Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:39 AM GMT

PDB ID	:	2DU4
Title	:	Crystal structure of Archaeoglobus fulgidus O-phosphoseryl-tRNA synthetase complexed with tRNACys
Authors	:	Fukunaga, R.
Deposited on	:	2006-07-20
Resolution	:	2.80 Å(reported)

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

The following versions of software and data (see references (1)) were used in the production of this report:

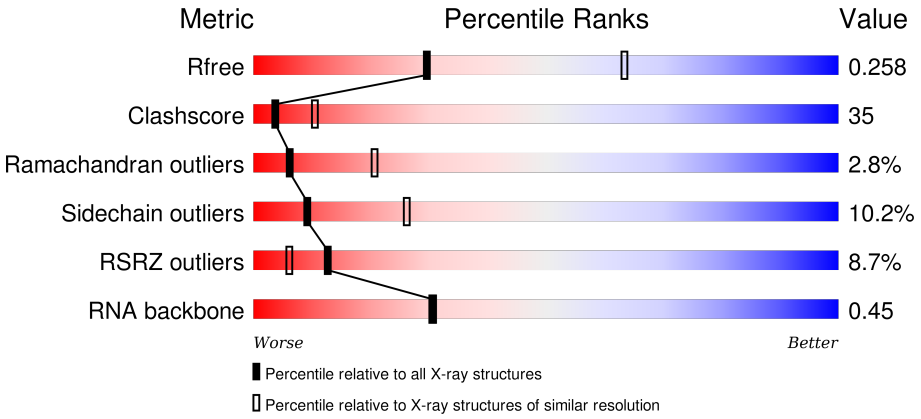
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)
RNA backbone	2183	1091 (3.20-2.40)

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

Mol	Chain	Length	Quality of chain
1	C	71	37% 28% 34% 38%
2	A	534	5% 42% 40% 5% 13%
2	B	534	7% 40% 40% 6% • 13%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9117 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	C	71	Total	C	N	O	P	0	0	0
			1520	675	272	502	71			

- Molecule 2 is a protein called O-phosphoseryl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	466	Total	C	N	O	S	0	0	0
			3777	2440	631	693	13			
2	B	465	Total	C	N	O	S	0	0	0
			3763	2429	630	691	13			

- Molecule 3 is water.

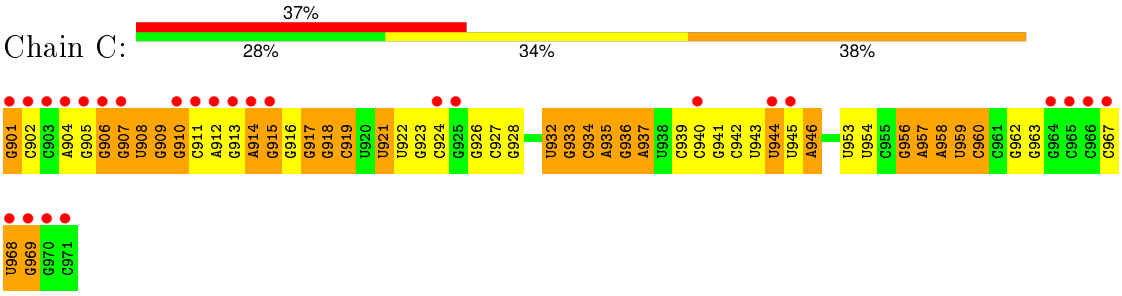
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	26	Total	O	0	0
			26	26		
3	B	31	Total	O	0	0
			31	31		

3 Residue-property plots (i)

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

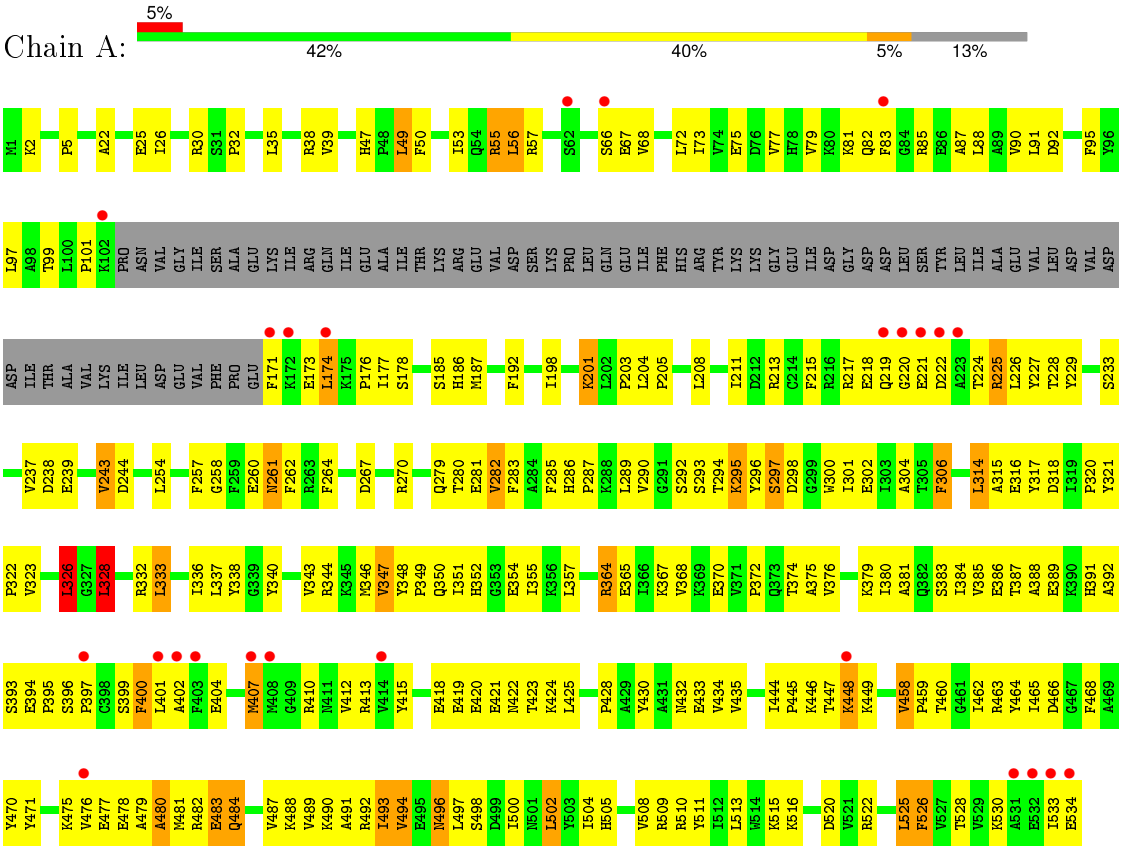
- Molecule 1: tRNA

Chain C:



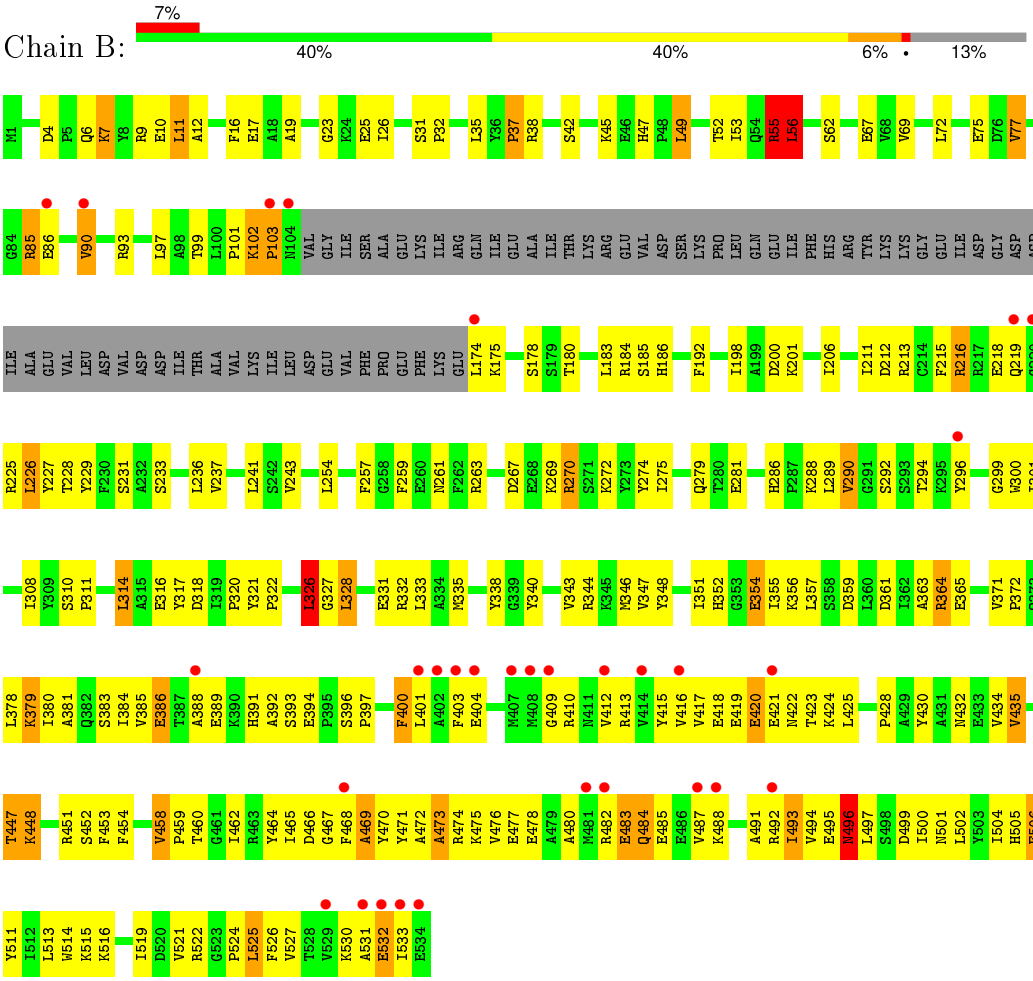
- Molecule 2: O-phosphoseryl-tRNA synthetase

