Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:33 PM GMT

PDB ID	:	1KOG
Title	:	Crystal structure of E. coli threonyl-tRNA synthetase interacting with the essential domain of its mRNA operator
Authors	:	Torres-Larrios, A.; Dock-Bregeon, A.C.; Romby, P.; Rees, B.; Sankaranarayanan, R.; Caillet, J.; Springer, M.; Ehresmann, C.; Ehresmann, B.; Moras, D.
Deposited on	:	2001-12-20
Resolution	:	3.50 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:

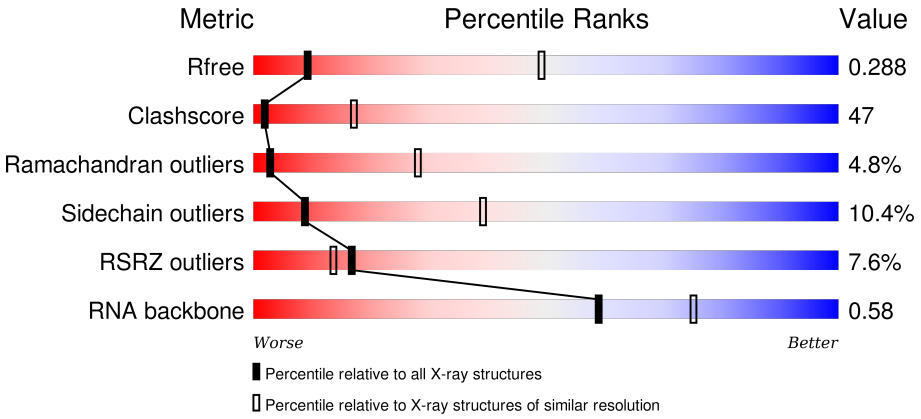
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.50 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	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)
RNA backbone	2183	1050 (4.20-2.80)

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	I	37	32% 30% 41% 22% 8%
1	J	37	16% 14% 57% 16% 14%
1	K	37	65% 11% 51% 32% 5%
1	L	37	35% 24% 46% 22% 8%

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Mol	Chain	Length	Quality of chain
1	M	37	16% 14% 51% 27% 8%
1	N	37	92% 22% 43% 27% 8%
1	O	37	3% 22% 41% 24% 14%
1	P	37	24% 19% 46% 24% 11%
2	A	401	% 32% 59% 8%
2	B	401	% 35% 55% 10%
2	C	401	5% 31% 59% 9%
2	D	401	11% 31% 61% 8%
2	E	401	13% 33% 58% 8%
2	F	401	9% 31% 59% 10%
2	G	401	31% 58% 10%
2	H	401	% 31% 58% 10%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	TSB	D	5002	-	-	-	X
4	TSB	E	6002	-	-	-	X
4	TSB	F	7002	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 32922 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 Threonyl-tRNA synthetase mRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	I	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	J	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	K	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	L	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	M	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	N	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	O	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			
1	P	37	Total	C	N	O	P	0	0	0
			785	349	132	267	37			

- Molecule 2 is a protein called Threonyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	B	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	C	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	D	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	E	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	F	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			

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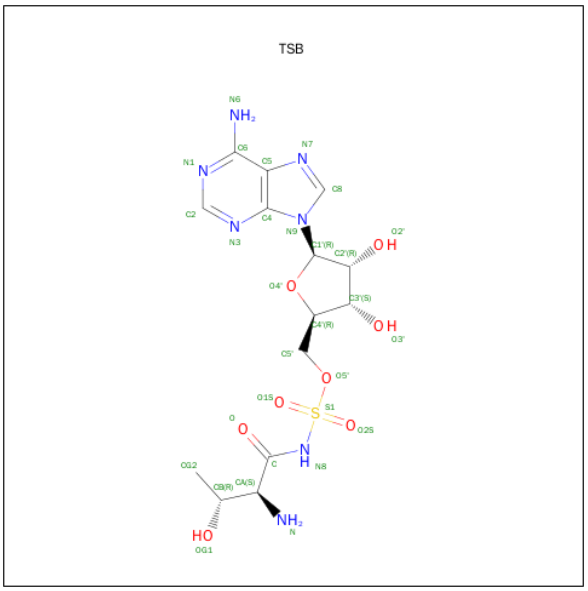
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			
2	H	401	Total	C	N	O	S	0	0	0
			3278	2069	576	610	23			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	H	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is 5'-O-(N-(L-THREONYL)-SULFAMOYL)ADENOSINE (three-letter code: TSB) (formula: $C_{14}H_{21}N_7O_8S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
4	B	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
4	C	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
4	D	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
4	E	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
4	F	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
4	G	1	Total	C	N	O	S	0	0
			30	14	7	8	1		
4	H	1	Total	C	N	O	S	0	0
			30	14	7	8	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	10	Total	O	0	0
			10	10		
5	B	15	Total	O	0	0
			15	15		
5	C	11	Total	O	0	0
			11	11		
5	D	14	Total	O	0	0
			14	14		
5	E	11	Total	O	0	0
			11	11		
5	F	13	Total	O	0	0
			13	13		
5	G	13	Total	O	0	0
			13	13		
5	H	16	Total	O	0	0
			16	16		
5	I	11	Total	O	0	0
			11	11		
5	J	12	Total	O	0	0
			12	12		
5	K	1	Total	O	0	0
			1	1		
5	L	8	Total	O	0	0
			8	8		

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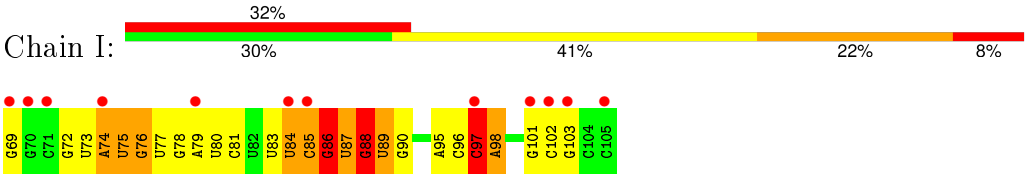
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	M	6	Total O 6 6	0	0
5	N	9	Total O 9 9	0	0
5	O	11	Total O 11 11	0	0
5	P	9	Total O 9 9	0	0

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.

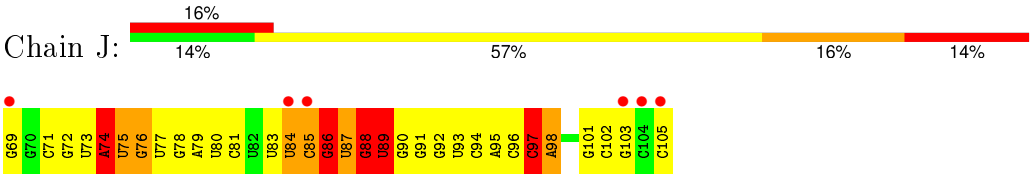
- Molecule 1: Threonyl-tRNA synthetase mRNA

Chain I:



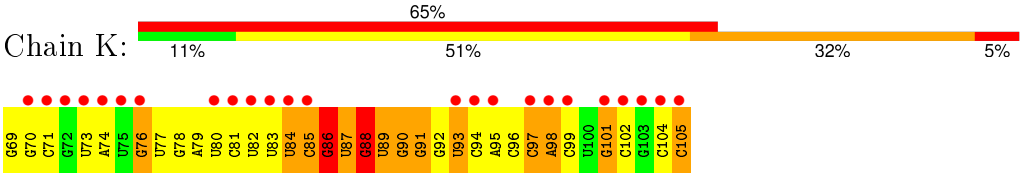
- Molecule 1: Threonyl-tRNA synthetase mRNA

Chain J:



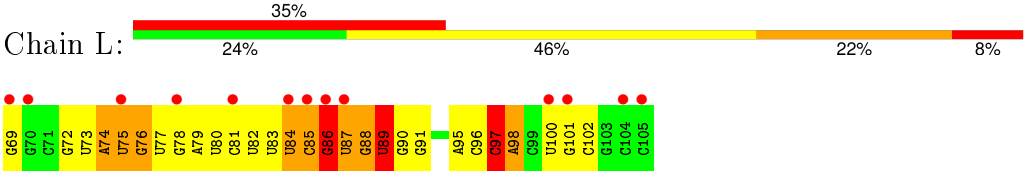
- Molecule 1: Threonyl-tRNA synthetase mRNA

Chain K:



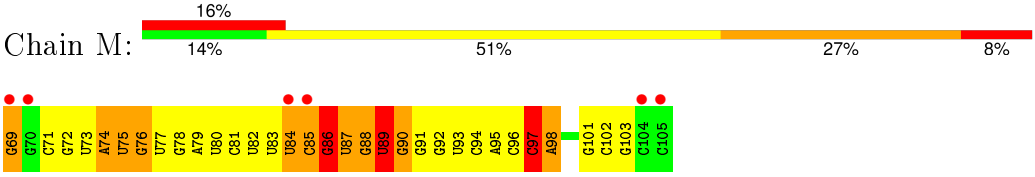
- Molecule 1: Threonyl-tRNA synthetase mRNA

Chain L:

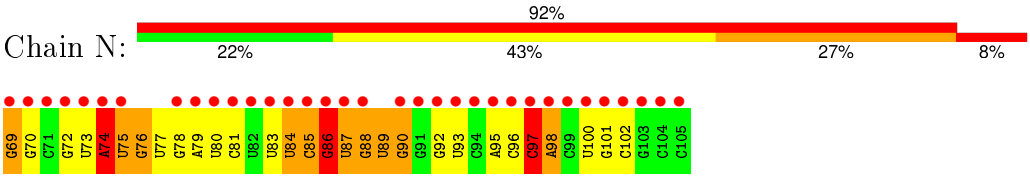


- Molecule 1: Threonyl-tRNA synthetase mRNA

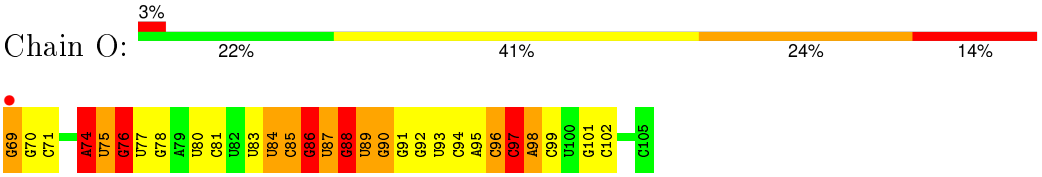
Chain M:



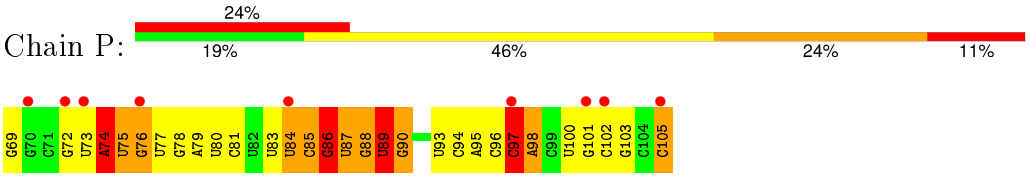
- Molecule 1: Threonyl-tRNA synthetase mRNA



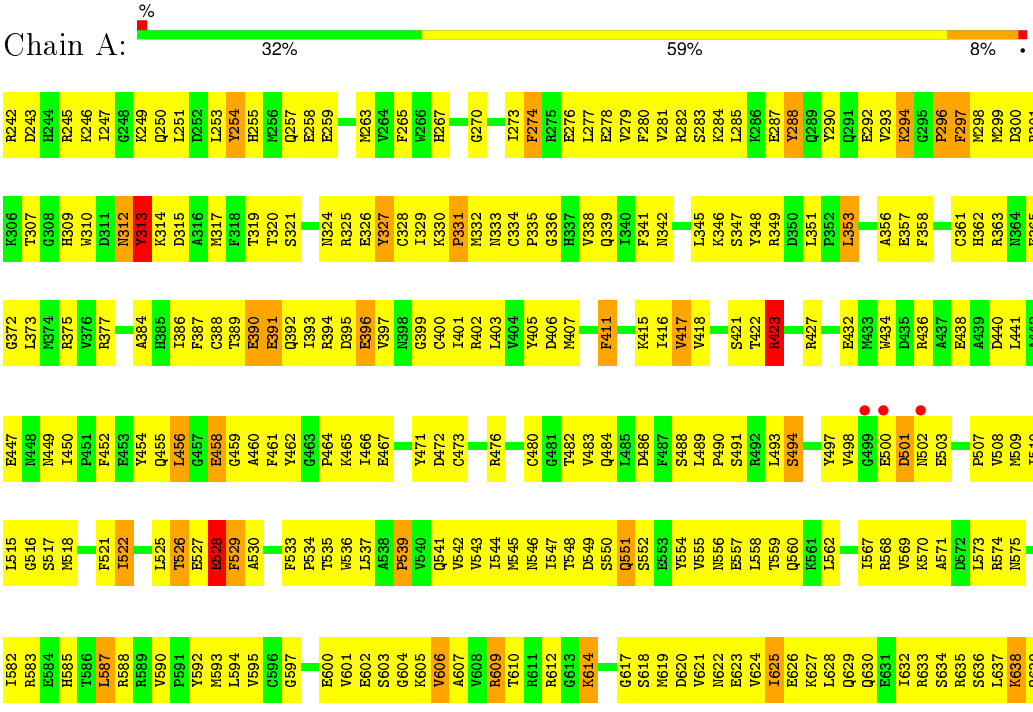
• Molecule 1: Threonyl-tRNA synthetase mRNA



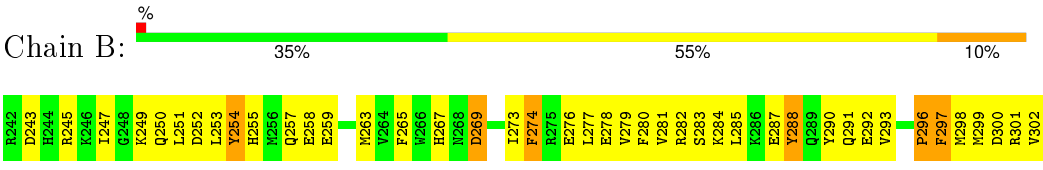
• Molecule 1: Threonyl-tRNA synthetase mRNA

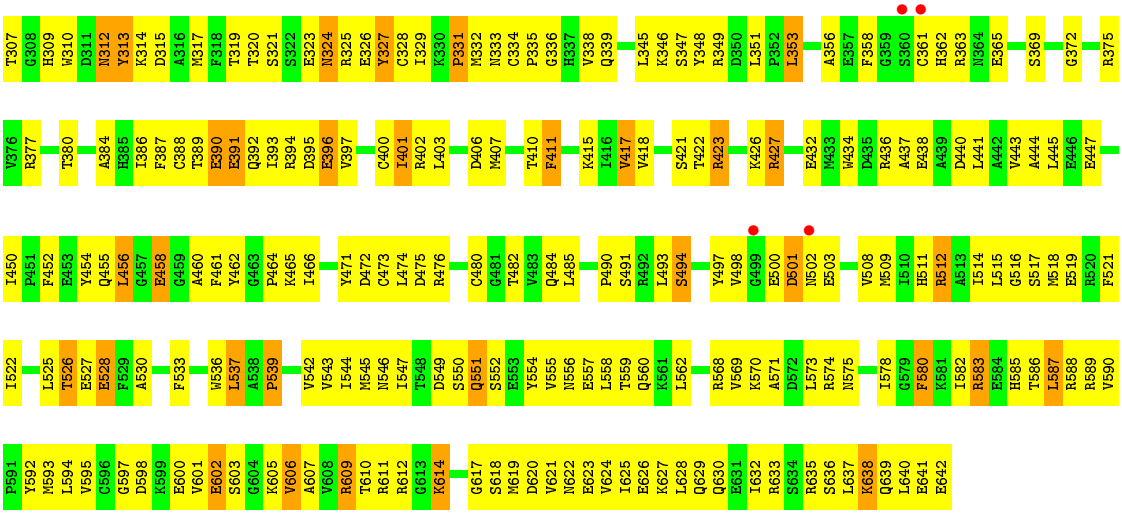


• Molecule 2: Threonyl-tRNA synthetase



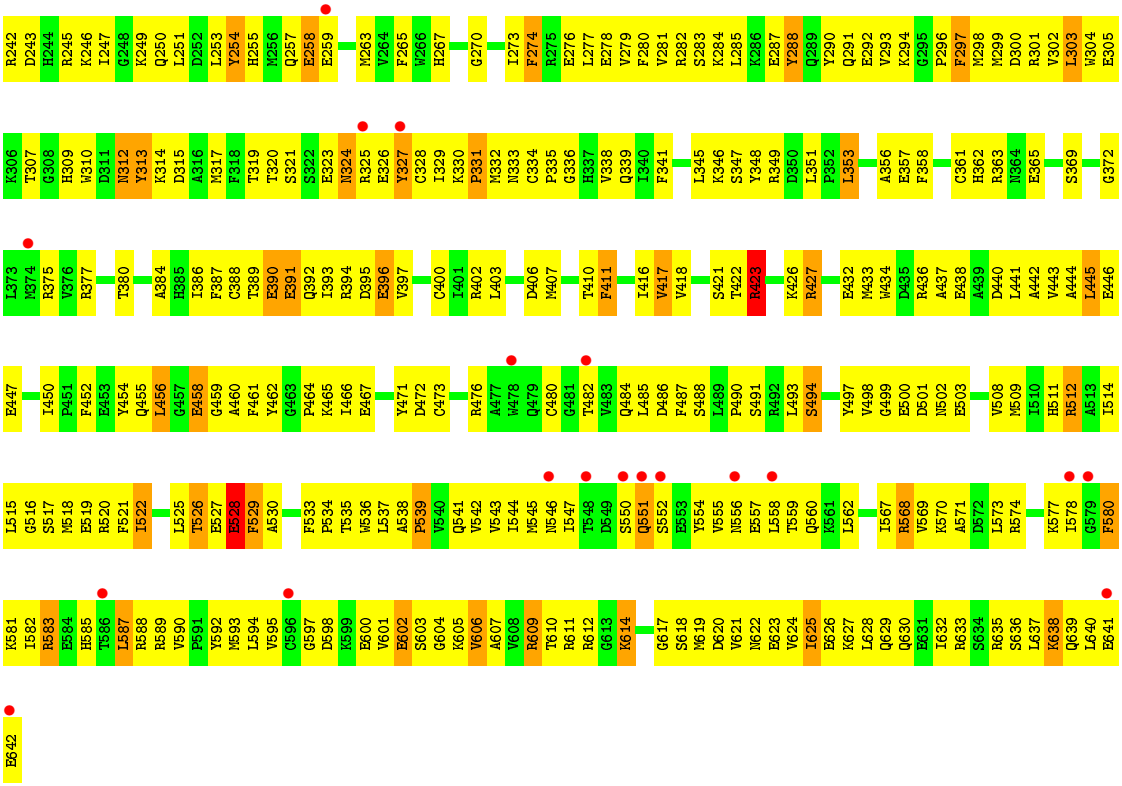
• Molecule 2: Threonyl-tRNA synthetase





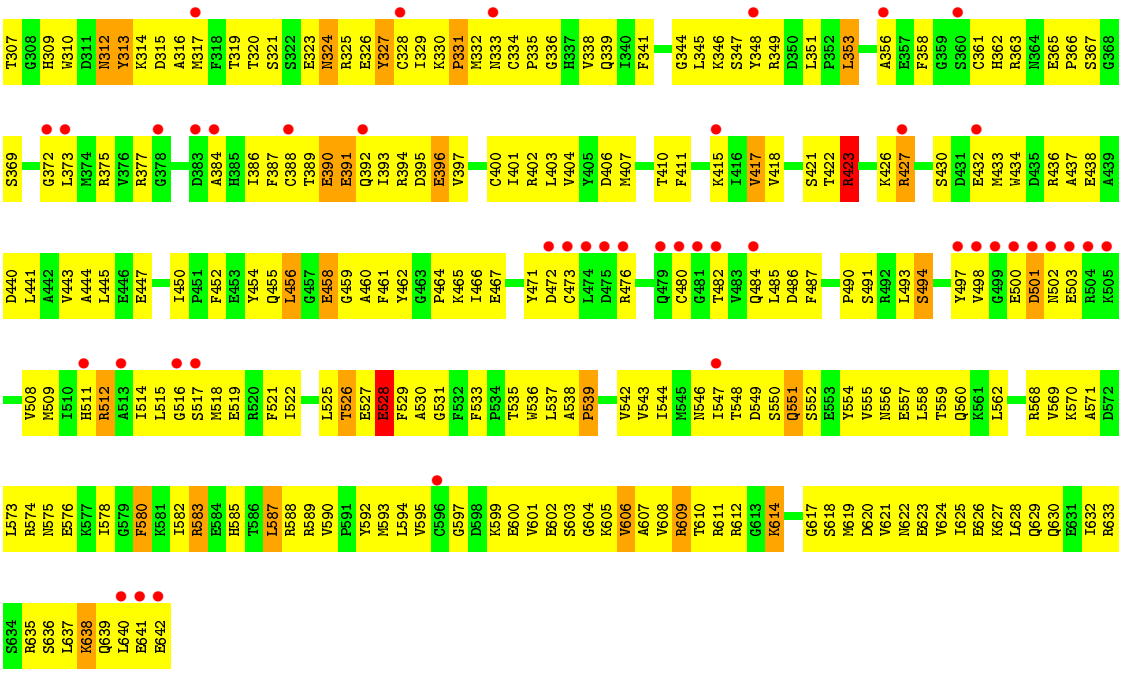
- Molecule 2: Threonyl-tRNA synthetase

Chain C:



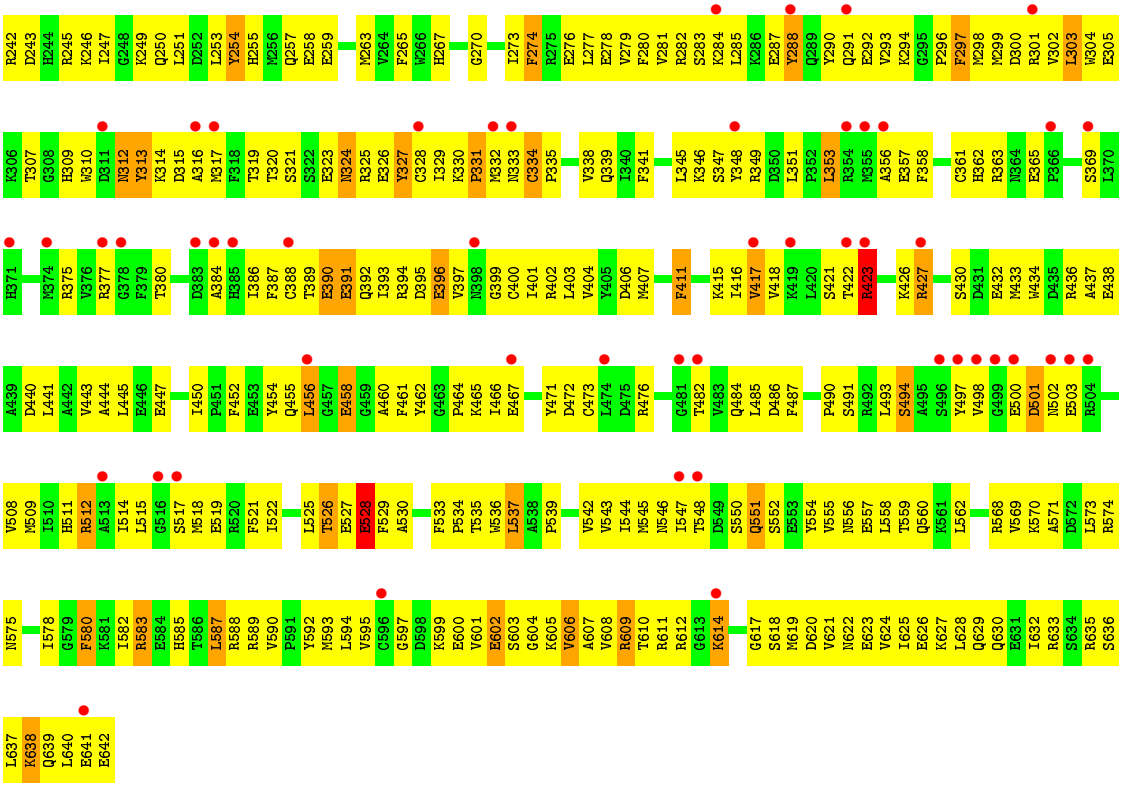
- Molecule 2: Threonyl-tRNA synthetase

Chain D:



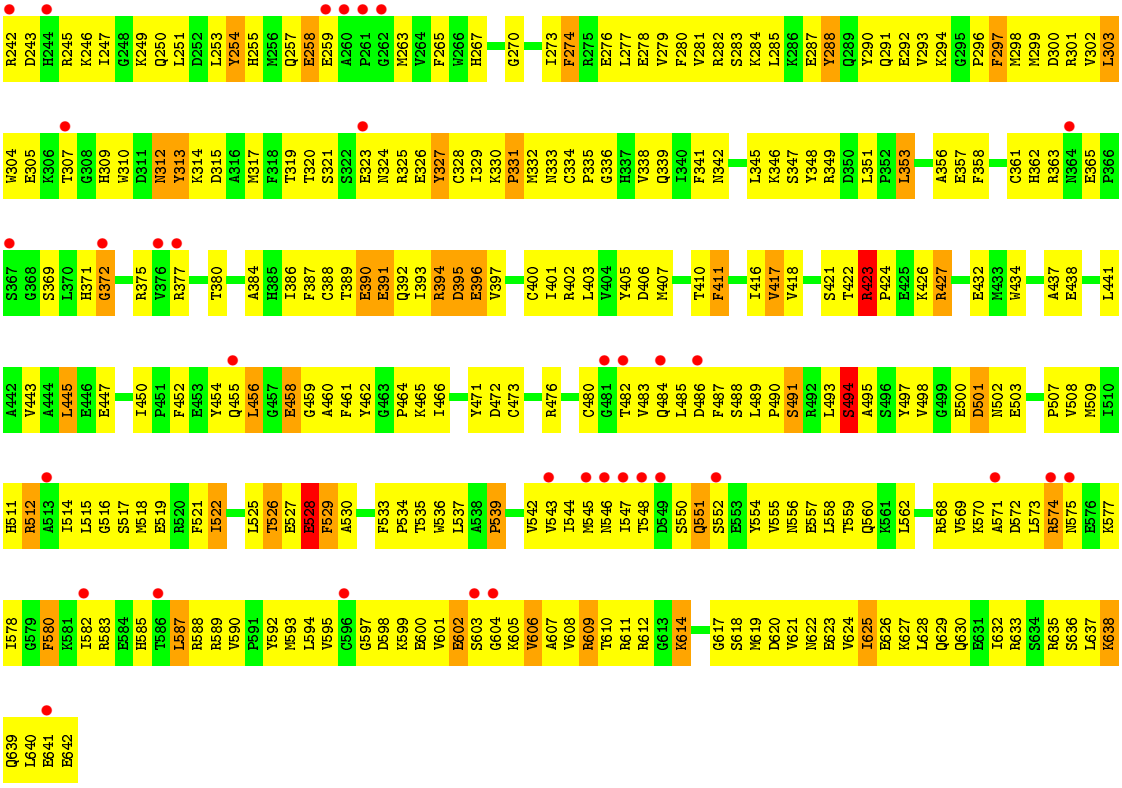
• Molecule 2: Threonyl-tRNA synthetase

Chain E:



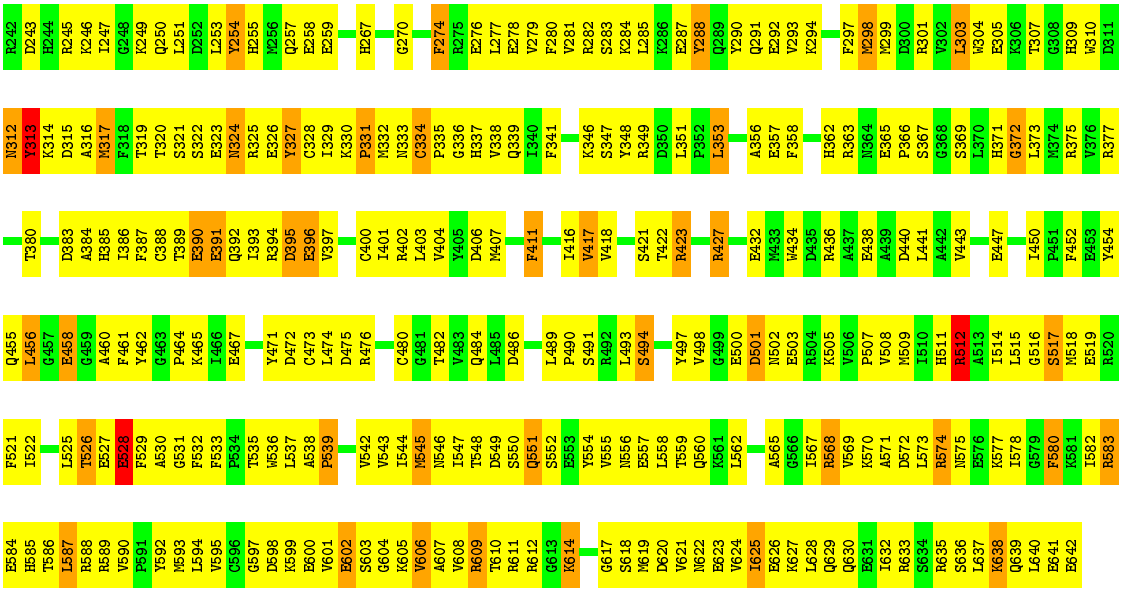
• Molecule 2: Threonyl-tRNA synthetase

Chain F:



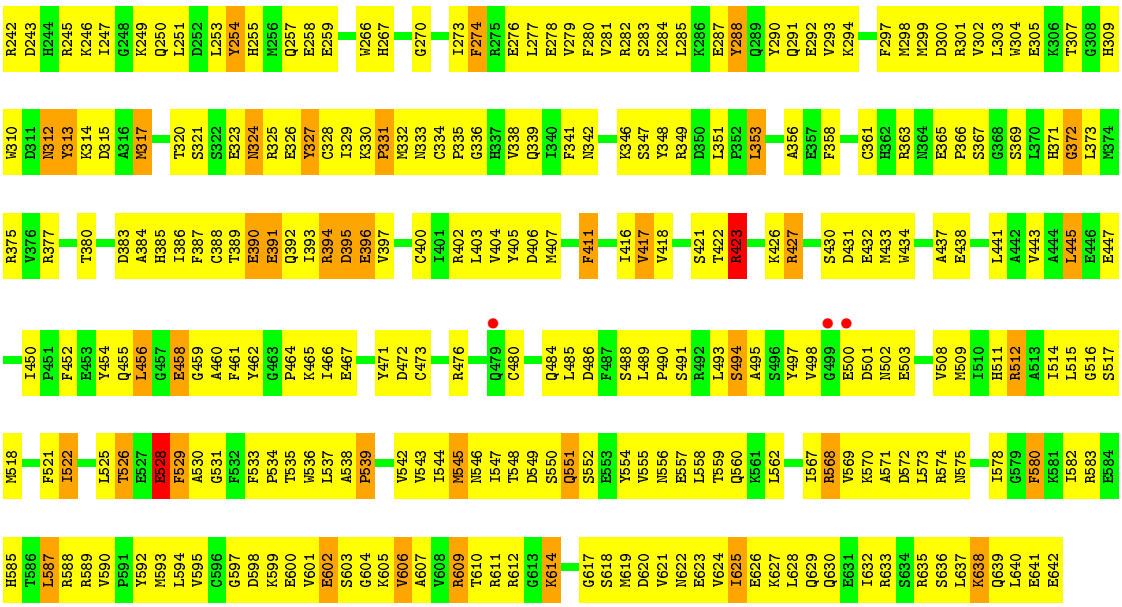
- Molecule 2: Threonyl-tRNA synthetase

Chain G:



- Molecule 2: Threonyl-tRNA synthetase

Chain H:


R242 D243 H244 R245 K246 I247 G248 K249 Q250 L251 D252 L253 Y254 H255 M256 Q257 E258 E259 W266 H267 G270 I273 F274 R275 E276 L277 E278 V279 F280 V281 R282 S283 K284 L285 K286 E287 Y288 Q289 Y290 Q291 E292 V293 K294 F297 M298 M299 D300 R301 V302 L303 W304 E305 K306 T307 G308 H309
W310 D311 M312 Y313 K314 D315 A316 M317 T320 S321 S322 E323 N324 R325 E326 Y327 C328 I329 K330 P331 M332 N333 C334 P335 G336 H337 V338 Q339 I340 F341 N342 K346 S347 Y348 R349 D350 L351 P352 L353 A356 E357 F358 C361 H362 R363 N364 E365 P366 S367 G368 S369 L370 H371 G372 L373 M374
R375 V376 R377 T380 D383 A384 H385 I386 F387 C388 T389 E390 E391 Q392 I393 R394 D395 E396 V397 C400 I401 R402 L403 V404 Y405 D406 M407 F411 I416 V417 V418 S421 T422 R423 K426 R427 S430 D431 E432 M433 W434 A437 E438 L441 A442 V443 A444 L445 E446 E447
I450 P451 F452 E453 Y454 Q455 L456 G457 E458 G459 A460 F461 Y462 G463 P464 K465 I466 E467 Y471 D472 C473 R476 Q479 C480 Q484 L485 D486 F487 S488 L489 P490 S491 R492 L493 S494 A495 S496 Y497 V498 G499 E500 D501 N502 E503 V508 M509 I510 H511 R512 A513 I514 L515 G516 S517
M518 F521 I522 L525 T526 E527 E528 F529 A530 G531 F532 F533 P534 T535 W536 L537 A538 P539 V542 V543 I544 M545 N546 I547 T548 D549 S550 Q551 S552 E553 Y554 V555 N556 E557 L558 T559 Q560 K561 L562 I567 R568 V569 K570 A571 D572 L573 R574 N575 I578 G579 F580 K581 I582 R583 E584
H585 T586 L587 R588 R589 V590 P591 Y592 M593 L594 V595 C596 G597 D598 K599 E600 V601 E602 S603 G604 K605 V606 A607 V608 R609 T610 R611 R612 G613 K614 G617 S618 M619 D620 V621 N622 E623 V624 I625 E626 K627 L628 Q629 Q630 E631 I632 R633 S634 R635 S636 L637 K638 Q639 L640 E641 E642

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	188.45Å 101.74Å 199.34Å 90.00° 114.40° 90.00°	Depositor
Resolution (Å)	29.80 – 3.50 29.80 – 3.46	Depositor EDS
% Data completeness (in resolution range)	90.0 (29.80-3.50) 92.6 (29.80-3.46)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.63 (at 3.47Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.251 , 0.287 0.256 , 0.288	Depositor DCC
R_{free} test set	8182 reflections (9.96%)	DCC
Wilson B-factor (Å^2)	96.2	Xtriage
Anisotropy	0.477	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 93.5	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	0 of 88408 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	32922	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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

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

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	I	0.71	1/874 (0.1%)	0.99	7/1358 (0.5%)
1	J	0.81	1/874 (0.1%)	1.01	7/1358 (0.5%)
1	K	0.94	1/874 (0.1%)	1.08	7/1358 (0.5%)
1	L	0.64	1/874 (0.1%)	0.96	5/1358 (0.4%)
1	M	0.79	1/874 (0.1%)	1.00	5/1358 (0.4%)
1	N	0.66	1/874 (0.1%)	0.94	4/1358 (0.3%)
1	O	0.99	3/874 (0.3%)	1.07	6/1358 (0.4%)
1	P	0.73	1/874 (0.1%)	0.99	6/1358 (0.4%)
2	A	0.64	0/3349	0.76	0/4508
2	B	0.70	1/3349 (0.0%)	0.78	0/4508
2	C	0.53	0/3349	0.71	0/4508
2	D	0.49	0/3349	0.68	0/4508
2	E	0.49	0/3349	0.69	0/4508
2	F	0.54	0/3349	0.73	0/4508
2	G	0.78	0/3349	0.85	2/4508 (0.0%)
2	H	0.66	0/3349	0.78	0/4508
All	All	0.65	11/33784 (0.0%)	0.81	49/46928 (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	I	0	2
1	J	0	4
1	K	0	1
1	L	0	3
1	M	0	2
1	N	0	2
1	O	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	3
All	All	0	20

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	69	G	OP3-P	-7.74	1.51	1.61
1	I	69	G	OP3-P	-7.56	1.52	1.61
1	K	69	G	OP3-P	-7.33	1.52	1.61
1	L	69	G	OP3-P	-7.26	1.52	1.61
1	P	69	G	OP3-P	-7.09	1.52	1.61
1	N	69	G	OP3-P	-7.04	1.52	1.61
1	O	69	G	OP3-P	-7.02	1.52	1.61
1	M	69	G	OP3-P	-6.75	1.53	1.61
1	O	76	G	C5-C6	5.84	1.48	1.42
1	O	88	G	C5-C6	5.49	1.47	1.42
2	B	269	ASP	CG-OD1	-5.00	1.13	1.25

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	74	A	N9-C1'-C2'	11.86	129.42	114.00
1	M	74	A	N9-C1'-C2'	10.30	127.39	114.00
1	P	74	A	N9-C1'-C2'	9.87	126.84	114.00
1	K	86	G	N9-C1'-C2'	9.58	126.46	114.00
1	L	74	A	N9-C1'-C2'	9.26	126.04	114.00
1	N	74	A	N9-C1'-C2'	9.06	125.77	114.00
1	I	74	A	N9-C1'-C2'	9.05	125.76	114.00
1	J	74	A	N9-C1'-C2'	8.90	125.57	114.00
2	G	512	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	O	97	C	N1-C1'-C2'	7.59	123.87	114.00
1	K	93	U	O4'-C1'-N1	7.52	114.21	108.20
1	P	86	G	N9-C1'-C2'	7.42	123.64	114.00
1	M	69	G	OP1-P-OP2	-7.17	108.85	119.60
1	P	105	C	C2'-C3'-O3'	7.13	125.18	109.50
1	O	87	U	N1-C1'-C2'	7.13	123.27	114.00
1	I	86	G	N9-C1'-C2'	6.86	122.91	114.00
1	M	97	C	N1-C1'-C2'	6.82	122.87	114.00
1	I	87	U	N1-C1'-C2'	6.66	122.66	114.00
1	J	86	G	N9-C1'-C2'	6.61	122.59	114.00
1	N	86	G	N9-C1'-C2'	6.41	122.33	114.00
1	P	97	C	N1-C1'-C2'	6.39	122.31	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	88	G	N9-C1'-C2'	6.28	122.17	114.00
1	J	87	U	N1-C1'-C2'	6.27	122.15	114.00
1	K	101	G	O4'-C1'-N9	6.25	113.20	108.20
1	J	97	C	N1-C1'-C2'	6.22	122.09	114.00
1	K	88	G	N9-C1'-C2'	6.08	121.90	114.00
1	M	87	U	N1-C1'-C2'	6.07	121.89	114.00
1	O	86	G	N9-C1'-C2'	6.07	121.89	114.00
1	M	86	G	N9-C1'-C2'	6.05	121.87	114.00
1	N	97	C	N1-C1'-C2'	6.04	121.85	114.00
1	J	88	G	O4'-C1'-N9	5.96	112.97	108.20
1	L	86	G	N9-C1'-C2'	5.95	121.73	114.00
1	J	69	G	OP1-P-OP2	-5.91	110.74	119.60
1	K	81	C	N1-C1'-C2'	-5.91	105.50	112.00
1	K	81	C	O4'-C1'-N1	5.86	112.89	108.20
1	L	97	C	N1-C1'-C2'	5.84	121.59	114.00
1	I	97	C	N1-C1'-C2'	5.83	121.59	114.00
1	N	87	U	N1-C1'-C2'	5.78	121.51	114.00
1	K	69	G	OP1-P-OP2	-5.74	110.99	119.60
1	L	74	A	O4'-C1'-N9	5.69	112.75	108.20
1	L	87	U	N1-C1'-C2'	5.56	121.22	114.00
1	P	87	U	N1-C1'-C2'	5.54	121.19	114.00
1	I	74	A	O4'-C1'-N9	5.51	112.61	108.20
1	I	88	G	O4'-C1'-N9	5.49	112.59	108.20
1	P	69	G	OP1-P-OP2	-5.26	111.71	119.60
1	J	74	A	O4'-C1'-N9	5.25	112.40	108.20
1	O	74	A	O4'-C1'-C2'	5.25	112.33	107.60
2	G	537	LEU	CB-CG-CD2	-5.10	102.33	111.00
1	O	88	G	N9-C1'-C2'	5.08	120.60	114.00

There are no chirality outliers.

