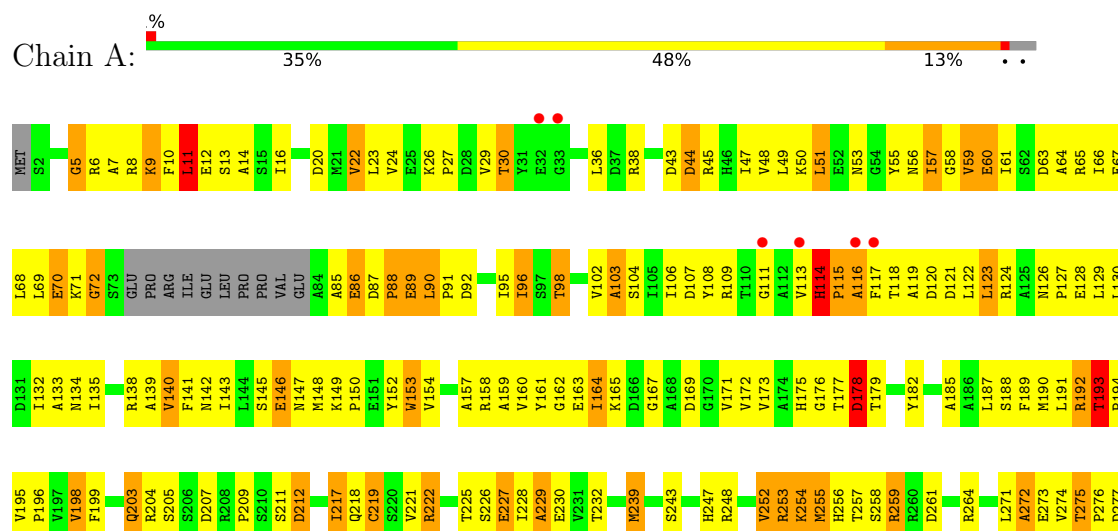
• Molecule 1: tRNA

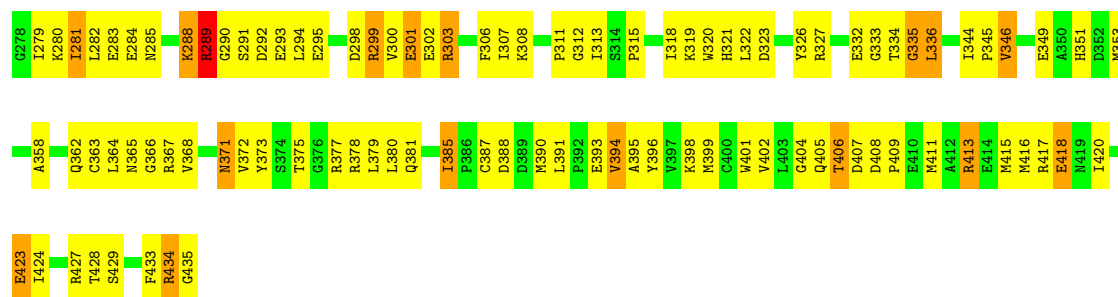


• Molecule 1: tRNA



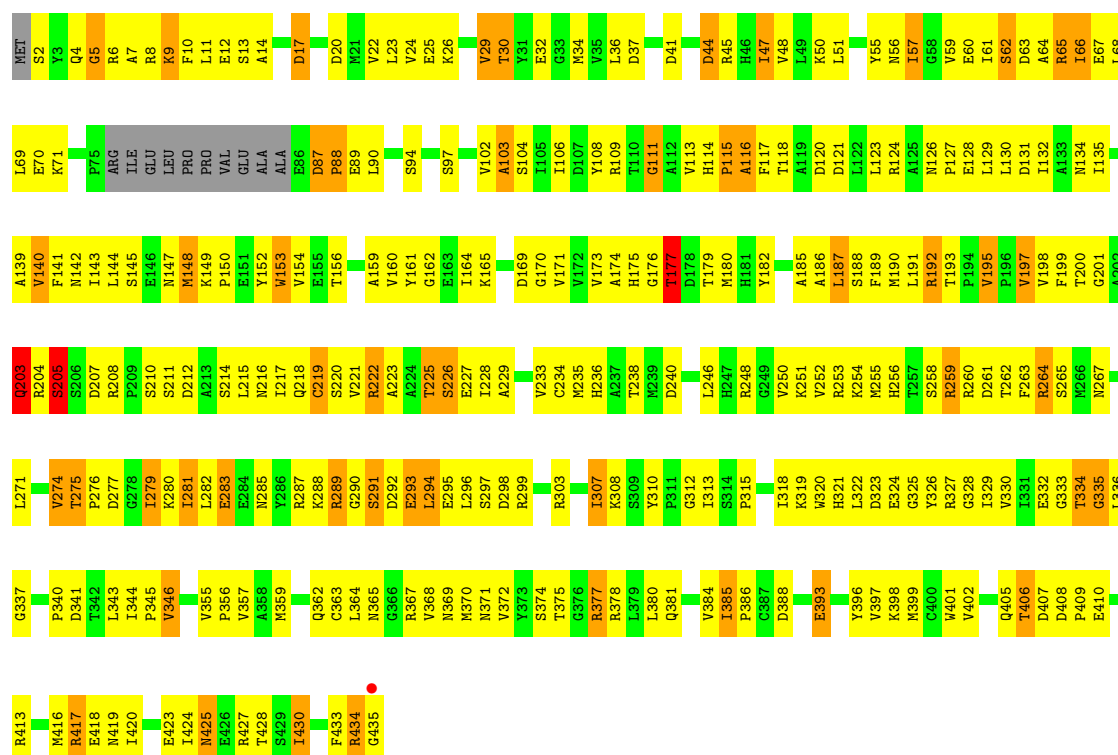
• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit D





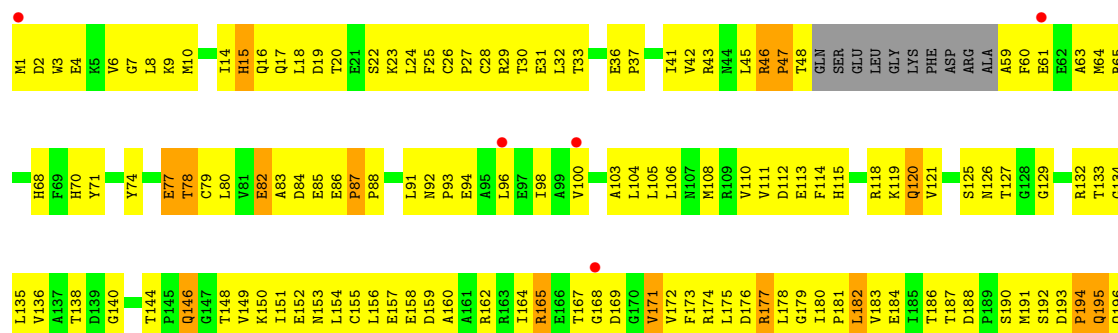
• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit D

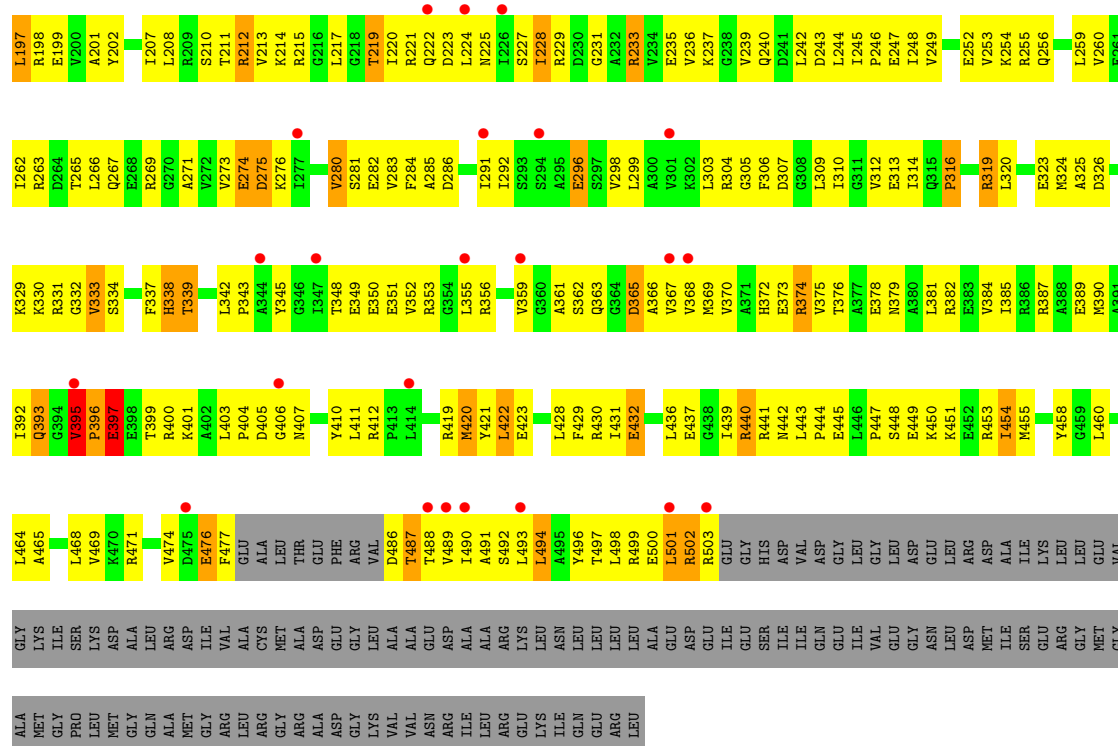
Chain B: 33% 52% 12% ..



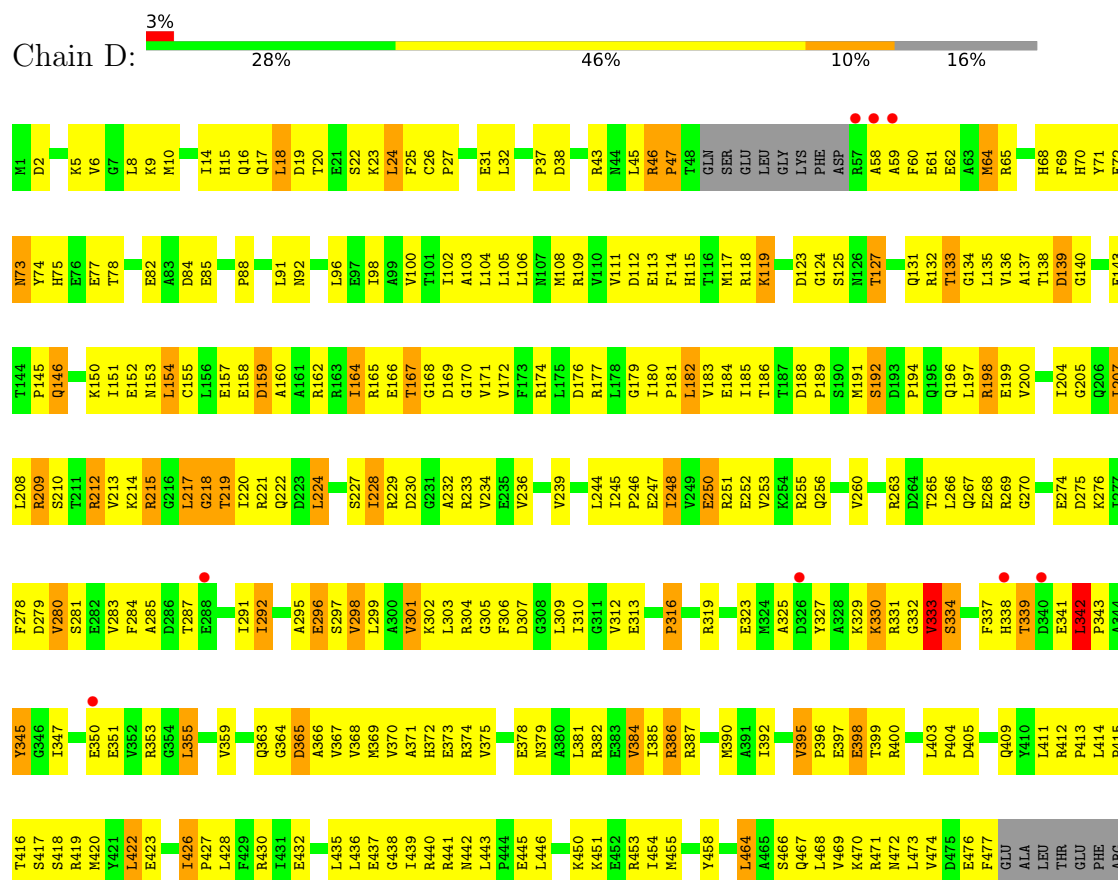
• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit E

Chain C: 5% 24% 47% 7% 22%





• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit E



ALA	VAL	ALA	VAL
GLU	ASN	GLU	VAL
ASP	ARG	T487	T486
ALA	ILE	V489	V489
ALA	LEU	T490	T490
ARG	ARG	A491	A491
GLU	GLU	S492	S492
LYS	LYS	L493	L493
ILE	ILE	L494	L494
GLN	GLN	A495	A495
GLU	GLU	Y496	Y496
ARG	ARG	T497	T497
LEU	LEU	L498	L498
	ALA	R499	R499
	GLU	E500	E500
ASP	ASP	L501	L501
GLU	GLU	R502	R502
ILE	ILE	R503	R503
GLU	GLU	E504	E504
SER	SER		
ILE	ILE	D507	D507
ILE	ILE	V508	V508
GLN	GLN	D509	D509
GLU	GLU	G510	G510
ILE	ILE	L511	L511
VAL	VAL	G512	G512
GLU	GLU	L513	L513
GLY	GLY	D514	D514
ASN	ASN	E515	E515
LEU	LEU	L516	L516
ASP	ASP	R517	R517
MET	MET	D518	D518
ILE	ILE	A519	A519
SER	SER	I520	I520
GLU	GLU	K521	K521
ARG	ARG	L522	L522
GLY	GLY	E523	E523
MET	MET	E524	E524
GLY	GLY	V525	V525
GLY	GLY	G526	G526
MET	MET	K527	K527
GLY	GLY	I528	I528
PRO	PRO	S529	S529
LEU	LEU	K530	K530
MET	MET	D531	D531
GLY	GLY	A532	A532
GLN	GLN	L533	L533
ALA	ALA	R534	R534
MET	MET	D535	D535
GLY	GLY	I536	I536
ARG	ARG	V537	V537
LEU	LEU	A538	A538
ARG	ARG	CYS	CYS
GLY	GLY	MET	MET
ARG	ARG	ALA	ALA
ALA	ALA	ASP	ASP
ASP	ASP	GLU	GLU
GLY	GLY	GLY	GLY
LYS	LYS	LEU	LEU

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	118.81Å 140.71Å 186.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.52 – 3.15 46.52 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.52-3.15) 98.9 (46.52-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.13Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.230 , 0.292 0.228 , 0.290	Depositor DCC
R_{free} test set	2728 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	60.0	Xtriage
Anisotropy	0.215	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	17816	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	E	0.33	0/1718	0.65	0/2676
1	F	0.34	0/1762	0.66	0/2744
2	A	0.59	0/3323	1.10	23/4501 (0.5%)
2	B	0.58	0/3330	1.08	19/4511 (0.4%)
3	C	0.44	0/3898	0.98	14/5265 (0.3%)
3	D	0.54	0/4179	1.03	18/5642 (0.3%)
All	All	0.50	0/18210	0.98	74/25339 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	1

There are no bond length outliers.

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	11	LEU	N-CA-C	-8.94	102.51	113.50
2	A	219	CYS	N-CA-C	-8.91	102.33	113.55
2	B	153	TRP	N-CA-C	-8.12	102.39	111.07
3	D	152	GLU	N-CA-C	8.06	119.76	110.97
3	D	522	LEU	N-CA-C	-8.00	103.00	114.12
3	D	18	LEU	N-CA-C	7.91	123.06	113.41
2	A	192	ARG	N-CA-C	-7.55	97.09	109.40
2	A	153	TRP	N-CA-C	-7.27	103.29	111.07
3	C	18	LEU	N-CA-C	7.13	122.07	113.23
3	C	30	THR	N-CA-C	7.10	120.89	112.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	494	LEU	N-CA-C	-7.09	105.24	114.04
3	D	46	ARG	CA-C-N	7.08	128.69	119.84
3	D	46	ARG	C-N-CA	7.08	128.69	119.84
2	B	219	CYS	N-CA-C	-7.07	104.78	113.41
3	D	395	VAL	CA-C-N	6.87	129.53	120.25
3	D	395	VAL	C-N-CA	6.87	129.53	120.25
2	B	385	ILE	N-CA-C	6.83	114.31	107.55
3	D	422	LEU	N-CA-C	6.80	120.24	110.10
2	A	366	GLY	N-CA-C	6.79	118.94	112.08
2	A	193	THR	N-CA-C	6.67	120.10	108.82
2	A	135	ILE	N-CA-C	6.64	118.14	109.58
2	B	177	THR	N-CA-C	6.54	118.09	110.97
3	C	152	GLU	N-CA-C	6.53	118.09	110.97
3	D	512	GLY	N-CA-C	-6.47	106.50	114.92
2	B	220	SER	N-CA-C	-6.31	104.48	111.36
2	B	192	ARG	N-CA-C	-6.24	98.22	108.76
2	B	193	THR	CA-C-N	6.18	127.56	119.84
2	B	193	THR	C-N-CA	6.18	127.56	119.84
2	A	198	VAL	N-CA-C	6.16	116.73	107.80
2	B	203	GLN	N-CA-C	-6.16	104.47	112.23
2	A	239	MET	N-CA-C	-6.14	105.75	113.18
2	A	203	GLN	N-CA-C	-6.14	104.49	112.23
3	D	426	ILE	CA-C-N	6.09	126.93	120.11
3	D	426	ILE	C-N-CA	6.09	126.93	120.11
3	C	63	ALA	N-CA-C	-6.07	104.59	111.14
2	B	265	SER	N-CA-C	-6.06	100.63	110.20
2	B	274	VAL	N-CA-C	6.01	117.81	109.45
2	B	111	GLY	N-CA-C	-5.96	107.46	115.21
3	D	24	LEU	N-CA-C	5.92	117.60	111.03
2	B	307	ILE	N-CA-C	5.85	116.28	107.80
2	B	198	VAL	N-CA-C	5.78	116.18	107.80
3	D	330	LYS	N-CA-C	-5.78	102.86	110.43
3	C	397	GLU	N-CA-C	-5.77	101.30	109.96
2	A	114	HIS	CA-C-N	5.72	126.99	119.84
2	A	114	HIS	C-N-CA	5.72	126.99	119.84
3	D	159	ASP	N-CA-C	-5.65	102.92	110.55
3	C	395	VAL	CA-C-N	-5.63	112.80	119.84
3	C	395	VAL	C-N-CA	-5.63	112.80	119.84
3	C	338	HIS	N-CA-C	5.62	118.35	108.75
2	A	385	ILE	CB-CA-C	-5.59	104.44	111.04
3	D	20	THR	N-CA-C	-5.58	101.48	110.14
3	D	523	LEU	N-CA-C	-5.56	106.54	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	87	PRO	CA-C-N	5.49	126.70	119.84
3	C	87	PRO	C-N-CA	5.49	126.70	119.84
3	C	454	ILE	CB-CA-C	-5.41	104.96	111.88
2	B	142	ASN	N-CA-C	5.41	116.90	107.49
3	D	170	GLY	N-CA-C	5.37	122.05	112.22
2	A	104	SER	N-CA-C	5.36	115.44	107.88
3	D	338	HIS	N-CA-C	5.33	117.86	108.75
2	A	372	VAL	N-CA-C	5.29	115.73	110.23
3	C	129	GLY	N-CA-C	-5.29	107.75	115.63
3	C	420	MET	N-CA-C	5.28	117.10	108.55
2	A	255	MET	N-CA-C	5.26	119.55	113.18
2	A	229	ALA	N-CA-C	5.21	116.52	109.11
2	B	283	GLU	N-CA-C	-5.20	102.58	110.28
2	A	89	GLU	N-CA-C	-5.19	106.34	113.56
2	A	272	ALA	N-CA-C	5.19	115.20	107.88
2	B	372	VAL	N-CA-C	5.18	115.33	110.30
2	B	135	ILE	N-CA-C	5.14	116.21	109.58
2	A	90	LEU	CA-C-N	5.09	125.08	119.89
2	A	90	LEU	C-N-CA	5.09	125.08	119.89
2	A	395	ALA	N-CA-C	-5.07	105.84	111.36
2	B	333	GLY	N-CA-C	5.04	120.19	111.98
2	A	243	SER	N-CA-C	5.02	117.49	109.81

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	960	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	E	1539	0	777	77	0
1	F	1579	0	799	68	0
2	A	3268	0	3217	345	0
2	B	3274	0	3220	340	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	3847	0	3861	447	1
3	D	4127	0	4152	414	1
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	31	0	0	11	0
5	B	24	0	0	5	0
5	C	36	0	0	9	0
5	D	49	0	0	14	0
5	E	16	0	0	2	0
5	F	24	0	0	6	0
All	All	17816	0	16026	1611	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 48.

