Full wwPDB X-ray Structure Validation Report (i)

Aug 6, 2023 – 09:15 PM EDT

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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

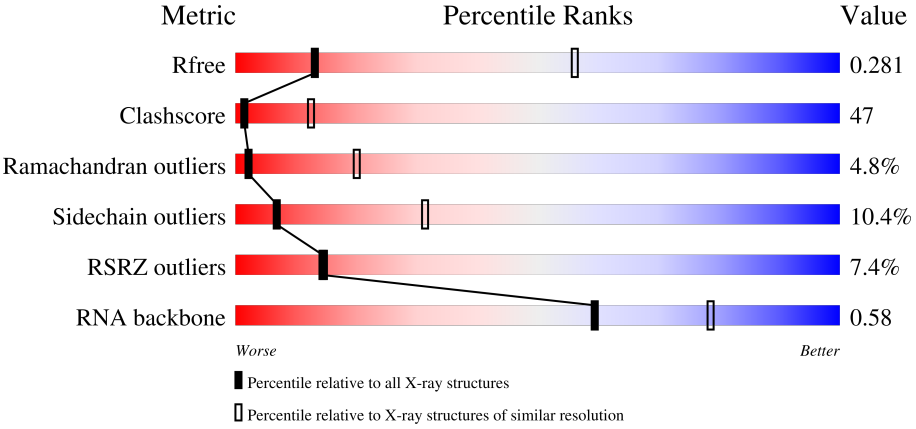
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)
RNA backbone	3102	1002 (4.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	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	10% 31% 61% 8%
2	E	401	12% 33% 58% 8%
2	F	401	8% 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

2 Entry composition (i)

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
			Total	C	N	O	P			
1	I	37	785	349	132	267	37	0	0	0
1	J	37	785	349	132	267	37	0	0	0
1	K	37	785	349	132	267	37	0	0	0
1	L	37	785	349	132	267	37	0	0	0
1	M	37	785	349	132	267	37	0	0	0
1	N	37	785	349	132	267	37	0	0	0
1	O	37	785	349	132	267	37	0	0	0
1	P	37	785	349	132	267	37	0	0	0

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

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

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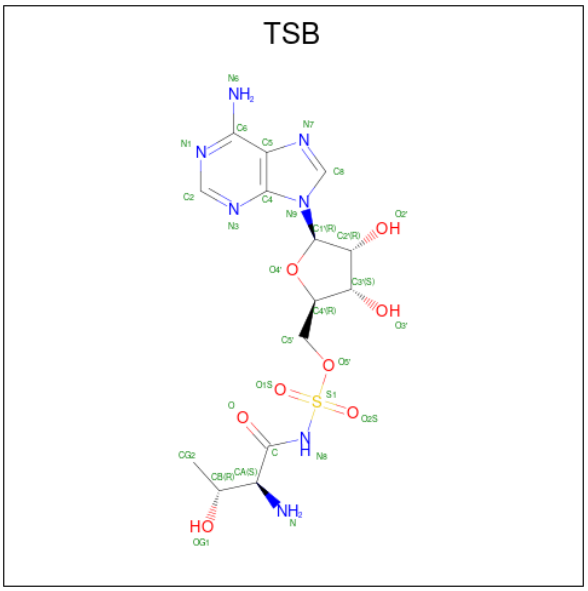
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	G	401	3278	2069	576	610	23	0	0	0
			Total	C	N	O	S			
2	H	401	3278	2069	576	610	23	0	0	0

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

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

- 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
			Total	C	N	O	S		
4	A	1	30	14	7	8	1	0	0
4	B	1	30	14	7	8	1	0	0
4	C	1	30	14	7	8	1	0	0
4	D	1	30	14	7	8	1	0	0
4	E	1	30	14	7	8	1	0	0
4	F	1	30	14	7	8	1	0	0
4	G	1	30	14	7	8	1	0	0
4	H	1	30	14	7	8	1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	I	11	11	11	0	0
5	J	12	12	12	0	0
5	K	1	1	1	0	0
5	L	8	8	8	0	0
5	M	6	6	6	0	0
5	N	9	9	9	0	0
5	O	11	11	11	0	0
5	P	9	9	9	0	0
5	A	10	10	10	0	0
5	B	15	15	15	0	0
5	C	11	11	11	0	0
5	D	14	14	14	0	0

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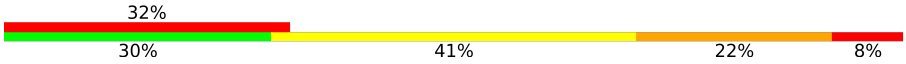
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	E	11	11	11	0	0
			Total	O		
5	F	13	13	13	0	0
			Total	O		
5	G	13	13	13	0	0
			Total	O		
5	H	16	16	16	0	0

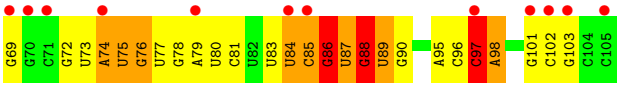
3 Residue-property plots (i)

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

• Molecule 1: Threonyl-tRNA synthetase mRNA

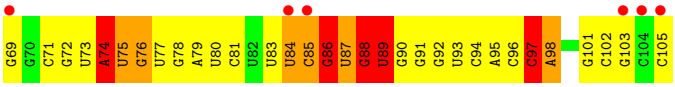
Chain I:





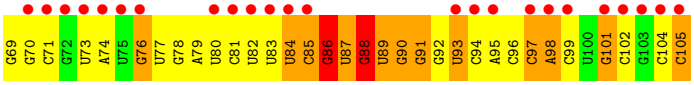
• Molecule 1: Threonyl-tRNA synthetase mRNA

Chain J:



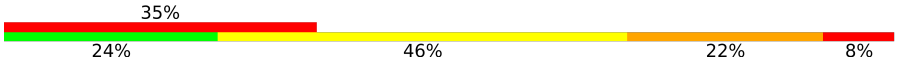
• Molecule 1: Threonyl-tRNA synthetase mRNA

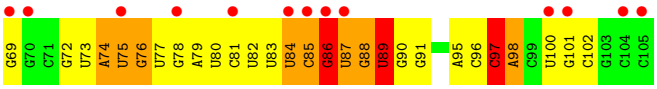
Chain K:



• Molecule 1: Threonyl-tRNA synthetase mRNA

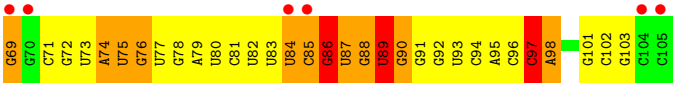
Chain L:





• Molecule 1: Threonyl-tRNA synthetase mRNA

Chain M:



• Molecule 1: Threonyl-tRNA synthetase mRNA

Chain N: 92% 22% 43% 27% 8%

G69 G70 C71 G72 U73 A74 U75 G76 U77 G78 A79 U80 C81 U82 U83 U84 C85 G86 U87 G88 U89 G90 G91 G92 U93 C94 A95 C96 C97 A98 C99 U100 G101 C102 G103 C104 C105

• Molecule 1: Threonyl-tRNA synthetase mRNA

Chain O: 3% 22% 41% 24% 14%

G69 G70 C71 A74 U75 G76 U77 G78 A79 U80 C81 U82 U83 U84 C85 G86 U87 G88 U89 G90 G91 G92 U93 C94 A95 C96 C97 A98 C99 U100 G101 C102 C105

• Molecule 1: Threonyl-tRNA synthetase mRNA

Chain P: 24% 19% 46% 24% 11%

G69 G70 C71 G72 U73 A74 U75 G76 U77 G78 A79 U80 C81 U82 U83 U84 C85 G86 U87 G88 U89 G90 U93 C94 A95 C96 C97 A98 C99 U100 G101 C102 G103 C104 C105

• Molecule 2: Threonyl-tRNA synthetase

Chain A: % 32% 59% 8%

R242 D243 H244 R245 K246 I247 G248 K249 Q250 L251 D252 L253 Y254 H255 M256 Q257 E258 E259 M263 V264 F265 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 G295 P296 F297 M298 M299 D300 R301 V302 L303 W304 E305

K306 T307 G308 H309 W310 D311 N312 Y313 K314 D315 A316 M317 F318 T319 T320 S321 N324 R325 E326 Y327 C328 I329 K330 P331 M332 N333 C334 P335 G336 H337 V338 Q339 I340 F341 N342 L345 K346 S347 Y348 R349 D350 L351 P352 L353 A356 E357 F358 C361 H362 R363 N364 E365 S369 L370 H371

G372 L373 M374 R375 V376 R377 A384 H385 I386 F387 C388 T389 E390 E391 Q392 I393 R394 D395 E396 V397 N398 G399 C400 I401 R402 L403 V404 Y405 D406 M407 F411 K415 I416 V417 V418 S421 T422 R423 R427 E432 M433 W434 D435 R436 A437 E438 A439 D440 L441 A442 V443 A444 L445 E446

E447 N448 N449 I450 P451 F452 E453 Y454 Q455 L456 G457 E458 G459 A460 F461 Y462 G463 P464 K465 I466 E467 Y471 D472 C473 R476 C480 G481 T482 V483 Q484 L485 D486 F487 S488 L489 P490 S491 R492 L493 S494 Y497 V498 G499 E500 D501 N502 E503 P507 V508 M509 I510 H511 R512 A513 I514

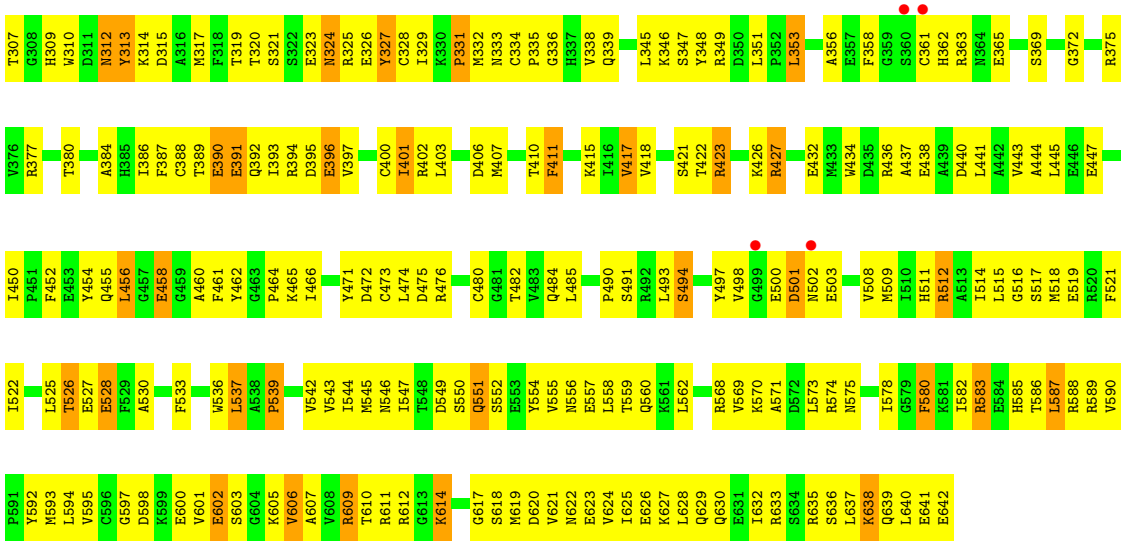
L515 G516 S517 M518 F521 I522 L525 T526 E527 E528 F529 A530 F533 P534 T535 W536 L537 A538 P539 V540 Q541 V542 V543 I544 M545 N546 I547 T548 D549 S550 Q551 S552 E553 Y554 V555 N556 E557 L558 T559 Q560 K561 L562 I567 R568 V569 K570 A571 D572 L573 R574 N575 I578 G579 F580 K581

I582 R583 E584 H585 T586 L587 R588 R589 V590 P591 Y592 M593 L594 V595 C596 G597 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

• Molecule 2: Threonyl-tRNA synthetase

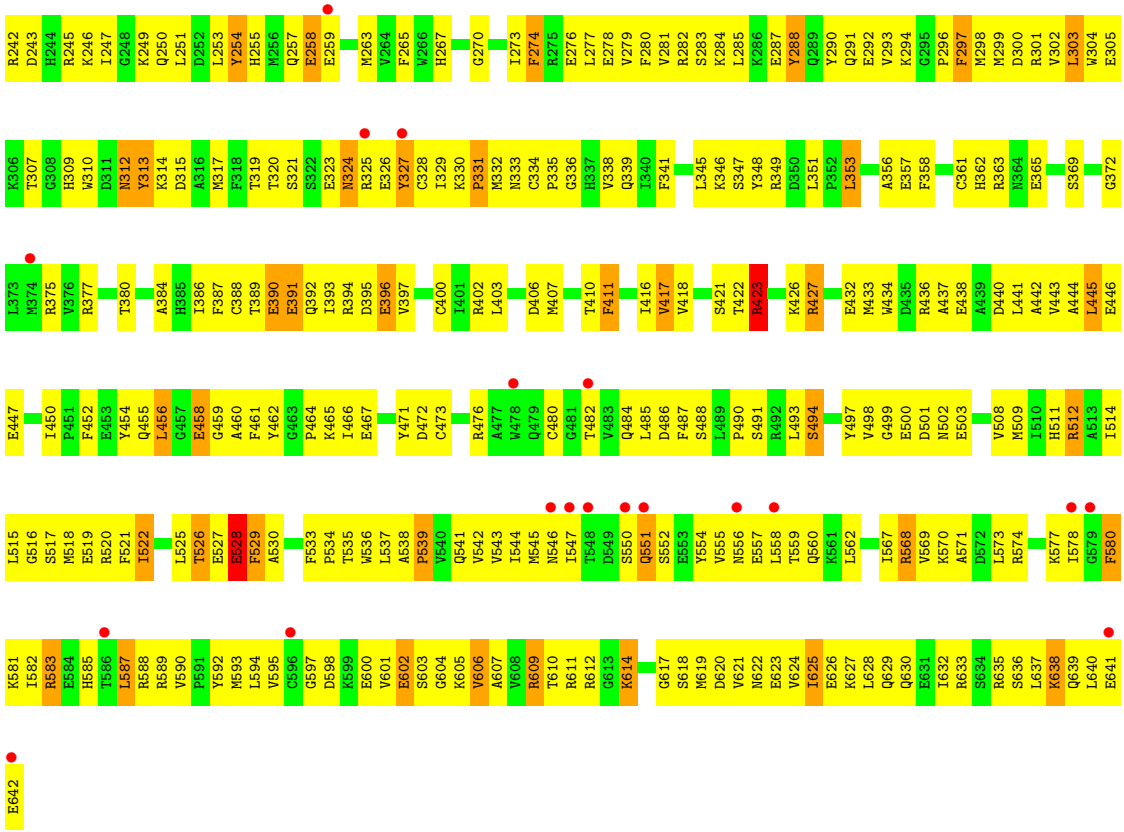
Chain B: % 35% 55% 10%

R242 D243 H244 R245 K246 I247 G248 K249 Q250 L251 D252 L253 Y254 H255 M256 Q257 E258 E259 M263 V264 F265 W266 H267 N268 D269 I273 F274 R275 E276 L277 E278 V279 F280 V281 R282 S283 K284 L285 K286 E287 Y288 Q289 Y290 Q291 E292 V293 P296 F297 M298 M299 D300 R301 V302 L303 W304 E305 K306



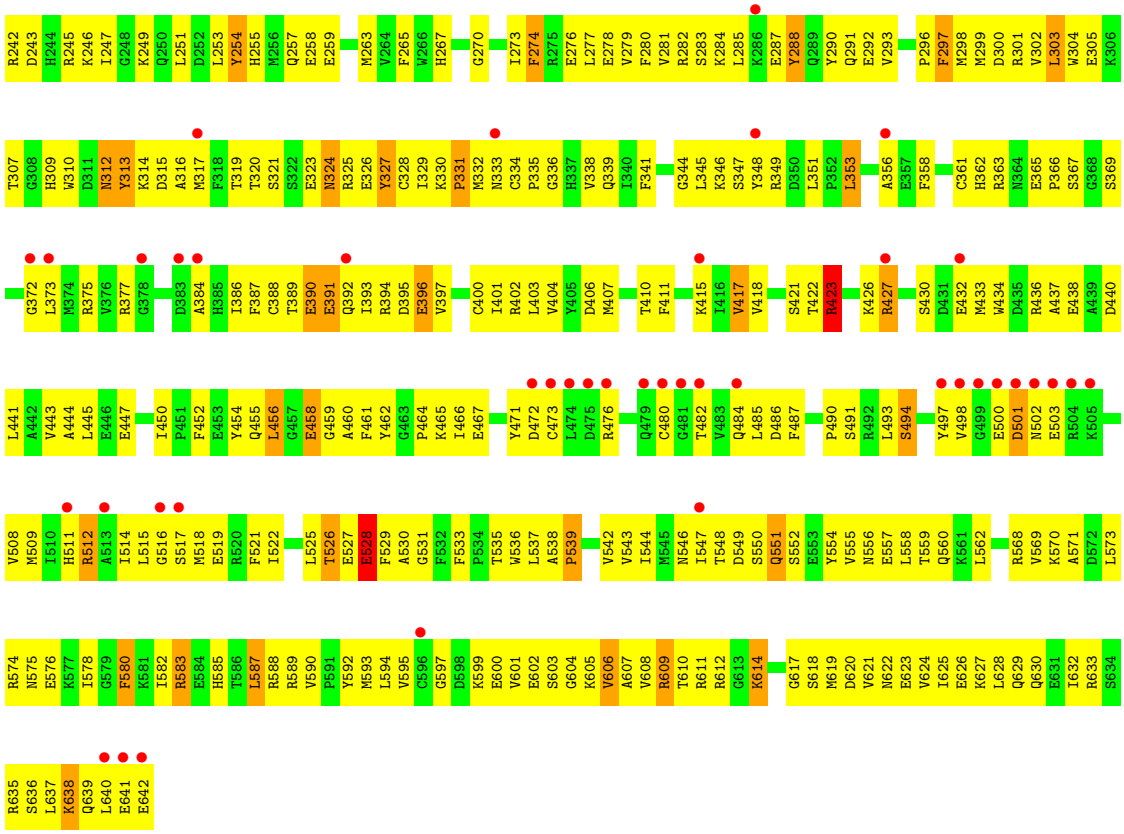
- Molecule 2: Threonyl-tRNA synthetase

Chain C:



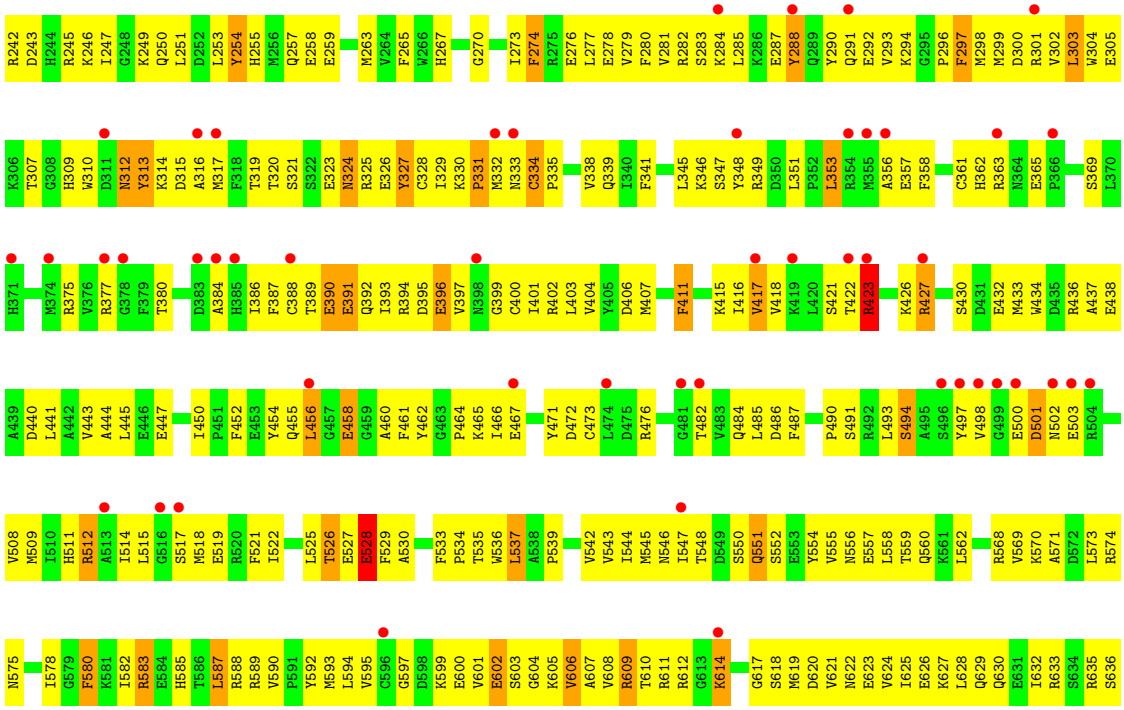
- Molecule 2: Threonyl-tRNA synthetase

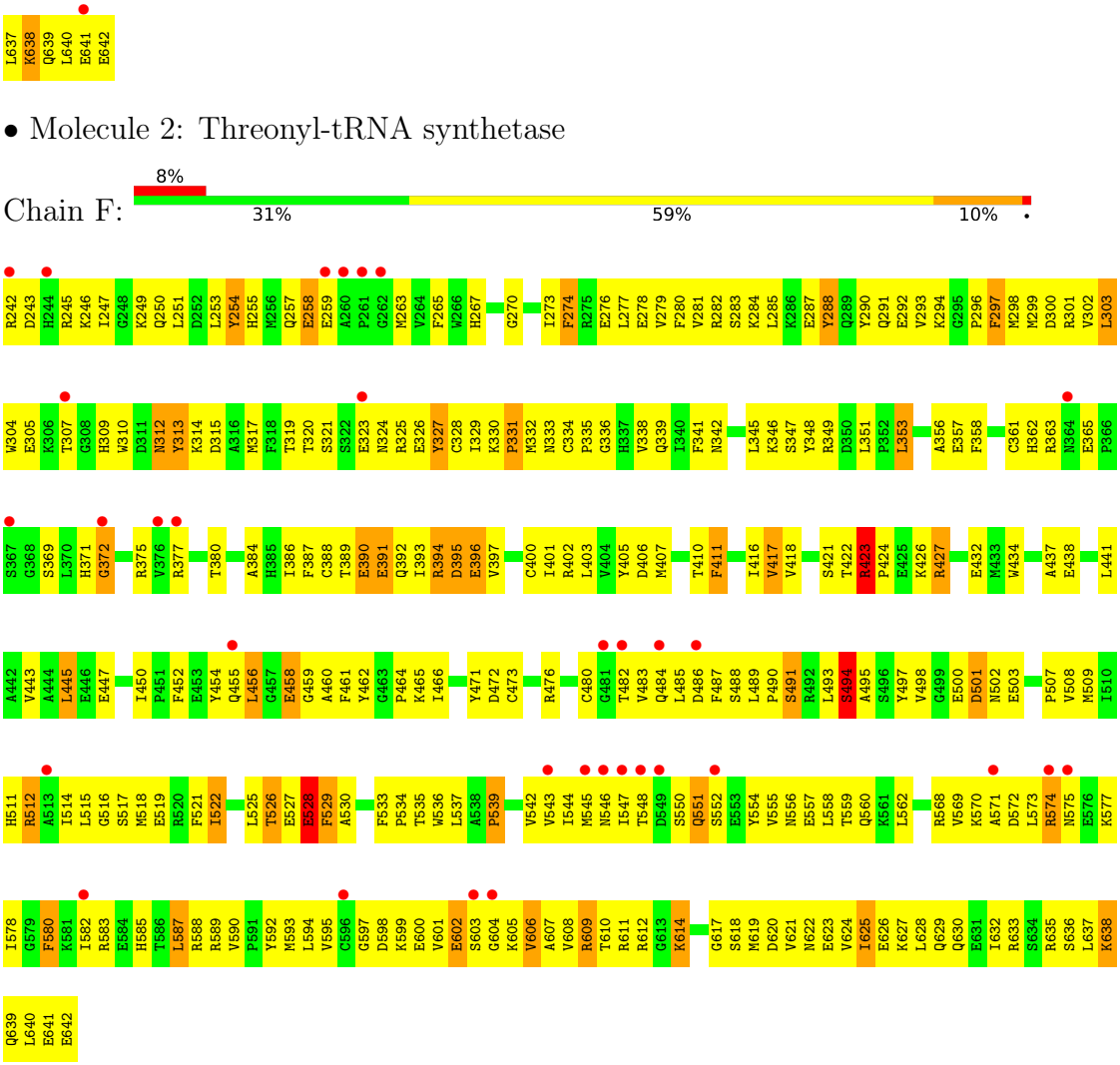
Chain D:



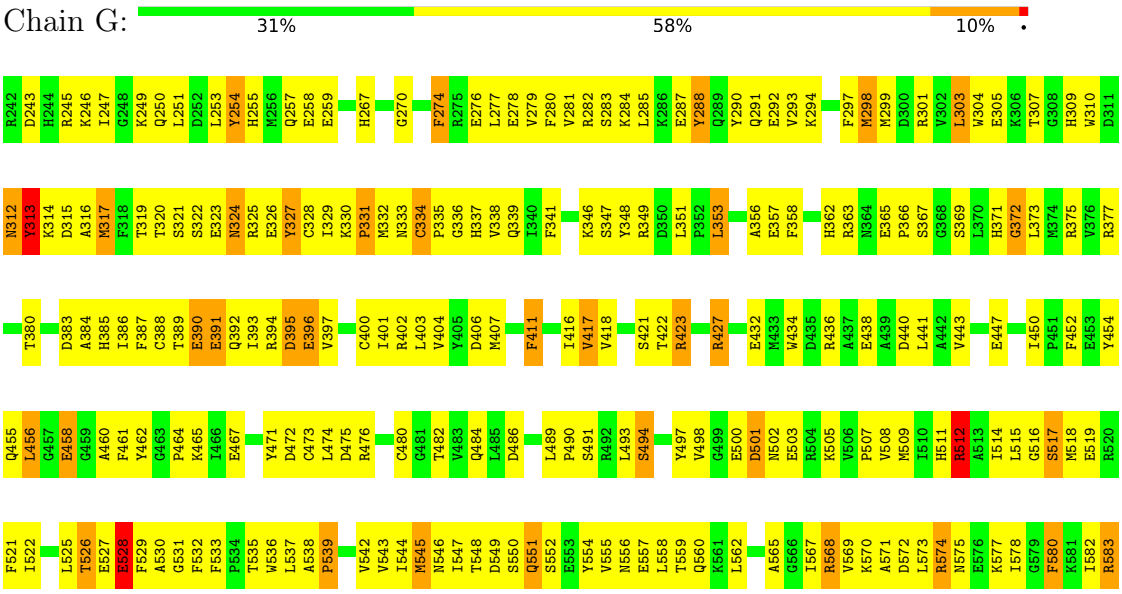
- Molecule 2: Threonyl-tRNA synthetase

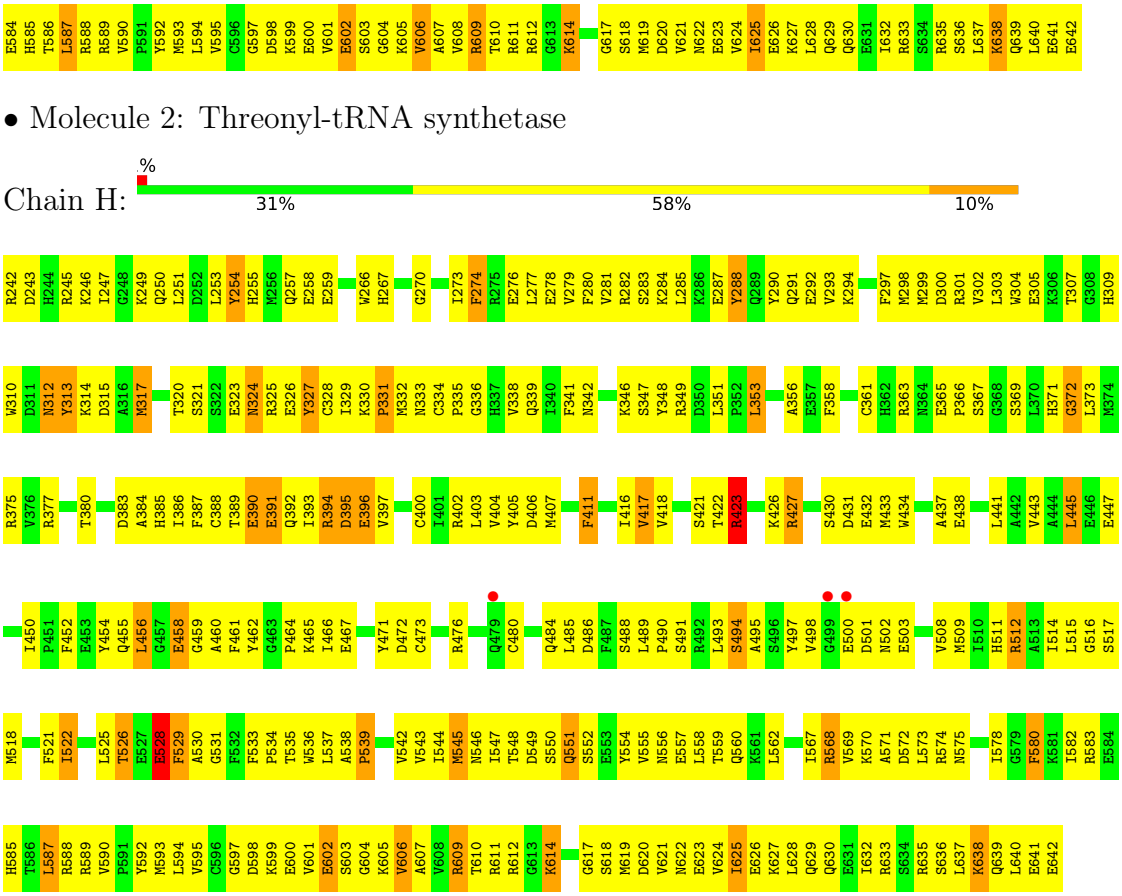
Chain E:





• Molecule 2: Threonyl-tRNA synthetase




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
• Molecule 2: Threonyl-tRNA synthetase
Chain H:
%
31%
58%
10%
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 N312 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 P580 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 0.248 , 0.281	Depositor DCC
R_{free} test set	8671 reflections (9.81%)	wwPDB-VP
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
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	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:F:559:THR:HG21	2:F:571:ALA:HB2	1.26	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:559:THR:HG21	2:H:571:ALA:HB2	1.31	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
1:I:103:G:H5"	5:I:113:HOH:O	1.68	0.92
2:D:421:SER:HB3	2:D:458:GLU:HB3	1.49	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:D:543:VAL:HG23	2:D:590:VAL:HG11	1.52	0.91
2:H:421:SER:HB3	2:H:458:GLU:HB3	1.50	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:C:411:PHE:HD2	2:C:525:LEU:HD21	1.39	0.88
2:D:582:ILE:HA	2:D:593:MET:HE1	1.53	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:H2'	1:K:87:U:O2	1.73	0.87
2:A:587:LEU:HD23	2:A:587:LEU:H	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
1:K:84:U:H4'	1:K:85:C:C5'	2.05	0.86
2:C:543:VAL:HG23	2:C:590:VAL:HG11	1.55	0.86
2:D:411:PHE:CE2	2:D:521:PHE:CZ	2.62	0.86
2:E:389:THR:OG1	2:E:392:GLN:HG3	1.75	0.86
2:H:411:PHE:CD2	2:H:525:LEU:HD21	2.09	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:G:587:LEU:HD23	2:G:587:LEU:H	1.40	0.86
2:C:307:THR:HG22	2:C:493:LEU:HD21	1.57	0.86
1:I:86:G:H2'	5:I:109:HOH:O	1.74	0.86
2:F:411:PHE:CD2	2:F:525:LEU:HD21	2.10	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
1:O:89:U:O2	1:O:89:U:H2'	1.78	0.84
2:D:411:PHE:HE2	2:D:521:PHE:HE1	1.25	0.84
2:F:389:THR:OG1	2:F:392:GLN:HG3	1.77	0.84
2:F:411:PHE:HD2	2:F:525:LEU:HD21	1.41	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:HD23	2:H:587:LEU:H	1.43	0.82
2:B:587:LEU:HD23	2:B:587:LEU:H	1.42	0.82
2:G:551:GLN:NE2	2:G:597:GLY:HA2	1.93	0.82
2:C:411:PHE:CE2	2:C:521:PHE:CE1	2.66	0.82
1:N:79:A:H1'	2:E:502:ASN:OD1	1.80	0.82
2:D:389:THR:OG1	2:D:392:GLN:HG3	1.80	0.82
1:N:100:U:H4'	5:F:7014:HOH:O	1.77	0.81
2:F:255:HIS:ND1	2:F:267:HIS:HE1	1.78	0.81
2:F:411:PHE:HE2	2:F:521:PHE:HE1	1.26	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:A:551:GLN:HE21	2:A:597:GLY:HA2	1.44	0.81
2:F:551:GLN:HE21	2:F: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
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
2:H:551:GLN:NE2	2:H:597:GLY:HA2	1.97	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:B:255:HIS:ND1	2:B:267:HIS:HE1	1.80	0.80
2:E:319:THR:O	2:F:320:THR:HG23	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:B:411:PHE:N	2:B:411:PHE:HD1	1.80	0.80
2:F:402:ARG:HH11	2:F:402:ARG:HB2	1.47	0.80
2:G:411:PHE:CD2	2:G:525:LEU:HD21	2.17	0.80
2:C:452:PHE:HE2	2:C:454:TYR:HE1	1.30	0.80
1:P:97:C:H5"	1:P:98:A:OP1	1.81	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)
2:F:307:THR:HG22	2:F:493:LEU:HD21	1.62	0.79
2:H:251:LEU:HA	2:H:588:ARG:HH12	1.47	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:255:HIS:ND1	2:D:267:HIS:HE1	1.80	0.79
2:D:501:ASP:OD2	2:D:503:GLU:HB2	1.82	0.79
2:A:320:THR:HG23	2:B:319:THR:O	1.83	0.79
2:F:582:ILE:HA	2:F:593:MET:HE2	1.62	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
1:P:89:U:O2	1:P:89:U:H2'	1.81	0.79
2:D:551:GLN:HE21	2:D:597:GLY:HA2	1.48	0.79
2:F:320:THR:HG22	2:F:321:SER:H	1.48	0.79
2:F:551:GLN:NE2	2:F:597:GLY:HA2	1.98	0.79
2:G:578:ILE:O	2:G:582:ILE:HG12	1.83	0.79
2:A:255:HIS:ND1	2:A:267:HIS:HE1	1.80	0.78
2:A:319:THR:O	2:B:320:THR:HG23	1.83	0.78
2:E:251:LEU:HA	2:E:588:ARG:HH12	1.48	0.78
2:E:411:PHE:N	2:E:411:PHE:HD1	1.80	0.78
2:G:403:LEU:HG	2:G:407:MET:CE	2.14	0.78
2:H:276:GLU:O	2:H:279:VAL:HG22	1.83	0.78
2:D:276:GLU:O	2:D:279:VAL:HG22	1.83	0.78
2:E:411:PHE:HE2	2:E:521:PHE:HE1	1.29	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:H	2:F:587:LEU:HD23	1.48	0.78
2:G:251:LEU:HA	2:G:588:ARG:NH1	1.99	0.78
2:G:402:ARG:HB2	2:G:402:ARG:HH11	1.49	0.78
2:B:251:LEU:HA	2:B:588:ARG:HH12	1.48	0.78
2:D:621:VAL:O	2:D:624:VAL:HG22	1.83	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:A:407:MET:SD	2:A:514:ILE:HG21	2.24	0.77
2:F:585:HIS:HB2	2:F:593:MET:CE	2.15	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
1:J:89:U:O2	1:J:89:U:H2'	1.82	0.77
2:A:303:LEU:HD11	2:A:339:GLN:HE21	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:551:GLN:HE21	2:E:597:GLY:HA2	1.50	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
1:N:89:U:H2'	1:N:89:U:O2	1.84	0.77
2:A:633:ARG:NH1	2:H:638:LYS:HZ1	1.82	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:B:452:PHE:HE2	2:B:454:TYR:HE1	1.30	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: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:D:452:PHE:HE2	2:D:454:TYR:HE1	1.31	0.76
2:F:251:LEU:HA	2:F:588:ARG:HH12	1.49	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:A:633:ARG:CZ	2:H:638:LYS:NZ	2.47	0.76
2:F:621:VAL:O	2:F:624:VAL:HG22	1.86	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:C:637:LEU:H	2:C:637:LEU:HD12	1.50	0.76
2:D:407:MET:SD	2:D:514:ILE:HG21	2.25	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: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:A:325:ARG:HH11	2:A:325:ARG:HG3	1.51	0.75
2:E:452:PHE:HE2	2:E:454:TYR:HE1	1.34	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:A:402:ARG:HH11	2:A:402:ARG:HB2	1.50	0.75
2:H:299:MET:O	2:H:327:TYR:HB3	1.86	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:E:473:CYS:HA	5:E:6010:HOH:O	1.86	0.74
2:H:411:PHE:HD2	2:H:525:LEU:CD2	1.99	0.74
2:A:411:PHE:HE2	2:A:521:PHE:HE1	1.33	0.74
1:L:88:G:H8	5:D:5016:HOH:O	1.69	0.74
2:A:452:PHE:HE2	2:A:454:TYR:HE1	1.33	0.74
2:E:411:PHE:N	2:E:411:PHE:CD1	2.54	0.74
2:F:321:SER:HB3	2:F:326:GLU:HA	1.70	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
1:J:103:G:OP2	5:J:1025:HOH:O	2.05	0.74
2:A:411:PHE:CE2	2:A:521:PHE:HE1	2.06	0.74
2:A:465:LYS:HG3	2:A:484:GLN:HG2	1.69	0.74
2:H:403:LEU:HG	2:H:407:MET:CE	2.18	0.74
2:C:251:LEU:HA	2:C:588:ARG:HH12	1.51	0.74
1:J:86:G:H3'	5:J:1013:HOH:O	1.88	0.74
2:C:621:VAL:O	2:C:624:VAL:HG22	1.86	0.74
1:K:77:U:H1'	1:K:98:A:N1	2.03	0.74
2:B:251:LEU:HA	2:B:588:ARG:NH1	2.02	0.74
2:B:585:HIS:HB2	2:B:593:MET:CE	2.17	0.74
2:C:411:PHE:N	2:C:411:PHE:HD1	1.85	0.74
2:H:452:PHE:HE2	2:H:454:TYR:HE1	1.35	0.74
2:D:390:GLU:HA	2:D:393:ILE:HG13	1.69	0.73
2:E:585:HIS:HB2	2:E:593:MET:CE	2.18	0.73
2:F:578:ILE:O	2:F:582:ILE:HG12	1.88	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:H	2:H:637:LEU:HD12	1.53	0.73
1:L:98:A:H4'	5:L:1227:HOH:O	1.87	0.73
2:G:249:LYS:HB3	2:G:249:LYS:NZ	2.02	0.73
2:C:263:MET:HE2	2:D:298:MET:HG2	1.69	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: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:E:321:SER:HB3	2:E:326:GLU:HA	1.70	0.73
2:A:633:ARG:NH1	2:H:638:LYS:NZ	2.37	0.73
2:D:637:LEU:H	2:D:637:LEU:HD12	1.53	0.73
2:A:583:ARG:O	2:A:587:LEU:HD23	1.88	0.73
2:D:402:ARG:HB2	2:D:402:ARG:HH11	1.53	0.73
2:D:551:GLN:NE2	2:D:597:GLY:HA2	2.03	0.73
2:D:625:ILE:O	2:D:629:GLN:HG3	1.89	0.73
2:E:251:LEU:HA	2:E:588:ARG:NH1	2.04	0.73
2:E:411:PHE:HD2	2:E:525:LEU:CD2	1.99	0.73
2:F:452:PHE:HE2	2:F:454:TYR:HE1	1.35	0.73
2:A:251:LEU:HA	2:A:588:ARG:HH12	1.53	0.72
2:C:411:PHE:N	2:C:411:PHE:CD1	2.57	0.72
2:H:621:VAL:O	2:H:624:VAL:HG22	1.88	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
1:M:69:G:OP3	1:P:105:C:O3'	2.08	0.72
2:F:501:ASP:OD2	2:F:503:GLU:HB2	1.89	0.72
1:L:78:G:O4'	2:C:345:LEU:HD23	1.89	0.72
1:M:88:G:H4'	1:M:89:U:OP1	1.87	0.72
2:B:411:PHE:N	2:B:411:PHE:CD1	2.51	0.72
2:D:578:ILE:O	2:D:582:ILE:HG12	1.89	0.72
2:F:637:LEU:HD12	2:F:637:LEU:H	1.54	0.72
2:G:547:ILE:HD12	2:G:597:GLY:HA3	1.71	0.72
2:H:390:GLU:HA	2:H:393:ILE:HG13	1.72	0.72
1:K:78:G:H2'	1:K:79:A:H8	1.54	0.72
2:C:403:LEU:HG	2:C:407:MET:CE	2.19	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:A:277:LEU:O	2:A:281:VAL:HG23	1.89	0.72
2:A:637:LEU:HD12	2:A:637:LEU:H	1.54	0.72
2:F:403:LEU:HG	2:F:407:MET:CE	2.20	0.72
1:O:86:G:H2'	5:O:1513:HOH:O	1.88	0.72
2:F:411:PHE:CE2	2:F:521:PHE:CZ	2.77	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
1:K:90:G:H8	2:C:577:LYS:CD	2.02	0.71
1:L:89:U:O2	1:L:89:U:H2'	1.88	0.71
1:P:86:G:C4	2:H:547:ILE:HD13	2.25	0.71
2:E:407:MET:SD	2:E:514:ILE:HG21	2.30	0.71
1:J:88:G:H4'	1:J:89:U:OP1	1.90	0.71
1:L:79:A:H1'	2:C:502:ASN:OD1	1.90	0.71
2:A:320:THR:HG22	2:A:321:SER:H	1.54	0.71
2:A:411:PHE:N	2:A:411:PHE:CD1	2.56	0.71
2:A:462:TYR:CE2	2:A:511:HIS:CE1	2.78	0.71
2:E:625:ILE:O	2:E:629:GLN:HG3	1.90	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
2:G:637:LEU:H	2:G:637:LEU:HD12	1.54	0.71
2:H:411:PHE:N	2:H:411:PHE:HD1	1.88	0.71
1:O:91:G:O3'	5:O:1518:HOH:O	2.08	0.71
2:A:585:HIS:HB2	2:A:593:MET:CE	2.21	0.71
2:E:299:MET:O	2:E:327:TYR:HB3	1.90	0.71
2:A:280:PHE:O	2:A:283:SER:HB3	1.91	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:251:LEU:HA	2:A:588:ARG:NH1	2.05	0.71
2:C:243:ASP:OD2	2:C:245:ARG:HB2	1.91	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:473:CYS:HA	5:C:4013:HOH:O	1.90	0.71
2:G:514:ILE:HG22	2:G:515:LEU:N	2.06	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
1:K:70:G:H22	1:K:105:C:H1'	1.56	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
2:B:637:LEU:H	2:B:637:LEU:HD12	1.56	0.71
2:E:402:ARG:HB2	2:E:402:ARG:HH11	1.54	0.71
1:K:97:C:H4'	1:K:98:A:OP1	1.91	0.70
1:O:89:U:C5	2:G:583:ARG:CZ	2.73	0.70
2:C:298:MET:HG2	2:D:263:MET:HE2	1.73	0.70
2:H:547:ILE:HD12	2:H:597:GLY:HA3	1.73	0.70
1:L:77:U:H1'	1:L:98:A:N1	2.06	0.70
2:E:637:LEU:H	2:E:637:LEU:HD12	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:321:SER:HB3	2:G:326:GLU:HA	1.72	0.70
2:C:517:SER:HB2	4:C:4002:TSB:H1'	1.72	0.70
1:M:84:U:H4'	1:M:85:C:C5'	2.22	0.70
2:C:411:PHE:CE2	2:C:521:PHE:CZ	2.79	0.70
2:H:320:THR:HG22	2:H:321:SER:H	1.53	0.70
1:L:97:C:H5"	1:L:98:A:OP1	1.91	0.70
2:C:585:HIS:HB2	2:C:593:MET:CE	2.20	0.70
2:A:621:VAL:O	2:A:624:VAL:HG22	1.92	0.70
2:B:276:GLU:O	2:B:279:VAL:HG22	1.91	0.70
2:B:578:ILE:O	2:B:582:ILE:HG12	1.92	0.70
2:F:411:PHE:N	2:F:411:PHE:HD1	1.89	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:C:544:ILE:HD11	2:C:562:LEU:HD22	1.72	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
1:J:91:G:H4'	5:J:1018:HOH:O	1.92	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
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:F:460:ALA:HB1	2:F:462:TYR:CE1	2.26	0.70
1:K:92:G:H2'	1:K:93:U:O4'	1.92	0.69
2:D:411:PHE:N	2:D:411:PHE:CD1	2.58	0.69
2:F:592:TYR:OH	2:F:639:GLN:HB3	1.92	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:NZ	2:H:249:LYS:HB3	2.06	0.69
2:H:411:PHE:N	2:H:411:PHE:CD1	2.59	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:HB2	2:B:402:ARG:NH1	2.07	0.69
1:I:89:U:H2'	1:I:89:U:O2	1.90	0.69
2:G:303:LEU:HD11	2:G:339:GLN:HE21	1.57	0.69
1:I:87:U:H2'	5:I:110:HOH:O	1.92	0.69
1:P:88:G:H4'	1:P:89:U:OP1	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
1:K:70:G:H2'	1:K:71:C:H6	1.56	0.69
2:D:585:HIS:HB2	2:D:593:MET:CE	2.23	0.69
2:F:402:ARG:HB2	2:F:402:ARG:NH1	2.06	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:G:411:PHE:HD2	2:G:525:LEU:CD2	2.04	0.69
2:H:554:TYR:O	2:H:558:LEU:HD13	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: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:K:70:G:N2	1:K:105:C:H1'	2.08	0.69
2:B:388:CYS:HB2	2:B:392:GLN:OE1	1.93	0.69
2:C:583:ARG:O	2:C:587:LEU:HD23	1.92	0.69
2:D:592:TYR:OH	2:D:639:GLN:HB3	1.93	0.69
2:F:421:SER:HA	2:F:455:GLN:HB3	1.75	0.69
2:B:551:GLN:NE2	2:B:597:GLY:HA2	2.08	0.68
1:J:78:G:O4'	2:A:345:LEU:HD23	1.93	0.68
2:B:411:PHE:CE2	2:B:521:PHE: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:F:462:TYR:CE2	2:F:511:HIS:CE1	2.81	0.68
2:F:544:ILE:HD11	2:F:562:LEU:HD22	1.75	0.68
1:M:77:U:H1'	1:M:98:A:N1	2.08	0.68
1:P:100:U:H4'	5:P:1630:HOH:O	1.93	0.68
2:D:321:SER:HB3	2:D:326:GLU:HA	1.75	0.68
2:E:421:SER:HA	2:E:455:GLN:HB3	1.74	0.68
1:L:91:G:H4'	5:L:1218:HOH:O	1.92	0.68
2:A:460:ALA:HB1	2:A:462:TYR:CE1	2.28	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
1:L:84:U:H4'	1:L:85:C:C5'	2.23	0.68
2:C:460:ALA:HB1	2:C:462:TYR:CE1	2.28	0.68
2:G:417:VAL:HG13	2:G:471:TYR:HE1	1.59	0.68
2:A:517:SER:CB	4:A:2002:TSB:H1'	2.24	0.68
1:I:98:A:H4'	5:I:114:HOH:O	1.93	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
2:F:465:LYS:HG3	2:F:484:GLN:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:595:VAL:HB	2:H:607:ALA:HB3	1.76	0.67
1:M:91:G:O3'	5:M:1318:HOH:O	2.12	0.67
1:O:89:U:H5	2:G:583:ARG:CZ	2.07	0.67
2:A:348:TYR:CD1	2:A:349:ARG:N	2.61	0.67
2:B:403:LEU:HG	2:B:407:MET:CE	2.22	0.67
2:B:622:ASN:ND2	5:B:226:HOH:O	2.26	0.67
2:G:411:PHE:N	2:G:411:PHE:CD1	2.62	0.67
2:C:421:SER:HA	2:C:455:GLN:HB3	1.75	0.67