Chain A:



- Molecule 2: O-phosphoseryl-tRNA synthetase

Chain B:


7%
40%
40%
6%
13%
M1 D4 P5 Q6 K7 Y8 R9 E10 L11 A12 F16 E17 A18 A19 G23 K24 E25 I26 S31 P32 L35 Y36 P37 R38 S42 K45 E46 H47 P48 L49 T52 I53 Q54 R55 L56 S62 E67 V68 V69 L72 E75 D76 V77 K80 K81 Q82 F83
G84 R85 E86 V90 R93 L97 A98 T99 L100 P101 K102 P103 N104 VAL GLY ILE SER ALA GLU LYS ILE ARG GLN ILE GLU ALA ILE THR LYS ARG GLU VAL ASP SER LYS PRO LEU GLN GLU ILE PHE HIS ARG TYR LYS LYS GLY GLU ILE ASP GLY ASP ASP LEU SER TYR LEU
ILE ALA GLU VAL LEU ASP VAL ASP ASP ILE THR ALA VAL LYS ILE LEU ASP GLU VAL PHE PRO GLU PHE LYS GLU L174 K175 S178 S179 T180 L183 R184 S185 H186 F192 I198 A199 D200 K201 I206 I211 D212 R213 C214 F215 R216 R217 E218 Q219 G220 E221 D222 A223 T224
R225 L226 Y227 T228 Y229 F230 S231 A232 S233 L236 V237 L241 S242 V243 L254 F257 G258 F259 E260 M261 F262 R263 D267 E268 K269 R270 S271 K272 Y273 Y274 I275 Q279 T280 E281 H286 P287 K288 L289 V290 G291 S292 S293 T294 K295 Y296 G299 W300 I301 E302 I303 A304 T305
I308 Y309 S310 P311 L314 A315 E316 Y317 D318 I319 P320 Y321 P322 L326 G327 L328 E331 R332 L333 A334 M335 Y338 G339 Y340 V343 R344 K345 M346 V347 Y348 I351 H352 G353 E354 I355 K356 L357 S358 D359 L360 D361 I362 A363 R364 E365 V371 P372 Q373 T374 A375 V376 G377
L378 K379 I380 A381 Q382 S383 I384 V385 E386 T387 A388 E389 K390 H391 A392 S393 E394 P395 S396 P397 F400 L401 A402 F403 E404 M407 N408 G409 R410 N411 V412 R413 V414 Y415 V416 V417 E418 E419 E420 E421 N422 T423 K424 L425 P428 A429 Y430 A431 N432 E433 V434 V435 Y442 G443 K446
T447 K448 R451 S452 F453 F454 V458 P459 T460 G461 I462 R463 Y464 I465 D466 G467 F468 A469 Y470 Y471 A472 A473 R474 K475 V476 E477 E478 A479 A480 M481 R482 E483 Q484 E485 E486 V487 K488 A491 R492 I493 V494 E495 N496 L497 S498 D499 I500 N501 L502 Y503 I504 H505 E506 N507 V508 R509 R510
Y511 I512 L513 W514 K515 K516 I519 D520 V521 R522 G523 P524 L525 F526 V527 T528 V529 K530 A531 E532 I533 E534

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α, β, γ	148.43Å 148.43Å 151.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	49.01 – 2.80 49.01 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.01-2.80) 98.6 (49.01-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.207 , 0.269 0.205 , 0.258	Depositor DCC
R_{free} test set	2362 reflections (5.00%)	DCC
Wilson B-factor (Å^2)	81.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 72.7	EDS
Estimated twinning fraction	0.020 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 47199 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9117	wwPDB-VP
Average B, all atoms (Å^2)	98.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	C	0.59	1/1697 (0.1%)	0.81	0/2644
2	A	0.63	0/3865	0.83	2/5218 (0.0%)
2	B	0.64	0/3851	0.85	5/5202 (0.1%)
All	All	0.63	1/9413 (0.0%)	0.84	7/13064 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	A	0	1
2	B	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	901	G	OP3-P	-6.95	1.52	1.61

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	326	LEU	CA-CB-CG	6.70	130.71	115.30
2	B	56	LEU	CA-CB-CG	6.18	129.51	115.30
2	A	326	LEU	CA-CB-CG	5.69	128.38	115.30
2	A	328	LEU	CA-CB-CG	5.65	128.31	115.30
2	B	443	GLY	N-CA-C	-5.48	99.39	113.10
2	B	212	ASP	CB-CG-OD1	5.12	122.91	118.30
2	B	55	ARG	NE-CZ-NH1	-5.07	117.77	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	338	TYR	Sidechain
2	B	274	TYR	Sidechain
2	B	338	TYR	Sidechain
1	C	956	G	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	C	1520	0	769	65	0
2	A	3777	0	3789	278	0
2	B	3763	0	3774	295	0
3	A	26	0	0	4	0
3	B	31	0	0	1	0
All	All	9117	0	8332	613	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 35.