All (20) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	I	74	A	Sidechain
1	I	86	G	Sidechain
1	J	74	A	Sidechain
1	J	86	G	Sidechain
1	J	89	U	Sidechain
1	J	97	C	Sidechain
1	K	86	G	Sidechain
1	L	74	A	Sidechain
1	L	86	G	Sidechain

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Mol	Chain	Res	Type	Group
1	L	89	U	Sidechain
1	M	86	G	Sidechain
1	M	89	U	Sidechain
1	N	74	A	Sidechain
1	N	86	G	Sidechain
1	O	74	A	Sidechain
1	O	86	G	Sidechain
1	O	88	G	Sidechain
1	P	74	A	Sidechain
1	P	86	G	Sidechain
1	P	89	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	I	785	0	397	45	0
1	J	785	0	397	53	0
1	K	785	0	397	76	0
1	L	785	0	397	42	0
1	M	785	0	397	72	0
1	N	785	0	397	44	0
1	O	785	0	397	56	0
1	P	785	0	397	65	0
2	A	3278	0	3208	336	0
2	B	3278	0	3208	316	0
2	C	3278	0	3208	340	0
2	D	3278	0	3208	331	0
2	E	3278	0	3208	333	0
2	F	3278	0	3208	346	0
2	G	3278	0	3208	314	0
2	H	3278	0	3208	313	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	30	0	21	3	0
4	B	30	0	20	4	0
4	C	30	0	21	3	0
4	D	30	0	21	4	0
4	E	30	0	21	4	0
4	F	30	0	21	5	0
4	G	30	0	21	4	0
4	H	30	0	21	4	0
5	A	10	0	0	0	0
5	B	15	0	0	8	0
5	C	11	0	0	3	0
5	D	14	0	0	4	0
5	E	11	0	0	5	0
5	F	13	0	0	2	0
5	G	13	0	0	4	0
5	H	16	0	0	3	0
5	I	11	0	0	10	0
5	J	12	0	0	8	0
5	K	1	0	0	0	0
5	L	8	0	0	3	0
5	M	6	0	0	10	0
5	N	9	0	0	2	0
5	O	11	0	0	9	0
5	P	9	0	0	14	0
All	All	32922	0	29007	2890	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 47.