2:C:535:THR:HG22	2:C:632:ILE:HG12	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:304:TRP:CZ3	2:H:328:CYS:HB2	2.28	0.67
2:H:346:LYS:O	2:H:497:TYR:HA	1.93	0.67
2:A:462:TYR:HE2	2:A:511:HIS:CE1	2.12	0.67
2:D:402:ARG:HB2	2:D:402:ARG:NH1	2.10	0.67
2:F:551:GLN:HE21	2:F:597:GLY:CA	2.08	0.67
2:E:460:ALA:HB1	2:E:462:TYR:CE1	2.30	0.67
2:E:554:TYR:O	2:E:557:GLU:HB3	1.94	0.67
2:F:290:TYR:CE2	2:F:512:ARG:NH1	2.62	0.67
2:G:407:MET:SD	2:G:514:ILE:HG21	2.34	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
1:N:97:C:H5"	1:N:98:A:OP1	1.94	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
2:D:411:PHE:HD2	2:D:525:LEU:HD21	1.59	0.67
2:E:460:ALA:HB1	2:E:462:TYR:CD1	2.30	0.67
2:F:411:PHE:N	2:F:411:PHE:CD1	2.59	0.67
2:A:346:LYS:O	2:A:497:TYR:HA	1.95	0.67
2:G:299:MET:O	2:G:327:TYR:HB3	1.95	0.67
2:G:402:ARG:HB2	2:G:402:ARG:NH1	2.09	0.67
2:A:402:ARG:HB2	2:A:402:ARG:NH1	2.10	0.67
2:A:403:LEU:HG	2:A:407:MET:CE	2.25	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:592:TYR:OH	2:A:639:GLN:HB3	1.94	0.67
2:B:390:GLU:HA	2:B:393:ILE:HG13	1.77	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
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:HB2	2:E:402:ARG:NH1	2.10	0.66
2:G:329:ILE:N	2:G:329:ILE:HD12	2.10	0.66
1:M:103:G:H5"	5:M:1325:HOH:O	1.95	0.66
1:O:84:U:H4'	1:O:85:C:C5'	2.25	0.66
1:P:84:U:H4'	1:P: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
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:G:585:HIS:HB2	2:G:593:MET:CE	2.25	0.66
1:L:75:U:O2'	1:L:76:G:OP1	2.13	0.66
2:B:441:LEU:HD12	2:B:464:PRO:HB2	1.77	0.66
2:B:621:VAL:O	2:B:624:VAL:HG22	1.94	0.66
2:E:298:MET:HG2	2:F:263:MET:HE2	1.76	0.66
2:G:304:TRP:CZ3	2:G:328:CYS:HB2	2.30	0.66
2:G:421:SER:CB	2:G:458:GLU:HB3	2.21	0.66
2:H:417:VAL:CG1	2:H:471:TYR:HE1	2.09	0.66
2:C:547:ILE:HD12	2:C:597:GLY:HA3	1.76	0.66
2:A:299:MET:O	2:A:327:TYR:HB3	1.96	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:E:544:ILE:HD11	2:E:562:LEU:HD22	1.78	0.66
2:G:625:ILE:O	2:G:629:GLN:HG3	1.96	0.66
1:O:89:U:O2	1:O:89:U:C2'	2.44	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
2:F:517:SER:CB	4:F:7002:TSB:H1'	2.25	0.66
2:G:421:SER:HA	2:G:455:GLN:HB3	1.78	0.66
2:H:402:ARG:HB2	2:H:402:ARG:NH1	2.10	0.66
2:A:332:MET:HE2	4:A:2002:TSB:HN12	1.60	0.66
2:D:517:SER:HB2	4:D:5002:TSB:H1'	1.78	0.66
2:E:348:TYR:CD1	2:E:349:ARG:N	2.64	0.66
2:F:514:ILE:HG22	2:F:515:LEU:N	2.11	0.66
1:I:87:U:H1'	2:A:582:ILE:HG13	1.77	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
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:O	2:G:580:PHE:HD1	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:332:MET:HG2	2:G:363:ARG:HH21	1.61	0.65
2:G:417:VAL:CG1	2:G:471:TYR:CE1	2.79	0.65
2:H:325:ARG:HH11	2:H:325:ARG:HG3	1.61	0.65
2:A:544:ILE:HD11	2:A:562:LEU:HD22	1.76	0.65
2:C:421:SER:CB	2:C:458:GLU:HB3	2.24	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:F:625:ILE:O	2:F:629:GLN:HG3	1.96	0.65
2:H:514:ILE:HG22	2:H:515:LEU:HD23	1.78	0.65
1:J:84:U:H4'	1:J:85:C:C5'	2.26	0.65
1:L:89:U:C5	2:D:583:ARG:CZ	2.79	0.65
2:B:243:ASP:OD2	2:B:245:ARG:HB2	1.96	0.65
2:B:325:ARG:HG3	2:B:325:ARG:HH11	1.61	0.65
2:B:547:ILE:HD12	2:B:597:GLY:HA3	1.78	0.65
2:E:434:TRP:O	2:E:438:GLU:HG3	1.97	0.65
1:O:77:U:H1'	1:O:98:A:N1	2.12	0.65
2:B:249:LYS:NZ	2:B:249:LYS:HB3	2.12	0.65
2:B:554:TYR:O	2:B:558:LEU:HD13	1.96	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: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
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
1:K:104:C:H2'	1:K:105:C:O4'	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
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
1:K:70:G:H2'	1:K:71:C:C6	2.31	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
2:B:411:PHE:CE2	2:B:521:PHE:HE1	2.14	0.65
2:E:441:LEU:HD12	2:E:464:PRO:HB2	1.78	0.65
2:E:554:TYR:O	2:E:558:LEU:HD13	1.96	0.65
2:E:580:PHE:HD1	2:E:580:PHE:O	1.78	0.65
2:G:403:LEU:HG	2:G:407:MET:HE3	1.78	0.65
2:F:403:LEU:HG	2:F:407:MET:HE3	1.79	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:G:280:PHE:CE2	2:G:407:MET:HG2	2.32	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:A:257:GLN:OE1	2:B:339:GLN:HB3	1.96	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: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:J:88:G:C8	5:J:1023:HOH:O	2.50	0.64
1:K:87:U:O2	1:K:87:U:C2'	2.45	0.64
1:K:88:G:C4'	1:K:89:U:OP1	2.45	0.64
2:A:249:LYS:NZ	2:A:249:LYS:HB3	2.11	0.64
2:B:334:CYS:N	2:B:335:PRO:HD2	2.12	0.64
1:K:90:G:H8	2:C:577:LYS:HD3	1.61	0.64
1:M:89:U:O2	1:M:89:U:C2'	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
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:A:514:ILE:HG22	2:A:515:LEU:N	2.11	0.64
2:E:585:HIS:HB2	2:E:593:MET:HE1	1.79	0.64
2:F:535:THR:HG22	2:F:632:ILE:HG12	1.79	0.64
2:H:391:GLU:OE1	2:H:391:GLU:N	2.30	0.64
2:H:417:VAL:HG13	2:H:471:TYR:HE1	1.62	0.64
2:B:392:GLN:O	2:B:396:GLU:HB2	1.98	0.64
2:D:339:GLN:OE1	2:D:339:GLN:HA	1.98	0.64
2:B:348:TYR:CD1	2:B:349:ARG:N	2.65	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:G:325:ARG:HG3	2:G:325:ARG:HH11	1.63	0.64
2:C:472:ASP:OD1	2:C:476:ARG:HB2	1.98	0.64
2:E:392:GLN:O	2:E:396:GLU:HB2	1.97	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:D:422:THR:OG1	2:D:456:LEU:HA	1.98	0.64
2:E:465:LYS:HG3	2:E:484:GLN:HG2	1.80	0.64
2:F:365:GLU:H	2:F:377:ARG:HD3	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:625:ILE:O	2:H:629:GLN:HG3	1.98	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:G:411:PHE:N	2:G:411:PHE:HD1	1.94	0.64
1:O:83:U:H3	2:G:575:ASN:HD21	1.45	0.63
2:D:348:TYR:CD1	2:D:349:ARG:N	2.67	0.63
2:F:253:LEU:O	2:F:254:TYR:HB3	1.98	0.63
2:F:411:PHE:CE2	2:F:521:PHE:HE1	2.11	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:HB2	2:C:402:ARG:NH1	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:D:417:VAL:HG13	2:D:471:TYR:HE1	1.63	0.63
2:G:334:CYS:N	2:G:335:PRO:HD2	2.13	0.63
1:J:87:U:H1'	2:B:582:ILE:HG13	1.81	0.63
1:P:84:U:H4'	1:P:85:C:O5'	1.99	0.63
2:B:417:VAL:HG13	2:B:471:TYR:HE1	1.64	0.63
2:C:257:GLN:HB3	2:C:259:GLU:OE2	1.98	0.63
2:D:554:TYR:O	2:D:558:LEU:HD13	1.98	0.63
2:F:500:GLU:C	2:F:502:ASN:H	2.02	0.63
2:C:612:ARG:HH11	2:C:612:ARG:HG3	1.63	0.63
1:N:78:G:O4'	2:E:345:LEU:HD23	1.98	0.63
1:O:89:U:O5'	5:O:1528:HOH:O	2.15	0.63
2:B:554:TYR:O	2:B:557:GLU:HB3	1.99	0.63
2:B:628:LEU:O	2:B:632:ILE:HG13	1.99	0.63
1:I:78:G:O2'	1:I:79:A:H5'	1.99	0.62
2:C:403:LEU:HG	2:C:407:MET:HE3	1.81	0.62
2:F:417:VAL:HG13	2:F:471:TYR:HE1	1.62	0.62
2:G:595:VAL:HB	2:G:607:ALA:HB3	1.80	0.62
1:I:77:U:H1'	1:I:98:A:N1	2.14	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
2:D:460:ALA:HB1	2:D:462:TYR:CD1	2.35	0.62
2:A:417:VAL:CG1	2:A:471:TYR:HE1	2.12	0.62
2:A:417:VAL:HG13	2:A:471:TYR:HE1	1.62	0.62
2:A:630:GLN:HA	2:A:633:ARG:NH1	2.14	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:595:VAL:HB	2:B:607:ALA:HB3	1.79	0.62
2:C:249:LYS:NZ	2:C:249:LYS:HB3	2.15	0.62
2:G:391:GLU:OE1	2:G:391:GLU:N	2.32	0.62
2:B:583:ARG:O	2:B:587:LEU:HD23	1.99	0.62
2:C:580:PHE:O	2:C:580:PHE:HD1	1.82	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:O	2:H:580:PHE:HD1	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:HH11	2:E:612:ARG:HG3	1.63	0.62
2:A:392:GLN:O	2:A:396:GLU:HB2	1.98	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:E:277:LEU:O	2:E:281:VAL:HG23	2.00	0.62
2:F:559:THR:HG21	2:F:571:ALA:CB	2.17	0.62
2:F:627:LYS:HB3	2:F:640:LEU:HD21	1.82	0.62
2:C:630:GLN:HA	2:C:633:ARG:NH1	2.14	0.62
2:F:277:LEU:O	2:F:281:VAL:HG23	2.00	0.62
2:H:388:CYS:HB2	2:H:392:GLN:OE1	2.00	0.62
2:H:418:VAL:HG21	2:H:450:ILE:HG21	1.82	0.62
2:H:421:SER:CB	2:H:458:GLU:HB3	2.26	0.62
1:I:84:U:H4'	1:I:85:C:O5'	2.00	0.62
2:E:417:VAL:HG13	2:E:471:TYR:HE1	1.64	0.62
2:G:554:TYR:O	2:G:557:GLU:HB3	1.99	0.62
2:D:585:HIS:HB2	2:D:593:MET:HE2	1.82	0.62
2:F:341:PHE:O	2:F:346:LYS:NZ	2.33	0.62
2:H:253:LEU:O	2:H:254:TYR:HB3	2.00	0.62
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
1:O:84:U:H4'	1:O:85:C:O5'	2.00	0.61
2:A:284:LYS:HG3	2:A:407:MET:HG3	1.82	0.61
2:B:542:VAL:HG12	2:B:543:VAL:N	2.15	0.61
2:E:627:LYS:HB3	2:E:640:LEU:HD21	1.81	0.61
2:F:249:LYS:NZ	2:F:249:LYS:HB3	2.13	0.61
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
2:A:580:PHE:O	2:A:580:PHE:HD1	1.83	0.61
2:B:465:LYS:HG3	2:B:484:GLN:HG2	1.82	0.61
2:E:253:LEU:O	2:E:254:TYR:HB3	1.99	0.61
2:H:592:TYR:OH	2:H:639:GLN:HB3	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:303:LEU:HD11	2:A:339:GLN:NE2	2.16	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:G:585:HIS:HB2	2:G:593:MET:HE3	1.83	0.61
1:K:86:G:C5'	1:K:87:U:OP1	2.45	0.61
1:M:69:G:O5'	1:P:105:C:O2'	2.18	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
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
1:N:75:U:O2'	1:N:76:G:OP1	2.19	0.61
2:C:543:VAL:HG11	2:C:585:HIS:CE1	2.36	0.61
2:D:580:PHE:O	2:D:580:PHE:HD1	1.84	0.61
2:B:257:GLN:HB3	2:B:259:GLU:OE2	2.01	0.61
2:H:500:GLU:C	2:H:502:ASN:H	2.05	0.61
2:B:580:PHE:HD1	2:B:580:PHE:O	1.83	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:D:257:GLN:HB3	2:D:259:GLU:OE2	2.01	0.61
2:E:422:THR:OG1	2:E:456:LEU:HA	2.00	0.61
2:F:375:ARG:NH2	5:F:7007:HOH:O	2.27	0.61
2:G:310:TRP:O	2:G:314:LYS:HB3	2.00	0.61
2:G:346:LYS:O	2:G:497:TYR:HA	2.01	0.61
2:G:517:SER:HB2	4:G:8002:TSB:H1'	1.81	0.61
2:G:544:ILE:HG22	2:G:555:VAL:HG13	1.81	0.61
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: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
2:G:583:ARG:O	2:G:587:LEU:HD23	2.01	0.60
2:A:500:GLU:C	2:A:502:ASN:H	2.03	0.60
2:C:296:PRO:HG2	2:D:265:PHE:CE1	2.35	0.60
2:E:339:GLN:OE1	2:E:339:GLN:HA	2.00	0.60
2:E:346:LYS:O	2:E:497:TYR:HA	2.01	0.60
1:M:87:U:H3'	5:M:1319:HOH:O	2.00	0.60
2:D:411:PHE:CE2	2:D:521:PHE:HZ	2.14	0.60
2:E:310:TRP:O	2:E:314:LYS:HB3	2.01	0.60
2:F:595:VAL:HB	2:F:607:ALA:HB3	1.82	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:H:609:ARG:O	2:H:609:ARG:HG3	2.01	0.60
2:A:585:HIS:HB2	2:A:593:MET:HE3	1.84	0.60
2:D:612:ARG:HG3	2:D:612:ARG:HH11	1.66	0.60
2:F:284:LYS:HG3	2:F:407:MET:HG3	1.83	0.60
2:F:422:THR:OG1	2:F:456:LEU:HA	2.00	0.60
2:F:554:TYR:O	2:F:558:LEU:HD13	2.01	0.60
1:M:83:U:H3	2:E:575:ASN:HD21	1.49	0.60
2:A:434:TRP:O	2:A:438:GLU:HG3	2.01	0.60
2:B:500:GLU:C	2:B:502:ASN:H	2.04	0.60
2:D:551:GLN:HE21	2:D:597:GLY:CA	2.14	0.60
2:H:369:SER:O	2:H:375:ARG:HD2	2.02	0.60
2:H:441:LEU:HD12	2:H:464:PRO:HB2	1.83	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:D:369:SER:O	2:D:375:ARG:HD2	2.01	0.60
2:E:403:LEU:HG	2:E:407:MET:HE3	1.84	0.60
2:F:606:VAL:O	2:F:618:SER:HA	2.01	0.60
2:G:281:VAL:HG12	2:G:285:LEU:HD12	1.82	0.60
1:M:86:G:O6	2:E:599:LYS:HB2	2.00	0.60
1:M:87:U:H2'	5:M:1319:HOH:O	2.00	0.60
1:P:87:U:H2'	5:P:1619:HOH:O	2.01	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:E:280:PHE:CE2	2:E:407:MET:HG2	2.37	0.60
2:F:462:TYR:HD2	2:F:486:ASP:OD2	1.85	0.60
2:F:543:VAL:HG11	2:F:585:HIS:CE1	2.36	0.60
2:E:417:VAL:CG1	2:E:471:TYR:HE1	2.14	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:339:GLN:OE1	2:H:339:GLN:HA	2.02	0.60
2:H:517:SER:CB	4:H:9002:TSB:H1'	2.31	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:280:PHE:CE2	2:H:407:MET:HG2	2.37	0.60
1:N:84:U:H4'	1:N:85:C:O5'	2.02	0.60
2:C:339:GLN:OE1	2:C:339:GLN:HA	2.02	0.60
2:C:627:LYS:HB3	2:C:640:LEU:HD21	1.82	0.60
2:D:393:ILE:HD11	2:D:508:VAL:HG11	1.82	0.60
2:E:303:LEU:HD11	2:E:339:GLN:HE21	1.67	0.60
2:G:254:TYR:CE1	2:G:373:LEU:HD21	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:620:ASP:HB3	2:G:623:GLU:HB2	1.84	0.60
2:H:403:LEU:HG	2:H:407:MET:HE3	1.83	0.60
1:I:101:G:O2'	1:I:102:C:H5'	2.02	0.59
1:M:69:G:P	1:P:105:C:O3'	2.60	0.59
2:A:325:ARG:HG3	2:A:325:ARG:NH1	2.10	0.59
2:A:423:ARG:HA	2:A:434:TRP:CZ3	2.37	0.59
2:A:484:GLN:HB2	2:A:511:HIS:HB2	1.84	0.59
2:D:346:LYS:O	2:D:497:TYR:HA	2.02	0.59
2:D:500:GLU:C	2:D:502:ASN:H	2.04	0.59
2:E:620:ASP:HB3	2:E:623:GLU:HB2	1.84	0.59
2:F:334:CYS:N	2:F:335:PRO:HD2	2.16	0.59
2:F:388:CYS:HB2	2:F:392:GLN:OE1	2.02	0.59
1:I:89:U:C5	2:A:583:ARG:NH1	2.70	0.59
1:P:101:G:O2'	1:P:102:C:H5'	2.02	0.59
2:H:517:SER:HB2	4:H:9002:TSB:H1'	1.83	0.59
2:A:472:ASP:OD1	2:A:476:ARG:HB2	2.01	0.59
2:A:606:VAL:O	2:A:618:SER:HA	2.02	0.59
2:B:592:TYR:OH	2:B:639:GLN:HB3	2.03	0.59
2:B:609:ARG:HG3	2:B:609:ARG:O	2.02	0.59
2:C:554:TYR:O	2:C:558:LEU:HD13	2.03	0.59
2:E:243:ASP:OD2	2:E:245:ARG:HB2	2.00	0.59
2:E:369:SER:O	2:E:375:ARG:HD2	2.00	0.59
2:E:500:GLU:C	2:E:502:ASN:H	2.04	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:G:253:LEU:O	2:G:254:TYR:HB3	2.01	0.59
2:H:257:GLN:HB3	2:H:259:GLU:OE2	2.00	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:H:535:THR:HG22	2:H:632:ILE:HG12	1.84	0.59
1:J:84:U:H4'	1:J:85:C:O5'	2.02	0.59
1:J:89:U:C6	2:B:583:ARG:CZ	2.85	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:388:CYS:HB2	2:E:392:GLN:OE1	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
2:A:514:ILE:HG22	2:A:515:LEU:HD23	1.84	0.59
2:B:514:ILE:HG22	2:B:515:LEU:N	2.18	0.59