All (613) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:55:ARG:HG2	2:A:55:ARG:HH21	1.10	1.07
2:B:55:ARG:HH21	2:B:55:ARG:HG2	1.18	1.01
2:B:47:HIS:HD2	2:B:49:LEU:H	1.12	0.97
2:B:85:ARG:H	2:B:85:ARG:HD2	1.33	0.94
1:C:942:C:H2'	1:C:943:U:H5'	1.48	0.93
2:B:292:SER:OG	2:B:294:THR:HG22	1.70	0.91
2:A:224:THR:O	2:A:225:ARG:HG3	1.71	0.91
2:B:488:LYS:HG2	2:B:530:LYS:HG2	1.53	0.90
2:A:397:PRO:HD3	2:A:421:GLU:HG2	1.54	0.89
2:A:55:ARG:HG2	2:A:55:ARG:NH2	1.86	0.89
1:C:967:C:H2'	1:C:968:U:O4'	1.73	0.88
2:A:494:VAL:HG21	2:A:500:ILE:HD13	1.55	0.87
2:A:101:PRO:HB3	2:A:177:ILE:HD11	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:SER:O	2:B:424:LYS:HD3	1.75	0.85
2:B:47:HIS:CD2	2:B:49:LEU:H	1.93	0.85
2:A:22:ALA:O	2:A:25:GLU:HG2	1.77	0.85
2:B:391:HIS:O	2:B:425:LEU:HD23	1.77	0.84
2:A:488:LYS:HD3	2:A:530:LYS:HE2	1.59	0.84
2:A:85:ARG:HG3	2:A:85:ARG:HH21	1.43	0.83
2:B:85:ARG:N	2:B:85:ARG:HD2	1.93	0.83
2:B:267:ASP:HB3	2:B:279:GLN:HG2	1.60	0.83
2:B:448:LYS:HD3	2:B:448:LYS:H	1.42	0.82
2:B:55:ARG:NH2	2:B:55:ARG:HG2	1.88	0.81
2:B:286:HIS:HD2	2:B:288:LYS:H	1.26	0.81
2:B:175:LYS:N	2:B:175:LYS:HD2	1.95	0.81
2:A:490:LYS:HB3	2:A:528:THR:HG23	1.61	0.81
2:A:448:LYS:H	2:A:448:LYS:HD3	1.45	0.80
2:B:289:LEU:O	2:B:292:SER:HB2	1.81	0.79
2:B:294:THR:HG23	2:B:296:TYR:H	1.47	0.79
2:A:267:ASP:HB3	2:A:279:GLN:HG2	1.63	0.79
2:A:374:THR:HG22	2:A:376:VAL:H	1.46	0.79
2:B:488:LYS:HE3	2:B:530:LYS:HE3	1.66	0.78
2:A:287:PRO:O	2:A:290:VAL:HG22	1.83	0.78
2:A:504:ILE:HB	2:A:508:VAL:HG21	1.65	0.78
2:B:394:GLU:HG3	2:B:400:PHE:HZ	1.49	0.78
2:A:47:HIS:CD2	2:A:49:LEU:H	2.01	0.78
2:A:430:TYR:HA	2:A:525:LEU:CD2	2.14	0.77
2:B:412:VAL:HG21	2:B:533:ILE:HG22	1.64	0.77
2:A:301:ILE:HD11	2:A:332:ARG:HD3	1.66	0.77
2:B:401:LEU:HD21	2:B:404:GLU:OE2	1.85	0.77
2:A:430:TYR:HA	2:A:525:LEU:HD23	1.67	0.77
1:C:909:G:H5'	1:C:910:G:OP2	1.85	0.77
2:A:434:VAL:O	2:A:460:THR:HG22	1.85	0.77
2:B:460:THR:HG23	2:B:462:ILE:H	1.49	0.76
2:B:448:LYS:CD	2:B:448:LYS:H	1.97	0.75
2:B:385:VAL:HG23	2:B:469:ALA:HB2	1.67	0.75
2:B:504:ILE:HB	2:B:508:VAL:HG21	1.68	0.75
1:C:907:G:H5'	1:C:908:U:OP2	1.86	0.75
2:B:7:LYS:N	2:B:7:LYS:HE2	2.01	0.75
2:B:7:LYS:O	2:B:11:LEU:HB2	1.87	0.74
2:A:430:TYR:HD2	2:A:465:ILE:HG21	1.52	0.74
2:A:391:HIS:HB3	2:A:394:GLU:HG3	1.68	0.74
2:B:464:TYR:HA	2:B:500:ILE:HD11	1.70	0.73
2:B:32:PRO:HA	2:B:35:LEU:HD12	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:VAL:HG21	2:B:530:LYS:NZ	2.03	0.73
2:A:434:VAL:HB	2:A:460:THR:HG21	1.70	0.73
2:A:99:THR:O	2:A:176:PRO:HA	1.89	0.73
2:A:479:ALA:HB2	2:A:487:VAL:HG11	1.70	0.73
2:B:401:LEU:HD13	2:B:415:TYR:CE1	2.24	0.72
2:A:75:GLU:HB3	2:A:77:VAL:HG12	1.71	0.72
2:A:85:ARG:HG3	2:A:85:ARG:NH2	2.03	0.72
2:B:385:VAL:HG23	2:B:469:ALA:CB	2.20	0.72
2:B:504:ILE:HD12	2:B:508:VAL:HG23	1.70	0.72
2:A:56:LEU:HD13	2:A:257:PHE:CZ	2.24	0.72
2:B:101:PRO:O	2:B:103:PRO:HD3	1.89	0.71
1:C:959:U:H5'	1:C:960:C:OP2	1.90	0.71
1:C:927:C:H2'	1:C:928:G:H8	1.55	0.71
2:B:464:TYR:CA	2:B:500:ILE:HD11	2.21	0.71
2:A:478:GLU:HB3	2:A:482:ARG:HH12	1.56	0.71
2:B:496:ASN:HD22	2:B:496:ASN:C	1.94	0.71
2:B:83:PHE:CD2	2:B:90:VAL:HG21	2.25	0.70
2:A:448:LYS:N	2:A:448:LYS:HD3	2.06	0.70
2:A:326:LEU:HD12	2:A:326:LEU:C	2.12	0.70
2:B:55:ARG:HH21	2:B:55:ARG:CG	2.03	0.69
2:B:448:LYS:N	2:B:448:LYS:HD3	2.07	0.69
2:B:374:THR:HG22	2:B:376:VAL:H	1.55	0.69
2:A:430:TYR:O	2:A:465:ILE:HG12	1.92	0.69
2:A:412:VAL:HG13	2:A:533:ILE:HG22	1.72	0.69
2:B:93:ARG:HD2	2:B:216:ARG:HD2	1.75	0.69
1:C:917:G:H2'	1:C:956:G:N2	2.07	0.69
2:B:23:GLY:O	2:B:26:ILE:HG12	1.93	0.69
2:A:401:LEU:HD13	2:A:415:TYR:CE1	2.28	0.69
2:A:219:GLN:HB2	2:A:221:GLU:OE2	1.92	0.69
1:C:933:G:H22	2:A:492:ARG:HD3	1.58	0.69
2:B:326:LEU:HD13	2:B:327:GLY:N	2.09	0.68
2:B:380:ILE:HG22	2:B:381:ALA:N	2.09	0.68
2:A:301:ILE:HD13	2:A:336:ILE:HD11	1.76	0.68
2:A:505:HIS:O	2:A:508:VAL:HG22	1.93	0.68
2:B:451:ARG:HG3	2:B:451:ARG:HH21	1.58	0.68
2:A:47:HIS:HD2	2:A:49:LEU:H	1.40	0.68
2:B:394:GLU:HG3	2:B:400:PHE:CZ	2.28	0.67
2:B:412:VAL:HG13	2:B:532:GLU:O	1.93	0.67
2:A:101:PRO:HD3	2:A:177:ILE:HG13	1.77	0.67
2:B:75:GLU:OE2	2:B:180:THR:HG23	1.94	0.67
1:C:941:G:H2'	1:C:942:C:H5'	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4:ASP:HB3	2:B:7:LYS:HD2	1.76	0.67
2:B:467:GLY:O	2:B:501:ASN:HB3	1.95	0.67
2:A:101:PRO:HB3	2:A:177:ILE:CD1	2.24	0.67
2:A:88:LEU:H	2:A:88:LEU:HD12	1.58	0.66
2:B:506:GLU:HB2	2:B:510:ARG:HH12	1.61	0.66
1:C:957:A:H4'	1:C:958:A:OP1	1.96	0.66
2:B:417:VAL:HG21	2:B:530:LYS:HZ2	1.60	0.66
2:B:420:GLU:HG3	2:B:421:GLU:H	1.61	0.66
2:A:101:PRO:CB	2:A:177:ILE:HD11	2.24	0.66
1:C:935:A:OP2	2:A:428:PRO:HG3	1.95	0.66
2:A:385:VAL:HG13	2:A:465:ILE:HD12	1.78	0.65
1:C:942:C:C2'	1:C:943:U:H5'	2.23	0.65
2:B:241:LEU:HD12	2:B:322:PRO:HB2	1.77	0.65
2:B:47:HIS:HD2	2:B:49:LEU:N	1.91	0.65
2:B:488:LYS:HE3	2:B:530:LYS:CE	2.27	0.65
2:B:290:VAL:HG12	2:B:299:GLY:HA3	1.78	0.65
2:B:412:VAL:HG12	2:B:413:ARG:N	2.12	0.65
2:A:368:VAL:HA	2:A:502:LEU:HD12	1.79	0.65
2:B:372:PRO:HB2	2:B:378:LEU:HD23	1.77	0.65
2:A:376:VAL:HG11	2:A:407:MET:HB3	1.78	0.65
2:A:447:THR:HG22	2:A:449:LYS:H	1.60	0.65
1:C:936:G:N2	2:A:522:ARG:H	1.95	0.64
2:A:368:VAL:HG22	2:A:502:LEU:HD11	1.78	0.64
2:A:475:LYS:HE2	2:A:475:LYS:HA	1.78	0.64
2:B:86:GLU:OE2	2:B:272:LYS:HG2	1.98	0.64
1:C:936:G:HO2'	1:C:937:A:P	2.21	0.64
2:B:286:HIS:CD2	2:B:288:LYS:H	2.12	0.64
2:B:286:HIS:NE2	2:B:288:LYS:HG3	2.13	0.64
2:A:391:HIS:O	2:A:425:LEU:HD23	1.98	0.64
2:B:381:ALA:HB2	2:B:473:ALA:CB	2.28	0.64
2:A:47:HIS:CD2	2:A:49:LEU:HB2	2.33	0.63
1:C:943:U:H2'	1:C:943:U:O2	1.96	0.63
1:C:936:G:H21	2:A:522:ARG:H	1.47	0.63
2:B:412:VAL:HG13	2:B:533:ILE:HA	1.81	0.63
2:A:88:LEU:N	2:A:88:LEU:HD12	2.13	0.63
2:B:224:THR:O	2:B:225:ARG:HG3	1.99	0.63
2:A:101:PRO:O	2:A:174:LEU:HD22	1.99	0.62
2:A:500:ILE:CG2	2:A:502:LEU:HD22	2.29	0.62
2:B:12:ALA:HB2	2:B:19:ALA:CB	2.28	0.62
2:A:447:THR:C	2:A:449:LYS:H	2.03	0.62
2:A:494:VAL:O	2:A:522:ARG:HA	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:902:C:O2	1:C:902:C:H2'	1.99	0.62
2:B:412:VAL:HG12	2:B:413:ARG:H	1.65	0.62
2:A:500:ILE:HG22	2:A:502:LEU:HB2	1.80	0.62
2:A:460:THR:HG23	2:A:462:ILE:H	1.64	0.62
2:B:90:VAL:O	2:B:93:ARG:HG2	1.99	0.62
2:A:413:ARG:HD2	2:A:415:TYR:OH	1.99	0.61
2:A:491:ALA:O	2:A:526:PHE:HA	2.00	0.61
2:B:351:ILE:HG22	2:B:351:ILE:O	1.99	0.61
2:A:500:ILE:HG23	2:A:502:LEU:HD22	1.81	0.61
2:B:396:SER:HB2	2:B:418:GLU:HG3	1.83	0.61
2:A:295:LYS:C	2:A:297:SER:H	2.04	0.61
2:A:320:PRO:HG2	2:A:321:TYR:CD1	2.35	0.61
2:A:32:PRO:O	2:A:38:ARG:NH1	2.34	0.61
1:C:933:G:H22	2:A:492:ARG:CD	2.14	0.61
2:A:380:ILE:O	2:A:384:ILE:HG13	2.01	0.61
1:C:942:C:H2'	1:C:942:C:O2	2.00	0.61