All (1611) 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)
3:D:133:THR:HG23	3:D:157:GLU:HB3	1.26	1.10
2:A:301:GLU:HG3	2:A:303:ARG:NH1	1.67	1.10
2:B:238:THR:HG23	2:B:240:ASP:H	1.12	1.08
3:D:43:ARG:HG2	3:D:43:ARG:HH11	1.19	1.06
3:C:233:ARG:HG3	3:C:397:GLU:HB3	1.37	1.06
2:A:178:ASP:OD2	2:B:334:THR:HB	1.53	1.05
2:B:315:PRO:HB3	2:B:346:VAL:HG21	1.40	1.04
1:F:958:A:H4'	1:F:959:C:OP1	1.56	1.03
2:A:264:ARG:HH21	2:B:435:GLY:HA2	1.24	1.03
3:C:450:LYS:HD2	3:C:474:VAL:HG11	1.38	1.02
3:D:305:GLY:H	3:D:365:ASP:HB3	1.23	1.01
3:C:259:LEU:HD23	3:C:262:ILE:HD12	1.43	1.01
2:A:435:GLY:HA2	2:B:264:ARG:HH21	1.26	0.99
3:D:454:ILE:HD12	3:D:474:VAL:HG13	1.45	0.98
1:E:958:A:H4'	1:E:959:C:OP1	1.64	0.97
1:E:919:U:H5''	1:E:920:A:H5''	1.43	0.96
2:A:275:THR:HG22	2:A:277:ASP:H	1.27	0.96
2:B:26:LYS:HB2	2:B:29:VAL:HG23	1.47	0.95
3:C:165:ARG:HH11	3:C:165:ARG:HB2	1.30	0.95
2:A:23:LEU:HB2	2:A:69:LEU:HD11	1.46	0.94
3:C:68:HIS:NE2	3:C:70:HIS:HE1	1.63	0.94
3:D:275:ASP:HA	3:D:385:ILE:HD13	1.47	0.94
3:D:146:GLN:HG3	3:D:196:GLN:HB2	1.50	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:256:HIS:HD2	2:A:259:ARG:H	1.05	0.93
3:D:291:ILE:H	3:D:291:ILE:HD12	1.32	0.93
3:C:195:GLN:HE22	3:C:198:ARG:HH21	1.14	0.93
3:D:224:LEU:HD11	3:D:239:VAL:HG21	1.52	0.92
3:D:164:ILE:HG22	3:D:165:ARG:HG3	1.51	0.92
3:C:16:GLN:HE21	3:C:16:GLN:HA	1.32	0.91
3:C:454:ILE:HD11	3:C:474:VAL:HG13	1.53	0.90
2:A:336:LEU:O	2:A:368:VAL:HG13	1.71	0.90
2:B:385:ILE:HG23	2:B:413:ARG:HH11	1.33	0.90
1:E:917:G:H2'	1:E:957:G:H22	1.36	0.90
1:F:917:G:H2'	1:F:957:G:H22	1.36	0.89
3:C:191:MET:HG3	3:C:197:LEU:HD12	1.54	0.89
1:F:969:G:H2'	1:F:970:A:H8	1.35	0.89
2:A:256:HIS:CD2	2:A:259:ARG:H	1.91	0.88
3:D:70:HIS:CE1	3:D:169:ASP:OD2	2.26	0.88
2:A:301:GLU:HG3	2:A:303:ARG:HH12	1.38	0.87
2:B:118:THR:HG22	2:B:120:ASP:H	1.39	0.87
3:C:133:THR:HG23	3:C:157:GLU:HB3	1.54	0.87
3:C:9:LYS:HB2	3:C:227:SER:HB3	1.55	0.87
2:B:275:THR:HG22	2:B:277:ASP:H	1.38	0.86
3:C:305:GLY:H	3:C:365:ASP:HB3	1.38	0.86
3:D:108:MET:HE3	3:D:151:ILE:HG22	1.55	0.86
3:D:305:GLY:N	3:D:365:ASP:HB3	1.89	0.86
1:F:917:G:H2'	1:F:957:G:N2	1.90	0.86
2:A:113:VAL:HG11	2:A:207:ASP:HB3	1.58	0.86
3:D:256:GLN:O	3:D:260:VAL:HG23	1.75	0.86
2:A:303:ARG:HH11	2:A:303:ARG:H	1.24	0.85
2:A:140:VAL:HG23	2:A:141:PHE:H	1.41	0.85
2:A:160:VAL:O	2:A:164:ILE:HG22	1.76	0.85
2:A:385:ILE:HD12	2:A:413:ARG:HB2	1.58	0.85
2:B:238:THR:HG23	2:B:240:ASP:N	1.91	0.85
1:F:918:G:O2'	1:F:919:U:H5'	1.75	0.85
2:B:25:GLU:HG2	2:B:65:ARG:HB3	1.59	0.84
2:A:8:ARG:HH12	2:A:9:LYS:HZ1	1.24	0.84
2:B:132:ILE:HG12	2:B:222:ARG:HH12	1.42	0.84
2:A:299:ARG:HG3	2:A:299:ARG:HH11	1.41	0.84
2:B:140:VAL:HG12	2:B:141:PHE:HD2	1.41	0.84
2:B:106:ILE:HD11	2:B:207:ASP:HB2	1.59	0.84
2:B:186:ALA:HB1	2:B:190:MET:HE2	1.59	0.84
2:B:344:ILE:HB	2:B:345:PRO:HD3	1.58	0.84
2:B:106:ILE:HG12	2:B:113:VAL:HG22	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:960:U:H5''	1:F:961:C:OP2	1.78	0.83
2:A:303:ARG:HH11	2:A:303:ARG:HG2	1.44	0.83
1:F:958:A:O2'	1:F:959:C:H5'	1.78	0.83
2:A:264:ARG:HH21	2:B:435:GLY:CA	1.91	0.83
3:D:70:HIS:HE1	3:D:169:ASP:OD2	1.62	0.83
3:C:195:GLN:NE2	3:C:198:ARG:HH21	1.76	0.82
3:C:1:MET:HE3	3:C:6:VAL:HG21	1.62	0.82
2:B:200:THR:HG22	2:B:201:GLY:N	1.94	0.82
3:C:437:GLU:HA	3:C:440:ARG:HB3	1.61	0.82
3:C:500:GLU:O	3:C:503:ARG:HB3	1.79	0.82
3:D:125:SER:HB2	3:D:160:ALA:HB1	1.61	0.82
1:F:921:A:N1	1:F:948:C:H1'	1.95	0.82
3:C:309:LEU:HA	3:C:312:VAL:HG23	1.62	0.82
1:E:947:A:H2'	1:E:948:C:H5'	1.60	0.81
3:C:493:LEU:O	3:C:498:LEU:HG	1.79	0.81
2:A:315:PRO:HB3	2:A:346:VAL:HG21	1.63	0.81
2:A:371:ASN:N	2:A:371:ASN:HD22	1.78	0.81
2:B:299:ARG:HB2	2:B:405:GLN:HE22	1.44	0.81
3:D:146:GLN:HG3	3:D:196:GLN:CB	2.10	0.81
3:C:70:HIS:CE1	3:C:169:ASP:OD2	2.33	0.81
3:C:368:VAL:HG11	3:C:384:VAL:HG21	1.63	0.80
3:D:84:ASP:HB2	3:D:127:THR:HG23	1.63	0.80
3:D:59:ALA:C	3:D:61:GLU:H	1.88	0.80
3:D:111:VAL:HG12	3:D:113:GLU:H	1.47	0.80
3:D:522:LEU:O	3:D:522:LEU:HD23	1.81	0.80
2:A:303:ARG:NH1	2:A:303:ARG:H	1.79	0.80
2:A:222:ARG:HG2	2:A:222:ARG:HH11	1.47	0.80
2:B:51:LEU:HD11	2:B:57:ILE:HD12	1.63	0.80
3:C:356:ARG:NH2	3:C:363:GLN:HA	1.97	0.80
2:A:264:ARG:NH2	2:B:435:GLY:HA2	1.95	0.80
3:D:43:ARG:HG2	3:D:43:ARG:NH1	1.93	0.80
3:C:454:ILE:HD11	3:C:474:VAL:CG1	2.13	0.79
3:C:165:ARG:HH11	3:C:165:ARG:CB	1.95	0.79
3:D:466:SER:O	3:D:470:LYS:HG3	1.82	0.79
2:A:319:LYS:HE3	2:A:323:ASP:OD2	1.82	0.79
2:B:180:MET:HE1	2:B:235:MET:HE2	1.65	0.79
1:E:947:A:C2'	1:E:948:C:H5'	2.13	0.79
2:A:193:THR:HG22	2:A:195:VAL:H	1.47	0.79
2:A:435:GLY:HA2	2:B:264:ARG:NH2	1.97	0.79
3:C:167:THR:HG22	3:C:168:GLY:H	1.45	0.79
3:C:105:LEU:HD21	3:C:443:LEU:HB3	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:125:SER:HB2	3:C:160:ALA:HB1	1.65	0.78
3:C:331:ARG:HH21	3:C:376:THR:HA	1.48	0.78
3:D:296:GLU:HB3	3:D:373:GLU:HA	1.64	0.78
2:A:303:ARG:NH1	2:A:303:ARG:HG2	1.98	0.78
3:C:471:ARG:HD3	3:C:499:ARG:NH2	1.99	0.78
2:A:118:THR:HG22	2:A:120:ASP:H	1.48	0.78
2:B:29:VAL:HG13	3:D:109:ARG:HG3	1.66	0.78
3:C:401:LYS:HB3	3:C:411:LEU:HD11	1.64	0.77
3:D:19:ASP:HA	3:D:214:LYS:HE2	1.66	0.77
3:D:368:VAL:HG11	3:D:384:VAL:HG21	1.67	0.77
3:D:342:LEU:HD13	3:D:342:LEU:O	1.85	0.77
2:A:9:LYS:HE3	2:A:9:LYS:HA	1.65	0.77
2:A:264:ARG:HE	2:B:435:GLY:C	1.92	0.77
2:A:391:LEU:HB2	2:A:394:VAL:HG12	1.63	0.77
3:C:356:ARG:HH21	3:C:363:GLN:HA	1.50	0.77
3:D:167:THR:HG22	3:D:169:ASP:H	1.50	0.77
3:C:65:ARG:HG3	3:C:65:ARG:HH11	1.50	0.76
2:B:177:THR:HG22	2:B:263:PHE:HE2	1.51	0.76
1:E:931:G:H1	1:E:939:C:H42	1.34	0.76
2:B:180:MET:HE3	2:B:233:VAL:HG13	1.65	0.76
2:B:203:GLN:HE21	2:B:203:GLN:HA	1.50	0.76
3:C:68:HIS:NE2	3:C:70:HIS:CE1	2.51	0.76
3:C:108:MET:HG2	3:C:140:GLY:HA3	1.68	0.76
3:C:445:GLU:OE2	3:C:450:LYS:HA	1.85	0.76
3:C:16:GLN:HA	3:C:16:GLN:NE2	2.00	0.76
3:C:1:MET:CE	3:C:6:VAL:HG21	2.15	0.75
2:B:315:PRO:HB3	2:B:346:VAL:CG2	2.16	0.75
3:D:105:LEU:HD21	3:D:443:LEU:HB3	1.68	0.75
3:D:228:ILE:HD11	3:D:253:VAL:HG13	1.68	0.75
1:F:948:C:H5''	1:F:949:A:H5''	1.67	0.75
3:C:114:PHE:CZ	3:C:134:GLY:HA3	2.20	0.75
3:C:20:THR:HG22	3:C:94:GLU:HG2	1.68	0.75
1:F:918:G:H3'	5:F:48:HOH:O	1.85	0.75
3:C:146:GLN:HG3	3:C:196:GLN:HB2	1.69	0.75
3:C:164:ILE:HG22	3:C:165:ARG:HD2	1.68	0.75
3:D:15:HIS:CE1	3:D:184:GLU:HG2	2.22	0.75
3:D:301:VAL:HG11	3:D:385:ILE:HD11	1.67	0.75
1:F:907:G:H5''	1:F:908:U:OP2	1.86	0.74
3:C:19:ASP:HA	3:C:214:LYS:NZ	2.01	0.74
1:E:932:C:H3'	1:E:933:U:H5''	1.69	0.74
3:D:105:LEU:HD23	3:D:443:LEU:HD13	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:145:SER:HB2	2:A:176:GLY:HA3	1.70	0.74
2:B:369:ASN:HD21	2:B:371:ASN:HB2	1.53	0.74
3:D:437:GLU:C	3:D:439:ILE:H	1.94	0.74
2:A:344:ILE:HB	2:A:345:PRO:HD3	1.69	0.74
3:D:132:ARG:HG3	3:D:158:GLU:OE2	1.88	0.74
2:B:145:SER:HB2	2:B:176:GLY:HA3	1.69	0.74
1:F:911:G:N2	1:F:925:U:H1'	2.03	0.74
2:A:147:ASN:ND2	2:B:341:ASP:H	1.85	0.74
3:C:110:VAL:HG21	3:C:436:LEU:HD11	1.70	0.74
2:A:301:GLU:OE2	2:A:327:ARG:HG3	1.88	0.73
2:A:6:ARG:HB2	2:A:44:ASP:OD2	1.87	0.73
3:C:319:ARG:HD2	3:C:319:ARG:N	2.03	0.73
1:F:969:G:H2'	1:F:970:A:C8	2.22	0.73
3:D:232:ALA:HB3	3:D:395:VAL:HG12	1.71	0.73
3:D:476:GLU:N	3:D:476:GLU:OE2	2.22	0.73
3:C:164:ILE:HG22	3:C:165:ARG:CD	2.19	0.73
3:C:331:ARG:NH2	3:C:379:ASN:HD22	1.87	0.73
2:A:177:THR:HG21	2:A:203:GLN:HE21	1.54	0.72
3:C:228:ILE:HD12	3:C:228:ILE:N	2.04	0.72
2:B:11:LEU:HD13	2:B:47:ILE:CD1	2.19	0.72
3:C:10:MET:HB2	3:C:191:MET:HB2	1.69	0.72
3:C:266:LEU:HD13	3:C:392:ILE:HD13	1.70	0.72
2:A:140:VAL:HG11	2:A:159:ALA:HB1	1.70	0.72
3:D:18:LEU:HB2	3:D:181:PRO:HB2	1.71	0.72
2:A:140:VAL:HG23	2:A:141:PHE:N	2.05	0.72
2:B:200:THR:HG22	2:B:201:GLY:H	1.54	0.72
3:C:59:ALA:C	3:C:61:GLU:H	1.98	0.72
3:D:250:GLU:HG3	3:D:251:ARG:N	2.04	0.72
2:B:170:GLY:HA2	2:B:195:VAL:HG13	1.70	0.72
2:A:257:THR:HG21	2:B:367:ARG:O	1.90	0.72
3:D:32:LEU:HD13	3:D:162:ARG:CZ	2.20	0.72
2:A:119:ALA:O	2:A:123:LEU:HD22	1.90	0.71
1:E:917:G:H2'	1:E:957:G:N2	2.05	0.71
2:A:222:ARG:HG2	2:A:222:ARG:NH1	2.04	0.71
3:D:191:MET:O	3:D:192:SER:HB3	1.88	0.71
2:A:204:ARG:HH22	2:A:258:SER:HB2	1.54	0.71
2:B:36:LEU:HD11	2:B:50:LYS:HB2	1.73	0.71
3:C:381:LEU:O	3:C:384:VAL:HG12	1.90	0.71
2:A:315:PRO:HB3	2:A:346:VAL:CG2	2.20	0.71
3:D:301:VAL:HG23	3:D:381:LEU:HD22	1.72	0.71
1:F:934:U:H1'	5:F:157:HOH:O	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:308:LYS:HA	2:A:332:GLU:HB3	1.73	0.71
2:B:318:ILE:HG13	2:B:343:LEU:CD1	2.21	0.71
3:D:533:LEU:HA	3:D:536:ILE:HD12	1.71	0.71
3:C:155:CYS:O	3:C:183:VAL:HA	1.90	0.71
2:A:123:LEU:HG	2:A:130:LEU:HD21	1.73	0.71
2:B:205:SER:O	2:B:211:SER:HB2	1.90	0.71
2:B:222:ARG:HH11	2:B:222:ARG:HG2	1.56	0.71
2:B:123:LEU:HD21	2:B:130:LEU:HD21	1.73	0.70
3:C:498:LEU:O	3:C:501:LEU:HB3	1.91	0.70
3:D:234:VAL:HG11	3:D:400:ARG:HD2	1.72	0.70
3:C:98:ILE:HG23	3:C:211:THR:HG21	1.72	0.70
3:D:319:ARG:HG3	3:D:319:ARG:HH11	1.53	0.70
2:B:320:TRP:O	2:B:324:GLU:HG2	1.92	0.70
3:C:342:LEU:HD13	3:C:342:LEU:O	1.91	0.70
2:B:335:GLY:O	2:B:336:LEU:HB2	1.90	0.70
2:B:385:ILE:HG23	2:B:413:ARG:NH1	2.05	0.70
2:B:217:ILE:HG23	2:B:218:GLN:N	2.07	0.70
2:B:434:ARG:HB3	2:B:434:ARG:NH1	2.06	0.70
3:C:228:ILE:HB	3:C:231:GLY:HA3	1.73	0.70
3:C:305:GLY:N	3:C:365:ASP:HB3	2.05	0.70
1:E:901:A:H3'	5:E:109:HOH:O	1.91	0.70
2:A:164:ILE:HD13	2:A:195:VAL:HG22	1.72	0.70
2:A:193:THR:CG2	2:A:194:PRO:HD2	2.22	0.70
2:A:333:GLY:O	2:A:362:GLN:HG3	1.91	0.70
3:D:342:LEU:N	3:D:343:PRO:HD3	2.07	0.70
3:C:275:ASP:HA	3:C:385:ILE:HD13	1.72	0.69
3:C:349:GLU:OE2	3:C:352:VAL:HG21	1.92	0.69
3:D:403:LEU:HB3	3:D:404:PRO:CD	2.22	0.69
2:B:256:HIS:HD2	2:B:259:ARG:H	1.39	0.69
3:D:6:VAL:HG12	3:D:228:ILE:HG23	1.74	0.69
3:D:174:ARG:HG2	3:D:176:ASP:OD1	1.91	0.69
3:D:518:ASP:HA	3:D:521:LYS:HG2	1.74	0.69
2:A:381:GLN:OE1	2:B:41:ASP:HA	1.92	0.69
3:C:19:ASP:HA	3:C:214:LYS:HZ3	1.55	0.69
3:C:256:GLN:O	3:C:260:VAL:HG23	1.92	0.69
1:E:960:U:H5''	1:E:961:C:OP2	1.93	0.69
2:B:11:LEU:HD13	2:B:47:ILE:HD11	1.72	0.69
3:C:9:LYS:HB2	3:C:227:SER:CB	2.23	0.69
2:B:417:ARG:HB3	2:B:417:ARG:NH1	2.08	0.69
3:C:219:THR:HG22	3:C:220:ILE:HG13	1.75	0.69
3:D:329:LYS:HE2	3:D:334:SER:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:435:GLY:C	2:B:264:ARG:HE	2.00	0.69
2:B:260:ARG:HD2	3:D:85:GLU:OE2	1.92	0.69
3:D:339:THR:HB	3:D:366:ALA:HB1	1.75	0.69
3:D:523:LEU:HB2	3:D:524:GLU:OE2	1.92	0.69
3:D:331:ARG:HE	3:D:331:ARG:HA	1.58	0.69
3:C:19:ASP:HB2	3:C:214:LYS:HG2	1.75	0.69
3:C:167:THR:HG22	3:C:168:GLY:N	2.07	0.68
2:A:145:SER:OG	2:A:179:THR:HG22	1.94	0.68
2:A:228:ILE:HD11	2:A:281:ILE:HG12	1.74	0.68
2:A:303:ARG:HH11	2:A:303:ARG:CG	2.06	0.68
3:C:184:GLU:HB3	5:C:902:HOH:O	1.93	0.68
3:C:191:MET:HG3	3:C:197:LEU:CD1	2.23	0.68
3:D:169:ASP:OD2	5:D:1906:HOH:O	2.10	0.68
3:C:422:LEU:N	3:C:422:LEU:HD12	2.08	0.68
3:D:309:LEU:HA	3:D:312:VAL:HG23	1.76	0.68
3:C:43:ARG:HG2	3:C:43:ARG:HH11	1.59	0.68
2:A:205:SER:O	2:A:211:SER:HB2	1.94	0.67
1:F:968:G:O2'	1:F:969:G:H5'	1.94	0.67
3:D:477:PHE:HZ	3:D:487:THR:HG23	1.60	0.67
2:B:154:VAL:HG13	2:B:298:ASP:HB2	1.76	0.67
3:C:225:ASN:ND2	3:C:235:GLU:HB3	2.09	0.67
3:D:98:ILE:HD11	3:D:212:ARG:NH1	2.08	0.67
1:F:954:U:H2'	1:F:955:U:H5'	1.76	0.67
3:D:472:ASN:O	3:D:473:LEU:HD23	1.94	0.67
3:D:18:LEU:O	3:D:19:ASP:HB3	1.93	0.67
3:D:266:LEU:HD13	3:D:392:ILE:HD13	1.77	0.67
3:D:244:LEU:HD12	3:D:247:GLU:HB3	1.77	0.67
3:D:520:ILE:O	3:D:523:LEU:HD13	1.95	0.67
2:A:68:LEU:HD21	2:A:71:LYS:HG2	1.77	0.67
3:D:304:ARG:HA	3:D:365:ASP:HB3	1.75	0.66
3:C:162:ARG:HA	3:C:177:ARG:HH21	1.60	0.66
3:C:492:SER:O	3:C:496:TYR:HB2	1.95	0.66
3:C:7:GLY:HA3	3:C:229:ARG:HB2	1.76	0.66
3:C:439:ILE:O	3:C:442:ASN:N	2.28	0.66
2:A:303:ARG:HH11	2:A:303:ARG:N	1.93	0.66
2:B:140:VAL:HG12	2:B:141:PHE:CD2	2.29	0.66
3:D:115:HIS:CE1	3:D:428:LEU:HD13	2.31	0.66
3:D:210:SER:OG	3:D:446:LEU:HA	1.95	0.66
1:E:932:C:H2'	1:E:933:U:H4'	1.77	0.66
3:C:304:ARG:HA	3:C:365:ASP:HB3	1.77	0.66
3:C:390:MET:SD	3:C:396:PRO:HG3	2.34	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:244:LEU:O	3:D:248:ILE:HG23	1.96	0.66
2:B:251:LYS:HE3	2:B:425:ASN:HD22	1.60	0.66
2:B:108:TYR:CD2	3:D:419:ARG:HB3	2.31	0.66
3:D:280:VAL:HG11	3:D:355:LEU:HD23	1.76	0.66
3:D:451:LYS:O	3:D:454:ILE:HG22	1.95	0.66
2:B:200:THR:CG2	2:B:201:GLY:N	2.59	0.65
2:A:29:VAL:HG12	2:A:30:THR:H	1.60	0.65
3:C:422:LEU:HD12	3:C:422:LEU:H	1.60	0.65
3:D:291:ILE:H	3:D:291:ILE:CD1	2.09	0.65
2:A:9:LYS:HA	2:A:9:LYS:CE	2.27	0.65
3:D:486:ASP:N	5:D:1902:HOH:O	2.28	0.65
1:F:912:G:H1	1:F:923:C:H42	1.44	0.65
2:B:68:LEU:HD21	2:B:71:LYS:HG2	1.78	0.65
2:B:169:ASP:O	2:B:195:VAL:HG22	1.97	0.65
3:C:184:GLU:OE1	5:C:905:HOH:O	2.14	0.65
3:D:65:ARG:NH1	3:D:65:ARG:HB3	2.12	0.65
1:E:909:G:H5'	1:E:910:G:OP2	1.97	0.65
1:F:920:A:H61	1:F:959:C:H5	1.45	0.65
2:B:10:PHE:HE2	2:B:66:ILE:HD11	1.61	0.65
3:C:16:GLN:HE22	3:C:220:ILE:HG12	1.61	0.65
3:D:331:ARG:HA	3:D:331:ARG:NE	2.12	0.65
3:C:303:LEU:HB3	3:C:306:PHE:CD1	2.31	0.64
3:D:292:ILE:HG23	3:D:371:ALA:HB2	1.79	0.64
3:C:224:LEU:HD23	3:C:236:VAL:HB	1.78	0.64
2:A:50:LYS:CD	2:A:56:ASN:HD21	2.10	0.64
3:C:115:HIS:CD2	3:C:428:LEU:HD22	2.31	0.64
3:C:104:LEU:HD13	3:C:440:ARG:HA	1.79	0.64
3:C:501:LEU:HD23	3:C:502:ARG:N	2.11	0.64
2:A:402:VAL:HG22	2:A:415:MET:HE2	1.78	0.64
2:A:435:GLY:CA	2:B:264:ARG:HE	2.09	0.64
2:B:256:HIS:CD2	2:B:259:ARG:H	2.15	0.64
2:B:274:VAL:HG22	2:B:279:ILE:HG23	1.77	0.64
3:C:448:SER:HA	3:C:451:LYS:HD2	1.80	0.64
3:D:96:LEU:O	3:D:100:VAL:HG23	1.97	0.64
2:A:164:ILE:HD13	2:A:195:VAL:CG2	2.27	0.64
2:A:8:ARG:NH2	2:A:9:LYS:HZ2	1.95	0.64
2:B:45:ARG:HH22	3:D:430:ARG:CZ	2.10	0.64
2:B:66:ILE:HG22	2:B:67:GLU:H	1.63	0.64
3:C:111:VAL:HG23	3:C:136:VAL:O	1.97	0.64
3:C:330:LYS:O	3:C:331:ARG:HB3	1.98	0.64
3:D:378:GLU:O	3:D:382:ARG:HG3	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:149:LYS:HG2	2:A:152:TYR:CD1	2.33	0.64
2:B:200:THR:CG2	2:B:201:GLY:H	2.10	0.64
3:D:445:GLU:HG3	3:D:450:LYS:HG2	1.79	0.64
2:A:68:LEU:HD12	2:A:69:LEU:H	1.64	0.63
2:A:96:ILE:HG13	2:A:140:VAL:HG13	1.81	0.63
2:A:108:TYR:CD2	3:C:419:ARG:HB2	2.32	0.63
2:A:177:THR:HB	2:A:254:LYS:NZ	2.13	0.63