2:E:411:PHE:CE2	2:E:521:PHE:CZ	2.90	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:612:ARG:HH11	2:F:612:ARG:HG3	1.67	0.59
2:G:281:VAL:HG12	2:G:285:LEU:CD1	2.32	0.59
2:G:434:TRP:O	2:G:438:GLU:HG3	2.02	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: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:D:325:ARG:HG3	2:D:325:ARG:HH11	1.66	0.59
2:H:304:TRP:CE3	2:H:328:CYS:HB2	2.38	0.59
1:P:87:U:C2'	5:P:1619:HOH:O	2.51	0.59
2:A:422:THR:OG1	2:A:456:LEU:HA	2.01	0.59
2:B:346:LYS:O	2:B:497:TYR:HA	2.03	0.59
2:B:407:MET:SD	2:B:514:ILE:HG21	2.43	0.59
2:D:411:PHE:CE2	2:D:521:PHE:HE1	2.05	0.59
2:D:434:TRP:O	2:D:438:GLU:HG3	2.02	0.59
2:E:393:ILE:HD11	2:E:508:VAL:HG11	1.85	0.59
2:E:517:SER:CB	4:E:6002:TSB:H1'	2.33	0.59
2:F:257:GLN:HB3	2:F:259:GLU:OE2	2.02	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:H:281:VAL:HG12	2:H:285:LEU:HD12	1.84	0.59
2:H:417:VAL:CG1	2:H:471:TYR:CE1	2.86	0.59
1:J:78:G:O2'	1:J:79:A:H5'	2.03	0.59
1:P:86:G:C4	2:H:547:ILE:CD1	2.85	0.59
2:A:329:ILE:HD12	2:A:329:ILE:N	2.17	0.59
2:B:310:TRP:O	2:B:314:LYS:HB3	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
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
1:M:75:U:O2'	1:M:76:G:OP1	2.21	0.59
2:A:365:GLU:H	2:A:377:ARG:HD3	1.67	0.59
2:A:554:TYR:O	2:A:558:LEU:HD13	2.03	0.59
2:B:585:HIS:HB2	2:B:593:MET:HE3	1.85	0.59
2:C:278:GLU:HB3	2:C:358:PHE:HE2	1.68	0.59
2:D:253:LEU:O	2:D:254:TYR:HB3	2.03	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
1:K:98:A:N6	2:D:345:LEU:HD22	2.18	0.58
2:B:627:LYS:HB3	2:B:640:LEU:HD21	1.85	0.58
2:C:556:ASN:ND2	2:C:573:LEU:HD11	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:610:THR:CG2	2:E:614:LYS:HB3	2.33	0.58
2:F:351:LEU:HD22	2:F:387:PHE:O	2.03	0.58
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
1:O:77:U:O5'	1:O:77:U:H6	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
1:M:78:G:H5'	5:M:1339:HOH:O	2.03	0.58
2:A:535:THR:HG22	2:A:632:ILE:HG12	1.84	0.58
2:A:587:LEU:HD23	2:A:587:LEU:N	2.14	0.58
2:A:625:ILE:O	2:A:629:GLN:HG3	2.03	0.58
2:C:369:SER:O	2:C:375:ARG:HD2	2.03	0.58
2:D:517:SER:CB	4:D:5002:TSB:H1'	2.33	0.58
2:E:551:GLN:HE21	2:E:597:GLY:CA	2.16	0.58
2:F:526:THR:HG23	2:F:533:PHE:HZ	1.68	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:411:PHE:CD2	2:D:521:PHE:CZ	2.91	0.58
2:D:418:VAL:HG21	2:D:450:ILE:HG21	1.85	0.58
2:E:257:GLN:HB3	2:E:259:GLU:OE2	2.02	0.58
1:L:89:U:C5	2:D:583:ARG:NH1	2.72	0.58
2:A:612:ARG:HG3	2:A:612:ARG:HH11	1.67	0.58
2:D:535:THR:HG22	2:D:632:ILE:HG12	1.83	0.58
2:F:325:ARG:HH11	2:F:325:ARG:HG3	1.67	0.58
2:F:369:SER:O	2:F:375:ARG:HD2	2.03	0.58
2:H:325:ARG:HG3	2:H:325:ARG:NH1	2.18	0.58
1:I:89:U:O2	1:I:89:U:C2'	2.51	0.58
1:N:75:U:O2'	1:N:89:U:O4	2.21	0.58
2:C:365:GLU:H	2:C:377:ARG:HD3	1.68	0.58
2:C:422:THR:OG1	2:C:456:LEU:HA	2.03	0.58
2:E:273:ILE:HG23	2:E:537:LEU:HD22	1.85	0.58
2:E:622:ASN:O	2:E:626:GLU:HG3	2.04	0.58
2:A:536:TRP:CZ3	2:A:635:ARG:HD3	2.38	0.58
2:B:612:ARG:HH11	2:B:612:ARG:HG3	1.69	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:F:472:ASP:OD1	2:F:476:ARG:HB2	2.03	0.58
2:F:630:GLN:HA	2:F:633:ARG:NH1	2.19	0.58
2:G:303:LEU:HD11	2:G:339:GLN:NE2	2.19	0.58
2:G:620:ASP:O	2:G:623:GLU:HB3	2.02	0.58
2:H:278:GLU:HB3	2:H:358:PHE:HE2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:G:OP2	1:P:105:C:C3'	2.52	0.58
1:O:87:U:O4	2:G:607:ALA:HB1	2.04	0.58
2:A:441:LEU:HD12	2:A:464:PRO:HB2	1.85	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
2:A:304:TRP:CZ3	2:A:328:CYS:HB2	2.39	0.58
2:C:500:GLU:C	2:C:502:ASN:H	2.06	0.58
2:D:422:THR:O	2:D:458:GLU:O	2.21	0.58
2:F:281:VAL:HG12	2:F:285:LEU:HD12	1.86	0.58
2:F:484:GLN:HB2	2:F:511:HIS:HB2	1.85	0.58
2:G:527:GLU:O	2:G:528:GLU:O	2.21	0.58
2:H:620:ASP:O	2:H:623:GLU:HB3	2.04	0.58
1:N:89:U:O2	1:N:89:U:C2'	2.50	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:B:278:GLU:HB3	2:B:358:PHE:HE2	1.69	0.57
2:B:403:LEU:HG	2:B:407:MET:HE3	1.86	0.57
2:F:554:TYR:O	2:F:557:GLU:HB3	2.02	0.57
2:G:421:SER:HB3	2:G:458:GLU:CB	2.26	0.57
2:H:536:TRP:O	2:H:568:ARG:NH2	2.36	0.57
2:H:610:THR:CG2	2:H:614:LYS:HB3	2.34	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:A:554:TYR:O	2:A:557:GLU:HB3	2.04	0.57
2:C:388:CYS:HB2	2:C:392:GLN:OE1	2.04	0.57
2:F:280:PHE:CE2	2:F:407:MET:HG2	2.38	0.57
2:G:441:LEU:HD12	2:G:464:PRO:HB2	1.84	0.57
2:G:528:GLU:O	2:G:530:ALA:N	2.37	0.57
2:H:620:ASP:HB3	2:H:623:GLU:HB2	1.84	0.57
1:L:89:U:O2	1:L:89:U:C2'	2.51	0.57
2:B:421:SER:HB3	2:B:458:GLU:CB	2.27	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: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: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:N	2:F:391:GLU:OE1	2.37	0.57
2:G:341:PHE:O	2:G:346:LYS:NZ	2.36	0.57
2:A:449:ASN:ND2	2:H:452:PHE:CD2	2.72	0.57
2:B:391:GLU:OE1	2:B:391:GLU:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:434:TRP:O	2:B:438:GLU:HG3	2.04	0.57
2:C:620:ASP:O	2:C:623:GLU:HB3	2.04	0.57
2:D:630:GLN:HA	2:D:633:ARG:NH1	2.19	0.57
1:I:79:A:O2'	2:B:500:GLU:O	2.23	0.57
1:L:84:U:H4'	1:L:85:C:O5'	2.04	0.57
1:P:85:C:H5	2:H:547:ILE:O	1.86	0.57
2:E:462:TYR:HE2	2:E:511:HIS:CE1	2.23	0.57
2:F:585:HIS:HB2	2:F:593:MET:HE1	1.86	0.57
2:H:332:MET:HG2	2:H:363:ARG:HH21	1.69	0.57
1:J:77:U:O5'	1:J:77:U:H6	1.87	0.57
1:L:89:U:H5	2:D:583:ARG:CZ	2.16	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:C:585:HIS:HB2	2:C:593:MET:HE3	1.85	0.57
2:D:606:VAL:O	2:D:618:SER:HA	2.05	0.57
2:E:403:LEU:O	2:E:407:MET:HB2	2.05	0.57
2:F:514:ILE:HG22	2:F:515:LEU:HD23	1.86	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:101:G:O2'	1:J:102:C:H5'	2.05	0.57
2:A:536:TRP:CE3	2:A:635:ARG:HD3	2.39	0.57
2:C:375:ARG:NH2	5:C:4008:HOH:O	2.36	0.57
2:D:411:PHE:CD2	2:D:521:PHE:HZ	2.23	0.57
2:D:620:ASP:O	2:D:624:VAL:HG13	2.04	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
1:L:101:G:O2'	1:L:102:C:H5'	2.05	0.57
2:A:403:LEU:HG	2:A:407:MET:HE3	1.85	0.57
2:B:325:ARG:HG3	2:B:325:ARG:NH1	2.19	0.57
2:G:403:LEU:O	2:G:407:MET:HB2	2.04	0.57
2:B:620:ASP:HB3	2:B:623:GLU:HB2	1.87	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: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:B:332:MET:HG2	2:B:363:ARG:HH21	1.70	0.56
2:B:417:VAL:CG1	2:B:471:TYR:HE1	2.18	0.56
2:B:500:GLU:OE1	2:B:500:GLU:N	2.37	0.56
2:B:610:THR:CG2	2:B:614:LYS:HB3	2.34	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:H:341:PHE:O	2:H:346:LYS:NZ	2.35	0.56
2:H:587:LEU:HD23	2:H:587:LEU:N	2.19	0.56
1:M:80:U:H2'	1:M:81:C:C6	2.40	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:B:638:LYS:HB2	2:B:642:GLU:HG3	1.87	0.56
2:C:536:TRP:O	2:C:568:ARG:NH2	2.38	0.56
2:D:484:GLN:HB2	2:D:511:HIS:HB2	1.87	0.56
2:E:418:VAL:HG21	2:E:450:ILE:HG21	1.86	0.56
2:G:285:LEU:HD22	2:G:290:TYR:CG	2.40	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
1:J:80:U:H2'	1:J:81:C:H6	1.70	0.56
1:J:89:U:O2	1:J:89:U:C2'	2.48	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:B:277:LEU:O	2:B:281:VAL:HG23	2.06	0.56
2:C:253:LEU:O	2:C:254:TYR:HB3	2.05	0.56
2:C:397:VAL:O	2:C:400:CYS:HB2	2.04	0.56
2:C:462:TYR:HE2	2:C:511:HIS:CE1	2.21	0.56
2:C:546:ASN:OD1	2:C:573:LEU:HA	2.05	0.56
2:D:542:VAL:HG12	2:D:543:VAL:N	2.21	0.56
2:D:620:ASP:HB3	2:D:623:GLU:HB2	1.87	0.56
2:F:309:HIS:HB3	2:F:317:MET:CE	2.35	0.56
2:G:332:MET:HG2	2:G:363:ARG:NH2	2.21	0.56
2:G:339:GLN:OE1	2:G:339:GLN:HA	2.05	0.56
2:G:411:PHE:CE2	2:G:521:PHE:CE1	2.94	0.56
2:G:542:VAL:HG12	2:G:543:VAL:N	2.20	0.56
2:G:624:VAL:HG23	2:G:625:ILE:N	2.20	0.56
2:H:309:HIS:HB3	2:H:317:MET:CE	2.36	0.56
2:H:472:ASP:OD1	2:H:476:ARG:HB2	2.04	0.56
2:A:304:TRP:CE3	2:A:328:CYS:HB2	2.40	0.56
2:A:620:ASP:HB3	2:A:623:GLU:HB2	1.87	0.56
2:E:312:ASN:O	2:E:313:TYR:HB2	2.06	0.56
2:F:278:GLU:HB3	2:F:358:PHE:HE2	1.70	0.56
2:F:332:MET:HG2	2:F:363:ARG:HH21	1.70	0.56
1:M:89:U:C5	2:E:583:ARG:NH1	2.73	0.56
2:D:391:GLU:OE1	2:D:391:GLU:N	2.38	0.56
2:D:514:ILE:HG22	2:D:515:LEU:N	2.20	0.56
2:E:304:TRP:CZ3	2:E:328:CYS:HB2	2.41	0.56
2:F:338:VAL:HG11	2:F:493:LEU:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:609:ARG:HG3	2:F:609:ARG:O	2.05	0.56
1:K:95:A:H1'	2:D:502:ASN:HD21	1.71	0.56
1:P:87:U:C2'	1:P:88:G:OP2	2.53	0.56
2:B:544:ILE:HG12	2:B:594:LEU:HD12	1.88	0.56
2:D:462:TYR:CE2	2:D:511:HIS:CE1	2.93	0.56
2:D:544:ILE:HG22	2:D:555:VAL:HG13	1.87	0.56
2:G:514:ILE:HG22	2:G:515:LEU:HD23	1.87	0.56
2:G:587:LEU:HD23	2:G:587:LEU:N	2.16	0.56
2:G:624:VAL:CG2	2:G:625:ILE:N	2.67	0.56
2:H:249:LYS:HB3	2:H:249:LYS:HZ3	1.69	0.56
1:M:75:U:O2'	1:M:89:U:O4	2.22	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
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: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
1:M:87:U:C2'	5:M:1319:HOH:O	2.54	0.56
2:B:369:SER:O	2:B:375:ARG:HD2	2.06	0.56
2:C:555:VAL:HB	2:C:573:LEU:HD21	1.88	0.56
2:D:312:ASN:O	2:D:313:TYR:HB2	2.05	0.56
2:F:418:VAL:HG21	2:F:450:ILE:HG21	1.88	0.56
1:I:78:G:O4'	2:B:345:LEU:HD23	2.06	0.56
1:M:77:U:H6	1:M:77:U:O5'	1.89	0.56
2:A:547:ILE:HD12	2:A:597:GLY:CA	2.36	0.56
2:C:312:ASN:O	2:C:313:TYR:HB2	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:G:312:ASN:O	2:G:313:TYR:HB2	2.05	0.56
2:H:403:LEU:O	2:H:407:MET:HB2	2.06	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:B:526:THR:O	2:B:530:ALA:N	2.37	0.56
2:D:332:MET:HG2	2:D:363:ARG:HH21	1.70	0.56
2:F:304:TRP:CZ3	2:F:328:CYS:HB2	2.40	0.56
2:G:609:ARG:HG3	2:G:609:ARG:O	2.06	0.56
2:A:301:ARG:O	2:A:305:GLU:HG3	2.06	0.55
2:B:259:GLU:H	2:B:259:GLU:CD	2.07	0.55
2:E:391:GLU:OE1	2:E:391:GLU:N	2.39	0.55
2:H:418:VAL:HG21	2:H:450:ILE:CG2	2.35	0.55
2:H:630:GLN:HA	2:H:633:ARG:NH1	2.21	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
1:M:78:G:C5'	5:M:1339:HOH:O	2.53	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: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
2:H:259:GLU:H	2:H:259:GLU:CD	2.07	0.55
1:K:73:U:O4	1:K:97:C:N3	2.39	0.55
2:C:310:TRP:O	2:C:314:LYS:HB3	2.06	0.55
2:C:547:ILE:HD12	2:C:597:GLY:CA	2.37	0.55
2:D:249:LYS:HB3	2:D:249:LYS:HZ3	1.68	0.55
2:E:386:ILE:HG21	2:E:396:GLU:HG3	1.89	0.55
2:E:472:ASP:OD1	2:E:476:ARG:HB2	2.06	0.55
2:G:309:HIS:HB3	2:G:317:MET:CE	2.36	0.55
2:G:411:PHE:CE2	2:G:521:PHE:HE1	2.24	0.55
2:A:310:TRP:O	2:A:314:LYS:HB3	2.06	0.55
2:A:578:ILE:HD11	2:A:595:VAL:CG2	2.36	0.55
2:B:556:ASN:HD21	2:B:573:LEU:HD11	1.72	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:G:422:THR:HB	2:G:438:GLU:OE2	2.06	0.55
2:H:397:VAL:O	2:H:400:CYS:HB2	2.07	0.55
2:H:443:VAL:O	2:H:447:GLU:HB2	2.05	0.55
1:K:97:C:C4'	1:K:98:A:OP1	2.55	0.55
1:M:93:U:H2'	1:M:94:C:H6	1.71	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:B:606:VAL:O	2:B:618:SER:HA	2.06	0.55
2:E:259:GLU:H	2:E:259:GLU:CD	2.08	0.55
2:F:546:ASN:OD1	2:F:573:LEU:HA	2.06	0.55
2:G:416:ILE:O	2:G:416:ILE:HG22	2.06	0.55
2:H:312:ASN:O	2:H:313:TYR:HB2	2.06	0.55
1:J:97:C:C5'	1:J:98:A:OP1	2.54	0.55
1:K:83:U:C2'	1:K:84:U:H5'	2.36	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
2:F:620:ASP:O	2:F:624:VAL:HG13	2.06	0.55
2:G:254:TYR:CD2	2:G:255:HIS:N	2.74	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:265:PHE:CE1	2:D:296:PRO:HG2	2.41	0.55
2:E:417:VAL:CG1	2:E:471:TYR:CE1	2.89	0.55
2:F:417:VAL:CG1	2:F:471:TYR:CE1	2.89	0.55
2:F:556:ASN:ND2	2:F:573:LEU:HD11	2.22	0.55
2:G:329:ILE:N	2:G:329:ILE:CD1	2.70	0.55
2:G:569:VAL:HG22	2:G:570:LYS:N	2.21	0.55
1:K:90:G:C8	2:C:577:LYS:CD	2.87	0.55
2:B:365:GLU:H	2:B:377:ARG:HD3	1.72	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
2:C:609:ARG:HG3	2:C:609:ARG:O	2.07	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:H:544:ILE:HG22	2:H:555:VAL:HG13	1.88	0.55
1:J:72:G:H2'	1:J:73:U:H6	1.72	0.55
1:K:83:U:O2'	1:K:84:U:H5'	2.07	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
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
2:E:339:GLN:HB3	2:F:257:GLN:OE1	2.06	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
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:D:304:TRP:CZ3	2:D:328:CYS:HB2	2.43	0.54
2:D:388:CYS:HB2	2:D:392:GLN:OE1	2.06	0.54
2:G:259:GLU:CD	2:G:259:GLU:H	2.11	0.54
2:G:627:LYS:HB3	2:G:640:LEU:HD21	1.89	0.54
1:M:97:C:C5'	1:M:98:A:OP1	2.52	0.54
2:C:334:CYS:N	2:C:335:PRO:HD2	2.22	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:F:547:ILE:HD12	2:F:597:GLY:CA	2.36	0.54
2:G:407:MET:CE	2:G:407:MET:CG	2.85	0.54
2:H:303:LEU:HD11	2:H:339:GLN:HE21	1.72	0.54
2:H:338:VAL:HG11	2:H:493:LEU:HB2	1.89	0.54
2:H:393:ILE:HD11	2:H:508:VAL:HG11	1.89	0.54
2:H:554:TYR:O	2:H:557:GLU:HB3	2.06	0.54
2:A:546:ASN:OD1	2:A:573:LEU:HA	2.08	0.54
2:B:441:LEU:O	2:B:444:ALA:HB3	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:D:417:VAL:CG1	2:D:471:TYR:CE1	2.91	0.54
2:E:263:MET:HE2	2:F:298:MET:HG2	1.89	0.54
2:E:638:LYS:HB2	2:E:642:GLU:HG3	1.89	0.54
2:F:597:GLY:O	2:F:601:VAL:HG23	2.06	0.54
2:F:638:LYS:HB2	2:F:642:GLU:HG3	1.90	0.54
2:G:257:GLN:HB3	2:G:259:GLU:OE2	2.07	0.54
2:G:484:GLN:HB2	2:G:511:HIS:HB2	1.88	0.54
2:H:334:CYS:N	2:H:335:PRO:HD2	2.23	0.54
2:A:341:PHE:O	2:A:346:LYS:NZ	2.38	0.54