2:A:504:ILE:HB	2:A:508:VAL:CG2	2.30	0.61
2:A:407:MET:O	2:A:407:MET:HG3	2.01	0.60
2:B:496:ASN:ND2	2:B:499:ASP:H	1.99	0.60
2:B:185:SER:O	2:B:229:TYR:OH	2.19	0.60
2:A:410:ARG:CD	2:A:533:ILE:HD12	2.30	0.60
2:A:220:GLY:HA2	2:A:227:TYR:OH	2.01	0.60
2:A:237:VAL:HG22	2:A:323:VAL:HG22	1.83	0.60
1:C:905:G:C2	1:C:906:G:H1'	2.36	0.60
2:B:505:HIS:O	2:B:508:VAL:HG22	2.01	0.60
2:A:432:ASN:O	2:A:463:ARG:HA	2.02	0.60
2:A:47:HIS:HD2	2:A:49:LEU:N	2.00	0.60
2:B:504:ILE:HB	2:B:508:VAL:CG2	2.31	0.60
2:B:183:LEU:HD13	2:B:215:PHE:CG	2.36	0.60
2:B:495:GLU:O	2:B:496:ASN:HB3	2.01	0.60
2:B:77:VAL:O	2:B:81:LYS:HG3	2.02	0.59
2:B:474:ARG:O	2:B:478:GLU:HG3	2.02	0.59
2:B:410:ARG:HH11	2:B:533:ILE:HD12	1.67	0.59
2:B:292:SER:C	2:B:294:THR:H	2.06	0.59
2:B:7:LYS:H	2:B:7:LYS:HE2	1.67	0.59
2:A:509:ARG:HD2	3:A:547:HOH:O	2.00	0.59
2:A:396:SER:HB2	2:A:420:GLU:O	2.03	0.59
2:A:484:GLN:O	2:A:533:ILE:HD11	2.03	0.59
2:B:434:VAL:HB	2:B:460:THR:HG21	1.84	0.59
2:B:7:LYS:O	2:B:11:LEU:CB	2.51	0.59
1:C:934:C:H4'	1:C:935:A:OP2	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:ALA:HA	2:B:533:ILE:HD12	1.85	0.59
1:C:917:G:H2'	1:C:956:G:H22	1.67	0.59
2:A:343:VAL:HG13	2:A:344:ARG:N	2.17	0.59
2:A:326:LEU:C	2:A:326:LEU:CD1	2.70	0.58
1:C:962:G:H2'	1:C:963:G:O4'	2.03	0.58
2:B:328:LEU:HD12	2:B:328:LEU:C	2.23	0.58
2:B:263:ARG:HG2	2:B:300:TRP:CZ3	2.39	0.58
2:A:448:LYS:CD	2:A:448:LYS:H	2.05	0.58
2:A:66:SER:OG	2:B:45:LYS:HE3	2.03	0.58
2:B:510:ARG:NH1	2:B:510:ARG:HB2	2.18	0.58
2:A:423:THR:HG23	2:A:424:LYS:N	2.19	0.58
2:A:185:SER:HA	2:A:215:PHE:O	2.02	0.58
2:B:286:HIS:HD2	2:B:288:LYS:N	1.99	0.58
2:B:465:ILE:HG13	2:B:466:ASP:N	2.19	0.58
2:A:494:VAL:HG12	2:A:522:ARG:HA	1.85	0.57
2:B:340:TYR:CD1	2:B:346:MET:HG3	2.39	0.57
2:B:85:ARG:CA	2:B:85:ARG:HH21	2.18	0.57
2:A:482:ARG:HB2	2:A:484:GLN:HE21	1.69	0.57
2:B:493:ILE:HD12	2:B:493:ILE:O	2.04	0.57
2:A:511:TYR:HB2	2:B:201:LYS:O	2.04	0.57
2:A:351:ILE:HG22	2:A:352:HIS:ND1	2.20	0.57
2:A:222:ASP:O	2:A:344:ARG:HD3	2.04	0.57
2:B:221:GLU:HB2	2:B:224:THR:HB	1.85	0.57
2:A:509:ARG:O	2:A:513:LEU:HD13	2.03	0.57
1:C:932:U:OP1	1:C:932:U:H6	1.87	0.57
2:B:335:MET:SD	2:B:343:VAL:HG22	2.44	0.57
2:B:289:LEU:O	2:B:292:SER:CB	2.51	0.57
2:B:380:ILE:HG12	2:B:403:PHE:CD1	2.39	0.57
2:B:192:PHE:HE2	2:B:314:LEU:HD13	1.70	0.57
2:A:480:ALA:HA	2:A:533:ILE:HD13	1.87	0.57
2:A:364:ARG:O	2:A:364:ARG:HG3	2.05	0.57
2:A:101:PRO:CG	2:A:177:ILE:HD11	2.35	0.57
2:B:303:ILE:O	2:B:303:ILE:HG13	2.05	0.56
2:B:47:HIS:CD2	2:B:49:LEU:HB2	2.41	0.56
2:A:301:ILE:CD1	2:A:332:ARG:HD3	2.35	0.56
2:B:468:PHE:O	2:B:471:TYR:N	2.38	0.56
2:B:506:GLU:O	2:B:510:ARG:NH1	2.39	0.56
2:B:468:PHE:CE2	2:B:491:ALA:HB2	2.40	0.56
2:A:395:PRO:HA	2:A:423:THR:O	2.05	0.56
2:A:218:GLU:HA	2:A:218:GLU:OE2	2.06	0.56
2:B:420:GLU:HG3	2:B:421:GLU:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:482:ARG:C	2:B:484:GLN:H	2.09	0.56
2:B:412:VAL:CG2	2:B:533:ILE:HG22	2.33	0.56
2:B:101:PRO:O	2:B:103:PRO:CD	2.54	0.56
2:B:343:VAL:HG23	3:B:549:HOH:O	2.06	0.56
2:A:292:SER:OG	2:A:294:THR:HG22	2.06	0.55
2:A:261:ASN:HD22	2:A:262:PHE:H	1.55	0.55
2:B:460:THR:CG2	2:B:462:ILE:H	2.16	0.55
1:C:926:G:H2'	1:C:927:C:C6	2.41	0.55
1:C:936:G:O2'	2:A:522:ARG:NH1	2.39	0.55
2:A:447:THR:HG22	2:A:449:LYS:N	2.21	0.55
2:B:404:GLU:HG2	2:B:413:ARG:HG2	1.89	0.55
2:B:381:ALA:HB2	2:B:473:ALA:HB3	1.89	0.55
2:B:397:PRO:HB3	2:B:419:GLU:HA	1.88	0.55
2:A:430:TYR:HD2	2:A:465:ILE:CG2	2.17	0.55
1:C:957:A:O2'	1:C:958:A:O5'	2.24	0.55
2:B:75:GLU:HB3	2:B:77:VAL:HG12	1.89	0.55
2:B:10:GLU:O	2:B:12:ALA:N	2.39	0.55
2:A:407:MET:HE1	2:A:476:VAL:HG23	1.89	0.54
2:B:301:ILE:HD11	2:B:332:ARG:HD3	1.88	0.54
2:A:292:SER:C	2:A:294:THR:H	2.11	0.54
2:A:497:LEU:HB3	2:A:502:LEU:O	2.07	0.54
2:B:484:GLN:O	2:B:533:ILE:HD11	2.07	0.54
2:A:394:GLU:HG3	2:A:400:PHE:CZ	2.43	0.54
2:B:519:ILE:HG22	2:B:521:VAL:HG23	1.89	0.54
2:B:428:PRO:HD2	2:B:524:PRO:HB2	1.90	0.54
2:A:368:VAL:HG22	2:A:502:LEU:CD1	2.38	0.54
2:A:376:VAL:HG11	2:A:407:MET:CB	2.37	0.54
2:B:430:TYR:HD2	2:B:465:ILE:HG21	1.73	0.54
2:A:264:PHE:HB3	2:A:280:THR:CG2	2.38	0.54
2:B:493:ILE:CD1	2:B:493:ILE:O	2.56	0.54
2:B:32:PRO:O	2:B:38:ARG:NH1	2.41	0.54
2:B:81:LYS:HB3	2:B:316:GLU:HG2	1.89	0.54
2:A:365:GLU:HG2	3:A:551:HOH:O	2.08	0.54
2:B:471:TYR:CZ	2:B:475:LYS:HE3	2.42	0.53
2:A:400:PHE:CD2	2:A:400:PHE:N	2.77	0.53
2:B:388:ALA:O	2:B:392:ALA:HB2	2.09	0.53
2:A:496:ASN:ND2	2:A:498:SER:HB3	2.23	0.53
2:B:494:VAL:O	2:B:522:ARG:HA	2.09	0.53
2:B:419:GLU:O	2:B:420:GLU:O	2.25	0.53
2:B:491:ALA:HB3	2:B:527:VAL:O	2.08	0.53
2:B:328:LEU:HD12	2:B:328:LEU:O	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:222:ASP:OD1	2:B:344:ARG:HD2	2.08	0.53
2:B:410:ARG:O	2:B:412:VAL:HG23	2.09	0.53
1:C:968:U:H2'	1:C:969:G:C8	2.43	0.53
2:A:264:PHE:HB3	2:A:280:THR:HG21	1.91	0.53
1:C:941:G:C2'	1:C:942:C:H5'	2.38	0.53
2:A:478:GLU:HB3	2:A:482:ARG:NH1	2.23	0.53
2:A:50:PHE:CE1	2:B:69:VAL:HG22	2.44	0.53
2:A:213:ARG:HG2	2:A:213:ARG:HH21	1.74	0.53
2:A:221:GLU:OE2	2:A:224:THR:HB	2.08	0.52
2:A:475:LYS:CA	2:A:475:LYS:HE2	2.39	0.52
2:B:10:GLU:C	2:B:12:ALA:H	2.11	0.52
1:C:918:G:O2'	1:C:919:C:OP1	2.22	0.52
2:A:347:VAL:CG2	2:A:348:TYR:CD2	2.91	0.52
2:B:432:ASN:HB2	2:B:464:TYR:CD1	2.44	0.52
2:B:388:ALA:HB2	2:B:416:VAL:HG11	1.90	0.52
2:B:37:PRO:O	2:B:364:ARG:HD3	2.09	0.52
2:B:492:ARG:HB3	2:B:526:PHE:CE2	2.45	0.52
2:B:415:TYR:N	2:B:530:LYS:O	2.32	0.52
2:A:381:ALA:O	2:A:385:VAL:HG23	2.08	0.52
2:B:218:GLU:HG3	2:B:225:ARG:HD2	1.91	0.52
2:A:343:VAL:CG1	2:A:344:ARG:N	2.72	0.52
2:B:428:PRO:HD2	2:B:524:PRO:CG	2.39	0.52
2:B:386:GLU:O	2:B:389:GLU:HB2	2.10	0.52
2:A:83:PHE:CE2	2:A:90:VAL:HG21	2.45	0.52
1:C:913:G:H21	1:C:921:U:H5	1.58	0.52
1:C:959:U:H5"	1:C:960:C:H5	1.75	0.52
2:A:387:THR:HG21	2:A:402:ALA:HA	1.91	0.52
2:B:85:ARG:HA	2:B:85:ARG:HH21	1.74	0.52
2:B:32:PRO:HA	2:B:35:LEU:CD1	2.38	0.52
2:A:404:GLU:HA	2:A:412:VAL:O	2.10	0.51
2:B:286:HIS:CD2	2:B:288:LYS:HG3	2.46	0.51
2:B:347:VAL:HG12	2:B:348:TYR:CD2	2.45	0.51
1:C:936:G:HO2'	2:A:522:ARG:NH1	2.08	0.51
2:A:494:VAL:CG2	2:A:500:ILE:HD13	2.35	0.51
2:B:185:SER:HB2	2:B:216:ARG:HD3	1.92	0.51
2:B:506:GLU:CB	2:B:510:ARG:HH12	2.23	0.51
2:B:222:ASP:CG	2:B:344:ARG:HD2	2.31	0.51
2:A:213:ARG:HH21	2:A:228:THR:CG2	2.23	0.51
1:C:909:G:C5'	1:C:910:G:OP2	2.56	0.51
2:B:359:ASP:HB3	2:B:458:VAL:HG13	1.92	0.51
2:A:282:VAL:HG13	2:A:304:ALA:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:488:LYS:HD3	2:A:530:LYS:CE	2.37	0.51
1:C:957:A:O2'	1:C:958:A:H3'	2.10	0.51
2:A:53:ILE:O	2:A:57:ARG:HG3	2.10	0.51
2:B:442:TYR:CE2	2:B:453:PHE:HE2	2.28	0.51
2:B:224:THR:HG22	2:B:225:ARG:N	2.25	0.51
2:A:511:TYR:CE1	2:A:515:LYS:HG3	2.46	0.51
2:B:259:PHE:CE2	2:B:286:HIS:HB2	2.45	0.50
