Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2024 – 01:28 AM EST

PDB ID	:	2D6F
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:

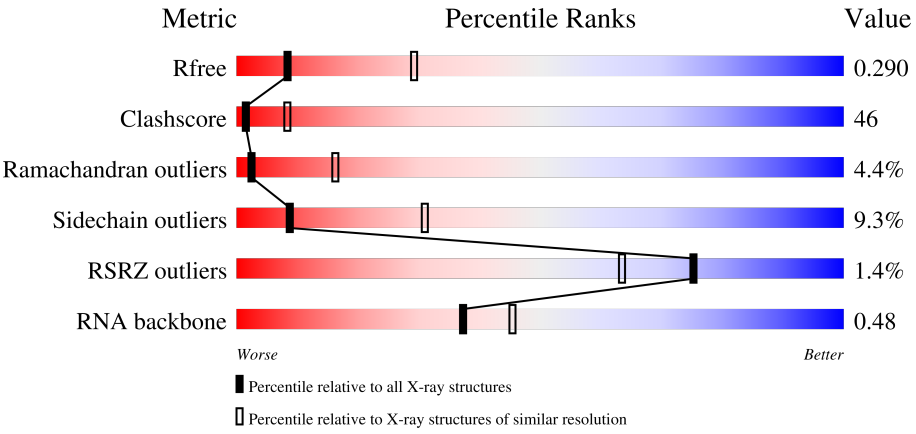
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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}	130704	1665 (3.20-3.12)
Clashscore	141614	1804 (3.20-3.12)
Ramachandran outliers	138981	1770 (3.20-3.12)
Sidechain outliers	138945	1769 (3.20-3.12)
RSRZ outliers	127900	1616 (3.20-3.12)
RNA backbone	3102	1073 (3.50-2.82)

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 <=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	7% 18% 58% 22% .
1	F	74	5% 27% 47% 24% .
2	A	435	% 37% 51% 9% .
2	B	435	37% 51% 9% .

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Mol	Chain	Length	Quality of chain
3	C	619	2% 26% 47% 6% 22%
3	D	619	% 30% 46% 8% 16%

2 Entry composition (i)

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 (three-letter code: 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.

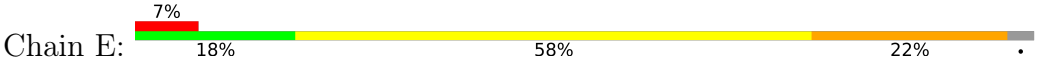
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	E	16	Total O 16 16	0	0
5	F	24	Total O 24 24	0	0
5	A	31	Total O 31 31	0	0
5	B	24	Total O 24 24	0	0
5	C	36	Total O 36 36	0	0
5	D	49	Total O 49 49	0	0

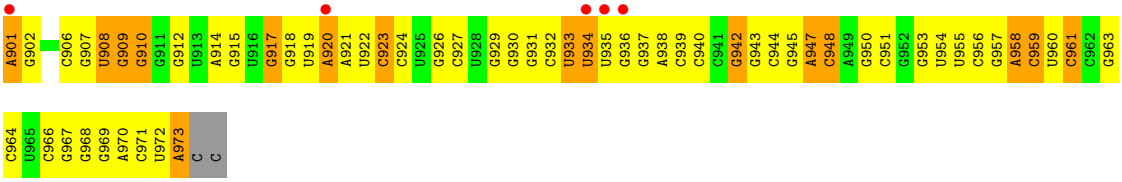
3 Residue-property plots (i)

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

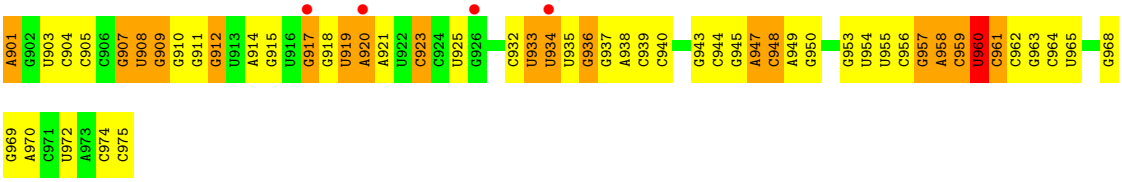
Chain E:





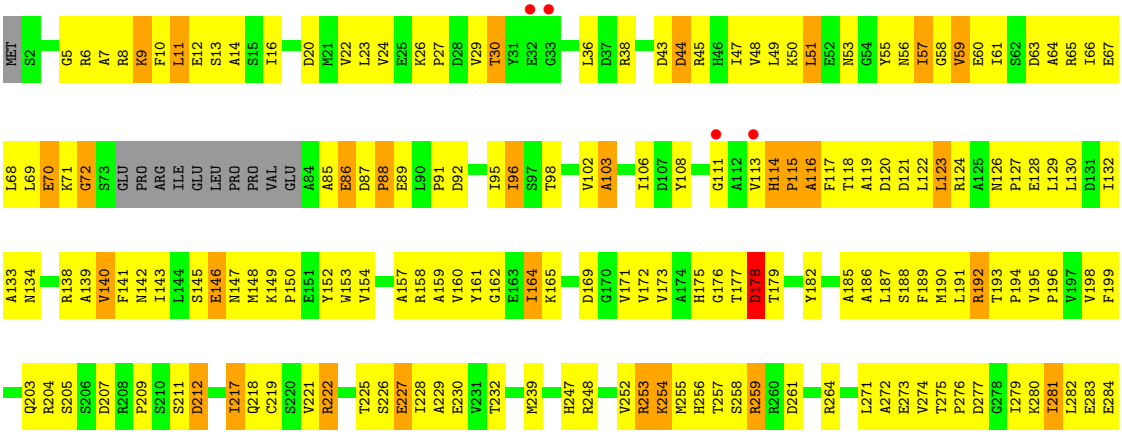
• Molecule 1: tRNA

Chain F:



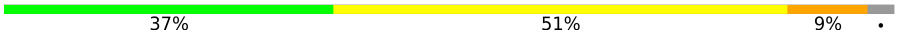
• Molecule 2: Glutamyl-tRNA(Gln) amidotransferase subunit D

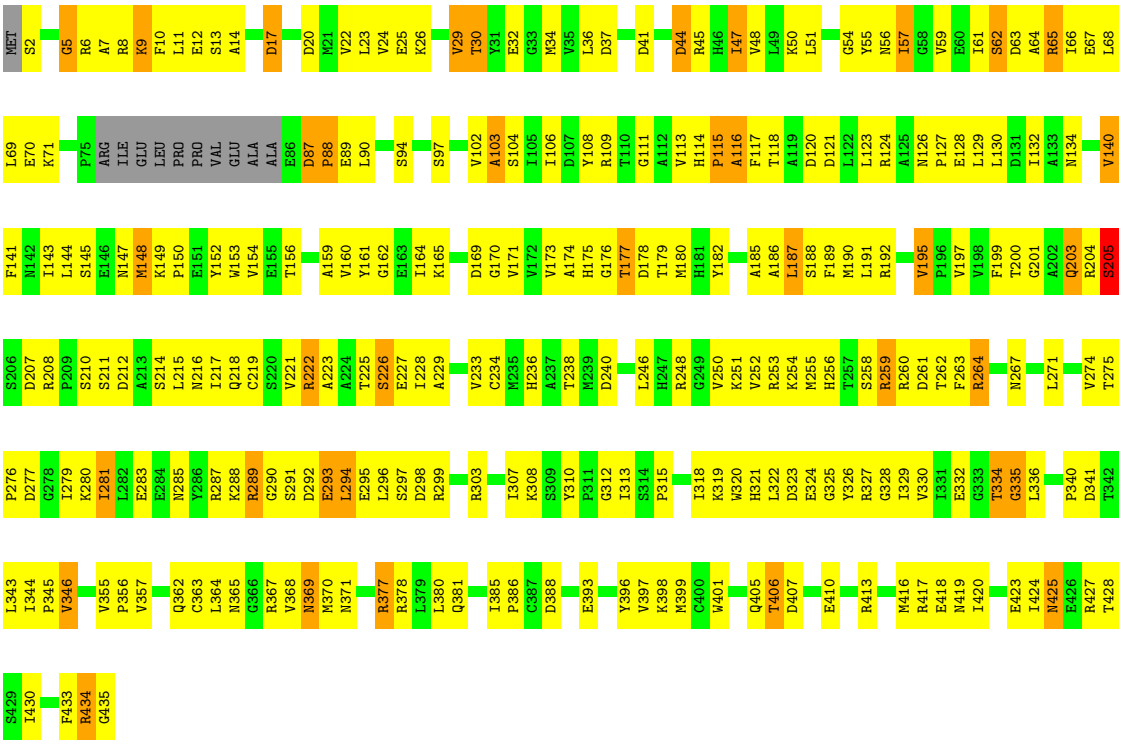
Chain A:



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

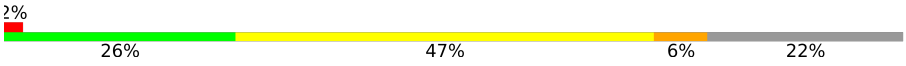
Chain B:

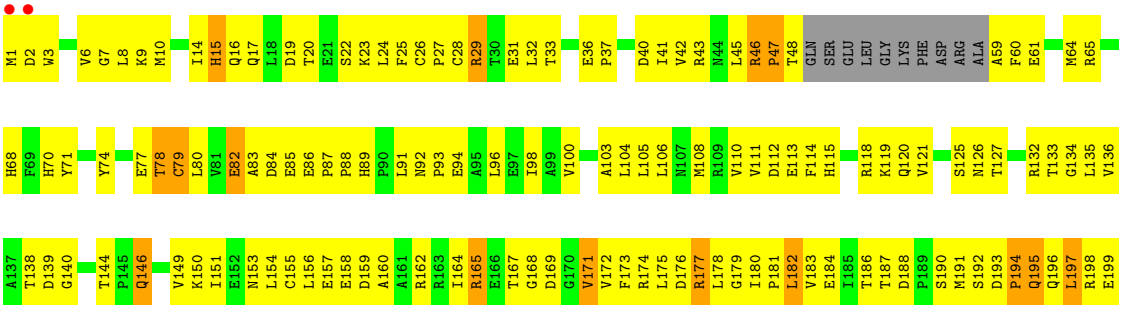


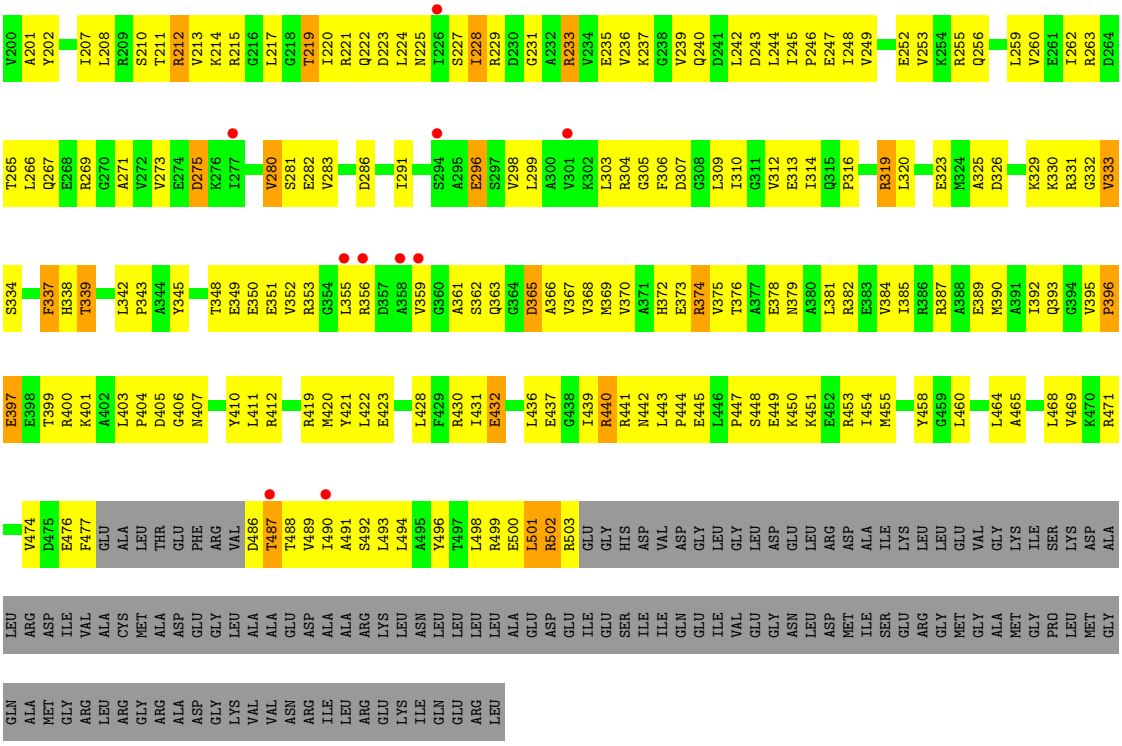


• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit E

Chain C:

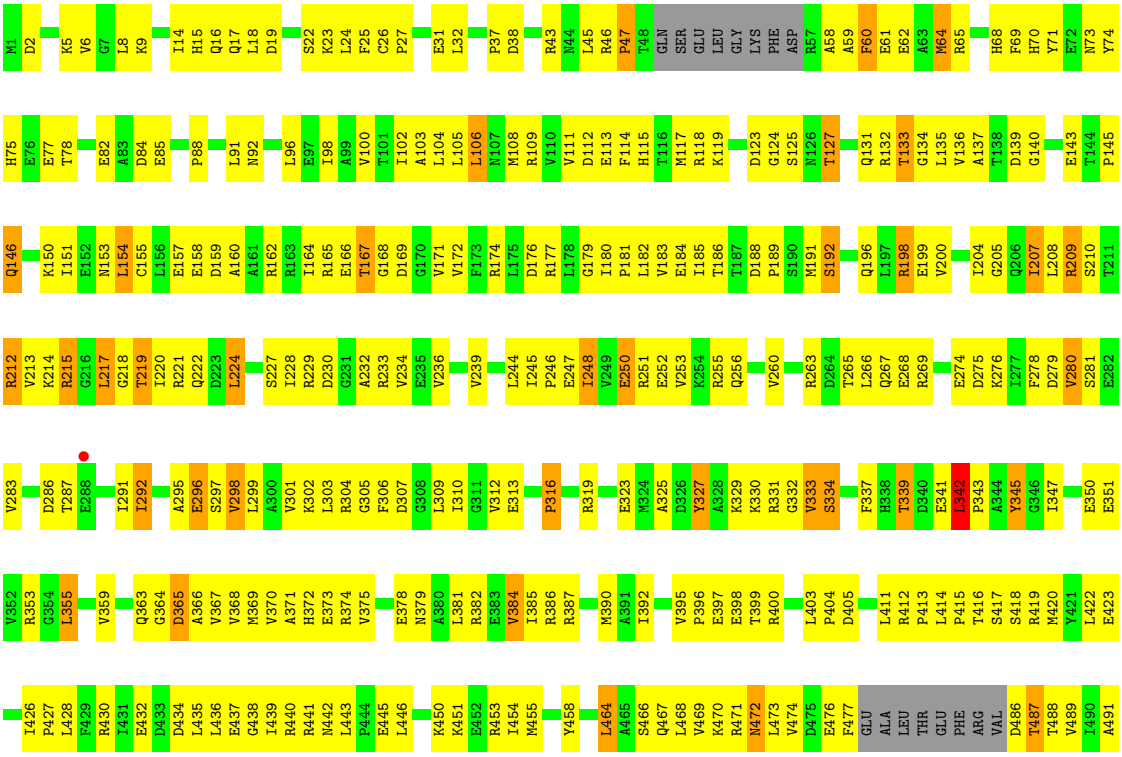


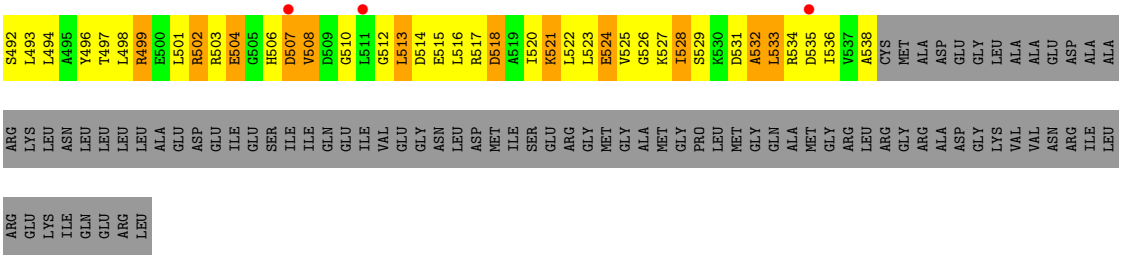




• Molecule 3: Glutamyl-tRNA(Gln) amidotransferase subunit E

Chain D:




S492 L493 L494 A495 Y496 T497 L498 R499 E500 L501 R502 R503 E504 G505 H506 D507 V508 D509 G510 L511 G512 L513 D514 E515 L516 R517 D518 A519 I520 K521 L522 L523 E524 V525 G526 K527 I528 S529 K530 D531 A532 L533 R534 D535 I536 V537 A538 CYS MET ALA ASP GLU GLY LEU ALA ALA GLU ASP ALA ALA
ARG LYS LEU ASN LEU LEU LEU LEU ALA GLU ASP GLU ILE GLU SER ILE ILE GLN GLU ILE VAL GLU GLY ASN LEU ASP MET ILE SER GLU ARG GLY MET GLY ALA MET GLY PRO LEU MET GLY GLN ALA MET GLY ARG LEU ARG GLY ARG ALA ASP GLY LYS VAL VAL ASN ARG ILE LEU
ARG GLU LYS ILE GLN GLU ARG LEU

4 Data and refinement statistics (i)

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 70.35 – 3.15	Depositor EDS
% Data completeness (in resolution range)	98.8 (46.52-3.15) 98.9 (70.35-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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)	0.24 , 55.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.37	1/1718 (0.1%)	0.69	0/2676
1	F	0.40	1/1762 (0.1%)	0.72	0/2744
2	A	0.44	0/3323	0.71	1/4501 (0.0%)
2	B	0.45	0/3330	0.71	0/4511
3	C	0.36	0/3898	0.64	0/5265
3	D	0.44	0/4179	0.68	0/5642
All	All	0.42	2/18210 (0.0%)	0.69	1/25339 (0.0%)

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

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	901	A	OP3-P	-7.11	1.52	1.61
1	F	901	A	OP3-P	-6.87	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	192	ARG	N-CA-C	-5.15	97.09	111.00

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 (i)

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	332	0
2	B	3274	0	3220	318	0
3	C	3847	0	3861	425	1
3	D	4127	0	4152	399	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	1543	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 46.