2:A:526:THR:HG23	2:A:533:PHE:HZ	1.72	0.54
2:A:578:ILE:HD11	2:A:595:VAL:HG22	1.88	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:E:365:GLU:H	2:E:377:ARG:HD3	1.71	0.54
2:E:386:ILE:HG21	2:E:396:GLU:CG	2.38	0.54
2:F:536:TRP:CE3	2:F:635:ARG:HD3	2.43	0.54
2:G:335:PRO:HG2	2:G:336:GLY:H	1.72	0.54
2:H:460:ALA:HB1	2:H:462:TYR:CD1	2.42	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:D:325:ARG:HG3	2:D:325:ARG:NH1	2.22	0.54
2:G:383:ASP:OD2	2:G:385:HIS:CE1	2.60	0.54
1:K:101:G:H2'	1:K:102:C:C6	2.41	0.54
2:A:312:ASN:O	2:A:313:TYR:HB2	2.06	0.54
2:A:351:LEU:HD22	2:A:387:PHE:O	2.07	0.54
2:B:284:LYS:HG3	2:B:407:MET:HG3	1.90	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:C:331:PRO:O	2:C:361:CYS:HB3	2.07	0.54
2:D:610:THR:HG21	2:D:614:LYS:HB3	1.90	0.54
2:F:556:ASN:HD21	2:F:573:LEU:HD11	1.73	0.54
2:G:278:GLU:HB3	2:G:358:PHE:HE2	1.72	0.54
2:G:422:THR:O	2:G:458:GLU:O	2.25	0.54
2:H:284:LYS:HG3	2:H:407:MET:HG3	1.90	0.54
2:H:434:TRP:O	2:H:438:GLU:HG3	2.08	0.54
2:A:288:TYR:N	2:A:288:TYR:CD1	2.76	0.54
2:C:332:MET:HG2	2:C:363:ARG:HH21	1.72	0.54
2:C:391:GLU:N	2:C:391:GLU:OE1	2.40	0.54
2:C:610:THR:CG2	2:C:614:LYS:HB3	2.38	0.54
2:D:290:TYR:CE2	2:D:512:ARG:NH1	2.75	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:606:VAL:O	2:E:618:SER:HA	2.08	0.54
2:F:539:PRO:O	2:F:568:ARG:HD2	2.07	0.54
2:F:557:GLU:O	2:F:560:GLN:HB3	2.08	0.54
2:B:273:ILE:HG23	2:B:537:LEU:HD22	1.90	0.54
2:E:330:LYS:O	5:E:6011:HOH:O	2.18	0.54
2:E:423:ARG:HA	2:E:434:TRP:CZ3	2.42	0.54
2:F:441:LEU:HD12	2:F:464:PRO:HB2	1.89	0.54
2:H:462:TYR:CE2	2:H:511:HIS:CE1	2.96	0.54
1:K:83:U:H1'	1:K:90:G:C6	2.43	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:A:544:ILE:HG12	2:A:594:LEU:HD12	1.89	0.54
2:A:627:LYS:HB3	2:A:640:LEU:HD21	1.90	0.54
2:B:423:ARG:HD2	2:B:438:GLU:OE2	2.07	0.54
2:C:585:HIS:HB2	2:C:593:MET:HE1	1.88	0.54
2:D:411:PHE:HE2	2:D:521:PHE:CZ	2.10	0.54
2:D:421:SER:HB3	2:D:458:GLU:C	2.28	0.54
2:D:536:TRP:CE3	2:D:635:ARG:HD3	2.43	0.54
2:E:362:HIS:HD2	5:E:6011:HOH:O	1.91	0.54
2:F:335:PRO:HG2	2:F:336:GLY:H	1.72	0.54
2:G:365:GLU:N	2:G:377:ARG:HD3	2.21	0.54
2:G:465:LYS:HG3	2:G:484:GLN:HG2	1.90	0.54
2:G:578:ILE:HD11	2:G:595:VAL:HG22	1.90	0.54
2:H:274:PHE:CE1	2:H:518:MET:HG3	2.43	0.54
1:J:75:U:O2'	1:J:89:U:O4	2.24	0.54
2:A:411:PHE:CE2	2:A:521:PHE:CZ	2.96	0.54
2:A:542:VAL:HG12	2:A:543:VAL:N	2.23	0.54
2:B:620:ASP:O	2:B:623:GLU:HB3	2.08	0.54
2:D:273:ILE:HG23	2:D:537:LEU:CD2	2.38	0.54
2:E:325:ARG:HH11	2:E:325:ARG:HG3	1.73	0.54
2:E:484:GLN:HB2	2:E:511:HIS:HB2	1.90	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:G:380:THR:N	2:G:519:GLU:OE2	2.41	0.54
2:H:578:ILE:HD11	2:H:595:VAL:HG22	1.90	0.54
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:284:LYS:HG3	2:E:407:MET:HG3	1.88	0.53
2:E:332:MET:HG2	2:E:363:ARG:HH21	1.72	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:E:604:GLY:O	2:E:621:VAL:HG23	2.09	0.53
2:H:335:PRO:HG2	2:H:336:GLY:H	1.73	0.53
2:H:461:PHE:C	2:H:461:PHE:CD1	2.81	0.53
1:O:75:U:O2'	1:O:89:U:O4	2.25	0.53
2:A:585:HIS:HB2	2:A:593:MET:HE1	1.90	0.53
2:A:622:ASN:O	2:A:626:GLU:HG3	2.07	0.53
2:D:338:VAL:HG11	2:D:493:LEU:HB2	1.89	0.53
2:E:281:VAL:HG12	2:E:285:LEU:HD12	1.91	0.53
2:F:310:TRP:O	2:F:314:LYS:HB3	2.08	0.53
2:G:400:CYS:SG	2:G:512:ARG:HG3	2.48	0.53
2:H:423:ARG:HA	2:H:434:TRP:CZ3	2.44	0.53
2:H:460:ALA:HB1	2:H:462:TYR:CE1	2.43	0.53
2:H:606:VAL:O	2:H:618:SER:HA	2.08	0.53
1:I:86:G:C2'	5:I:109:HOH:O	2.45	0.53
2:G:422:THR:OG1	2:G:456:LEU:HA	2.08	0.53
1:M:89:U:C6	2:E:583:ARG:CZ	2.92	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:A:583:ARG:O	2:A:587:LEU:CD2	2.55	0.53
2:B:338:VAL:HG11	2:B:493:LEU:HB2	1.91	0.53
2:B:422:THR:OG1	2:B:456:LEU:HA	2.09	0.53
2:B:637:LEU:HD12	2:B:637:LEU:N	2.22	0.53
2:C:325:ARG:HG3	2:C:325:ARG:NH1	2.23	0.53
2:D:473:CYS:HB2	2:D:527:GLU:OE1	2.09	0.53
2:E:624:VAL:CG2	2:E:625:ILE:N	2.72	0.53
2:F:572:ASP:OD2	2:F:574:ARG:NH2	2.31	0.53
2:G:278:GLU:CB	2:G:358:PHE:HE2	2.22	0.53
1:O:80:U:H2'	1:O:81:C:C6	2.44	0.53
1:P:86:G:O6	2:H:599:LYS:HB2	2.09	0.53
1:P:103:G:H5"	5:P:1625:HOH:O	2.08	0.53
2:B:375:ARG:NH1	5:B:210:HOH:O	2.35	0.53
2:B:386:ILE:HG21	2:B:396:GLU:HG3	1.90	0.53
2:C:559:THR:HG21	2:C:571:ALA:CB	2.20	0.53
2:C:600:GLU:HB3	2:C:605:LYS:O	2.09	0.53
2:C:638:LYS:HB2	2:C:642:GLU:HG3	1.90	0.53
2:F:325:ARG:HG3	2:F:325:ARG:NH1	2.23	0.53
2:F:403:LEU:O	2:F:407:MET:HB2	2.08	0.53
2:G:547:ILE:HD12	2:G:597:GLY:CA	2.37	0.53
2:H:348:TYR:CD1	2:H:348:TYR:C	2.82	0.53
2:H:422:THR:O	2:H:458:GLU:O	2.26	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:622:ASN:ND2	5:H:826:HOH:O	2.36	0.53
1:I:88:G:H1'	2:A:583:ARG:HG2	1.90	0.53
1:K:84:U:H4'	1:K:85:C:O5'	2.09	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:B:620:ASP:O	2:B:624:VAL:HG13	2.08	0.53
2:D:556:ASN:ND2	2:D:573:LEU:HD11	2.23	0.53
2:E:620:ASP:O	2:E:623:GLU:HB3	2.08	0.53
2:F:339:GLN:HA	2:F:339:GLN:OE1	2.08	0.53
2:F:410:THR:C	2:F:411:PHE:HD1	2.12	0.53
2:F:555:VAL:HB	2:F:573:LEU:HD21	1.89	0.53
2:G:301:ARG:O	2:G:305:GLU:HG3	2.08	0.53
2:H:624:VAL:CG2	2:H:625:ILE:N	2.71	0.53
2:H:637:LEU:HD12	2:H:637:LEU:N	2.22	0.53
1:K:98:A:C6	2:D:345:LEU:HB2	2.42	0.53
1:P:77:U:H6	1:P:77:U:O5'	1.92	0.53
2:A:620:ASP:O	2:A:624:VAL:HG13	2.08	0.53
2:B:288:TYR:N	2:B:288:TYR:HD1	2.07	0.53
2:B:550:SER:C	2:B:552:SER:H	2.12	0.53
2:C:539:PRO:O	2:C:568:ARG:HD2	2.08	0.53
2:F:288:TYR:N	2:F:288:TYR:CD1	2.77	0.53
2:A:356:ALA:HA	2:A:384:ALA:HA	1.91	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:CD1	2.77	0.53
2:D:288:TYR:N	2:D:288:TYR:HD1	2.06	0.53
2:E:600:GLU:HB3	2:E:605:LYS:O	2.09	0.53
2:H:278:GLU:CB	2:H:358:PHE:HE2	2.22	0.53
2:A:339:GLN:OE1	2:A:339:GLN:HA	2.09	0.53
2:B:472:ASP:OD1	2:B:476:ARG:HB2	2.09	0.53
2:D:329:ILE:HD12	2:D:329:ILE:N	2.24	0.53
2:E:334:CYS:N	2:E:335:PRO:HD2	2.24	0.53
2:E:421:SER:HB3	2:E:458:GLU:C	2.28	0.53
2:H:329:ILE:HD12	2:H:329:ILE:N	2.24	0.53
1:M:69:G:OP2	1:P:105:C:H2'	2.09	0.53
2:A:254:TYR:CZ	2:A:373:LEU:HD21	2.44	0.53
2:A:338:VAL:HG11	2:A:493:LEU:HB2	1.91	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:B:281:VAL:HG12	2:B:285:LEU:HD12	1.90	0.53
2:B:288:TYR:N	2:B:288:TYR:CD1	2.76	0.53
2:B:298:MET:HE2	2:B:327:TYR:CD1	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:259:GLU:H	2:C:259:GLU:CD	2.12	0.53
2:C:284:LYS:HG3	2:C:407:MET:HG3	1.90	0.53
2:C:403:LEU:O	2:C:407:MET:HB2	2.08	0.53
2:D:259:GLU:CD	2:D:259:GLU:H	2.10	0.53
2:G:243:ASP:OD2	2:G:245:ARG:HB2	2.08	0.53
2:H:627:LYS:HB3	2:H:640:LEU:HD21	1.89	0.53
1:P:75:U:O2'	1:P:89:U:O4	2.26	0.52
1:P:80:U:H2'	1:P:81:C:C6	2.44	0.52
2:A:334:CYS:N	2:A:335:PRO:HD2	2.24	0.52
2:C:423:ARG:HD2	2:C:438:GLU:OE2	2.08	0.52
2:D:281:VAL:HG12	2:D:285:LEU:HD12	1.91	0.52
2:E:288:TYR:CD1	2:E:288:TYR:N	2.77	0.52
2:F:421:SER:HB3	2:F:458:GLU:C	2.30	0.52
2:G:462:TYR:CE2	2:G:511:HIS:CE1	2.96	0.52
2:H:247:ILE:O	2:H:250:GLN:HB2	2.09	0.52
2:H:375:ARG:NH2	5:H:810:HOH:O	2.17	0.52
1:O:93:U:C2	1:O:94:C:C5	2.97	0.52
2:A:288:TYR:N	2:A:288:TYR:HD1	2.07	0.52
2:A:362:HIS:CE1	2:B:297:PHE:CG	2.97	0.52
2:A:416:ILE:O	2:A:416:ILE:HG22	2.09	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:D:301:ARG:O	2:D:305:GLU:HG3	2.09	0.52
2:D:536:TRP:O	2:D:568:ARG:NH2	2.42	0.52
2:D:556:ASN:HD21	2:D:573:LEU:HD11	1.74	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:F:423:ARG:O	2:F:423:ARG:HG2	2.10	0.52
2:G:418:VAL:HG21	2:G:450:ILE:HG21	1.90	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:C:288:TYR:N	2:C:288:TYR:CD1	2.78	0.52
2:C:422:THR:O	2:C:458:GLU:O	2.27	0.52
2:D:622:ASN:O	2:D:626:GLU:HG3	2.09	0.52
2:E:288:TYR:N	2:E:288:TYR:HD1	2.07	0.52
2:E:332:MET:HE2	4:E:6002:TSB:HN12	1.74	0.52
2:E:543:VAL:HG11	2:E:585:HIS:CE1	2.44	0.52
2:F:331:PRO:O	2:F:361:CYS:HB3	2.09	0.52
2:F:473:CYS:HB2	2:F:527:GLU:OE1	2.08	0.52
2:G:460:ALA:C	2:G:462:TYR:H	2.13	0.52
2:G:535:THR:HG22	2:G:632:ILE:HG12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:578:ILE:HD11	2:H:595:VAL:CG2	2.38	0.52
2:H:580:PHE:CD1	2:H:580:PHE:C	2.82	0.52
1:N:86:G:H1'	2:F:547:ILE:HG21	1.92	0.52
2:A:529:PHE:CD2	2:A:534:PRO:HD3	2.45	0.52
2:B:587:LEU:HD23	2:B:587:LEU:N	2.19	0.52
2:F:329:ILE:HD12	2:F:329:ILE:N	2.25	0.52
1:L:100:U:H4'	5:L:1230:HOH:O	2.08	0.52
1:M:93:U:C2	1:M:94:C:C6	2.97	0.52
2:A:254:TYR:CD2	2:A:255:HIS:N	2.77	0.52
2:A:500:GLU:OE1	2:A:500:GLU:N	2.41	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:C:622:ASN:O	2:C:626:GLU:HG3	2.10	0.52
2:E:557:GLU:O	2:E:560:GLN:HB3	2.09	0.52
2:E:569:VAL:HG22	2:E:570:LYS:N	2.25	0.52
2:G:284:LYS:HG3	2:G:407:MET:HG3	1.91	0.52
2:G:348:TYR:CD1	2:G:348:TYR:C	2.82	0.52
2:G:386:ILE:HG21	2:G:396:GLU:CG	2.39	0.52
1:J:87:U:H3'	5:J:1019:HOH:O	2.10	0.52
1:P:88:G:P	5:P:1623:HOH:O	2.66	0.52
2:C:462:TYR:HD2	2:C:486:ASP:OD2	1.93	0.52
2:D:386:ILE:HG21	2:D:396:GLU:HG3	1.90	0.52
2:D:536:TRP:CZ3	2:D:635:ARG:HD3	2.44	0.52
2:G:313:TYR:HB3	2:G:317:MET:HE1	1.91	0.52
2:H:282:ARG:HD3	2:H:292:GLU:OE1	2.10	0.52
2:H:557:GLU:O	2:H:560:GLN:HB3	2.09	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:A:569:VAL:HG22	2:A:570:LYS:N	2.25	0.52
2:C:536:TRP:CE3	2:C:635:ARG:HD3	2.44	0.52
2:C:544:ILE:HG12	2:C:594:LEU:HD12	1.91	0.52
2:C:597:GLY:O	2:C:601:VAL:HG23	2.08	0.52
2:D:365:GLU:H	2:D:377:ARG:HD3	1.73	0.52
2:D:543:VAL:HG11	2:D:585:HIS:CE1	2.44	0.52
2:F:259:GLU:CD	2:F:259:GLU:H	2.12	0.52
2:F:536:TRP:CZ3	2:F:635:ARG:HD3	2.44	0.52
2:F:578:ILE:HD11	2:F:595:VAL:CG2	2.40	0.52
2:G:580:PHE:C	2:G:580:PHE:CD1	2.81	0.52
2:G:637:LEU:HD12	2:G:637:LEU:N	2.24	0.52
2:H:544:ILE:HG12	2:H:594:LEU:HD12	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:93:U:C2	1:O:94:C:C6	2.98	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:B:636:SER:OG	2:B:638:LYS:HD3	2.10	0.52
2:C:606:VAL:O	2:C:618:SER:HA	2.10	0.52
2:C:620:ASP:HB3	2:C:623:GLU:CB	2.40	0.52
2:D:638:LYS:HB2	2:D:642:GLU:HG3	1.91	0.52
2:E:329:ILE:N	2:E:329:ILE:HD12	2.25	0.52
2:E:556:ASN:ND2	2:E:573:LEU:HD11	2.25	0.52
2:G:386:ILE:HG21	2:G:396:GLU:HG3	1.92	0.52
2:H:421:SER:HB3	2:H:458:GLU:C	2.31	0.52
2:D:620:ASP:O	2:D:623:GLU:HB3	2.10	0.52
2:E:544:ILE:HG22	2:E:555:VAL:HG13	1.91	0.52
2:F:288:TYR:N	2:F:288:TYR:HD1	2.07	0.52
2:F:624:VAL:CG2	2:F:625:ILE:N	2.73	0.52
2:G:375:ARG:NH1	5:G:710:HOH:O	2.32	0.52
1:K:78:G:H2'	1:K:79:A:C8	2.42	0.51
2:C:421:SER:HB3	2:C:458:GLU:C	2.31	0.51
2:D:544:ILE:HG12	2:D:594:LEU:HD12	1.91	0.51
2:D:636:SER:OG	2:D:638:LYS:HD3	2.10	0.51
2:E:610:THR:HG21	2:E:614:LYS:HB3	1.92	0.51
2:F:628:LEU:O	2:F:632:ILE:HG13	2.10	0.51
2:G:443:VAL:O	2:G:447:GLU:HB2	2.09	0.51
1:O:89:U:H2'	1:O:90:G:OP1	2.10	0.51
2:A:362:HIS:HE1	2:B:297:PHE:CG	2.28	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:C:309:HIS:HB3	2:C:317:MET:CE	2.39	0.51
2:D:418:VAL:HG21	2:D:450:ILE:CG2	2.39	0.51
2:D:423:ARG:HD2	2:D:438:GLU:OE2	2.11	0.51
2:D:624:VAL:CG2	2:D:625:ILE:N	2.72	0.51
2:E:290:TYR:CE2	2:E:512:ARG:NH1	2.78	0.51
2:E:462:TYR:HD2	2:E:486:ASP:OD2	1.92	0.51
2:F:278:GLU:HG2	2:F:518:MET:HE2	1.93	0.51
2:F:622:ASN:O	2:F:626:GLU:HG3	2.09	0.51
2:G:578:ILE:HD11	2:G:595:VAL:CG2	2.39	0.51
2:H:273:ILE:HG23	2:H:537:LEU:HD22	1.91	0.51
2:A:280:PHE:CE2	2:A:407:MET:HG2	2.44	0.51
2:A:559:THR:HG21	2:A:571:ALA:CB	2.19	0.51
2:C:278:GLU:CB	2:C:358:PHE:HE2	2.22	0.51
2:D:285:LEU:HD22	2:D:290:TYR:CG	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:555:VAL:HB	2:D:573:LEU:HD21	1.91	0.51
2:E:304:TRP:CE3	2:E:328:CYS:HB2	2.45	0.51
2:G:620:ASP:O	2:G:624:VAL:HG13	2.10	0.51
1:N:89:U:HO2'	2:F:580:PHE:CB	2.23	0.51
2:B:557:GLU:O	2:B:560:GLN:HB3	2.10	0.51
2:D:514:ILE:HG22	2:D:515:LEU:HD23	1.92	0.51
2:E:296:PRO:HG2	2:F:265:PHE:CE1	2.45	0.51
2:E:418:VAL:HG21	2:E:450:ILE:CG2	2.40	0.51
2:E:482:THR:HG21	4:E:6002:TSB:H5'2	1.92	0.51
2:G:515:LEU:HD22	2:G:521:PHE:CE2	2.46	0.51
2:H:636:SER:OG	2:H:638:LYS:HD3	2.11	0.51
1:I:89:U:C6	2:A:583:ARG:CZ	2.93	0.51
2:A:331:PRO:O	2:A:361:CYS:HB3	2.09	0.51
2:A:339:GLN:HB3	2:B:257:GLN:OE1	2.11	0.51
2:A:624:VAL:CG2	2:A:625:ILE:N	2.72	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:E:547:ILE:HD12	2:E:597:GLY:CA	2.41	0.51
2:F:287:GLU:HB2	2:F:288:TYR:HD1	1.75	0.51
2:G:338:VAL:HG11	2:G:493:LEU:HB2	1.92	0.51
2:G:606:VAL:O	2:G:618:SER:HA	2.11	0.51
2:H:301:ARG:O	2:H:305:GLU:HG3	2.09	0.51
1:I:84:U:O2'	1:I:85:C:OP2	2.28	0.51
1:J:95:A:H2'	1:J:96:C:C6	2.46	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
2:B:247:ILE:O	2:B:250:GLN:HB2	2.11	0.51
2:D:443:VAL:O	2:D:447:GLU:HB2	2.10	0.51
2:E:620:ASP:HB3	2:E:623:GLU:CB	2.41	0.51
2:F:620:ASP:O	2:F:623:GLU:HB3	2.11	0.51
2:H:313:TYR:HB3	2:H:317:MET:HE1	1.92	0.51
1:M:80:U:H2'	1:M:81:C:H6	1.75	0.51
2:B:543:VAL:HG11	2:B:585:HIS:CE1	2.46	0.51
2:B:562:LEU:HD12	2:B:625:ILE:HD11	1.93	0.51
2:C:280:PHE:O	2:C:283:SER:HB3	2.09	0.51
2:C:297:PHE:CD1	2:D:362:HIS:HE1	2.28	0.51
2:C:462:TYR:HE2	2:C:511:HIS:NE2	2.09	0.51
2:C:578:ILE:HD11	2:C:595:VAL:CG2	2.41	0.51
2:G:461:PHE:CD1	2:G:461:PHE:C	2.84	0.51
2:G:622:ASN:O	2:G:626:GLU:HG3	2.10	0.51
2:H:251:LEU:O	2:H:253:LEU:HD23	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:75:U:O2'	1:I:89:U:O4	2.28	0.51