2:A:479:ALA:C	2:A:481:MET:H	2.14	0.50
2:A:410:ARG:HD3	2:A:533:ILE:HD12	1.93	0.50
2:B:465:ILE:HG13	2:B:466:ASP:H	1.75	0.50
2:B:491:ALA:O	2:B:526:PHE:HA	2.12	0.50
2:B:56:LEU:HB3	2:B:211:ILE:CD1	2.41	0.50
2:B:510:ARG:HB2	2:B:510:ARG:HH11	1.75	0.50
2:A:370:GLU:HA	3:A:554:HOH:O	2.11	0.50
2:A:187:MET:HG2	2:A:233:SER:HB3	1.93	0.50
2:A:326:LEU:HD12	2:A:326:LEU:O	2.11	0.50
2:B:412:VAL:HG13	2:B:532:GLU:C	2.30	0.50
2:A:85:ARG:HH21	2:A:85:ARG:CG	2.19	0.50
2:B:263:ARG:HG2	2:B:300:TRP:CH2	2.46	0.50
2:A:494:VAL:HG21	2:A:500:ILE:CD1	2.36	0.50
2:B:447:THR:HG22	2:B:448:LYS:HE2	1.94	0.50
1:C:908:U:H5"	1:C:909:G:OP1	2.12	0.50
2:A:434:VAL:HB	2:A:460:THR:CG2	2.39	0.50
2:B:294:THR:HG23	2:B:296:TYR:N	2.23	0.50
2:B:482:ARG:O	2:B:484:GLN:N	2.44	0.50
2:A:260:GLU:OE2	2:A:287:PRO:HG2	2.12	0.50
2:A:418:GLU:HB2	2:A:425:LEU:HA	1.94	0.50
2:B:496:ASN:ND2	2:B:496:ASN:C	2.64	0.50
2:B:396:SER:HB3	2:B:418:GLU:HG2	1.92	0.50
2:A:315:ALA:O	2:A:317:TYR:N	2.45	0.50
2:A:289:LEU:HD22	2:A:296:TYR:HB2	1.94	0.50
2:B:497:LEU:O	2:B:500:ILE:HG22	2.11	0.49
2:A:511:TYR:CZ	2:A:515:LYS:HG3	2.46	0.49
2:A:460:THR:HG23	2:A:462:ILE:N	2.26	0.49
2:A:496:ASN:HD21	2:A:498:SER:HB3	1.77	0.49
2:A:173:GLU:O	2:A:174:LEU:O	2.30	0.49
2:B:497:LEU:HG	2:B:521:VAL:HG21	1.94	0.49
2:A:376:VAL:O	2:A:380:ILE:HG13	2.13	0.49
2:B:464:TYR:O	2:B:500:ILE:HD11	2.13	0.49
1:C:917:G:O2'	1:C:918:G:O5'	2.30	0.49
2:B:381:ALA:HB2	2:B:473:ALA:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:914:A:H2'	1:C:915:G:O4'	2.12	0.49
2:B:377:GLY:HA3	2:B:477:GLU:OE1	2.12	0.49
2:B:496:ASN:HD21	2:B:499:ASP:H	1.60	0.49
2:B:77:VAL:HA	2:B:80:LYS:HD2	1.94	0.49
2:A:201:LYS:HD3	2:B:514:TRP:CG	2.48	0.49
2:B:378:LEU:O	2:B:380:ILE:N	2.46	0.49
2:A:464:TYR:N	2:A:464:TYR:CD1	2.79	0.48
2:B:504:ILE:HD11	2:B:509:ARG:HB2	1.95	0.48
2:B:383:SER:O	2:B:386:GLU:N	2.46	0.48
2:A:75:GLU:OE2	2:A:75:GLU:HA	2.13	0.48
1:C:934:C:H5"	1:C:935:A:O5'	2.14	0.48
2:A:258:GLY:HA3	2:A:286:HIS:HE1	1.79	0.48
2:A:203:PRO:CG	2:B:357:LEU:HD11	2.43	0.48
2:B:409:GLY:O	2:B:410:ARG:HG2	2.12	0.48
1:C:944:U:O2	1:C:946:A:H5'	2.14	0.48
2:A:394:GLU:HG3	2:A:400:PHE:HZ	1.76	0.48
2:B:464:TYR:HA	2:B:500:ILE:CD1	2.41	0.48
2:A:477:GLU:O	2:A:481:MET:HE2	2.13	0.48
1:C:916:G:H2'	1:C:959:U:O2'	2.14	0.48
2:B:383:SER:O	2:B:384:ILE:C	2.52	0.48
2:B:488:LYS:HG2	2:B:530:LYS:CG	2.34	0.48
2:B:391:HIS:HB3	2:B:400:PHE:CZ	2.49	0.48
2:B:446:LYS:HG3	2:B:454:PHE:CE2	2.49	0.47
2:A:347:VAL:HG22	2:A:348:TYR:CD2	2.49	0.47
2:A:346:MET:CE	2:A:347:VAL:HG12	2.43	0.47
2:A:464:TYR:HB3	2:A:500:ILE:HD11	1.96	0.47
2:B:340:TYR:CG	2:B:346:MET:HG3	2.49	0.47
2:B:31:SER:HB2	2:B:32:PRO:HD2	1.95	0.47
2:B:267:ASP:HB2	2:B:281:GLU:HG3	1.97	0.47
1:C:922:U:H2'	1:C:923:G:C8	2.49	0.47
2:A:95:PHE:HD2	2:B:97:LEU:HB3	1.80	0.47
2:B:448:LYS:HA	2:B:451:ARG:HG2	1.96	0.47
2:A:447:THR:C	2:A:449:LYS:N	2.67	0.47
2:B:213:ARG:HD3	2:B:228:THR:HG21	1.96	0.47
2:A:30:ARG:HB2	2:A:35:LEU:CD1	2.44	0.47
2:A:198:ILE:HG22	2:B:355:ILE:HG21	1.96	0.47
2:B:311:PRO:HA	2:B:314:LEU:HB2	1.96	0.47
2:A:430:TYR:HB2	2:A:465:ILE:HG23	1.96	0.47
2:A:482:ARG:C	2:A:484:GLN:H	2.17	0.47
2:A:483:GLU:O	2:A:484:GLN:O	2.33	0.47
2:A:204:LEU:HD23	2:A:239:GLU:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:496:ASN:C	2:A:496:ASN:HD22	2.19	0.47
2:A:494:VAL:O	2:A:494:VAL:HG12	2.14	0.47
2:A:72:LEU:HD21	2:A:215:PHE:HE1	1.80	0.47
2:A:83:PHE:CD2	2:A:90:VAL:HG21	2.50	0.47
2:A:192:PHE:HE2	2:A:314:LEU:CD1	2.28	0.47
1:C:911:C:C4	1:C:912:A:N7	2.83	0.46
2:A:224:THR:O	2:A:225:ARG:CG	2.55	0.46
2:B:478:GLU:O	2:B:482:ARG:NH2	2.48	0.46
2:B:412:VAL:HG22	2:B:533:ILE:HA	1.97	0.46
2:A:388:ALA:O	2:A:392:ALA:HB2	2.15	0.46
2:B:397:PRO:HB3	2:B:419:GLU:O	2.15	0.46
2:B:10:GLU:C	2:B:12:ALA:N	2.68	0.46
2:B:451:ARG:HH21	2:B:451:ARG:CG	2.28	0.46
2:A:267:ASP:HB2	2:A:281:GLU:HG3	1.97	0.46
2:A:238:ASP:O	2:A:322:PRO:HD2	2.15	0.46
2:A:493:ILE:H	2:A:493:ILE:HD12	1.80	0.46
2:B:6:GLN:HG2	2:B:9:ARG:HH11	1.79	0.46
2:B:332:ARG:HB2	2:B:332:ARG:HE	1.43	0.46
2:B:290:VAL:HG12	2:B:299:GLY:CA	2.46	0.46
2:B:363:ALA:HB2	2:B:458:VAL:HG22	1.97	0.46
2:B:434:VAL:O	2:B:460:THR:HG22	2.15	0.46
2:B:213:ARG:HH21	2:B:228:THR:CG2	2.29	0.46
2:A:458:VAL:HA	2:A:459:PRO:HD3	1.71	0.46
2:A:82:GLN:CD	2:A:192:PHE:CD1	2.89	0.46
2:A:221:GLU:OE2	2:A:224:THR:CB	2.63	0.46
2:A:88:LEU:CD1	2:A:88:LEU:H	2.25	0.46
2:A:295:LYS:C	2:A:297:SER:N	2.68	0.46
2:B:183:LEU:HD13	2:B:215:PHE:CD1	2.50	0.46
2:B:378:LEU:C	2:B:380:ILE:N	2.69	0.46
1:C:904:A:H2'	1:C:905:G:C8	2.51	0.46
1:C:916:G:O5'	1:C:916:G:H8	1.98	0.46
2:B:351:ILE:O	2:B:351:ILE:CG2	2.62	0.46
2:A:39:VAL:O	2:A:364:ARG:NH2	2.49	0.46
2:A:82:GLN:CD	2:A:192:PHE:HD1	2.19	0.46
2:B:417:VAL:HG21	2:B:530:LYS:HZ3	1.77	0.45
2:A:349:PRO:HG2	2:A:350:GLN:OE1	2.16	0.45
2:B:174:LEU:HB3	2:B:175:LYS:H	1.55	0.45
2:A:407:MET:CE	2:A:476:VAL:HG23	2.46	0.45
2:A:47:HIS:H	2:B:67:GLU:HB3	1.82	0.45
1:C:907:G:C5'	1:C:908:U:OP2	2.59	0.45
2:B:468:PHE:O	2:B:470:TYR:N	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:376:VAL:HA	2:B:379:LYS:HE3	1.99	0.45
2:A:468:PHE:O	2:A:471:TYR:N	2.49	0.45
2:B:16:PHE:O	2:B:19:ALA:N	2.50	0.45
2:A:468:PHE:CD2	2:A:491:ALA:HB2	2.52	0.45
2:A:68:VAL:HG21	2:A:208:LEU:HD13	1.98	0.45
2:A:243:VAL:HG22	2:A:306:PHE:HE1	1.81	0.45
2:A:47:HIS:CE1	2:A:347:VAL:HA	2.51	0.45
1:C:902:C:O2	1:C:902:C:C2'	2.65	0.45
1:C:922:U:H2'	1:C:923:G:H8	1.80	0.45
2:B:259:PHE:CD2	2:B:286:HIS:HB2	2.52	0.45
2:B:174:LEU:HD23	2:B:175:LYS:NZ	2.32	0.45
2:B:460:THR:HG23	2:B:462:ILE:N	2.26	0.45
2:A:404:GLU:HG3	2:A:413:ARG:CG	2.46	0.45
1:C:904:A:H2'	1:C:905:G:H8	1.81	0.45
2:B:301:ILE:HG12	2:B:302:GLU:N	2.31	0.45
2:A:466:ASP:O	2:A:470:TYR:CD2	2.69	0.45
2:A:298:ASP:OD2	2:A:298:ASP:N	2.49	0.45
2:A:333:LEU:HD22	2:A:337:LEU:HG	1.99	0.45
2:B:483:GLU:O	2:B:484:GLN:O	2.33	0.45
2:B:72:LEU:HA	2:B:184:ARG:HG2	1.98	0.45
2:B:404:GLU:HA	2:B:412:VAL:O	2.17	0.45
2:A:283:PHE:CE1	2:A:302:GLU:HB2	2.52	0.45
2:A:217:ARG:HH22	2:B:102:LYS:HZ2	1.64	0.45
2:B:85:ARG:CD	2:B:85:ARG:N	2.73	0.45
2:B:292:SER:C	2:B:294:THR:N	2.71	0.45
2:B:434:VAL:HB	2:B:460:THR:CG2	2.47	0.45
2:A:500:ILE:HG23	2:A:500:ILE:O	2.16	0.44
2:A:448:LYS:CD	2:A:448:LYS:N	2.75	0.44
2:B:396:SER:CB	2:B:418:GLU:HG3	2.47	0.44
2:B:225:ARG:HH21	2:B:225:ARG:HG3	1.82	0.44
2:A:515:LYS:O	2:A:516:LYS:HB2	2.17	0.44
2:A:79:VAL:HG21	2:A:91:LEU:HD21	1.99	0.44
2:A:488:LYS:HD3	2:A:530:LYS:HG2	1.99	0.44
2:A:383:SER:O	2:A:387:THR:HG23	2.17	0.44
2:A:328:LEU:HD12	2:A:328:LEU:C	2.37	0.44
2:B:218:GLU:OE2	2:B:218:GLU:HA	2.17	0.44
2:A:286:HIS:HB3	2:A:289:LEU:HD12	1.99	0.44
1:C:936:G:H21	2:A:522:ARG:N	2.12	0.44
2:B:7:LYS:CA	2:B:7:LYS:HE2	2.47	0.44
2:A:410:ARG:HB2	2:A:534:GLU:OXT	2.17	0.44