2:B:208:ARG:HD3	5:D:1907:HOH:O	1.97	0.63
3:D:82:GLU:O	3:D:127:THR:HG21	1.98	0.63
2:A:273:GLU:HB3	2:A:280:LYS:HB3	1.79	0.63
3:C:14:ILE:HG12	3:C:222:GLN:HG2	1.78	0.63
3:C:32:LEU:HD21	3:C:177:ARG:HG3	1.80	0.63
1:E:939:C:O2'	1:E:940:C:H5'	1.97	0.63
3:D:167:THR:CG2	3:D:168:GLY:N	2.62	0.63
3:D:184:GLU:OE1	5:D:1901:HOH:O	2.15	0.63
3:D:323:GLU:CD	3:D:400:ARG:HH22	2.07	0.63
2:A:289:ARG:HG3	2:A:289:ARG:HH11	1.64	0.63
2:A:280:LYS:HG2	2:A:280:LYS:O	1.97	0.63
2:A:399:MET:HA	2:A:416:MET:HE1	1.81	0.63
2:B:192:ARG:HG3	2:B:295:GLU:HB2	1.79	0.63
3:C:211:THR:O	3:C:213:VAL:HG23	1.99	0.63
2:A:8:ARG:NH1	2:A:9:LYS:HZ1	1.94	0.63
1:E:953:G:H21	3:C:496:TYR:HE2	1.46	0.62
2:A:192:ARG:HG3	2:A:295:GLU:HB2	1.81	0.62
2:B:175:HIS:CD2	2:B:180:MET:HA	2.34	0.62
3:C:223:ASP:OD1	3:C:237:LYS:HD3	1.99	0.62
3:D:514:ASP:OD2	3:D:535:ASP:HA	1.99	0.62
1:F:963:G:H5'	3:D:471:ARG:HH22	1.63	0.62
2:B:132:ILE:HG12	2:B:222:ARG:NH1	2.11	0.62
3:C:77:GLU:CD	3:C:77:GLU:H	2.06	0.62
2:A:301:GLU:OE2	2:A:303:ARG:CZ	2.48	0.62
2:B:222:ARG:HG3	2:B:275:THR:O	2.00	0.62
2:B:417:ARG:HB3	2:B:417:ARG:HH11	1.64	0.62
2:B:228:ILE:HD11	2:B:281:ILE:HD13	1.80	0.62
3:C:263:ARG:HD3	3:C:393:GLN:O	2.00	0.62
3:C:381:LEU:O	3:C:385:ILE:HG13	1.99	0.62
3:D:516:LEU:O	3:D:520:ILE:HG13	1.99	0.62
1:E:908:U:H3	1:E:914:A:H62	1.44	0.62
3:C:320:LEU:CD1	3:C:387:ARG:HH21	2.12	0.62
1:E:918:G:O2'	1:E:919:U:H5'	1.99	0.62
1:E:933:U:O5'	1:E:934:U:H5''	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:933:U:H3	1:F:936:G:H5''	1.63	0.62
1:F:939:C:O2'	1:F:940:C:H5'	2.00	0.62
2:A:98:THR:HG21	2:A:148:MET:HE1	1.80	0.62
2:A:147:ASN:HD22	2:B:340:PRO:HA	1.62	0.62
2:A:177:THR:HB	2:A:254:LYS:HZ2	1.65	0.62
2:B:177:THR:HB	2:B:254:LYS:NZ	2.14	0.62
2:A:129:LEU:HD23	2:A:132:ILE:HD12	1.81	0.62
2:B:385:ILE:HD13	2:B:413:ARG:HA	1.81	0.62
3:D:62:GLU:HA	3:D:65:ARG:NH1	2.14	0.62
3:D:381:LEU:HA	3:D:384:VAL:CG1	2.30	0.62
2:A:175:HIS:HD2	2:A:176:GLY:O	1.83	0.62
2:A:190:MET:HE2	2:A:300:VAL:HG21	1.82	0.62
2:B:388:ASP:OD1	2:B:424:ILE:HD13	2.00	0.62
3:C:471:ARG:NH2	3:C:499:ARG:HB2	2.14	0.62
3:D:136:VAL:HG22	3:D:154:LEU:O	2.00	0.61
3:D:224:LEU:HD12	3:D:236:VAL:HB	1.81	0.61
3:D:466:SER:OG	3:D:470:LYS:HE3	2.00	0.61
3:D:102:ILE:O	3:D:106:LEU:HD12	2.00	0.61
2:A:86:GLU:O	2:A:86:GLU:HG2	2.00	0.61
3:C:267:GLN:HA	5:C:920:HOH:O	2.00	0.61
3:D:59:ALA:C	3:D:61:GLU:N	2.57	0.61
3:D:62:GLU:HA	3:D:65:ARG:HH12	1.65	0.61
3:D:111:VAL:HG12	3:D:113:GLU:N	2.14	0.61
3:C:223:ASP:OD1	3:C:237:LYS:HA	2.01	0.61
2:A:29:VAL:HG12	2:A:30:THR:N	2.16	0.61
3:C:16:GLN:HE21	3:C:16:GLN:CA	2.02	0.61
3:C:162:ARG:CA	3:C:177:ARG:HH21	2.12	0.61
3:C:331:ARG:NH2	3:C:379:ASN:ND2	2.48	0.61
3:D:145:PRO:HD2	3:D:146:GLN:HE21	1.64	0.61
1:E:955:U:H2'	1:E:957:G:OP2	1.98	0.61
2:A:161:TYR:CD1	2:A:294:LEU:HD21	2.35	0.61
2:A:402:VAL:HG21	2:A:416:MET:HE2	1.82	0.61
2:B:204:ARG:NH2	2:B:258:SER:O	2.32	0.61
3:C:319:ARG:HG3	3:C:319:ARG:HH11	1.64	0.61
3:D:15:HIS:NE2	3:D:184:GLU:HG2	2.16	0.61
3:D:330:LYS:O	3:D:331:ARG:HB3	2.00	0.61
3:D:432:GLU:HG3	3:D:435:LEU:HG	1.82	0.61
2:B:222:ARG:HG2	2:B:222:ARG:NH1	2.12	0.61
3:C:105:LEU:CD2	3:C:443:LEU:HB3	2.30	0.61
3:C:215:ARG:HD3	5:C:922:HOH:O	2.00	0.61
3:C:245:ILE:HB	3:C:246:PRO:HD3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:319:ARG:HD2	3:C:319:ARG:H	1.63	0.61
3:C:339:THR:HB	3:C:366:ALA:HB1	1.81	0.61
1:E:926:G:H2'	1:E:927:C:C6	2.36	0.61
2:B:177:THR:HG22	2:B:263:PHE:CE2	2.35	0.61
3:C:65:ARG:HG3	3:C:65:ARG:NH1	2.13	0.61
3:D:15:HIS:HE1	5:D:1901:HOH:O	1.83	0.61
3:D:517:ARG:HH21	3:D:521:LYS:NZ	1.97	0.61
2:A:68:LEU:HD11	2:A:70:GLU:C	2.26	0.61
3:D:278:PHE:CD1	3:D:359:VAL:HG23	2.36	0.61
2:A:36:LEU:HD11	2:A:50:LYS:HB2	1.83	0.61
2:A:44:ASP:O	2:A:45:ARG:HB2	1.99	0.61
2:A:55:TYR:CE1	3:C:420:MET:HE1	2.35	0.61
2:A:239:MET:O	3:C:43:ARG:NH1	2.32	0.61
2:A:427:ARG:NH2	2:A:429:SER:HB2	2.15	0.61
2:A:427:ARG:NH2	3:D:75:HIS:O	2.33	0.61
2:B:308:LYS:HA	2:B:332:GLU:HB3	1.81	0.61
3:C:191:MET:O	3:C:192:SER:HB3	2.00	0.61
3:C:208:LEU:O	3:C:213:VAL:HG21	1.99	0.61
3:C:355:LEU:O	3:C:359:VAL:HG12	2.00	0.61
2:A:182:TYR:O	2:A:185:ALA:HB3	2.01	0.60
3:C:296:GLU:HB2	3:C:373:GLU:HA	1.83	0.60
3:C:248:ILE:HG22	3:C:406:GLY:HA2	1.82	0.60
3:C:265:THR:O	3:C:269:ARG:HG2	2.02	0.60
3:D:469:VAL:HG22	3:D:474:VAL:HG21	1.83	0.60
2:B:124:ARG:HG3	2:B:124:ARG:HH11	1.65	0.60
2:B:165:LYS:HE2	2:B:294:LEU:HD23	1.82	0.60
3:C:98:ILE:HD11	3:C:212:ARG:HB2	1.82	0.60
3:C:149:VAL:HG11	3:C:191:MET:HE1	1.84	0.60
3:D:14:ILE:HG12	3:D:222:GLN:HG2	1.83	0.60
2:A:12:GLU:C	2:A:14:ALA:H	2.09	0.60
2:A:158:ARG:HG3	2:A:158:ARG:HH11	1.66	0.60
2:A:164:ILE:HG13	2:A:294:LEU:HD22	1.83	0.60
2:A:320:TRP:CD1	2:B:320:TRP:CD1	2.90	0.60
3:C:430:ARG:HB3	3:C:430:ARG:NH1	2.16	0.60
3:C:437:GLU:HA	3:C:440:ARG:CB	2.32	0.60
3:D:397:GLU:HB3	3:D:414:LEU:HD22	1.82	0.60
2:A:256:HIS:HD2	2:A:259:ARG:N	1.89	0.60
2:B:36:LEU:N	2:B:36:LEU:HD12	2.17	0.60
2:B:200:THR:CG2	2:B:216:ASN:HB3	2.32	0.60
3:C:136:VAL:CG1	3:C:154:LEU:HD22	2.31	0.60
2:B:36:LEU:HD13	2:B:48:VAL:HG12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:299:LEU:HD11	3:D:374:ARG:HD3	1.83	0.60
2:A:95:ILE:HG22	2:A:117:PHE:CE2	2.37	0.60
2:A:175:HIS:CD2	2:A:176:GLY:N	2.70	0.60
2:A:222:ARG:HG3	2:A:275:THR:O	2.02	0.60
2:A:256:HIS:CD2	2:A:258:SER:H	2.20	0.60
3:D:19:ASP:HA	3:D:214:LYS:CE	2.31	0.60
3:D:45:LEU:HD23	3:D:69:PHE:CE1	2.37	0.60
2:A:399:MET:HA	2:A:416:MET:CE	2.31	0.59
3:D:468:LEU:HD21	3:D:477:PHE:HB2	1.83	0.59
1:E:943:G:O2'	1:E:944:C:H5'	2.02	0.59
3:C:325:ALA:O	3:C:329:LYS:HG3	2.02	0.59
2:B:26:LYS:CB	2:B:29:VAL:HG23	2.26	0.59
2:B:287:ARG:HD2	2:B:292:ASP:OD2	2.03	0.59
3:C:350:GLU:HA	3:C:353:ARG:HD3	1.84	0.59
3:D:280:VAL:HG11	3:D:355:LEU:CD2	2.32	0.59
3:C:233:ARG:O	3:C:397:GLU:HA	2.02	0.59
3:D:437:GLU:C	3:D:439:ILE:N	2.59	0.59
1:E:972:U:H2'	1:E:973:A:C8	2.37	0.59
2:B:9:LYS:HA	2:B:9:LYS:HZ2	1.67	0.59
2:B:108:TYR:CE2	3:D:419:ARG:HB3	2.37	0.59
2:B:195:VAL:HG22	2:B:289:ARG:HH12	1.68	0.59
3:C:307:ASP:O	3:C:309:LEU:HD12	2.03	0.59
3:C:323:GLU:O	3:C:326:ASP:HB2	2.02	0.59
3:C:195:GLN:HE22	3:C:198:ARG:NH2	1.92	0.59
2:A:169:ASP:O	2:A:195:VAL:HB	2.02	0.59
2:A:434:ARG:HB2	5:B:446:HOH:O	2.03	0.59
2:B:45:ARG:HH22	3:D:430:ARG:NH2	2.00	0.59
2:B:222:ARG:O	2:B:225:THR:HB	2.03	0.59
3:C:489:VAL:HA	3:C:492:SER:OG	2.02	0.59
2:A:192:ARG:CG	2:A:295:GLU:HB2	2.33	0.59
3:D:374:ARG:HD2	3:D:378:GLU:OE2	2.03	0.59
2:A:161:TYR:HD1	2:A:294:LEU:HD21	1.67	0.59
3:C:120:GLN:HE21	3:C:419:ARG:HD2	1.67	0.59
3:C:378:GLU:O	3:C:382:ARG:HG3	2.03	0.59
3:C:437:GLU:HB3	3:C:441:ARG:NH2	2.18	0.59
1:F:964:C:H2'	1:F:965:U:O4'	2.03	0.59
3:C:374:ARG:HH22	3:C:378:GLU:CB	2.15	0.59
1:E:931:G:H1	1:E:939:C:N4	2.00	0.58
2:B:274:VAL:HG12	2:B:275:THR:N	2.18	0.58
2:B:369:ASN:C	2:B:369:ASN:HD22	2.10	0.58
3:C:499:ARG:O	3:C:502:ARG:HG3	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:154:LEU:HD22	3:D:185:ILE:HG12	1.84	0.58
3:D:8:LEU:O	3:D:9:LYS:HD3	2.02	0.58
3:D:247:GLU:OE2	3:D:251:ARG:HG3	2.04	0.58
3:D:274:GLU:HB3	3:D:276:LYS:HG3	1.85	0.58
1:E:909:G:O2'	1:E:945:G:O2'	2.17	0.58
1:E:967:G:H2'	1:E:968:G:H8	1.69	0.58
3:C:120:GLN:NE2	3:C:419:ARG:HD2	2.17	0.58
3:C:342:LEU:CD1	3:C:352:VAL:HG22	2.34	0.58
3:D:205:GLY:O	3:D:209:ARG:HG2	2.02	0.58
2:B:111:GLY:HA3	5:B:455:HOH:O	2.03	0.58
1:F:974:C:O2	3:D:412:ARG:NH2	2.37	0.58
3:D:275:ASP:HA	3:D:385:ILE:CD1	2.28	0.58
2:A:299:ARG:HG3	2:A:299:ARG:NH1	2.16	0.58
3:C:448:SER:HA	3:C:451:LYS:CE	2.34	0.58
3:D:143:GLU:HB3	5:D:1948:HOH:O	2.02	0.58
3:D:341:GLU:C	3:D:343:PRO:HD3	2.28	0.58
2:B:56:ASN:HD22	2:B:56:ASN:N	2.00	0.58
1:E:914:A:H2'	1:E:915:G:O4'	2.04	0.58
2:A:435:GLY:HA2	2:B:264:ARG:HE	1.67	0.58
3:C:331:ARG:NE	3:C:379:ASN:HB2	2.18	0.58
3:C:496:TYR:O	3:C:499:ARG:HB3	2.04	0.58
3:D:19:ASP:HB2	3:D:214:LYS:HD3	1.84	0.58
3:D:454:ILE:CD1	3:D:474:VAL:HG13	2.29	0.58
1:E:932:C:H2'	1:E:933:U:C4'	2.34	0.58
1:F:919:U:H5''	1:F:920:A:O5'	2.04	0.58
3:D:212:ARG:CB	3:D:212:ARG:HH11	2.16	0.58
3:D:386:ARG:O	3:D:390:MET:HG3	2.03	0.58
2:B:170:GLY:HA2	2:B:195:VAL:CG1	2.34	0.57
3:C:202:TYR:HB2	3:C:242:LEU:HD21	1.85	0.57
3:D:16:GLN:HG2	3:D:208:LEU:HD13	1.86	0.57
2:A:142:ASN:C	2:A:143:ILE:HG13	2.28	0.57
2:B:264:ARG:HH11	2:B:264:ARG:HG2	1.69	0.57
3:D:68:HIS:HE1	3:D:169:ASP:OD2	1.86	0.57
2:B:144:LEU:HB2	2:B:147:ASN:ND2	2.19	0.57
3:C:178:LEU:HD23	3:C:179:GLY:N	2.20	0.57
3:D:133:THR:HG23	3:D:157:GLU:CB	2.18	0.57
1:E:926:G:H2'	1:E:927:C:H6	1.68	0.57
3:C:349:GLU:O	3:C:353:ARG:HG2	2.04	0.57
3:D:32:LEU:HD13	3:D:162:ARG:NH1	2.19	0.57
3:D:111:VAL:HG12	3:D:112:ASP:N	2.19	0.57
2:A:193:THR:HG22	2:A:194:PRO:HD2	1.84	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:336:LEU:HB2	5:A:459:HOH:O	2.04	0.57
2:B:385:ILE:HD11	2:B:413:ARG:HB2	1.86	0.57
3:C:219:THR:HG22	3:C:220:ILE:N	2.18	0.57
1:F:962:C:O3'	3:D:499:ARG:HD3	2.04	0.57
2:B:204:ARG:O	2:B:205:SER:C	2.48	0.57
3:D:32:LEU:HD22	3:D:176:ASP:CG	2.30	0.57
2:A:138:ARG:HH12	2:A:140:VAL:HG12	1.69	0.57
2:A:391:LEU:HB2	2:A:394:VAL:CG1	2.33	0.57
3:C:228:ILE:HG12	3:C:256:GLN:HG2	1.87	0.57
3:C:369:MET:HG2	3:C:370:VAL:N	2.20	0.57
1:E:950:G:O2'	1:E:951:C:H5'	2.04	0.57
2:A:378:ARG:O	2:A:378:ARG:NH1	2.38	0.57
2:B:179:THR:HG23	2:B:182:TYR:HB2	1.87	0.57
2:B:248:ARG:HB2	2:B:271:LEU:HD11	1.87	0.57
3:C:71:TYR:CD2	3:C:127:THR:HG22	2.40	0.57
3:C:211:THR:HG22	3:C:212:ARG:H	1.69	0.57
3:C:348:THR:OG1	3:C:351:GLU:HG3	2.05	0.57
3:D:155:CYS:O	3:D:183:VAL:HA	2.04	0.57
3:D:228:ILE:CD1	3:D:253:VAL:HG13	2.34	0.57
2:A:371:ASN:N	2:A:371:ASN:ND2	2.49	0.57
3:C:132:ARG:NH1	3:C:158:GLU:OE2	2.37	0.57
3:C:201:ALA:HB3	3:C:242:LEU:HD13	1.86	0.57
3:C:332:GLY:O	3:C:333:VAL:HB	2.04	0.57
3:C:211:THR:HG22	3:C:212:ARG:N	2.20	0.56
2:A:318:ILE:HB	2:A:346:VAL:HG11	1.87	0.56
2:B:124:ARG:HH11	2:B:124:ARG:CG	2.18	0.56
3:C:1:MET:HE2	3:C:3:TRP:CZ3	2.40	0.56
3:D:332:GLY:O	3:D:333:VAL:HG23	2.05	0.56
1:F:901:A:H2'	5:F:137:HOH:O	2.05	0.56
1:F:954:U:C2'	1:F:955:U:H5'	2.35	0.56
2:A:9:LYS:HE3	2:A:9:LYS:CA	2.35	0.56
2:A:283:GLU:CD	2:A:285:ASN:H	2.13	0.56
5:A:463:HOH:O	3:C:64:MET:HE1	2.05	0.56
3:C:16:GLN:HB3	3:C:183:VAL:CG2	2.35	0.56
3:C:194:PRO:HG3	3:C:249:VAL:HG11	1.86	0.56
3:C:299:LEU:HB2	3:C:381:LEU:CD1	2.35	0.56
3:D:104:LEU:HD11	3:D:436:LEU:HD11	1.87	0.56
3:D:464:LEU:HD22	3:D:491:ALA:HB1	1.86	0.56
3:D:531:ASP:C	3:D:533:LEU:H	2.12	0.56
1:E:929:G:N3	1:E:929:G:H2'	2.20	0.56
2:B:401:TRP:O	2:B:405:GLN:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:118:ARG:HE	3:C:423:GLU:CD	2.14	0.56
3:C:195:GLN:NE2	3:C:198:ARG:NH2	2.51	0.56
3:C:471:ARG:HH11	3:C:499:ARG:CZ	2.17	0.56
3:D:331:ARG:HG2	3:D:379:ASN:HB3	1.87	0.56
2:A:55:TYR:OH	3:C:133:THR:HG21	2.06	0.56
3:D:32:LEU:HD21	3:D:177:ARG:HB2	1.87	0.56
3:C:489:VAL:HA	3:C:492:SER:HG	1.70	0.56
3:D:337:PHE:CE2	3:D:345:TYR:CD2	2.94	0.56
1:E:908:U:H3	1:E:914:A:N6	2.04	0.56
2:B:410:GLU:H	2:B:410:GLU:CD	2.13	0.56
3:C:448:SER:HA	3:C:451:LYS:CD	2.36	0.56
2:B:217:ILE:CG2	2:B:218:GLN:N	2.69	0.56
3:D:451:LYS:O	3:D:455:MET:HG3	2.06	0.56
2:A:299:ARG:HA	5:A:465:HOH:O	2.05	0.56
2:B:5:GLY:O	2:B:8:ARG:HG2	2.06	0.56
3:C:174:ARG:HG2	3:C:176:ASP:OD1	2.05	0.56
2:A:363:CYS:O	2:A:364:LEU:HB2	2.06	0.55
3:D:6:VAL:HG11	3:D:228:ILE:HD13	1.88	0.55
3:D:58:ALA:HA	5:D:1905:HOH:O	2.04	0.55
2:B:149:LYS:HB2	2:B:150:PRO:HD2	1.88	0.55
2:B:275:THR:HG23	2:B:276:PRO:HD2	1.88	0.55
2:B:318:ILE:HG13	2:B:343:LEU:HD12	1.88	0.55
3:C:146:GLN:CD	3:C:146:GLN:N	2.64	0.55
3:D:281:SER:HA	3:D:298:VAL:HG13	1.87	0.55
2:A:8:ARG:NH1	2:A:9:LYS:NZ	2.54	0.55
2:A:98:THR:CG2	2:A:148:MET:HE1	2.35	0.55
2:A:114:HIS:O	2:A:115:PRO:O	2.24	0.55
3:D:403:LEU:HB3	3:D:404:PRO:HD2	1.88	0.55
3:D:526:GLY:HA3	3:D:534:ARG:NH1	2.21	0.55
2:A:281:ILE:HG22	2:A:281:ILE:O	2.06	0.55
2:A:427:ARG:HB3	3:D:27:PRO:HG2	1.88	0.55
2:B:434:ARG:HB3	2:B:434:ARG:CZ	2.36	0.55
3:C:23:LYS:HG3	3:C:28:CYS:O	2.06	0.55
3:C:74:TYR:CB	3:C:77:GLU:HG2	2.35	0.55
3:C:291:ILE:HD12	3:C:291:ILE:H	1.72	0.55
1:E:907:G:H1'	1:E:967:G:N2	2.21	0.55
2:A:51:LEU:HD11	2:A:57:ILE:HG21	1.88	0.55
2:A:132:ILE:HG12	2:A:222:ARG:HH12	1.70	0.55
2:B:192:ARG:CG	2:B:295:GLU:HB2	2.36	0.55
3:C:374:ARG:HH22	3:C:378:GLU:HB2	1.72	0.55
2:A:113:VAL:HG11	2:A:207:ASP:CB	2.33	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:59:ALA:O	3:D:61:GLU:N	2.30	0.55
3:D:68:HIS:CE1	3:D:169:ASP:OD2	2.60	0.55
3:D:331:ARG:HE	3:D:331:ARG:CA	2.18	0.55
3:D:342:LEU:N	3:D:343:PRO:CD	2.69	0.55
1:E:958:A:C4'	1:E:959:C:OP1	2.49	0.55
2:A:50:LYS:HD2	2:A:56:ASN:HD21	1.72	0.55
2:A:189:PHE:CE2	2:A:423:GLU:HG2	2.42	0.55
3:C:1:MET:HE1	3:C:253:VAL:CG1	2.36	0.55
3:D:98:ILE:HD11	3:D:212:ARG:HH12	1.69	0.55
3:D:531:ASP:O	3:D:533:LEU:N	2.28	0.55
3:C:309:LEU:HA	3:C:312:VAL:CG2	2.34	0.55
3:D:477:PHE:CZ	3:D:487:THR:HG23	2.39	0.55
3:D:510:GLY:O	3:D:513:LEU:HB3	2.06	0.55
2:A:95:ILE:HG22	2:A:117:PHE:HE2	1.71	0.55
2:B:7:ALA:HA	2:B:61:ILE:CD1	2.37	0.55
3:C:494:LEU:HA	3:C:498:LEU:HD12	1.89	0.55
3:D:486:ASP:O	3:D:488:THR:N	2.40	0.55
2:B:55:TYR:CZ	3:D:420:MET:HE1	2.42	0.55
2:A:204:ARG:NH2	2:A:258:SER:HB2	2.22	0.54
3:D:119:LYS:NZ	3:D:131:GLN:OE1	2.40	0.54
3:D:224:LEU:HD21	3:D:245:ILE:HG12	1.88	0.54
1:F:963:G:C4'	3:D:467:GLN:HE22	2.20	0.54
3:D:319:ARG:HG3	3:D:319:ARG:NH1	2.21	0.54
3:D:418:SER:HA	5:D:1945:HOH:O	2.06	0.54
2:A:102:VAL:O	2:A:103:ALA:HB2	2.07	0.54
2:A:146:GLU:OE1	2:A:146:GLU:N	2.38	0.54
3:D:119:LYS:HA	3:D:420:MET:HB3	1.89	0.54
3:D:303:LEU:HD12	3:D:310:ILE:HD11	1.90	0.54
2:B:9:LYS:HA	2:B:9:LYS:NZ	2.22	0.54
3:C:16:GLN:NE2	3:C:220:ILE:HG12	2.21	0.54
3:C:136:VAL:HG11	3:C:154:LEU:HD22	1.90	0.54
3:C:164:ILE:O	3:C:165:ARG:HG3	2.07	0.54
1:F:912:G:H1	1:F:923:C:N4	2.06	0.54
2:A:187:LEU:HD12	2:A:191:LEU:HD12	1.89	0.54
3:C:8:LEU:HD12	3:C:227:SER:O	2.07	0.54
3:C:136:VAL:HG12	3:C:154:LEU:O	2.07	0.54
3:C:198:ARG:HG3	3:C:242:LEU:CD1	2.38	0.54
3:C:501:LEU:C	3:C:503:ARG:H	2.15	0.54
3:D:523:LEU:C	3:D:524:GLU:HG3	2.32	0.54
2:A:132:ILE:HG23	2:A:222:ARG:NH1	2.22	0.54
2:A:172:VAL:HG22	2:A:198:VAL:CG2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:335:GLY:O	2:A:336:LEU:HB2	2.07	0.54