2:A:421:SER:CA	2:A:455:GLN:HB3	2.40	0.51
2:B:452:PHE:CE2	2:B:454:TYR:HE1	2.20	0.51
2:C:304:TRP:CZ3	2:C:328:CYS:HB2	2.46	0.51
2:C:410:THR:C	2:C:411:PHE:HD1	2.13	0.51
2:D:462:TYR:HD2	2:D:486:ASP:OD2	1.93	0.51
2:F:610:THR:HG21	2:F:614:LYS:HB3	1.93	0.51
2:A:423:ARG:O	2:A:423:ARG:HG2	2.10	0.51
2:C:290:TYR:CE2	2:C:512:ARG:NH1	2.79	0.51
2:D:526:THR:HG23	2:D:533:PHE:HZ	1.75	0.51
2:D:604:GLY:O	2:D:621:VAL:HG23	2.10	0.51
2:G:638:LYS:HB2	2:G:642:GLU:HG3	1.93	0.51
2:H:555:VAL:HB	2:H:573:LEU:HD21	1.92	0.51
2:A:637:LEU:HD12	2:A:637:LEU:N	2.23	0.51
2:C:624:VAL:CG2	2:C:625:ILE:N	2.74	0.51
2:C:636:SER:OG	2:C:638:LYS:HD3	2.11	0.51
2:D:452:PHE:HE2	2:D:454:TYR:CE1	2.22	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:G:580:PHE:HD1	2:G:580:PHE:C	2.14	0.51
2:H:638:LYS:HB2	2:H:642:GLU:HG3	1.92	0.51
1:M:86:G:O6	2:E:599:LYS:CB	2.59	0.50
2:B:332:MET:HE2	4:B:3002:TSB:HN12	1.75	0.50
2:C:249:LYS:HB3	2:C:249:LYS:HZ3	1.74	0.50
2:C:257:GLN:OE1	2:D:339:GLN:HB3	2.10	0.50
2:D:278:GLU:CB	2:D:358:PHE:HE2	2.24	0.50
2:D:580:PHE:C	2:D:580:PHE:CD1	2.84	0.50
2:E:351:LEU:HD22	2:E:387:PHE:O	2.10	0.50
2:E:578:ILE:HD11	2:E:595:VAL:HG22	1.93	0.50
2:F:301:ARG:O	2:F:305:GLU:HG3	2.10	0.50
2:G:421:SER:HB3	2:G:458:GLU:C	2.31	0.50
2:H:620:ASP:O	2:H:624:VAL:HG13	2.11	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:E:461:PHE:C	2:E:461:PHE:CD1	2.85	0.50
2:F:332:MET:HE2	4:F:7002:TSB:HN12	1.76	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:A:609:ARG:HG3	2:A:609:ARG:O	2.11	0.50
2:C:329:ILE:HD12	2:C:329:ILE:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:529:PHE:CD2	2:C:534:PRO:HD3	2.47	0.50
2:C:547:ILE:HG12	2:C:578:ILE:HD12	1.92	0.50
2:D:341:PHE:O	2:D:346:LYS:NZ	2.38	0.50
2:E:305:GLU:HA	2:E:310:TRP:HB3	1.94	0.50
2:F:461:PHE:CD1	2:F:461:PHE:C	2.83	0.50
2:G:636:SER:OG	2:G:638:LYS:HD3	2.11	0.50
1:J:105:C:H2'	1:O:69:G:O4'	2.12	0.50
1:K:104:C:H2'	1:K:105:C:C4'	2.42	0.50
2:B:335:PRO:HG2	2:B:336:GLY:H	1.76	0.50
2:C:557:GLU:O	2:C:560:GLN:HB3	2.11	0.50
2:C:580:PHE:CD1	2:C:580:PHE:C	2.84	0.50
2:D:578:ILE:HD11	2:D:595:VAL:HG22	1.93	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
2:F:462:TYR:CD2	2:F:486:ASP:OD2	2.64	0.50
2:H:331:PRO:O	2:H:361:CYS:HB3	2.12	0.50
1:P:78:G:O2'	1:P:79:A:H5'	2.12	0.50
2:A:411:PHE:HE2	2:A:521:PHE:CE1	2.17	0.50
2:A:418:VAL:HG21	2:A:450:ILE:HG21	1.93	0.50
2:B:422:THR:O	2:B:423:ARG:C	2.50	0.50
2:C:441:LEU:HD12	2:C:464:PRO:HB2	1.93	0.50
2:E:280:PHE:O	2:E:283:SER:HB3	2.11	0.50
2:E:580:PHE:HD1	2:E:580:PHE:C	2.15	0.50
2:F:529:PHE:H	2:F:529:PHE:HD1	1.58	0.50
2:F:551:GLN:HG2	2:F:597:GLY:C	2.32	0.50
2:H:342:ASN:HD21	2:H:495:ALA:HA	1.75	0.50
2:H:548:THR:HG23	2:H:551:GLN:OE1	2.12	0.50
2:B:417:VAL:CG1	2:B:471:TYR:CE1	2.94	0.50
2:C:288:TYR:N	2:C:288:TYR:HD1	2.08	0.50
2:C:473:CYS:HB2	2:C:527:GLU:OE1	2.12	0.50
2:D:637:LEU:HD12	2:D:637:LEU:N	2.23	0.50
2:E:325:ARG:NH2	2:F:258:GLU:O	2.45	0.50
2:E:331:PRO:O	2:E:361:CYS:HB3	2.12	0.50
2:F:411:PHE:CE2	2:F:521:PHE:HZ	2.27	0.50
2:F:544:ILE:HG12	2:F:594:LEU:HD12	1.92	0.50
2:F:580:PHE:CD1	2:F:580:PHE:C	2.83	0.50
2:G:460:ALA:C	2:G:462:TYR:N	2.65	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
1:K:85:C:C2	2:C:577:LYS:HG3	2.46	0.50
2:A:278:GLU:HG2	2:A:518:MET:HE2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:297:PHE:CG	2:B:362:HIS:CE1	3.00	0.50
2:A:329:ILE:N	2:A:329:ILE:CD1	2.75	0.50
2:B:243:ASP:O	2:B:247:ILE:HG13	2.12	0.50
2:B:362:HIS:HD2	5:B:232:HOH:O	1.94	0.50
2:B:600:GLU:HB3	2:B:605:LYS:O	2.11	0.50
2:C:434:TRP:O	2:C:438:GLU:HG3	2.11	0.50
2:D:397:VAL:O	2:D:401:ILE:HG12	2.12	0.50
1:I:89:U:C5	2:A:583:ARG:CZ	2.95	0.50
1:O:92:G:H2'	1:O:93:U:H6	1.76	0.50
2:B:285:LEU:HD22	2:B:290:TYR:CG	2.47	0.50
2:B:536:TRP:CE3	2:B:635:ARG:HD3	2.47	0.50
2:B:569:VAL:HG22	2:B:570:LYS:N	2.26	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:D:304:TRP:CE3	2:D:328:CYS:HB2	2.46	0.50
2:D:500:GLU:OE1	2:D:500:GLU:N	2.44	0.50
2:E:273:ILE:HG23	2:E:537:LEU:CD2	2.41	0.50
2:H:620:ASP:HB3	2:H:623:GLU:CB	2.42	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:B:578:ILE:HD11	2:B:595:VAL:HG22	1.94	0.50
2:C:445:LEU:HD21	2:C:466:ILE:HG12	1.94	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:F:624:VAL:HG23	2:F:625:ILE:N	2.27	0.50
2:H:624:VAL:HG23	2:H:625:ILE:N	2.26	0.50
1:N:89:U:O3'	2:F:577:LYS:NZ	2.44	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:C:461:PHE:CD1	2:C:461:PHE:C	2.86	0.49
2:C:484:GLN:HB2	2:C:511:HIS:HB2	1.94	0.49
2:D:578:ILE:HD11	2:D:595:VAL:CG2	2.42	0.49
2:E:514:ILE:HG22	2:E:515:LEU:HD23	1.93	0.49
2:E:536:TRP:CE3	2:E:635:ARG:HD3	2.47	0.49
2:E:637:LEU:HD12	2:E:637:LEU:N	2.26	0.49
2:F:247:ILE:O	2:F:250:GLN:HB2	2.11	0.49
1:L:80:U:H2'	1:L:81:C:C6	2.47	0.49
2:B:249:LYS:HB3	2:B:249:LYS:HZ3	1.77	0.49
2:B:393:ILE:HD11	2:B:508:VAL:HG11	1.94	0.49
2:C:348:TYR:CD1	2:C:348:TYR:C	2.84	0.49
2:D:461:PHE:CD1	2:D:461:PHE:C	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:483:VAL:HG22	2:F:512:ARG:HB2	1.94	0.49
2:G:280:PHE:CZ	2:G:407:MET:HG2	2.47	0.49
2:G:472:ASP:OD1	2:G:476:ARG:HB2	2.12	0.49
2:G:536:TRP:CZ3	2:G:635:ARG:HD3	2.47	0.49
2:G:620:ASP:HB3	2:G:623:GLU:CB	2.42	0.49
2:H:356:ALA:HA	2:H:384:ALA:HA	1.93	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
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
2:F:542:VAL:HG12	2:F:543:VAL:N	2.27	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
1:K:93:U:H2'	1:K:94:C:C6	2.46	0.49
2:A:473:CYS:HB2	2:A:527:GLU:OE1	2.12	0.49
2:C:393:ILE:HD11	2:C:508:VAL:HG11	1.95	0.49
2:C:480:CYS:O	2:C:516:GLY:HA3	2.12	0.49
2:D:557:GLU:O	2:D:560:GLN:HB3	2.12	0.49
2:E:624:VAL:HG23	2:E:625:ILE:N	2.27	0.49
2:F:402:ARG:NH1	2:F:402:ARG:CB	2.75	0.49
2:G:291:GLN:NE2	2:G:353:LEU:HD21	2.26	0.49
2:H:254:TYR:CZ	2:H:373:LEU:HD21	2.48	0.49
2:C:587:LEU:HD23	2:C:587:LEU:N	2.20	0.49
2:C:637:LEU:HD12	2:C:637:LEU:N	2.21	0.49
2:D:280:PHE:O	2:D:283:SER:HB3	2.12	0.49
2:D:313:TYR:HB3	2:D:317:MET:HE1	1.93	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: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:H:280:PHE:CZ	2:H:407:MET:HG2	2.48	0.49
2:H:291:GLN:NE2	2:H:353:LEU:HD21	2.28	0.49
2:A:305:GLU:HA	2:A:310:TRP:HB3	1.94	0.49
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:C:536:TRP:CZ3	2:C:635:ARG:HD3	2.47	0.49
2:D:423:ARG:HA	2:D:434:TRP:CZ3	2.47	0.49
2:D:620:ASP:HB3	2:D:623:GLU:CB	2.42	0.49
2:E:590:VAL:O	2:E:611:ARG:HB3	2.13	0.49
2:G:418:VAL:HG21	2:G:450:ILE:CG2	2.43	0.49
2:G:427:ARG:HB2	2:G:434:TRP:CZ2	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:J:84:U:O2'	1:J:85:C:OP2	2.31	0.49
2:A:263:MET:CE	2:B:298:MET:HG2	2.38	0.49
2:A:421:SER:HB3	2:A:458:GLU:C	2.32	0.49
2:B:415:LYS:HG2	2:B:471:TYR:CD1	2.48	0.49
2:C:243:ASP:O	2:C:247:ILE:HG13	2.13	0.49
2:D:600:GLU:HB3	2:D:605:LYS:O	2.12	0.49
2:D:624:VAL:HG23	2:D:625:ILE:N	2.27	0.49
2:F:416:ILE:O	2:F:416:ILE:HG22	2.10	0.49
2:F:578:ILE:HD11	2:F:595:VAL:HG22	1.93	0.49
2:B:329:ILE:N	2:B:329:ILE:HD12	2.27	0.49
2:B:460:ALA:C	2:B:462:TYR:H	2.16	0.49
2:B:590:VAL:O	2:B:611:ARG:HB3	2.12	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:F:580:PHE:HD1	2:F:580:PHE:C	2.16	0.49
2:F:620:ASP:HB3	2:F:623:GLU:CB	2.43	0.49
1:K:105:C:O2	1:K:105:C:C2'	2.60	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
2:A:297:PHE:CG	2:B:362:HIS:HE1	2.31	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: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:E:313:TYR:HB3	2:E:317:MET:HE1	1.95	0.49
2:E:609:ARG:O	2:E:609:ARG:HG3	2.13	0.49
2:G:621:VAL:HG12	2:G:622:ASN:N	2.28	0.49
2:H:580:PHE:HD1	2:H:580:PHE:C	2.15	0.49
2:H:610:THR:HG21	2:H:614:LYS:HB3	1.94	0.49
1:M:88:G:H8	5:E:6013:HOH:O	1.96	0.49
2:B:624:VAL:CG2	2:B:625:ILE:N	2.75	0.49
2:C:304:TRP:CE3	2:C:328:CYS:HB2	2.48	0.49
2:C:624:VAL:O	2:C:628:LEU:HG	2.12	0.49
2:D:309:HIS:HB3	2:D:317:MET:CE	2.43	0.49
2:F:282:ARG:HD3	2:F:292:GLU:OE1	2.13	0.49
1:I:86:G:P	1:I:86:G:O4'	2.71	0.48
2:A:277:LEU:O	2:A:280:PHE:HB3	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:421:SER:HB3	2:A:458:GLU:CB	2.30	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:C:529:PHE:H	2:C:529:PHE:HD1	1.58	0.48
2:D:597:GLY:O	2:D:601:VAL:HG23	2.12	0.48
2:F:313:TYR:HB3	2:F:317:MET:HE1	1.94	0.48
2:F:460:ALA:C	2:F:462:TYR:H	2.15	0.48
2:G:555:VAL:HB	2:G:573:LEU:HD21	1.94	0.48
2:H:330:LYS:HA	2:H:331:PRO:HD3	1.60	0.48
2:A:348:TYR:CD1	2:A:348:TYR:C	2.86	0.48
2:A:403:LEU:O	2:A:407:MET:HB2	2.12	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:D:609:ARG:HG3	2:D:609:ARG:O	2.13	0.48
2:E:500:GLU:OE1	2:E:500:GLU:N	2.43	0.48
2:F:500:GLU:OE1	2:F:500:GLU:N	2.42	0.48
2:F:512:ARG:NE	2:F:512:ARG:O	2.45	0.48
1:M:69:G:P	1:P:105:C:HO3'	2.31	0.48
1:O:87:U:C2'	1:O:88:G:OP2	2.60	0.48
2:A:624:VAL:HG23	2:A:625:ILE:N	2.26	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:C:462:TYR:CE2	2:C:511:HIS:NE2	2.81	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
2:E:274:PHE:CD1	2:E:274:PHE:C	2.86	0.48
2:E:285:LEU:HD22	2:E:290:TYR:CG	2.49	0.48
2:E:325:ARG:HG3	2:E:325:ARG:NH1	2.27	0.48
2:G:282:ARG:HD3	2:G:292:GLU:OE1	2.13	0.48
2:G:351:LEU:HD22	2:G:387:PHE:O	2.13	0.48
1:K:78:G:O2'	1:K:79:A:H5'	2.12	0.48
1:O:89:U:O3'	2:G:577:LYS:NZ	2.46	0.48
2:B:303:LEU:HD11	2:B:339:GLN:HE21	1.78	0.48
2:B:422:THR:O	2:B:458:GLU:O	2.31	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:D:462:TYR:HE2	2:D:511:HIS:CE1	2.31	0.48
2:E:278:GLU:CB	2:E:358:PHE:HE2	2.26	0.48
2:E:427:ARG:HB2	2:E:434:TRP:CZ2	2.49	0.48
2:E:597:GLY:O	2:E:601:VAL:HG23	2.14	0.48
2:F:491:SER:O	2:F:494:SER:N	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:251:LEU:O	2:G:253:LEU:HD23	2.14	0.48
2:G:462:TYR:HD2	2:G:486:ASP:OD2	1.97	0.48
2:G:500:GLU:OE1	2:G:500:GLU:N	2.44	0.48
2:H:253:LEU:HD23	2:H:253:LEU:N	2.29	0.48
2:H:351:LEU:HD22	2:H:387:PHE:O	2.13	0.48
2:H:386:ILE:HG21	2:H:396:GLU:HG3	1.95	0.48
2:H:423:ARG:O	2:H:423:ARG:HG2	2.13	0.48
1:N:89:U:O2'	2:F:580:PHE:HB2	2.13	0.48
1:P:86:G:C2'	5:P:1613:HOH:O	2.61	0.48
2:A:288:TYR:CZ	2:A:403:LEU:HD13	2.48	0.48
2:A:620:ASP:HB3	2:A:623:GLU:CB	2.43	0.48
2:B:365:GLU:OE1	2:B:365:GLU:HA	2.13	0.48
2:B:610:THR:HG21	2:B:614:LYS:HB3	1.96	0.48
2:C:320:THR:HG22	2:C:321:SER:N	2.22	0.48
2:C:628:LEU:O	2:C:632:ILE:HG13	2.13	0.48
2:D:331:PRO:O	2:D:361:CYS:HB3	2.14	0.48
2:E:636:SER:OG	2:E:638:LYS:HD3	2.11	0.48
2:F:348:TYR:CD1	2:F:348:TYR:C	2.86	0.48
2:H:480:CYS:O	2:H:516:GLY:HA3	2.13	0.48
1:J:93:U:H2'	1:J:94:C:H6	1.79	0.48
1:L:88:G:H1'	2:D:583:ARG:HG2	1.96	0.48
1:N:77:U:O5'	1:N:77:U:H6	1.96	0.48
1:N:84:U:H4'	1:N:85:C:H5'	1.96	0.48
2:A:319:THR:H	2:B:320:THR:CG2	2.26	0.48
2:A:580:PHE:HD1	2:A:580:PHE:C	2.16	0.48
2:A:597:GLY:O	2:A:601:VAL:HG23	2.13	0.48
2:A:610:THR:CG2	2:A:614:LYS:HB3	2.42	0.48
2:B:320:THR:HG22	2:B:321:SER:N	2.25	0.48
2:B:403:LEU:O	2:B:407:MET:HB2	2.14	0.48
2:B:461:PHE:C	2:B:461:PHE:CD1	2.86	0.48
2:B:536:TRP:CZ3	2:B:635:ARG:HD3	2.48	0.48
2:C:512:ARG:O	2:C:512:ARG:NE	2.44	0.48
2:E:265:PHE:CZ	2:F:296:PRO:HG2	2.48	0.48
2:E:362:HIS:CE1	2:F:297:PHE:CG	3.02	0.48
2:F:305:GLU:HA	2:F:310:TRP:HB3	1.94	0.48
2:F:411:PHE:CD2	2:F:521:PHE:CZ	3.01	0.48
2:F:418:VAL:HG21	2:F:450:ILE:CG2	2.44	0.48
2:G:280:PHE:O	2:G:283:SER:HB3	2.12	0.48
1:M:80:U:OP2	2:F:349:ARG:NH2	2.47	0.48
2:A:441:LEU:O	2:A:444:ALA:HB3	2.13	0.48
2:A:539:PRO:O	2:A:568:ARG:HD2	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:339:GLN:OE1	2:B:339:GLN:CA	2.60	0.48
2:C:400:CYS:SG	2:C:512:ARG:HG3	2.54	0.48
2:C:452:PHE:HE2	2:C:454:TYR:CE1	2.20	0.48
2:C:465:LYS:HG3	2:C:484:GLN:CG	2.42	0.48
2:C:604:GLY:O	2:C:621:VAL:HG23	2.13	0.48
2:D:254:TYR:HA	2:D:267:HIS:ND1	2.27	0.48
2:D:303:LEU:HD11	2:D:339:GLN:NE2	2.28	0.48
2:E:555:VAL:HB	2:E:573:LEU:HD21	1.95	0.48
2:F:545:MET:SD	2:F:582:ILE:HD13	2.54	0.48
2:G:362:HIS:CD2	5:G:732:HOH:O	2.56	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
1:I:88:G:C8	5:I:112:HOH:O	2.48	0.48
1:I:95:A:H2'	1:I:96:C:O4'	2.14	0.48
1:K:98:A:O2'	2:D:344:GLY:N	2.28	0.48
2:B:389:THR:HG1	2:B:392:GLN:HG3	1.74	0.48
2:B:580:PHE:CD1	2:B:580:PHE:C	2.85	0.48
2:C:254:TYR:HA	2:C:267:HIS:ND1	2.29	0.48
2:C:273:ILE:HG23	2:C:537:LEU:HD22	1.96	0.48
2:E:554:TYR:CE1	2:E:558:LEU:HD11	2.49	0.48
2:E:578:ILE:HD11	2:E:595:VAL:CG2	2.43	0.48
2:F:386:ILE:HG21	2:F:396:GLU:HG3	1.95	0.48
2:G:556:ASN:HD21	2:G:573:LEU:HD11	1.79	0.48
2:G:572:ASP:OD2	2:G:574:ARG:NH2	2.37	0.48
1:I:72:G:H2'	1:I:73:U:H6	1.78	0.48
1:K:79:A:N1	1:K:94:C:N3	2.62	0.48
1:M:69:G:C8	1:P:105:C:O2	2.67	0.48
1:O:95:A:H2'	1:O:96:C:O4'	2.14	0.48
2:A:335:PRO:HG2	2:A:336:GLY:H	1.79	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: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:E:515:LEU:HD22	2:E:521:PHE:CE2	2.48	0.48
2:E:536:TRP:CD1	2:E:635:ARG:HA	2.49	0.48
2:G:397:VAL:O	2:G:400:CYS:HB2	2.13	0.48
2:G:423:ARG:HD2	2:G:438:GLU:OE2	2.14	0.48
2:H:254:TYR:CD2	2:H:255:HIS:N	2.82	0.48
1:L:75:U:O2'	1:L:89:U:O4	2.28	0.48
1:L:87:U:H1'	2:D:582:ILE:HG13	1.96	0.48
2:C:437:ALA:HA	2:C:485:LEU:HD23	1.96	0.48