All (2890) 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:G:407:MET:CE	2:G:407:MET:SD	2.05	1.44
2:D:559:THR:HG21	2:D:571:ALA:HB2	1.29	1.15
2:G:559:THR:HG21	2:G:571:ALA:HB2	1.27	1.12
2:E:559:THR:HG21	2:E:571:ALA:HB2	1.30	1.12
2:A:559:THR:HG21	2:A:571:ALA:HB2	1.27	1.11
2:C:559:THR:HG21	2:C:571:ALA:HB2	1.30	1.10
2:H:559:THR:HG21	2:H:571:ALA:HB2	1.31	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:559:THR:HG21	2:F:571:ALA:HB2	1.26	1.09
2:B:559:THR:HG21	2:B:571:ALA:HB2	1.32	1.07
2:E:411:PHE:HD2	2:E:525:LEU:HD21	1.21	1.06
2:D:411:PHE:HE2	2:D:521:PHE:CE1	1.74	1.05
2:B:473:CYS:HA	5:B:221:HOH:O	1.57	1.05
1:O:87:U:H2'	5:O:1519:HOH:O	1.58	1.03
2:B:411:PHE:HD2	2:B:525:LEU:HD21	1.23	1.02
2:A:411:PHE:HD2	2:A:525:LEU:HD21	1.25	1.02
2:G:421:SER:HB3	2:G:458:GLU:HB3	1.40	1.01
1:K:86:G:H5'	1:K:87:U:OP1	1.63	0.97
2:E:421:SER:HB3	2:E:458:GLU:HB3	1.47	0.97
2:H:411:PHE:HD2	2:H:525:LEU:HD21	1.28	0.96
2:A:298:MET:HG2	2:B:263:MET:HE2	1.48	0.96
2:B:421:SER:HB3	2:B:458:GLU:HB3	1.45	0.95
2:A:421:SER:HB3	2:A:458:GLU:HB3	1.45	0.93
2:G:582:ILE:HA	2:G:593:MET:HE1	1.50	0.92
2:D:421:SER:HB3	2:D:458:GLU:HB3	1.49	0.92
1:I:103:G:H5"	5:I:113:HOH:O	1.68	0.92
2:D:411:PHE:CE2	2:D:521:PHE:CE1	2.57	0.92
2:E:411:PHE:CD2	2:E:525:LEU:HD21	2.04	0.92
2:C:421:SER:HB3	2:C:458:GLU:HB3	1.50	0.91
2:H:421:SER:HB3	2:H:458:GLU:HB3	1.50	0.91
2:D:543:VAL:HG23	2:D:590:VAL:HG11	1.52	0.91
1:K:84:U:H4'	1:K:85:C:H5'	1.53	0.91
1:O:77:U:O3'	5:O:1539:HOH:O	1.89	0.91
2:C:389:THR:OG1	2:C:392:GLN:HG3	1.71	0.91
2:C:411:PHE:HE2	2:C:521:PHE:CE1	1.87	0.90
2:C:411:PHE:HE2	2:C:521:PHE:HE1	1.18	0.90
2:F:411:PHE:HE2	2:F:521:PHE:CE1	1.88	0.90
1:K:88:G:H4'	1:K:89:U:OP1	1.71	0.90
2:B:411:PHE:CD2	2:B:525:LEU:HD21	2.06	0.89
1:O:85:C:H5	2:G:547:ILE:O	1.55	0.89
2:G:543:VAL:HG23	2:G:590:VAL:HG11	1.55	0.89
2:A:389:THR:OG1	2:A:392:GLN:HG3	1.71	0.89
2:B:389:THR:OG1	2:B:392:GLN:HG3	1.72	0.89
2:F:543:VAL:HG23	2:F:590:VAL:HG11	1.54	0.88
2:A:411:PHE:CD2	2:A:525:LEU:HD21	2.08	0.88
2:E:582:ILE:HA	2:E:593:MET:HE2	1.53	0.88
2:D:582:ILE:HA	2:D:593:MET:HE1	1.53	0.88
2:C:411:PHE:HD2	2:C:525:LEU:HD21	1.39	0.88
1:K:101:G:O2'	1:K:102:C:H5'	1.73	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:543:VAL:HG23	2:H:590:VAL:HG11	1.53	0.88
1:J:98:A:H4'	5:J:1027:HOH:O	1.74	0.88
1:K:87:U:O2	1:K:87:U:H2'	1.73	0.87
2:A:587:LEU:H	2:A:587:LEU:HD23	1.38	0.87
2:G:452:PHE:HE2	2:G:454:TYR:HE1	1.22	0.87
2:G:551:GLN:HE21	2:G:597:GLY:HA2	1.39	0.87
2:F:421:SER:HB3	2:F:458:GLU:HB3	1.55	0.87
2:A:633:ARG:CZ	2:H:638:LYS:HZ3	1.88	0.87
2:A:307:THR:HG22	2:A:493:LEU:HD21	1.54	0.87
2:A:543:VAL:HG23	2:A:590:VAL:HG11	1.56	0.86
2:E:307:THR:HG22	2:E:493:LEU:HD21	1.57	0.86
2:H:389:THR:OG1	2:H:392:GLN:HG3	1.75	0.86
2:D:411:PHE:CE2	2:D:521:PHE:CZ	2.62	0.86
2:C:543:VAL:HG23	2:C:590:VAL:HG11	1.55	0.86
1:K:84:U:H4'	1:K:85:C:C5'	2.05	0.86
2:H:411:PHE:CD2	2:H:525:LEU:HD21	2.09	0.86
2:E:389:THR:OG1	2:E:392:GLN:HG3	1.75	0.86
2:G:587:LEU:H	2:G:587:LEU:HD23	1.40	0.86
2:A:276:GLU:O	2:A:279:VAL:HG22	1.75	0.86
2:G:389:THR:OG1	2:G:392:GLN:HG3	1.75	0.86
2:C:307:THR:HG22	2:C:493:LEU:HD21	1.57	0.86
2:F:411:PHE:CD2	2:F:525:LEU:HD21	2.10	0.86
1:I:86:G:H2'	5:I:109:HOH:O	1.74	0.86
2:H:582:ILE:HA	2:H:593:MET:HE1	1.56	0.85
2:B:582:ILE:HA	2:B:593:MET:HE2	1.57	0.85
2:C:255:HIS:ND1	2:C:267:HIS:HE1	1.75	0.85
2:H:473:CYS:HA	5:H:821:HOH:O	1.76	0.85
2:G:276:GLU:O	2:G:279:VAL:HG22	1.77	0.84
2:H:551:GLN:HE21	2:H:597:GLY:HA2	1.41	0.84
2:E:543:VAL:HG23	2:E:590:VAL:HG11	1.59	0.84
2:C:411:PHE:CD2	2:C:525:LEU:HD21	2.12	0.84
2:D:411:PHE:HE2	2:D:521:PHE:HE1	1.25	0.84
1:O:89:U:O2	1:O:89:U:H2'	1.78	0.84
2:F:411:PHE:HD2	2:F:525:LEU:HD21	1.41	0.84
2:F:389:THR:OG1	2:F:392:GLN:HG3	1.77	0.84
2:G:411:PHE:HD2	2:G:525:LEU:HD21	1.43	0.84
1:M:89:U:O2	1:M:89:U:H2'	1.75	0.83
2:H:407:MET:SD	2:H:514:ILE:HG21	2.18	0.83
2:A:263:MET:HE2	2:B:298:MET:HG2	1.61	0.83
2:D:307:THR:HG22	2:D:493:LEU:HD21	1.58	0.83
1:I:88:G:H8	5:I:112:HOH:O	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:582:ILE:HA	2:C:593:MET:HE2	1.60	0.82
2:C:587:LEU:HD23	2:C:587:LEU:H	1.43	0.82
2:H:587:LEU:H	2:H:587:LEU:HD23	1.43	0.82
2:G:551:GLN:NE2	2:G:597:GLY:HA2	1.93	0.82
2:B:587:LEU:HD23	2:B:587:LEU:H	1.42	0.82
2:C:411:PHE:CE2	2:C:521:PHE:CE1	2.66	0.82
2:D:389:THR:OG1	2:D:392:GLN:HG3	1.80	0.82
1:N:79:A:H1'	2:E:502:ASN:OD1	1.80	0.82
1:N:100:U:H4'	5:F:7014:HOH:O	1.77	0.81
2:F:411:PHE:HE2	2:F:521:PHE:HE1	1.26	0.81
2:F:255:HIS:ND1	2:F:267:HIS:HE1	1.78	0.81
2:C:276:GLU:O	2:C:279:VAL:HG22	1.80	0.81
2:E:411:PHE:CE2	2:E:521:PHE:CE1	2.69	0.81
2:C:551:GLN:HE21	2:C:597:GLY:HA2	1.43	0.81
2:F:551:GLN:HE21	2:F:597:GLY:HA2	1.44	0.81
2:A:551:GLN:HE21	2:A:597:GLY:HA2	1.44	0.81
1:O:86:G:O6	2:G:599:LYS:CB	2.29	0.81
2:H:307:THR:HG22	2:H:493:LEU:HD21	1.63	0.81
1:N:86:G:H2'	5:N:1413:HOH:O	1.81	0.81
2:H:255:HIS:ND1	2:H:267:HIS:HE1	1.79	0.81
2:B:501:ASP:OD2	2:B:503:GLU:HB2	1.81	0.80
2:B:543:VAL:HG23	2:B:590:VAL:HG11	1.63	0.80
2:E:587:LEU:HD23	2:E:587:LEU:H	1.46	0.80
2:H:348:TYR:CD1	2:H:349:ARG:N	2.49	0.80
1:O:97:C:H5"	1:O:98:A:OP1	1.81	0.80
2:C:320:THR:HG22	2:C:321:SER:H	1.45	0.80
2:H:551:GLN:NE2	2:H:597:GLY:HA2	1.97	0.80
1:P:83:U:H3	2:H:575:ASN:HD21	1.30	0.80
2:B:307:THR:HG22	2:B:493:LEU:HD21	1.61	0.80
1:N:88:G:H4'	1:N:89:U:OP1	1.80	0.80
2:G:621:VAL:O	2:G:624:VAL:HG22	1.80	0.80
2:F:411:PHE:CE2	2:F:521:PHE:CE1	2.69	0.80
2:G:254:TYR:CZ	2:G:373:LEU:HD21	2.16	0.80
2:E:319:THR:O	2:F:320:THR:HG23	1.80	0.80
2:B:255:HIS:ND1	2:B:267:HIS:HE1	1.80	0.80
2:B:411:PHE:HD1	2:B:411:PHE:N	1.80	0.80
2:G:411:PHE:CD2	2:G:525:LEU:HD21	2.17	0.80
2:F:402:ARG:HH11	2:F:402:ARG:HB2	1.47	0.80
2:C:452:PHE:HE2	2:C:454:TYR:HE1	1.30	0.80
2:H:251:LEU:HA	2:H:588:ARG:HH12	1.47	0.79
2:A:321:SER:HB3	2:A:326:GLU:HA	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:97:C:H5"	1:P:98:A:OP1	1.81	0.79
2:F:307:THR:HG22	2:F:493:LEU:HD21	1.62	0.79
2:G:251:LEU:HA	2:G:588:ARG:HH12	1.47	0.79
1:M:98:A:O3'	5:M:1327:HOH:O	1.99	0.79
2:A:501:ASP:OD2	2:A:503:GLU:HB2	1.81	0.79
2:D:501:ASP:OD2	2:D:503:GLU:HB2	1.82	0.79
2:D:255:HIS:ND1	2:D:267:HIS:HE1	1.80	0.79
2:F:582:ILE:HA	2:F:593:MET:HE2	1.62	0.79
2:A:320:THR:HG23	2:B:319:THR:O	1.83	0.79
2:B:320:THR:HG22	2:B:321:SER:H	1.48	0.79
2:E:501:ASP:OD2	2:E:503:GLU:HB2	1.83	0.79
2:D:551:GLN:HE21	2:D:597:GLY:HA2	1.48	0.79
1:P:89:U:H2'	1:P:89:U:O2	1.81	0.79
2:G:578:ILE:O	2:G:582:ILE:HG12	1.83	0.79
2:F:551:GLN:NE2	2:F:597:GLY:HA2	1.98	0.79
2:F:320:THR:HG22	2:F:321:SER:H	1.48	0.79
2:G:403:LEU:HG	2:G:407:MET:CE	2.14	0.78
2:E:411:PHE:N	2:E:411:PHE:HD1	1.80	0.78
2:H:276:GLU:O	2:H:279:VAL:HG22	1.83	0.78
2:A:319:THR:O	2:B:320:THR:HG23	1.83	0.78
2:A:255:HIS:ND1	2:A:267:HIS:HE1	1.80	0.78
2:E:251:LEU:HA	2:E:588:ARG:HH12	1.48	0.78
2:E:411:PHE:HE2	2:E:521:PHE:HE1	1.29	0.78
2:D:276:GLU:O	2:D:279:VAL:HG22	1.83	0.78
2:E:255:HIS:ND1	2:E:267:HIS:HE1	1.80	0.78
2:G:348:TYR:CD1	2:G:349:ARG:N	2.52	0.78
1:M:89:U:C5	2:E:583:ARG:CZ	2.66	0.78
2:C:501:ASP:OD2	2:C:503:GLU:HB2	1.83	0.78
2:F:587:LEU:HD23	2:F:587:LEU:H	1.48	0.78
2:G:251:LEU:HA	2:G:588:ARG:NH1	1.99	0.78
2:G:402:ARG:HH11	2:G:402:ARG:HB2	1.49	0.78
2:D:621:VAL:O	2:D:624:VAL:HG22	1.83	0.78
2:B:251:LEU:HA	2:B:588:ARG:HH12	1.48	0.78
2:D:411:PHE:CD2	2:D:525:LEU:HD21	2.18	0.77
2:G:320:THR:HG22	2:G:321:SER:H	1.49	0.77
2:F:585:HIS:HB2	2:F:593:MET:CE	2.15	0.77
2:A:407:MET:SD	2:A:514:ILE:HG21	2.24	0.77
2:C:407:MET:SD	2:C:514:ILE:HG21	2.24	0.77
2:E:320:THR:HG22	2:E:321:SER:H	1.49	0.77
2:E:551:GLN:HE21	2:E:597:GLY:HA2	1.50	0.77
1:J:89:U:O2	1:J:89:U:H2'	1.82	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:303:LEU:HD11	2:A:339:GLN:HE21	1.48	0.77
2:H:578:ILE:O	2:H:582:ILE:HG12	1.84	0.77
2:H:501:ASP:OD2	2:H:503:GLU:HB2	1.84	0.77
2:A:390:GLU:HA	2:A:393:ILE:HG13	1.66	0.77
1:O:85:C:C5	2:G:547:ILE:O	2.37	0.77
2:A:578:ILE:O	2:A:582:ILE:HG12	1.83	0.77
2:H:402:ARG:HB2	2:H:402:ARG:HH11	1.50	0.77
2:A:633:ARG:NH1	2:H:638:LYS:HZ1	1.82	0.77
1:N:89:U:O2	1:N:89:U:H2'	1.84	0.77
2:G:307:THR:HG22	2:G:493:LEU:HD21	1.67	0.77
2:H:585:HIS:HB2	2:H:593:MET:CE	2.15	0.77
2:E:411:PHE:CE2	2:E:521:PHE:HE1	2.02	0.76
2:F:276:GLU:O	2:F:279:VAL:HG22	1.84	0.76
2:C:551:GLN:NE2	2:C:597:GLY:HA2	1.98	0.76
2:F:251:LEU:HA	2:F:588:ARG:NH1	2.00	0.76
2:B:452:PHE:HE2	2:B:454:TYR:HE1	1.30	0.76
2:D:587:LEU:HD23	2:D:587:LEU:H	1.50	0.76
2:G:365:GLU:H	2:G:377:ARG:HD3	1.50	0.76
1:O:86:G:O6	2:G:599:LYS:HB2	1.86	0.76
2:F:251:LEU:HA	2:F:588:ARG:HH12	1.49	0.76
2:D:452:PHE:HE2	2:D:454:TYR:HE1	1.31	0.76
2:A:411:PHE:N	2:A:411:PHE:HD1	1.83	0.76
2:D:320:THR:HG22	2:D:321:SER:H	1.50	0.76
2:F:621:VAL:O	2:F:624:VAL:HG22	1.86	0.76
2:A:633:ARG:CZ	2:H:638:LYS:NZ	2.47	0.76
2:G:255:HIS:ND1	2:G:267:HIS:HE1	1.82	0.76
1:J:75:U:O2'	1:J:76:G:OP1	2.02	0.76
1:M:97:C:H5"	1:M:98:A:OP1	1.84	0.76
2:A:551:GLN:NE2	2:A:597:GLY:HA2	2.01	0.76
1:I:88:G:H4'	1:I:89:U:OP1	1.85	0.76
2:A:411:PHE:CE2	2:A:521:PHE:CE1	2.74	0.76
2:A:582:ILE:HA	2:A:593:MET:HE2	1.67	0.76
2:E:320:THR:HG23	2:F:319:THR:O	1.86	0.76
2:E:390:GLU:HA	2:E:393:ILE:HG13	1.68	0.76
2:D:407:MET:SD	2:D:514:ILE:HG21	2.25	0.76
2:C:637:LEU:HD12	2:C:637:LEU:H	1.50	0.76
2:D:251:LEU:HA	2:D:588:ARG:HH12	1.51	0.76
2:F:460:ALA:HB1	2:F:462:TYR:CD1	2.21	0.76
1:L:88:G:H4'	1:L:89:U:OP1	1.85	0.75
2:E:452:PHE:HE2	2:E:454:TYR:HE1	1.34	0.75
2:A:325:ARG:HG3	2:A:325:ARG:HH11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:517:SER:HB2	4:A:2002:TSB:H1'	1.68	0.75
2:E:621:VAL:O	2:E:624:VAL:HG22	1.85	0.75
1:J:97:C:H5"	1:J:98:A:OP1	1.86	0.75
2:H:299:MET:O	2:H:327:TYR:HB3	1.86	0.75
2:A:402:ARG:HH11	2:A:402:ARG:HB2	1.50	0.75
2:B:421:SER:CB	2:B:458:GLU:HB3	2.17	0.75
1:I:84:U:H4'	1:I:85:C:C5'	2.16	0.75
2:C:251:LEU:HA	2:C:588:ARG:NH1	2.02	0.75
1:K:76:G:N2	1:K:97:C:C2	2.55	0.75
2:A:298:MET:HG2	2:B:263:MET:CE	2.16	0.74
2:H:251:LEU:HA	2:H:588:ARG:NH1	2.03	0.74
2:H:411:PHE:HD2	2:H:525:LEU:CD2	1.99	0.74
2:E:473:CYS:HA	5:E:6010:HOH:O	1.86	0.74
2:A:411:PHE:HE2	2:A:521:PHE:HE1	1.33	0.74
2:E:411:PHE:N	2:E:411:PHE:CD1	2.54	0.74
1:L:88:G:H8	5:D:5016:HOH:O	1.69	0.74
2:F:321:SER:HB3	2:F:326:GLU:HA	1.70	0.74
2:A:452:PHE:HE2	2:A:454:TYR:HE1	1.33	0.74
2:H:465:LYS:HG3	2:H:484:GLN:HG2	1.68	0.74
1:P:86:G:H3'	5:P:1613:HOH:O	1.86	0.74
2:F:390:GLU:HA	2:F:393:ILE:HG13	1.69	0.74
2:A:411:PHE:CE2	2:A:521:PHE:HE1	2.06	0.74
2:H:403:LEU:HG	2:H:407:MET:CE	2.18	0.74
2:A:465:LYS:HG3	2:A:484:GLN:HG2	1.69	0.74
1:J:103:G:OP2	5:J:1025:HOH:O	2.05	0.74
2:C:251:LEU:HA	2:C:588:ARG:HH12	1.51	0.74
2:C:621:VAL:O	2:C:624:VAL:HG22	1.86	0.74
1:J:86:G:H3'	5:J:1013:HOH:O	1.88	0.74
2:C:411:PHE:HD1	2:C:411:PHE:N	1.85	0.74
2:B:585:HIS:HB2	2:B:593:MET:CE	2.17	0.74
2:B:251:LEU:HA	2:B:588:ARG:NH1	2.02	0.74
1:K:77:U:H1'	1:K:98:A:N1	2.03	0.74
2:H:452:PHE:HE2	2:H:454:TYR:HE1	1.35	0.74
2:F:578:ILE:O	2:F:582:ILE:HG12	1.88	0.73
2:E:585:HIS:HB2	2:E:593:MET:CE	2.18	0.73
2:D:390:GLU:HA	2:D:393:ILE:HG13	1.69	0.73
2:G:390:GLU:HA	2:G:393:ILE:HG13	1.68	0.73
1:O:88:G:H4'	1:O:89:U:OP1	1.86	0.73
2:G:362:HIS:HD2	5:G:732:HOH:O	1.71	0.73
1:K:82:U:H2'	1:K:83:U:H5'	1.70	0.73
2:E:276:GLU:O	2:E:279:VAL:HG22	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:637:LEU:HD12	2:H:637:LEU:H	1.53	0.73
1:L:98:A:H4'	5:L:1227:HOH:O	1.87	0.73
2:G:249:LYS:NZ	2:G:249:LYS:HB3	2.02	0.73
2:C:411:PHE:CE2	2:C:521:PHE:HE1	2.05	0.73
2:F:348:TYR:CD1	2:F:349:ARG:N	2.57	0.73
2:C:263:MET:HE2	2:D:298:MET:HG2	1.69	0.73
2:E:321:SER:HB3	2:E:326:GLU:HA	1.70	0.73
2:B:402:ARG:HB2	2:B:402:ARG:HH11	1.52	0.73
2:C:402:ARG:HH11	2:C:402:ARG:HB2	1.54	0.73
2:A:633:ARG:NH1	2:H:638:LYS:NZ	2.37	0.73
2:D:637:LEU:HD12	2:D:637:LEU:H	1.53	0.73
2:D:625:ILE:O	2:D:629:GLN:HG3	1.89	0.73
2:E:411:PHE:HD2	2:E:525:LEU:CD2	1.99	0.73
2:D:551:GLN:NE2	2:D:597:GLY:HA2	2.03	0.73
2:A:583:ARG:O	2:A:587:LEU:HD23	1.88	0.73
2:E:251:LEU:HA	2:E:588:ARG:NH1	2.04	0.73
2:F:452:PHE:HE2	2:F:454:TYR:HE1	1.35	0.73
2:D:402:ARG:HB2	2:D:402:ARG:HH11	1.53	0.73
2:H:621:VAL:O	2:H:624:VAL:HG22	1.88	0.72
2:C:411:PHE:CD1	2:C:411:PHE:N	2.57	0.72
2:A:251:LEU:HA	2:A:588:ARG:HH12	1.53	0.72
2:D:251:LEU:HA	2:D:588:ARG:NH1	2.04	0.72
2:B:411:PHE:HD2	2:B:525:LEU:CD2	2.02	0.72
2:F:501:ASP:OD2	2:F:503:GLU:HB2	1.89	0.72
1:M:69:G:OP3	1:P:105:C:O3'	2.08	0.72
2:B:411:PHE:CD1	2:B:411:PHE:N	2.51	0.72
2:D:578:ILE:O	2:D:582:ILE:HG12	1.89	0.72
2:G:547:ILE:HD12	2:G:597:GLY:HA3	1.71	0.72
1:M:88:G:H4'	1:M:89:U:OP1	1.87	0.72
1:L:78:G:O4'	2:C:345:LEU:HD23	1.89	0.72
2:F:637:LEU:HD12	2:F:637:LEU:H	1.54	0.72
2:H:390:GLU:HA	2:H:393:ILE:HG13	1.72	0.72
2:E:403:LEU:HG	2:E:407:MET:CE	2.20	0.72
2:F:517:SER:HB2	4:F:7002:TSB:H1'	1.72	0.72
2:C:403:LEU:HG	2:C:407:MET:CE	2.19	0.72
1:K:78:G:H2'	1:K:79:A:H8	1.54	0.72
2:A:277:LEU:O	2:A:281:VAL:HG23	1.89	0.72
2:F:403:LEU:HG	2:F:407:MET:CE	2.20	0.72
2:A:637:LEU:H	2:A:637:LEU:HD12	1.54	0.72
2:F:411:PHE:CE2	2:F:521:PHE:CZ	2.77	0.72
1:O:86:G:H2'	5:O:1513:HOH:O	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:578:ILE:O	2:C:582:ILE:HG12	1.90	0.72
2:G:417:VAL:CG1	2:G:471:TYR:HE1	2.03	0.72
2:E:407:MET:SD	2:E:514:ILE:HG21	2.30	0.71
1:L:89:U:O2	1:L:89:U:H2'	1.88	0.71
1:K:90:G:H8	2:C:577:LYS:CD	2.02	0.71
1:P:86:G:C4	2:H:547:ILE:HD13	2.25	0.71
2:A:411:PHE:N	2:A:411:PHE:CD1	2.56	0.71
2:H:411:PHE:N	2:H:411:PHE:HD1	1.88	0.71
2:F:547:ILE:HD12	2:F:597:GLY:HA3	1.72	0.71
2:G:392:GLN:O	2:G:396:GLU:HB2	1.89	0.71
1:J:88:G:H4'	1:J:89:U:OP1	1.90	0.71
2:A:320:THR:HG22	2:A:321:SER:H	1.54	0.71
2:E:625:ILE:O	2:E:629:GLN:HG3	1.90	0.71
2:A:462:TYR:CE2	2:A:511:HIS:CE1	2.78	0.71
1:L:79:A:H1'	2:C:502:ASN:OD1	1.90	0.71
2:G:637:LEU:H	2:G:637:LEU:HD12	1.54	0.71
2:A:585:HIS:HB2	2:A:593:MET:CE	2.21	0.71
1:O:91:G:O3'	5:O:1518:HOH:O	2.08	0.71
2:E:299:MET:O	2:E:327:TYR:HB3	1.90	0.71
2:B:625:ILE:O	2:B:629:GLN:HG3	1.91	0.71
2:C:321:SER:HB3	2:C:326:GLU:HA	1.73	0.71
2:A:280:PHE:O	2:A:283:SER:HB3	1.91	0.71
2:G:514:ILE:HG22	2:G:515:LEU:N	2.06	0.71
2:A:251:LEU:HA	2:A:588:ARG:NH1	2.05	0.71
2:C:319:THR:O	2:D:320:THR:HG23	1.91	0.71
2:C:390:GLU:HA	2:C:393:ILE:HG13	1.72	0.71
2:C:243:ASP:OD2	2:C:245:ARG:HB2	1.91	0.71
2:C:473:CYS:HA	5:C:4013:HOH:O	1.90	0.71
1:K:82:U:C2'	1:K:83:U:H5'	2.21	0.71
2:E:578:ILE:O	2:E:582:ILE:HG12	1.91	0.71
2:G:551:GLN:HE21	2:G:597:GLY:CA	2.03	0.71
2:H:277:LEU:O	2:H:281:VAL:HG23	1.91	0.71
1:K:70:G:H22	1:K:105:C:H1'	1.56	0.71
2:E:402:ARG:HB2	2:E:402:ARG:HH11	1.54	0.71
2:B:637:LEU:HD12	2:B:637:LEU:H	1.56	0.71
1:O:89:U:C5	2:G:583:ARG:CZ	2.73	0.70
2:H:547:ILE:HD12	2:H:597:GLY:HA3	1.73	0.70
1:K:97:C:H4'	1:K:98:A:OP1	1.91	0.70
2:C:298:MET:HG2	2:D:263:MET:HE2	1.73	0.70
2:G:321:SER:HB3	2:G:326:GLU:HA	1.72	0.70
1:L:77:U:H1'	1:L:98:A:N1	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:637:LEU:H	2:E:637:LEU:HD12	1.56	0.70
2:C:517:SER:HB2	4:C:4002:TSB:H1'	1.72	0.70
2:C:411:PHE:CE2	2:C:521:PHE:CZ	2.79	0.70
1:M:84:U:H4'	1:M:85:C:C5'	2.22	0.70
2:H:320:THR:HG22	2:H:321:SER:H	1.53	0.70
2:C:585:HIS:HB2	2:C:593:MET:CE	2.20	0.70
1:L:97:C:H5"	1:L:98:A:OP1	1.91	0.70
2:B:276:GLU:O	2:B:279:VAL:HG22	1.91	0.70
2:F:411:PHE:N	2:F:411:PHE:HD1	1.89	0.70
2:B:578:ILE:O	2:B:582:ILE:HG12	1.92	0.70
2:A:621:VAL:O	2:A:624:VAL:HG22	1.92	0.70
2:C:544:ILE:HD11	2:C:562:LEU:HD22	1.72	0.70
1:J:77:U:H1'	1:J:98:A:N1	2.06	0.70
2:A:462:TYR:HD2	2:A:486:ASP:OD2	1.73	0.70
2:G:501:ASP:OD2	2:G:503:GLU:HB2	1.92	0.70
1:N:84:U:H4'	1:N:85:C:C5'	2.22	0.70
2:C:460:ALA:HB1	2:C:462:TYR:CD1	2.27	0.70
2:B:321:SER:HB3	2:B:326:GLU:HA	1.72	0.70
2:D:299:MET:O	2:D:327:TYR:HB3	1.91	0.70
2:H:321:SER:HB3	2:H:326:GLU:HA	1.74	0.70
1:J:91:G:H4'	5:J:1018:HOH:O	1.92	0.70
2:F:460:ALA:HB1	2:F:462:TYR:CE1	2.26	0.70
2:A:290:TYR:CE2	2:A:512:ARG:NH1	2.60	0.70
2:D:249:LYS:NZ	2:D:249:LYS:HB3	2.07	0.70
2:D:411:PHE:N	2:D:411:PHE:CD1	2.58	0.69
1:K:92:G:H2'	1:K:93:U:O4'	1.92	0.69
2:F:592:TYR:OH	2:F:639:GLN:HB3	1.92	0.69
2:H:411:PHE:CD1	2:H:411:PHE:N	2.59	0.69
2:A:421:SER:HA	2:A:455:GLN:HB3	1.74	0.69
2:C:465:LYS:HG3	2:C:484:GLN:HG2	1.72	0.69
2:H:249:LYS:HB3	2:H:249:LYS:NZ	2.06	0.69
2:B:551:GLN:HE21	2:B:597:GLY:HA2	1.56	0.69
2:B:583:ARG:NH2	5:B:216:HOH:O	2.26	0.69
2:F:583:ARG:O	2:F:587:LEU:HD23	1.92	0.69
1:I:75:U:O2'	1:I:76:G:OP1	2.09	0.69
2:A:547:ILE:HD12	2:A:597:GLY:HA3	1.72	0.69
2:B:402:ARG:NH1	2:B:402:ARG:HB2	2.07	0.69
1:I:89:U:O2	1:I:89:U:H2'	1.90	0.69
2:G:303:LEU:HD11	2:G:339:GLN:HE21	1.57	0.69
1:P:88:G:H4'	1:P:89:U:OP1	1.92	0.69
1:I:87:U:H2'	5:I:110:HOH:O	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:460:ALA:HB1	2:A:462:TYR:CD1	2.28	0.69
2:D:585:HIS:HB2	2:D:593:MET:CE	2.23	0.69
2:F:402:ARG:NH1	2:F:402:ARG:HB2	2.06	0.69
1:K:70:G:H2'	1:K:71:C:H6	1.56	0.69
2:G:411:PHE:HD2	2:G:525:LEU:CD2	2.04	0.69
2:D:547:ILE:HD12	2:D:597:GLY:HA3	1.74	0.69
2:E:551:GLN:NE2	2:E:597:GLY:HA2	2.06	0.69
2:F:346:LYS:O	2:F:497:TYR:HA	1.93	0.69
2:H:554:TYR:O	2:H:558:LEU:HD13	1.92	0.69
2:E:421:SER:CB	2:E:458:GLU:HB3	2.21	0.69
2:E:583:ARG:O	2:E:587:LEU:HD23	1.92	0.69
1:P:77:U:H1'	1:P:98:A:N1	2.08	0.69
2:C:592:TYR:OH	2:C:639:GLN:HB3	1.92	0.69
2:B:388:CYS:HB2	2:B:392:GLN:OE1	1.93	0.69
2:F:421:SER:HA	2:F:455:GLN:HB3	1.75	0.69
2:C:583:ARG:O	2:C:587:LEU:HD23	1.92	0.69
1:K:70:G:N2	1:K:105:C:H1'	2.08	0.69
2:D:592:TYR:OH	2:D:639:GLN:HB3	1.93	0.69
2:B:551:GLN:NE2	2:B:597:GLY:HA2	2.08	0.68
2:B:411:PHE:CE2	2:B:521:PHE:CE1	2.81	0.68
1:J:78:G:O4'	2:A:345:LEU:HD23	1.93	0.68
2:F:544:ILE:HD11	2:F:562:LEU:HD22	1.75	0.68
2:F:462:TYR:CE2	2:F:511:HIS:CE1	2.81	0.68
1:J:88:G:H1'	2:B:583:ARG:HG2	1.76	0.68
1:K:105:C:H2'	1:K:105:C:O2	1.91	0.68
2:E:421:SER:HA	2:E:455:GLN:HB3	1.74	0.68
1:M:77:U:H1'	1:M:98:A:N1	2.08	0.68
2:D:321:SER:HB3	2:D:326:GLU:HA	1.75	0.68
1:P:100:U:H4'	5:P:1630:HOH:O	1.93	0.68
2:A:460:ALA:HB1	2:A:462:TYR:CE1	2.28	0.68
1:L:91:G:H4'	5:L:1218:HOH:O	1.92	0.68
2:D:421:SER:CB	2:D:458:GLU:HB3	2.22	0.68
2:H:551:GLN:HE21	2:H:597:GLY:CA	2.07	0.68
2:G:417:VAL:HG13	2:G:471:TYR:HE1	1.59	0.68
2:C:460:ALA:HB1	2:C:462:TYR:CE1	2.28	0.68
1:L:84:U:H4'	1:L:85:C:C5'	2.23	0.68
2:A:517:SER:CB	4:A:2002:TSB:H1'	2.24	0.68
1:K:91:G:O2'	1:K:92:G:H5'	1.94	0.68
1:N:77:U:H1'	1:N:98:A:N1	2.09	0.68
1:I:98:A:H4'	5:I:114:HOH:O	1.93	0.68
2:H:595:VAL:HB	2:H:607:ALA:HB3	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:465:LYS:HG3	2:F:484:GLN:HG2	1.75	0.67
2:G:411:PHE:CD1	2:G:411:PHE:N	2.62	0.67
2:B:622:ASN:ND2	5:B:226:HOH:O	2.26	0.67
1:O:89:U:H5	2:G:583:ARG:CZ	2.07	0.67
2:B:403:LEU:HG	2:B:407:MET:CE	2.22	0.67
2:A:348:TYR:CD1	2:A:349:ARG:N	2.61	0.67
1:M:91:G:O3'	5:M:1318:HOH:O	2.12	0.67
2:C:535:THR:HG22	2:C:632:ILE:HG12	1.75	0.67
2:C:421:SER:HA	2:C:455:GLN:HB3	1.75	0.67
2:D:595:VAL:HB	2:D:607:ALA:HB3	1.77	0.67
2:G:544:ILE:HD11	2:G:562:LEU:HD22	1.76	0.67
2:H:346:LYS:O	2:H:497:TYR:HA	1.93	0.67
2:H:304:TRP:CZ3	2:H:328:CYS:HB2	2.28	0.67
2:F:551:GLN:HE21	2:F:597:GLY:CA	2.08	0.67
2:A:462:TYR:HE2	2:A:511:HIS:CE1	2.12	0.67
2:D:402:ARG:NH1	2:D:402:ARG:HB2	2.10	0.67
2:G:407:MET:SD	2:G:514:ILE:HG21	2.34	0.67
2:F:290:TYR:CE2	2:F:512:ARG:NH1	2.62	0.67
2:E:554:TYR:O	2:E:557:GLU:HB3	1.94	0.67
2:E:460:ALA:HB1	2:E:462:TYR:CE1	2.30	0.67
1:J:89:U:C5	2:B:583:ARG:NH1	2.62	0.67
2:C:277:LEU:O	2:C:281:VAL:HG23	1.95	0.67
2:C:348:TYR:CD1	2:C:349:ARG:N	2.63	0.67
2:D:411:PHE:HD2	2:D:525:LEU:HD21	1.59	0.67
2:F:411:PHE:N	2:F:411:PHE:CD1	2.59	0.67
2:B:339:GLN:OE1	2:B:339:GLN:HA	1.93	0.67
2:D:403:LEU:HG	2:D:407:MET:CE	2.25	0.67
1:N:97:C:H5"	1:N:98:A:OP1	1.94	0.67
2:E:460:ALA:HB1	2:E:462:TYR:CD1	2.30	0.67
2:G:402:ARG:HB2	2:G:402:ARG:NH1	2.09	0.67
2:G:299:MET:O	2:G:327:TYR:HB3	1.95	0.67
2:A:346:LYS:O	2:A:497:TYR:HA	1.95	0.67
2:A:411:PHE:HD2	2:A:525:LEU:CD2	2.04	0.67
2:H:421:SER:HA	2:H:455:GLN:HB3	1.77	0.67
2:A:403:LEU:HG	2:A:407:MET:CE	2.25	0.67
2:A:402:ARG:NH1	2:A:402:ARG:HB2	2.10	0.67
2:D:421:SER:HA	2:D:455:GLN:HB3	1.75	0.67
2:H:392:GLN:O	2:H:396:GLU:HB2	1.95	0.67
2:B:390:GLU:HA	2:B:393:ILE:HG13	1.77	0.67
2:A:592:TYR:OH	2:A:639:GLN:HB3	1.94	0.67
1:J:89:U:C5	2:B:583:ARG:CZ	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:402:ARG:NH1	2:E:402:ARG:HB2	2.10	0.66
2:G:329:ILE:HD12	2:G:329:ILE:N	2.10	0.66
1:O:84:U:H4'	1:O:85:C:C5'	2.25	0.66
2:F:585:HIS:HB2	2:F:593:MET:HE3	1.76	0.66
2:H:585:HIS:HB2	2:H:593:MET:HE2	1.77	0.66
1:P:84:U:H4'	1:P:85:C:C5'	2.25	0.66
1:M:103:G:H5"	5:M:1325:HOH:O	1.95	0.66
2:G:585:HIS:HB2	2:G:593:MET:CE	2.25	0.66
2:C:320:THR:HG23	2:D:319:THR:O	1.95	0.66
2:F:299:MET:O	2:F:327:TYR:HB3	1.95	0.66
2:B:621:VAL:O	2:B:624:VAL:HG22	1.94	0.66
2:G:421:SER:CB	2:G:458:GLU:HB3	2.21	0.66
1:L:75:U:O2'	1:L:76:G:OP1	2.13	0.66
2:E:298:MET:HG2	2:F:263:MET:HE2	1.76	0.66
2:B:441:LEU:HD12	2:B:464:PRO:HB2	1.77	0.66
2:H:417:VAL:CG1	2:H:471:TYR:HE1	2.09	0.66
2:G:304:TRP:CZ3	2:G:328:CYS:HB2	2.30	0.66
2:C:547:ILE:HD12	2:C:597:GLY:HA3	1.76	0.66
2:B:517:SER:HB2	4:B:3002:TSB:H1'	1.78	0.66
2:C:551:GLN:HE21	2:C:597:GLY:CA	2.09	0.66
2:G:625:ILE:O	2:G:629:GLN:HG3	1.96	0.66
2:E:544:ILE:HD11	2:E:562:LEU:HD22	1.78	0.66
2:A:299:MET:O	2:A:327:TYR:HB3	1.96	0.66
2:B:544:ILE:HD11	2:B:562:LEU:HD22	1.77	0.66
2:E:411:PHE:HE2	2:E:521:PHE:CE1	2.10	0.66
1:O:89:U:O2	1:O:89:U:C2'	2.44	0.66
2:G:421:SER:HA	2:G:455:GLN:HB3	1.78	0.66
2:F:517:SER:CB	4:F:7002:TSB:H1'	2.25	0.66
2:H:402:ARG:HB2	2:H:402:ARG:NH1	2.10	0.66
2:E:348:TYR:CD1	2:E:349:ARG:N	2.64	0.66
2:D:517:SER:HB2	4:D:5002:TSB:H1'	1.78	0.66
2:A:332:MET:HE2	4:A:2002:TSB:HN12	1.60	0.66
2:F:514:ILE:HG22	2:F:515:LEU:N	2.11	0.66
2:D:583:ARG:O	2:D:587:LEU:HD23	1.95	0.66
2:E:547:ILE:HD12	2:E:597:GLY:HA3	1.77	0.66
1:I:87:U:H1'	2:A:582:ILE:HG13	1.77	0.66
2:E:592:TYR:OH	2:E:639:GLN:HB3	1.95	0.66
2:F:243:ASP:OD2	2:F:245:ARG:HB2	1.95	0.66
1:K:101:G:H2'	1:K:102:C:H6	1.61	0.66
2:C:462:TYR:CE2	2:C:511:HIS:CE1	2.84	0.66
2:G:580:PHE:HD1	2:G:580:PHE:O	1.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:544:ILE:HD11	2:D:562:LEU:HD22	1.77	0.65
2:G:417:VAL:CG1	2:G:471:TYR:CE1	2.79	0.65
2:G:332:MET:HG2	2:G:363:ARG:HH21	1.61	0.65
2:H:325:ARG:HG3	2:H:325:ARG:HH11	1.61	0.65
2:F:625:ILE:O	2:F:629:GLN:HG3	1.96	0.65
2:D:411:PHE:N	2:D:411:PHE:HD1	1.94	0.65
2:D:465:LYS:HG3	2:D:484:GLN:HG2	1.77	0.65
2:C:421:SER:CB	2:C:458:GLU:HB3	2.24	0.65
2:H:514:ILE:HG22	2:H:515:LEU:HD23	1.78	0.65
2:A:544:ILE:HD11	2:A:562:LEU:HD22	1.76	0.65
2:E:434:TRP:O	2:E:438:GLU:HG3	1.97	0.65
1:L:89:U:C5	2:D:583:ARG:CZ	2.79	0.65
2:B:547:ILE:HD12	2:B:597:GLY:HA3	1.78	0.65
2:B:243:ASP:OD2	2:B:245:ARG:HB2	1.96	0.65
1:J:84:U:H4'	1:J:85:C:C5'	2.26	0.65
2:B:325:ARG:HH11	2:B:325:ARG:HG3	1.61	0.65
1:O:77:U:H1'	1:O:98:A:N1	2.12	0.65
2:E:595:VAL:HB	2:E:607:ALA:HB3	1.79	0.65
2:F:580:PHE:O	2:F:580:PHE:HD1	1.79	0.65
2:B:554:TYR:O	2:B:558:LEU:HD13	1.96	0.65
2:B:249:LYS:NZ	2:B:249:LYS:HB3	2.12	0.65
2:H:544:ILE:HD11	2:H:562:LEU:HD22	1.78	0.65
2:H:612:ARG:HH11	2:H:612:ARG:HG3	1.62	0.65
2:B:299:MET:O	2:B:327:TYR:HB3	1.96	0.65
2:C:554:TYR:O	2:C:557:GLU:HB3	1.97	0.65
1:M:85:C:H5	2:E:547:ILE:O	1.79	0.65
2:F:407:MET:SD	2:F:514:ILE:HG21	2.35	0.65
1:K:104:C:H2'	1:K:105:C:O4'	1.97	0.65
2:G:554:TYR:O	2:G:558:LEU:HD13	1.97	0.65
1:K:90:G:OP2	2:C:577:LYS:HB2	1.96	0.65
1:N:83:U:H3	2:F:575:ASN:HD21	1.45	0.65
2:D:441:LEU:HD12	2:D:464:PRO:HB2	1.78	0.65
2:G:403:LEU:HG	2:G:407:MET:HE3	1.78	0.65
2:B:411:PHE:CE2	2:B:521:PHE:HE1	2.14	0.65
1:N:86:G:O6	2:F:599:LYS:HB2	1.97	0.65
2:A:253:LEU:O	2:A:254:TYR:HB3	1.97	0.65
1:K:70:G:H2'	1:K:71:C:C6	2.31	0.65
2:E:554:TYR:O	2:E:558:LEU:HD13	1.96	0.65
2:E:441:LEU:HD12	2:E:464:PRO:HB2	1.78	0.65
2:E:580:PHE:O	2:E:580:PHE:HD1	1.78	0.65
2:G:280:PHE:CE2	2:G:407:MET:HG2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:421:SER:CB	2:F:458:GLU:HB3	2.27	0.65
2:G:277:LEU:O	2:G:281:VAL:HG23	1.96	0.65
2:F:403:LEU:HG	2:F:407:MET:HE3	1.79	0.65
2:E:517:SER:HB2	4:E:6002:TSB:H1'	1.79	0.65
1:M:89:U:H5	2:E:583:ARG:CZ	2.10	0.64
2:H:514:ILE:HG22	2:H:515:LEU:N	2.12	0.64
2:H:583:ARG:O	2:H:587:LEU:HD23	1.97	0.64
2:A:257:GLN:OE1	2:B:339:GLN:HB3	1.96	0.64
2:C:595:VAL:HB	2:C:607:ALA:HB3	1.78	0.64
2:F:392:GLN:O	2:F:396:GLU:HB2	1.97	0.64
1:K:87:U:C2'	1:K:87:U:O2	2.45	0.64
1:K:88:G:C4'	1:K:89:U:OP1	2.45	0.64
1:J:88:G:C8	5:J:1023:HOH:O	2.50	0.64
2:B:334:CYS:N	2:B:335:PRO:HD2	2.12	0.64
2:A:249:LYS:HB3	2:A:249:LYS:NZ	2.11	0.64
1:K:90:G:H8	2:C:577:LYS:HD3	1.61	0.64
1:M:89:U:C2'	1:M:89:U:O2	2.43	0.64
2:C:299:MET:O	2:C:327:TYR:HB3	1.97	0.64
2:E:462:TYR:CE2	2:E:511:HIS:CE1	2.85	0.64
2:F:303:LEU:HD11	2:F:339:GLN:HE21	1.62	0.64
2:F:535:THR:HG22	2:F:632:ILE:HG12	1.79	0.64
1:K:86:G:C4	2:C:547:ILE:HD13	2.33	0.64
2:A:421:SER:CB	2:A:458:GLU:HB3	2.23	0.64
2:E:585:HIS:HB2	2:E:593:MET:HE1	1.79	0.64
2:A:514:ILE:HG22	2:A:515:LEU:N	2.11	0.64
2:H:417:VAL:HG13	2:H:471:TYR:HE1	1.62	0.64
2:H:391:GLU:OE1	2:H:391:GLU:N	2.30	0.64
2:B:392:GLN:O	2:B:396:GLU:HB2	1.98	0.64
2:D:339:GLN:HA	2:D:339:GLN:OE1	1.98	0.64
2:C:625:ILE:O	2:C:629:GLN:HG3	1.98	0.64
2:D:473:CYS:HA	5:D:5013:HOH:O	1.97	0.64
2:B:348:TYR:CD1	2:B:349:ARG:N	2.65	0.64
2:G:325:ARG:HG3	2:G:325:ARG:HH11	1.63	0.64
2:E:392:GLN:O	2:E:396:GLU:HB2	1.97	0.64
2:C:472:ASP:OD1	2:C:476:ARG:HB2	1.98	0.64
2:H:625:ILE:O	2:H:629:GLN:HG3	1.98	0.64
2:D:422:THR:OG1	2:D:456:LEU:HA	1.98	0.64
1:P:89:U:O2	1:P:89:U:C2'	2.46	0.64
2:A:551:GLN:HE21	2:A:597:GLY:CA	2.11	0.64
2:C:339:GLN:HB3	2:D:257:GLN:OE1	1.98	0.64
2:E:465:LYS:HG3	2:E:484:GLN:HG2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:365:GLU:H	2:F:377:ARG:HD3	1.63	0.64
2:G:411:PHE:HD1	2:G:411:PHE:N	1.94	0.64
1:N:86:G:C4	2:F:547:ILE:HD13	2.33	0.64
2:B:253:LEU:O	2:B:254:TYR:HB3	1.97	0.64
2:F:411:PHE:CE2	2:F:521:PHE:HE1	2.11	0.63
2:F:253:LEU:O	2:F:254:TYR:HB3	1.98	0.63
2:D:348:TYR:CD1	2:D:349:ARG:N	2.67	0.63
1:O:83:U:H3	2:G:575:ASN:HD21	1.45	0.63
2:D:460:ALA:HB1	2:D:462:TYR:CE1	2.33	0.63
2:F:462:TYR:HE2	2:F:511:HIS:CE1	2.16	0.63
1:O:97:C:C5'	1:O:98:A:OP1	2.45	0.63
2:A:369:SER:O	2:A:375:ARG:HD2	1.98	0.63
2:C:346:LYS:O	2:C:497:TYR:HA	1.98	0.63
2:D:243:ASP:OD2	2:D:245:ARG:HB2	1.98	0.63
2:C:402:ARG:NH1	2:C:402:ARG:HB2	2.14	0.63
2:B:411:PHE:HE2	2:B:521:PHE:HE1	1.47	0.63
2:B:421:SER:HA	2:B:455:GLN:HB3	1.80	0.63
2:G:334:CYS:N	2:G:335:PRO:HD2	2.13	0.63
2:D:417:VAL:HG13	2:D:471:TYR:HE1	1.63	0.63
1:P:84:U:H4'	1:P:85:C:O5'	1.99	0.63
1:J:87:U:H1'	2:B:582:ILE:HG13	1.81	0.63
2:C:257:GLN:HB3	2:C:259:GLU:OE2	1.98	0.63
2:F:500:GLU:C	2:F:502:ASN:H	2.02	0.63
2:B:417:VAL:HG13	2:B:471:TYR:HE1	1.64	0.63
2:D:554:TYR:O	2:D:558:LEU:HD13	1.98	0.63
2:C:612:ARG:HG3	2:C:612:ARG:HH11	1.63	0.63
2:B:628:LEU:O	2:B:632:ILE:HG13	1.99	0.63
1:O:89:U:O5'	5:O:1528:HOH:O	2.15	0.63
1:N:78:G:O4'	2:E:345:LEU:HD23	1.98	0.63
2:B:554:TYR:O	2:B:557:GLU:HB3	1.99	0.63
2:G:595:VAL:HB	2:G:607:ALA:HB3	1.80	0.62
2:C:403:LEU:HG	2:C:407:MET:HE3	1.81	0.62
1:I:78:G:O2'	1:I:79:A:H5'	1.99	0.62
2:F:417:VAL:HG13	2:F:471:TYR:HE1	1.62	0.62
2:D:460:ALA:HB1	2:D:462:TYR:CD1	2.35	0.62
1:K:79:A:C2	1:K:94:C:C2	2.87	0.62
2:C:526:THR:HG23	2:C:533:PHE:HZ	1.63	0.62
1:I:77:U:H1'	1:I:98:A:N1	2.14	0.62
2:A:630:GLN:HA	2:A:633:ARG:NH1	2.14	0.62
2:B:595:VAL:HB	2:B:607:ALA:HB3	1.79	0.62
2:A:417:VAL:HG13	2:A:471:TYR:HE1	1.62	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:417:VAL:CG1	2:A:471:TYR:HE1	2.12	0.62
2:C:249:LYS:HB3	2:C:249:LYS:NZ	2.15	0.62
2:G:391:GLU:N	2:G:391:GLU:OE1	2.32	0.62
2:C:580:PHE:HD1	2:C:580:PHE:O	1.82	0.62
2:B:583:ARG:O	2:B:587:LEU:HD23	1.99	0.62
1:K:98:A:C5	2:D:345:LEU:HB2	2.34	0.62
2:C:517:SER:CB	4:C:4002:TSB:H1'	2.28	0.62
2:H:580:PHE:HD1	2:H:580:PHE:O	1.81	0.62
1:M:84:U:H4'	1:M:85:C:O5'	2.00	0.62
2:D:392:GLN:O	2:D:396:GLU:HB2	1.98	0.62
2:E:612:ARG:HG3	2:E:612:ARG:HH11	1.63	0.62
2:F:559:THR:HG21	2:F:571:ALA:CB	2.17	0.62
2:E:277:LEU:O	2:E:281:VAL:HG23	2.00	0.62
2:A:392:GLN:O	2:A:396:GLU:HB2	1.98	0.62
2:F:627:LYS:HB3	2:F:640:LEU:HD21	1.82	0.62
2:D:610:THR:CG2	2:D:614:LYS:HB3	2.29	0.62
2:E:249:LYS:NZ	2:E:249:LYS:HB3	2.15	0.62
2:H:421:SER:CB	2:H:458:GLU:HB3	2.26	0.62
2:H:388:CYS:HB2	2:H:392:GLN:OE1	2.00	0.62
2:F:277:LEU:O	2:F:281:VAL:HG23	2.00	0.62
2:H:418:VAL:HG21	2:H:450:ILE:HG21	1.82	0.62
2:C:630:GLN:HA	2:C:633:ARG:NH1	2.14	0.62
1:I:84:U:H4'	1:I:85:C:O5'	2.00	0.62
2:G:554:TYR:O	2:G:557:GLU:HB3	1.99	0.62
2:E:417:VAL:HG13	2:E:471:TYR:HE1	1.64	0.62
2:D:585:HIS:HB2	2:D:593:MET:HE2	1.82	0.62
2:H:253:LEU:O	2:H:254:TYR:HB3	2.00	0.62
2:F:341:PHE:O	2:F:346:LYS:NZ	2.33	0.62
2:H:411:PHE:CE2	2:H:521:PHE:CE1	2.88	0.61
2:H:411:PHE:CE2	2:H:521:PHE:HE1	2.17	0.61
1:O:84:U:H4'	1:O:85:C:O5'	2.00	0.61
2:B:542:VAL:HG12	2:B:543:VAL:N	2.15	0.61
2:A:284:LYS:HG3	2:A:407:MET:HG3	1.82	0.61
1:K:73:U:C5	1:K:97:C:N4	2.67	0.61
1:K:95:A:C1'	2:D:502:ASN:HD21	2.13	0.61
2:F:249:LYS:HB3	2:F:249:LYS:NZ	2.13	0.61
2:E:627:LYS:HB3	2:E:640:LEU:HD21	1.81	0.61
2:E:253:LEU:O	2:E:254:TYR:HB3	1.99	0.61
2:B:465:LYS:HG3	2:B:484:GLN:HG2	1.82	0.61
2:H:592:TYR:OH	2:H:639:GLN:HB3	2.00	0.61
2:A:580:PHE:O	2:A:580:PHE:HD1	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:585:HIS:HB2	2:G:593:MET:HE3	1.83	0.61
2:A:595:VAL:HB	2:A:607:ALA:HB3	1.80	0.61
2:D:303:LEU:HD11	2:D:339:GLN:HE21	1.65	0.61
2:A:303:LEU:HD11	2:A:339:GLN:NE2	2.16	0.61
1:K:86:G:C5'	1:K:87:U:OP1	2.45	0.61
2:A:388:CYS:HB2	2:A:392:GLN:OE1	2.00	0.61
2:D:277:LEU:O	2:D:281:VAL:HG23	2.00	0.61
1:M:69:G:O5'	1:P:105:C:O2'	2.18	0.61
2:G:517:SER:CB	4:G:8002:TSB:H1'	2.30	0.61
2:H:310:TRP:O	2:H:314:LYS:HB3	2.01	0.61
2:G:500:GLU:C	2:G:502:ASN:H	2.03	0.61
2:C:543:VAL:HG11	2:C:585:HIS:CE1	2.36	0.61
2:D:580:PHE:HD1	2:D:580:PHE:O	1.84	0.61
1:N:75:U:O2'	1:N:76:G:OP1	2.19	0.61
2:H:500:GLU:C	2:H:502:ASN:H	2.05	0.61
2:B:257:GLN:HB3	2:B:259:GLU:OE2	2.01	0.61
2:E:422:THR:OG1	2:E:456:LEU:HA	2.00	0.61
2:G:544:ILE:HG22	2:G:555:VAL:HG13	1.81	0.61
2:D:257:GLN:HB3	2:D:259:GLU:OE2	2.01	0.61
2:G:517:SER:HB2	4:G:8002:TSB:H1'	1.81	0.61
2:G:346:LYS:O	2:G:497:TYR:HA	2.01	0.61
2:F:375:ARG:NH2	5:F:7007:HOH:O	2.27	0.61
2:C:417:VAL:CG1	2:C:471:TYR:HE1	2.14	0.61
2:C:417:VAL:HG13	2:C:471:TYR:HE1	1.66	0.61
2:G:310:TRP:O	2:G:314:LYS:HB3	2.00	0.61
2:B:580:PHE:O	2:B:580:PHE:HD1	1.83	0.61
2:G:583:ARG:O	2:G:587:LEU:HD23	2.01	0.60
2:B:280:PHE:CE2	2:B:407:MET:HG2	2.36	0.60
2:B:517:SER:CB	4:B:3002:TSB:H1'	2.31	0.60
2:C:392:GLN:O	2:C:396:GLU:HB2	2.01	0.60
1:O:86:G:O6	2:G:599:LYS:HB3	1.99	0.60
1:O:86:G:C2'	5:O:1513:HOH:O	2.45	0.60
1:O:101:G:O2'	1:O:102:C:H5'	2.01	0.60
2:E:339:GLN:HA	2:E:339:GLN:OE1	2.00	0.60
2:A:500:GLU:C	2:A:502:ASN:H	2.03	0.60
2:E:346:LYS:O	2:E:497:TYR:HA	2.01	0.60
2:C:296:PRO:HG2	2:D:265:PHE:CE1	2.35	0.60
2:D:411:PHE:CE2	2:D:521:PHE:HZ	2.14	0.60
2:F:595:VAL:HB	2:F:607:ALA:HB3	1.82	0.60
1:M:87:U:H3'	5:M:1319:HOH:O	2.00	0.60
2:H:609:ARG:O	2:H:609:ARG:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:630:GLN:HA	2:G:633:ARG:NH1	2.15	0.60
2:E:310:TRP:O	2:E:314:LYS:HB3	2.01	0.60
2:A:585:HIS:HB2	2:A:593:MET:HE3	1.84	0.60
2:F:422:THR:OG1	2:F:456:LEU:HA	2.00	0.60
2:F:284:LYS:HG3	2:F:407:MET:HG3	1.83	0.60
2:F:554:TYR:O	2:F:558:LEU:HD13	2.01	0.60
2:D:612:ARG:HH11	2:D:612:ARG:HG3	1.66	0.60
2:A:434:TRP:O	2:A:438:GLU:HG3	2.01	0.60
2:D:551:GLN:HE21	2:D:597:GLY:CA	2.14	0.60
2:B:500:GLU:C	2:B:502:ASN:H	2.04	0.60
1:M:83:U:H3	2:E:575:ASN:HD21	1.49	0.60
2:H:441:LEU:HD12	2:H:464:PRO:HB2	1.83	0.60
2:H:369:SER:O	2:H:375:ARG:HD2	2.02	0.60
2:E:403:LEU:HG	2:E:407:MET:HE3	1.84	0.60
2:A:257:GLN:HB3	2:A:259:GLU:OE2	2.02	0.60
2:A:462:TYR:CD2	2:A:486:ASP:OD2	2.54	0.60
2:G:281:VAL:HG12	2:G:285:LEU:HD12	1.82	0.60
2:F:606:VAL:O	2:F:618:SER:HA	2.01	0.60
2:D:369:SER:O	2:D:375:ARG:HD2	2.01	0.60
2:E:280:PHE:CE2	2:E:407:MET:HG2	2.37	0.60
2:F:543:VAL:HG11	2:F:585:HIS:CE1	2.36	0.60
1:M:86:G:O6	2:E:599:LYS:HB2	2.00	0.60
1:P:87:U:H2'	5:P:1619:HOH:O	2.01	0.60
2:F:462:TYR:HD2	2:F:486:ASP:OD2	1.85	0.60
1:M:87:U:H2'	5:M:1319:HOH:O	2.00	0.60
2:D:310:TRP:O	2:D:314:LYS:HB3	2.02	0.60
2:D:627:LYS:HB3	2:D:640:LEU:HD21	1.82	0.60
2:G:452:PHE:CE2	2:G:454:TYR:HE1	2.13	0.60
2:H:280:PHE:O	2:H:283:SER:HB3	2.01	0.60
2:H:517:SER:CB	4:H:9002:TSB:H1'	2.31	0.60
2:E:417:VAL:CG1	2:E:471:TYR:HE1	2.14	0.60
2:H:339:GLN:OE1	2:H:339:GLN:HA	2.02	0.60
2:H:280:PHE:CE2	2:H:407:MET:HG2	2.37	0.60
1:J:80:U:H2'	1:J:81:C:C6	2.37	0.60
2:B:630:GLN:HA	2:B:633:ARG:NH1	2.17	0.60
2:H:403:LEU:HG	2:H:407:MET:HE3	1.83	0.60
2:E:303:LEU:HD11	2:E:339:GLN:HE21	1.67	0.60
2:G:620:ASP:HB3	2:G:623:GLU:HB2	1.84	0.60
2:G:254:TYR:CE1	2:G:373:LEU:HD21	2.37	0.60
2:C:339:GLN:HA	2:C:339:GLN:OE1	2.02	0.60
2:D:393:ILE:HD11	2:D:508:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:84:U:H4'	1:N:85:C:O5'	2.02	0.60
2:C:627:LYS:HB3	2:C:640:LEU:HD21	1.82	0.60
2:A:423:ARG:HA	2:A:434:TRP:CZ3	2.37	0.59
2:F:388:CYS:HB2	2:F:392:GLN:OE1	2.02	0.59
2:A:325:ARG:HG3	2:A:325:ARG:NH1	2.10	0.59
2:E:620:ASP:HB3	2:E:623:GLU:HB2	1.84	0.59
2:A:484:GLN:HB2	2:A:511:HIS:HB2	1.84	0.59
1:M:69:G:P	1:P:105:C:O3'	2.60	0.59
2:D:500:GLU:C	2:D:502:ASN:H	2.04	0.59
2:D:346:LYS:O	2:D:497:TYR:HA	2.02	0.59
2:F:334:CYS:N	2:F:335:PRO:HD2	2.16	0.59
1:I:101:G:O2'	1:I:102:C:H5'	2.02	0.59
1:I:89:U:C5	2:A:583:ARG:NH1	2.70	0.59
2:H:517:SER:HB2	4:H:9002:TSB:H1'	1.83	0.59
1:P:101:G:O2'	1:P:102:C:H5'	2.02	0.59
2:E:500:GLU:C	2:E:502:ASN:H	2.04	0.59
2:H:257:GLN:HB3	2:H:259:GLU:OE2	2.00	0.59
2:G:253:LEU:O	2:G:254:TYR:HB3	2.01	0.59
2:E:546:ASN:OD1	2:E:573:LEU:HA	2.02	0.59
2:F:280:PHE:O	2:F:283:SER:HB3	2.02	0.59
2:C:554:TYR:O	2:C:558:LEU:HD13	2.03	0.59
2:E:369:SER:O	2:E:375:ARG:HD2	2.00	0.59
2:A:606:VAL:O	2:A:618:SER:HA	2.02	0.59
2:B:609:ARG:HG3	2:B:609:ARG:O	2.02	0.59
2:B:592:TYR:OH	2:B:639:GLN:HB3	2.03	0.59
2:A:472:ASP:OD1	2:A:476:ARG:HB2	2.01	0.59
2:E:243:ASP:OD2	2:E:245:ARG:HB2	2.00	0.59
2:H:535:THR:HG22	2:H:632:ILE:HG12	1.84	0.59
2:A:332:MET:HG2	2:A:363:ARG:HH21	1.67	0.59
2:E:535:THR:HG22	2:E:632:ILE:HG12	1.85	0.59
2:F:417:VAL:CG1	2:F:471:TYR:HE1	2.15	0.59
2:E:388:CYS:HB2	2:E:392:GLN:OE1	2.02	0.59
1:J:89:U:C6	2:B:583:ARG:CZ	2.85	0.59
1:J:84:U:H4'	1:J:85:C:O5'	2.02	0.59
2:G:247:ILE:O	2:G:250:GLN:HB2	2.02	0.59
2:G:369:SER:O	2:G:375:ARG:HD2	2.01	0.59
1:N:101:G:O2'	1:N:102:C:H5'	2.02	0.59
2:C:325:ARG:HH11	2:C:325:ARG:HG3	1.67	0.59
2:E:411:PHE:CE2	2:E:521:PHE:CZ	2.90	0.59
2:B:514:ILE:HG22	2:B:515:LEU:N	2.18	0.59
2:G:434:TRP:O	2:G:438:GLU:HG3	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:514:ILE:HG22	2:A:515:LEU:HD23	1.84	0.59
2:G:281:VAL:HG12	2:G:285:LEU:CD1	2.32	0.59
2:F:612:ARG:HH11	2:F:612:ARG:HG3	1.67	0.59
2:G:612:ARG:HH11	2:G:612:ARG:HG3	1.66	0.59
2:A:544:ILE:HG22	2:A:555:VAL:HG13	1.85	0.59
2:H:304:TRP:CE3	2:H:328:CYS:HB2	2.38	0.59
2:D:325:ARG:HH11	2:D:325:ARG:HG3	1.66	0.59
2:B:278:GLU:CB	2:B:358:PHE:HE2	2.15	0.59
2:D:273:ILE:HG23	2:D:537:LEU:HD22	1.85	0.59
2:E:517:SER:CB	4:E:6002:TSB:H1'	2.33	0.59
2:D:411:PHE:CE2	2:D:521:PHE:HE1	2.05	0.59
2:B:407:MET:SD	2:B:514:ILE:HG21	2.43	0.59
2:A:422:THR:OG1	2:A:456:LEU:HA	2.01	0.59
2:D:434:TRP:O	2:D:438:GLU:HG3	2.02	0.59
1:P:87:U:C2'	5:P:1619:HOH:O	2.51	0.59
2:H:281:VAL:HG12	2:H:285:LEU:HD12	1.84	0.59
2:F:257:GLN:HB3	2:F:259:GLU:OE2	2.02	0.59
2:E:393:ILE:HD11	2:E:508:VAL:HG11	1.85	0.59
2:H:417:VAL:CG1	2:H:471:TYR:CE1	2.86	0.59
2:F:610:THR:CG2	2:F:614:LYS:HB3	2.33	0.59
2:G:592:TYR:OH	2:G:639:GLN:HB3	2.03	0.59
2:B:346:LYS:O	2:B:497:TYR:HA	2.03	0.59
2:C:544:ILE:HG22	2:C:555:VAL:HG13	1.85	0.59
2:C:620:ASP:HB3	2:C:623:GLU:HB2	1.84	0.59
1:P:86:G:C4	2:H:547:ILE:CD1	2.85	0.59
1:J:78:G:O2'	1:J:79:A:H5'	2.03	0.59
2:D:417:VAL:CG1	2:D:471:TYR:HE1	2.16	0.59
2:D:554:TYR:O	2:D:557:GLU:HB3	2.02	0.59
2:A:329:ILE:N	2:A:329:ILE:HD12	2.17	0.59
2:B:310:TRP:O	2:B:314:LYS:HB3	2.03	0.59
2:B:585:HIS:HB2	2:B:593:MET:HE3	1.85	0.59
1:M:75:U:O2'	1:M:76:G:OP1	2.21	0.59
2:D:253:LEU:O	2:D:254:TYR:HB3	2.03	0.59
2:C:278:GLU:HB3	2:C:358:PHE:HE2	1.68	0.59
2:A:554:TYR:O	2:A:558:LEU:HD13	2.03	0.59
2:A:365:GLU:H	2:A:377:ARG:HD3	1.67	0.59
2:B:546:ASN:OD1	2:B:573:LEU:HA	2.03	0.58
2:C:303:LEU:HD11	2:C:339:GLN:HE21	1.68	0.58
2:C:556:ASN:ND2	2:C:573:LEU:HD11	2.18	0.58
2:F:351:LEU:HD22	2:F:387:PHE:O	2.03	0.58
1:K:98:A:N6	2:D:345:LEU:HD22	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:290:TYR:CE2	2:G:512:ARG:NH1	2.71	0.58
2:G:375:ARG:NH2	5:G:710:HOH:O	2.26	0.58
2:E:610:THR:CG2	2:E:614:LYS:HB3	2.33	0.58
2:B:627:LYS:HB3	2:B:640:LEU:HD21	1.85	0.58
1:O:77:U:H6	1:O:77:U:O5'	1.85	0.58
2:F:434:TRP:O	2:F:438:GLU:HG3	2.02	0.58
2:G:546:ASN:OD1	2:G:573:LEU:HA	2.04	0.58
2:E:551:GLN:HE21	2:E:597:GLY:CA	2.16	0.58
2:A:587:LEU:N	2:A:587:LEU:HD23	2.14	0.58
2:D:517:SER:CB	4:D:5002:TSB:H1'	2.33	0.58
2:A:625:ILE:O	2:A:629:GLN:HG3	2.03	0.58
2:A:535:THR:HG22	2:A:632:ILE:HG12	1.84	0.58
2:F:526:THR:HG23	2:F:533:PHE:HZ	1.68	0.58
2:C:369:SER:O	2:C:375:ARG:HD2	2.03	0.58
1:M:78:G:H5'	5:M:1339:HOH:O	2.03	0.58
2:D:411:PHE:CD2	2:D:521:PHE:CZ	2.91	0.58
2:E:257:GLN:HB3	2:E:259:GLU:OE2	2.02	0.58
2:A:417:VAL:CG1	2:A:471:TYR:CE1	2.87	0.58
2:B:418:VAL:HG21	2:B:450:ILE:HG21	1.86	0.58
2:D:418:VAL:HG21	2:D:450:ILE:HG21	1.85	0.58
2:D:535:THR:HG22	2:D:632:ILE:HG12	1.83	0.58
1:L:89:U:C5	2:D:583:ARG:NH1	2.72	0.58
2:H:325:ARG:HG3	2:H:325:ARG:NH1	2.18	0.58
2:F:369:SER:O	2:F:375:ARG:HD2	2.03	0.58
2:F:325:ARG:HG3	2:F:325:ARG:HH11	1.67	0.58
2:A:612:ARG:HH11	2:A:612:ARG:HG3	1.67	0.58
2:C:422:THR:OG1	2:C:456:LEU:HA	2.03	0.58
1:I:89:U:C2'	1:I:89:U:O2	2.51	0.58
1:N:75:U:O2'	1:N:89:U:O4	2.21	0.58
2:E:622:ASN:O	2:E:626:GLU:HG3	2.04	0.58
2:E:273:ILE:HG23	2:E:537:LEU:HD22	1.85	0.58
2:C:365:GLU:H	2:C:377:ARG:HD3	1.68	0.58
2:C:280:PHE:CE2	2:C:407:MET:HG2	2.38	0.58
2:C:514:ILE:HG22	2:C:515:LEU:N	2.19	0.58
2:G:620:ASP:O	2:G:623:GLU:HB3	2.02	0.58
2:G:303:LEU:HD11	2:G:339:GLN:NE2	2.19	0.58
2:F:630:GLN:HA	2:F:633:ARG:NH1	2.19	0.58
2:A:536:TRP:CZ3	2:A:635:ARG:HD3	2.38	0.58
2:F:472:ASP:OD1	2:F:476:ARG:HB2	2.03	0.58
2:H:278:GLU:HB3	2:H:358:PHE:HE2	1.68	0.58
2:B:612:ARG:HH11	2:B:612:ARG:HG3	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:87:U:O4	2:G:607:ALA:HB1	2.04	0.58
2:E:542:VAL:HG12	2:E:543:VAL:N	2.18	0.58
2:H:290:TYR:CE2	2:H:512:ARG:NH1	2.71	0.58
1:M:69:G:OP2	1:P:105:C:C3'	2.52	0.58
2:A:441:LEU:HD12	2:A:464:PRO:HB2	1.85	0.58
2:H:620:ASP:O	2:H:623:GLU:HB3	2.04	0.58
2:D:422:THR:O	2:D:458:GLU:O	2.21	0.58
2:F:484:GLN:HB2	2:F:511:HIS:HB2	1.85	0.58
2:C:500:GLU:C	2:C:502:ASN:H	2.06	0.58
2:F:281:VAL:HG12	2:F:285:LEU:HD12	1.86	0.58
2:A:304:TRP:CZ3	2:A:328:CYS:HB2	2.39	0.58
2:G:527:GLU:O	2:G:528:GLU:O	2.21	0.58
2:B:403:LEU:HG	2:B:407:MET:HE3	1.86	0.57
2:G:421:SER:HB3	2:G:458:GLU:CB	2.26	0.57
1:N:89:U:C2'	1:N:89:U:O2	2.50	0.57
2:H:610:THR:CG2	2:H:614:LYS:HB3	2.34	0.57
2:F:554:TYR:O	2:F:557:GLU:HB3	2.02	0.57
2:B:278:GLU:HB3	2:B:358:PHE:HE2	1.69	0.57
2:H:536:TRP:O	2:H:568:ARG:NH2	2.36	0.57
2:A:362:HIS:HE1	2:B:297:PHE:CD1	2.22	0.57
2:A:391:GLU:OE1	2:A:391:GLU:N	2.36	0.57
2:H:620:ASP:HB3	2:H:623:GLU:HB2	1.84	0.57
2:C:388:CYS:HB2	2:C:392:GLN:OE1	2.04	0.57
1:M:89:U:H5	2:E:583:ARG:NH2	2.01	0.57
1:P:97:C:C5'	1:P:98:A:OP1	2.51	0.57
2:F:280:PHE:CE2	2:F:407:MET:HG2	2.38	0.57
2:G:528:GLU:O	2:G:530:ALA:N	2.37	0.57
2:A:554:TYR:O	2:A:557:GLU:HB3	2.04	0.57
2:G:441:LEU:HD12	2:G:464:PRO:HB2	1.84	0.57
2:C:556:ASN:HD21	2:C:573:LEU:HD11	1.69	0.57
2:E:514:ILE:HG22	2:E:515:LEU:N	2.18	0.57
2:B:421:SER:HB3	2:B:458:GLU:CB	2.27	0.57
1:L:89:U:O2	1:L:89:U:C2'	2.51	0.57
2:F:423:ARG:HA	2:F:434:TRP:CZ3	2.38	0.57
2:C:338:VAL:HG11	2:C:493:LEU:HB2	1.85	0.57
2:G:341:PHE:O	2:G:346:LYS:NZ	2.36	0.57
2:D:472:ASP:OD1	2:D:476:ARG:HB2	2.04	0.57
2:E:265:PHE:CE1	2:F:296:PRO:HG2	2.39	0.57
2:F:391:GLU:OE1	2:F:391:GLU:N	2.37	0.57
2:C:620:ASP:O	2:C:623:GLU:HB3	2.04	0.57
2:B:434:TRP:O	2:B:438:GLU:HG3	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:449:ASN:ND2	2:H:452:PHE:CD2	2.72	0.57
2:D:630:GLN:HA	2:D:633:ARG:NH1	2.19	0.57
2:B:391:GLU:OE1	2:B:391:GLU:N	2.38	0.57
2:F:585:HIS:HB2	2:F:593:MET:HE1	1.86	0.57
1:P:85:C:H5	2:H:547:ILE:O	1.86	0.57
1:I:79:A:O2'	2:B:500:GLU:O	2.23	0.57
2:H:332:MET:HG2	2:H:363:ARG:HH21	1.69	0.57
1:L:84:U:H4'	1:L:85:C:O5'	2.04	0.57
2:E:462:TYR:HE2	2:E:511:HIS:CE1	2.23	0.57
2:E:403:LEU:O	2:E:407:MET:HB2	2.05	0.57
2:C:585:HIS:HB2	2:C:593:MET:HE3	1.85	0.57
1:L:89:U:H5	2:D:583:ARG:CZ	2.16	0.57
2:H:542:VAL:HG12	2:H:543:VAL:N	2.20	0.57
2:H:585:HIS:HB2	2:H:593:MET:HE3	1.85	0.57
1:J:77:U:O5'	1:J:77:U:H6	1.87	0.57
2:F:514:ILE:HG22	2:F:515:LEU:HD23	1.86	0.57
2:A:243:ASP:OD2	2:A:245:ARG:HB2	2.04	0.57
2:A:636:SER:OG	2:A:638:LYS:HD3	2.04	0.57
2:D:606:VAL:O	2:D:618:SER:HA	2.05	0.57
2:D:620:ASP:O	2:D:624:VAL:HG13	2.04	0.57
2:D:411:PHE:CD2	2:D:521:PHE:HZ	2.23	0.57
2:C:375:ARG:NH2	5:C:4008:HOH:O	2.36	0.57
2:A:536:TRP:CE3	2:A:635:ARG:HD3	2.39	0.57
1:J:101:G:O2'	1:J:102:C:H5'	2.05	0.57
2:G:403:LEU:O	2:G:407:MET:HB2	2.04	0.57
2:A:403:LEU:HG	2:A:407:MET:HE3	1.85	0.57
1:I:84:U:H4'	1:I:85:C:H5'	1.86	0.57
1:K:79:A:O2'	2:D:500:GLU:O	2.22	0.57
2:B:325:ARG:NH1	2:B:325:ARG:HG3	2.19	0.57
1:L:101:G:O2'	1:L:102:C:H5'	2.05	0.57
2:B:620:ASP:HB3	2:B:623:GLU:HB2	1.87	0.57
2:H:422:THR:OG1	2:H:456:LEU:HA	2.05	0.57
2:H:547:ILE:HD12	2:H:597:GLY:CA	2.35	0.57
2:D:403:LEU:HG	2:D:407:MET:HE3	1.87	0.57
2:E:620:ASP:O	2:E:624:VAL:HG13	2.05	0.57
2:H:243:ASP:OD2	2:H:245:ARG:HB2	2.04	0.57
2:B:332:MET:HG2	2:B:363:ARG:HH21	1.70	0.56
2:H:587:LEU:HD23	2:H:587:LEU:N	2.19	0.56
2:B:500:GLU:OE1	2:B:500:GLU:N	2.37	0.56
2:H:341:PHE:O	2:H:346:LYS:NZ	2.35	0.56
2:G:325:ARG:HG3	2:G:325:ARG:NH1	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:417:VAL:CG1	2:B:471:TYR:HE1	2.18	0.56
2:B:610:THR:CG2	2:B:614:LYS:HB3	2.34	0.56
2:D:484:GLN:HB2	2:D:511:HIS:HB2	1.87	0.56
1:P:75:U:O2'	1:P:76:G:OP1	2.23	0.56
2:A:633:ARG:NH2	2:H:638:LYS:HD2	2.18	0.56
2:G:285:LEU:HD22	2:G:290:TYR:CG	2.40	0.56
1:M:80:U:H2'	1:M:81:C:C6	2.40	0.56
2:E:418:VAL:HG21	2:E:450:ILE:HG21	1.86	0.56
2:G:536:TRP:O	2:G:568:ARG:NH2	2.38	0.56
2:H:365:GLU:H	2:H:377:ARG:HD3	1.69	0.56
2:C:536:TRP:O	2:C:568:ARG:NH2	2.38	0.56