3:D:167:THR:HG23	3:D:168:GLY:N	2.23	0.54
3:D:301:VAL:CG2	3:D:381:LEU:HD22	2.38	0.54
3:D:304:ARG:HA	3:D:365:ASP:CB	2.38	0.54
2:B:356:PRO:HB2	2:B:399:MET:HE1	1.89	0.54
3:C:80:LEU:HD22	3:C:85:GLU:HB2	1.89	0.54
3:C:374:ARG:HH11	3:C:374:ARG:HG2	1.71	0.54
3:D:64:MET:HG2	3:D:65:ARG:N	2.22	0.54
3:D:265:THR:O	3:D:269:ARG:HG2	2.08	0.54
3:D:458:TYR:O	3:D:487:THR:HG21	2.07	0.54
2:A:257:THR:HG23	2:B:336:LEU:HA	1.89	0.54
2:B:186:ALA:HB1	2:B:190:MET:CE	2.33	0.54
3:C:375:VAL:O	3:C:379:ASN:ND2	2.41	0.54
3:D:337:PHE:HB2	3:D:369:MET:HG2	1.89	0.54
1:E:932:C:C3'	1:E:933:U:H5''	2.37	0.54
2:A:264:ARG:NE	2:B:435:GLY:C	2.64	0.54
2:B:55:TYR:CE2	3:D:420:MET:HE1	2.43	0.54
3:C:118:ARG:HG3	3:C:423:GLU:HB2	1.90	0.54
1:F:903:U:H2'	1:F:904:C:O4'	2.07	0.53
2:A:61:ILE:HA	2:A:64:ALA:HB2	1.88	0.53
3:C:33:THR:O	3:C:162:ARG:NH2	2.42	0.53
3:C:291:ILE:H	3:C:291:ILE:CD1	2.21	0.53
3:D:45:LEU:HD23	3:D:69:PHE:CD1	2.42	0.53
3:D:287:THR:HG22	5:D:1925:HOH:O	2.06	0.53
1:E:910:G:OP2	1:E:910:G:H3'	2.09	0.53
2:A:8:ARG:HH22	2:A:9:LYS:HZ2	1.56	0.53
2:A:49:LEU:HD12	2:A:59:VAL:HG11	1.89	0.53
2:A:158:ARG:NE	2:A:298:ASP:OD2	2.37	0.53
2:A:175:HIS:CD2	2:A:176:GLY:H	2.25	0.53
2:B:150:PRO:HA	2:B:153:TRP:CE3	2.43	0.53
3:C:59:ALA:O	3:C:61:GLU:N	2.32	0.53
3:C:111:VAL:O	3:C:431:ILE:HD12	2.08	0.53
3:D:157:GLU:OE2	3:D:184:GLU:OE1	2.26	0.53
1:F:958:A:C4'	1:F:959:C:OP1	2.45	0.53
2:A:68:LEU:HD11	2:A:70:GLU:O	2.07	0.53
2:A:275:THR:HG23	2:A:276:PRO:HD2	1.89	0.53
2:B:195:VAL:HG22	2:B:289:ARG:NH1	2.22	0.53
2:B:293:GLU:O	2:B:295:GLU:HG3	2.09	0.53
3:C:3:TRP:HZ3	3:C:253:VAL:HG11	1.72	0.53
2:B:180:MET:HE2	2:B:263:PHE:CZ	2.43	0.53
2:B:214:SER:O	2:B:217:ILE:HG22	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:271:LEU:HD22	2:B:283:GLU:HG2	1.91	0.53
3:D:119:LYS:HD2	3:D:418:SER:HB3	1.91	0.53
3:D:200:VAL:O	3:D:204:ILE:HG13	2.09	0.53
3:D:365:ASP:OD2	3:D:365:ASP:N	2.40	0.53
3:D:486:ASP:HB3	3:D:489:VAL:CG2	2.37	0.53
1:E:937:G:H2'	1:E:938:A:O4'	2.09	0.53
2:A:47:ILE:HD12	2:A:61:ILE:HG21	1.90	0.53
2:A:157:ALA:HA	2:A:187:LEU:CD1	2.39	0.53
2:A:194:PRO:O	2:A:289:ARG:HD3	2.08	0.53
2:A:365:ASN:HB2	2:B:255:MET:O	2.08	0.53
2:B:380:LEU:HD21	2:B:386:PRO:CG	2.38	0.53
2:A:8:ARG:HH12	2:A:9:LYS:NZ	2.01	0.53
2:B:205:SER:HB2	2:B:207:ASP:OD1	2.09	0.53
3:C:10:MET:O	3:C:191:MET:HG2	2.07	0.53
3:C:299:LEU:HB2	3:C:381:LEU:HD12	1.90	0.53
1:E:922:U:H2'	1:E:923:C:N1	2.23	0.53
3:C:15:HIS:ND1	3:C:184:GLU:HG2	2.23	0.53
3:C:121:VAL:HB	3:C:126:ASN:HD21	1.74	0.53
3:C:146:GLN:HG3	3:C:196:GLN:CB	2.39	0.53
3:C:162:ARG:HA	3:C:177:ARG:NH2	2.23	0.53
2:B:123:LEU:CD2	2:B:130:LEU:HD21	2.38	0.53
2:B:203:GLN:HA	2:B:203:GLN:NE2	2.22	0.53
3:C:259:LEU:CD2	3:C:262:ILE:HD12	2.29	0.53
3:D:486:ASP:O	3:D:486:ASP:CG	2.52	0.53
3:D:488:THR:HG23	5:D:1921:HOH:O	2.07	0.53
3:D:515:GLU:HA	3:D:518:ASP:OD1	2.09	0.53
2:B:66:ILE:HG22	2:B:67:GLU:N	2.24	0.53
3:D:15:HIS:CE1	3:D:184:GLU:CG	2.91	0.53
1:E:922:U:H2'	1:E:923:C:C6	2.44	0.52
2:A:158:ARG:HG3	2:A:158:ARG:NH1	2.25	0.52
2:A:193:THR:HG23	2:A:194:PRO:HD2	1.91	0.52
2:A:232:THR:HG22	2:A:248:ARG:HA	1.90	0.52
2:B:23:LEU:HB2	2:B:69:LEU:HD11	1.91	0.52
3:C:121:VAL:HG12	3:C:121:VAL:O	2.09	0.52
3:C:201:ALA:HB3	3:C:242:LEU:CD1	2.38	0.52
3:C:306:PHE:CZ	3:C:392:ILE:HD11	2.43	0.52
3:C:342:LEU:HD13	3:C:352:VAL:HG22	1.90	0.52
2:A:198:VAL:HG12	2:A:232:THR:OG1	2.09	0.52
2:B:12:GLU:C	2:B:14:ALA:H	2.16	0.52
2:B:140:VAL:HG11	2:B:159:ALA:HB2	1.92	0.52
3:C:146:GLN:CD	3:C:146:GLN:H	2.15	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:15:HIS:CE1	3:D:184:GLU:OE1	2.62	0.52
2:A:12:GLU:O	2:A:14:ALA:N	2.42	0.52
3:D:307:ASP:HB3	3:D:364:GLY:O	2.09	0.52
1:E:930:G:O2'	1:E:931:G:H5'	2.09	0.52
2:A:154:VAL:HG13	2:A:298:ASP:HB2	1.91	0.52
3:C:228:ILE:CG1	3:C:256:GLN:HG2	2.39	0.52
3:C:292:ILE:HD11	3:C:369:MET:HE1	1.90	0.52
3:C:441:ARG:O	3:C:442:ASN:ND2	2.42	0.52
3:D:177:ARG:HG3	3:D:180:ILE:HD12	1.91	0.52
3:D:468:LEU:HD21	3:D:477:PHE:CB	2.39	0.52
3:D:503:ARG:O	3:D:504:GLU:HG3	2.08	0.52
2:A:247:HIS:HB3	2:A:252:VAL:HG22	1.91	0.52
2:B:325:GLY:O	2:B:327:ARG:NH1	2.43	0.52
3:C:59:ALA:C	3:C:61:GLU:N	2.63	0.52
3:D:105:LEU:CD2	3:D:443:LEU:HB3	2.38	0.52
3:D:224:LEU:CD1	3:D:248:ILE:HD11	2.38	0.52
3:D:381:LEU:HD23	3:D:384:VAL:HG11	1.92	0.52
2:A:95:ILE:HD13	2:A:217:ILE:HD11	1.92	0.52
2:B:102:VAL:O	2:B:103:ALA:HB2	2.09	0.52
3:C:183:VAL:O	3:C:183:VAL:HG23	2.10	0.52
3:C:454:ILE:CD1	3:C:474:VAL:HG13	2.34	0.52
2:A:229:ALA:HB3	2:A:288:LYS:O	2.09	0.52
2:A:344:ILE:HD13	2:A:379:LEU:HD23	1.91	0.52
2:B:10:PHE:CB	2:B:61:ILE:HD12	2.40	0.52
3:C:74:TYR:CG	3:C:77:GLU:HG2	2.45	0.52
3:C:324:MET:HE2	3:C:384:VAL:HG22	1.92	0.52
3:D:62:GLU:CG	3:D:65:ARG:HH12	2.22	0.52
3:D:162:ARG:HB3	3:D:177:ARG:HH21	1.75	0.52
3:D:263:ARG:O	3:D:267:GLN:HG3	2.08	0.52
1:F:914:A:H2'	1:F:915:G:O4'	2.10	0.52
2:B:204:ARG:HB2	2:B:211:SER:HA	1.92	0.52
3:C:313:GLU:HG3	3:C:319:ARG:NH1	2.25	0.52
3:D:68:HIS:CE1	5:D:1906:HOH:O	2.63	0.52
3:D:191:MET:O	3:D:192:SER:CB	2.55	0.52
3:C:355:LEU:HD22	3:C:367:VAL:HG11	1.90	0.52
3:D:22:SER:OG	3:D:27:PRO:HA	2.10	0.52
3:D:65:ARG:HB3	3:D:65:ARG:HH11	1.72	0.52
3:D:440:ARG:HA	3:D:443:LEU:HD21	1.92	0.52
1:F:962:C:OP1	3:D:503:ARG:NH1	2.43	0.52
2:B:161:TYR:CE1	2:B:294:LEU:HG	2.45	0.52
3:C:471:ARG:NH1	3:C:499:ARG:NE	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:292:ILE:HG23	3:D:371:ALA:CB	2.40	0.52
2:A:299:ARG:HH11	2:A:299:ARG:CG	2.18	0.51
3:D:416:THR:HG22	3:D:417:SER:N	2.25	0.51
3:C:22:SER:HB2	3:C:27:PRO:HA	1.91	0.51
3:C:437:GLU:C	3:C:439:ILE:H	2.18	0.51
1:F:949:A:OP1	1:F:959:C:H1'	2.10	0.51
2:A:196:PRO:HG3	2:A:228:ILE:O	2.10	0.51
1:F:932:C:H2'	1:F:933:U:H4'	1.91	0.51
2:A:221:VAL:O	2:A:225:THR:HG23	2.10	0.51
3:D:43:ARG:NH1	3:D:43:ARG:CG	2.62	0.51
3:D:114:PHE:CZ	3:D:134:GLY:HA3	2.45	0.51
2:B:175:HIS:HD2	2:B:176:GLY:O	1.94	0.51
3:C:355:LEU:CD2	3:C:367:VAL:HG11	2.39	0.51
2:B:87:ASP:OD1	2:B:90:LEU:HD23	2.10	0.51
2:B:274:VAL:CG1	2:B:275:THR:N	2.74	0.51
2:B:418:GLU:O	2:B:420:ILE:HG13	2.11	0.51
3:D:88:PRO:HG3	3:D:132:ARG:NH2	2.26	0.51
1:F:911:G:C2	1:F:925:U:H1'	2.45	0.51
2:A:68:LEU:HD12	2:A:69:LEU:N	2.26	0.51
2:A:283:GLU:OE1	2:A:285:ASN:N	2.42	0.51
2:B:111:GLY:C	3:D:422:LEU:HD12	2.36	0.51
2:B:321:HIS:O	2:B:326:TYR:HB2	2.10	0.51
3:C:262:ILE:HG23	3:C:309:LEU:HD23	1.92	0.51
2:A:367:ARG:NH2	2:A:428:THR:HG23	2.25	0.51
2:B:153:TRP:HB3	2:B:190:MET:HE1	1.93	0.51
2:B:363:CYS:O	2:B:364:LEU:HB2	2.11	0.51
3:C:319:ARG:HG3	3:C:319:ARG:NH1	2.23	0.51
3:D:177:ARG:HA	3:D:180:ILE:CD1	2.41	0.51
1:E:917:G:C2'	1:E:957:G:H22	2.18	0.51
2:B:61:ILE:O	2:B:62:SER:C	2.54	0.51
3:C:29:ARG:NH1	3:C:29:ARG:HB2	2.26	0.51
3:D:278:PHE:HD1	3:D:359:VAL:HA	1.75	0.51
1:F:960:U:OP2	1:F:960:U:H6	1.94	0.50
2:A:68:LEU:CD1	2:A:70:GLU:H	2.24	0.50
2:A:190:MET:HE2	2:A:300:VAL:CG2	2.40	0.50
2:A:362:GLN:NE2	5:A:447:HOH:O	2.43	0.50
2:B:344:ILE:HB	2:B:345:PRO:CD	2.35	0.50
3:C:138:THR:HG22	3:C:153:ASN:OD1	2.11	0.50
3:D:106:LEU:HB2	3:D:108:MET:HG3	1.92	0.50
1:F:960:U:C5'	1:F:961:C:OP2	2.56	0.50
2:A:162:GLY:O	2:A:165:LYS:N	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:10:PHE:C	2:B:10:PHE:CD2	2.89	0.50
2:B:161:TYR:O	2:B:164:ILE:HG22	2.11	0.50
2:B:189:PHE:CE2	2:B:398:LYS:HG3	2.46	0.50
3:C:167:THR:CG2	3:C:168:GLY:H	2.22	0.50
3:C:228:ILE:N	3:C:228:ILE:CD1	2.73	0.50
2:A:124:ARG:HG3	2:A:124:ARG:HH11	1.76	0.50
2:B:88:PRO:O	2:B:89:GLU:HB3	2.11	0.50
2:B:149:LYS:HB2	2:B:150:PRO:CD	2.41	0.50
2:B:260:ARG:NH2	3:D:84:ASP:OD2	2.44	0.50
2:B:430:ILE:HD11	3:C:41:ILE:HD11	1.94	0.50
3:C:10:MET:HE2	3:C:197:LEU:HD22	1.94	0.50
3:C:111:VAL:HG12	3:C:113:GLU:H	1.75	0.50
3:D:278:PHE:HE1	3:D:359:VAL:O	1.94	0.50
1:E:926:G:H2'	1:E:927:C:O4'	2.11	0.50
1:E:958:A:H1'	1:E:960:U:H5	1.77	0.50
2:A:274:VAL:HG12	2:A:275:THR:N	2.26	0.50
2:B:417:ARG:HH11	2:B:417:ARG:CB	2.24	0.50
3:C:489:VAL:HG23	3:C:490:ILE:N	2.26	0.50
2:A:27:PRO:HD2	2:A:63:ASP:OD2	2.11	0.50
2:A:259:ARG:NH1	2:A:261:ASP:OD1	2.45	0.50
2:B:29:VAL:HG13	3:D:109:ARG:CG	2.39	0.50
2:B:281:ILE:HG22	2:B:283:GLU:O	2.11	0.50
3:C:31:GLU:OE2	3:C:32:LEU:O	2.30	0.50
3:C:228:ILE:HD13	3:C:256:GLN:CD	2.36	0.50
3:D:191:MET:HE3	3:D:197:LEU:CD1	2.41	0.50
2:A:150:PRO:HA	2:A:153:TRP:CD2	2.46	0.50
2:B:219:CYS:O	2:B:274:VAL:HG11	2.11	0.50
3:C:149:VAL:HG21	3:C:191:MET:HE1	1.93	0.50
3:C:343:PRO:HA	3:C:349:GLU:OE2	2.11	0.50
3:D:108:MET:HG2	3:D:140:GLY:HA3	1.92	0.50
3:D:278:PHE:CD1	3:D:359:VAL:HA	2.47	0.50
2:B:369:ASN:C	2:B:369:ASN:ND2	2.67	0.50
3:C:291:ILE:HD12	3:C:291:ILE:N	2.27	0.50
2:B:8:ARG:HG3	2:B:9:LYS:N	2.26	0.50
3:D:111:VAL:CG1	3:D:112:ASP:N	2.75	0.50
3:D:441:ARG:C	3:D:442:ASN:OD1	2.55	0.50
1:E:906:C:O2'	1:E:907:G:H5'	2.12	0.50
1:E:960:U:H6	1:E:960:U:O5'	1.95	0.50
1:F:957:G:N3	1:F:957:G:H2'	2.26	0.50
3:C:1:MET:HE1	3:C:253:VAL:HG11	1.93	0.50
3:C:16:GLN:OE1	3:C:213:VAL:CG1	2.60	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:111:VAL:HG23	3:C:136:VAL:C	2.36	0.50
3:D:207:ILE:HG22	3:D:208:LEU:N	2.26	0.50
2:A:248:ARG:CZ	2:A:271:LEU:HD21	2.42	0.49
2:B:17:ASP:OD2	2:B:71:LYS:NZ	2.41	0.49
2:B:128:GLU:CD	2:B:128:GLU:H	2.20	0.49
3:C:20:THR:CG2	3:C:94:GLU:HG2	2.40	0.49
3:C:98:ILE:HD13	3:C:212:ARG:O	2.12	0.49
3:D:108:MET:HB3	3:D:137:ALA:HB1	1.93	0.49
3:D:341:GLU:C	3:D:343:PRO:CD	2.85	0.49
3:D:499:ARG:CB	3:D:499:ARG:HH11	2.25	0.49
2:B:90:LEU:O	2:B:134:ASN:ND2	2.45	0.49
2:B:393:GLU:H	2:B:393:GLU:CD	2.20	0.49
3:D:501:LEU:C	3:D:503:ARG:H	2.20	0.49
2:A:87:ASP:HB3	5:A:446:HOH:O	2.12	0.49
2:A:319:LYS:O	2:A:320:TRP:C	2.55	0.49
2:B:44:ASP:O	2:B:45:ARG:HB2	2.11	0.49
2:B:140:VAL:HG11	2:B:159:ALA:CB	2.42	0.49
2:B:222:ARG:NH2	2:B:277:ASP:O	2.45	0.49
1:E:914:A:C2	1:E:915:G:H1'	2.48	0.49
2:B:328:GLY:HA3	2:B:399:MET:HE3	1.94	0.49
2:B:428:THR:HG21	3:C:80:LEU:HD12	1.95	0.49
3:C:71:TYR:CE2	3:C:127:THR:HG22	2.48	0.49
3:C:339:THR:O	3:C:343:PRO:HD3	2.12	0.49
3:C:471:ARG:NH1	3:C:499:ARG:CZ	2.75	0.49
3:C:471:ARG:HH22	3:C:499:ARG:HB2	1.78	0.49
3:D:43:ARG:HD2	3:D:71:TYR:CE1	2.48	0.49
3:D:68:HIS:HE1	5:D:1906:HOH:O	1.96	0.49
1:E:918:G:H5'	1:E:920:A:C2	2.47	0.49
2:A:11:LEU:HG	2:A:47:ILE:HD13	1.93	0.49
2:A:111:GLY:O	3:C:421:TYR:HB2	2.13	0.49
3:C:46:ARG:HG3	3:C:46:ARG:HH11	1.77	0.49
3:C:165:ARG:CB	3:C:165:ARG:NH1	2.72	0.49
3:C:207:ILE:O	3:C:210:SER:OG	2.20	0.49
3:D:118:ARG:HG3	3:D:423:GLU:HB2	1.94	0.49
3:D:313:GLU:OE2	3:D:316:PRO:HA	2.13	0.49
1:E:948:C:N3	1:E:959:C:N4	2.60	0.49
2:B:212:ASP:HB2	2:B:236:HIS:CE1	2.47	0.49
2:B:393:GLU:O	2:B:397:VAL:HG23	2.12	0.49
3:C:100:VAL:O	3:C:103:ALA:HB3	2.12	0.49
3:C:187:THR:O	3:C:188:ASP:C	2.56	0.49
3:D:347:ILE:HG22	3:D:351:GLU:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:116:ALA:HB1	2:A:121:ASP:OD2	2.12	0.49
2:A:148:MET:HE2	2:A:175:HIS:CE1	2.47	0.49
3:D:298:VAL:C	3:D:299:LEU:HD23	2.37	0.49
3:D:454:ILE:O	3:D:458:TYR:HD1	1.95	0.49
1:F:963:G:O4'	3:D:467:GLN:NE2	2.39	0.49
2:A:193:THR:HG22	2:A:194:PRO:CD	2.43	0.49
3:D:108:MET:SD	3:D:154:LEU:HB2	2.53	0.49
3:D:417:SER:N	5:D:1909:HOH:O	2.44	0.49
3:D:502:ARG:HD2	3:D:507:ASP:OD1	2.12	0.49
2:B:160:VAL:O	2:B:164:ILE:HG22	2.13	0.49
3:C:77:GLU:CD	3:C:77:GLU:N	2.71	0.49
3:D:17:GLN:O	3:D:213:VAL:HG13	2.13	0.49
3:D:62:GLU:HG2	3:D:65:ARG:HH12	1.78	0.49
3:D:207:ILE:O	3:D:210:SER:HB2	2.12	0.49
3:D:303:LEU:HB3	3:D:306:PHE:CD1	2.48	0.49
3:D:325:ALA:O	3:D:329:LYS:HG3	2.13	0.49
3:D:520:ILE:C	3:D:522:LEU:H	2.20	0.49
2:A:115:PRO:O	2:A:116:ALA:HB2	2.13	0.49
2:A:146:GLU:CD	2:A:146:GLU:H	2.20	0.49
2:A:164:ILE:O	2:A:164:ILE:HD12	2.12	0.49
2:A:306:PHE:HB3	2:B:310:TYR:CE2	2.47	0.49
2:A:435:GLY:HA2	2:B:264:ARG:NE	2.28	0.49
3:C:201:ALA:CB	3:C:242:LEU:HD13	2.42	0.49
3:D:252:GLU:OE2	3:D:255:ARG:NH2	2.46	0.49
1:E:954:U:H2'	1:E:955:U:H5'	1.95	0.48
1:F:921:A:H61	1:F:947:A:H2'	1.78	0.48
2:A:280:LYS:O	2:A:281:ILE:C	2.55	0.48
2:A:402:VAL:C	2:A:404:GLY:H	2.20	0.48
3:C:79:CYS:H	3:C:82:GLU:HG3	1.78	0.48
3:C:159:ASP:OD2	3:C:177:ARG:HD2	2.13	0.48
3:C:271:ALA:HB1	3:C:304:ARG:O	2.13	0.48
3:D:274:GLU:OE1	3:D:276:LYS:HE2	2.12	0.48
3:D:493:LEU:HD12	3:D:497:THR:HB	1.94	0.48
2:B:22:VAL:HB	2:B:66:ILE:CG2	2.43	0.48
2:B:55:TYR:HA	3:D:117:MET:HE2	1.95	0.48
3:C:16:GLN:NE2	3:C:16:GLN:CA	2.67	0.48
3:C:337:PHE:HB2	3:C:369:MET:HE2	1.94	0.48
1:E:912:G:N2	1:E:924:C:N3	2.61	0.48
1:E:947:A:C3'	1:E:948:C:H5'	2.43	0.48
2:A:334:THR:O	2:A:335:GLY:C	2.56	0.48
3:C:256:GLN:OE1	3:C:395:VAL:HG11	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:365:ASP:OD2	3:C:365:ASP:N	2.34	0.48
3:C:486:ASP:C	3:C:487:THR:HG1	2.21	0.48
3:D:6:VAL:HG12	3:D:228:ILE:CG2	2.43	0.48
3:D:46:ARG:O	3:D:47:PRO:O	2.31	0.48
3:D:176:ASP:OD1	3:D:176:ASP:N	2.45	0.48
3:D:219:THR:HG22	3:D:220:ILE:N	2.28	0.48
3:D:309:LEU:HA	3:D:312:VAL:CG2	2.44	0.48
3:D:494:LEU:HD22	3:D:498:LEU:HD11	1.94	0.48
1:E:920:A:N6	1:E:959:C:H5	2.10	0.48
1:E:957:G:N3	1:E:957:G:H2'	2.27	0.48
1:E:966:C:H2'	1:E:967:G:H8	1.79	0.48
1:F:918:G:H5'	5:F:107:HOH:O	2.13	0.48
2:A:253:ARG:HG3	2:A:391:LEU:HD13	1.94	0.48
2:B:161:TYR:C	2:B:164:ILE:HG22	2.38	0.48
2:B:418:GLU:HG2	2:B:420:ILE:HG13	1.95	0.48
3:C:486:ASP:O	3:C:488:THR:N	2.46	0.48
3:D:91:LEU:HD22	3:D:114:PHE:CD2	2.49	0.48
3:D:167:THR:HG23	3:D:168:GLY:H	1.78	0.48
3:D:227:SER:HB2	3:D:233:ARG:HD3	1.94	0.48
2:A:248:ARG:HB2	2:A:271:LEU:HD11	1.94	0.48
2:B:161:TYR:CB	2:B:296:LEU:HD22	2.43	0.48
2:B:200:THR:HG21	2:B:216:ASN:HB3	1.94	0.48
3:C:319:ARG:HD3	5:C:936:HOH:O	2.13	0.48
3:D:135:LEU:HD11	3:D:153:ASN:OD1	2.14	0.48
3:D:396:PRO:O	3:D:398:GLU:HG2	2.13	0.48
2:A:319:LYS:O	2:A:322:LEU:N	2.46	0.48
3:C:96:LEU:O	3:C:100:VAL:HG23	2.14	0.48
3:C:113:GLU:CD	3:C:428:LEU:HD13	2.39	0.48
3:D:62:GLU:HA	3:D:65:ARG:NH2	2.28	0.48
3:D:104:LEU:HD11	3:D:436:LEU:CD1	2.43	0.48
3:D:224:LEU:HD11	3:D:248:ILE:HD11	1.95	0.48
3:D:527:LYS:O	3:D:528:ILE:C	2.56	0.48
2:A:7:ALA:HA	2:A:61:ILE:HD11	1.95	0.48
2:A:48:VAL:HG22	3:C:115:HIS:HE1	1.79	0.48
2:A:193:THR:CG2	2:A:195:VAL:O	2.62	0.48
2:B:115:PRO:O	2:B:116:ALA:HB2	2.13	0.48
3:C:299:LEU:HD11	3:C:374:ARG:NH1	2.28	0.48
3:C:331:ARG:HH21	3:C:379:ASN:HD22	1.60	0.48
3:C:342:LEU:HD13	3:C:342:LEU:C	2.38	0.48