All (1543) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:186:ALA:HB1	2:B:190:MET:HE2	1.57	0.87
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:A:399:MET:HA	2:A:416:MET:HE3	1.66	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: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: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:D:59:ALA:C	3:D:61:GLU:H	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
2:A:264:ARG:HE	2:B:435:GLY:C	1.92	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:MET:HE1	3:C:253:VAL:HG11	1.72	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
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
3:D:437:GLU:C	3:D:439:ILE:H	1.94	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:260:ARG:HD2	3:D:85:GLU:OE2	1.92	0.69
3:C:149:VAL:HG21	3:C:191:MET:HE3	1.73	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:D:18:LEU:O	3:D:19:ASP:HB3	1.93	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
2:A:402:VAL:HG22	2:A:415:MET:HE2	1.76	0.67
1:F:968:G:O2'	1:F:969:G:H5'	1.94	0.67
3:C:59:ALA:C	3:C:61:GLU:H	1.98	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:1:MET:HE3	3:C:6:VAL:HG21	1.75	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:266:LEU:HD13	3:D:392:ILE:HD13	1.77	0.67
3:C:1:MET:HE1	3:C:253:VAL:CG1	2.25	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:435:GLY:C	2:B:264:ARG:HE	2.00	0.63
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:132:ILE:HG12	2:B:222:ARG:NH1	2.11	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
2:A:44:ASP:O	2:A:45:ARG:HB2	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
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:147:ASN:HD22	2:B:340:PRO:HA	1.62	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: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: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:B:204:ARG:NH2	2:B:258:SER:O	2.32	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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: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:D:14:ILE:HG12	3:D:222:GLN:HG2	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:371:ASN:N	2:A:371:ASN:ND2	2.49	0.59
3:C:233:ARG:O	3:C:397:GLU:HA	2.02	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
2:B:141:PHE:HZ	2:B:156:THR:HG1	1.51	0.59
3:C:374:ARG:HH22	3:C:378:GLU:CB	2.15	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:499:ARG:O	3:C:502:ARG:HG3	2.03	0.58
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
3:D:323:GLU:CD	3:D:400:ARG:HH22	2.07	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:77:GLU:CD	3:C:77:GLU:H	2.06	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
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
2:A:177:THR:HB	2:A:254:LYS:HZ2	1.69	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
2:A:98:THR:HG21	2:A:148:MET:HE1	1.86	0.58
2:B:149:LYS:HZ3	2:B:152:TYR:HE1	1.51	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: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
2:B:186:ALA:HB1	2:B:190:MET:CE	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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
3:D:59:ALA:C	3:D:61:GLU:N	2.57	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: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
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
1:E:929:G:N3	1:E:929:G:H2'	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:401:TRP:O	2:B:405:GLN:HG2	2.05	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:D:437:GLU:C	3:D:439:ILE:N	2.59	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:A:68:LEU:HD11	2:A:70:GLU:C	2.26	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:C:489:VAL:HA	3:C:492:SER:HG	1.70	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:A:12:GLU:C	2:A:14:ALA:H	2.09	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: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: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:D:98:ILE:HD11	3:D:212:ARG:HH12	1.69	0.55
3:D:108:MET:CE	3:D:151:ILE:HG22	2.37	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: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
2:A:387:CYS:HB3	2:A:390:MET:HE3	1.90	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
2:B:369:ASN:C	2:B:369:ASN:HD22	2.10	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
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
2:A:335:GLY:O	2:A:336:LEU:HB2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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
3:D:341:GLU:C	3:D:343:PRO:HD3	2.28	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:68:LEU:HD11	2:A:70:GLU:O	2.07	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: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:214:SER:O	2:B:217:ILE:HG22	2.08	0.53
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:142:ASN:C	2:A:143:ILE:HG13	2.28	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:102:VAL:O	2:B:103:ALA:HB2	2.09	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: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:140:VAL:HG11	2:B:159:ALA:HB2	1.92	0.52
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
2:B:204:ARG:O	2:B:205:SER:C	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:228:ILE:CG1	3:C:256:GLN:HG2	2.39	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: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
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
3:D:32:LEU:HD22	3:D:176:ASP:CG	2.30	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: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
2:B:410:GLU:H	2:B:410:GLU:CD	2.13	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
3:D:531:ASP:C	3:D:533:LEU:H	2.12	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