2:B:638:LYS:HB2	2:B:642:GLU:HG3	1.87	0.56
2:G:411:PHE:CE2	2:G:521:PHE:CE1	2.94	0.56
2:D:620:ASP:HB3	2:D:623:GLU:HB2	1.87	0.56
2:C:546:ASN:OD1	2:C:573:LEU:HA	2.05	0.56
2:G:542:VAL:HG12	2:G:543:VAL:N	2.20	0.56
2:B:277:LEU:O	2:B:281:VAL:HG23	2.06	0.56
2:D:542:VAL:HG12	2:D:543:VAL:N	2.21	0.56
1:J:89:U:O2	1:J:89:U:C2'	2.48	0.56
2:C:253:LEU:O	2:C:254:TYR:HB3	2.05	0.56
2:G:624:VAL:HG23	2:G:625:ILE:N	2.20	0.56
2:C:462:TYR:HE2	2:C:511:HIS:CE1	2.21	0.56
2:G:339:GLN:OE1	2:G:339:GLN:HA	2.05	0.56
2:G:332:MET:HG2	2:G:363:ARG:NH2	2.21	0.56
1:J:80:U:H2'	1:J:81:C:H6	1.70	0.56
2:H:309:HIS:HB3	2:H:317:MET:CE	2.36	0.56
1:O:93:U:N3	1:O:94:C:C5	2.74	0.56
2:A:297:PHE:CD1	2:B:362:HIS:HE1	2.22	0.56
2:H:472:ASP:OD1	2:H:476:ARG:HB2	2.04	0.56
2:C:397:VAL:O	2:C:400:CYS:HB2	2.04	0.56
2:F:309:HIS:HB3	2:F:317:MET:CE	2.35	0.56
2:F:332:MET:HG2	2:F:363:ARG:HH21	1.70	0.56
2:A:620:ASP:HB3	2:A:623:GLU:HB2	1.87	0.56
2:A:304:TRP:CE3	2:A:328:CYS:HB2	2.40	0.56
2:F:278:GLU:HB3	2:F:358:PHE:HE2	1.70	0.56
2:E:312:ASN:O	2:E:313:TYR:HB2	2.06	0.56
1:M:89:U:C5	2:E:583:ARG:NH1	2.73	0.56
2:F:338:VAL:HG11	2:F:493:LEU:HB2	1.88	0.56
2:D:514:ILE:HG22	2:D:515:LEU:N	2.20	0.56
2:F:609:ARG:HG3	2:F:609:ARG:O	2.05	0.56
2:E:304:TRP:CZ3	2:E:328:CYS:HB2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:391:GLU:OE1	2:D:391:GLU:N	2.38	0.56
2:G:514:ILE:HG22	2:G:515:LEU:HD23	1.87	0.56
2:D:544:ILE:HG22	2:D:555:VAL:HG13	1.87	0.56
2:B:544:ILE:HG12	2:B:594:LEU:HD12	1.88	0.56
2:G:587:LEU:HD23	2:G:587:LEU:N	2.16	0.56
2:D:462:TYR:CE2	2:D:511:HIS:CE1	2.93	0.56
1:P:87:U:C2'	1:P:88:G:OP2	2.53	0.56
2:G:624:VAL:CG2	2:G:625:ILE:N	2.67	0.56
1:K:95:A:H1'	2:D:502:ASN:HD21	1.71	0.56
2:H:249:LYS:HB3	2:H:249:LYS:HZ3	1.69	0.56
2:C:620:ASP:O	2:C:624:VAL:HG13	2.06	0.56
2:E:338:VAL:HG11	2:E:493:LEU:HB2	1.88	0.56
1:M:75:U:O2'	1:M:89:U:O4	2.22	0.56
2:H:281:VAL:HG12	2:H:285:LEU:CD1	2.35	0.56
2:H:400:CYS:SG	2:H:512:ARG:HG3	2.46	0.56
2:F:312:ASN:O	2:F:313:TYR:HB2	2.06	0.56
2:H:273:ILE:HG23	2:H:537:LEU:CD2	2.36	0.56
2:C:555:VAL:HB	2:C:573:LEU:HD21	1.88	0.56
1:M:87:U:C2'	5:M:1319:HOH:O	2.54	0.56
2:F:418:VAL:HG21	2:F:450:ILE:HG21	1.88	0.56
2:D:312:ASN:O	2:D:313:TYR:HB2	2.05	0.56
2:B:369:SER:O	2:B:375:ARG:HD2	2.06	0.56
1:M:77:U:H6	1:M:77:U:O5'	1.89	0.56
2:H:403:LEU:O	2:H:407:MET:HB2	2.06	0.56
2:A:547:ILE:HD12	2:A:597:GLY:CA	2.36	0.56
1:I:78:G:O4'	2:B:345:LEU:HD23	2.06	0.56
2:D:280:PHE:CE2	2:D:407:MET:HG2	2.41	0.56
2:D:334:CYS:N	2:D:335:PRO:HD2	2.21	0.56
2:C:312:ASN:O	2:C:313:TYR:HB2	2.06	0.56
2:G:312:ASN:O	2:G:313:TYR:HB2	2.05	0.56
2:D:332:MET:HG2	2:D:363:ARG:HH21	1.70	0.56
1:I:97:C:H5"	1:I:98:A:OP1	2.05	0.56
2:A:249:LYS:HB3	2:A:249:LYS:HZ3	1.69	0.56
2:G:609:ARG:O	2:G:609:ARG:HG3	2.06	0.56
2:B:526:THR:O	2:B:530:ALA:N	2.37	0.56
2:F:304:TRP:CZ3	2:F:328:CYS:HB2	2.40	0.56
2:B:259:GLU:CD	2:B:259:GLU:H	2.07	0.55
2:H:418:VAL:HG21	2:H:450:ILE:CG2	2.35	0.55
2:A:301:ARG:O	2:A:305:GLU:HG3	2.06	0.55
2:H:630:GLN:HA	2:H:633:ARG:NH1	2.21	0.55
2:E:391:GLU:OE1	2:E:391:GLU:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:86:G:O6	2:H:599:LYS:CB	2.54	0.55
2:F:422:THR:O	2:F:458:GLU:O	2.22	0.55
2:G:304:TRP:CE3	2:G:328:CYS:HB2	2.41	0.55
2:B:556:ASN:ND2	2:B:573:LEU:HD11	2.21	0.55
2:B:585:HIS:HB2	2:B:593:MET:HE1	1.86	0.55
2:H:259:GLU:H	2:H:259:GLU:CD	2.07	0.55
2:E:628:LEU:O	2:E:632:ILE:HG13	2.07	0.55
2:E:630:GLN:HA	2:E:633:ARG:NH1	2.21	0.55
1:M:78:G:C5'	5:M:1339:HOH:O	2.53	0.55
2:G:411:PHE:CE2	2:G:521:PHE:HE1	2.24	0.55
2:C:547:ILE:HD12	2:C:597:GLY:CA	2.37	0.55
2:E:386:ILE:HG21	2:E:396:GLU:HG3	1.89	0.55
1:K:73:U:O4	1:K:97:C:N3	2.39	0.55
2:D:249:LYS:HZ3	2:D:249:LYS:HB3	1.68	0.55
2:G:309:HIS:HB3	2:G:317:MET:CE	2.36	0.55
2:E:472:ASP:OD1	2:E:476:ARG:HB2	2.06	0.55
2:C:310:TRP:O	2:C:314:LYS:HB3	2.06	0.55
2:B:556:ASN:HD21	2:B:573:LEU:HD11	1.72	0.55
2:G:422:THR:HB	2:G:438:GLU:OE2	2.06	0.55
2:A:578:ILE:HD11	2:A:595:VAL:CG2	2.36	0.55
2:H:397:VAL:O	2:H:400:CYS:HB2	2.07	0.55
2:D:386:ILE:HG21	2:D:396:GLU:CG	2.37	0.55
2:E:362:HIS:HE1	2:F:297:PHE:CD1	2.24	0.55
2:F:304:TRP:CE3	2:F:328:CYS:HB2	2.42	0.55
2:A:310:TRP:O	2:A:314:LYS:HB3	2.06	0.55
2:H:443:VAL:O	2:H:447:GLU:HB2	2.05	0.55
2:F:546:ASN:OD1	2:F:573:LEU:HA	2.06	0.55
2:E:259:GLU:H	2:E:259:GLU:CD	2.08	0.55
1:K:97:C:C4'	1:K:98:A:OP1	2.55	0.55
2:A:620:ASP:O	2:A:623:GLU:HB3	2.07	0.55
2:B:418:VAL:HG21	2:B:450:ILE:CG2	2.36	0.55
2:H:312:ASN:O	2:H:313:TYR:HB2	2.06	0.55
2:B:606:VAL:O	2:B:618:SER:HA	2.06	0.55
2:G:416:ILE:O	2:G:416:ILE:HG22	2.06	0.55
1:M:93:U:H2'	1:M:94:C:H6	1.71	0.55
2:F:620:ASP:O	2:F:624:VAL:HG13	2.06	0.55
1:K:83:U:C2'	1:K:84:U:H5'	2.36	0.55
1:J:97:C:C5'	1:J:98:A:OP1	2.54	0.55
2:G:254:TYR:CD2	2:G:255:HIS:N	2.74	0.55
2:C:301:ARG:O	2:C:305:GLU:HG3	2.07	0.55
2:F:536:TRP:O	2:F:568:ARG:NH2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:556:ASN:ND2	2:F:573:LEU:HD11	2.22	0.55
2:G:569:VAL:HG22	2:G:570:LYS:N	2.21	0.55
2:G:329:ILE:CD1	2:G:329:ILE:N	2.70	0.55
2:F:417:VAL:CG1	2:F:471:TYR:CE1	2.89	0.55
2:E:417:VAL:CG1	2:E:471:TYR:CE1	2.89	0.55
2:C:265:PHE:CE1	2:D:296:PRO:HG2	2.41	0.55
2:H:544:ILE:HG22	2:H:555:VAL:HG13	1.88	0.55
2:B:421:SER:HB3	2:B:458:GLU:C	2.27	0.55
2:C:423:ARG:HA	2:C:434:TRP:CZ3	2.41	0.55
1:K:90:G:C8	2:C:577:LYS:CD	2.87	0.55
2:G:388:CYS:HB2	2:G:392:GLN:OE1	2.05	0.55
2:G:610:THR:CG2	2:G:614:LYS:HB3	2.37	0.55
2:C:609:ARG:HG3	2:C:609:ARG:O	2.07	0.55
2:B:365:GLU:H	2:B:377:ARG:HD3	1.72	0.55
1:O:75:U:O2'	1:O:76:G:OP1	2.24	0.55
2:A:298:MET:CG	2:B:263:MET:HE2	2.32	0.55
1:K:83:U:O2'	1:K:84:U:H5'	2.07	0.55
2:E:585:HIS:HB2	2:E:593:MET:HE3	1.88	0.55
2:G:452:PHE:HE2	2:G:454:TYR:CE1	2.13	0.55
2:E:339:GLN:HB3	2:F:257:GLN:OE1	2.06	0.55
2:A:462:TYR:HE2	2:A:511:HIS:NE2	2.04	0.55
2:D:351:LEU:HD22	2:D:387:PHE:O	2.07	0.55
1:J:72:G:H2'	1:J:73:U:H6	1.72	0.55
2:D:388:CYS:HB2	2:D:392:GLN:OE1	2.06	0.54
2:G:259:GLU:H	2:G:259:GLU:CD	2.11	0.54
1:L:78:G:O2'	1:L:79:A:H5'	2.06	0.54
2:B:484:GLN:HB2	2:B:511:HIS:HB2	1.89	0.54
2:G:627:LYS:HB3	2:G:640:LEU:HD21	1.89	0.54
2:D:304:TRP:CZ3	2:D:328:CYS:HB2	2.43	0.54
2:G:407:MET:CE	2:G:407:MET:CG	2.85	0.54
2:F:547:ILE:HD12	2:F:597:GLY:CA	2.36	0.54
2:H:393:ILE:HD11	2:H:508:VAL:HG11	1.89	0.54
1:M:97:C:C5'	1:M:98:A:OP1	2.52	0.54
2:H:338:VAL:HG11	2:H:493:LEU:HB2	1.89	0.54
2:D:284:LYS:HG3	2:D:407:MET:HG3	1.90	0.54
2:E:298:MET:HG2	2:F:263:MET:CE	2.36	0.54
2:C:334:CYS:N	2:C:335:PRO:HD2	2.22	0.54
2:H:554:TYR:O	2:H:557:GLU:HB3	2.06	0.54
2:H:303:LEU:HD11	2:H:339:GLN:HE21	1.72	0.54
2:F:597:GLY:O	2:F:601:VAL:HG23	2.06	0.54
2:G:257:GLN:HB3	2:G:259:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:403:LEU:O	2:D:407:MET:HB2	2.07	0.54
2:A:546:ASN:OD1	2:A:573:LEU:HA	2.08	0.54
2:E:263:MET:HE2	2:F:298:MET:HG2	1.89	0.54
2:B:441:LEU:O	2:B:444:ALA:HB3	2.07	0.54
2:E:638:LYS:HB2	2:E:642:GLU:HG3	1.89	0.54
2:D:417:VAL:CG1	2:D:471:TYR:CE1	2.91	0.54
2:F:638:LYS:HB2	2:F:642:GLU:HG3	1.90	0.54
2:H:334:CYS:N	2:H:335:PRO:HD2	2.23	0.54
2:G:484:GLN:HB2	2:G:511:HIS:HB2	1.88	0.54
2:A:578:ILE:HD11	2:A:595:VAL:HG22	1.88	0.54
2:E:386:ILE:HG21	2:E:396:GLU:CG	2.38	0.54
2:H:460:ALA:HB1	2:H:462:TYR:CD1	2.42	0.54
2:A:341:PHE:O	2:A:346:LYS:NZ	2.38	0.54
2:G:335:PRO:HG2	2:G:336:GLY:H	1.72	0.54
2:C:417:VAL:CG1	2:C:471:TYR:CE1	2.89	0.54
2:E:309:HIS:HB3	2:E:317:MET:CE	2.38	0.54
2:F:536:TRP:CE3	2:F:635:ARG:HD3	2.43	0.54
2:E:365:GLU:H	2:E:377:ARG:HD3	1.71	0.54
2:A:526:THR:HG23	2:A:533:PHE:HZ	1.72	0.54
2:D:325:ARG:NH1	2:D:325:ARG:HG3	2.22	0.54
1:M:78:G:O4'	2:F:345:LEU:HD23	2.08	0.54
2:A:536:TRP:O	2:A:568:ARG:NH2	2.40	0.54
2:G:383:ASP:OD2	2:G:385:HIS:CE1	2.60	0.54
2:F:556:ASN:HD21	2:F:573:LEU:HD11	1.73	0.54
2:B:284:LYS:HG3	2:B:407:MET:HG3	1.90	0.54
2:G:422:THR:O	2:G:458:GLU:O	2.25	0.54
2:H:434:TRP:O	2:H:438:GLU:HG3	2.08	0.54
2:A:351:LEU:HD22	2:A:387:PHE:O	2.07	0.54
1:K:101:G:H2'	1:K:102:C:C6	2.41	0.54
2:H:284:LYS:HG3	2:H:407:MET:HG3	1.90	0.54
2:D:610:THR:HG21	2:D:614:LYS:HB3	1.90	0.54
2:C:331:PRO:O	2:C:361:CYS:HB3	2.07	0.54
2:G:278:GLU:HB3	2:G:358:PHE:HE2	1.72	0.54
2:B:309:HIS:HB3	2:B:317:MET:CE	2.37	0.54
2:B:313:TYR:HB3	2:B:317:MET:HE1	1.89	0.54
2:A:312:ASN:O	2:A:313:TYR:HB2	2.06	0.54
2:D:546:ASN:OD1	2:D:573:LEU:HA	2.08	0.54
2:E:422:THR:O	2:E:458:GLU:O	2.25	0.54
2:A:288:TYR:CD1	2:A:288:TYR:N	2.76	0.54
2:D:290:TYR:CE2	2:D:512:ARG:NH1	2.75	0.54
2:C:332:MET:HG2	2:C:363:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:557:GLU:O	2:F:560:GLN:HB3	2.08	0.54
2:F:539:PRO:O	2:F:568:ARG:HD2	2.07	0.54
2:C:610:THR:CG2	2:C:614:LYS:HB3	2.38	0.54
2:E:606:VAL:O	2:E:618:SER:HA	2.08	0.54
2:C:391:GLU:N	2:C:391:GLU:OE1	2.40	0.54
2:E:423:ARG:HA	2:E:434:TRP:CZ3	2.42	0.54
2:H:462:TYR:CE2	2:H:511:HIS:CE1	2.96	0.54
2:E:330:LYS:O	5:E:6011:HOH:O	2.18	0.54
2:F:441:LEU:HD12	2:F:464:PRO:HB2	1.89	0.54
2:B:273:ILE:HG23	2:B:537:LEU:HD22	1.90	0.54
2:D:411:PHE:HE2	2:D:521:PHE:CZ	2.10	0.54
2:G:578:ILE:HD11	2:G:595:VAL:HG22	1.90	0.54
2:C:585:HIS:HB2	2:C:593:MET:HE1	1.88	0.54
2:B:423:ARG:HD2	2:B:438:GLU:OE2	2.07	0.54
2:D:421:SER:HB3	2:D:458:GLU:C	2.28	0.54
1:K:83:U:H1'	1:K:90:G:C6	2.43	0.54
2:A:627:LYS:HB3	2:A:640:LEU:HD21	1.90	0.54
2:A:259:GLU:CD	2:A:259:GLU:H	2.09	0.54
2:A:281:VAL:HG12	2:A:285:LEU:HD12	1.90	0.54
2:G:365:GLU:N	2:G:377:ARG:HD3	2.21	0.54
2:A:544:ILE:HG12	2:A:594:LEU:HD12	1.89	0.54
2:F:335:PRO:HG2	2:F:336:GLY:H	1.72	0.54
2:E:362:HIS:HD2	5:E:6011:HOH:O	1.91	0.54
2:G:465:LYS:HG3	2:G:484:GLN:HG2	1.90	0.54
2:H:274:PHE:CE1	2:H:518:MET:HG3	2.43	0.54
2:D:536:TRP:CE3	2:D:635:ARG:HD3	2.43	0.54
2:F:544:ILE:HG22	2:F:555:VAL:HG13	1.89	0.54
2:F:620:ASP:HB3	2:F:623:GLU:HB2	1.89	0.54
2:B:620:ASP:O	2:B:623:GLU:HB3	2.08	0.54
2:A:411:PHE:CE2	2:A:521:PHE:CZ	2.96	0.54
2:H:578:ILE:HD11	2:H:595:VAL:HG22	1.90	0.54
2:A:542:VAL:HG12	2:A:543:VAL:N	2.23	0.54
1:J:75:U:O2'	1:J:89:U:O4	2.24	0.54
2:E:484:GLN:HB2	2:E:511:HIS:HB2	1.90	0.54
2:D:273:ILE:HG23	2:D:537:LEU:CD2	2.38	0.54
2:G:380:THR:N	2:G:519:GLU:OE2	2.41	0.54
2:E:325:ARG:HH11	2:E:325:ARG:HG3	1.73	0.54
2:E:332:MET:HG2	2:E:363:ARG:HH21	1.72	0.53
2:E:284:LYS:HG3	2:E:407:MET:HG3	1.88	0.53
2:H:461:PHE:C	2:H:461:PHE:CD1	2.81	0.53
2:E:604:GLY:O	2:E:621:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:580:PHE:CD1	2:E:580:PHE:C	2.82	0.53
2:H:335:PRO:HG2	2:H:336:GLY:H	1.73	0.53
2:A:309:HIS:HB3	2:A:317:MET:CE	2.37	0.53
2:D:278:GLU:HB3	2:D:358:PHE:HE2	1.73	0.53
2:E:281:VAL:HG12	2:E:285:LEU:HD12	1.91	0.53
1:O:75:U:O2'	1:O:89:U:O4	2.25	0.53
2:H:423:ARG:HA	2:H:434:TRP:CZ3	2.44	0.53
2:A:585:HIS:HB2	2:A:593:MET:HE1	1.90	0.53
2:D:338:VAL:HG11	2:D:493:LEU:HB2	1.89	0.53
2:H:460:ALA:HB1	2:H:462:TYR:CE1	2.43	0.53
2:G:400:CYS:SG	2:G:512:ARG:HG3	2.48	0.53
2:A:622:ASN:O	2:A:626:GLU:HG3	2.07	0.53
2:H:606:VAL:O	2:H:618:SER:HA	2.08	0.53
2:F:310:TRP:O	2:F:314:LYS:HB3	2.08	0.53
2:G:422:THR:OG1	2:G:456:LEU:HA	2.08	0.53
1:I:86:G:C2'	5:I:109:HOH:O	2.45	0.53
2:B:422:THR:OG1	2:B:456:LEU:HA	2.09	0.53
2:A:583:ARG:O	2:A:587:LEU:CD2	2.55	0.53
1:M:89:U:C6	2:E:583:ARG:CZ	2.92	0.53
2:B:338:VAL:HG11	2:B:493:LEU:HB2	1.91	0.53
2:E:624:VAL:CG2	2:E:625:ILE:N	2.72	0.53
2:B:637:LEU:HD12	2:B:637:LEU:N	2.22	0.53
2:D:473:CYS:HB2	2:D:527:GLU:OE1	2.09	0.53
2:C:325:ARG:NH1	2:C:325:ARG:HG3	2.23	0.53
2:G:278:GLU:CB	2:G:358:PHE:HE2	2.22	0.53
1:P:103:G:C5'	5:P:1625:HOH:O	2.56	0.53
2:A:278:GLU:HB3	2:A:358:PHE:HE2	1.74	0.53
2:F:572:ASP:OD2	2:F:574:ARG:NH2	2.31	0.53
2:C:559:THR:HG21	2:C:571:ALA:CB	2.20	0.53
2:H:622:ASN:ND2	5:H:826:HOH:O	2.36	0.53
2:H:422:THR:O	2:H:458:GLU:O	2.26	0.53
2:G:547:ILE:HD12	2:G:597:GLY:CA	2.37	0.53
2:B:386:ILE:HG21	2:B:396:GLU:HG3	1.90	0.53
1:P:86:G:O6	2:H:599:LYS:HB2	2.09	0.53
2:H:348:TYR:CD1	2:H:348:TYR:C	2.82	0.53
2:F:403:LEU:O	2:F:407:MET:HB2	2.08	0.53
2:F:325:ARG:HG3	2:F:325:ARG:NH1	2.23	0.53
2:B:375:ARG:NH1	5:B:210:HOH:O	2.35	0.53
1:P:103:G:H5"	5:P:1625:HOH:O	2.08	0.53
1:O:80:U:H2'	1:O:81:C:C6	2.44	0.53
2:C:600:GLU:HB3	2:C:605:LYS:O	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:638:LYS:HB2	2:C:642:GLU:HG3	1.90	0.53
2:D:556:ASN:ND2	2:D:573:LEU:HD11	2.23	0.53
2:H:624:VAL:CG2	2:H:625:ILE:N	2.71	0.53
2:F:555:VAL:HB	2:F:573:LEU:HD21	1.89	0.53
2:B:620:ASP:O	2:B:624:VAL:HG13	2.08	0.53
1:K:84:U:H4'	1:K:85:C:O5'	2.09	0.53
2:F:410:THR:C	2:F:411:PHE:HD1	2.12	0.53
1:I:88:G:H1'	2:A:583:ARG:HG2	1.90	0.53
1:N:79:A:O2'	2:E:502:ASN:HB2	2.07	0.53
2:A:320:THR:CG2	2:B:319:THR:H	2.22	0.53
2:E:620:ASP:O	2:E:623:GLU:HB3	2.08	0.53
2:H:637:LEU:HD12	2:H:637:LEU:N	2.22	0.53
2:F:339:GLN:OE1	2:F:339:GLN:HA	2.08	0.53
2:G:301:ARG:O	2:G:305:GLU:HG3	2.08	0.53
1:P:77:U:O5'	1:P:77:U:H6	1.92	0.53
1:K:98:A:C6	2:D:345:LEU:HB2	2.42	0.53
2:A:620:ASP:O	2:A:624:VAL:HG13	2.08	0.53
2:C:539:PRO:O	2:C:568:ARG:HD2	2.08	0.53
2:F:288:TYR:CD1	2:F:288:TYR:N	2.77	0.53
2:B:550:SER:C	2:B:552:SER:H	2.12	0.53
2:B:288:TYR:HD1	2:B:288:TYR:N	2.07	0.53
2:B:422:THR:HB	2:B:438:GLU:OE2	2.09	0.53
2:D:288:TYR:N	2:D:288:TYR:HD1	2.06	0.53
2:D:288:TYR:N	2:D:288:TYR:CD1	2.77	0.53
2:H:278:GLU:CB	2:H:358:PHE:HE2	2.22	0.53
2:A:356:ALA:HA	2:A:384:ALA:HA	1.91	0.53
2:E:600:GLU:HB3	2:E:605:LYS:O	2.09	0.53
2:E:421:SER:HB3	2:E:458:GLU:C	2.28	0.53
2:A:339:GLN:OE1	2:A:339:GLN:HA	2.09	0.53
2:E:334:CYS:N	2:E:335:PRO:HD2	2.24	0.53
2:B:472:ASP:OD1	2:B:476:ARG:HB2	2.09	0.53
2:H:329:ILE:N	2:H:329:ILE:HD12	2.24	0.53
2:D:329:ILE:N	2:D:329:ILE:HD12	2.24	0.53
2:B:281:VAL:HG12	2:B:285:LEU:HD12	1.90	0.53
2:A:338:VAL:HG11	2:A:493:LEU:HB2	1.91	0.53
2:C:259:GLU:CD	2:C:259:GLU:H	2.12	0.53
2:B:298:MET:HE2	2:B:327:TYR:CD1	2.44	0.53
2:C:403:LEU:O	2:C:407:MET:HB2	2.08	0.53
2:C:284:LYS:HG3	2:C:407:MET:HG3	1.90	0.53
2:D:259:GLU:CD	2:D:259:GLU:H	2.10	0.53
2:A:254:TYR:CZ	2:A:373:LEU:HD21	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:G:OP2	1:P:105:C:H2'	2.09	0.53
2:A:555:VAL:HB	2:A:573:LEU:HD21	1.90	0.53
2:A:638:LYS:HB2	2:A:642:GLU:HG3	1.90	0.53
2:H:627:LYS:HB3	2:H:640:LEU:HD21	1.89	0.53
2:B:288:TYR:CD1	2:B:288:TYR:N	2.76	0.53
2:G:243:ASP:OD2	2:G:245:ARG:HB2	2.08	0.53
2:C:423:ARG:HD2	2:C:438:GLU:OE2	2.08	0.52
1:P:75:U:O2'	1:P:89:U:O4	2.26	0.52
2:F:421:SER:HB3	2:F:458:GLU:C	2.30	0.52
2:D:281:VAL:HG12	2:D:285:LEU:HD12	1.91	0.52
2:H:375:ARG:NH2	5:H:810:HOH:O	2.17	0.52
2:H:247:ILE:O	2:H:250:GLN:HB2	2.09	0.52
2:G:462:TYR:CE2	2:G:511:HIS:CE1	2.96	0.52
2:A:334:CYS:N	2:A:335:PRO:HD2	2.24	0.52
2:E:288:TYR:CD1	2:E:288:TYR:N	2.77	0.52
1:P:80:U:H2'	1:P:81:C:C6	2.44	0.52
2:D:556:ASN:HD21	2:D:573:LEU:HD11	1.74	0.52
2:F:423:ARG:HG2	2:F:423:ARG:O	2.10	0.52
2:B:551:GLN:HE21	2:B:597:GLY:CA	2.20	0.52
2:C:281:VAL:HG12	2:C:285:LEU:HD12	1.91	0.52
2:A:288:TYR:HD1	2:A:288:TYR:N	2.07	0.52
2:D:301:ARG:O	2:D:305:GLU:HG3	2.09	0.52
2:A:362:HIS:CE1	2:B:297:PHE:CG	2.97	0.52
1:O:93:U:C2	1:O:94:C:C5	2.97	0.52
2:D:536:TRP:O	2:D:568:ARG:NH2	2.42	0.52
2:E:278:GLU:HB3	2:E:358:PHE:HE2	1.74	0.52
2:E:297:PHE:CD1	2:F:362:HIS:HE1	2.27	0.52
2:G:418:VAL:HG21	2:G:450:ILE:HG21	1.90	0.52
2:A:416:ILE:HG22	2:A:416:ILE:O	2.09	0.52
2:D:622:ASN:O	2:D:626:GLU:HG3	2.09	0.52
2:E:332:MET:HE2	4:E:6002:TSB:HN12	1.74	0.52
2:C:422:THR:O	2:C:458:GLU:O	2.27	0.52
2:E:543:VAL:HG11	2:E:585:HIS:CE1	2.44	0.52
2:H:578:ILE:HD11	2:H:595:VAL:CG2	2.38	0.52
1:P:87:U:H2'	1:P:88:G:OP2	2.09	0.52
2:A:462:TYR:CE2	2:A:511:HIS:NE2	2.77	0.52
2:H:580:PHE:C	2:H:580:PHE:CD1	2.82	0.52
2:F:473:CYS:HB2	2:F:527:GLU:OE1	2.08	0.52
2:F:331:PRO:O	2:F:361:CYS:HB3	2.09	0.52
2:G:460:ALA:C	2:G:462:TYR:H	2.13	0.52
2:E:288:TYR:HD1	2:E:288:TYR:N	2.07	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:288:TYR:N	2:C:288:TYR:CD1	2.78	0.52
2:G:535:THR:HG22	2:G:632:ILE:HG12	1.92	0.52
1:N:86:G:H1'	2:F:547:ILE:HG21	1.92	0.52
2:B:587:LEU:HD23	2:B:587:LEU:N	2.19	0.52
2:A:529:PHE:CD2	2:A:534:PRO:HD3	2.45	0.52
2:F:329:ILE:HD12	2:F:329:ILE:N	2.25	0.52
2:G:284:LYS:HG3	2:G:407:MET:HG3	1.91	0.52
2:C:622:ASN:O	2:C:626:GLU:HG3	2.10	0.52
2:C:542:VAL:HG12	2:C:543:VAL:N	2.25	0.52
2:C:578:ILE:HD11	2:C:595:VAL:HG22	1.92	0.52
2:G:386:ILE:HG21	2:G:396:GLU:CG	2.39	0.52
2:A:254:TYR:CD2	2:A:255:HIS:N	2.77	0.52
2:G:348:TYR:CD1	2:G:348:TYR:C	2.82	0.52
2:A:500:GLU:OE1	2:A:500:GLU:N	2.41	0.52
2:E:557:GLU:O	2:E:560:GLN:HB3	2.09	0.52
1:M:93:U:C2	1:M:94:C:C6	2.97	0.52
2:E:569:VAL:HG22	2:E:570:LYS:N	2.25	0.52
1:L:100:U:H4'	5:L:1230:HOH:O	2.08	0.52
1:P:88:G:P	5:P:1623:HOH:O	2.66	0.52
1:J:87:U:H3'	5:J:1019:HOH:O	2.10	0.52
2:D:386:ILE:HG21	2:D:396:GLU:HG3	1.90	0.52
2:C:462:TYR:HD2	2:C:486:ASP:OD2	1.93	0.52
2:H:557:GLU:O	2:H:560:GLN:HB3	2.09	0.52
2:G:313:TYR:HB3	2:G:317:MET:HE1	1.91	0.52
2:D:536:TRP:CZ3	2:D:635:ARG:HD3	2.44	0.52
2:H:282:ARG:HD3	2:H:292:GLU:OE1	2.10	0.52
2:A:580:PHE:CD1	2:A:580:PHE:C	2.83	0.52
2:C:258:GLU:O	2:D:325:ARG:NH2	2.42	0.52
2:H:365:GLU:HA	2:H:365:GLU:OE1	2.10	0.52
2:C:544:ILE:HG12	2:C:594:LEU:HD12	1.91	0.52
2:H:544:ILE:HG12	2:H:594:LEU:HD12	1.91	0.52
2:C:597:GLY:O	2:C:601:VAL:HG23	2.08	0.52
2:D:543:VAL:HG11	2:D:585:HIS:CE1	2.44	0.52
2:F:578:ILE:HD11	2:F:595:VAL:CG2	2.40	0.52
2:F:259:GLU:CD	2:F:259:GLU:H	2.12	0.52
2:G:637:LEU:N	2:G:637:LEU:HD12	2.24	0.52
2:A:569:VAL:HG22	2:A:570:LYS:N	2.25	0.52
2:G:580:PHE:C	2:G:580:PHE:CD1	2.81	0.52
2:C:536:TRP:CE3	2:C:635:ARG:HD3	2.44	0.52
2:F:536:TRP:CZ3	2:F:635:ARG:HD3	2.44	0.52
2:D:365:GLU:H	2:D:377:ARG:HD3	1.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:620:ASP:HB3	2:C:623:GLU:CB	2.40	0.52
2:H:421:SER:HB3	2:H:458:GLU:C	2.31	0.52
1:P:84:U:O2	2:H:549:ASP:OD1	2.28	0.52
2:A:543:VAL:HG11	2:A:585:HIS:CE1	2.45	0.52
2:G:386:ILE:HG21	2:G:396:GLU:HG3	1.92	0.52
2:E:556:ASN:ND2	2:E:573:LEU:HD11	2.25	0.52
2:B:636:SER:OG	2:B:638:LYS:HD3	2.10	0.52
1:O:93:U:C2	1:O:94:C:C6	2.98	0.52
2:C:606:VAL:O	2:C:618:SER:HA	2.10	0.52
2:D:638:LYS:HB2	2:D:642:GLU:HG3	1.91	0.52
2:E:329:ILE:HD12	2:E:329:ILE:N	2.25	0.52
2:D:620:ASP:O	2:D:623:GLU:HB3	2.10	0.52
2:F:624:VAL:CG2	2:F:625:ILE:N	2.73	0.52
2:E:544:ILE:HG22	2:E:555:VAL:HG13	1.91	0.52
2:G:375:ARG:NH1	5:G:710:HOH:O	2.32	0.52
2:F:288:TYR:N	2:F:288:TYR:HD1	2.07	0.52
2:D:544:ILE:HG12	2:D:594:LEU:HD12	1.91	0.51
2:F:628:LEU:O	2:F:632:ILE:HG13	2.10	0.51
2:C:421:SER:HB3	2:C:458:GLU:C	2.31	0.51
1:K:78:G:H2'	1:K:79:A:C8	2.42	0.51
2:E:610:THR:HG21	2:E:614:LYS:HB3	1.92	0.51
2:D:636:SER:OG	2:D:638:LYS:HD3	2.10	0.51
2:G:443:VAL:O	2:G:447:GLU:HB2	2.09	0.51
2:D:624:VAL:CG2	2:D:625:ILE:N	2.72	0.51
2:F:622:ASN:O	2:F:626:GLU:HG3	2.09	0.51
2:E:290:TYR:CE2	2:E:512:ARG:NH1	2.78	0.51
2:G:578:ILE:HD11	2:G:595:VAL:CG2	2.39	0.51
1:O:89:U:H2'	1:O:90:G:OP1	2.10	0.51
2:D:423:ARG:HD2	2:D:438:GLU:OE2	2.11	0.51
2:B:304:TRP:CZ3	2:B:328:CYS:HB2	2.45	0.51
2:C:263:MET:CE	2:D:298:MET:HG2	2.39	0.51
2:E:462:TYR:HD2	2:E:486:ASP:OD2	1.92	0.51
2:D:418:VAL:HG21	2:D:450:ILE:CG2	2.39	0.51
2:A:362:HIS:HE1	2:B:297:PHE:CG	2.28	0.51
2:F:278:GLU:HG2	2:F:518:MET:HE2	1.93	0.51
2:H:273:ILE:HG23	2:H:537:LEU:HD22	1.91	0.51
2:C:309:HIS:HB3	2:C:317:MET:CE	2.39	0.51
2:D:555:VAL:HB	2:D:573:LEU:HD21	1.91	0.51
2:A:559:THR:HG21	2:A:571:ALA:CB	2.19	0.51
2:G:620:ASP:O	2:G:624:VAL:HG13	2.10	0.51
2:A:280:PHE:CE2	2:A:407:MET:HG2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:LEU:HD22	2:D:290:TYR:CG	2.45	0.51
2:C:278:GLU:CB	2:C:358:PHE:HE2	2.22	0.51
2:E:304:TRP:CE3	2:E:328:CYS:HB2	2.45	0.51
2:G:515:LEU:HD22	2:G:521:PHE:CE2	2.46	0.51
2:E:482:THR:HG21	4:E:6002:TSB:H5'2	1.92	0.51
2:H:636:SER:OG	2:H:638:LYS:HD3	2.11	0.51
1:N:89:U:HO2'	2:F:580:PHE:CB	2.23	0.51
2:D:514:ILE:HG22	2:D:515:LEU:HD23	1.92	0.51
2:B:557:GLU:O	2:B:560:GLN:HB3	2.10	0.51
2:E:418:VAL:HG21	2:E:450:ILE:CG2	2.40	0.51
2:E:296:PRO:HG2	2:F:265:PHE:CE1	2.45	0.51
2:E:547:ILE:HD12	2:E:597:GLY:CA	2.41	0.51
1:I:89:U:C6	2:A:583:ARG:CZ	2.93	0.51
2:A:339:GLN:HB3	2:B:257:GLN:OE1	2.11	0.51
2:G:338:VAL:HG11	2:G:493:LEU:HB2	1.92	0.51
2:A:624:VAL:CG2	2:A:625:ILE:N	2.72	0.51
2:H:301:ARG:O	2:H:305:GLU:HG3	2.09	0.51
2:F:287:GLU:HB2	2:F:288:TYR:HD1	1.75	0.51
2:G:606:VAL:O	2:G:618:SER:HA	2.11	0.51
2:A:331:PRO:O	2:A:361:CYS:HB3	2.09	0.51
2:B:269:ASP:HB3	2:B:539:PRO:HB3	1.92	0.51
2:C:442:ALA:O	2:C:446:GLU:HG2	2.11	0.51
2:F:620:ASP:O	2:F:623:GLU:HB3	2.11	0.51
1:K:85:C:C1'	2:C:577:LYS:HG2	2.40	0.51
1:P:89:U:O5'	5:P:1628:HOH:O	2.19	0.51
1:J:95:A:H2'	1:J:96:C:C6	2.46	0.51
2:E:620:ASP:HB3	2:E:623:GLU:CB	2.41	0.51
1:I:84:U:O2'	1:I:85:C:OP2	2.28	0.51
2:B:247:ILE:O	2:B:250:GLN:HB2	2.11	0.51
2:H:313:TYR:HB3	2:H:317:MET:HE1	1.92	0.51
2:D:443:VAL:O	2:D:447:GLU:HB2	2.10	0.51
2:B:562:LEU:HD12	2:B:625:ILE:HD11	1.93	0.51
2:C:578:ILE:HD11	2:C:595:VAL:CG2	2.41	0.51
2:B:543:VAL:HG11	2:B:585:HIS:CE1	2.46	0.51
2:C:280:PHE:O	2:C:283:SER:HB3	2.09	0.51
2:H:251:LEU:O	2:H:253:LEU:HD23	2.11	0.51
2:G:622:ASN:O	2:G:626:GLU:HG3	2.10	0.51
1:M:80:U:H2'	1:M:81:C:H6	1.75	0.51
2:C:462:TYR:HE2	2:C:511:HIS:NE2	2.09	0.51
2:C:297:PHE:CD1	2:D:362:HIS:HE1	2.28	0.51
2:G:461:PHE:CD1	2:G:461:PHE:C	2.84	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:421:SER:CA	2:A:455:GLN:HB3	2.40	0.51
2:D:462:TYR:HD2	2:D:486:ASP:OD2	1.93	0.51
2:C:410:THR:C	2:C:411:PHE:HD1	2.13	0.51
1:I:75:U:O2'	1:I:89:U:O4	2.28	0.51
2:B:452:PHE:CE2	2:B:454:TYR:HE1	2.20	0.51
2:F:610:THR:HG21	2:F:614:LYS:HB3	1.93	0.51
2:C:304:TRP:CZ3	2:C:328:CYS:HB2	2.46	0.51
2:D:604:GLY:O	2:D:621:VAL:HG23	2.10	0.51
2:H:555:VAL:HB	2:H:573:LEU:HD21	1.92	0.51
2:A:423:ARG:HG2	2:A:423:ARG:O	2.10	0.51
2:C:290:TYR:CE2	2:C:512:ARG:NH1	2.79	0.51
2:G:638:LYS:HB2	2:G:642:GLU:HG3	1.93	0.51
2:D:526:THR:HG23	2:D:533:PHE:HZ	1.75	0.51
2:C:624:VAL:CG2	2:C:625:ILE:N	2.74	0.51
2:D:547:ILE:HD12	2:D:597:GLY:CA	2.39	0.51
2:F:462:TYR:HE2	2:F:511:HIS:NE2	2.09	0.51
2:H:638:LYS:HB2	2:H:642:GLU:HG3	1.92	0.51
2:D:452:PHE:HE2	2:D:454:TYR:CE1	2.22	0.51
2:A:637:LEU:HD12	2:A:637:LEU:N	2.23	0.51
2:G:580:PHE:C	2:G:580:PHE:HD1	2.14	0.51
2:C:636:SER:OG	2:C:638:LYS:HD3	2.11	0.51
2:H:620:ASP:O	2:H:624:VAL:HG13	2.11	0.50
2:B:332:MET:HE2	4:B:3002:TSB:HN12	1.75	0.50
2:G:421:SER:HB3	2:G:458:GLU:C	2.31	0.50
2:D:580:PHE:C	2:D:580:PHE:CD1	2.84	0.50
2:E:578:ILE:HD11	2:E:595:VAL:HG22	1.93	0.50
1:M:86:G:O6	2:E:599:LYS:CB	2.59	0.50
2:C:257:GLN:OE1	2:D:339:GLN:HB3	2.10	0.50
2:C:249:LYS:HB3	2:C:249:LYS:HZ3	1.74	0.50
2:D:278:GLU:CB	2:D:358:PHE:HE2	2.24	0.50
2:F:301:ARG:O	2:F:305:GLU:HG3	2.10	0.50
2:E:351:LEU:HD22	2:E:387:PHE:O	2.10	0.50
2:E:461:PHE:CD1	2:E:461:PHE:C	2.85	0.50
2:H:411:PHE:HE2	2:H:521:PHE:HE1	1.56	0.50
2:H:422:THR:HB	2:H:438:GLU:OE2	2.12	0.50
2:F:332:MET:HE2	4:F:7002:TSB:HN12	1.76	0.50
1:K:78:G:N3	1:K:79:A:C8	2.78	0.50
2:E:274:PHE:O	2:E:518:MET:HE3	2.11	0.50
2:E:443:VAL:O	2:E:447:GLU:HB2	2.11	0.50
2:C:547:ILE:HG12	2:C:578:ILE:HD12	1.92	0.50
2:E:305:GLU:HA	2:E:310:TRP:HB3	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:341:PHE:O	2:D:346:LYS:NZ	2.38	0.50
2:G:636:SER:OG	2:G:638:LYS:HD3	2.11	0.50
2:A:609:ARG:HG3	2:A:609:ARG:O	2.11	0.50
2:C:529:PHE:CD2	2:C:534:PRO:HD3	2.47	0.50
2:F:461:PHE:C	2:F:461:PHE:CD1	2.83	0.50
2:C:329:ILE:N	2:C:329:ILE:HD12	2.26	0.50
2:D:578:ILE:HD11	2:D:595:VAL:HG22	1.93	0.50
2:C:580:PHE:C	2:C:580:PHE:CD1	2.84	0.50
2:F:462:TYR:CD2	2:F:486:ASP:OD2	2.64	0.50
2:E:556:ASN:HD21	2:E:573:LEU:HD11	1.77	0.50
2:F:281:VAL:HG12	2:F:285:LEU:CD1	2.42	0.50
1:K:104:C:H2'	1:K:105:C:C4'	2.42	0.50
2:C:557:GLU:O	2:C:560:GLN:HB3	2.11	0.50
2:B:335:PRO:HG2	2:B:336:GLY:H	1.76	0.50
2:H:331:PRO:O	2:H:361:CYS:HB3	2.12	0.50
1:J:105:C:H2'	1:O:69:G:O4'	2.12	0.50
2:E:280:PHE:O	2:E:283:SER:HB3	2.11	0.50
2:A:411:PHE:HE2	2:A:521:PHE:CE1	2.17	0.50
2:B:422:THR:O	2:B:423:ARG:C	2.50	0.50
2:F:551:GLN:HG2	2:F:597:GLY:C	2.32	0.50
2:H:548:THR:HG23	2:H:551:GLN:OE1	2.12	0.50
2:E:580:PHE:C	2:E:580:PHE:HD1	2.15	0.50
2:C:441:LEU:HD12	2:C:464:PRO:HB2	1.93	0.50
2:F:529:PHE:H	2:F:529:PHE:HD1	1.58	0.50
1:P:78:G:O2'	1:P:79:A:H5'	2.12	0.50
2:A:418:VAL:HG21	2:A:450:ILE:HG21	1.93	0.50
2:H:342:ASN:HD21	2:H:495:ALA:HA	1.75	0.50
2:F:544:ILE:HG12	2:F:594:LEU:HD12	1.92	0.50
2:F:411:PHE:CE2	2:F:521:PHE:HZ	2.27	0.50
2:F:580:PHE:C	2:F:580:PHE:CD1	2.83	0.50
2:G:556:ASN:ND2	2:G:573:LEU:HD11	2.27	0.50
2:H:452:PHE:HE2	2:H:454:TYR:CE1	2.23	0.50
2:D:637:LEU:HD12	2:D:637:LEU:N	2.23	0.50
2:C:473:CYS:HB2	2:C:527:GLU:OE1	2.12	0.50
2:B:417:VAL:CG1	2:B:471:TYR:CE1	2.94	0.50
2:E:331:PRO:O	2:E:361:CYS:HB3	2.12	0.50
2:G:460:ALA:C	2:G:462:TYR:N	2.65	0.50
2:E:325:ARG:NH2	2:F:258:GLU:O	2.45	0.50
2:C:288:TYR:N	2:C:288:TYR:HD1	2.08	0.50
2:C:434:TRP:O	2:C:438:GLU:HG3	2.11	0.50
1:K:85:C:C2	2:C:577:LYS:HG3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ASP:O	2:B:247:ILE:HG13	2.12	0.50
2:A:329:ILE:N	2:A:329:ILE:CD1	2.75	0.50
2:A:297:PHE:CG	2:B:362:HIS:CE1	3.00	0.50
2:B:362:HIS:HD2	5:B:232:HOH:O	1.94	0.50
2:A:278:GLU:HG2	2:A:518:MET:HE2	1.94	0.50
2:B:600:GLU:HB3	2:B:605:LYS:O	2.11	0.50
2:D:397:VAL:O	2:D:401:ILE:HG12	2.12	0.50
2:H:620:ASP:HB3	2:H:623:GLU:CB	2.42	0.50
2:B:285:LEU:HD22	2:B:290:TYR:CG	2.47	0.50
1:I:89:U:C5	2:A:583:ARG:CZ	2.95	0.50
2:D:500:GLU:N	2:D:500:GLU:OE1	2.44	0.50
2:C:247:ILE:O	2:C:250:GLN:HB2	2.12	0.50
2:C:332:MET:HE2	4:C:4002:TSB:HN12	1.77	0.50
2:E:273:ILE:HG23	2:E:537:LEU:CD2	2.41	0.50
1:O:92:G:H2'	1:O:93:U:H6	1.76	0.50
2:D:304:TRP:CE3	2:D:328:CYS:HB2	2.46	0.50
2:B:569:VAL:HG22	2:B:570:LYS:N	2.26	0.50
2:B:536:TRP:CE3	2:B:635:ARG:HD3	2.47	0.50
2:H:624:VAL:HG23	2:H:625:ILE:N	2.26	0.50
2:F:624:VAL:HG23	2:F:625:ILE:N	2.27	0.50
2:B:578:ILE:HD11	2:B:595:VAL:HG22	1.94	0.50
1:L:77:U:O5'	1:L:77:U:H6	1.95	0.50
1:M:92:G:H2'	1:M:93:U:H6	1.77	0.50
2:D:278:GLU:HG2	2:D:518:MET:HE2	1.94	0.50
2:E:536:TRP:O	2:E:568:ARG:NH2	2.45	0.50
2:C:445:LEU:HD21	2:C:466:ILE:HG12	1.94	0.50
2:E:514:ILE:HG22	2:E:515:LEU:HD23	1.93	0.49
2:C:461:PHE:CD1	2:C:461:PHE:C	2.86	0.49
2:D:578:ILE:HD11	2:D:595:VAL:CG2	2.42	0.49
1:N:89:U:O3'	2:F:577:LYS:NZ	2.44	0.49
2:E:637:LEU:N	2:E:637:LEU:HD12	2.26	0.49
2:C:484:GLN:HB2	2:C:511:HIS:HB2	1.94	0.49
2:F:247:ILE:O	2:F:250:GLN:HB2	2.11	0.49
2:B:334:CYS:SG	2:B:511:HIS:HE1	2.34	0.49
2:C:313:TYR:HB3	2:C:317:MET:HE1	1.94	0.49
2:E:536:TRP:CE3	2:E:635:ARG:HD3	2.47	0.49
2:G:280:PHE:CZ	2:G:407:MET:HG2	2.47	0.49
2:D:461:PHE:CD1	2:D:461:PHE:C	2.86	0.49
2:G:620:ASP:HB3	2:G:623:GLU:CB	2.42	0.49
2:F:483:VAL:HG22	2:F:512:ARG:HB2	1.94	0.49
2:C:348:TYR:C	2:C:348:TYR:CD1	2.84	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:393:ILE:HD11	2:B:508:VAL:HG11	1.94	0.49
2:B:249:LYS:HZ3	2:B:249:LYS:HB3	1.77	0.49
2:G:536:TRP:CZ3	2:G:635:ARG:HD3	2.47	0.49
2:H:356:ALA:HA	2:H:384:ALA:HA	1.93	0.49
2:G:472:ASP:OD1	2:G:476:ARG:HB2	2.12	0.49
1:L:80:U:H2'	1:L:81:C:C6	2.47	0.49
2:G:559:THR:HG21	2:G:571:ALA:CB	2.20	0.49
2:H:621:VAL:HG12	2:H:622:ASN:N	2.27	0.49
2:F:542:VAL:HG12	2:F:543:VAL:N	2.27	0.49
1:N:79:A:C1'	2:E:502:ASN:OD1	2.57	0.49
2:B:348:TYR:CD1	2:B:348:TYR:C	2.86	0.49
1:J:72:G:H2'	1:J:73:U:C6	2.47	0.49
1:M:101:G:O2'	1:M:102:C:H5'	2.12	0.49
2:H:254:TYR:CZ	2:H:373:LEU:HD21	2.48	0.49
2:F:402:ARG:CB	2:F:402:ARG:NH1	2.75	0.49
2:E:624:VAL:HG23	2:E:625:ILE:N	2.27	0.49
1:K:93:U:H2'	1:K:94:C:C6	2.46	0.49
2:C:393:ILE:HD11	2:C:508:VAL:HG11	1.95	0.49
2:D:557:GLU:O	2:D:560:GLN:HB3	2.12	0.49
2:A:473:CYS:HB2	2:A:527:GLU:OE1	2.12	0.49
2:G:291:GLN:NE2	2:G:353:LEU:HD21	2.26	0.49
2:C:480:CYS:O	2:C:516:GLY:HA3	2.12	0.49
2:D:619:MET:HG3	2:D:624:VAL:HG12	1.94	0.49
2:F:460:ALA:C	2:F:462:TYR:N	2.64	0.49
2:H:280:PHE:CZ	2:H:407:MET:HG2	2.48	0.49
2:C:587:LEU:HD23	2:C:587:LEU:N	2.20	0.49
2:D:280:PHE:O	2:D:283:SER:HB3	2.12	0.49
2:C:637:LEU:N	2:C:637:LEU:HD12	2.21	0.49
2:G:526:THR:HG23	2:G:533:PHE:HZ	1.77	0.49
2:G:539:PRO:O	2:G:568:ARG:HD2	2.13	0.49
2:D:313:TYR:HB3	2:D:317:MET:HE1	1.93	0.49
2:H:291:GLN:NE2	2:H:353:LEU:HD21	2.28	0.49
2:D:620:ASP:HB3	2:D:623:GLU:CB	2.42	0.49
2:G:427:ARG:HB2	2:G:434:TRP:CZ2	2.47	0.49
2:D:423:ARG:HA	2:D:434:TRP:CZ3	2.47	0.49
2:E:590:VAL:O	2:E:611:ARG:HB3	2.13	0.49
2:H:386:ILE:HG21	2:H:396:GLU:CG	2.43	0.49
2:H:400:CYS:O	2:H:404:VAL:HG23	2.13	0.49
2:C:536:TRP:CZ3	2:C:635:ARG:HD3	2.47	0.49
2:A:305:GLU:HA	2:A:310:TRP:HB3	1.94	0.49
2:G:418:VAL:HG21	2:G:450:ILE:CG2	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:443:VAL:O	2:A:447:GLU:HB2	2.13	0.49
2:A:461:PHE:CD1	2:A:461:PHE:C	2.85	0.49
2:D:624:VAL:HG23	2:D:625:ILE:N	2.27	0.49
2:A:421:SER:HB3	2:A:458:GLU:C	2.32	0.49
2:F:578:ILE:HD11	2:F:595:VAL:HG22	1.93	0.49
2:A:263:MET:CE	2:B:298:MET:HG2	2.38	0.49
2:C:243:ASP:O	2:C:247:ILE:HG13	2.13	0.49
1:J:84:U:O2'	1:J:85:C:OP2	2.31	0.49
2:B:415:LYS:HG2	2:B:471:TYR:CD1	2.48	0.49
2:F:416:ILE:HG22	2:F:416:ILE:O	2.10	0.49
2:D:600:GLU:HB3	2:D:605:LYS:O	2.12	0.49
2:F:620:ASP:HB3	2:F:623:GLU:CB	2.43	0.49
2:B:590:VAL:O	2:B:611:ARG:HB3	2.12	0.49
2:F:580:PHE:HD1	2:F:580:PHE:C	2.16	0.49
2:C:298:MET:HG2	2:D:263:MET:CE	2.41	0.49
2:F:480:CYS:O	2:F:516:GLY:HA3	2.13	0.49
2:B:460:ALA:C	2:B:462:TYR:H	2.16	0.49
2:B:329:ILE:N	2:B:329:ILE:HD12	2.27	0.49
2:C:619:MET:HG3	2:C:624:VAL:HG12	1.93	0.49
2:D:410:THR:C	2:D:411:PHE:HD1	2.15	0.49
2:E:300:ASP:OD2	2:E:302:VAL:HB	2.13	0.49
2:G:621:VAL:HG12	2:G:622:ASN:N	2.28	0.49
1:L:97:C:C5'	1:L:98:A:OP1	2.60	0.49
1:M:69:G:OP2	1:P:105:C:O3'	2.31	0.49
1:M:69:G:OP2	1:P:105:C:C2'	2.61	0.49
1:K:105:C:C2'	1:K:105:C:O2	2.60	0.49
2:H:580:PHE:C	2:H:580:PHE:HD1	2.15	0.49
2:H:610:THR:HG21	2:H:614:LYS:HB3	1.94	0.49
2:E:609:ARG:O	2:E:609:ARG:HG3	2.13	0.49
2:A:297:PHE:CG	2:B:362:HIS:HE1	2.31	0.49
2:E:313:TYR:HB3	2:E:317:MET:HE1	1.95	0.49
2:B:443:VAL:O	2:B:447:GLU:HB2	2.11	0.49
2:C:443:VAL:O	2:C:447:GLU:HB2	2.13	0.49
2:C:624:VAL:O	2:C:628:LEU:HG	2.12	0.49
2:B:624:VAL:CG2	2:B:625:ILE:N	2.75	0.49
1:M:88:G:H8	5:E:6013:HOH:O	1.96	0.49
2:F:282:ARG:HD3	2:F:292:GLU:OE1	2.13	0.49
2:D:309:HIS:HB3	2:D:317:MET:CE	2.43	0.49
2:C:304:TRP:CE3	2:C:328:CYS:HB2	2.48	0.49
2:A:421:SER:HB3	2:A:458:GLU:CB	2.30	0.48
2:D:597:GLY:O	2:D:601:VAL:HG23	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:460:ALA:C	2:F:462:TYR:H	2.15	0.48
1:I:86:G:O4'	1:I:86:G:P	2.71	0.48
2:B:298:MET:HE3	2:B:327:TYR:HB2	1.95	0.48
2:C:514:ILE:HG22	2:C:515:LEU:HD23	1.94	0.48
2:G:555:VAL:HB	2:G:573:LEU:HD21	1.94	0.48
2:A:277:LEU:O	2:A:280:PHE:HB3	2.12	0.48
2:F:313:TYR:HB3	2:F:317:MET:HE1	1.94	0.48
2:C:529:PHE:H	2:C:529:PHE:HD1	1.58	0.48
2:H:330:LYS:HA	2:H:331:PRO:HD3	1.60	0.48
2:B:547:ILE:HD12	2:B:597:GLY:CA	2.43	0.48
2:C:583:ARG:O	2:C:587:LEU:CD2	2.60	0.48
2:E:500:GLU:N	2:E:500:GLU:OE1	2.43	0.48
2:A:403:LEU:O	2:A:407:MET:HB2	2.12	0.48
2:F:500:GLU:OE1	2:F:500:GLU:N	2.42	0.48
2:F:512:ARG:O	2:F:512:ARG:NE	2.45	0.48
2:A:348:TYR:C	2:A:348:TYR:CD1	2.86	0.48
2:D:609:ARG:HG3	2:D:609:ARG:O	2.13	0.48
2:E:285:LEU:HD22	2:E:290:TYR:CG	2.49	0.48
1:O:87:U:C2'	1:O:88:G:OP2	2.60	0.48
2:C:545:MET:SD	2:C:582:ILE:HD13	2.52	0.48
2:D:460:ALA:C	2:D:462:TYR:H	2.16	0.48
1:M:69:G:P	1:P:105:C:HO3'	2.31	0.48
2:A:624:VAL:HG23	2:A:625:ILE:N	2.26	0.48
2:C:462:TYR:CE2	2:C:511:HIS:NE2	2.81	0.48
2:E:325:ARG:HG3	2:E:325:ARG:NH1	2.27	0.48
2:E:274:PHE:CD1	2:E:274:PHE:C	2.86	0.48
2:G:351:LEU:HD22	2:G:387:PHE:O	2.13	0.48
2:B:460:ALA:C	2:B:462:TYR:N	2.66	0.48
2:B:519:GLU:CD	2:B:519:GLU:H	2.17	0.48
2:G:282:ARG:HD3	2:G:292:GLU:OE1	2.13	0.48
1:O:89:U:O3'	2:G:577:LYS:NZ	2.46	0.48
2:E:427:ARG:HB2	2:E:434:TRP:CZ2	2.49	0.48
2:B:422:THR:O	2:B:458:GLU:O	2.31	0.48
2:D:462:TYR:HE2	2:D:511:HIS:CE1	2.31	0.48
2:H:423:ARG:HG2	2:H:423:ARG:O	2.13	0.48
2:E:597:GLY:O	2:E:601:VAL:HG23	2.14	0.48
2:H:386:ILE:HG21	2:H:396:GLU:HG3	1.95	0.48
2:H:253:LEU:N	2:H:253:LEU:HD23	2.29	0.48
2:G:251:LEU:O	2:G:253:LEU:HD23	2.14	0.48
2:B:303:LEU:HD11	2:B:339:GLN:HE21	1.78	0.48
2:G:500:GLU:OE1	2:G:500:GLU:N	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:78:G:O2'	1:K:79:A:H5'	2.12	0.48
2:B:610:THR:HG22	2:B:614:LYS:O	2.13	0.48
2:C:278:GLU:HG2	2:C:518:MET:HE2	1.95	0.48
2:G:462:TYR:HD2	2:G:486:ASP:OD2	1.97	0.48
2:E:278:GLU:CB	2:E:358:PHE:HE2	2.26	0.48
2:H:351:LEU:HD22	2:H:387:PHE:O	2.13	0.48
2:F:491:SER:O	2:F:494:SER:N	2.41	0.48
2:C:628:LEU:O	2:C:632:ILE:HG13	2.13	0.48
1:P:86:G:C2'	5:P:1613:HOH:O	2.61	0.48
2:C:320:THR:HG22	2:C:321:SER:N	2.22	0.48
1:N:89:U:O2'	2:F:580:PHE:HB2	2.13	0.48
2:A:288:TYR:CZ	2:A:403:LEU:HD13	2.48	0.48
2:F:348:TYR:C	2:F:348:TYR:CD1	2.86	0.48
2:A:620:ASP:HB3	2:A:623:GLU:CB	2.43	0.48
2:E:636:SER:OG	2:E:638:LYS:HD3	2.11	0.48
2:B:610:THR:HG21	2:B:614:LYS:HB3	1.96	0.48
2:D:331:PRO:O	2:D:361:CYS:HB3	2.14	0.48
2:B:365:GLU:OE1	2:B:365:GLU:HA	2.13	0.48
2:H:480:CYS:O	2:H:516:GLY:HA3	2.13	0.48
2:G:280:PHE:O	2:G:283:SER:HB3	2.12	0.48
2:B:403:LEU:O	2:B:407:MET:HB2	2.14	0.48
1:L:88:G:H1'	2:D:583:ARG:HG2	1.96	0.48
2:F:411:PHE:CD2	2:F:521:PHE:CZ	3.01	0.48
1:J:93:U:H2'	1:J:94:C:H6	1.79	0.48
2:A:597:GLY:O	2:A:601:VAL:HG23	2.13	0.48
2:A:319:THR:H	2:B:320:THR:CG2	2.26	0.48
2:B:320:THR:HG22	2:B:321:SER:N	2.25	0.48
1:N:84:U:H4'	1:N:85:C:H5'	1.96	0.48
1:N:77:U:O5'	1:N:77:U:H6	1.96	0.48
2:A:580:PHE:HD1	2:A:580:PHE:C	2.16	0.48
2:E:265:PHE:CZ	2:F:296:PRO:HG2	2.48	0.48
2:C:512:ARG:O	2:C:512:ARG:NE	2.44	0.48
2:E:362:HIS:CE1	2:F:297:PHE:CG	3.02	0.48
2:F:418:VAL:HG21	2:F:450:ILE:CG2	2.44	0.48
2:F:305:GLU:HA	2:F:310:TRP:HB3	1.94	0.48
2:A:610:THR:CG2	2:A:614:LYS:HB3	2.42	0.48
2:B:536:TRP:CZ3	2:B:635:ARG:HD3	2.48	0.48
2:B:461:PHE:CD1	2:B:461:PHE:C	2.86	0.48
2:C:604:GLY:O	2:C:621:VAL:HG23	2.13	0.48
2:H:546:ASN:OD1	2:H:573:LEU:HA	2.13	0.48
2:H:569:VAL:HG22	2:H:570:LYS:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:545:MET:SD	2:F:582:ILE:HD13	2.54	0.48
2:D:303:LEU:HD11	2:D:339:GLN:NE2	2.28	0.48
2:C:452:PHE:HE2	2:C:454:TYR:CE1	2.20	0.48
2:D:254:TYR:HA	2:D:267:HIS:ND1	2.27	0.48
2:B:339:GLN:OE1	2:B:339:GLN:CA	2.60	0.48
2:E:555:VAL:HB	2:E:573:LEU:HD21	1.95	0.48
2:G:362:HIS:CD2	5:G:732:HOH:O	2.56	0.48
1:M:80:U:OP2	2:F:349:ARG:NH2	2.47	0.48
2:C:465:LYS:HG3	2:C:484:GLN:CG	2.42	0.48
2:A:539:PRO:O	2:A:568:ARG:HD2	2.12	0.48
2:A:441:LEU:O	2:A:444:ALA:HB3	2.13	0.48
2:C:400:CYS:SG	2:C:512:ARG:HG3	2.54	0.48
2:B:389:THR:HG1	2:B:392:GLN:HG3	1.74	0.48
2:E:578:ILE:HD11	2:E:595:VAL:CG2	2.43	0.48
1:I:88:G:C8	5:I:112:HOH:O	2.48	0.48
2:C:254:TYR:HA	2:C:267:HIS:ND1	2.29	0.48
2:F:386:ILE:HG21	2:F:396:GLU:HG3	1.95	0.48
1:I:95:A:H2'	1:I:96:C:O4'	2.14	0.48
2:G:556:ASN:HD21	2:G:573:LEU:HD11	1.79	0.48
1:K:98:A:O2'	2:D:344:GLY:N	2.28	0.48
2:E:554:TYR:CE1	2:E:558:LEU:HD11	2.49	0.48
2:B:580:PHE:C	2:B:580:PHE:CD1	2.85	0.48
2:C:273:ILE:HG23	2:C:537:LEU:HD22	1.96	0.48
2:G:572:ASP:OD2	2:G:574:ARG:NH2	2.37	0.48
2:E:515:LEU:HD22	2:E:521:PHE:CE2	2.48	0.48
2:G:423:ARG:HD2	2:G:438:GLU:OE2	2.14	0.48
2:C:421:SER:CA	2:C:455:GLN:HB3	2.43	0.48
2:D:585:HIS:HB2	2:D:593:MET:HE3	1.95	0.48
2:A:386:ILE:O	2:A:509:MET:HA	2.13	0.48
2:C:253:LEU:O	2:C:270:GLY:HA3	2.14	0.48
2:H:254:TYR:CD2	2:H:255:HIS:N	2.82	0.48
2:G:397:VAL:O	2:G:400:CYS:HB2	2.13	0.48
1:M:69:G:C8	1:P:105:C:O2	2.67	0.48
1:K:79:A:N1	1:K:94:C:N3	2.62	0.48
2:A:335:PRO:HG2	2:A:336:GLY:H	1.79	0.48
2:E:536:TRP:CD1	2:E:635:ARG:HA	2.49	0.48
1:I:72:G:H2'	1:I:73:U:H6	1.78	0.48
1:O:95:A:H2'	1:O:96:C:O4'	2.14	0.48
2:E:411:PHE:CD2	2:E:525:LEU:CD2	2.85	0.48
2:E:423:ARG:HD2	2:E:438:GLU:OE2	2.14	0.48
1:L:87:U:H1'	2:D:582:ILE:HG13	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:75:U:O2'	1:L:89:U:O4	2.28	0.48
2:H:526:THR:O	2:H:530:ALA:HA	2.14	0.48
2:C:437:ALA:HA	2:C:485:LEU:HD23	1.96	0.48
1:I:79:A:H1'	2:B:502:ASN:OD1	2.13	0.47
2:G:544:ILE:HG12	2:G:594:LEU:HD12	1.96	0.47
1:J:103:G:P	5:J:1025:HOH:O	2.71	0.47
2:C:298:MET:HE2	2:C:327:TYR:CD1	2.48	0.47
2:B:555:VAL:HB	2:B:573:LEU:HD21	1.95	0.47
2:B:473:CYS:HB2	2:B:527:GLU:OE1	2.14	0.47
2:D:460:ALA:C	2:D:462:TYR:N	2.65	0.47
2:C:291:GLN:NE2	2:C:353:LEU:HD21	2.29	0.47
2:C:386:ILE:HG21	2:C:396:GLU:CG	2.44	0.47
2:F:547:ILE:HG12	2:F:578:ILE:HD12	1.96	0.47
1:J:92:G:H2'	1:J:93:U:H6	1.79	0.47
2:H:484:GLN:HB2	2:H:511:HIS:HB2	1.96	0.47
2:F:637:LEU:HD12	2:F:637:LEU:N	2.26	0.47
2:F:278:GLU:CB	2:F:358:PHE:HE2	2.26	0.47
2:G:278:GLU:HG2	2:G:518:MET:HE2	1.95	0.47
2:B:331:PRO:O	2:B:361:CYS:HB3	2.14	0.47
2:E:287:GLU:HB2	2:E:288:TYR:HD1	1.79	0.47
2:B:282:ARG:HD3	2:B:292:GLU:OE1	2.14	0.47
2:D:580:PHE:C	2:D:580:PHE:HD1	2.17	0.47
2:H:288:TYR:N	2:H:288:TYR:CD1	2.82	0.47
1:M:78:G:O2'	1:M:79:A:H5'	2.14	0.47
2:H:536:TRP:CZ3	2:H:635:ARG:HD3	2.49	0.47
2:C:609:ARG:HD3	2:C:610:THR:O	2.14	0.47
2:F:636:SER:OG	2:F:638:LYS:HD3	2.14	0.47
2:A:356:ALA:CB	2:A:384:ALA:HB2	2.44	0.47
2:A:356:ALA:HA	2:A:384:ALA:CB	2.45	0.47
2:C:624:VAL:HG23	2:C:625:ILE:N	2.29	0.47
2:B:621:VAL:HG12	2:B:622:ASN:N	2.29	0.47
2:H:423:ARG:HD2	2:H:438:GLU:OE2	2.15	0.47
1:K:85:C:O2	1:K:90:G:N7	2.47	0.47
2:H:500:GLU:N	2:H:500:GLU:OE1	2.45	0.47
2:G:569:VAL:O	2:G:570:LYS:HG2	2.14	0.47
2:G:253:LEU:O	2:G:270:GLY:HA3	2.14	0.47
1:K:98:A:H2'	1:K:98:A:N3	2.30	0.47
2:E:298:MET:HE3	2:E:327:TYR:HB2	1.96	0.47
2:A:556:ASN:ND2	2:A:573:LEU:HD11	2.28	0.47
2:G:557:GLU:O	2:G:560:GLN:HB3	2.14	0.47
2:E:301:ARG:O	2:E:305:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:556:ASN:ND2	2:H:573:LEU:HD11	2.29	0.47
2:B:423:ARG:HA	2:B:434:TRP:CZ3	2.49	0.47
2:C:411:PHE:CD2	2:C:521:PHE:CZ	3.03	0.47
2:B:578:ILE:HD11	2:B:595:VAL:CG2	2.45	0.47
1:J:88:G:H1'	2:B:583:ARG:CG	2.43	0.47
2:E:544:ILE:HG12	2:E:594:LEU:HD12	1.96	0.47
2:E:621:VAL:HG12	2:E:622:ASN:N	2.29	0.47
2:F:393:ILE:HD11	2:F:508:VAL:HG11	1.97	0.47
2:G:536:TRP:CE3	2:G:635:ARG:HD3	2.49	0.47
2:G:366:PRO:O	2:G:367:SER:C	2.53	0.47
2:A:296:PRO:HG2	2:B:265:PHE:CE1	2.50	0.47
2:H:421:SER:HB3	2:H:458:GLU:CB	2.35	0.47
1:N:78:G:O2'	1:N:79:A:H5'	2.15	0.47
2:C:281:VAL:HG12	2:C:285:LEU:CD1	2.45	0.47
1:I:95:A:H2'	1:I:96:C:C6	2.48	0.47
2:A:287:GLU:HB2	2:A:288:TYR:HD1	1.80	0.47
2:D:281:VAL:HG12	2:D:285:LEU:CD1	2.45	0.47
2:C:526:THR:HG23	2:C:533:PHE:CZ	2.46	0.47
2:H:539:PRO:O	2:H:568:ARG:HD2	2.15	0.47
2:C:287:GLU:HB2	2:C:288:TYR:HD1	1.79	0.47
2:E:569:VAL:O	2:E:570:LYS:HG2	2.14	0.47
2:A:273:ILE:HG22	2:A:522:ILE:HD11	1.96	0.47
2:F:624:VAL:O	2:F:628:LEU:HG	2.14	0.47
2:G:543:VAL:HG11	2:G:585:HIS:CE1	2.50	0.47
2:B:280:PHE:O	2:B:283:SER:HB3	2.15	0.47
2:G:423:ARG:HA	2:G:434:TRP:CZ3	2.50	0.47
2:D:580:PHE:HE1	5:D:5014:HOH:O	1.96	0.47
1:K:88:G:H5"	1:K:89:U:P	2.55	0.47
2:E:473:CYS:HB2	2:E:527:GLU:OE1	2.15	0.47
2:A:562:LEU:HD12	2:A:625:ILE:HD11	1.96	0.47
2:A:619:MET:HG3	2:A:624:VAL:HG12	1.96	0.47
2:F:298:MET:CE	2:F:327:TYR:HB2	2.45	0.47
2:F:243:ASP:O	2:F:247:ILE:HG13	2.15	0.47
2:B:554:TYR:CE1	2:B:558:LEU:HD11	2.50	0.47
2:B:609:ARG:HD3	2:B:610:THR:O	2.15	0.47
2:G:246:LYS:O	2:G:250:GLN:HG2	2.15	0.47
2:B:278:GLU:HB3	2:B:358:PHE:CE2	2.49	0.47
2:B:375:ARG:NH2	5:B:208:HOH:O	2.26	0.47
2:B:550:SER:O	2:B:552:SER:N	2.47	0.47
2:D:397:VAL:O	2:D:400:CYS:HB2	2.15	0.47
2:A:247:ILE:O	2:A:250:GLN:HB2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:443:VAL:O	2:F:447:GLU:HB2	2.15	0.47
2:H:603:SER:C	2:H:605:LYS:H	2.18	0.47
2:C:418:VAL:HG21	2:C:450:ILE:HG21	1.97	0.47
2:D:445:LEU:HD21	2:D:466:ILE:HG12	1.97	0.47
2:B:411:PHE:CE2	2:B:521:PHE:CZ	3.03	0.47
2:E:421:SER:CA	2:E:455:GLN:HB3	2.43	0.47
2:A:386:ILE:HG21	2:A:396:GLU:HG3	1.95	0.47
2:H:288:TYR:N	2:H:288:TYR:HD1	2.12	0.47
2:A:548:THR:HG23	2:A:551:GLN:OE1	2.15	0.47
1:K:79:A:C2	1:K:94:C:O2	2.68	0.47
2:B:301:ARG:O	2:B:305:GLU:HG3	2.14	0.47
2:G:278:GLU:OE2	2:G:358:PHE:HD2	1.98	0.47
2:E:436:ARG:HG2	2:E:440:ASP:OD2	2.15	0.47
2:C:562:LEU:HD12	2:C:625:ILE:HD11	1.96	0.47
2:H:624:VAL:O	2:H:628:LEU:HG	2.15	0.47
2:G:421:SER:OG	2:G:467:GLU:OE2	2.33	0.47
2:B:423:ARG:NE	2:B:438:GLU:OE1	2.48	0.47
2:F:543:VAL:HG11	2:F:585:HIS:ND1	2.30	0.47
1:N:86:G:C4	2:F:547:ILE:CD1	2.97	0.47
2:H:589:ARG:O	2:H:611:ARG:HD3	2.15	0.47
2:A:281:VAL:HG12	2:A:285:LEU:CD1	2.45	0.47
2:F:303:LEU:HD11	2:F:339:GLN:NE2	2.27	0.47
2:E:365:GLU:HA	2:E:365:GLU:OE1	2.15	0.47
1:N:80:U:H2'	1:N:81:C:C6	2.50	0.47
2:H:416:ILE:HG22	2:H:416:ILE:O	2.14	0.47
2:G:600:GLU:HB3	2:G:605:LYS:O	2.14	0.47
2:H:266:TRP:CH2	2:H:522:ILE:HD12	2.50	0.47
2:A:265:PHE:CE1	2:B:296:PRO:HG2	2.50	0.47
2:H:628:LEU:O	2:H:632:ILE:HG13	2.14	0.47
1:L:86:G:C4	2:D:547:ILE:HD13	2.49	0.47
1:P:84:U:O2'	1:P:85:C:OP2	2.29	0.47
2:E:583:ARG:O	2:E:587:LEU:CD2	2.63	0.47
2:G:562:LEU:HB3	2:G:569:VAL:HG11	1.97	0.47
2:C:501:ASP:O	2:C:503:GLU:HG2	2.15	0.47
2:H:484:GLN:HE22	4:H:9002:TSB:HN8	1.62	0.47
2:F:452:PHE:HE2	2:F:454:TYR:CE1	2.24	0.47
2:H:526:THR:HG23	2:H:533:PHE:HZ	1.80	0.47
2:G:460:ALA:HB1	2:G:462:TYR:CE1	2.50	0.47
2:E:526:THR:HG23	2:E:533:PHE:HZ	1.79	0.47
2:D:624:VAL:O	2:D:628:LEU:HG	2.15	0.46
2:B:624:VAL:O	2:B:628:LEU:HG	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:281:VAL:HG12	2:E:285:LEU:CD1	2.43	0.46
2:G:421:SER:CA	2:G:455:GLN:HB3	2.44	0.46
1:K:89:U:O2	1:K:89:U:H2'	2.15	0.46
2:G:597:GLY:O	2:G:601:VAL:HG23	2.15	0.46
2:E:547:ILE:HG12	2:E:578:ILE:HD12	1.97	0.46
2:F:583:ARG:O	2:F:587:LEU:CD2	2.61	0.46
2:E:619:MET:HG3	2:E:624:VAL:HG12	1.97	0.46
2:C:335:PRO:HG2	2:C:336:GLY:H	1.79	0.46
2:F:528:GLU:O	2:F:530:ALA:N	2.48	0.46
1:M:93:U:N3	1:M:94:C:C5	2.82	0.46
2:C:529:PHE:N	2:C:529:PHE:CD1	2.78	0.46
2:B:536:TRP:O	2:B:568:ARG:NH2	2.48	0.46
2:E:536:TRP:CZ3	2:E:635:ARG:HD3	2.50	0.46
2:G:356:ALA:HA	2:G:384:ALA:HA	1.97	0.46
2:G:531:GLY:O	2:G:589:ARG:HG3	2.16	0.46
2:D:559:THR:HG21	2:D:571:ALA:CB	2.21	0.46
2:B:281:VAL:HG12	2:B:285:LEU:CD1	2.44	0.46
2:A:422:THR:O	2:A:423:ARG:C	2.53	0.46
2:H:545:MET:CE	2:H:593:MET:HB3	2.45	0.46
2:F:386:ILE:HG21	2:F:396:GLU:CG	2.45	0.46
2:A:397:VAL:O	2:A:400:CYS:HB2	2.14	0.46
2:F:280:PHE:CZ	2:F:407:MET:HG2	2.50	0.46
2:A:600:GLU:HB3	2:A:605:LYS:O	2.15	0.46
1:N:95:A:H2'	1:N:96:C:O4'	2.15	0.46
2:E:400:CYS:SG	2:E:512:ARG:HG3	2.55	0.46
2:C:580:PHE:HD1	2:C:580:PHE:C	2.18	0.46
2:B:386:ILE:HG21	2:B:396:GLU:CG	2.45	0.46
1:O:93:U:H2'	1:O:94:C:H6	1.80	0.46
1:M:71:C:N3	1:M:72:G:N7	2.64	0.46
2:B:482:THR:O	2:B:512:ARG:HA	2.16	0.46
2:B:515:LEU:HD22	2:B:521:PHE:CE2	2.50	0.46
2:B:455:GLN:O	2:B:456:LEU:C	2.53	0.46
2:H:287:GLU:HB2	2:H:288:TYR:HD1	1.79	0.46
2:E:348:TYR:C	2:E:348:TYR:CD1	2.89	0.46