3:C:437:GLU:HB3	3:C:441:ARG:CZ	2.44	0.48
3:C:445:GLU:OE1	3:C:453:ARG:NH1	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:370:VAL:HG21	3:D:381:LEU:HG	1.96	0.48
1:E:918:G:C1'	1:E:957:G:N2	2.77	0.48
3:C:331:ARG:NH2	3:C:376:THR:HA	2.23	0.48
1:F:953:G:O2'	1:F:954:U:H5'	2.14	0.48
2:A:299:ARG:HB2	2:A:405:GLN:HE22	1.79	0.48
2:B:143:ILE:HD11	2:B:152:TYR:CE2	2.49	0.48
2:B:165:LYS:HE2	2:B:294:LEU:CD2	2.44	0.48
2:B:328:GLY:HA3	2:B:399:MET:CE	2.43	0.48
2:B:330:VAL:HG21	2:B:396:TYR:HA	1.94	0.48
3:C:42:VAL:HG22	3:C:70:HIS:CD2	2.49	0.48
3:C:291:ILE:HG21	3:C:337:PHE:HZ	1.79	0.48
1:E:931:G:H2'	1:E:932:C:O4'	2.14	0.47
2:A:301:GLU:OE2	2:A:303:ARG:NH2	2.47	0.47
2:B:336:LEU:O	2:B:368:VAL:HG13	2.14	0.47
2:B:428:THR:CG2	3:C:80:LEU:HD12	2.44	0.47
3:C:46:ARG:HH11	3:C:46:ARG:CG	2.27	0.47
3:D:25:PHE:CE2	3:D:426:ILE:HD13	2.49	0.47
3:D:191:MET:HE3	3:D:197:LEU:HD13	1.96	0.47
2:A:264:ARG:HE	2:B:435:GLY:CA	2.28	0.47
3:C:281:SER:HA	3:C:298:VAL:CG1	2.44	0.47
3:C:468:LEU:HD11	3:C:491:ALA:HB1	1.95	0.47
3:D:108:MET:CE	3:D:151:ILE:HG22	2.37	0.47
3:D:355:LEU:O	3:D:359:VAL:HG12	2.15	0.47
1:F:921:A:N1	1:F:948:C:C1'	2.75	0.47
2:A:102:VAL:O	2:A:102:VAL:HG23	2.14	0.47
2:A:157:ALA:HA	2:A:187:LEU:HD11	1.95	0.47
3:C:106:LEU:HD13	3:C:151:ILE:HD13	1.96	0.47
3:C:303:LEU:HB3	3:C:306:PHE:CG	2.48	0.47
3:D:159:ASP:HB2	3:D:182:LEU:HD13	1.95	0.47
3:D:486:ASP:O	3:D:486:ASP:OD2	2.32	0.47
2:B:88:PRO:C	2:B:90:LEU:H	2.21	0.47
3:D:437:GLU:O	3:D:439:ILE:N	2.47	0.47
2:B:12:GLU:O	2:B:14:ALA:N	2.47	0.47
2:B:114:HIS:O	2:B:115:PRO:O	2.33	0.47
2:B:320:TRP:CZ2	2:B:324:GLU:HG3	2.49	0.47
3:C:111:VAL:HG12	3:C:112:ASP:N	2.28	0.47
3:C:156:LEU:HA	3:C:182:LEU:O	2.14	0.47
3:C:337:PHE:N	3:C:337:PHE:CD1	2.82	0.47
3:D:62:GLU:CA	3:D:65:ARG:HH12	2.26	0.47
3:D:493:LEU:O	3:D:493:LEU:HG	2.14	0.47
2:A:387:CYS:HB3	2:A:390:MET:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:11:LEU:HD13	2:B:47:ILE:HD13	1.93	0.47
2:B:124:ARG:CG	2:B:124:ARG:NH1	2.76	0.47
2:B:150:PRO:HA	2:B:153:TRP:CD2	2.49	0.47
2:B:327:ARG:O	2:B:356:PRO:HD2	2.14	0.47
3:C:98:ILE:CD1	3:C:212:ARG:HB2	2.44	0.47
3:D:2:ASP:HB3	3:D:5:LYS:CG	2.45	0.47
3:D:454:ILE:HD12	3:D:474:VAL:CG1	2.32	0.47
1:E:930:G:H2'	1:E:931:G:C8	2.50	0.47
1:F:954:U:H5''	3:D:488:THR:HG22	1.97	0.47
2:A:106:ILE:HG12	2:A:113:VAL:HG22	1.97	0.47
2:A:161:TYR:CD1	2:A:294:LEU:HD11	2.49	0.47
2:A:332:GLU:CD	5:A:450:HOH:O	2.57	0.47
2:A:387:CYS:HB3	2:A:390:MET:HE3	1.97	0.47
2:B:50:LYS:NZ	2:B:56:ASN:HD21	2.12	0.47
2:B:56:ASN:N	2:B:56:ASN:ND2	2.63	0.47
2:B:87:ASP:OD1	2:B:87:ASP:O	2.32	0.47
2:B:128:GLU:HG2	2:B:218:GLN:HE22	1.80	0.47
2:B:320:TRP:CE2	2:B:324:GLU:HG3	2.50	0.47
3:C:32:LEU:HD13	3:C:162:ARG:CZ	2.44	0.47
3:C:193:ASP:OD2	3:C:196:GLN:HB2	2.15	0.47
3:D:105:LEU:HD23	3:D:443:LEU:CD1	2.41	0.47
1:E:908:U:OP2	1:E:908:U:H6	1.97	0.47
1:E:921:A:H8	1:E:921:A:OP2	1.97	0.47
1:F:954:U:H4'	3:D:492:SER:HB3	1.97	0.47
2:A:139:ALA:O	2:A:140:VAL:C	2.58	0.47
2:B:89:GLU:C	2:B:90:LEU:HD22	2.40	0.47
3:D:502:ARG:C	3:D:503:ARG:HG3	2.39	0.47
2:A:435:GLY:HA2	2:B:264:ARG:CZ	2.45	0.47
2:B:25:GLU:OE1	2:B:65:ARG:HG2	2.15	0.47
2:B:104:SER:HA	2:B:116:ALA:HB3	1.97	0.47
2:B:402:VAL:HG21	2:B:416:MET:HE2	1.97	0.47
2:A:147:ASN:ND2	2:B:340:PRO:HA	2.29	0.47
2:A:307:ILE:HD13	2:A:318:ILE:HD13	1.97	0.47
2:A:373:TYR:C	2:A:377:ARG:NH1	2.73	0.47
2:A:388:ASP:HB2	2:A:424:ILE:HG23	1.97	0.47
3:C:374:ARG:HH22	3:C:378:GLU:CD	2.22	0.47
3:D:10:MET:HE1	3:D:194:PRO:HA	1.97	0.47
3:D:171:VAL:HG12	3:D:172:VAL:N	2.30	0.47
3:D:220:ILE:HG12	3:D:221:ARG:H	1.80	0.47
3:D:228:ILE:HG22	3:D:229:ARG:O	2.15	0.47
3:D:423:GLU:HG2	3:D:426:ILE:HD12	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:468:LEU:HD12	3:D:473:LEU:HB2	1.96	0.47
2:B:57:ILE:CD1	3:D:135:LEU:HD23	2.45	0.46
2:B:312:GLY:O	2:B:313:ILE:C	2.57	0.46
3:C:171:VAL:CG2	3:C:172:VAL:N	2.78	0.46
3:C:280:VAL:HG11	3:C:355:LEU:HG	1.97	0.46
3:C:355:LEU:O	3:C:355:LEU:HD23	2.15	0.46
3:D:43:ARG:HD2	3:D:71:TYR:HE1	1.80	0.46
3:D:426:ILE:HA	3:D:427:PRO:HD3	1.76	0.46
1:E:906:C:C2'	1:E:907:G:H5'	2.45	0.46
2:A:175:HIS:CD2	2:A:176:GLY:O	2.68	0.46
2:A:189:PHE:CE1	2:A:398:LYS:HG3	2.49	0.46
2:B:299:ARG:HB2	2:B:405:GLN:NE2	2.21	0.46
3:C:3:TRP:CZ3	3:C:253:VAL:HG21	2.50	0.46
3:C:19:ASP:HA	3:C:214:LYS:HZ2	1.80	0.46
3:C:20:THR:HG22	3:C:94:GLU:CG	2.41	0.46
3:C:220:ILE:HG22	3:C:221:ARG:N	2.30	0.46
3:C:498:LEU:C	3:C:501:LEU:HB3	2.40	0.46
3:D:145:PRO:HB2	3:D:146:GLN:NE2	2.30	0.46
3:D:331:ARG:NE	3:D:331:ARG:CA	2.78	0.46
3:D:526:GLY:HA3	3:D:534:ARG:HH12	1.80	0.46
1:E:907:G:H5''	1:E:908:U:OP2	2.15	0.46
2:A:212:ASP:OD1	2:A:212:ASP:N	2.39	0.46
2:A:351:HIS:HB2	5:A:457:HOH:O	2.14	0.46
2:B:118:THR:HB	2:B:121:ASP:OD2	2.15	0.46
2:B:293:GLU:O	2:B:293:GLU:HG3	2.16	0.46
3:C:24:LEU:O	3:C:92:ASN:HB2	2.15	0.46
3:C:313:GLU:HG3	3:C:319:ARG:HH12	1.80	0.46
2:A:189:PHE:CZ	2:A:398:LYS:HG3	2.51	0.46
2:A:363:CYS:O	2:A:364:LEU:CB	2.63	0.46
3:C:361:ALA:N	5:C:917:HOH:O	2.48	0.46
3:D:73:ASN:HD22	3:D:73:ASN:N	2.13	0.46
3:D:115:HIS:NE2	3:D:428:LEU:HD13	2.30	0.46
3:D:125:SER:CB	3:D:160:ALA:HB1	2.38	0.46
2:A:408:ASP:HB3	2:A:411:MET:HB3	1.98	0.46
3:D:70:HIS:HB2	3:D:172:VAL:HG22	1.98	0.46
2:A:274:VAL:CG1	2:A:275:THR:N	2.79	0.46
2:A:281:ILE:HG22	2:A:284:GLU:OE2	2.15	0.46
2:B:111:GLY:HA3	3:D:422:LEU:HD12	1.98	0.46
2:B:203:GLN:O	2:B:204:ARG:NH1	2.49	0.46
3:C:19:ASP:HB2	3:C:214:LYS:CG	2.45	0.46
3:C:198:ARG:HG3	3:C:242:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:233:ARG:HG3	3:C:397:GLU:CB	2.26	0.46
3:D:150:LYS:C	3:D:151:ILE:HD12	2.40	0.46
3:D:487:THR:C	3:D:489:VAL:N	2.72	0.46
3:D:532:ALA:O	3:D:533:LEU:HG	2.16	0.46
1:F:959:C:O2	1:F:959:C:H2'	2.16	0.46
2:A:47:ILE:CD1	2:A:61:ILE:HG21	2.46	0.46
2:A:91:PRO:O	2:A:133:ALA:HB1	2.16	0.46
2:B:161:TYR:HB2	2:B:296:LEU:HD22	1.98	0.46
3:D:487:THR:C	3:D:489:VAL:H	2.24	0.46
1:F:943:G:O2'	1:F:944:C:H5'	2.15	0.46
2:A:205:SER:CB	2:A:207:ASP:OD1	2.64	0.46
2:B:23:LEU:HD12	2:B:32:GLU:CG	2.46	0.46
2:B:253:ARG:NH1	2:B:393:GLU:OE1	2.48	0.46
2:B:369:ASN:ND2	2:B:371:ASN:HB2	2.27	0.46
3:C:74:TYR:H	3:C:78:THR:HB	1.81	0.46
3:C:451:LYS:CB	5:C:915:HOH:O	2.63	0.46
3:D:146:GLN:HG3	3:D:196:GLN:CA	2.45	0.46
2:A:434:ARG:H	2:A:434:ARG:HG2	1.56	0.46
2:B:171:VAL:O	2:B:197:VAL:HA	2.15	0.46
3:C:1:MET:O	3:C:1:MET:HG2	2.16	0.46
3:C:16:GLN:HB3	3:C:183:VAL:HG22	1.98	0.46
3:D:59:ALA:O	3:D:62:GLU:N	2.41	0.46
3:D:501:LEU:HD21	3:D:536:ILE:CD1	2.46	0.46
1:E:970:A:H2'	1:E:971:C:C6	2.51	0.46
2:A:255:MET:O	2:B:365:ASN:HB2	2.16	0.46
2:B:20:ASP:HB3	2:B:68:LEU:CD1	2.46	0.46
2:B:280:LYS:O	2:B:281:ILE:C	2.59	0.46
3:D:280:VAL:HG13	3:D:283:VAL:HG21	1.97	0.46
3:D:302:LYS:NZ	3:D:304:ARG:HE	2.14	0.46
3:D:518:ASP:HA	3:D:521:LYS:CG	2.43	0.46
1:F:918:G:HO2'	1:F:919:U:H5'	1.80	0.45
1:F:954:U:H2'	1:F:955:U:C5'	2.43	0.45
2:A:88:PRO:HA	5:A:453:HOH:O	2.16	0.45
2:A:118:THR:C	2:A:120:ASP:N	2.73	0.45
2:A:204:ARG:O	2:A:205:SER:C	2.59	0.45
2:A:218:GLN:HG3	2:A:276:PRO:HG3	1.97	0.45
2:A:358:ALA:HB1	2:A:387:CYS:SG	2.56	0.45
3:C:8:LEU:HA	3:C:227:SER:O	2.15	0.45
3:C:324:MET:HE2	3:C:384:VAL:CG2	2.46	0.45
3:D:62:GLU:HA	3:D:65:ARG:CZ	2.45	0.45
3:D:145:PRO:HD2	3:D:146:GLN:NE2	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:213:VAL:HG12	3:D:214:LYS:N	2.31	0.45
1:E:950:G:H2'	1:E:951:C:H6	1.82	0.45
1:F:950:G:N2	1:F:965:U:C2	2.83	0.45
2:B:256:HIS:HD2	2:B:258:SER:H	1.64	0.45
2:B:303:ARG:NH1	2:B:324:GLU:O	2.49	0.45
2:B:419:ASN:ND2	2:B:424:ILE:O	2.49	0.45
3:C:227:SER:C	3:C:228:ILE:HD12	2.41	0.45
3:C:310:ILE:HG22	3:C:338:HIS:CD2	2.51	0.45
3:D:19:ASP:CA	3:D:214:LYS:HE2	2.43	0.45
2:A:346:VAL:HG23	5:A:439:HOH:O	2.16	0.45
2:B:175:HIS:CD2	2:B:176:GLY:O	2.69	0.45
3:C:135:LEU:CD1	3:C:153:ASN:HB3	2.45	0.45
3:C:228:ILE:HG12	3:C:256:GLN:CG	2.46	0.45
3:C:359:VAL:HG22	3:C:359:VAL:O	2.17	0.45
3:D:58:ALA:HB3	5:D:1917:HOH:O	2.16	0.45
3:D:274:GLU:C	3:D:276:LYS:H	2.25	0.45
1:E:960:U:H3'	5:E:146:HOH:O	2.16	0.45
2:A:312:GLY:O	2:A:313:ILE:C	2.56	0.45
2:A:349:GLU:O	2:A:353:MET:HG3	2.15	0.45
2:A:362:GLN:O	2:A:364:LEU:HG	2.17	0.45
2:B:45:ARG:NH2	3:D:430:ARG:CZ	2.78	0.45
2:B:223:ALA:C	2:B:225:THR:N	2.74	0.45
2:B:262:THR:HG23	2:B:263:PHE:CD2	2.51	0.45
3:D:164:ILE:CG2	3:D:165:ARG:HG3	2.33	0.45
3:D:198:ARG:HG3	3:D:199:GLU:N	2.32	0.45
3:D:234:VAL:CG1	3:D:400:ARG:HD2	2.44	0.45
3:D:468:LEU:CD1	3:D:473:LEU:HB2	2.46	0.45
2:A:66:ILE:HG22	2:A:67:GLU:H	1.81	0.45
3:C:17:GLN:HB3	3:C:214:LYS:HG3	1.99	0.45
3:C:80:LEU:HD22	3:C:85:GLU:CB	2.45	0.45
3:C:98:ILE:HG23	3:C:211:THR:CG2	2.43	0.45
3:C:144:THR:HB	3:C:199:GLU:HG2	1.99	0.45
3:C:223:ASP:CG	3:C:237:LYS:HD3	2.42	0.45
3:C:273:VAL:HB	3:C:389:GLU:OE1	2.16	0.45
3:C:372:HIS:CD2	3:C:373:GLU:H	2.34	0.45
3:C:439:ILE:O	3:C:440:ARG:C	2.59	0.45
3:D:146:GLN:CD	3:D:146:GLN:H	2.25	0.45
3:D:160:ALA:O	3:D:177:ARG:HG2	2.17	0.45
3:D:331:ARG:HG3	3:D:331:ARG:O	2.15	0.45
2:A:367:ARG:HG3	2:A:367:ARG:HH11	1.81	0.45
2:B:423:GLU:HG2	2:B:424:ILE:HG13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:498:LEU:O	3:C:501:LEU:HD22	2.17	0.45
3:D:520:ILE:O	3:D:522:LEU:N	2.47	0.45
1:E:958:A:H1'	1:E:960:U:C5	2.52	0.45
2:A:160:VAL:O	2:A:161:TYR:C	2.60	0.45
2:B:61:ILE:O	2:B:63:ASP:N	2.49	0.45
2:B:371:ASN:O	2:B:377:ARG:HD3	2.17	0.45
3:C:29:ARG:HB2	3:C:29:ARG:HH11	1.80	0.45
3:C:135:LEU:HD21	3:C:138:THR:CG2	2.46	0.45
3:C:262:ILE:HD11	3:C:314:ILE:HG22	1.99	0.45
3:D:132:ARG:HG3	3:D:132:ARG:NH1	2.32	0.45
3:D:491:ALA:C	3:D:493:LEU:H	2.25	0.45
1:F:963:G:OP1	3:D:499:ARG:HD3	2.17	0.45
2:A:7:ALA:O	2:A:11:LEU:HB2	2.17	0.45
2:A:88:PRO:O	2:A:89:GLU:CB	2.65	0.45
2:A:161:TYR:HD1	2:A:294:LEU:HD11	1.82	0.45
2:B:143:ILE:HG21	2:B:148:MET:HE3	1.98	0.45
2:B:149:LYS:HZ3	2:B:152:TYR:HE1	1.64	0.45
3:C:211:THR:C	3:C:213:VAL:HG23	2.42	0.45
3:C:342:LEU:HD12	3:C:352:VAL:HG13	1.99	0.45
3:C:374:ARG:HH12	3:C:378:GLU:HB2	1.81	0.45
1:E:930:G:H2'	1:E:931:G:H8	1.82	0.45
2:A:141:PHE:HD1	2:A:143:ILE:HD12	1.82	0.45
2:A:378:ARG:NH1	2:A:378:ARG:HG3	2.32	0.45
2:B:6:ARG:HB2	2:B:44:ASP:OD2	2.17	0.45
2:B:223:ALA:C	2:B:225:THR:H	2.25	0.45
3:C:454:ILE:O	3:C:458:TYR:HB2	2.17	0.45
3:C:494:LEU:HD23	3:C:498:LEU:HD11	1.98	0.45
3:D:476:GLU:O	3:D:477:PHE:C	2.58	0.45
2:A:49:LEU:CD1	2:A:59:VAL:HG11	2.47	0.45
2:A:256:HIS:HA	2:B:365:ASN:O	2.17	0.45
2:B:139:ALA:O	2:B:140:VAL:C	2.59	0.45
2:B:253:ARG:HH11	2:B:393:GLU:CD	2.25	0.45
3:C:105:LEU:HD23	3:C:443:LEU:HD13	1.99	0.45
3:D:18:LEU:HD22	3:D:98:ILE:HG21	1.99	0.45
3:D:38:ASP:OD2	3:D:75:HIS:N	2.35	0.45
1:F:908:U:O2'	1:F:947:A:H2'	2.17	0.44
1:F:920:A:C6	1:F:948:C:N3	2.86	0.44
2:B:10:PHE:CZ	2:B:64:ALA:HB3	2.52	0.44
2:B:89:GLU:OE1	2:B:89:GLU:HA	2.18	0.44
2:B:385:ILE:CG2	2:B:417:ARG:HD3	2.47	0.44
3:C:26:CYS:SG	3:C:27:PRO:CD	3.06	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:451:LYS:O	3:C:455:MET:HG3	2.17	0.44
3:D:68:HIS:CE1	3:D:169:ASP:OD1	2.70	0.44
2:A:88:PRO:O	2:A:89:GLU:HB3	2.17	0.44
2:A:289:ARG:HB3	2:A:290:GLY:H	1.61	0.44
2:B:180:MET:HE3	2:B:233:VAL:CG1	2.39	0.44
3:C:164:ILE:CD1	3:C:174:ARG:HB2	2.47	0.44
3:C:284:PHE:O	3:C:285:ALA:C	2.60	0.44
2:A:92:ASP:OD1	2:A:134:ASN:HB2	2.17	0.44
2:A:147:ASN:ND2	2:B:341:ASP:N	2.58	0.44
3:C:177:ARG:HG2	3:C:180:ILE:HD12	1.99	0.44
3:C:191:MET:O	3:C:192:SER:CB	2.64	0.44
3:D:46:ARG:HA	3:D:47:PRO:HD3	1.80	0.44
2:A:38:ARG:HD3	2:A:48:VAL:HG23	1.99	0.44
2:A:160:VAL:HG13	2:A:171:VAL:HG11	1.99	0.44
2:A:275:THR:HG22	2:A:277:ASP:N	2.11	0.44
2:B:275:THR:HG23	2:B:276:PRO:CD	2.48	0.44
3:C:450:LYS:CD	3:C:474:VAL:HG11	2.28	0.44
3:C:460:LEU:HD22	3:C:464:LEU:HD13	1.99	0.44
3:C:497:THR:C	3:C:499:ARG:N	2.75	0.44
3:D:399:THR:HG22	3:D:411:LEU:HD12	2.00	0.44
2:A:8:ARG:HH11	2:A:12:GLU:CD	2.26	0.44
2:B:87:ASP:OD2	2:B:90:LEU:HD23	2.16	0.44
2:B:217:ILE:CG2	2:B:218:GLN:H	2.31	0.44
2:B:307:ILE:HD13	2:B:318:ILE:HD13	2.00	0.44
3:C:339:THR:HG1	3:C:367:VAL:H	1.63	0.44
3:C:454:ILE:CG2	3:C:460:LEU:HD12	2.47	0.44
2:A:336:LEU:HD23	2:A:336:LEU:HA	1.77	0.44
2:B:406:THR:OG1	2:B:407:ASP:N	2.51	0.44
3:C:242:LEU:HD12	3:C:245:ILE:HD12	1.98	0.44
3:C:477:PHE:HE1	3:C:487:THR:HA	1.82	0.44
1:E:942:G:C2	1:E:943:G:C8	3.06	0.44
2:A:50:LYS:HG3	2:A:56:ASN:ND2	2.32	0.44
2:A:149:LYS:HG2	2:A:152:TYR:CE1	2.52	0.44
2:A:417:ARG:HG2	2:A:417:ARG:HH11	1.83	0.44
2:B:87:ASP:CG	2:B:90:LEU:HD23	2.42	0.44
3:C:132:ARG:NH2	5:C:935:HOH:O	2.51	0.44
3:D:16:GLN:CG	3:D:208:LEU:HD13	2.47	0.44
3:D:297:SER:OG	3:D:374:ARG:HB2	2.17	0.44
1:F:962:C:H1'	3:D:496:TYR:CD1	2.53	0.44
2:A:68:LEU:HD22	2:A:71:LYS:HE2	1.99	0.44
2:A:141:PHE:CD1	2:A:143:ILE:HD12	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:148:MET:HE3	2:B:148:MET:HA	1.98	0.44
2:B:210:SER:O	2:B:211:SER:C	2.59	0.44
3:C:8:LEU:HD21	3:C:10:MET:SD	2.57	0.44
3:C:46:ARG:O	3:C:47:PRO:O	2.36	0.44
3:C:119:LYS:O	3:C:121:VAL:HG23	2.17	0.44
3:C:342:LEU:N	3:C:343:PRO:CD	2.81	0.44
3:D:70:HIS:HE1	3:D:169:ASP:CG	2.22	0.44
1:F:955:U:H3'	5:F:35:HOH:O	2.18	0.44
2:A:38:ARG:HG2	2:A:38:ARG:HH11	1.83	0.44
3:C:16:GLN:OE1	3:C:213:VAL:HG12	2.17	0.44
3:C:471:ARG:HH12	3:C:499:ARG:HA	1.82	0.44
3:D:43:ARG:HH11	3:D:43:ARG:CG	2.00	0.44
3:D:299:LEU:HB2	3:D:381:LEU:HD12	1.99	0.44
2:B:9:LYS:HZ3	2:B:9:LYS:HB2	1.83	0.43
2:B:130:LEU:HD23	2:B:130:LEU:HA	1.79	0.43
2:B:212:ASP:OD1	2:B:212:ASP:N	2.36	0.43
2:B:217:ILE:HG23	2:B:218:GLN:H	1.81	0.43
3:D:104:LEU:HD23	3:D:104:LEU:HA	1.86	0.43
3:D:305:GLY:H	3:D:365:ASP:CB	2.12	0.43
3:D:494:LEU:HD21	3:D:515:GLU:OE1	2.17	0.43
1:E:901:A:H1'	3:C:240:GLN:HB3	1.99	0.43
2:A:53:ASN:OD1	2:A:55:TYR:HB2	2.18	0.43
2:A:60:GLU:HB3	3:C:112:ASP:OD1	2.18	0.43
2:A:138:ARG:HG2	2:A:139:ALA:H	1.83	0.43
2:A:165:LYS:C	2:A:167:GLY:H	2.25	0.43
2:A:175:HIS:HD2	2:A:176:GLY:N	2.13	0.43
2:A:177:THR:O	2:A:178:ASP:C	2.61	0.43
2:A:185:ALA:O	2:A:188:SER:HB2	2.18	0.43
2:A:264:ARG:NH1	2:B:433:PHE:HE2	2.16	0.43
2:A:272:ALA:HA	2:A:282:LEU:HG	2.00	0.43
2:A:407:ASP:O	2:A:409:PRO:HD3	2.17	0.43
2:B:148:MET:HE2	2:B:152:TYR:CB	2.47	0.43
2:B:215:LEU:O	2:B:219:CYS:HB2	2.17	0.43
2:B:308:LYS:HE3	2:B:362:GLN:HE21	1.83	0.43
3:C:82:GLU:H	3:C:82:GLU:HG2	1.30	0.43