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:C:10:MET:HE2	3:C:197:LEU:HD22	1.92	0.51
3:C:118:ARG:HE	3:C:423:GLU:CD	2.14	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:146:GLN:CD	3:C:146:GLN:N	2.64	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: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: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
3:C:29:ARG:NH1	3:C:29:ARG:HB2	2.26	0.51
3:C:59:ALA:C	3:C:61:GLU:N	2.63	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:283:GLU:CD	2:A:285:ASN:H	2.13	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
3:D:108:MET:HE1	3:D:151:ILE:HG22	1.92	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
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: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
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:C:501:LEU:C	3:C:503:ARG:H	2.15	0.50
3:D:111:VAL:CG1	3:D:112:ASP:N	2.75	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:16:GLN:OE1	3:C:213:VAL:CG1	2.60	0.50
3:D:176:ASP:OD1	3:D:176:ASP:N	2.45	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
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: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
3:D:523:LEU:C	3:D:524:GLU:HG3	2.32	0.49
2:A:87:ASP:HB3	5:A:446:HOH:O	2.12	0.49
2:B:44:ASP:O	2:B:45:ARG:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:54:GLY:O	3:D:117:MET:HE2	2.12	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: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
2:B:55:TYR:HA	3:D:117:MET:HE2	1.94	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:D:347:ILE:HG22	3:D:351:GLU:HB2	1.95	0.49
2:A:115:PRO:O	2:A:116:ALA:HB2	2.13	0.49
2:A:116:ALA:HB1	2:A:121:ASP:OD2	2.12	0.49
2:A:264:ARG:NE	2:B:435:GLY:C	2.64	0.49
2:B:12:GLU:C	2:B:14:ALA:H	2.16	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:186:ALA:HB1	2:A:190:MET:HE3	1.94	0.49
2:A:193:THR:HG22	2:A:194:PRO:CD	2.43	0.49
3:C:1:MET:HE2	3:C:6:VAL:HG21	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:146:GLN:CD	3:C:146:GLN:H	2.15	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
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
3:C:16:GLN:NE2	3:C:16:GLN:CA	2.67	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
3:C:256:GLN:OE1	3:C:395:VAL:HG11	2.12	0.48
3:C:365:ASP:OD2	3:C:365:ASP:N	2.34	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: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:55:TYR:CE2	3:D:420:MET:HE1	2.49	0.48
2:B:143:ILE:CG2	2:B:148:MET:HE3	2.43	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:486:ASP:O	3:D:486:ASP:CG	2.52	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: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
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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:437:GLU:C	3:C:439:ILE:H	2.18	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
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: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: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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:388:ASP:HB2	2:A:424:ILE:HG23	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
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
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: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
2:B:143:ILE:HG21	2:B:148:MET:HE3	1.97	0.46
2:B:369:ASN:C	2:B:369:ASN:ND2	2.67	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
2:B:111:GLY:C	3:D:422:LEU:HD12	2.36	0.46
3:D:70:HIS:HB2	3:D:172:VAL:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:233:ARG:HG3	3:C:397:GLU:CB	2.26	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:61:ILE:O	2:B:62:SER:C	2.54	0.46
2:B:161:TYR:HB2	2:B:296:LEU:HD22	1.98	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:10:PHE:C	2:B:10:PHE:CD2	2.89	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
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: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
2:A:387:CYS:HB3	2:A:390:MET:CE	2.45	0.45
3:C:8:LEU:HA	3:C:227:SER:O	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:228:ILE:HD13	3:C:256:GLN:CD	2.36	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
1:E:960:U:H3'	5:E:146:HOH:O	2.16	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: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: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:D:160:ALA:O	3:D:177:ARG:HG2	2.17	0.45
3:D:298:VAL:C	3:D:299:LEU:HD23	2.37	0.45
3:D:331:ARG:HG3	3:D:331:ARG:O	2.15	0.45
3:D:441:ARG:C	3:D:442:ASN:OD1	2.55	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
3:C:111:VAL:HG23	3:C:136:VAL:C	2.36	0.45
3:C:498:LEU:O	3:C:501:LEU:HD22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:61:ILE:O	2:B:63:ASP:N	2.49	0.45
2:B:128:GLU:CD	2:B:128:GLU:H	2.20	0.45
2:B:371:ASN:O	2:B:377:ARG:HD3	2.17	0.45
2:B:393:GLU:H	2:B:393:GLU:CD	2.20	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:341:GLU:C	3:D:343:PRO:CD	2.85	0.45
3:D:501:LEU:C	3:D:503:ARG:H	2.20	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
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:319:LYS:O	2:A:320:TRP:C	2.55	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
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
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
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
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:A:413:ARG:HG3	2:A:414:GLU:N	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:164:ILE:CD1	3:C:174:ARG:HB2	2.47	0.44
3:C:187:THR:O	3:C:188:ASP:C	2.56	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:77:GLU:CD	3:C:77:GLU:N	2.71	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:D:399:THR:HG22	3:D:411:LEU:HD12	2.00	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: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:A:402:VAL:C	2:A:404:GLY:H	2.20	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:146:GLU:H	2:A:146:GLU:CD	2.20	0.44