2:A:449:ASN:ND2	2:H:452:PHE:CE2	2.83	0.46
2:F:285:LEU:HD21	2:F:512:ARG:HH12	1.80	0.46
2:D:305:GLU:HA	2:D:310:TRP:HB3	1.97	0.46
2:C:610:THR:HG21	2:C:614:LYS:HB3	1.97	0.46
2:D:365:GLU:HA	2:D:365:GLU:OE1	2.15	0.46
2:B:291:GLN:NE2	2:B:353:LEU:HD21	2.30	0.46
2:D:569:VAL:HG22	2:D:570:LYS:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:621:VAL:HG12	2:D:622:ASN:N	2.31	0.46
2:C:386:ILE:HG21	2:C:396:GLU:HG3	1.96	0.46
2:B:547:ILE:HG12	2:B:578:ILE:HD12	1.97	0.46
1:J:89:U:H5	2:B:583:ARG:CZ	2.27	0.46
2:B:501:ASP:O	2:B:503:GLU:HG2	2.16	0.46
1:L:95:A:H2'	1:L:96:C:C6	2.50	0.46
2:C:298:MET:HE3	2:C:327:TYR:HB2	1.98	0.46
2:C:305:GLU:HA	2:C:310:TRP:HB3	1.98	0.46
2:B:536:TRP:CD1	2:B:635:ARG:HA	2.50	0.46
2:F:600:GLU:HB3	2:F:605:LYS:O	2.15	0.46
2:F:619:MET:HG3	2:F:624:VAL:HG12	1.96	0.46
2:G:545:MET:HE3	2:G:593:MET:HB3	1.96	0.46
2:H:421:SER:OG	2:H:467:GLU:OE2	2.33	0.46
2:A:545:MET:SD	2:A:582:ILE:HD13	2.56	0.46
2:B:542:VAL:CG1	2:B:543:VAL:N	2.77	0.46
1:I:95:A:H1'	2:B:502:ASN:HD21	1.81	0.46
2:B:580:PHE:HD1	2:B:580:PHE:C	2.19	0.46
1:M:93:U:C2	1:M:94:C:C5	3.03	0.46
2:G:460:ALA:HB1	2:G:462:TYR:CD1	2.50	0.46
2:H:274:PHE:CZ	2:H:518:MET:HG3	2.51	0.46
2:H:488:SER:C	2:H:490:PRO:HD2	2.35	0.46
2:F:445:LEU:HD21	2:F:466:ILE:HG12	1.98	0.46
2:C:356:ALA:HA	2:C:384:ALA:HA	1.98	0.46
2:B:423:ARG:HE	2:B:438:GLU:CD	2.19	0.46
1:O:86:G:O4'	1:O:86:G:P	2.73	0.46
1:M:86:G:C4	2:E:547:ILE:HD13	2.51	0.46
2:E:548:THR:HG23	2:E:551:GLN:OE1	2.15	0.46
2:F:423:ARG:HD2	2:F:438:GLU:OE2	2.16	0.46
2:H:285:LEU:HD21	2:H:512:ARG:HH12	1.81	0.46
2:E:255:HIS:HE2	2:E:257:GLN:CG	2.29	0.46
2:G:500:GLU:C	2:G:502:ASN:N	2.69	0.46
1:K:93:U:C4	1:K:94:C:N4	2.84	0.46
2:C:612:ARG:CG	2:C:612:ARG:HH11	2.29	0.46
2:E:341:PHE:O	2:E:346:LYS:NZ	2.40	0.46
2:A:527:GLU:O	2:A:528:GLU:O	2.34	0.46
2:G:347:SER:HA	2:G:498:VAL:H	1.81	0.46
2:B:274:PHE:C	2:B:274:PHE:CD1	2.89	0.46
2:H:300:ASP:OD2	2:H:302:VAL:HB	2.16	0.46
2:D:628:LEU:O	2:D:632:ILE:HG13	2.14	0.46
2:C:621:VAL:HG12	2:C:622:ASN:N	2.31	0.46
2:H:562:LEU:HD12	2:H:625:ILE:HD11	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:423:ARG:NE	2:A:438:GLU:OE1	2.48	0.46
2:C:422:THR:HB	2:C:438:GLU:OE2	2.15	0.46
2:A:288:TYR:CE2	2:A:403:LEU:HD13	2.51	0.46
2:B:452:PHE:HE2	2:B:454:TYR:CE1	2.21	0.46
1:I:84:U:O2'	1:I:85:C:P	2.73	0.46
2:H:462:TYR:HD2	2:H:486:ASP:OD2	1.98	0.46
2:D:348:TYR:CD1	2:D:348:TYR:C	2.88	0.46
1:K:95:A:C2	1:K:96:C:C2	3.03	0.46
2:E:247:ILE:O	2:E:250:GLN:HB2	2.16	0.46
2:F:356:ALA:HA	2:F:384:ALA:CB	2.46	0.46
2:H:602:GLU:OE1	2:H:602:GLU:N	2.49	0.46
2:E:422:THR:O	2:E:423:ARG:C	2.54	0.46
1:L:86:G:P	1:L:86:G:O4'	2.73	0.46
1:P:86:G:C3'	5:P:1613:HOH:O	2.54	0.46
2:G:562:LEU:HD12	2:G:625:ILE:HD11	1.98	0.46
2:G:402:ARG:CB	2:G:402:ARG:NH1	2.77	0.46
2:A:512:ARG:O	2:A:512:ARG:NE	2.48	0.46
2:F:397:VAL:O	2:F:401:ILE:HG12	2.15	0.46
2:D:274:PHE:O	2:D:518:MET:HE3	2.15	0.46
2:H:329:ILE:N	2:H:329:ILE:CD1	2.79	0.46
2:E:329:ILE:CD1	2:E:329:ILE:N	2.79	0.46
2:C:297:PHE:CG	2:D:362:HIS:HE1	2.34	0.46
2:C:273:ILE:HG22	2:C:522:ILE:HD11	1.98	0.46
2:A:488:SER:C	2:A:490:PRO:HD2	2.36	0.46
2:H:619:MET:HG3	2:H:624:VAL:HG12	1.98	0.46
2:E:277:LEU:O	2:E:280:PHE:HB3	2.16	0.46
2:B:280:PHE:CZ	2:B:407:MET:HG2	2.51	0.46
2:D:548:THR:HG23	2:D:551:GLN:OE1	2.16	0.46
2:E:386:ILE:O	2:E:509:MET:HA	2.16	0.46
2:A:462:TYR:CD1	2:A:462:TYR:N	2.84	0.46
1:J:86:G:O4'	1:J:86:G:P	2.73	0.46
2:E:299:MET:HE1	2:E:335:PRO:HB2	1.97	0.46
2:A:621:VAL:HG12	2:A:622:ASN:N	2.29	0.46
2:G:298:MET:HE2	2:G:327:TYR:CD1	2.51	0.46
2:B:526:THR:HG23	2:B:533:PHE:HZ	1.81	0.46
2:A:278:GLU:CB	2:A:358:PHE:HE2	2.29	0.46
2:E:550:SER:C	2:E:552:SER:H	2.18	0.46
2:D:347:SER:HA	2:D:498:VAL:H	1.80	0.46
2:B:602:GLU:N	2:B:602:GLU:OE1	2.49	0.46
2:E:602:GLU:N	2:E:602:GLU:OE1	2.49	0.46
2:B:555:VAL:O	2:B:559:THR:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:620:ASP:HB3	2:B:623:GLU:CB	2.46	0.45
2:G:585:HIS:HB2	2:G:593:MET:HE2	1.94	0.45
1:O:87:U:C2'	5:O:1519:HOH:O	2.39	0.45
2:H:411:PHE:HE2	2:H:525:LEU:HD11	1.81	0.45
1:P:87:U:H3'	5:P:1619:HOH:O	2.16	0.45
1:I:87:U:C2'	1:I:88:G:OP2	2.64	0.45
2:D:339:GLN:CA	2:D:339:GLN:OE1	2.64	0.45
2:D:490:PRO:HD3	2:D:509:MET:CE	2.46	0.45
2:C:500:GLU:N	2:C:500:GLU:OE1	2.48	0.45
2:F:298:MET:HE2	2:F:327:TYR:CD1	2.51	0.45
2:F:330:LYS:HA	2:F:331:PRO:HD3	1.64	0.45
2:A:528:GLU:O	2:A:530:ALA:N	2.49	0.45
1:I:80:U:H2'	1:I:81:C:C6	2.51	0.45
2:E:423:ARG:HG2	2:E:423:ARG:O	2.15	0.45
2:D:427:ARG:HB2	2:D:434:TRP:CZ2	2.51	0.45
2:G:569:VAL:CG2	2:G:570:LYS:N	2.79	0.45
2:A:402:ARG:NH1	2:A:402:ARG:CB	2.78	0.45
2:F:290:TYR:CZ	2:F:512:ARG:NH1	2.85	0.45
2:A:500:GLU:C	2:A:502:ASN:N	2.70	0.45
2:B:375:ARG:NH2	5:B:210:HOH:O	2.36	0.45
2:D:356:ALA:HA	2:D:384:ALA:HA	1.98	0.45
2:F:273:ILE:HG22	2:F:522:ILE:HD11	1.97	0.45
2:C:589:ARG:O	2:C:611:ARG:HD3	2.16	0.45
1:O:97:C:C4'	1:O:98:A:OP1	2.64	0.45
2:F:422:THR:HB	2:F:438:GLU:OE2	2.17	0.45
2:B:545:MET:SD	2:B:582:ILE:HD13	2.56	0.45
1:M:87:U:C3'	5:M:1319:HOH:O	2.62	0.45
2:F:253:LEU:O	2:F:270:GLY:HA3	2.16	0.45
2:H:298:MET:HE3	2:H:327:TYR:HB2	1.98	0.45
2:B:278:GLU:CA	2:B:358:PHE:HE2	2.29	0.45
2:H:526:THR:O	2:H:530:ALA:N	2.49	0.45
2:D:526:THR:O	2:D:530:ALA:N	2.50	0.45
2:D:526:THR:O	2:D:530:ALA:HA	2.16	0.45
2:B:329:ILE:N	2:B:329:ILE:CD1	2.80	0.45
2:D:300:ASP:OD2	2:D:302:VAL:HB	2.16	0.45
2:F:488:SER:C	2:F:490:PRO:HD2	2.36	0.45
2:A:294:LYS:HA	2:A:357:GLU:HG3	1.98	0.45
2:G:279:VAL:CG2	2:G:280:PHE:N	2.80	0.45
2:G:280:PHE:HE2	2:G:407:MET:HG2	1.78	0.45
2:C:588:ARG:C	2:C:589:ARG:HG2	2.36	0.45
2:F:462:TYR:CE2	2:F:511:HIS:NE2	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:320:THR:HG22	2:G:321:SER:N	2.25	0.45
2:A:462:TYR:HE2	2:A:511:HIS:CD2	2.35	0.45
2:A:541:GLN:HE22	2:A:632:ILE:HD13	1.82	0.45
2:D:536:TRP:CD1	2:D:635:ARG:HA	2.52	0.45
2:G:550:SER:C	2:G:552:SER:H	2.19	0.45
2:E:285:LEU:HD21	2:E:512:ARG:HH12	1.82	0.45
1:K:85:C:C2'	2:C:577:LYS:HG2	2.46	0.45
1:I:88:G:H1'	2:A:583:ARG:CG	2.46	0.45
2:G:490:PRO:HD3	2:G:509:MET:CE	2.46	0.45
2:F:386:ILE:O	2:F:509:MET:HA	2.17	0.45
2:B:304:TRP:CE3	2:B:328:CYS:HB2	2.52	0.45
2:E:500:GLU:C	2:E:502:ASN:N	2.70	0.45
2:C:282:ARG:HD3	2:C:292:GLU:OE1	2.16	0.45
2:E:624:VAL:O	2:E:628:LEU:HG	2.17	0.45
1:M:81:C:O2'	1:M:82:U:H5'	2.16	0.45
1:K:93:U:H2'	1:K:94:C:H6	1.82	0.45
2:E:462:TYR:CE2	2:E:511:HIS:NE2	2.85	0.45
2:A:471:TYR:CD1	2:A:471:TYR:N	2.85	0.45
2:G:627:LYS:O	2:G:630:GLN:HB3	2.16	0.45
1:M:71:C:C2	1:M:72:G:C8	3.04	0.45
2:F:380:THR:N	2:F:519:GLU:OE2	2.50	0.45
2:H:550:SER:C	2:H:552:SER:H	2.20	0.45
2:D:437:ALA:HA	2:D:485:LEU:HD23	1.97	0.45
2:D:519:GLU:H	2:D:519:GLU:CD	2.20	0.45
2:C:569:VAL:HG22	2:C:570:LYS:N	2.31	0.45
2:E:397:VAL:O	2:E:400:CYS:HB2	2.16	0.45
2:B:277:LEU:O	2:B:280:PHE:HB3	2.17	0.45
2:C:551:GLN:HG2	2:C:597:GLY:C	2.37	0.45
2:D:421:SER:HB3	2:D:458:GLU:CB	2.35	0.45
2:C:411:PHE:CE2	2:C:521:PHE:HZ	2.31	0.45
1:K:98:A:N7	2:D:345:LEU:HD13	2.31	0.45
2:E:362:HIS:HE1	2:F:297:PHE:CG	2.34	0.45
2:G:330:LYS:HA	2:G:331:PRO:HD3	1.63	0.45
2:A:445:LEU:HD21	2:A:466:ILE:HG12	1.98	0.45
2:H:380:THR:HG22	2:H:380:THR:O	2.17	0.45
1:J:96:C:H2'	1:J:97:C:C6	2.51	0.45
2:B:251:LEU:HD22	2:B:588:ARG:O	2.17	0.45
2:F:397:VAL:O	2:F:400:CYS:HB2	2.17	0.45
2:H:554:TYR:CE1	2:H:558:LEU:HD11	2.51	0.45
2:B:312:ASN:O	2:B:313:TYR:HB2	2.16	0.45
2:A:405:TYR:HE1	2:A:416:ILE:HG21	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:273:ILE:HG23	2:A:537:LEU:CD2	2.46	0.45
2:F:294:LYS:HA	2:F:357:GLU:HG3	1.98	0.45
2:B:300:ASP:OD2	2:B:302:VAL:HB	2.16	0.45
2:F:555:VAL:O	2:F:559:THR:HG23	2.17	0.45
2:A:422:THR:HB	2:A:438:GLU:OE2	2.17	0.45
2:G:551:GLN:HG2	2:G:597:GLY:C	2.36	0.45
2:B:551:GLN:HE21	2:B:598:ASP:N	2.14	0.45
2:A:482:THR:O	2:A:512:ARG:HA	2.16	0.45
2:D:332:MET:HE2	4:D:5002:TSB:HN12	1.81	0.45
2:E:460:ALA:C	2:E:462:TYR:H	2.19	0.45
2:D:609:ARG:HD3	2:D:610:THR:O	2.17	0.45
2:E:610:THR:HG22	2:E:614:LYS:O	2.17	0.45
2:C:441:LEU:O	2:C:444:ALA:HB3	2.16	0.45
2:E:445:LEU:HD21	2:E:466:ILE:HG12	1.98	0.45
2:F:562:LEU:HB3	2:F:569:VAL:HG11	1.97	0.45
2:E:280:PHE:CZ	2:E:407:MET:HG2	2.51	0.45
1:O:89:U:P	5:O:1528:HOH:O	2.75	0.45
2:C:585:HIS:HA	2:C:588:ARG:HB2	1.99	0.45
2:B:427:ARG:HB2	2:B:434:TRP:CZ2	2.52	0.45
2:A:422:THR:O	2:A:458:GLU:O	2.34	0.45
2:B:490:PRO:HD3	2:B:509:MET:CE	2.47	0.45
1:N:86:G:O6	2:F:599:LYS:CB	2.65	0.45
1:J:93:U:C2	1:J:94:C:C6	3.05	0.45
2:G:567:ILE:O	2:G:569:VAL:N	2.50	0.45
2:D:253:LEU:O	2:D:270:GLY:HA3	2.17	0.45
2:D:299:MET:HE1	2:D:335:PRO:HB2	1.99	0.45
2:A:417:VAL:HG13	2:A:471:TYR:CE1	2.47	0.45
2:D:610:THR:HG22	2:D:614:LYS:O	2.17	0.45
2:F:526:THR:HG23	2:F:533:PHE:CZ	2.50	0.45
2:G:383:ASP:OD2	2:G:385:HIS:HE1	2.00	0.45
1:P:80:U:H2'	1:P:81:C:H6	1.80	0.45
2:C:294:LYS:HA	2:C:294:LYS:HD2	1.84	0.45
2:B:279:VAL:CG2	2:B:280:PHE:N	2.80	0.45
2:B:423:ARG:O	2:B:423:ARG:HG2	2.17	0.45
2:A:455:GLN:O	2:A:456:LEU:C	2.55	0.45
1:K:90:G:C8	2:C:577:LYS:HD2	2.51	0.45
2:F:421:SER:CA	2:F:455:GLN:HB3	2.45	0.45
1:M:87:U:C2'	1:M:88:G:OP2	2.65	0.45
2:E:251:LEU:HD22	2:E:588:ARG:O	2.17	0.45
2:A:628:LEU:O	2:A:632:ILE:HG13	2.17	0.45
2:C:297:PHE:CG	2:D:362:HIS:CE1	3.05	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:294:LYS:HA	2:C:357:GLU:HG3	1.99	0.45
2:A:480:CYS:O	2:A:516:GLY:HA3	2.17	0.45
2:A:282:ARG:HD3	2:A:292:GLU:OE1	2.16	0.45
2:C:436:ARG:HG2	2:C:440:ASP:OD2	2.17	0.45
2:H:569:VAL:O	2:H:570:LYS:HG2	2.17	0.44
2:C:543:VAL:HG11	2:C:585:HIS:ND1	2.31	0.44
2:H:551:GLN:HG2	2:H:597:GLY:C	2.37	0.44
2:F:465:LYS:HG3	2:F:484:GLN:CG	2.44	0.44
2:F:255:HIS:HE2	2:F:257:GLN:CG	2.30	0.44
1:N:87:U:H2'	5:N:1419:HOH:O	2.16	0.44
2:C:303:LEU:HD11	2:C:339:GLN:NE2	2.31	0.44
2:E:320:THR:HG22	2:E:321:SER:N	2.25	0.44
2:G:397:VAL:O	2:G:401:ILE:HG12	2.17	0.44
2:E:460:ALA:C	2:E:462:TYR:N	2.68	0.44
2:E:243:ASP:O	2:E:247:ILE:HG13	2.17	0.44
2:G:309:HIS:HB3	2:G:317:MET:HE1	1.99	0.44
2:B:603:SER:C	2:B:605:LYS:H	2.20	0.44
2:B:624:VAL:HG23	2:B:625:ILE:N	2.32	0.44
1:O:89:U:H5	2:G:583:ARG:NH2	2.14	0.44
2:A:423:ARG:HD2	2:A:438:GLU:OE2	2.18	0.44
2:C:421:SER:HB3	2:C:458:GLU:CB	2.35	0.44
2:H:551:GLN:HE21	2:H:598:ASP:N	2.16	0.44
2:B:253:LEU:HD23	2:B:253:LEU:N	2.32	0.44
2:F:285:LEU:HD22	2:F:290:TYR:CG	2.52	0.44
1:L:84:U:H4'	1:L:85:C:H5'	1.97	0.44
2:D:329:ILE:CD1	2:D:329:ILE:N	2.80	0.44
2:H:323:GLU:H	2:H:323:GLU:CD	2.19	0.44
2:C:323:GLU:O	2:C:324:ASN:O	2.35	0.44
2:C:242:ARG:HE	2:C:246:LYS:HD3	1.82	0.44
2:G:474:LEU:O	2:G:475:ASP:C	2.55	0.44
1:I:83:U:H3	2:A:575:ASN:HD21	1.65	0.44
2:B:421:SER:CA	2:B:455:GLN:HB3	2.47	0.44
2:C:423:ARG:NE	2:C:438:GLU:OE1	2.49	0.44
2:D:585:HIS:HA	2:D:588:ARG:HB2	1.98	0.44
1:O:84:U:C2'	2:G:548:THR:HG1	2.30	0.44
2:F:588:ARG:C	2:F:589:ARG:HG2	2.37	0.44
1:M:84:U:H4'	1:M:85:C:H5'	1.96	0.44
1:I:86:G:H3'	5:I:109:HOH:O	2.17	0.44
2:F:291:GLN:NE2	2:F:353:LEU:HD21	2.32	0.44
2:D:389:THR:HG1	2:D:392:GLN:HG3	1.80	0.44
2:G:604:GLY:O	2:G:621:VAL:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:501:ASP:O	2:H:503:GLU:HG2	2.18	0.44
2:G:400:CYS:O	2:G:404:VAL:HG23	2.17	0.44
2:A:556:ASN:HD21	2:A:573:LEU:HD11	1.82	0.44
2:F:365:GLU:N	2:F:377:ARG:HD3	2.30	0.44
2:D:353:LEU:HB3	2:D:387:PHE:HB2	1.98	0.44
2:C:437:ALA:HB2	2:C:487:PHE:CD2	2.52	0.44
2:B:274:PHE:O	2:B:518:MET:HE3	2.17	0.44
2:G:288:TYR:N	2:G:288:TYR:CD1	2.85	0.44
2:D:426:LYS:HB3	2:D:426:LYS:HE2	1.84	0.44
2:D:550:SER:C	2:D:552:SER:H	2.20	0.44
2:C:590:VAL:O	2:C:611:ARG:HB3	2.17	0.44
2:C:351:LEU:HD22	2:C:387:PHE:O	2.17	0.44
2:F:411:PHE:CD2	2:F:521:PHE:HZ	2.35	0.44
2:H:542:VAL:CG1	2:H:543:VAL:N	2.80	0.44
1:P:85:C:C5	2:H:547:ILE:O	2.68	0.44
2:F:455:GLN:O	2:F:456:LEU:C	2.56	0.44
2:C:254:TYR:CD2	2:C:255:HIS:N	2.85	0.44
2:G:251:LEU:CA	2:G:588:ARG:HH12	2.25	0.44
2:D:501:ASP:O	2:D:503:GLU:HG2	2.18	0.44
2:A:285:LEU:HD21	2:A:512:ARG:HH12	1.83	0.44
2:C:298:MET:O	2:C:298:MET:HG2	2.16	0.44
2:H:305:GLU:HA	2:H:310:TRP:HB3	1.98	0.44
2:B:278:GLU:HA	2:B:358:PHE:HE2	1.83	0.44
2:C:362:HIS:HE1	2:D:297:PHE:CD1	2.35	0.44
1:N:72:G:H2'	1:N:73:U:H6	1.82	0.44
2:E:421:SER:OG	2:E:467:GLU:OE2	2.36	0.44
1:K:89:U:O2'	2:C:580:PHE:CG	2.69	0.44
2:E:303:LEU:HD11	2:E:339:GLN:NE2	2.31	0.44
2:A:255:HIS:HE2	2:A:257:GLN:CG	2.30	0.44
2:D:287:GLU:HB2	2:D:288:TYR:HD1	1.82	0.44
1:L:96:C:H2'	1:L:97:C:C6	2.52	0.44
2:E:399:GLY:HA2	2:E:402:ARG:HH11	1.82	0.44
2:F:471:TYR:N	2:F:471:TYR:CD1	2.86	0.44
2:E:609:ARG:HD3	2:E:610:THR:O	2.18	0.44
2:H:274:PHE:C	2:H:274:PHE:CD1	2.90	0.44
2:B:287:GLU:HB2	2:B:288:TYR:HD1	1.83	0.44
2:H:323:GLU:O	2:H:324:ASN:O	2.36	0.44
2:F:569:VAL:HG22	2:F:570:LYS:N	2.33	0.44
2:B:619:MET:HG3	2:B:624:VAL:HG12	2.00	0.44
2:F:548:THR:HG23	2:F:551:GLN:OE1	2.18	0.44
1:J:88:G:H8	5:J:1023:HOH:O	1.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:395:ASP:N	2:H:395:ASP:OD1	2.47	0.44
2:B:588:ARG:C	2:B:589:ARG:HG2	2.38	0.44
2:G:365:GLU:HA	2:G:365:GLU:OE1	2.18	0.44
2:A:562:LEU:HB3	2:A:569:VAL:HG11	2.00	0.44
1:P:103:G:H5'	5:P:1625:HOH:O	2.18	0.44
2:E:603:SER:C	2:E:605:LYS:H	2.19	0.44
2:A:273:ILE:HG23	2:A:537:LEU:HD22	1.99	0.44
2:E:526:THR:O	2:E:530:ALA:HA	2.18	0.44
2:D:437:ALA:HB2	2:D:487:PHE:CD2	2.53	0.44
1:P:72:G:H2'	1:P:73:U:H6	1.83	0.44
2:F:437:ALA:HA	2:F:485:LEU:HD23	1.99	0.44
2:G:274:PHE:C	2:G:274:PHE:CD1	2.90	0.44
2:D:562:LEU:HB3	2:D:569:VAL:HG11	2.00	0.44
2:F:562:LEU:HD12	2:F:625:ILE:HD11	2.00	0.44
2:H:427:ARG:HB2	2:H:434:TRP:CZ2	2.52	0.44
2:A:386:ILE:HG21	2:A:396:GLU:CG	2.48	0.44
1:M:86:G:O4'	1:M:86:G:P	2.76	0.44
1:P:86:G:N9	2:H:547:ILE:HD13	2.31	0.44
2:A:551:GLN:HG2	2:A:597:GLY:C	2.38	0.44
2:D:255:HIS:HE2	2:D:257:GLN:CG	2.31	0.44
2:A:285:LEU:HD22	2:A:290:TYR:CG	2.52	0.44
2:H:609:ARG:HD3	2:H:610:THR:O	2.18	0.44
2:D:274:PHE:C	2:D:274:PHE:CD1	2.91	0.44
2:A:356:ALA:HB2	2:A:384:ALA:HB2	2.00	0.44
2:H:405:TYR:HE1	2:H:416:ILE:HG21	1.83	0.44
2:G:287:GLU:HB2	2:G:288:TYR:HD1	1.82	0.44
2:G:288:TYR:HD1	2:G:288:TYR:N	2.15	0.44
2:C:427:ARG:HA	2:C:461:PHE:O	2.18	0.44
2:F:551:GLN:HE21	2:F:598:ASP:N	2.16	0.44
2:F:459:GLY:HA2	2:F:465:LYS:HE2	1.99	0.44
2:C:255:HIS:ND1	2:C:267:HIS:CE1	2.67	0.44
1:M:98:A:H4'	5:M:1327:HOH:O	2.17	0.44
2:E:339:GLN:CA	2:E:339:GLN:OE1	2.66	0.44
2:F:277:LEU:O	2:F:280:PHE:HB3	2.17	0.44
2:H:471:TYR:N	2:H:471:TYR:CD1	2.86	0.44
2:D:291:GLN:NE2	2:D:353:LEU:HD21	2.33	0.44
2:D:528:GLU:O	2:D:530:ALA:N	2.51	0.44
2:H:603:SER:C	2:H:605:LYS:N	2.71	0.44
2:E:347:SER:HA	2:E:498:VAL:H	1.83	0.44
2:H:612:ARG:HH11	2:H:612:ARG:CG	2.28	0.44
2:B:290:TYR:CE2	2:B:512:ARG:NH1	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:422:THR:O	2:G:423:ARG:C	2.56	0.44
2:D:547:ILE:HG12	2:D:578:ILE:HD12	2.00	0.44
1:N:86:G:N3	2:F:547:ILE:CD1	2.81	0.44
1:J:94:C:C2	1:J:95:A:C8	3.06	0.44
1:J:75:U:O2'	1:J:76:G:P	2.76	0.44
2:E:587:LEU:HD23	2:E:587:LEU:N	2.24	0.44
2:A:320:THR:HG23	2:B:319:THR:H	1.83	0.44
2:A:332:MET:HG2	2:A:363:ARG:NH2	2.31	0.44
2:F:500:GLU:C	2:F:502:ASN:N	2.69	0.44
2:E:462:TYR:HE2	2:E:511:HIS:NE2	2.14	0.44
2:F:527:GLU:O	2:F:528:GLU:O	2.36	0.44
2:C:482:THR:O	2:C:512:ARG:HA	2.17	0.44
2:G:462:TYR:CD2	2:G:486:ASP:OD2	2.70	0.44
2:A:313:TYR:HB3	2:A:317:MET:HE1	2.00	0.44
2:H:600:GLU:HB3	2:H:605:LYS:O	2.17	0.44
2:B:351:LEU:HD22	2:B:387:PHE:O	2.17	0.44
1:J:83:U:H3	2:B:575:ASN:HD21	1.66	0.44
2:G:395:ASP:N	2:G:395:ASP:OD1	2.48	0.44
2:D:282:ARG:HD3	2:D:292:GLU:OE1	2.17	0.44
2:H:556:ASN:HD21	2:H:573:LEU:HD11	1.83	0.43
2:F:587:LEU:N	2:F:587:LEU:HD23	2.25	0.43
2:D:298:MET:HE2	2:D:327:TYR:CD1	2.53	0.43
2:D:441:LEU:O	2:D:444:ALA:HB3	2.18	0.43
2:C:278:GLU:HB3	2:C:358:PHE:CE2	2.52	0.43
2:A:557:GLU:O	2:A:560:GLN:HB3	2.18	0.43
2:D:317:MET:HG3	2:D:331:PRO:HG3	2.00	0.43
2:B:569:VAL:O	2:B:570:LYS:HG2	2.17	0.43
2:A:250:GLN:HA	2:A:250:GLN:NE2	2.33	0.43
2:F:300:ASP:OD2	2:F:302:VAL:HB	2.18	0.43
2:D:555:VAL:O	2:D:559:THR:HG23	2.18	0.43
2:B:473:CYS:CA	5:B:221:HOH:O	2.35	0.43
2:D:551:GLN:HG2	2:D:597:GLY:C	2.38	0.43
2:A:388:CYS:O	2:A:508:VAL:HG23	2.18	0.43
2:E:542:VAL:CG1	2:E:543:VAL:N	2.80	0.43
2:F:332:MET:HG2	2:F:363:ARG:NH2	2.33	0.43
2:H:388:CYS:O	2:H:508:VAL:HG23	2.18	0.43
2:G:386:ILE:O	2:G:509:MET:HA	2.18	0.43
2:F:353:LEU:HB3	2:F:387:PHE:HB2	1.99	0.43
2:B:500:GLU:C	2:B:502:ASN:N	2.70	0.43
2:C:298:MET:CE	2:C:327:TYR:HB2	2.47	0.43
2:A:418:VAL:HG21	2:A:450:ILE:CG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:480:CYS:O	2:B:516:GLY:HA3	2.18	0.43
2:C:347:SER:HA	2:C:498:VAL:H	1.83	0.43
2:F:604:GLY:O	2:F:621:VAL:HG23	2.18	0.43
1:P:86:G:P	1:P:86:G:O4'	2.76	0.43
1:M:89:U:H2'	1:M:90:G:OP1	2.18	0.43
2:D:254:TYR:CD2	2:D:255:HIS:N	2.85	0.43
2:B:402:ARG:NH1	2:B:402:ARG:CB	2.79	0.43
2:A:529:PHE:H	2:A:529:PHE:HD1	1.55	0.43
2:A:348:TYR:CE2	2:A:500:GLU:HG3	2.53	0.43
1:I:77:U:O5'	1:I:77:U:H6	2.01	0.43
2:E:639:GLN:O	2:E:642:GLU:HG2	2.18	0.43
2:F:627:LYS:CB	2:F:640:LEU:HD21	2.47	0.43
2:H:528:GLU:O	2:H:530:ALA:N	2.51	0.43
2:C:330:LYS:HA	2:C:331:PRO:HD3	1.61	0.43
2:E:353:LEU:HA	2:E:353:LEU:HD22	1.82	0.43
2:F:356:ALA:HA	2:F:384:ALA:HA	2.00	0.43
2:F:342:ASN:HD21	2:F:495:ALA:HA	1.83	0.43
2:E:437:ALA:HA	2:E:485:LEU:HD23	2.00	0.43
1:L:72:G:H2'	1:L:73:U:H6	1.81	0.43
2:A:387:PHE:CE1	2:A:509:MET:SD	3.11	0.43
2:F:585:HIS:CB	2:F:593:MET:HE3	2.47	0.43
2:F:353:LEU:HA	2:F:353:LEU:HD22	1.78	0.43
2:F:254:TYR:HA	2:F:267:HIS:ND1	2.33	0.43
1:N:87:U:C2'	1:N:88:G:OP2	2.66	0.43
2:G:348:TYR:CE2	2:G:500:GLU:HG3	2.53	0.43
2:D:482:THR:HG21	4:D:5002:TSB:H5'2	1.99	0.43
2:D:335:PRO:HG2	2:D:336:GLY:H	1.81	0.43
2:D:500:GLU:C	2:D:502:ASN:N	2.70	0.43
2:F:482:THR:O	2:F:512:ARG:HA	2.18	0.43
2:A:569:VAL:O	2:A:570:LYS:HG2	2.19	0.43
2:G:319:THR:HG22	2:G:328:CYS:HA	1.99	0.43
2:F:417:VAL:HG13	2:F:471:TYR:CE1	2.49	0.43
2:H:610:THR:HG22	2:H:614:LYS:O	2.18	0.43
1:I:72:G:H2'	1:I:73:U:C6	2.52	0.43
2:D:436:ARG:HG2	2:D:440:ASP:OD2	2.19	0.43
2:E:282:ARG:HD3	2:E:292:GLU:OE1	2.19	0.43
2:G:436:ARG:HG2	2:G:440:ASP:OD2	2.18	0.43
2:G:521:PHE:HE1	2:G:525:LEU:HD11	1.84	0.43
2:D:562:LEU:HD12	2:D:625:ILE:HD11	2.00	0.43
2:D:521:PHE:HE1	2:D:525:LEU:HD11	1.82	0.43
2:G:583:ARG:O	2:G:586:THR:N	2.50	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:285:LEU:HD21	2:B:512:ARG:HH12	1.83	0.43
2:A:423:ARG:HB3	2:A:434:TRP:CE3	2.54	0.43
1:J:87:U:C2'	1:J:88:G:OP2	2.66	0.43
2:E:254:TYR:HA	2:E:267:HIS:ND1	2.34	0.43
2:D:554:TYR:CE1	2:D:558:LEU:HD11	2.54	0.43
2:C:471:TYR:N	2:C:471:TYR:CD1	2.86	0.43
2:F:612:ARG:HH11	2:F:612:ARG:CG	2.32	0.43
2:F:609:ARG:HD3	2:F:610:THR:O	2.18	0.43
2:C:309:HIS:HB3	2:C:317:MET:HE1	2.01	0.43
1:J:71:C:C2	1:J:72:G:C8	3.06	0.43
2:E:291:GLN:NE2	2:E:353:LEU:HD21	2.32	0.43
2:C:300:ASP:OD2	2:C:302:VAL:HB	2.19	0.43
2:H:445:LEU:HD21	2:H:466:ILE:HG12	2.01	0.43
2:C:274:PHE:C	2:C:274:PHE:CD1	2.92	0.43
2:D:459:GLY:HA2	2:D:465:LYS:HE2	2.01	0.43
2:D:421:SER:OG	2:D:467:GLU:OE2	2.37	0.43
1:L:86:G:O6	2:D:599:LYS:HB2	2.18	0.43
2:F:423:ARG:NE	2:F:438:GLU:OE1	2.52	0.43
2:F:320:THR:HG22	2:F:321:SER:N	2.25	0.43
2:G:249:LYS:HZ3	2:G:249:LYS:HB3	1.80	0.43
2:E:402:ARG:CB	2:E:402:ARG:NH1	2.80	0.43
1:N:84:U:O2'	1:N:85:C:OP2	2.30	0.43
2:E:462:TYR:CD2	2:E:486:ASP:OD2	2.71	0.43
2:D:243:ASP:O	2:D:247:ILE:HG13	2.19	0.43
2:E:612:ARG:CG	2:E:612:ARG:HH11	2.30	0.43
2:F:526:THR:O	2:F:530:ALA:HA	2.18	0.43
2:G:609:ARG:HD3	2:G:610:THR:O	2.18	0.43
2:C:610:THR:HG22	2:C:614:LYS:O	2.19	0.43
2:D:603:SER:C	2:D:605:LYS:H	2.21	0.43
1:P:72:G:H2'	1:P:73:U:C6	2.54	0.43
1:N:69:G:O2'	1:N:70:G:H5'	2.18	0.43
2:H:242:ARG:HE	2:H:246:LYS:HD3	1.84	0.43
2:C:380:THR:N	2:C:519:GLU:OE2	2.50	0.43
2:B:622:ASN:O	2:B:626:GLU:HG3	2.18	0.43
2:E:521:PHE:HE1	2:E:525:LEU:HD11	1.84	0.43
2:D:423:ARG:HE	2:D:438:GLU:CD	2.22	0.43
2:H:597:GLY:O	2:H:601:VAL:HG23	2.17	0.43
1:P:87:U:O2'	1:P:88:G:P	2.77	0.43
2:F:484:GLN:HE22	4:F:7002:TSB:HN8	1.67	0.43
1:M:95:A:H2'	1:M:96:C:O4'	2.18	0.43
2:D:254:TYR:CZ	2:D:373:LEU:HD21	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:402:ARG:CB	2:H:402:ARG:NH1	2.79	0.43
2:A:465:LYS:HG3	2:A:484:GLN:CG	2.44	0.43
2:H:320:THR:HG22	2:H:321:SER:N	2.29	0.43
2:F:298:MET:HE3	2:F:327:TYR:HB2	1.99	0.43
2:A:327:TYR:CD1	2:A:327:TYR:N	2.87	0.43
2:B:323:GLU:O	2:B:324:ASN:O	2.36	0.43
2:B:347:SER:HA	2:B:498:VAL:H	1.84	0.43
2:D:323:GLU:CD	2:D:323:GLU:H	2.22	0.43
2:B:445:LEU:HD21	2:B:466:ILE:HG12	2.00	0.43
2:B:544:ILE:HG22	2:B:555:VAL:HG13	2.00	0.43
1:O:86:G:H1'	2:G:547:ILE:HD13	2.01	0.43
2:A:263:MET:HE2	2:B:298:MET:CG	2.40	0.43
2:B:255:HIS:HE2	2:B:257:GLN:CG	2.32	0.43
2:A:254:TYR:CE1	2:A:373:LEU:HD21	2.54	0.43
2:E:594:LEU:CD2	2:E:608:VAL:HG22	2.48	0.43
2:E:415:LYS:HG2	2:E:471:TYR:CD1	2.54	0.43
2:C:520:ARG:NH1	5:C:4008:HOH:O	2.50	0.43
2:A:634:SER:O	2:A:635:ARG:C	2.57	0.43
2:H:538:ALA:O	2:H:539:PRO:C	2.57	0.43
2:F:426:LYS:HE2	2:F:426:LYS:HB3	1.88	0.43
2:B:622:ASN:HB3	2:H:612:ARG:O	2.19	0.43
2:G:542:VAL:CG1	2:G:543:VAL:N	2.82	0.43
1:K:89:U:C2'	1:K:89:U:O2	2.66	0.43
2:A:351:LEU:HD13	2:A:388:CYS:HA	2.00	0.43
1:P:87:U:H1'	2:H:582:ILE:HG13	2.00	0.43
1:J:89:U:H5	2:B:583:ARG:NH2	2.16	0.43
2:C:280:PHE:CZ	2:C:407:MET:HG2	2.53	0.43
1:N:87:U:H2'	1:N:88:G:OP2	2.19	0.43
2:D:280:PHE:CZ	2:D:407:MET:HG2	2.53	0.43
2:A:452:PHE:CE2	2:A:454:TYR:HE1	2.24	0.43
1:L:95:A:H2'	1:L:96:C:O4'	2.19	0.43
1:J:79:A:H1'	2:A:502:ASN:OD1	2.19	0.43
1:N:97:C:C5'	1:N:98:A:OP1	2.64	0.43
2:F:242:ARG:HE	2:F:246:LYS:HD3	1.83	0.43
2:B:358:PHE:N	2:B:358:PHE:CD1	2.86	0.43
2:H:243:ASP:O	2:H:247:ILE:HG13	2.19	0.43
2:F:371:HIS:O	2:F:372:GLY:C	2.56	0.43
2:H:430:SER:O	2:H:431:ASP:C	2.55	0.43
2:E:242:ARG:HE	2:E:246:LYS:HD3	1.83	0.43
2:B:410:THR:HB	2:B:411:PHE:CD1	2.53	0.43
1:L:88:G:H1'	2:D:583:ARG:CG	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:U:C2'	1:L:88:G:OP2	2.66	0.43
2:G:551:GLN:HE21	2:G:598:ASP:N	2.16	0.43
2:A:630:GLN:HA	2:A:633:ARG:HH12	1.84	0.43
2:H:279:VAL:CG2	2:H:280:PHE:N	2.82	0.43
2:G:417:VAL:HG11	2:G:471:TYR:CE1	2.52	0.43
2:A:567:ILE:O	2:A:569:VAL:N	2.52	0.43
2:G:313:TYR:CE1	2:G:316:ALA:HB3	2.54	0.43
2:G:628:LEU:O	2:G:632:ILE:HG13	2.19	0.43
2:F:405:TYR:HE1	2:F:416:ILE:HG21	1.84	0.43
2:E:526:THR:O	2:E:530:ALA:N	2.51	0.43
2:B:353:LEU:HB3	2:B:387:PHE:HB2	2.00	0.43
2:B:323:GLU:CD	2:B:323:GLU:H	2.22	0.43
2:F:394:ARG:O	2:F:395:ASP:C	2.57	0.43
2:G:480:CYS:O	2:G:516:GLY:HA3	2.19	0.43
2:H:383:ASP:OD2	2:H:385:HIS:CE1	2.72	0.43
2:F:621:VAL:HG12	2:F:622:ASN:N	2.33	0.42
2:D:421:SER:CA	2:D:455:GLN:HB3	2.45	0.42
2:A:353:LEU:HB3	2:A:387:PHE:HB2	1.99	0.42
2:F:585:HIS:HA	2:F:588:ARG:HB2	2.01	0.42
2:F:251:LEU:CA	2:F:588:ARG:HH12	2.25	0.42
2:F:590:VAL:O	2:F:611:ARG:HB3	2.19	0.42
1:M:84:U:O2'	1:M:85:C:OP2	2.27	0.42
2:A:585:HIS:HA	2:A:588:ARG:HB2	2.01	0.42
2:F:254:TYR:CD2	2:F:255:HIS:N	2.87	0.42
2:H:255:HIS:HE2	2:H:257:GLN:CG	2.31	0.42
2:C:462:TYR:CD2	2:C:486:ASP:OD2	2.71	0.42
2:A:299:MET:O	2:A:304:TRP:HZ3	2.02	0.42
2:H:609:ARG:O	2:H:609:ARG:CG	2.67	0.42
2:D:627:LYS:O	2:D:630:GLN:HB3	2.19	0.42
2:G:250:GLN:HA	2:G:250:GLN:NE2	2.34	0.42
2:C:603:SER:C	2:C:605:LYS:H	2.21	0.42
2:A:330:LYS:HA	2:A:331:PRO:HD3	1.60	0.42
2:F:529:PHE:CD2	2:F:534:PRO:HD3	2.54	0.42
2:G:572:ASP:OD1	2:G:574:ARG:HB2	2.18	0.42
2:F:273:ILE:HG23	2:F:537:LEU:HD22	2.01	0.42
2:B:397:VAL:O	2:B:400:CYS:HB2	2.19	0.42
2:D:531:GLY:O	2:D:589:ARG:HG3	2.19	0.42
2:C:541:GLN:HE22	2:C:632:ILE:HD13	1.84	0.42
2:H:567:ILE:O	2:H:569:VAL:N	2.52	0.42
2:C:423:ARG:HE	2:C:438:GLU:CD	2.22	0.42
2:E:545:MET:SD	2:E:582:ILE:HD13	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:79:A:O2'	2:C:500:GLU:O	2.35	0.42
2:F:281:VAL:O	2:F:282:ARG:C	2.56	0.42
2:E:399:GLY:HA2	2:E:402:ARG:NH1	2.35	0.42
2:G:332:MET:HE2	4:G:8002:TSB:HN12	1.84	0.42
2:C:249:LYS:HA	2:C:249:LYS:HE2	2.01	0.42
2:F:274:PHE:CD1	2:F:274:PHE:C	2.91	0.42
2:B:550:SER:C	2:B:552:SER:N	2.72	0.42
2:G:337:HIS:NE2	2:G:357:GLU:OE1	2.47	0.42
2:C:416:ILE:O	2:C:416:ILE:HG22	2.18	0.42
2:E:356:ALA:HA	2:E:384:ALA:HA	2.00	0.42
2:D:423:ARG:NE	2:D:438:GLU:OE1	2.52	0.42
2:B:386:ILE:O	2:B:509:MET:HA	2.19	0.42
2:A:280:PHE:CZ	2:A:407:MET:HG2	2.54	0.42
2:A:400:CYS:SG	2:A:512:ARG:HG3	2.60	0.42
2:A:290:TYR:CZ	2:A:512:ARG:NH1	2.86	0.42
2:G:393:ILE:O	2:G:397:VAL:HG23	2.19	0.42
2:F:365:GLU:HA	2:F:365:GLU:OE1	2.19	0.42
2:C:627:LYS:CB	2:C:640:LEU:HD21	2.47	0.42
2:H:247:ILE:HD12	2:H:526:THR:HG22	2.00	0.42
2:G:610:THR:HG21	2:G:614:LYS:HB3	2.00	0.42
1:M:72:G:H2'	1:M:73:U:H6	1.84	0.42
2:F:347:SER:HA	2:F:498:VAL:H	1.84	0.42
1:N:92:G:H2'	1:N:93:U:H6	1.84	0.42
2:A:242:ARG:HE	2:A:246:LYS:HD3	1.85	0.42
2:F:569:VAL:O	2:F:570:LYS:HG2	2.20	0.42
2:D:422:THR:HB	2:D:438:GLU:OE2	2.19	0.42
2:E:490:PRO:HD3	2:E:509:MET:HE2	2.02	0.42
1:P:94:C:C2	1:P:95:A:C8	3.07	0.42
1:K:78:G:H21	2:D:502:ASN:CG	2.20	0.42
2:A:604:GLY:O	2:A:621:VAL:HG23	2.20	0.42
2:D:610:THR:HG22	2:D:614:LYS:HB3	2.00	0.42
2:E:417:VAL:HG13	2:E:471:TYR:CE1	2.50	0.42
2:E:627:LYS:CB	2:E:640:LEU:HD21	2.47	0.42
2:G:497:TYR:OH	2:G:505:LYS:HE2	2.19	0.42
2:G:526:THR:HG23	2:G:533:PHE:CZ	2.55	0.42
2:G:612:ARG:HH11	2:G:612:ARG:CG	2.32	0.42
2:C:365:GLU:HA	2:C:365:GLU:OE1	2.19	0.42
2:E:330:LYS:HA	2:E:331:PRO:HD3	1.61	0.42
2:H:529:PHE:CD2	2:H:534:PRO:HD3	2.55	0.42
2:H:347:SER:HA	2:H:498:VAL:H	1.85	0.42
1:O:89:U:C2'	1:O:90:G:OP1	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:411:PHE:CD2	2:A:525:LEU:CD2	2.90	0.42
1:O:78:G:P	5:O:1539:HOH:O	2.73	0.42
2:C:411:PHE:CD2	2:C:521:PHE:HZ	2.37	0.42
1:I:86:G:C3'	5:I:109:HOH:O	2.66	0.42
1:M:87:U:H2'	1:M:88:G:OP2	2.19	0.42
1:N:78:G:C1'	2:E:345:LEU:HD23	2.49	0.42
2:H:589:ARG:O	2:H:611:ARG:NH1	2.48	0.42
1:P:93:U:N3	1:P:94:C:C5	2.88	0.42
2:A:501:ASP:O	2:A:503:GLU:HG2	2.19	0.42
2:E:588:ARG:C	2:E:589:ARG:HG2	2.40	0.42
2:G:393:ILE:HD11	2:G:508:VAL:HG11	2.02	0.42
2:C:460:ALA:C	2:C:462:TYR:N	2.72	0.42
2:C:459:GLY:HA2	2:C:465:LYS:HE2	2.01	0.42
2:B:305:GLU:HA	2:B:310:TRP:HB3	2.01	0.42
2:H:278:GLU:OE2	2:H:358:PHE:HD2	2.02	0.42
2:E:317:MET:HG3	2:E:331:PRO:HG3	2.02	0.42
2:E:274:PHE:HD1	2:E:274:PHE:C	2.22	0.42
2:E:278:GLU:HG2	2:E:518:MET:HE2	2.01	0.42
2:C:488:SER:C	2:C:490:PRO:HD2	2.40	0.42
2:A:436:ARG:HG2	2:A:440:ASP:OD2	2.20	0.42
2:E:416:ILE:HG22	2:E:416:ILE:O	2.18	0.42
2:C:422:THR:O	2:C:423:ARG:C	2.57	0.42
2:C:353:LEU:HB3	2:C:387:PHE:HB2	2.02	0.42
2:G:548:THR:HG23	2:G:551:GLN:OE1	2.20	0.42
2:A:386:ILE:HB	2:A:510:ILE:HB	2.01	0.42
2:E:545:MET:HE1	2:E:593:MET:HB3	2.00	0.42
2:F:427:ARG:HB2	2:F:434:TRP:CZ2	2.55	0.42
1:P:96:C:H2'	1:P:97:C:C6	2.54	0.42
2:A:254:TYR:HA	2:A:267:HIS:ND1	2.34	0.42
2:A:397:VAL:O	2:A:401:ILE:HG12	2.20	0.42
2:D:332:MET:HG2	2:D:363:ARG:NH2	2.34	0.42
2:H:459:GLY:HA2	2:H:465:LYS:HE2	2.02	0.42
1:M:69:G:N7	1:P:105:C:C2	2.87	0.42
2:D:400:CYS:O	2:D:404:VAL:HG23	2.19	0.42
2:C:273:ILE:HG23	2:C:537:LEU:CD2	2.50	0.42
2:G:603:SER:C	2:G:605:LYS:H	2.22	0.42
2:D:242:ARG:HE	2:D:246:LYS:HD3	1.85	0.42
2:B:474:LEU:O	2:B:475:ASP:C	2.57	0.42
2:F:602:GLU:N	2:F:602:GLU:OE1	2.53	0.42
2:H:604:GLY:O	2:H:621:VAL:HG23	2.20	0.42
2:E:400:CYS:O	2:E:404:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:590:VAL:O	2:G:611:ARG:HB3	2.19	0.42
2:D:422:THR:O	2:D:423:ARG:C	2.58	0.42
2:C:386:ILE:O	2:C:509:MET:HA	2.20	0.42
2:C:387:PHE:CE1	2:C:509:MET:SD	3.13	0.42
2:H:543:VAL:HG11	2:H:585:HIS:CE1	2.53	0.42
1:J:87:U:H2'	1:J:88:G:OP2	2.19	0.42
2:D:402:ARG:NH1	2:D:402:ARG:CB	2.80	0.42
1:M:69:G:N7	1:P:105:C:O2	2.52	0.42
1:K:70:G:C4	1:K:71:C:C5	3.07	0.42
2:E:441:LEU:O	2:E:444:ALA:HB3	2.19	0.42
2:C:341:PHE:O	2:C:346:LYS:NZ	2.45	0.42
2:F:610:THR:HG22	2:F:614:LYS:O	2.19	0.42
2:C:365:GLU:N	2:C:377:ARG:HD3	2.33	0.42
2:E:297:PHE:CG	2:F:362:HIS:CE1	3.07	0.42
2:F:329:ILE:CD1	2:F:329:ILE:N	2.83	0.42
2:E:426:LYS:HB3	2:E:426:LYS:HE2	1.85	0.42
2:C:562:LEU:HB3	2:C:569:VAL:HG11	2.01	0.42
2:C:427:ARG:HB2	2:C:434:TRP:CZ2	2.55	0.42
2:D:542:VAL:CG1	2:D:543:VAL:N	2.82	0.42
1:N:86:G:O4'	1:N:86:G:P	2.78	0.42
1:I:89:U:C6	2:A:583:ARG:NH1	2.88	0.42
2:H:285:LEU:HD22	2:H:290:TYR:CG	2.54	0.42
2:E:349:ARG:HE	2:E:349:ARG:HB2	1.61	0.42
2:H:531:GLY:O	2:H:589:ARG:HG3	2.20	0.42
1:N:90:G:O5'	2:F:577:LYS:HD3	2.20	0.42
2:D:452:PHE:CE2	2:D:454:TYR:HE1	2.22	0.42
2:H:462:TYR:CD2	2:H:486:ASP:OD2	2.72	0.42
2:D:249:LYS:HE2	2:D:249:LYS:HA	2.02	0.42
2:D:415:LYS:HG2	2:D:471:TYR:CD1	2.55	0.42
2:G:305:GLU:HA	2:G:310:TRP:HB3	2.01	0.42
2:B:400:CYS:O	2:B:401:ILE:C	2.58	0.42
2:C:550:SER:C	2:C:552:SER:H	2.23	0.42
2:E:323:GLU:H	2:E:323:GLU:CD	2.23	0.42
2:C:602:GLU:N	2:C:602:GLU:OE1	2.53	0.42
2:C:541:GLN:NE2	2:C:632:ILE:HD13	2.35	0.42
2:H:621:VAL:O	2:H:622:ASN:C	2.57	0.42
2:E:482:THR:O	2:E:512:ARG:HA	2.19	0.42
2:B:411:PHE:HE2	2:B:521:PHE:CE1	2.27	0.42
2:D:423:ARG:HG2	2:D:423:ARG:O	2.19	0.42
2:D:462:TYR:CD2	2:D:486:ASP:OD2	2.72	0.42
2:D:590:VAL:O	2:D:611:ARG:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:84:U:H3	2:G:549:ASP:CG	2.23	0.42
2:F:421:SER:HB3	2:F:459:GLY:N	2.35	0.42
2:F:517:SER:HB3	4:F:7002:TSB:H1'	2.01	0.42
2:H:394:ARG:O	2:H:397:VAL:N	2.53	0.42
2:G:619:MET:HG3	2:G:624:VAL:HG12	2.01	0.42
2:B:252:ASP:OD1	2:B:267:HIS:CD2	2.72	0.42
2:A:483:VAL:HG22	2:A:512:ARG:HB2	2.01	0.42
2:E:534:PRO:O	2:E:535:THR:C	2.58	0.42
1:M:81:C:H2'	1:M:82:U:O4'	2.20	0.42
1:K:80:U:C6	1:K:80:U:H3'	2.55	0.42
2:E:298:MET:CG	2:F:263:MET:HE2	2.48	0.42
2:A:624:VAL:O	2:A:628:LEU:HG	2.20	0.42
2:F:327:TYR:CD1	2:F:327:TYR:N	2.87	0.42
2:E:441:LEU:HA	2:E:441:LEU:HD23	1.90	0.42
2:F:317:MET:HG3	2:F:331:PRO:HG3	2.01	0.42
2:C:317:MET:HG3	2:C:331:PRO:HG3	2.02	0.42
2:E:603:SER:C	2:E:605:LYS:N	2.73	0.42
1:L:81:C:C4	1:L:82:U:C4	3.07	0.42
2:G:353:LEU:HB3	2:G:387:PHE:HB2	2.01	0.42
2:F:603:SER:C	2:F:605:LYS:H	2.23	0.42
2:B:426:LYS:HB3	2:B:426:LYS:HE2	1.87	0.42
2:G:411:PHE:HE2	2:G:521:PHE:HE1	1.67	0.42
2:F:626:GLU:HG3	2:F:626:GLU:H	1.73	0.42
2:E:397:VAL:O	2:E:401:ILE:HG12	2.19	0.42
2:C:551:GLN:HE21	2:C:598:ASP:N	2.18	0.42
2:C:421:SER:OG	2:C:467:GLU:OE2	2.37	0.42
1:J:95:A:H2'	1:J:96:C:O4'	2.20	0.42
2:B:597:GLY:O	2:B:601:VAL:HG23	2.20	0.42
2:A:621:VAL:O	2:A:622:ASN:C	2.57	0.42
1:J:84:U:H4'	1:J:85:C:H5'	2.01	0.42
2:D:471:TYR:CD1	2:D:471:TYR:N	2.87	0.42
2:E:358:PHE:N	2:E:358:PHE:CD1	2.88	0.42
2:A:610:THR:HG21	2:A:614:LYS:HB3	2.02	0.42
2:C:519:GLU:H	2:C:519:GLU:CD	2.22	0.42
2:B:437:ALA:HA	2:B:485:LEU:HD23	2.02	0.42
2:H:622:ASN:O	2:H:626:GLU:HG3	2.19	0.41
2:D:583:ARG:HD3	5:D:5014:HOH:O	2.19	0.41
2:D:587:LEU:N	2:D:587:LEU:HD23	2.27	0.41
2:F:462:TYR:N	2:F:462:TYR:CD1	2.88	0.41
2:E:627:LYS:O	2:E:630:GLN:HB3	2.20	0.41
2:H:627:LYS:O	2:H:630:GLN:HB3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:92:G:H2'	1:M:93:U:C6	2.53	0.41
2:F:287:GLU:HB2	2:F:288:TYR:CD1	2.54	0.41
2:E:380:THR:N	2:E:519:GLU:OE2	2.52	0.41
2:F:594:LEU:CD2	2:F:608:VAL:HG22	2.50	0.41
1:K:90:G:P	2:C:577:LYS:NZ	2.93	0.41
1:O:77:U:O2'	1:O:98:A:N1	2.45	0.41
2:H:253:LEU:O	2:H:270:GLY:HA3	2.20	0.41
2:H:500:GLU:C	2:H:502:ASN:N	2.71	0.41
2:A:325:ARG:CG	2:A:325:ARG:HH11	2.24	0.41
2:H:460:ALA:C	2:H:462:TYR:N	2.72	0.41
1:K:80:U:OP2	2:D:349:ARG:NH2	2.53	0.41
2:F:249:LYS:HZ3	2:F:249:LYS:HB3	1.84	0.41
2:E:313:TYR:CE1	2:E:316:ALA:HB3	2.55	0.41
1:M:93:U:H2'	1:M:94:C:C6	2.53	0.41
2:B:603:SER:C	2:B:605:LYS:N	2.72	0.41
2:A:347:SER:HA	2:A:498:VAL:H	1.84	0.41
2:D:569:VAL:O	2:D:570:LYS:HG2	2.19	0.41
1:O:90:G:C8	2:G:577:LYS:HD3	2.55	0.41
2:C:545:MET:SD	2:C:581:LYS:HB3	2.61	0.41
2:E:423:ARG:HE	2:E:438:GLU:CD	2.23	0.41
2:H:277:LEU:O	2:H:280:PHE:HB3	2.21	0.41
2:H:394:ARG:O	2:H:395:ASP:C	2.59	0.41
2:G:562:LEU:O	2:G:565:ALA:HB3	2.20	0.41
2:A:460:ALA:C	2:A:462:TYR:N	2.72	0.41
2:G:473:CYS:HB2	2:G:527:GLU:OE1	2.21	0.41
2:C:358:PHE:CD1	2:C:358:PHE:N	2.88	0.41
2:F:274:PHE:O	2:F:518:MET:HE3	2.20	0.41
2:E:365:GLU:N	2:E:377:ARG:HD3	2.35	0.41
1:L:83:U:H3	2:D:575:ASN:HD21	1.68	0.41
2:A:342:ASN:HA	2:A:342:ASN:HD22	1.63	0.41
2:D:594:LEU:CD2	2:D:608:VAL:HG22	2.51	0.41
1:M:76:G:N2	1:M:97:C:C2	2.89	0.41
2:D:285:LEU:HD21	2:D:512:ARG:HH12	1.85	0.41
2:G:285:LEU:HD21	2:G:512:ARG:HH12	1.85	0.41
2:F:349:ARG:HB2	2:F:349:ARG:HE	1.59	0.41
2:C:299:MET:HE1	2:C:335:PRO:HB2	2.03	0.41
2:C:298:MET:CG	2:D:263:MET:HE2	2.46	0.41
1:K:99:C:O3'	2:C:249:LYS:NZ	2.54	0.41
2:H:536:TRP:CE3	2:H:635:ARG:HD3	2.55	0.41
1:J:74:A:C2	1:J:101:G:C2	3.09	0.41
2:F:536:TRP:CD1	2:F:635:ARG:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:353:LEU:HB3	2:E:387:PHE:HB2	2.01	0.41
2:G:532:PHE:CZ	2:G:589:ARG:NH1	2.89	0.41
2:A:371:HIS:O	2:A:372:GLY:C	2.57	0.41
2:A:455:GLN:O	2:A:456:LEU:O	2.38	0.41
1:L:89:U:H5	2:D:583:ARG:NH2	2.18	0.41
2:C:277:LEU:O	2:C:280:PHE:HB3	2.21	0.41
2:H:349:ARG:HB2	2:H:349:ARG:HE	1.64	0.41
2:E:254:TYR:CD2	2:E:255:HIS:N	2.88	0.41
2:H:465:LYS:HG3	2:H:484:GLN:CG	2.46	0.41
1:K:95:A:H2'	1:K:96:C:O4'	2.20	0.41
2:F:246:LYS:O	2:F:250:GLN:HG2	2.21	0.41
2:E:249:LYS:HB3	2:E:249:LYS:HZ3	1.83	0.41
2:G:526:THR:O	2:G:530:ALA:N	2.53	0.41
2:F:609:ARG:CG	2:F:609:ARG:O	2.69	0.41
2:B:627:LYS:CB	2:B:640:LEU:HD21	2.51	0.41
2:A:526:THR:HG23	2:A:533:PHE:CZ	2.53	0.41
2:B:317:MET:HG3	2:B:331:PRO:HG3	2.03	0.41
2:E:569:VAL:CG2	2:E:570:LYS:N	2.84	0.41
2:F:437:ALA:HB2	2:F:487:PHE:CD2	2.55	0.41
2:D:366:PRO:O	2:D:367:SER:C	2.59	0.41
2:G:323:GLU:O	2:G:324:ASN:O	2.38	0.41
2:C:555:VAL:O	2:C:559:THR:HG23	2.21	0.41
2:H:422:THR:O	2:H:423:ARG:C	2.58	0.41
2:H:455:GLN:O	2:H:456:LEU:C	2.59	0.41
1:P:89:U:H2'	1:P:90:G:OP1	2.21	0.41
2:A:542:VAL:CG1	2:A:543:VAL:N	2.84	0.41
2:E:389:THR:HG1	2:E:392:GLN:HG3	1.84	0.41
2:E:253:LEU:O	2:E:270:GLY:HA3	2.20	0.41
2:D:482:THR:O	2:D:512:ARG:HA	2.20	0.41
2:G:610:THR:HG22	2:G:614:LYS:HB3	2.02	0.41
2:G:278:GLU:HB3	2:G:358:PHE:CE2	2.54	0.41
2:G:322:SER:O	2:G:323:GLU:C	2.57	0.41
2:F:550:SER:C	2:F:552:SER:H	2.23	0.41
2:H:366:PRO:O	2:H:367:SER:C	2.59	0.41
2:G:543:VAL:HG21	2:G:590:VAL:HG21	2.03	0.41
2:B:514:ILE:HG22	2:B:515:LEU:HD23	2.02	0.41
1:K:101:G:O2'	1:K:102:C:C5'	2.58	0.41
2:F:421:SER:HB3	2:F:458:GLU:CB	2.40	0.41
2:C:255:HIS:HE2	2:C:257:GLN:CG	2.34	0.41
2:F:351:LEU:HD13	2:F:388:CYS:HA	2.02	0.41
1:M:96:C:H2'	1:M:97:C:C6	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:584:GLU:O	2:G:588:ARG:HB2	2.20	0.41
2:C:339:GLN:OE1	2:C:339:GLN:CA	2.67	0.41
2:E:562:LEU:HD12	2:E:625:ILE:HD11	2.02	0.41
2:C:263:MET:HE2	2:D:298:MET:CG	2.45	0.41
2:E:298:MET:HE2	2:E:327:TYR:CD1	2.56	0.41
2:F:554:TYR:CE1	2:F:558:LEU:HD11	2.56	0.41
2:B:609:ARG:CG	2:B:609:ARG:O	2.69	0.41
2:A:365:GLU:N	2:A:377:ARG:HD3	2.33	0.41
2:D:330:LYS:HA	2:D:331:PRO:HD3	1.62	0.41
1:O:70:G:O2'	1:O:71:C:H5'	2.21	0.41
2:E:294:LYS:HA	2:E:357:GLU:HG3	2.02	0.41
2:G:371:HIS:O	2:G:372:GLY:C	2.59	0.41
2:A:274:PHE:CD1	2:A:274:PHE:C	2.94	0.41
1:O:87:U:H2'	1:O:88:G:OP2	2.20	0.41
2:E:421:SER:HB3	2:E:458:GLU:CB	2.32	0.41
2:H:547:ILE:HG12	2:H:578:ILE:HD12	2.02	0.41
1:P:86:G:H2'	5:P:1613:HOH:O	2.20	0.41
2:H:386:ILE:O	2:H:509:MET:HA	2.20	0.41
2:B:299:MET:O	2:B:304:TRP:HZ3	2.04	0.41
2:D:288:TYR:CZ	2:D:403:LEU:HD13	2.56	0.41
2:A:452:PHE:HE2	2:A:454:TYR:CE1	2.23	0.41
2:H:462:TYR:CE2	2:H:511:HIS:NE2	2.89	0.41
2:H:332:MET:HE2	4:H:9002:TSB:HN12	1.86	0.41
2:B:365:GLU:N	2:B:377:ARG:HD3	2.35	0.41
2:G:358:PHE:CD1	2:G:358:PHE:N	2.87	0.41
2:F:441:LEU:HD23	2:F:441:LEU:HA	1.91	0.41
2:H:274:PHE:HD1	2:H:274:PHE:C	2.24	0.41
2:D:526:THR:HG23	2:D:533:PHE:CZ	2.56	0.41
2:C:329:ILE:N	2:C:329:ILE:CD1	2.84	0.41
2:H:353:LEU:HB3	2:H:387:PHE:HB2	2.02	0.41
2:E:323:GLU:O	2:E:324:ASN:O	2.38	0.41
2:H:555:VAL:O	2:H:559:THR:HG23	2.20	0.41
2:B:280:PHE:HE2	2:B:407:MET:HG2	1.85	0.41
2:E:455:GLN:O	2:E:456:LEU:C	2.59	0.41
2:D:421:SER:HB3	2:D:459:GLY:N	2.35	0.41
2:H:427:ARG:HA	2:H:461:PHE:O	2.21	0.41
1:L:89:U:C6	2:D:583:ARG:CZ	3.03	0.41
1:N:86:G:N3	2:F:547:ILE:HD13	2.36	0.41
1:J:93:U:N3	1:J:94:C:C5	2.89	0.41
1:I:88:G:N2	5:I:111:HOH:O	2.47	0.41
2:F:462:TYR:HE2	2:F:511:HIS:CD2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:348:TYR:CE2	2:E:500:GLU:HG3	2.56	0.41
2:G:594:LEU:CD2	2:G:608:VAL:HG22	2.51	0.41
2:A:300:ASP:OD2	2:A:302:VAL:HB	2.20	0.41
2:A:300:ASP:HB2	2:B:259:GLU:O	2.21	0.41
2:C:452:PHE:CE2	2:C:454:TYR:HE1	2.22	0.41
1:P:97:C:C4'	1:P:98:A:OP1	2.69	0.41
2:F:493:LEU:HD23	2:F:493:LEU:N	2.35	0.41
2:A:501:ASP:CG	2:A:503:GLU:HB2	2.42	0.41
2:A:253:LEU:O	2:A:270:GLY:HA3	2.21	0.41
2:G:377:ARG:HH11	2:G:377:ARG:HG3	1.86	0.41
2:A:459:GLY:HA2	2:A:465:LYS:HE2	2.03	0.41
2:F:348:TYR:CE2	2:F:500:GLU:HG3	2.55	0.41
2:C:527:GLU:O	2:C:528:GLU:O	2.39	0.41
2:C:528:GLU:O	2:C:530:ALA:N	2.53	0.41
2:G:298:MET:HG2	2:G:298:MET:O	2.21	0.41
2:G:517:SER:HB3	4:G:8002:TSB:H1'	2.00	0.41
2:E:247:ILE:HA	2:E:250:GLN:HB2	2.03	0.41
2:E:250:GLN:NE2	2:E:250:GLN:HA	2.36	0.41
2:C:538:ALA:O	2:C:539:PRO:C	2.59	0.41
2:F:358:PHE:N	2:F:358:PHE:CD1	2.88	0.41
1:O:80:U:H2'	1:O:81:C:H6	1.84	0.41
1:O:69:G:O2'	1:O:70:G:H5'	2.21	0.41
1:P:78:G:H5'	5:P:1639:HOH:O	2.21	0.41
2:C:480:CYS:O	2:C:516:GLY:CA	2.69	0.41
2:E:528:GLU:O	2:E:530:ALA:N	2.53	0.41
2:G:602:GLU:OE1	2:G:602:GLU:N	2.54	0.41
2:A:550:SER:C	2:A:552:SER:H	2.24	0.41
1:O:76:G:H21	1:O:99:C:N4	2.19	0.41
2:B:482:THR:HG21	4:B:3002:TSB:H5'2	2.02	0.41
2:E:427:ARG:HA	2:E:461:PHE:O	2.21	0.41
2:E:422:THR:HB	2:E:438:GLU:OE2	2.21	0.41
2:H:421:SER:CA	2:H:455:GLN:HB3	2.48	0.41
2:H:572:ASP:OD2	2:H:585:HIS:HE1	2.04	0.41
2:F:423:ARG:HB3	2:F:434:TRP:CE3	2.56	0.41
2:E:300:ASP:HB3	2:F:259:GLU:HB2	2.03	0.41
2:H:588:ARG:C	2:H:589:ARG:HG2	2.40	0.41
2:G:255:HIS:HE2	2:G:257:GLN:CG	2.33	0.41
2:B:254:TYR:CD2	2:B:255:HIS:N	2.89	0.41
2:D:320:THR:HG22	2:D:321:SER:N	2.26	0.41
2:D:277:LEU:O	2:D:280:PHE:HB3	2.20	0.41
2:A:399:GLY:HA2	2:A:402:ARG:HH11	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:390:GLU:H	2:D:390:GLU:HG2	1.71	0.41
2:C:500:GLU:C	2:C:502:ASN:N	2.72	0.41
2:G:417:VAL:HG13	2:G:471:TYR:CE1	2.46	0.41
2:C:526:THR:O	2:C:530:ALA:HA	2.20	0.41
2:A:529:PHE:N	2:A:529:PHE:CD1	2.76	0.41
2:A:626:GLU:H	2:A:626:GLU:HG3	1.70	0.41
2:H:358:PHE:N	2:H:358:PHE:CD1	2.89	0.41
2:D:538:ALA:O	2:D:539:PRO:C	2.58	0.41
1:L:72:G:H2'	1:L:73:U:C6	2.56	0.41
2:B:397:VAL:O	2:B:401:ILE:HG12	2.21	0.41
2:E:519:GLU:CD	2:E:519:GLU:H	2.22	0.41
2:H:562:LEU:HB3	2:H:569:VAL:HG11	2.02	0.40
2:G:545:MET:CE	2:G:593:MET:HB3	2.51	0.40
2:A:421:SER:OG	2:A:467:GLU:OE2	2.39	0.40
1:I:87:U:H2'	1:I:88:G:OP2	2.20	0.40
2:F:424:PRO:HD2	2:F:434:TRP:CH2	2.55	0.40
2:B:298:MET:CE	2:B:327:TYR:HB2	2.51	0.40
1:M:69:G:P	1:P:105:C:C2'	3.09	0.40
2:C:462:TYR:HE2	2:C:511:HIS:CD2	2.38	0.40
2:A:441:LEU:HD23	2:A:441:LEU:HA	1.91	0.40
1:L:80:U:H2'	1:L:81:C:H6	1.85	0.40
2:E:294:LYS:HA	2:E:294:LYS:HD2	1.85	0.40
2:H:426:LYS:HB3	2:H:426:LYS:HE2	1.90	0.40
2:G:294:LYS:HA	2:G:294:LYS:HD2	1.76	0.40
2:C:567:ILE:O	2:C:569:VAL:N	2.54	0.40
2:C:353:LEU:HA	2:C:353:LEU:HD22	1.81	0.40
2:A:353:LEU:HD22	2:A:353:LEU:HA	1.83	0.40
2:A:627:LYS:O	2:A:630:GLN:HB3	2.21	0.40
2:D:386:ILE:O	2:D:509:MET:HA	2.21	0.40
2:C:281:VAL:O	2:C:282:ARG:C	2.60	0.40
1:N:89:U:O2'	2:F:580:PHE:CB	2.69	0.40
2:G:567:ILE:O	2:G:569:VAL:HG12	2.22	0.40
2:E:501:ASP:O	2:E:503:GLU:HG2	2.22	0.40
2:C:499:GLY:HA3	2:C:501:ASP:OD1	2.20	0.40
2:H:339:GLN:CA	2:H:339:GLN:OE1	2.69	0.40
2:G:247:ILE:HD12	2:G:526:THR:HG22	2.02	0.40
2:E:362:HIS:CD2	5:E:6011:HOH:O	2.70	0.40
2:D:313:TYR:CE1	2:D:316:ALA:HB3	2.56	0.40
2:B:380:THR:N	2:B:519:GLU:OE2	2.54	0.40
2:E:437:ALA:HB2	2:E:487:PHE:CD2	2.56	0.40
2:G:323:GLU:CD	2:G:323:GLU:H	2.24	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:436:ARG:HG2	2:B:440:ASP:OD2	2.21	0.40
2:E:430:SER:O	2:E:433:MET:HB2	2.20	0.40
2:A:423:ARG:HE	2:A:438:GLU:CD	2.23	0.40
2:D:576:GLU:HG2	2:D:580:PHE:CD2	2.56	0.40
2:H:288:TYR:CZ	2:H:403:LEU:HD13	2.57	0.40
2:G:544:ILE:CG2	2:G:555:VAL:HG13	2.49	0.40
1:P:93:U:C2	1:P:94:C:C6	3.10	0.40
2:F:400:CYS:SG	2:F:512:ARG:HG3	2.61	0.40
2:G:538:ALA:O	2:G:539:PRO:C	2.59	0.40
2:D:539:PRO:O	2:D:568:ARG:HD2	2.21	0.40
2:A:609:ARG:HD3	2:A:610:THR:O	2.22	0.40
2:A:603:SER:C	2:A:605:LYS:H	2.24	0.40
2:C:356:ALA:HB2	2:C:384:ALA:HB2	2.03	0.40
2:C:323:GLU:CD	2:C:323:GLU:H	2.23	0.40
2:H:437:ALA:HA	2:H:485:LEU:HD23	2.03	0.40
2:H:371:HIS:O	2:H:372:GLY:C	2.59	0.40
2:D:430:SER:O	2:D:433:MET:HB2	2.21	0.40
2:C:426:LYS:HE2	2:C:426:LYS:HB3	1.89	0.40
2:C:621:VAL:O	2:C:622:ASN:C	2.59	0.40
2:D:427:ARG:HA	2:D:461:PHE:O	2.22	0.40
2:C:423:ARG:O	2:C:423:ARG:HG2	2.21	0.40
2:A:393:ILE:HD11	2:A:508:VAL:HG11	2.02	0.40
1:M:84:U:O2'	1:M:85:C:P	2.79	0.40
2:A:545:MET:SD	2:A:581:LYS:HB3	2.61	0.40
2:B:551:GLN:H	2:B:551:GLN:CD	2.22	0.40
2:B:583:ARG:O	2:B:586:THR:N	2.54	0.40
2:C:279:VAL:CG2	2:C:280:PHE:N	2.84	0.40
2:H:251:LEU:CA	2:H:588:ARG:HH12	2.27	0.40
2:H:348:TYR:CE2	2:H:500:GLU:HG3	2.56	0.40
1:P:95:A:H2'	1:P:96:C:O4'	2.20	0.40
2:G:349:ARG:HE	2:G:349:ARG:HB2	1.64	0.40
2:H:460:ALA:C	2:H:462:TYR:H	2.25	0.40
1:K:79:A:OP1	2:D:349:ARG:NH2	2.54	0.40
2:C:460:ALA:C	2:C:462:TYR:H	2.24	0.40
2:B:249:LYS:HA	2:B:249:LYS:HE2	2.03	0.40
2:C:554:TYR:CE1	2:C:558:LEU:HD11	2.56	0.40
2:G:554:TYR:CE1	2:G:558:LEU:HD11	2.56	0.40
2:B:358:PHE:HD1	2:B:358:PHE:N	2.19	0.40
1:O:92:G:H2'	1:O:93:U:C6	2.55	0.40
2:D:356:ALA:HA	2:D:384:ALA:CB	2.52	0.40
2:B:356:ALA:HA	2:B:384:ALA:HA	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:323:GLU:H	2:F:323:GLU:CD	2.22	0.40
2:C:433:MET:HE2	2:C:433:MET:HB3	1.97	0.40
2:E:548:THR:HG22	2:E:551:GLN:HE22	1.86	0.40
2:E:490:PRO:HD3	2:E:509:MET:CE	2.51	0.40
2:B:501:ASP:O	2:B:502:ASN:C	2.58	0.40
2:G:482:THR:O	2:G:512:ARG:HA	2.21	0.40
2:A:534:PRO:O	2:A:535:THR:C	2.59	0.40
2:A:415:LYS:HG2	2:A:471:TYR:CD1	2.57	0.40
2:F:356:ALA:CB	2:F:384:ALA:HB2	2.51	0.40
2:F:294:LYS:HD2	2:F:294:LYS:HA	1.83	0.40
2:D:323:GLU:O	2:D:324:ASN:O	2.39	0.40
2:D:480:CYS:O	2:D:516:GLY:HA3	2.22	0.40
2:H:433:MET:HE2	2:H:433:MET:HB3	1.95	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	399/401 (100%)	327 (82%)	53 (13%)	19 (5%)	3	28
2	B	399/401 (100%)	325 (82%)	57 (14%)	17 (4%)	3	31
2	C	399/401 (100%)	327 (82%)	52 (13%)	20 (5%)	3	27
2	D	399/401 (100%)	327 (82%)	54 (14%)	18 (4%)	3	30
2	E	399/401 (100%)	327 (82%)	55 (14%)	17 (4%)	3	31
2	F	399/401 (100%)	327 (82%)	52 (13%)	20 (5%)	3	27
2	G	399/401 (100%)	323 (81%)	55 (14%)	21 (5%)	2	25
2	H	399/401 (100%)	323 (81%)	55 (14%)	21 (5%)	2	25
All	All	3192/3208 (100%)	2606 (82%)	433 (14%)	153 (5%)	3	28