3:C:144:THR:OG1	3:C:196:GLN:HG3	2.19	0.43
3:C:245:ILE:O	3:C:249:VAL:HG23	2.18	0.43
3:C:307:ASP:HA	3:C:366:ALA:HB2	1.99	0.43
3:C:374:ARG:NH2	3:C:378:GLU:HB2	2.34	0.43
3:D:280:VAL:O	3:D:280:VAL:HG12	2.18	0.43
3:D:375:VAL:O	3:D:379:ASN:ND2	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:512:GLY:O	3:D:516:LEU:HB2	2.18	0.43
3:D:517:ARG:HH21	3:D:521:LYS:HZ3	1.62	0.43
3:D:531:ASP:C	3:D:533:LEU:N	2.75	0.43
2:A:16:ILE:HG21	2:A:22:VAL:HG11	1.99	0.43
2:A:140:VAL:CG2	2:A:141:PHE:H	2.22	0.43
2:A:217:ILE:CG2	2:A:218:GLN:N	2.80	0.43
2:B:238:THR:CG2	2:B:240:ASP:HB2	2.48	0.43
2:B:385:ILE:HG12	2:B:413:ARG:HD3	1.99	0.43
3:C:332:GLY:O	3:C:333:VAL:CB	2.66	0.43
3:C:445:GLU:OE2	3:C:450:LYS:CA	2.62	0.43
3:D:337:PHE:HE2	3:D:345:TYR:CD2	2.35	0.43
1:E:956:C:C2	1:E:957:G:C8	3.06	0.43
2:A:66:ILE:O	2:A:67:GLU:HG3	2.18	0.43
2:A:128:GLU:OE2	3:C:46:ARG:NH2	2.49	0.43
2:A:398:LYS:NZ	2:A:418:GLU:O	2.52	0.43
2:B:64:ALA:O	2:B:65:ARG:HB2	2.18	0.43
3:C:87:PRO:HA	3:C:88:PRO:HD3	1.78	0.43
3:C:437:GLU:C	3:C:439:ILE:N	2.75	0.43
2:A:55:TYR:HH	3:C:133:THR:HG21	1.83	0.43
2:A:204:ARG:NH2	2:A:258:SER:O	2.50	0.43
2:A:256:HIS:CD2	2:A:259:ARG:HB2	2.54	0.43
2:B:208:ARG:NH2	3:D:118:ARG:HH22	2.16	0.43
2:B:378:ARG:O	2:B:381:GLN:HB3	2.17	0.43
3:C:15:HIS:CD2	3:C:15:HIS:N	2.87	0.43
3:C:410:TYR:O	3:C:411:LEU:HD23	2.18	0.43
3:D:69:PHE:CE2	3:D:124:GLY:HA3	2.53	0.43
3:D:162:ARG:HH21	3:D:174:ARG:HD2	1.82	0.43
3:D:502:ARG:CZ	3:D:508:VAL:HG22	2.48	0.43
2:B:12:GLU:C	2:B:14:ALA:N	2.77	0.43
2:B:179:THR:O	2:B:180:MET:C	2.61	0.43
2:B:259:ARG:NH1	2:B:261:ASP:OD2	2.51	0.43
3:C:28:CYS:SG	3:C:79:CYS:HB3	2.59	0.43
3:D:517:ARG:HH21	3:D:521:LYS:HZ2	1.64	0.43
1:E:909:G:O2'	1:E:945:G:C2'	2.67	0.43
2:A:58:GLY:HA3	3:C:113:GLU:HB3	2.01	0.43
2:A:126:ASN:N	2:A:127:PRO:HD3	2.34	0.43
2:A:344:ILE:CB	2:A:345:PRO:HD3	2.45	0.43
2:A:365:ASN:ND2	2:A:433:PHE:HE1	2.17	0.43
2:B:102:VAL:HG21	2:B:217:ILE:HD13	1.99	0.43
2:B:259:ARG:HB3	2:B:261:ASP:OD1	2.19	0.43
3:C:36:GLU:OE1	3:C:37:PRO:HD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:159:ASP:HA	3:C:182:LEU:HD22	2.01	0.43
3:C:451:LYS:HB3	5:C:915:HOH:O	2.19	0.43
3:D:62:GLU:HA	3:D:65:ARG:HH22	1.82	0.43
3:D:212:ARG:HH11	3:D:212:ARG:HB3	1.83	0.43
2:A:205:SER:HB2	2:A:207:ASP:OD1	2.19	0.43
2:A:209:PRO:HB2	3:C:45:LEU:HD12	2.00	0.43
2:A:222:ARG:HH11	2:A:222:ARG:CG	2.22	0.43
2:A:307:ILE:CD1	2:A:318:ILE:HD13	2.49	0.43
2:B:256:HIS:CD2	2:B:259:ARG:HB2	2.53	0.43
2:B:385:ILE:CD1	2:B:413:ARG:HA	2.49	0.43
3:C:252:GLU:CD	3:C:255:ARG:HH21	2.26	0.43
3:C:400:ARG:HG2	3:C:410:TYR:HA	2.01	0.43
3:D:37:PRO:HA	3:D:74:TYR:CE2	2.54	0.43
2:B:10:PHE:HE2	2:B:66:ILE:CD1	2.31	0.43
3:C:1:MET:HE1	3:C:253:VAL:HG12	2.00	0.43
3:C:244:LEU:HD12	3:C:247:GLU:HB3	2.01	0.43
3:C:283:VAL:O	3:C:283:VAL:HG12	2.18	0.43
1:F:901:A:H61	1:F:972:U:H3	1.66	0.43
1:F:909:G:O2'	1:F:945:G:C2'	2.67	0.43
2:A:406:THR:OG1	2:A:407:ASP:N	2.51	0.43
2:B:129:LEU:HD22	2:B:221:VAL:HG21	2.01	0.43
2:B:143:ILE:HB	2:B:148:MET:HE1	2.01	0.43
2:B:173:VAL:HB	2:B:199:PHE:CD1	2.54	0.43
2:B:188:SER:HA	5:B:449:HOH:O	2.19	0.43
2:B:226:SER:OG	2:B:227:GLU:N	2.51	0.43
3:C:348:THR:O	3:C:352:VAL:HG23	2.18	0.43
3:C:374:ARG:HG2	3:C:374:ARG:NH1	2.33	0.43
3:C:430:ARG:HB3	3:C:430:ARG:HH11	1.83	0.43
3:C:447:PRO:O	3:C:451:LYS:HG3	2.18	0.43
3:D:16:GLN:CD	3:D:213:VAL:HG11	2.43	0.43
3:D:77:GLU:OE2	3:D:77:GLU:N	2.46	0.43
1:F:907:G:C6	1:F:949:A:N6	2.88	0.42
2:A:187:LEU:HG	2:A:199:PHE:HZ	1.84	0.42
2:A:380:LEU:HD23	2:A:380:LEU:HA	1.87	0.42
3:C:178:LEU:HD23	3:C:178:LEU:C	2.44	0.42
2:A:20:ASP:OD1	2:A:72:GLY:N	2.49	0.42
2:A:87:ASP:CB	5:A:446:HOH:O	2.66	0.42
2:B:55:TYR:HE2	3:D:133:THR:HB	1.83	0.42
2:B:335:GLY:O	2:B:336:LEU:CB	2.64	0.42
3:C:14:ILE:CD1	3:C:222:GLN:HE21	2.32	0.42
3:C:439:ILE:O	3:C:441:ARG:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:465:ALA:O	3:C:469:VAL:HG23	2.19	0.42
3:D:224:LEU:CD1	3:D:239:VAL:HG21	2.35	0.42
2:A:24:VAL:HG21	2:A:49:LEU:HD11	2.01	0.42
2:B:321:HIS:O	2:B:326:TYR:HD1	2.02	0.42
3:C:240:GLN:H	3:C:240:GLN:HG2	1.55	0.42
3:C:331:ARG:O	3:C:331:ARG:HG3	2.19	0.42
3:C:331:ARG:HE	3:C:379:ASN:HB2	1.83	0.42
3:D:229:ARG:O	3:D:230:ASP:OD1	2.38	0.42
1:E:939:C:H2'	1:E:940:C:H6	1.84	0.42
1:F:975:C:H5'	5:F:60:HOH:O	2.18	0.42
2:A:49:LEU:HD12	2:A:59:VAL:CG1	2.49	0.42
2:B:97:SER:HA	2:B:174:ALA:HB3	2.00	0.42
2:B:187:LEU:CD1	2:B:191:LEU:HD22	2.50	0.42
3:C:14:ILE:HD13	3:C:222:GLN:HE21	1.85	0.42
3:C:252:GLU:OE2	3:C:255:ARG:NH2	2.53	0.42
3:C:274:GLU:C	3:C:276:LYS:H	2.26	0.42
3:D:103:ALA:HB1	3:D:137:ALA:CB	2.50	0.42
3:D:108:MET:SD	3:D:154:LEU:HD23	2.58	0.42
3:D:188:ASP:HA	3:D:189:PRO:HD3	1.83	0.42
3:D:414:LEU:HG	3:D:415:PRO:HD2	2.02	0.42
1:F:959:C:C5	1:F:960:U:C4	3.07	0.42
2:A:50:LYS:CG	2:A:56:ASN:ND2	2.83	0.42
2:A:367:ARG:HH21	2:A:428:THR:HG23	1.84	0.42
2:B:34:MET:O	2:B:36:LEU:HD12	2.19	0.42
2:B:126:ASN:N	2:B:127:PRO:HD3	2.34	0.42
2:B:177:THR:HB	2:B:254:LYS:CE	2.50	0.42
2:B:367:ARG:HG3	2:B:367:ARG:HH11	1.85	0.42
3:C:108:MET:HE3	3:C:151:ILE:HG22	2.01	0.42
3:C:339:THR:CB	3:C:366:ALA:HB1	2.49	0.42
3:D:23:LYS:HD3	3:D:179:GLY:HA3	2.02	0.42
3:D:339:THR:CB	3:D:366:ALA:HB1	2.47	0.42
2:A:378:ARG:HG3	2:A:378:ARG:HH11	1.85	0.42
2:B:251:LYS:NZ	2:B:267:ASN:HB2	2.34	0.42
2:B:263:PHE:HB2	5:B:437:HOH:O	2.18	0.42
2:B:290:GLY:O	2:B:292:ASP:N	2.53	0.42
2:B:318:ILE:O	2:B:321:HIS:HB2	2.18	0.42
3:C:164:ILE:HD11	3:C:174:ARG:HB2	2.02	0.42
3:C:171:VAL:HG22	3:C:173:PHE:CE2	2.55	0.42
3:C:228:ILE:CB	3:C:256:GLN:HG2	2.50	0.42
3:C:362:SER:HB2	3:C:365:ASP:OD2	2.19	0.42
3:C:430:ARG:CZ	3:C:430:ARG:CB	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:6:VAL:CG1	3:D:228:ILE:HD13	2.50	0.42
3:D:24:LEU:HD11	3:D:91:LEU:HD12	2.01	0.42
3:D:138:THR:O	3:D:139:ASP:C	2.62	0.42
3:D:217:LEU:O	3:D:218:GLY:C	2.62	0.42
3:D:327:TYR:CE1	3:D:387:ARG:HD3	2.55	0.42
2:A:107:ASP:C	2:A:109:ARG:H	2.28	0.42
2:B:319:LYS:O	2:B:322:LEU:N	2.52	0.42
3:C:16:GLN:CG	3:C:213:VAL:HG11	2.50	0.42
3:C:349:GLU:HA	3:C:352:VAL:HB	2.02	0.42
3:D:6:VAL:HG12	3:D:6:VAL:O	2.20	0.42
3:D:68:HIS:CE1	3:D:169:ASP:CG	2.97	0.42
3:D:269:ARG:O	3:D:270:GLY:C	2.61	0.42
3:D:299:LEU:HD21	3:D:374:ARG:HE	1.85	0.42
3:D:332:GLY:O	3:D:333:VAL:CB	2.68	0.42
3:D:471:ARG:HH11	3:D:471:ARG:HG2	1.84	0.42
2:A:293:GLU:HA	2:A:293:GLU:OE1	2.19	0.42
2:A:391:LEU:CB	2:A:394:VAL:HG12	2.44	0.42
2:A:415:MET:HE2	2:A:415:MET:HB3	1.86	0.42
2:B:114:HIS:HA	2:B:115:PRO:HD3	1.95	0.42
2:B:234:CYS:HB2	2:B:246:LEU:HD12	2.02	0.42
3:C:9:LYS:O	3:C:227:SER:HB3	2.20	0.42
3:C:25:PHE:CE2	3:C:91:LEU:HD12	2.55	0.42
3:C:171:VAL:HG23	3:C:172:VAL:N	2.34	0.42
3:C:291:ILE:HG21	3:C:337:PHE:CZ	2.55	0.42
3:C:403:LEU:HB3	3:C:404:PRO:CD	2.50	0.42
3:D:132:ARG:HG3	3:D:132:ARG:HH11	1.83	0.42
3:D:177:ARG:HA	3:D:180:ILE:HD11	2.02	0.42
3:D:342:LEU:HD22	3:D:342:LEU:HA	1.85	0.42
1:F:932:C:H3'	1:F:933:U:H5''	2.00	0.42
1:F:956:C:C4	1:F:957:G:N7	2.88	0.42
2:A:8:ARG:HH22	2:A:9:LYS:NZ	2.18	0.42
2:A:122:LEU:O	2:A:126:ASN:N	2.53	0.42
2:A:402:VAL:C	2:A:404:GLY:N	2.75	0.42
2:A:427:ARG:HH22	2:A:429:SER:HB2	1.81	0.42
2:B:204:ARG:O	2:B:205:SER:O	2.38	0.42
3:C:91:LEU:O	3:C:93:PRO:HD3	2.20	0.42
3:D:217:LEU:HA	3:D:217:LEU:HD23	1.84	0.42
3:D:372:HIS:CD2	3:D:373:GLU:H	2.38	0.42
3:D:469:VAL:CG2	3:D:474:VAL:HG21	2.48	0.42
2:A:189:PHE:HE2	2:A:423:GLU:HG2	1.81	0.42
2:A:272:ALA:HB2	2:A:281:ILE:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:385:ILE:CD1	2:A:413:ARG:HB2	2.37	0.42
2:B:156:THR:HG22	2:B:187:LEU:HD21	2.01	0.42
2:B:256:HIS:CD2	2:B:258:SER:H	2.38	0.42
2:B:329:ILE:HB	2:B:357:VAL:HG22	2.01	0.42
3:C:422:LEU:N	3:C:422:LEU:CD1	2.79	0.42
3:C:429:PHE:C	3:C:429:PHE:CD2	2.98	0.42
3:D:162:ARG:HB3	3:D:177:ARG:NH2	2.33	0.42
3:D:523:LEU:N	3:D:523:LEU:HD12	2.35	0.42
1:E:963:G:O2'	1:E:964:C:H5'	2.20	0.41
2:A:5:GLY:O	2:A:6:ARG:C	2.63	0.41
2:A:306:PHE:HB2	2:A:396:TYR:CD1	2.55	0.41
2:B:10:PHE:CD1	2:B:61:ILE:HB	2.56	0.41
2:B:111:GLY:O	3:D:422:LEU:HD12	2.20	0.41
2:B:228:ILE:HD12	2:B:246:LEU:HD23	2.02	0.41
3:C:42:VAL:HG22	3:C:70:HIS:NE2	2.35	0.41
3:C:214:LYS:O	3:C:219:THR:HG21	2.20	0.41
3:C:323:GLU:OE1	3:C:400:ARG:NH2	2.53	0.41
3:D:164:ILE:HD13	3:D:174:ARG:HB2	2.02	0.41
3:D:269:ARG:HD2	3:D:305:GLY:O	2.20	0.41
3:D:509:ASP:CG	3:D:510:GLY:N	2.78	0.41
3:D:535:ASP:CG	3:D:536:ILE:N	2.78	0.41
2:A:96:ILE:HG22	2:A:173:VAL:HG13	2.02	0.41
2:A:227:GLU:HA	2:A:227:GLU:OE1	2.20	0.41
2:B:374:SER:O	2:B:375:THR:C	2.64	0.41
3:C:108:MET:HG2	3:C:140:GLY:CA	2.46	0.41
3:C:342:LEU:O	3:C:342:LEU:HD22	2.20	0.41
3:C:422:LEU:H	3:C:422:LEU:CD1	2.29	0.41
2:A:148:MET:CB	2:A:179:THR:HG21	2.50	0.41
2:A:162:GLY:O	2:A:163:GLU:C	2.62	0.41
2:A:289:ARG:HG3	2:A:289:ARG:NH1	2.32	0.41
3:C:3:TRP:HA	3:C:3:TRP:CE3	2.55	0.41
3:C:16:GLN:CG	3:C:213:VAL:CG1	2.98	0.41
3:D:37:PRO:HG2	3:D:72:GLU:CD	2.45	0.41
3:D:215:ARG:HD3	3:D:215:ARG:N	2.36	0.41
3:D:350:GLU:O	3:D:353:ARG:HG2	2.20	0.41
2:A:401:TRP:CZ3	2:A:420:ILE:HD13	2.55	0.41
2:B:337:GLY:O	2:B:359:MET:HE3	2.20	0.41
2:B:370:MET:O	2:B:380:LEU:HD12	2.19	0.41
3:C:430:ARG:NH2	3:C:432:GLU:OE2	2.48	0.41
3:D:227:SER:O	3:D:228:ILE:HG13	2.20	0.41
2:B:229:ALA:HB3	2:B:288:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:319:LYS:HD2	2:B:323:ASP:OD1	2.20	0.41
3:C:83:ALA:O	3:C:84:ASP:CB	2.69	0.41
3:D:292:ILE:O	3:D:295:ALA:HB3	2.20	0.41
3:D:342:LEU:HD11	3:D:347:ILE:HD12	2.02	0.41
3:D:523:LEU:N	3:D:523:LEU:CD1	2.83	0.41
1:F:914:A:C2'	1:F:915:G:H5'	2.51	0.41
2:A:138:ARG:NH1	2:A:140:VAL:HG12	2.35	0.41
2:A:193:THR:HG21	2:A:195:VAL:O	2.20	0.41
2:A:283:GLU:OE1	2:A:285:ASN:O	2.38	0.41
2:A:299:ARG:NH1	2:A:299:ARG:CG	2.79	0.41
2:B:55:TYR:OH	3:D:133:THR:HG21	2.21	0.41
2:B:145:SER:HB2	2:B:176:GLY:CA	2.44	0.41
2:B:179:THR:O	2:B:179:THR:CG2	2.68	0.41
3:C:127:THR:CG2	3:C:175:LEU:HD21	2.50	0.41
3:C:149:VAL:CG1	3:C:191:MET:HE1	2.49	0.41
3:C:180:ILE:HA	3:C:181:PRO:HD3	1.92	0.41
3:C:225:ASN:HD22	3:C:235:GLU:HB3	1.82	0.41
3:C:471:ARG:CZ	3:C:499:ARG:HB2	2.51	0.41
3:D:24:LEU:O	3:D:92:ASN:HB2	2.20	0.41
3:D:304:ARG:CA	3:D:365:ASP:HB3	2.49	0.41
3:D:491:ALA:C	3:D:493:LEU:N	2.79	0.41
1:E:966:C:H2'	1:E:967:G:C8	2.55	0.41
1:F:907:G:N1	1:F:949:A:C6	2.89	0.41
1:F:963:G:O2'	1:F:964:C:H5'	2.21	0.41
2:A:55:TYR:HD2	3:C:135:LEU:HB2	1.85	0.41
2:A:311:PRO:O	2:B:396:TYR:OH	2.37	0.41
2:B:370:MET:HE1	2:B:384:VAL:HG11	2.03	0.41
2:B:408:ASP:O	2:B:409:PRO:C	2.63	0.41
3:C:10:MET:HB3	3:C:197:LEU:HD13	2.03	0.41
3:C:15:HIS:HD2	3:C:221:ARG:O	2.03	0.41
3:C:105:LEU:HD11	3:C:444:PRO:HD2	2.03	0.41
3:C:405:ASP:OD2	3:C:407:ASN:ND2	2.53	0.41
3:C:497:THR:C	3:C:499:ARG:H	2.27	0.41
3:D:16:GLN:O	3:D:182:LEU:HA	2.19	0.41
1:E:926:G:O2'	1:E:927:C:H5'	2.20	0.41
2:A:102:VAL:HG21	2:A:217:ILE:HG12	2.02	0.41
2:A:124:ARG:HG3	2:A:124:ARG:NH1	2.34	0.41
2:A:275:THR:C	2:A:277:ASP:N	2.78	0.41
2:B:57:ILE:HD11	3:D:135:LEU:HD23	2.02	0.41
2:B:285:ASN:C	2:B:285:ASN:ND2	2.79	0.41
3:C:47:PRO:O	3:C:48:THR:OG1	2.27	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:GLN:HB3	3:C:419:ARG:HG3	2.03	0.41
3:C:120:GLN:CB	3:C:419:ARG:HG3	2.51	0.41
3:C:157:GLU:OE2	3:C:184:GLU:OE1	2.39	0.41
3:C:255:ARG:HE	3:C:255:ARG:HB3	1.71	0.41
3:C:403:LEU:HB3	3:C:404:PRO:HD2	2.03	0.41
1:E:931:G:N2	1:E:940:C:C2	2.89	0.41
1:F:940:C:H6	1:F:940:C:O5'	2.03	0.41
2:A:36:LEU:HB2	2:A:48:VAL:CG1	2.51	0.41
2:A:108:TYR:HD2	3:C:420:MET:N	2.19	0.41
2:A:219:CYS:O	2:A:274:VAL:HG11	2.21	0.41
2:A:321:HIS:O	2:A:326:TYR:HB2	2.21	0.41
2:B:2:SER:N	2:B:37:ASP:OD2	2.54	0.41
2:B:182:TYR:O	2:B:185:ALA:HB3	2.20	0.41
2:B:191:LEU:C	2:B:192:ARG:HD3	2.45	0.41
3:C:46:ARG:CG	3:C:46:ARG:NH1	2.83	0.41
3:C:154:LEU:C	3:C:154:LEU:HD23	2.46	0.41
3:C:239:VAL:HG12	3:C:239:VAL:O	2.21	0.41
3:C:476:GLU:O	3:C:477:PHE:C	2.64	0.41
3:D:9:LYS:O	3:D:227:SER:HB3	2.21	0.41
3:D:284:PHE:O	3:D:285:ALA:C	2.64	0.41
3:D:291:ILE:HD12	3:D:291:ILE:N	2.15	0.41
1:E:968:G:O2'	1:E:969:G:H5'	2.21	0.41
2:A:7:ALA:H	2:A:44:ASP:HB2	1.86	0.41
2:A:345:PRO:HB2	5:A:439:HOH:O	2.19	0.41
2:B:118:THR:C	2:B:120:ASP:N	2.77	0.41
2:B:327:ARG:O	2:B:355:VAL:HG13	2.21	0.41
3:C:198:ARG:HD2	3:C:243:ASP:HA	2.02	0.41
3:D:245:ILE:N	3:D:246:PRO:CD	2.83	0.41
3:D:279:ASP:O	3:D:281:SER:N	2.50	0.41
3:D:337:PHE:HE2	3:D:345:TYR:HD2	1.69	0.41
2:B:148:MET:HE2	2:B:152:TYR:HB2	2.03	0.40
3:C:399:THR:O	3:C:411:LEU:HB2	2.21	0.40
3:C:445:GLU:HB2	3:C:449:GLU:HB2	2.02	0.40
3:C:490:ILE:O	3:C:494:LEU:HG	2.20	0.40
3:D:535:ASP:O	3:D:538:ALA:N	2.54	0.40
1:E:967:G:H2'	1:E:968:G:C8	2.52	0.40
2:A:118:THR:O	2:A:120:ASP:N	2.55	0.40
2:A:161:TYR:O	2:A:164:ILE:HG23	2.21	0.40
2:B:24:VAL:O	2:B:30:THR:HA	2.22	0.40
2:B:162:GLY:O	2:B:165:LYS:N	2.53	0.40
2:B:234:CYS:HB2	2:B:246:LEU:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:135:LEU:HD11	3:C:153:ASN:HB3	2.02	0.40
3:C:237:LYS:NZ	3:C:412:ARG:HH22	2.20	0.40
1:E:918:G:H8	1:E:918:G:O5'	2.03	0.40
2:A:279:ILE:HG12	2:A:281:ILE:H	1.87	0.40
2:A:353:MET:HE2	2:A:353:MET:HB3	1.89	0.40
2:B:109:ARG:HA	2:B:109:ARG:HD2	1.88	0.40
2:B:161:TYR:O	2:B:164:ILE:CG2	2.70	0.40
3:C:164:ILE:CG2	3:C:165:ARG:HD2	2.44	0.40
3:C:197:LEU:HD22	3:C:224:LEU:HD12	2.03	0.40
3:C:249:VAL:O	3:C:253:VAL:HG23	2.21	0.40
3:C:254:LYS:HZ2	3:C:316:PRO:HG2	1.86	0.40
1:E:902:G:C2	1:E:972:U:C2	3.09	0.40
1:F:937:G:C4	1:F:938:A:C8	3.08	0.40
2:A:26:LYS:HB3	2:A:27:PRO:HD2	2.04	0.40
2:A:148:MET:CE	2:A:175:HIS:CE1	3.04	0.40
2:B:370:MET:SD	2:B:386:PRO:HG3	2.61	0.40
2:B:380:LEU:HD21	2:B:386:PRO:HG3	2.02	0.40
2:B:398:LYS:C	2:B:416:MET:HE1	2.47	0.40
3:C:47:PRO:O	3:C:48:THR:CB	2.68	0.40
3:D:15:HIS:CD2	3:D:184:GLU:HG2	2.56	0.40
3:D:102:ILE:HD13	3:D:208:LEU:CD2	2.51	0.40
3:D:370:VAL:CG2	3:D:381:LEU:HG	2.51	0.40
2:A:264:ARG:NH1	2:B:433:PHE:CE2	2.89	0.40
2:B:55:TYR:CE1	3:D:420:MET:HE1	2.57	0.40
2:B:140:VAL:CG1	2:B:141:PHE:HD2	2.20	0.40
2:B:254:LYS:HB3	5:B:440:HOH:O	2.22	0.40
3:C:273:VAL:CG1	3:C:385:ILE:HG23	2.51	0.40
3:C:447:PRO:O	3:C:448:SER:C	2.64	0.40
3:C:469:VAL:HG22	3:C:474:VAL:HG21	2.03	0.40
3:D:499:ARG:HH11	3:D:499:ARG:CG	2.34	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:169:ASP:OD2	3:D:268:GLU:OE1[4_556]	2.08	0.12