2:A:384:ILE:O	2:A:388:ALA:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:492:ARG:HB3	2:B:526:PHE:HE2	1.83	0.44
2:B:501:ASN:O	2:B:502:LEU:HD12	2.17	0.44
2:A:239:GLU:HG2	2:A:321:TYR:CE2	2.52	0.44
2:B:435:VAL:HB	2:B:459:PRO:HA	1.99	0.44
2:A:433:GLU:N	2:A:444:ILE:O	2.44	0.44
2:B:432:ASN:HB3	2:B:464:TYR:CE1	2.52	0.44
2:A:282:VAL:HG13	2:A:304:ALA:C	2.38	0.44
2:B:85:ARG:HH21	2:B:85:ARG:N	2.16	0.44
2:A:171:PHE:O	2:A:174:LEU:HG	2.18	0.44
1:C:908:U:OP2	1:C:908:U:H6	2.01	0.44
1:C:957:A:H1'	1:C:959:U:C5	2.53	0.44
2:B:275:ILE:HG13	2:B:310:SER:HA	1.99	0.44
2:A:55:ARG:NH2	2:A:55:ARG:CG	2.66	0.44
2:B:174:LEU:C	2:B:175:LYS:HD2	2.36	0.44
2:A:306:PHE:CD1	2:A:306:PHE:C	2.90	0.44
2:A:101:PRO:HD3	2:A:177:ILE:CG1	2.48	0.43
2:A:315:ALA:C	2:A:317:TYR:H	2.21	0.43
2:B:391:HIS:CG	2:B:400:PHE:CE1	3.06	0.43
2:A:347:VAL:CG2	2:A:348:TYR:CE2	3.01	0.43
2:A:203:PRO:HG3	2:B:357:LEU:HD11	1.99	0.43
1:C:912:A:H1'	1:C:923:G:N2	2.33	0.43
2:A:430:TYR:HA	2:A:525:LEU:HD21	1.95	0.43
2:A:228:THR:HG22	2:A:229:TYR:N	2.33	0.43
2:A:213:ARG:HH21	2:A:228:THR:HG21	1.83	0.43
2:A:410:ARG:NE	2:A:533:ILE:HD12	2.33	0.43
2:B:294:THR:HG21	2:B:296:TYR:CD1	2.54	0.43
2:A:399:SER:C	2:A:400:PHE:CD2	2.92	0.43
2:B:487:VAL:O	2:B:488:LYS:HG3	2.19	0.43
2:B:4:ASP:CB	2:B:7:LYS:HD2	2.45	0.43
2:B:331:GLU:O	2:B:335:MET:HG3	2.18	0.43
2:B:303:ILE:HD12	2:B:332:ARG:HG2	2.00	0.43
2:B:428:PRO:HD2	2:B:524:PRO:CB	2.48	0.43
2:B:347:VAL:CG1	2:B:348:TYR:CE2	3.02	0.43
2:B:52:THR:O	2:B:53:ILE:C	2.56	0.43
2:B:56:LEU:HD13	2:B:257:PHE:CZ	2.54	0.43
2:A:509:ARG:NH1	3:A:535:HOH:O	2.50	0.43
1:C:939:C:H2'	1:C:940:C:C6	2.54	0.43
2:B:211:ILE:HA	2:B:231:SER:O	2.19	0.43
2:B:380:ILE:HG22	2:B:473:ALA:HB2	2.01	0.43
2:A:481:MET:C	2:A:483:GLU:H	2.21	0.43
2:B:374:THR:HG22	2:B:376:VAL:N	2.29	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:285:PHE:HB2	2:A:300:TRP:CZ2	2.53	0.43
1:C:953:U:C4	1:C:954:U:C4	3.07	0.43
2:B:413:ARG:O	2:B:531:ALA:HA	2.19	0.43
1:C:906:G:H2'	1:C:906:G:N3	2.34	0.43
2:A:510:ARG:HE	2:B:200:ASP:HB2	1.84	0.43
2:B:55:ARG:HB3	2:B:257:PHE:HE1	1.83	0.42
2:B:383:SER:HA	2:B:386:GLU:HB3	2.01	0.42
2:B:412:VAL:CG1	2:B:413:ARG:N	2.81	0.42
2:A:464:TYR:HD1	2:A:464:TYR:N	2.16	0.42
2:B:451:ARG:NH2	2:B:451:ARG:HG3	2.31	0.42
2:A:385:VAL:O	2:A:389:GLU:HG3	2.19	0.42
2:B:475:LYS:HA	2:B:475:LYS:HD3	1.89	0.42
2:A:404:GLU:HG3	2:A:413:ARG:HG3	2.01	0.42
2:A:2:LYS:HB2	2:A:2:LYS:HE3	1.70	0.42
2:B:447:THR:CG2	2:B:448:LYS:HE2	2.49	0.42
2:A:290:VAL:O	2:A:290:VAL:HG23	2.20	0.42
2:A:479:ALA:CB	2:A:487:VAL:HG11	2.45	0.42
2:A:468:PHE:CE2	2:A:491:ALA:HB2	2.55	0.42
2:B:31:SER:CB	2:B:32:PRO:HD2	2.48	0.42
2:A:383:SER:HA	2:A:386:GLU:HB3	2.01	0.42
2:B:347:VAL:HG11	2:B:348:TYR:CE2	2.54	0.42
2:B:56:LEU:HD13	2:B:257:PHE:CE2	2.54	0.42
2:A:218:GLU:HG3	2:A:225:ARG:CB	2.50	0.42
2:A:397:PRO:HD3	2:A:421:GLU:CG	2.38	0.42
2:A:340:TYR:CG	2:A:346:MET:HG3	2.55	0.42
2:A:364:ARG:O	2:A:367:LYS:HE2	2.19	0.42
2:B:511:TYR:CZ	2:B:515:LYS:HG3	2.55	0.42
2:A:346:MET:HE1	2:A:347:VAL:HG12	2.00	0.42
2:B:269:LYS:O	2:B:270:ARG:C	2.58	0.42
2:A:500:ILE:HA	2:A:500:ILE:HD12	1.85	0.42
2:A:497:LEU:HD22	2:A:502:LEU:HB3	2.02	0.42
2:A:315:ALA:C	2:A:317:TYR:N	2.73	0.42
2:B:513:LEU:O	2:B:516:LYS:N	2.49	0.42
2:B:380:ILE:O	2:B:383:SER:N	2.51	0.42
2:B:281:GLU:HA	2:B:305:THR:HG22	2.01	0.42
2:A:445:PRO:O	2:A:447:THR:N	2.53	0.42
2:B:12:ALA:HB2	2:B:19:ALA:HB1	2.01	0.42
2:B:364:ARG:HG3	2:B:364:ARG:O	2.18	0.42
1:C:923:G:O2'	1:C:924:C:H5'	2.20	0.42
2:B:361:ASP:O	2:B:365:GLU:HG2	2.19	0.42
2:B:206:ILE:HB	2:B:237:VAL:HB	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:419:GLU:OE2	2:A:530:LYS:NZ	2.53	0.42
2:A:88:LEU:CD1	2:A:88:LEU:N	2.82	0.42
2:A:494:VAL:HG12	2:A:522:ARG:CA	2.49	0.42
2:B:400:PHE:N	2:B:400:PHE:CD2	2.87	0.42
2:A:292:SER:O	2:A:294:THR:N	2.52	0.42
2:B:458:VAL:HA	2:B:459:PRO:HD3	1.77	0.42
2:A:92:ASP:O	2:A:217:ARG:HD3	2.20	0.42
2:B:56:LEU:HB3	2:B:211:ILE:HD11	2.01	0.41
2:A:500:ILE:CG2	2:A:502:LEU:HB2	2.48	0.41
2:A:396:SER:HB3	2:A:418:GLU:HG2	2.02	0.41
2:B:218:GLU:C	2:B:219:GLN:HG2	2.41	0.41
2:A:53:ILE:HG23	2:A:211:ILE:HG21	2.02	0.41
1:C:944:U:H2'	1:C:946:A:OP1	2.20	0.41
2:A:67:GLU:HB3	2:B:47:HIS:HB2	2.01	0.41
2:B:403:PHE:CG	2:B:404:GLU:N	2.87	0.41
2:B:394:GLU:HA	2:B:394:GLU:OE2	2.20	0.41
1:C:909:G:C4'	1:C:910:G:OP2	2.68	0.41
2:A:95:PHE:CD2	2:B:97:LEU:HB3	2.55	0.41
2:B:401:LEU:HA	2:B:415:TYR:CD1	2.55	0.41
2:A:464:TYR:HA	2:A:500:ILE:HG13	2.02	0.41
2:A:520:ASP:OD1	2:A:522:ARG:NH2	2.52	0.41
2:A:401:LEU:CD1	2:A:415:TYR:CE1	3.00	0.41
2:A:201:LYS:O	2:B:511:TYR:HB2	2.20	0.41
2:B:378:LEU:C	2:B:380:ILE:H	2.23	0.41
2:B:525:LEU:HD22	2:B:527:VAL:CG1	2.51	0.41
2:B:371:VAL:HA	2:B:372:PRO:HD3	1.89	0.41
1:C:917:G:O2'	1:C:918:G:P	2.79	0.41
2:A:292:SER:C	2:A:294:THR:N	2.73	0.41
2:A:375:ALA:O	2:A:379:LYS:HG3	2.20	0.41
2:B:352:HIS:O	2:B:354:GLU:OE1	2.38	0.41
2:A:218:GLU:HG3	2:A:225:ARG:HD2	2.01	0.41
2:B:451:ARG:O	2:B:452:SER:C	2.59	0.41
2:A:176:PRO:HB2	2:B:178:SER:CB	2.50	0.41
2:A:479:ALA:O	2:A:481:MET:N	2.54	0.41
2:A:393:SER:HA	2:A:424:LYS:CD	2.50	0.41
2:B:317:TYR:O	2:B:318:ASP:HB2	2.20	0.41
2:B:192:PHE:CE2	2:B:314:LEU:HD13	2.52	0.41
2:B:226:LEU:CD2	2:B:344:ARG:HG2	2.51	0.41
1:C:901:G:N3	1:C:901:G:H2'	2.35	0.41
2:B:403:PHE:O	2:B:404:GLU:HG3	2.20	0.41
2:B:401:LEU:HA	2:B:415:TYR:HD1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:85:ARG:C	2:A:87:ALA:N	2.73	0.41
1:C:933:G:H3'	1:C:933:G:C8	2.55	0.41
2:B:468:PHE:O	2:B:469:ALA:C	2.59	0.41
2:A:394:GLU:CG	2:A:400:PHE:HZ	2.34	0.41
2:B:432:ASN:O	2:B:464:TYR:HD1	2.04	0.41
2:A:77:VAL:O	2:A:81:LYS:HG3	2.20	0.41
2:A:432:ASN:O	2:A:463:ARG:CA	2.68	0.41
1:C:911:C:H2'	1:C:912:A:O4'	2.21	0.41
1:C:936:G:O2'	1:C:937:A:P	2.75	0.41
2:B:432:ASN:CB	2:B:464:TYR:CD1	3.04	0.41
2:A:239:GLU:O	2:A:322:PRO:HG3	2.20	0.41
2:A:72:LEU:HD21	2:A:215:PHE:CE1	2.56	0.40
2:B:320:PRO:HG2	2:B:321:TYR:CE1	2.56	0.40
2:A:73:ILE:CD1	2:B:227:TYR:HB3	2.51	0.40
2:A:101:PRO:HG3	2:A:177:ILE:HD11	2.02	0.40
2:A:490:LYS:CD	2:A:492:ARG:HH12	2.35	0.40
2:B:472:ALA:O	2:B:475:LYS:N	2.50	0.40
2:A:400:PHE:CE2	2:A:425:LEU:HD22	2.56	0.40
2:B:396:SER:HA	2:B:397:PRO:HA	1.73	0.40
2:A:55:ARG:HH21	2:A:55:ARG:CG	1.99	0.40
2:A:492:ARG:HH11	2:A:492:ARG:CG	2.34	0.40
2:B:464:TYR:C	2:B:500:ILE:HD11	2.42	0.40
2:A:401:LEU:HA	2:A:415:TYR:CD1	2.56	0.40
2:A:355:ILE:HG21	2:B:198:ILE:HG22	2.04	0.40
1:C:957:A:H1'	1:C:959:U:H5	1.87	0.40
2:B:374:THR:HG22	2:B:375:ALA:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	A	462/534 (86%)	403 (87%)	48 (10%)	11 (2%)	7 25
2	B	461/534 (86%)	399 (87%)	47 (10%)	15 (3%)	5 16
All	All	923/1068 (86%)	802 (87%)	95 (10%)	26 (3%)	6 21