All (153) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	313	TYR
2	A	324	ASN
2	A	456	LEU
2	A	528	GLU
2	A	574	ARG
2	B	313	TYR
2	B	324	ASN
2	B	456	LEU
2	B	528	GLU
2	C	313	TYR
2	C	324	ASN
2	C	456	LEU
2	C	528	GLU
2	D	313	TYR
2	D	324	ASN
2	D	456	LEU
2	D	528	GLU
2	E	313	TYR
2	E	324	ASN
2	E	456	LEU
2	E	528	GLU
2	E	574	ARG
2	F	313	TYR
2	F	324	ASN
2	F	456	LEU
2	F	528	GLU
2	G	313	TYR
2	G	324	ASN
2	G	456	LEU
2	G	528	GLU
2	G	529	PHE
2	H	313	TYR
2	H	324	ASN
2	H	456	LEU
2	H	528	GLU
2	A	394	ARG
2	A	494	SER
2	A	529	PHE
2	B	394	ARG
2	B	551	GLN
2	B	574	ARG
2	C	394	ARG

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Mol	Chain	Res	Type
2	C	494	SER
2	C	529	PHE
2	C	574	ARG
2	C	617	GLY
2	D	394	ARG
2	D	529	PHE
2	D	574	ARG
2	D	614	LYS
2	E	394	ARG
2	F	394	ARG
2	F	494	SER
2	F	529	PHE
2	F	574	ARG
2	F	614	LYS
2	G	394	ARG
2	G	574	ARG
2	G	617	GLY
2	H	394	ARG
2	H	494	SER
2	H	529	PHE
2	H	574	ARG
2	H	614	LYS
2	A	254	TYR
2	A	614	LYS
2	B	254	TYR
2	B	494	SER
2	C	614	LYS
2	D	254	TYR
2	D	494	SER
2	D	617	GLY
2	E	254	TYR
2	E	494	SER
2	E	529	PHE
2	E	551	GLN
2	E	614	LYS
2	E	617	GLY
2	F	617	GLY
2	G	254	TYR
2	G	494	SER
2	G	551	GLN
2	G	568	ARG
2	G	614	LYS