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	420/435 (97%)	349 (83%)	50 (12%)	21 (5%)	1	10
2	B	420/435 (97%)	337 (80%)	65 (16%)	18 (4%)	2	13
3	C	479/619 (77%)	411 (86%)	52 (11%)	16 (3%)	3	17
3	D	516/619 (83%)	436 (84%)	55 (11%)	25 (5%)	2	11
All	All	1835/2108 (87%)	1533 (84%)	222 (12%)	80 (4%)	2	12

All (80) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	13	SER
2	A	115	PRO
2	A	140	VAL
2	A	281	ILE
2	B	44	ASP
2	B	115	PRO
2	B	140	VAL
2	B	226	SER
2	B	291	SER
3	C	47	PRO
3	C	217	LEU
3	C	333	VAL
3	D	47	PRO
3	D	219	THR
3	D	296	GLU
3	D	333	VAL
3	D	532	ALA
2	A	5	GLY
2	A	44	ASP
2	A	65	ARG
2	A	103	ALA
2	A	116	ALA

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Mol	Chain	Res	Type
2	A	178	ASP
2	A	288	LYS
2	A	289	ARG
2	A	291	SER
2	A	335	GLY
2	B	13	SER
2	B	65	ARG
2	B	116	ALA
2	B	205	SER
2	B	281	ILE
2	B	289	ARG
2	B	335	GLY
3	C	296	GLU
3	C	316	PRO
3	C	487	THR
3	D	217	LEU
3	D	316	PRO
3	D	528	ILE
2	A	70	GLU
2	A	85	ALA
2	A	226	SER
2	B	5	GLY
2	B	62	SER
2	B	294	LEU
3	C	60	PHE
3	C	440	ARG
3	D	60	PHE
3	D	192	SER
3	D	280	VAL
3	D	339	THR
3	D	507	ASP
3	D	513	LEU
3	D	521	LYS
2	A	51	LEU
2	A	86	GLU
3	C	219	THR
3	C	339	THR
3	C	432	GLU
3	D	139	ASP
3	D	334	SER
3	D	487	THR
2	B	70	GLU