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	174	LEU
2	A	484	GLN
2	B	102	LYS
2	B	420	GLU
2	B	484	GLN
2	A	178	SER
2	A	316	GLU
2	A	480	ALA
2	B	11	LEU
2	B	17	GLU
2	B	270	ARG
2	B	423	THR
2	B	469	ALA
2	A	293	SER
2	A	483	GLU
2	B	379	LYS
2	B	473	ALA
2	B	483	GLU
2	A	225	ARG
2	B	496	ASN
2	A	270	ARG
2	A	446	LYS
2	A	526	PHE
2	B	386	GLU
2	B	90	VAL
2	B	103	PRO

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	403/464 (87%)	363 (90%)	40 (10%)	10 28
2	B	402/464 (87%)	360 (90%)	42 (10%)	9 25
All	All	805/928 (87%)	723 (90%)	82 (10%)	9 26

All (82) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	5	PRO
2	A	26	ILE
2	A	49	LEU
2	A	55	ARG
2	A	56	LEU
2	A	97	LEU
2	A	186	HIS
2	A	201	LYS
2	A	205	PRO
2	A	226	LEU
2	A	243	VAL
2	A	244	ASP
2	A	254	LEU
2	A	261	ASN
2	A	282	VAL
2	A	295	LYS
2	A	297	SER
2	A	306	PHE
2	A	314	LEU
2	A	318	ASP
2	A	326	LEU
2	A	328	LEU
2	A	333	LEU
2	A	347	VAL
2	A	354	GLU
2	A	357	LEU
2	A	364	ARG
2	A	372	PRO
2	A	400	PHE
2	A	407	MET
2	A	422	ASN
2	A	435	VAL
2	A	448	LYS
2	A	458	VAL
2	A	489	VAL