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Mol	Chain	Res	Type
2	H	294	LYS
2	H	551	GLN
2	A	551	GLN
2	A	617	GLY
2	B	583	ARG
2	B	617	GLY
2	C	254	TYR
2	C	551	GLN
2	D	551	GLN
2	F	254	TYR
2	F	551	GLN
2	G	331	PRO
2	G	372	GLY
2	G	583	ARG
2	H	254	TYR
2	H	331	PRO
2	H	617	GLY
2	A	294	LYS
2	A	331	PRO
2	A	501	ASP
2	B	331	PRO
2	B	401	ILE
2	B	614	LYS
2	C	331	PRO
2	C	445	LEU
2	D	331	PRO
2	D	501	ASP
2	D	583	ARG
2	E	331	PRO
2	E	501	ASP
2	E	583	ARG
2	F	445	LEU
2	G	298	MET
2	G	501	ASP
2	H	568	ARG
2	B	501	ASP
2	C	568	ARG
2	C	583	ARG
2	F	331	PRO
2	F	372	GLY
2	F	501	ASP
2	H	293	VAL

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Mol	Chain	Res	Type
2	H	445	LEU
2	A	423	ARG
2	A	489	LEU
2	B	293	VAL
2	C	293	VAL
2	C	372	GLY
2	C	423	ARG
2	D	372	GLY
2	A	293	VAL
2	A	625	ILE
2	D	293	VAL
2	D	423	ARG
2	E	293	VAL
2	E	423	ARG
2	F	423	ARG
2	H	423	ARG
2	H	489	LEU
2	B	372	GLY
2	F	293	VAL
2	F	489	LEU
2	G	293	VAL
2	G	625	ILE
2	H	372	GLY
2	H	625	ILE
2	C	625	ILE
2	F	625	ILE
2	G	489	LEU