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Mol	Chain	Res	Type
2	B	103	ALA
3	C	2	ASP
3	C	212	ARG
3	C	334	SER
3	D	413	PRO
3	D	508	VAL
3	D	525	VAL
3	D	533	LEU
2	A	72	GLY
2	A	88	PRO
3	C	396	PRO
2	B	88	PRO
3	C	280	VAL
3	D	342	LEU
3	D	438	GLY
3	D	218	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	356/367 (97%)	311 (87%)	45 (13%)	4	18
2	B	358/367 (98%)	315 (88%)	43 (12%)	5	20
3	C	423/529 (80%)	386 (91%)	37 (9%)	9	32
3	D	452/529 (85%)	404 (89%)	48 (11%)	6	24
All	All	1589/1792 (89%)	1416 (89%)	173 (11%)	6	23

All (173) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	9	LYS
2	A	10	PHE
2	A	11	LEU
2	A	22	VAL
2	A	30	THR

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Mol	Chain	Res	Type
2	A	43	ASP
2	A	57	ILE
2	A	59	VAL
2	A	60	GLU
2	A	90	LEU
2	A	96	ILE
2	A	98	THR
2	A	114	HIS
2	A	123	LEU
2	A	146	GLU
2	A	164	ILE
2	A	178	ASP
2	A	193	THR
2	A	212	ASP
2	A	217	ILE
2	A	222	ARG
2	A	227	GLU
2	A	230	GLU
2	A	252	VAL
2	A	253	ARG
2	A	254	LYS
2	A	259	ARG
2	A	275	THR
2	A	289	ARG
2	A	292	ASP
2	A	299	ARG
2	A	301	GLU
2	A	302	GLU
2	A	303	ARG
2	A	336	LEU
2	A	346	VAL
2	A	371	ASN
2	A	375	THR
2	A	393	GLU
2	A	394	VAL
2	A	406	THR
2	A	413	ARG
2	A	418	GLU
2	A	423	GLU
2	A	434	ARG
2	B	4	GLN
2	B	9	LYS

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Mol	Chain	Res	Type
2	B	17	ASP
2	B	29	VAL
2	B	30	THR
2	B	47	ILE
2	B	57	ILE
2	B	59	VAL
2	B	60	GLU
2	B	66	ILE
2	B	87	ASP
2	B	94	SER
2	B	117	PHE
2	B	131	ASP
2	B	148	MET
2	B	177	THR
2	B	187	LEU
2	B	195	VAL
2	B	197	VAL
2	B	203	GLN
2	B	205	SER
2	B	222	ARG
2	B	225	THR
2	B	250	VAL
2	B	252	VAL
2	B	259	ARG
2	B	264	ARG
2	B	275	THR
2	B	279	ILE
2	B	282	LEU
2	B	291	SER
2	B	293	GLU
2	B	297	SER
2	B	334	THR
2	B	346	VAL
2	B	377	ARG
2	B	393	GLU
2	B	406	THR
2	B	417	ARG
2	B	425	ASN
2	B	427	ARG
2	B	430	ILE
2	B	434	ARG
3	C	4	GLU

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Mol	Chain	Res	Type
3	C	15	HIS
3	C	46	ARG
3	C	77	GLU
3	C	78	THR
3	C	82	GLU
3	C	86	GLU
3	C	120	GLN
3	C	146	GLN
3	C	148	THR
3	C	150	LYS
3	C	165	ARG
3	C	171	VAL
3	C	177	ARG
3	C	182	LEU
3	C	186	THR
3	C	190	SER
3	C	194	PRO
3	C	195	GLN
3	C	197	LEU
3	C	228	ILE
3	C	233	ARG
3	C	274	GLU
3	C	275	ASP
3	C	282	GLU
3	C	286	ASP
3	C	319	ARG
3	C	345	TYR
3	C	365	ASP
3	C	374	ARG
3	C	393	GLN
3	C	395	VAL
3	C	397	GLU
3	C	422	LEU
3	C	476	GLU
3	C	501	LEU
3	C	502	ARG
3	D	26	CYS
3	D	31	GLU
3	D	64	MET
3	D	73	ASN
3	D	78	THR
3	D	119	LYS

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Mol	Chain	Res	Type
3	D	123	ASP
3	D	127	THR
3	D	133	THR
3	D	146	GLN
3	D	154	LEU
3	D	164	ILE
3	D	166	GLU
3	D	167	THR
3	D	182	LEU
3	D	186	THR
3	D	198	ARG
3	D	207	ILE
3	D	209	ARG
3	D	212	ARG
3	D	215	ARG
3	D	224	LEU
3	D	228	ILE
3	D	248	ILE
3	D	250	GLU
3	D	292	ILE
3	D	298	VAL
3	D	301	VAL
3	D	333	VAL
3	D	342	LEU
3	D	345	TYR
3	D	355	LEU
3	D	363	GLN
3	D	365	ASP
3	D	367	VAL
3	D	384	VAL
3	D	386	ARG
3	D	398	GLU
3	D	405	ASP
3	D	409	GLN
3	D	453	ARG
3	D	464	LEU
3	D	499	ARG
3	D	504	GLU
3	D	518	ASP
3	D	523	LEU
3	D	524	GLU
3	D	529	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	56	ASN
2	A	147	ASN
2	A	175	HIS
2	A	203	GLN
2	A	218	GLN
2	A	256	HIS
2	A	338	HIS
2	A	362	GLN
2	A	365	ASN
2	A	371	ASN
2	A	405	GLN
2	B	56	ASN
2	B	134	ASN
2	B	175	HIS
2	B	203	GLN
2	B	218	GLN
2	B	256	HIS
2	B	285	ASN
2	B	362	GLN
2	B	369	ASN
2	B	405	GLN
2	B	425	ASN
3	C	15	HIS
3	C	70	HIS
3	C	73	ASN
3	C	89	HIS
3	C	115	HIS
3	C	126	ASN
3	C	146	GLN
3	C	195	GLN
3	C	196	GLN
3	C	222	GLN
3	C	225	ASN
3	C	267	GLN
3	C	372	HIS
3	C	379	ASN
3	C	442	ASN
3	C	472	ASN
3	D	15	HIS
3	D	39	HIS
3	D	68	HIS

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Mol	Chain	Res	Type
3	D	70	HIS
3	D	73	ASN
3	D	107	ASN
3	D	115	HIS
3	D	146	GLN
3	D	196	GLN
3	D	203	GLN
3	D	222	GLN
3	D	372	HIS
3	D	379	ASN
3	D	393	GLN
3	D	409	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	E	71/74 (95%)	16 (22%)	1 (1%)
1	F	73/74 (98%)	19 (26%)	4 (5%)
All	All	144/148 (97%)	35 (24%)	5 (3%)

All (35) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	E	908	U
1	E	909	G
1	E	910	G
1	E	917	G
1	E	920	A
1	E	923	C
1	E	933	U
1	E	934	U
1	E	935	U
1	E	936	G
1	E	942	G
1	E	947	A
1	E	948	C
1	E	959	C
1	E	961	C
1	E	973	A
1	F	905	C
1	F	908	U

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Mol	Chain	Res	Type
1	F	909	G
1	F	910	G
1	F	912	G
1	F	917	G
1	F	919	U
1	F	920	A
1	F	923	C
1	F	933	U
1	F	934	U
1	F	935	U
1	F	936	G
1	F	947	A
1	F	948	C
1	F	957	G
1	F	959	C
1	F	960	U
1	F	961	C

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	E	958	A
1	F	907	G
1	F	909	G
1	F	958	A
1	F	960	U

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	E	72/74 (97%)	0.87	7 (9%)	13 8	83, 122, 174, 192	0
1	F	74/74 (100%)	0.37	3 (4%)	41 24	55, 88, 139, 152	0
2	A	424/435 (97%)	-0.35	6 (1%)	73 53	7, 33, 81, 113	0
2	B	424/435 (97%)	-0.36	1 (0%)	91 84	12, 36, 68, 93	0
3	C	485/619 (78%)	0.38	28 (5%)	29 16	23, 76, 133, 142	0
3	D	522/619 (84%)	-0.11	16 (3%)	51 31	9, 41, 102, 122	0
All	All	2001/2256 (88%)	-0.04	61 (3%)	52 32	7, 46, 127, 192	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	935	U	8.3
3	D	511	LEU	7.5
2	A	113	VAL	7.0
1	E	936	G	6.1
2	B	435	GLY	5.8
1	E	934	U	5.3
1	E	901	A	5.1
3	C	359	VAL	4.7
3	C	355	LEU	4.1
3	D	58	ALA	4.1
3	C	501	LEU	4.0
3	C	367	VAL	4.0
2	A	111	GLY	3.6
3	C	226	ILE	3.4
3	D	528	ILE	3.4
3	C	488	THR	3.3
2	A	117	PHE	3.2
3	C	490	ILE	3.1
3	D	512	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	F	926	G	3.1
3	C	493	LEU	3.1
1	F	925	U	3.0
3	D	535	ASP	2.9
1	F	975	C	2.9
3	D	515	GLU	2.9
3	D	492	SER	2.8
1	E	937	G	2.8
2	A	32	GLU	2.8
2	A	33	GLY	2.7
1	E	920	A	2.7
3	D	518	ASP	2.7
3	C	414	LEU	2.7
3	C	347	ILE	2.6
3	C	222	GLN	2.6
3	D	59	ALA	2.6
3	D	538	ALA	2.6
3	C	503	ARG	2.6
3	C	1	MET	2.6
3	D	326	ASP	2.5
3	C	224	LEU	2.5
3	C	301	VAL	2.5
3	D	338	HIS	2.4
2	A	116	ALA	2.4
3	D	288	GLU	2.4
3	C	344	ALA	2.3
3	C	294	SER	2.3
1	E	938	A	2.3
3	C	395	VAL	2.3
3	D	350	GLU	2.3
3	C	61	GLU	2.2
3	C	406	GLY	2.2
3	C	277	ILE	2.2
3	C	291	ILE	2.2
3	C	100	VAL	2.2
3	C	475	ASP	2.2
3	D	57	ARG	2.2
3	C	368	VAL	2.1
3	C	96	LEU	2.1
3	C	168	GLY	2.1
3	D	340	ASP	2.0
3	C	489	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ZN	C	900	1/1	1.00	0.01	41,41,41,41	0
4	ZN	D	1900	1/1	1.00	0.01	35,35,35,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.