2:A:149:LYS:HG2	2:A:152:TYR:CE1	2.52	0.44
2:A:280:LYS:O	2:A:281:ILE:C	2.55	0.44
2:A:417:ARG:HG2	2:A:417:ARG:HH11	1.83	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
3:D:520:ILE:C	3:D:522:LEU:H	2.20	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:98:THR:CG2	2:A:148:MET:HE1	2.48	0.44
2:A:141:PHE:CD1	2:A:143:ILE:HD12	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:LEU:N	3:C:343:PRO:CD	2.81	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
2:A:334:THR:O	2:A:335:GLY:C	2.56	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:C:486:ASP:C	3:C:487:THR:HG1	2.21	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:175:HIS:HD2	2:A:176:GLY:N	2.13	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:161:TYR:C	2:B:164:ILE:HG22	2.38	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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:113:GLU:CD	3:C:428:LEU:HD13	2.39	0.43
3:D:527:LYS:O	3:D:528:ILE:C	2.56	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:342:LEU:HD13	3:C:342:LEU:C	2.38	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
3:D:502:ARG:C	3:D:503:ARG:HG3	2.39	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:88:PRO:C	2:B:90:LEU:H	2.21	0.43
2:B:129:LEU:HD22	2:B:221:VAL:HG21	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
2:B:399:MET:N	2:B:416:MET:HE1	2.34	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: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
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
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:A:332:GLU:CD	5:A:450:HOH:O	2.57	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:180:MET:CE	2:B:233:VAL:HG13	2.49	0.42
2:B:367:ARG:HG3	2:B:367:ARG:HH11	1.85	0.42
3:C:339:THR:CB	3:C:366:ALA:HB1	2.49	0.42
3:C:420:MET:HB2	3:C:420:MET:HE3	1.97	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:139:ALA:O	2:A:140:VAL:C	2.58	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
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:327:TYR:CE1	3:D:387:ARG:HD3	2.55	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:C:374:ARG:HH22	3:C:378:GLU:CD	2.22	0.42
3:D:6:VAL:HG12	3:D:6:VAL:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:148:MET:HE3	2:A:175:HIS:CE1	2.54	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
5:A:463:HOH:O	3:C:64:MET:HE1	2.19	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: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
2:B:312:GLY:O	2:B:313:ILE:C	2.57	0.42
2:B:356:PRO:HB2	2:B:399:MET:HE1	2.01	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
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:498:LEU:C	3:C:501:LEU:HB3	2.40	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:306:PHE:HB2	2:A:396:TYR:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:89:GLU:C	2:B:90:LEU:HD22	2.40	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:289:ARG:HG3	2:A:289:ARG:NH1	2.32	0.41
2:B:223:ALA:C	2:B:225:THR:N	2.74	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:150:LYS:C	3:D:151:ILE:HD12	2.40	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
3:D:487:THR:C	3:D:489:VAL:N	2.72	0.41
2:A:401:TRP:CZ3	2:A:420:ILE:HD13	2.55	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
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:487:THR:C	3:D:489:VAL:H	2.24	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:A:373:TYR:C	2:A:377:ARG:NH1	2.73	0.41
2:B:55:TYR:OH	3:D:133:THR:HG21	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:506:HIS:CG	3:D:506:HIS:O	2.73	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
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: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:B:57:ILE:HD11	3:D:135:LEU:HD23	2.02	0.41
3:C:47:PRO:O	3:C:48:THR:OG1	2.27	0.41
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:98:THR:CG2	2:A:98:THR:O	2.69	0.41
2:A:108:TYR:HD2	3:C:420:MET:N	2.19	0.41
2:A:118:THR:C	2:A:120:ASP:N	2.73	0.41
2:A:204:ARG:O	2:A:205:SER:C	2.59	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:280:LYS:O	2:B:281:ILE:C	2.59	0.41
3:C:46:ARG:CG	3:C:46:ARG:NH1	2.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:239:VAL:HG12	3:C:239:VAL:O	2.21	0.41
3:D:9:LYS:O	3:D:227:SER:HB3	2.21	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:327:ARG:O	2:B:355:VAL:HG13	2.21	0.41
3:C:149:VAL:CG2	3:C:191:MET:HE3	2.46	0.41
3:C:198:ARG:HD2	3:C:243:ASP:HA	2.02	0.41
3:C:227:SER:C	3:C:228:ILE:HD12	2.41	0.41
3:D:245:ILE:N	3:D:246:PRO:CD	2.83	0.41
3:D:274:GLU:C	3:D:276:LYS:H	2.25	0.41
3:D:279:ASP:O	3:D:281:SER:N	2.50	0.41
3:D:302:LYS:HZ1	3:D:304:ARG:HE	1.67	0.41
3:D:337:PHE:HE2	3:D:345:TYR:HD2	1.69	0.41
2:A:312:GLY:O	2:A:313:ILE:C	2.56	0.40
2:B:210:SER:O	2:B:211:SER:C	2.59	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:359:VAL:O	3:D:359:VAL:HG22	2.21	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
3:C:135:LEU:HD11	3:C:153:ASN:HB3	2.02	0.40
3:C:223:ASP:CG	3:C:237:LYS:HD3	2.42	0.40
3:C:237:LYS:NZ	3:C:412:ARG:HH22	2.20	0.40
3:C:439:ILE:O	3:C:440:ARG:C	2.59	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:160:VAL:O	2:A:161:TYR:C	2.60	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
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
3:D:491:ALA:C	3:D:493:LEU:H	2.25	0.40
2:A:264:ARG:NH1	2:B:433:PHE:CE2	2.89	0.40
2:B:140:VAL:CG1	2:B:141:PHE:HD2	2.20	0.40
2:B:223:ALA:C	2:B:225:THR:H	2.25	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: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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	420/435 (97%)	349 (83%)	50 (12%)	21 (5%)	2 14
2	B	420/435 (97%)	337 (80%)	65 (16%)	18 (4%)	2 17
3	C	479/619 (77%)	411 (86%)	52 (11%)	16 (3%)	4 22