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	356/356 (100%)	317 (89%)	39 (11%)	8 36
2	B	356/356 (100%)	318 (89%)	38 (11%)	8 37
2	C	356/356 (100%)	321 (90%)	35 (10%)	10 42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	D	356/356 (100%)	321 (90%)	35 (10%)	10 42
2	E	356/356 (100%)	319 (90%)	37 (10%)	9 39
2	F	356/356 (100%)	320 (90%)	36 (10%)	9 40
2	G	356/356 (100%)	315 (88%)	41 (12%)	7 33
2	H	356/356 (100%)	320 (90%)	36 (10%)	9 40
All	All	2848/2848 (100%)	2551 (90%)	297 (10%)	9 39

All (297) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	258	GLU
2	A	274	PHE
2	A	288	TYR
2	A	296	PRO
2	A	297	PHE
2	A	303	LEU
2	A	312	ASN
2	A	313	TYR
2	A	315	ASP
2	A	327	TYR
2	A	333	ASN
2	A	353	LEU
2	A	390	GLU
2	A	391	GLU
2	A	395	ASP
2	A	396	GLU
2	A	406	ASP
2	A	411	PHE
2	A	417	VAL
2	A	423	ARG
2	A	427	ARG
2	A	432	GLU
2	A	458	GLU
2	A	491	SER
2	A	494	SER
2	A	507	PRO
2	A	512	ARG
2	A	522	ILE
2	A	526	THR
2	A	528	GLU

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Mol	Chain	Res	Type
2	A	539	PRO
2	A	549	ASP
2	A	580	PHE
2	A	587	LEU
2	A	602	GLU
2	A	606	VAL
2	A	609	ARG
2	A	638	LYS
2	A	641	GLU
2	B	258	GLU
2	B	274	PHE
2	B	288	TYR
2	B	296	PRO
2	B	297	PHE
2	B	303	LEU
2	B	312	ASN
2	B	315	ASP
2	B	327	TYR
2	B	333	ASN
2	B	353	LEU
2	B	390	GLU
2	B	391	GLU
2	B	395	ASP
2	B	396	GLU
2	B	406	ASP
2	B	411	PHE
2	B	417	VAL
2	B	423	ARG
2	B	427	ARG
2	B	432	GLU
2	B	458	GLU
2	B	491	SER
2	B	494	SER
2	B	512	ARG
2	B	522	ILE
2	B	526	THR
2	B	528	GLU
2	B	537	LEU
2	B	539	PRO
2	B	549	ASP
2	B	580	PHE
2	B	587	LEU

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Mol	Chain	Res	Type
2	B	602	GLU
2	B	606	VAL
2	B	609	ARG
2	B	638	LYS
2	B	641	GLU
2	C	258	GLU
2	C	274	PHE
2	C	288	TYR
2	C	297	PHE
2	C	303	LEU
2	C	312	ASN
2	C	315	ASP
2	C	327	TYR
2	C	333	ASN
2	C	353	LEU
2	C	390	GLU
2	C	391	GLU
2	C	395	ASP
2	C	396	GLU
2	C	406	ASP
2	C	411	PHE
2	C	417	VAL
2	C	423	ARG
2	C	427	ARG
2	C	432	GLU
2	C	458	GLU
2	C	491	SER
2	C	494	SER
2	C	512	ARG
2	C	522	ILE
2	C	526	THR
2	C	528	GLU
2	C	539	PRO
2	C	580	PHE
2	C	587	LEU
2	C	602	GLU
2	C	606	VAL
2	C	609	ARG
2	C	638	LYS
2	C	641	GLU
2	D	258	GLU
2	D	274	PHE

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Mol	Chain	Res	Type
2	D	288	TYR
2	D	297	PHE
2	D	303	LEU
2	D	312	ASN
2	D	315	ASP
2	D	327	TYR
2	D	333	ASN
2	D	353	LEU
2	D	390	GLU
2	D	391	GLU
2	D	395	ASP
2	D	396	GLU
2	D	406	ASP
2	D	417	VAL
2	D	423	ARG
2	D	427	ARG
2	D	432	GLU
2	D	458	GLU
2	D	491	SER
2	D	494	SER
2	D	512	ARG
2	D	522	ILE
2	D	526	THR
2	D	528	GLU
2	D	539	PRO
2	D	549	ASP
2	D	580	PHE
2	D	587	LEU
2	D	602	GLU
2	D	606	VAL
2	D	609	ARG
2	D	638	LYS
2	D	641	GLU
2	E	258	GLU
2	E	274	PHE
2	E	288	TYR
2	E	297	PHE
2	E	303	LEU
2	E	312	ASN
2	E	315	ASP
2	E	327	TYR
2	E	333	ASN

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Mol	Chain	Res	Type
2	E	334	CYS
2	E	353	LEU
2	E	390	GLU
2	E	391	GLU
2	E	395	ASP
2	E	396	GLU
2	E	406	ASP
2	E	411	PHE
2	E	417	VAL
2	E	423	ARG
2	E	427	ARG
2	E	432	GLU
2	E	458	GLU
2	E	491	SER
2	E	494	SER
2	E	512	ARG
2	E	522	ILE
2	E	526	THR
2	E	528	GLU
2	E	537	LEU
2	E	539	PRO
2	E	580	PHE
2	E	587	LEU
2	E	602	GLU
2	E	606	VAL
2	E	609	ARG
2	E	638	LYS
2	E	641	GLU
2	F	258	GLU
2	F	274	PHE
2	F	288	TYR
2	F	297	PHE
2	F	303	LEU
2	F	312	ASN
2	F	315	ASP
2	F	327	TYR
2	F	333	ASN
2	F	353	LEU
2	F	390	GLU
2	F	391	GLU
2	F	395	ASP
2	F	396	GLU

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Mol	Chain	Res	Type
2	F	406	ASP
2	F	411	PHE
2	F	417	VAL
2	F	423	ARG
2	F	427	ARG
2	F	432	GLU
2	F	458	GLU
2	F	491	SER
2	F	494	SER
2	F	507	PRO
2	F	512	ARG
2	F	522	ILE
2	F	526	THR
2	F	528	GLU
2	F	539	PRO
2	F	580	PHE
2	F	587	LEU
2	F	602	GLU
2	F	606	VAL
2	F	609	ARG
2	F	638	LYS
2	F	641	GLU
2	G	258	GLU
2	G	274	PHE
2	G	288	TYR
2	G	297	PHE
2	G	303	LEU
2	G	312	ASN
2	G	313	TYR
2	G	315	ASP
2	G	317	MET
2	G	327	TYR
2	G	333	ASN
2	G	334	CYS
2	G	353	LEU
2	G	390	GLU
2	G	391	GLU
2	G	395	ASP
2	G	396	GLU
2	G	406	ASP
2	G	411	PHE
2	G	417	VAL

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Mol	Chain	Res	Type
2	G	423	ARG
2	G	427	ARG
2	G	432	GLU
2	G	458	GLU
2	G	491	SER
2	G	494	SER
2	G	507	PRO
2	G	512	ARG
2	G	517	SER
2	G	522	ILE
2	G	526	THR
2	G	528	GLU
2	G	539	PRO
2	G	545	MET
2	G	580	PHE
2	G	587	LEU
2	G	602	GLU
2	G	606	VAL
2	G	609	ARG
2	G	638	LYS
2	G	641	GLU
2	H	258	GLU
2	H	274	PHE
2	H	288	TYR
2	H	297	PHE
2	H	312	ASN
2	H	315	ASP
2	H	317	MET
2	H	327	TYR
2	H	333	ASN
2	H	353	LEU
2	H	390	GLU
2	H	391	GLU
2	H	395	ASP
2	H	396	GLU
2	H	406	ASP
2	H	411	PHE
2	H	417	VAL
2	H	423	ARG
2	H	427	ARG
2	H	432	GLU
2	H	458	GLU

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Mol	Chain	Res	Type
2	H	491	SER
2	H	494	SER
2	H	512	ARG
2	H	522	ILE
2	H	526	THR
2	H	528	GLU
2	H	539	PRO
2	H	545	MET
2	H	580	PHE
2	H	587	LEU
2	H	602	GLU
2	H	606	VAL
2	H	609	ARG
2	H	638	LYS
2	H	641	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	250	GLN
2	A	257	GLN
2	A	267	HIS
2	A	268	ASN
2	A	291	GLN
2	A	342	ASN
2	A	362	HIS
2	A	371	HIS
2	A	381	GLN
2	A	449	ASN
2	A	479	GLN
2	A	556	ASN
2	A	560	GLN
2	A	564	ASN
2	A	575	ASN
2	A	585	HIS
2	B	250	GLN
2	B	257	GLN
2	B	267	HIS
2	B	291	GLN
2	B	342	ASN
2	B	362	HIS
2	B	371	HIS

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Mol	Chain	Res	Type
2	B	381	GLN
2	B	479	GLN
2	B	556	ASN
2	B	560	GLN
2	B	564	ASN
2	B	575	ASN
2	B	585	HIS
2	B	629	GLN
2	B	639	GLN
2	C	250	GLN
2	C	257	GLN
2	C	267	HIS
2	C	291	GLN
2	C	342	ASN
2	C	362	HIS
2	C	371	HIS
2	C	381	GLN
2	C	479	GLN
2	C	556	ASN
2	C	560	GLN
2	C	564	ASN
2	C	575	ASN
2	C	585	HIS
2	C	629	GLN
2	D	250	GLN
2	D	257	GLN
2	D	267	HIS
2	D	268	ASN
2	D	291	GLN
2	D	342	ASN
2	D	362	HIS
2	D	371	HIS
2	D	381	GLN
2	D	479	GLN
2	D	556	ASN
2	D	560	GLN
2	D	564	ASN
2	D	575	ASN
2	D	585	HIS
2	D	629	GLN
2	D	639	GLN
2	E	250	GLN

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Mol	Chain	Res	Type
2	E	257	GLN
2	E	267	HIS
2	E	291	GLN
2	E	333	ASN
2	E	342	ASN
2	E	362	HIS
2	E	371	HIS
2	E	381	GLN
2	E	479	GLN
2	E	556	ASN
2	E	560	GLN
2	E	564	ASN
2	E	575	ASN
2	E	585	HIS
2	E	629	GLN
2	F	250	GLN
2	F	257	GLN
2	F	267	HIS
2	F	268	ASN
2	F	291	GLN
2	F	342	ASN
2	F	362	HIS
2	F	371	HIS
2	F	381	GLN
2	F	479	GLN
2	F	484	GLN
2	F	556	ASN
2	F	560	GLN
2	F	564	ASN
2	F	575	ASN
2	F	585	HIS
2	F	629	GLN
2	F	639	GLN
2	G	250	GLN
2	G	257	GLN
2	G	267	HIS
2	G	291	GLN
2	G	342	ASN
2	G	362	HIS
2	G	371	HIS
2	G	381	GLN
2	G	479	GLN

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Mol	Chain	Res	Type
2	G	556	ASN
2	G	560	GLN
2	G	564	ASN
2	G	575	ASN
2	G	585	HIS
2	G	629	GLN
2	H	250	GLN
2	H	257	GLN
2	H	267	HIS
2	H	291	GLN
2	H	342	ASN
2	H	362	HIS
2	H	371	HIS
2	H	381	GLN
2	H	479	GLN
2	H	484	GLN
2	H	556	ASN
2	H	560	GLN
2	H	575	ASN
2	H	585	HIS
2	H	629	GLN
2	H	639	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	I	36/37 (97%)	6 (16%)	4 (11%)
1	J	36/37 (97%)	9 (25%)	5 (13%)
1	K	36/37 (97%)	11 (30%)	4 (11%)
1	L	36/37 (97%)	7 (19%)	4 (11%)
1	M	36/37 (97%)	8 (22%)	5 (13%)
1	N	36/37 (97%)	8 (22%)	4 (11%)
1	O	36/37 (97%)	9 (25%)	5 (13%)
1	P	36/37 (97%)	8 (22%)	5 (13%)
All	All	288/296 (97%)	66 (22%)	36 (12%)

All (66) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	I	76	G
1	I	85	C

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Mol	Chain	Res	Type
1	I	86	G
1	I	89	U
1	I	90	G
1	I	98	A
1	J	74	A
1	J	75	U
1	J	76	G
1	J	85	C
1	J	86	G
1	J	88	G
1	J	89	U
1	J	90	G
1	J	98	A
1	K	74	A
1	K	76	G
1	K	85	C
1	K	86	G
1	K	87	U
1	K	88	G
1	K	89	U
1	K	90	G
1	K	91	G
1	K	98	A
1	K	105	C
1	L	76	G
1	L	85	C
1	L	86	G
1	L	88	G
1	L	89	U
1	L	90	G
1	L	98	A
1	M	75	U
1	M	76	G
1	M	85	C
1	M	86	G
1	M	88	G
1	M	89	U
1	M	90	G
1	M	98	A
1	N	74	A
1	N	76	G
1	N	85	C

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Mol	Chain	Res	Type
1	N	86	G
1	N	88	G
1	N	89	U
1	N	90	G
1	N	98	A
1	O	74	A
1	O	76	G
1	O	85	C
1	O	86	G
1	O	88	G
1	O	89	U
1	O	90	G
1	O	96	C
1	O	98	A
1	P	75	U
1	P	76	G
1	P	85	C
1	P	86	G
1	P	88	G
1	P	89	U
1	P	90	G
1	P	98	A

All (36) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	I	75	U
1	I	84	U
1	I	88	G
1	I	97	C
1	J	74	A
1	J	75	U
1	J	84	U
1	J	88	G
1	J	97	C
1	K	84	U
1	K	86	G
1	K	88	G
1	K	97	C
1	L	75	U
1	L	84	U
1	L	88	G

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Mol	Chain	Res	Type
1	L	97	C
1	M	74	A
1	M	75	U
1	M	84	U
1	M	88	G
1	M	97	C
1	N	75	U
1	N	84	U
1	N	88	G
1	N	97	C
1	O	74	A
1	O	75	U
1	O	84	U
1	O	88	G
1	O	97	C
1	P	74	A
1	P	75	U
1	P	84	U
1	P	88	G
1	P	97	C

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 (i)

Of 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	TSB	A	2002	3	24,32,32	2.05	3 (12%)	31,48,48	1.14	1 (3%)
4	TSB	B	3002	3	24,32,32	3.06	2 (8%)	31,48,48	0.64	0
4	TSB	C	4002	3	24,32,32	2.28	2 (8%)	31,48,48	0.83	0
4	TSB	D	5002	3	24,32,32	2.57	2 (8%)	31,48,48	0.67	0
4	TSB	E	6002	3	24,32,32	2.83	2 (8%)	31,48,48	0.70	0
4	TSB	F	7002	3	24,32,32	2.06	2 (8%)	31,48,48	0.96	1 (3%)
4	TSB	G	8002	3	24,32,32	2.62	3 (12%)	31,48,48	1.20	2 (6%)
4	TSB	H	9002	3	24,32,32	2.33	2 (8%)	31,48,48	1.06	2 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	TSB	A	2002	3	-	0/17/39/39	0/3/3/3
4	TSB	B	3002	3	-	0/17/39/39	0/3/3/3
4	TSB	C	4002	3	-	0/17/39/39	0/3/3/3
4	TSB	D	5002	3	-	0/17/39/39	0/3/3/3
4	TSB	E	6002	3	-	0/17/39/39	0/3/3/3
4	TSB	F	7002	3	-	0/17/39/39	0/3/3/3
4	TSB	G	8002	3	-	0/17/39/39	0/3/3/3
4	TSB	H	9002	3	-	0/17/39/39	0/3/3/3

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2002	TSB	C-N8	-2.56	1.33	1.37
4	G	8002	TSB	C2-N3	2.65	1.36	1.32
4	A	2002	TSB	O1S-S1	5.68	1.47	1.42
4	F	7002	TSB	O1S-S1	6.26	1.47	1.42
4	G	8002	TSB	O1S-S1	6.78	1.48	1.42
4	C	4002	TSB	O1S-S1	6.81	1.48	1.42
4	H	9002	TSB	O1S-S1	6.93	1.48	1.42
4	A	2002	TSB	O2S-S1	7.09	1.48	1.42
4	F	7002	TSB	O2S-S1	7.46	1.48	1.42
4	D	5002	TSB	O2S-S1	8.00	1.49	1.42
4	C	4002	TSB	O2S-S1	8.36	1.49	1.42
4	H	9002	TSB	O2S-S1	8.49	1.49	1.42
4	E	6002	TSB	O2S-S1	8.76	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	5002	TSB	O1S-S1	9.20	1.50	1.42
4	B	3002	TSB	O2S-S1	9.44	1.50	1.42
4	G	8002	TSB	O2S-S1	9.71	1.50	1.42
4	E	6002	TSB	O1S-S1	10.18	1.51	1.42
4	B	3002	TSB	O1S-S1	11.24	1.52	1.42

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	8002	TSB	O2S-S1-N8	-4.12	103.00	108.50
4	H	9002	TSB	O2S-S1-N8	-2.84	104.70	108.50
4	F	7002	TSB	O2S-S1-O1S	-2.19	118.15	120.77
4	H	9002	TSB	C2'-C1'-N9	-2.03	111.19	114.29
4	G	8002	TSB	CA-C-N8	2.06	120.68	116.08
4	A	2002	TSB	O1S-S1-N8	3.79	113.56	108.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2002	TSB	3	0
4	B	3002	TSB	4	0
4	C	4002	TSB	3	0
4	D	5002	TSB	4	0
4	E	6002	TSB	4	0
4	F	7002	TSB	5	0
4	G	8002	TSB	4	0
4	H	9002	TSB	4	0

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	I	37/37 (100%)	1.51	12 (32%) 1 0	82, 115, 150, 153	0
1	J	37/37 (100%)	0.93	6 (16%) 3 3	55, 88, 135, 152	0
1	K	37/37 (100%)	2.67	24 (64%) 0 0	119, 148, 168, 184	0
1	L	37/37 (100%)	1.62	13 (35%) 0 0	110, 134, 170, 180	0
1	M	37/37 (100%)	1.08	6 (16%) 3 3	60, 86, 153, 166	0
1	N	37/37 (100%)	3.65	34 (91%) 0 0	140, 163, 181, 184	0
1	O	37/37 (100%)	0.47	1 (2%) 58 47	45, 67, 115, 124	0
1	P	37/37 (100%)	1.22	9 (24%) 1 1	46, 104, 155, 159	0
2	A	401/401 (100%)	-0.20	4 (0%) 84 76	15, 68, 109, 136	0
2	B	401/401 (100%)	-0.11	4 (0%) 84 76	17, 62, 105, 137	0
2	C	401/401 (100%)	0.30	19 (4%) 35 28	55, 101, 146, 160	0
2	D	401/401 (100%)	0.56	45 (11%) 7 7	80, 123, 147, 158	0
2	E	401/401 (100%)	0.69	51 (12%) 5 5	75, 126, 150, 168	0
2	F	401/401 (100%)	0.46	35 (8%) 13 12	47, 105, 148, 168	0
2	G	401/401 (100%)	-0.26	0 100 100	7, 48, 98, 132	0
2	H	401/401 (100%)	-0.17	3 (0%) 89 82	14, 68, 105, 135	0
All	All	3504/3504 (100%)	0.28	266 (7%) 17 14	7, 91, 147, 184	0

All (266) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	546	ASN	8.3
2	F	546	ASN	8.1
2	C	596	CYS	7.5
1	N	97	C	7.2
2	F	571	ALA	6.8

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Mol	Chain	Res	Type	RSRZ
1	N	85	C	6.6
1	N	84	U	6.5
1	N	94	C	6.4
1	N	83	U	6.3
1	K	74	A	6.2
2	F	596	CYS	6.1
1	K	72	G	5.9
2	D	642	GLU	5.9
1	N	80	U	5.6
2	E	498	VAL	5.4
2	D	427	ARG	5.3
2	F	260	ALA	5.1
1	K	84	U	4.9
1	L	85	C	4.9
2	D	641	GLU	4.9
1	K	73	U	4.8
1	K	85	C	4.7
1	M	69	G	4.6
1	K	71	C	4.6
1	N	87	U	4.5
2	D	482	THR	4.5
2	D	484	GLN	4.5
1	N	79	A	4.4
1	K	76	G	4.4
1	I	70	G	4.4
2	C	551	GLN	4.4
1	K	80	U	4.4
1	M	85	C	4.4
1	N	78	G	4.3
1	I	85	C	4.2
1	N	70	G	4.1
1	M	105	C	4.0
2	E	356	ALA	4.0
1	L	78	G	3.9
1	N	75	U	3.8
2	B	360	SER	3.6
1	K	70	G	3.6
2	E	504	ARG	3.6
1	N	102	C	3.6
2	E	547	ILE	3.6
1	J	85	C	3.6
1	K	82	U	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	317	MET	3.5
1	N	82	U	3.5
1	N	96	C	3.5
2	D	481	GLY	3.5
1	K	101	G	3.4
1	N	81	C	3.4
1	I	69	G	3.4
1	N	86	G	3.4
2	D	472	ASP	3.4
2	E	316	ALA	3.4
2	F	259	GLU	3.4
1	I	103	G	3.4
1	N	98	A	3.3
1	N	101	G	3.3
2	E	499	GLY	3.3
1	K	94	C	3.3
2	D	640	LEU	3.3
1	L	70	G	3.3
1	N	91	G	3.3
1	N	103	G	3.3
2	D	348	TYR	3.3
1	K	97	C	3.3
2	E	371	HIS	3.3
2	E	384	ALA	3.3
2	E	427	ARG	3.3
1	I	71	C	3.2
1	N	92	G	3.2
2	F	364	ASN	3.2
1	N	99	C	3.2
2	F	484	GLN	3.2
1	K	75	U	3.2
2	E	377	ARG	3.2
2	D	503	GLU	3.1
1	J	84	U	3.1
2	D	474	LEU	3.1
2	D	415	LYS	3.1
1	N	73	U	3.0
2	D	596	CYS	3.0
1	N	93	U	3.0
1	N	90	G	3.0
1	I	101	G	3.0
1	I	102	C	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	105	C	3.0
2	F	575	ASN	2.9
2	D	501	ASP	2.9
1	K	103	G	2.9
1	K	83	U	2.9
2	C	259	GLU	2.9
2	E	366	PRO	2.9
2	E	383	ASP	2.9
2	F	482	THR	2.8
1	N	74	A	2.8
2	F	242	ARG	2.8
2	C	548	THR	2.8
2	C	327	TYR	2.8
2	E	291	GLN	2.8
2	F	545	MET	2.8
2	C	550	SER	2.8
1	K	104	C	2.8
1	N	71	C	2.7
2	D	286	LYS	2.7
2	D	498	VAL	2.7
2	F	261	PRO	2.7
1	N	104	C	2.7
2	D	511	HIS	2.7
1	N	95	A	2.7
2	F	549	ASP	2.7
1	L	84	U	2.7
1	N	72	G	2.7
2	D	499	GLY	2.7
2	D	356	ALA	2.7
2	D	504	ARG	2.7
2	E	374	MET	2.7
2	C	642	GLU	2.7
2	E	482	THR	2.7
2	D	372	GLY	2.7
2	D	502	ASN	2.7
2	E	333	ASN	2.7
1	P	76	G	2.7
2	D	516	GLY	2.7
2	B	502	ASN	2.6
1	N	100	U	2.6
2	C	482	THR	2.6
2	E	288	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	E	497	TYR	2.6
2	F	377	ARG	2.6
2	B	499	GLY	2.6
2	C	579	GLY	2.6
1	I	74	A	2.6
1	O	69	G	2.6
2	D	392	GLN	2.6
1	K	102	C	2.6
2	D	480	CYS	2.6
2	F	481	GLY	2.6
2	E	423	ARG	2.6
2	D	476	ARG	2.5
1	L	101	G	2.5
1	J	105	C	2.5
2	E	355	MET	2.5
1	P	70	G	2.5
2	E	419	LYS	2.5
2	D	383	ASP	2.5
1	K	81	C	2.5
2	E	596	CYS	2.5
2	H	500	GLU	2.5
1	I	105	C	2.5
2	C	478	TRP	2.5
2	F	513	ALA	2.5
2	E	641	GLU	2.5
2	E	481	GLY	2.5
2	D	333	ASN	2.5
2	E	388	CYS	2.5
2	D	475	ASP	2.5
1	K	105	C	2.5
1	L	87	U	2.5
2	E	398	ASN	2.4
2	D	473	CYS	2.4
1	L	69	G	2.4
2	F	543	VAL	2.4
2	E	513	ALA	2.4
1	J	104	C	2.4
1	J	103	G	2.4
2	D	378	GLY	2.4
2	F	376	VAL	2.4
2	D	513	ALA	2.4
2	D	500	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
2	E	417	VAL	2.4
2	D	505	LYS	2.4
1	N	69	G	2.4
1	M	84	U	2.4
2	E	496	SER	2.4
1	P	97	C	2.4
2	F	548	THR	2.4
2	F	574	ARG	2.4
2	F	372	GLY	2.4
2	A	642	GLU	2.4
2	E	385	HIS	2.4
1	L	100	U	2.4
2	E	354	ARG	2.4
2	D	517	SER	2.4
2	F	367	SER	2.4
1	P	101	G	2.4
2	F	307	THR	2.3
2	D	317	MET	2.3
1	L	105	C	2.3
1	M	104	C	2.3
2	C	374	MET	2.3
1	P	105	C	2.3
1	P	72	G	2.3
2	E	516	GLY	2.3
2	F	582	ILE	2.3
2	D	547	ILE	2.3
2	E	378	GLY	2.3
2	A	500	GLU	2.3
2	F	486	ASP	2.3
2	F	547	ILE	2.3
1	N	88	G	2.3
2	C	556	ASN	2.3
1	L	81	C	2.3
2	E	503	GLU	2.3
2	F	552	SER	2.3
2	E	502	ASN	2.3
2	H	499	GLY	2.3
2	B	361	CYS	2.3
2	C	586	THR	2.3
2	D	388	CYS	2.2
2	E	422	THR	2.2
2	F	244	HIS	2.2

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Mol	Chain	Res	Type	RSRZ
1	L	86	G	2.2
1	M	70	G	2.2
2	E	456	LEU	2.2
2	C	552	SER	2.2
2	D	497	TYR	2.2
2	E	467	GLU	2.2
2	E	474	LEU	2.2
1	K	99	C	2.2
1	P	73	U	2.2
2	C	578	ILE	2.2
2	F	455	GLN	2.2
2	C	641	GLU	2.2
1	I	84	U	2.2
2	D	373	LEU	2.2
2	E	348	TYR	2.2
2	E	500	GLU	2.2
2	E	332	MET	2.2
2	A	499	GLY	2.1
2	F	323	GLU	2.1
2	E	517	SER	2.1
2	C	325	ARG	2.1
2	F	641	GLU	2.1
2	C	558	LEU	2.1
2	D	432	GLU	2.1
2	E	614	LYS	2.1
2	F	603	SER	2.1
1	K	95	A	2.1
2	E	311	ASP	2.1
2	H	479	GLN	2.1
1	K	93	U	2.1
1	P	84	U	2.1
2	E	301	ARG	2.1
2	F	604	GLY	2.1
2	E	548	THR	2.1
1	P	102	C	2.1
1	L	75	U	2.1
2	D	328	CYS	2.1
1	I	97	C	2.1
2	E	369	SER	2.1
1	I	79	A	2.1
1	K	98	A	2.1
2	E	328	CYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	479	GLN	2.1
2	E	284	LYS	2.1
2	A	502	ASN	2.0
1	L	104	C	2.0
2	D	360	SER	2.0
2	F	262	GLY	2.0
2	D	384	ALA	2.0
2	F	586	THR	2.0
1	J	69	G	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{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	LLDF	B-factors(Å^2)	Q<0.9
4	TSB	G	8002	30/30	0.94	0.31	0.55	0,18,49,50	0
4	TSB	D	5002	30/30	0.75	0.57	0.49	94,112,119,120	0
4	TSB	H	9002	30/30	0.91	0.39	0.48	30,48,71,72	0
4	TSB	B	3002	30/30	0.95	0.38	0.48	32,50,57,58	0
4	TSB	E	6002	30/30	0.65	0.51	0.12	86,122,126,127	0
4	TSB	A	2002	30/30	0.96	0.29	0.11	31,44,58,65	0
4	TSB	F	7002	30/30	0.81	0.42	0.10	89,103,111,112	0
3	ZN	B	1	1/1	0.99	0.32	-0.10	52,52,52,52	0
4	TSB	C	4002	30/30	0.87	0.36	-0.29	73,88,100,102	0
3	ZN	G	1	1/1	0.95	0.24	-0.61	27,27,27,27	0
3	ZN	F	1	1/1	0.81	0.26	-0.80	101,101,101,101	0
3	ZN	A	1	1/1	0.99	0.23	-0.93	42,42,42,42	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	ZN	H	1	1/1	0.98	0.27	-0.98	54,54,54,54	0
3	ZN	D	1	1/1	0.77	0.30	-1.76	135,135,135,135	0
3	ZN	E	1	1/1	0.73	0.26	-1.94	185,185,185,185	0
3	ZN	C	1	1/1	0.95	0.27	-2.07	95,95,95,95	0

6.5 Other polymers

There are no such residues in this entry.