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Mol	Chain	Res	Type
2	A	493	ILE
2	A	494	VAL
2	A	496	ASN
2	A	502	LEU
2	A	525	LEU
2	B	7	LYS
2	B	25	GLU
2	B	37	PRO
2	B	42	SER
2	B	49	LEU
2	B	55	ARG
2	B	56	LEU
2	B	62	SER
2	B	77	VAL
2	B	85	ARG
2	B	99	THR
2	B	186	HIS
2	B	216	ARG
2	B	224	THR
2	B	226	LEU
2	B	233	SER
2	B	236	LEU
2	B	243	VAL
2	B	254	LEU
2	B	261	ASN
2	B	290	VAL
2	B	308	ILE
2	B	314	LEU
2	B	326	LEU
2	B	328	LEU
2	B	333	LEU
2	B	354	GLU
2	B	356	LYS
2	B	364	ARG
2	B	400	PHE
2	B	422	ASN
2	B	435	VAL
2	B	447	THR
2	B	448	LYS
2	B	458	VAL
2	B	476	VAL
2	B	485	GLU

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Mol	Chain	Res	Type
2	B	493	ILE
2	B	496	ASN
2	B	506	GLU
2	B	525	LEU
2	B	532	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	47	HIS
2	A	186	HIS
2	A	261	ASN
2	A	286	HIS
2	A	382	GLN
2	A	391	HIS
2	A	422	ASN
2	A	484	GLN
2	A	496	ASN
2	B	47	HIS
2	B	186	HIS
2	B	261	ASN
2	B	286	HIS
2	B	382	GLN
2	B	391	HIS
2	B	422	ASN
2	B	496	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	70/71 (98%)	22 (31%)	8 (11%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	906	G
1	C	907	G
1	C	908	U
1	C	909	G
1	C	910	G

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Mol	Chain	Res	Type
1	C	914	A
1	C	915	G
1	C	917	G
1	C	918	G
1	C	919	C
1	C	921	U
1	C	932	U
1	C	933	G
1	C	935	A
1	C	937	A
1	C	944	U
1	C	945	U
1	C	946	A
1	C	958	A
1	C	960	C
1	C	968	U
1	C	969	G

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	907	G
1	C	909	G
1	C	917	G
1	C	918	G
1	C	934	C
1	C	936	G
1	C	957	A
1	C	959	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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{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	C	71/71 (100%)	1.96	26 (36%) 0 0	107, 182, 200, 200	0
2	A	466/534 (87%)	0.48	25 (5%) 29 19	40, 76, 137, 201	0
2	B	465/534 (87%)	0.52	36 (7%) 16 8	39, 74, 157, 199	0
All	All	1002/1139 (87%)	0.60	87 (8%) 13 6	39, 78, 178, 201	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	222	ASP	10.8
2	B	223	ALA	10.1
2	A	220	GLY	8.7
2	A	223	ALA	7.9
1	C	971	C	6.7
2	A	222	ASP	6.7
2	B	220	GLY	6.6
2	A	171	PHE	6.3
1	C	970	G	6.0
1	C	969	G	5.8
1	C	901	G	5.7
2	A	219	GLN	5.6
2	B	221	GLU	5.6
2	B	407	MET	5.5
1	C	902	C	5.5
1	C	904	A	5.0
1	C	903	C	5.0
2	B	104	ASN	4.9
2	A	533	ILE	4.8
2	B	487	VAL	4.6
2	A	221	GLU	4.4
1	C	906	G	4.3
1	C	944	U	4.3

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Mol	Chain	Res	Type	RSRZ
2	A	172	LYS	4.3
2	B	414	VAL	4.3
2	B	533	ILE	4.0
1	C	905	G	4.0
2	B	529	VAL	3.8
1	C	925	G	3.7
2	B	408	MET	3.7
1	C	966	C	3.7
1	C	907	G	3.6
2	B	403	PHE	3.6
1	C	968	U	3.5
2	B	224	THR	3.4
1	C	913	G	3.4
2	B	90	VAL	3.4
1	C	910	G	3.4
2	B	219	GLN	3.3
1	C	945	U	3.3
2	A	174	LEU	3.2
2	B	404	GLU	3.1
2	A	402	ALA	3.1
2	A	408	MET	3.1
2	A	102	LYS	3.1
2	A	403	PHE	3.0
2	A	397	PRO	3.0
2	B	174	LEU	3.0
1	C	964	G	3.0
1	C	965	C	3.0
2	B	412	VAL	2.8
2	B	409	GLY	2.8
2	B	481	MET	2.8
2	B	531	ALA	2.8
2	B	468	PHE	2.8
1	C	967	C	2.7
2	A	407	MET	2.7
1	C	924	C	2.7
1	C	914	A	2.7
2	B	402	ALA	2.7
2	B	296	TYR	2.6
2	A	531	ALA	2.6
2	A	62	SER	2.6
2	B	86	GLU	2.6
2	B	103	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
2	A	401	LEU	2.5
2	B	421	GLU	2.4
1	C	940	C	2.4
2	A	476	VAL	2.4
2	A	414	VAL	2.4
2	A	534	GLU	2.4
2	B	532	GLU	2.4
2	B	534	GLU	2.4
2	B	488	LYS	2.3
1	C	911	C	2.3
2	A	83	PHE	2.3
1	C	915	G	2.3
2	B	416	VAL	2.2
2	B	376	VAL	2.2
2	A	532	GLU	2.2
2	A	66	SER	2.1
1	C	912	A	2.1
2	B	401	LEU	2.1
2	B	388	ALA	2.1
2	B	482	ARG	2.1
2	B	492	ARG	2.0
2	A	448	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.