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	D	516/619 (83%)	436 (84%)	55 (11%)	25 (5%)	2 15
All	All	1835/2108 (87%)	1533 (84%)	222 (12%)	80 (4%)	2 16

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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
3	D	438	GLY
3	D	218	GLY

5.3.2 Protein sidechains (i)

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%)	320 (90%)	36 (10%)	7 27
2	B	358/367 (98%)	325 (91%)	33 (9%)	9 31
3	C	423/529 (80%)	388 (92%)	35 (8%)	11 37
3	D	452/529 (85%)	408 (90%)	44 (10%)	8 29
All	All	1589/1792 (89%)	1441 (91%)	148 (9%)	9 31

All (148) 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	30	THR
2	A	43	ASP
2	A	57	ILE
2	A	59	VAL
2	A	96	ILE
2	A	114	HIS
2	A	123	LEU
2	A	146	GLU
2	A	164	ILE
2	A	178	ASP
2	A	212	ASP
2	A	217	ILE
2	A	222	ARG
2	A	227	GLU
2	A	230	GLU
2	A	253	ARG

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Mol	Chain	Res	Type
2	A	254	LYS
2	A	259	ARG
2	A	289	ARG
2	A	292	ASP
2	A	302	GLU
2	A	303	ARG
2	A	316	ASP
2	A	327	ARG
2	A	371	ASN
2	A	375	THR
2	A	394	VAL
2	A	406	THR
2	A	413	ARG
2	A	418	GLU
2	A	423	GLU
2	A	425	ASN
2	A	434	ARG
2	B	9	LYS
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	87	ASP
2	B	94	SER
2	B	117	PHE
2	B	148	MET
2	B	177	THR
2	B	178	ASP
2	B	187	LEU
2	B	195	VAL
2	B	203	GLN
2	B	205	SER
2	B	222	ARG
2	B	250	VAL
2	B	252	VAL
2	B	259	ARG
2	B	264	ARG
2	B	285	ASN
2	B	293	GLU
2	B	297	SER

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Mol	Chain	Res	Type
2	B	334	THR
2	B	346	VAL
2	B	369	ASN
2	B	377	ARG
2	B	406	THR
2	B	425	ASN
2	B	427	ARG
2	B	434	ARG
3	C	15	HIS
3	C	29	ARG
3	C	40	ASP
3	C	46	ARG
3	C	78	THR
3	C	79	CYS
3	C	82	GLU
3	C	86	GLU
3	C	89	HIS
3	C	139	ASP
3	C	146	GLN
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	275	ASP
3	C	282	GLU
3	C	286	ASP
3	C	319	ARG
3	C	337	PHE
3	C	345	TYR
3	C	365	ASP
3	C	374	ARG
3	C	397	GLU
3	C	476	GLU
3	C	501	LEU

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Mol	Chain	Res	Type
3	C	502	ARG
3	D	26	CYS
3	D	31	GLU
3	D	60	PHE
3	D	64	MET
3	D	78	THR
3	D	106	LEU
3	D	123	ASP
3	D	127	THR
3	D	133	THR
3	D	146	GLN
3	D	154	LEU
3	D	166	GLU
3	D	167	THR
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	248	ILE
3	D	250	GLU
3	D	286	ASP
3	D	292	ILE
3	D	298	VAL
3	D	327	TYR
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	405	ASP
3	D	434	ASP
3	D	453	ARG
3	D	464	LEU
3	D	472	ASN
3	D	499	ARG
3	D	502	ARG
3	D	504	GLU

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Mol	Chain	Res	Type
3	D	518	ASP
3	D	524	GLU
3	D	529	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (49) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	4	GLN
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	371	ASN
2	A	405	GLN
2	B	46	HIS
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	70	HIS
3	C	73	ASN
3	C	115	HIS
3	C	126	ASN
3	C	131	GLN
3	C	146	GLN
3	C	195	GLN
3	C	222	GLN
3	C	225	ASN
3	C	267	GLN
3	C	372	HIS
3	C	379	ASN

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Mol	Chain	Res	Type
3	C	442	ASN
3	D	15	HIS
3	D	39	HIS
3	D	68	HIS
3	D	70	HIS
3	D	73	ASN
3	D	115	HIS
3	D	146	GLN
3	D	203	GLN
3	D	222	GLN
3	D	267	GLN
3	D	372	HIS
3	D	379	ASN
3	D	393	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

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Mol	Chain	Res	Type
1	F	905	C
1	F	908	U
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 monosaccharides 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, 95^{th} 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%)	0.29	5 (6%) 16 9	83, 122, 174, 192	0
1	F	74/74 (100%)	0.33	4 (5%) 25 13	55, 88, 139, 152	0
2	A	424/435 (97%)	-0.48	4 (0%) 84 75	7, 33, 81, 113	0
2	B	424/435 (97%)	-0.49	0 100 100	12, 36, 68, 93	0
3	C	485/619 (78%)	-0.07	12 (2%) 57 42	23, 76, 133, 142	0
3	D	522/619 (84%)	-0.43	4 (0%) 86 78	9, 41, 102, 122	0
All	All	2001/2256 (88%)	-0.31	29 (1%) 75 63	7, 46, 127, 192	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	935	U	13.7
3	D	511	LEU	8.4
1	E	934	U	6.5
3	C	359	VAL	6.4
1	E	936	G	5.3
3	C	355	LEU	3.8
1	E	920	A	3.7
3	C	1	MET	3.6
2	A	113	VAL	3.1
3	C	490	ILE	2.7
1	F	920	A	2.7
1	F	917	G	2.7
3	C	277	ILE	2.5
2	A	33	GLY	2.5
2	A	32	GLU	2.5
3	C	2	ASP	2.5
3	C	294	SER	2.4
2	A	111	GLY	2.3
3	D	507	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
3	C	487	THR	2.2
3	C	226	ILE	2.2
3	C	301	VAL	2.2
3	D	535	ASP	2.2
3	D	288	GLU	2.2
3	C	358	ALA	2.1
1	F	926	G	2.1
3	C	356	ARG	2.1
1	F	934	U	2.1
1	E	901	A	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 monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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(Å^2)	Q<0.9
4	ZN	C	900	1/1	1.00	0.14	41,41,41,41	0
4	ZN	D	1900	1/1	1.00	0.13	35,35,35,35	0

6.5 Other polymers (i)

There are no such residues in this entry.