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:88:G:H1'	2:B:583:ARG:CG	2.43	0.47
2:A:296:PRO:HG2	2:B:265:PHE:CE1	2.50	0.47
2:B:423:ARG:HA	2:B:434:TRP:CZ3	2.49	0.47
2:B:578:ILE:HD11	2:B:595:VAL:CG2	2.45	0.47
2:C:411:PHE:CD2	2:C:521:PHE:CZ	3.03	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:366:PRO:O	2:G:367:SER:C	2.53	0.47
2:G:536:TRP:CE3	2:G:635:ARG:HD3	2.49	0.47
2:H:556:ASN:ND2	2:H:573:LEU:HD11	2.29	0.47
1:I:95:A:H2'	1:I:96:C:C6	2.48	0.47
1:N:78:G:O2'	1:N:79:A:H5'	2.15	0.47
2:A:273:ILE:HG22	2:A:522:ILE:HD11	1.96	0.47
2:A:287:GLU:HB2	2:A:288:TYR:HD1	1.80	0.47
2:C:281:VAL:HG12	2:C:285:LEU:CD1	2.45	0.47
2:C:287:GLU:HB2	2:C:288:TYR:HD1	1.79	0.47
2:C:526:THR:HG23	2:C:533:PHE:CZ	2.46	0.47
2:D:281:VAL:HG12	2:D:285:LEU:CD1	2.45	0.47
2:E:569:VAL:O	2:E:570:LYS:HG2	2.14	0.47
2:H:421:SER:HB3	2:H:458:GLU:CB	2.35	0.47
2:H:539:PRO:O	2:H:568:ARG:HD2	2.15	0.47
1:K:88:G:H5"	1:K:89:U:P	2.55	0.47
2:A:247:ILE:O	2:A:250:GLN:HB2	2.14	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:B:278:GLU:HB3	2:B:358:PHE:CE2	2.49	0.47
2:B:280:PHE:O	2:B:283:SER:HB3	2.15	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: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:C:418:VAL:HG21	2:C:450:ILE:HG21	1.97	0.47
2:D:397:VAL:O	2:D:400:CYS:HB2	2.15	0.47
2:D:445:LEU:HD21	2:D:466:ILE:HG12	1.97	0.47
2:D:580:PHE:HE1	5:D:5014:HOH:O	1.96	0.47
2:E:473:CYS:HB2	2:E:527:GLU:OE1	2.15	0.47
2:F:243:ASP:O	2:F:247:ILE:HG13	2.15	0.47
2:F:298:MET:CE	2:F:327:TYR:HB2	2.45	0.47
2:F:443:VAL:O	2:F:447:GLU:HB2	2.15	0.47
2:F:624:VAL:O	2:F:628:LEU:HG	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:246:LYS:O	2:G:250:GLN:HG2	2.15	0.47
2:G:423:ARG:HA	2:G:434:TRP:CZ3	2.50	0.47
2:G:543:VAL:HG11	2:G:585:HIS:CE1	2.50	0.47
2:H:603:SER:C	2:H:605:LYS:H	2.18	0.47
1:K:79:A:C2	1:K:94:C:O2	2.68	0.47
2:A:386:ILE:HG21	2:A:396:GLU:HG3	1.95	0.47
2:A:548:THR:HG23	2:A:551:GLN:OE1	2.15	0.47
2:B:301:ARG:O	2:B:305:GLU:HG3	2.14	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:E:436:ARG:HG2	2:E:440:ASP:OD2	2.15	0.47
2:G:278:GLU:OE2	2:G:358:PHE:HD2	1.98	0.47
2:H:288:TYR:N	2:H:288:TYR:HD1	2.12	0.47
1:N:80:U:H2'	1:N:81:C:C6	2.50	0.47
1:N:86:G:C4	2:F:547:ILE:CD1	2.97	0.47
2:A:265:PHE:CE1	2:B:296:PRO:HG2	2.50	0.47
2:A:281:VAL:HG12	2:A:285:LEU:CD1	2.45	0.47
2:B:423:ARG:NE	2:B:438:GLU:OE1	2.48	0.47
2:C:562:LEU:HD12	2:C:625:ILE:HD11	1.96	0.47
2:E:365:GLU:HA	2:E:365:GLU:OE1	2.15	0.47
2:F:303:LEU:HD11	2:F:339:GLN:NE2	2.27	0.47
2:F:543:VAL:HG11	2:F:585:HIS:ND1	2.30	0.47
2:G:421:SER:OG	2:G:467:GLU:OE2	2.33	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:H:416:ILE:HG22	2:H:416:ILE:O	2.14	0.47
2:H:589:ARG:O	2:H:611:ARG:HD3	2.15	0.47
2:H:624:VAL:O	2:H:628:LEU:HG	2.15	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:C:501:ASP:O	2:C:503:GLU:HG2	2.15	0.47
2:E:526:THR:HG23	2:E:533:PHE:HZ	1.79	0.47
2:E:583:ARG:O	2:E:587:LEU:CD2	2.63	0.47
2:F:452:PHE:HE2	2:F:454:TYR:CE1	2.24	0.47
2:G:460:ALA:HB1	2:G:462:TYR:CE1	2.50	0.47
2:G:562:LEU:HB3	2:G:569:VAL:HG11	1.97	0.47
2:H:484:GLN:HE22	4:H:9002:TSB:HN8	1.62	0.47
2:H:526:THR:HG23	2:H:533:PHE:HZ	1.80	0.47
2:H:628:LEU:O	2:H:632:ILE:HG13	2.14	0.47
1:K:89:U:O2	1:K:89:U:H2'	2.15	0.46
1:M:93:U:N3	1:M:94:C:C5	2.82	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:536:TRP:O	2:B:568:ARG:NH2	2.48	0.46
2:B:624:VAL:O	2:B:628:LEU:HG	2.14	0.46
2:C:335:PRO:HG2	2:C:336:GLY:H	1.79	0.46
2:C:529:PHE:CD1	2:C:529:PHE:N	2.78	0.46
2:D:624:VAL:O	2:D:628:LEU:HG	2.15	0.46
2:E:281:VAL:HG12	2:E:285:LEU:CD1	2.43	0.46
2:E:536:TRP:CZ3	2:E:635:ARG:HD3	2.50	0.46
2:E:547:ILE:HG12	2:E:578:ILE:HD12	1.97	0.46
2:E:619:MET:HG3	2:E:624:VAL:HG12	1.97	0.46
2:F:528:GLU:O	2:F:530:ALA:N	2.48	0.46
2:F:583:ARG:O	2:F:587:LEU:CD2	2.61	0.46
2:G:356:ALA:HA	2:G:384:ALA:HA	1.97	0.46
2:G:421:SER:CA	2:G:455:GLN:HB3	2.44	0.46
2:G:531:GLY:O	2:G:589:ARG:HG3	2.16	0.46
2:G:597:GLY:O	2:G:601:VAL:HG23	2.15	0.46
1:N:95:A:H2'	1:N:96:C:O4'	2.15	0.46
2:A:397:VAL:O	2:A:400:CYS:HB2	2.14	0.46
2:A:422:THR:O	2:A:423:ARG:C	2.53	0.46
2:A:600:GLU:HB3	2:A:605:LYS:O	2.15	0.46
2:B:281:VAL:HG12	2:B:285:LEU:CD1	2.44	0.46
2:D:559:THR:HG21	2:D:571:ALA:CB	2.21	0.46
2:F:280:PHE:CZ	2:F:407:MET:HG2	2.50	0.46
2:F:386:ILE:HG21	2:F:396:GLU:CG	2.45	0.46
2:H:545:MET:CE	2:H:593:MET:HB3	2.45	0.46
1:M:71:C:N3	1:M:72:G:N7	2.64	0.46
1:O:93:U:H2'	1:O:94:C:H6	1.80	0.46
2:B:386:ILE:HG21	2:B:396:GLU:CG	2.45	0.46
2:C:580:PHE:HD1	2:C:580:PHE:C	2.18	0.46
2:E:400:CYS:SG	2:E:512:ARG:HG3	2.55	0.46
2:A:449:ASN:ND2	2:H:452:PHE:CE2	2.83	0.46
2:B:291:GLN:NE2	2:B:353:LEU:HD21	2.30	0.46
2:B:455:GLN:O	2:B:456:LEU:C	2.53	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:C:610:THR:HG21	2:C:614:LYS:HB3	1.97	0.46
2:D:305:GLU:HA	2:D:310:TRP:HB3	1.97	0.46
2:D:365:GLU:OE1	2:D:365:GLU:HA	2.15	0.46
2:E:348:TYR:CD1	2:E:348:TYR:C	2.89	0.46
2:F:285:LEU:HD21	2:F:512:ARG:HH12	1.80	0.46
2:H:287:GLU:HB2	2:H:288:TYR:HD1	1.79	0.46
1:J:89:U:H5	2:B:583:ARG:CZ	2.27	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:95:A:H2'	1:L:96:C:C6	2.50	0.46
2:B:501:ASP:O	2:B:503:GLU:HG2	2.16	0.46
2:B:536:TRP:CD1	2:B:635:ARG:HA	2.50	0.46
2:B:547:ILE:HG12	2:B:578:ILE:HD12	1.97	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:C:386:ILE:HG21	2:C:396:GLU:HG3	1.96	0.46
2:D:569:VAL:HG22	2:D:570:LYS:N	2.30	0.46
2:D:621:VAL:HG12	2:D:622:ASN:N	2.31	0.46
2:F:600:GLU:HB3	2:F:605:LYS:O	2.15	0.46
1:I:95:A:H1'	2:B:502:ASN:HD21	1.81	0.46
1:M:93:U:C2	1:M:94:C:C5	3.03	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
2:B:580:PHE:HD1	2:B:580:PHE:C	2.19	0.46
2:C:356:ALA:HA	2:C:384:ALA:HA	1.98	0.46
2:F:445:LEU:HD21	2:F:466:ILE:HG12	1.98	0.46
2:F:619:MET:HG3	2:F:624:VAL:HG12	1.96	0.46
2:G:460:ALA:HB1	2:G:462:TYR:CD1	2.50	0.46
2:G:545:MET:HE3	2:G:593:MET:HB3	1.96	0.46
2:H:274:PHE:CZ	2:H:518:MET:HG3	2.51	0.46
2:H:421:SER:OG	2:H:467:GLU:OE2	2.33	0.46
2:H:488:SER:C	2:H:490:PRO:HD2	2.35	0.46
1:K:93:U:C4	1:K:94:C:N4	2.84	0.46
1:M:86:G:C4	2:E:547:ILE:HD13	2.51	0.46
1:O:86:G:P	1:O:86:G:O4'	2.73	0.46
2:A:527:GLU:O	2:A:528:GLU:O	2.34	0.46
2:B:274:PHE:CD1	2:B:274:PHE:C	2.89	0.46
2:B:423:ARG:HE	2:B:438:GLU:CD	2.19	0.46
2:C:612:ARG:HH11	2:C:612:ARG:CG	2.29	0.46
2:E:255:HIS:HE2	2:E:257:GLN:CG	2.29	0.46
2:E:341:PHE:O	2:E:346:LYS:NZ	2.40	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:G:347:SER:HA	2:G:498:VAL:H	1.81	0.46
2:G:500:GLU:C	2:G:502:ASN:N	2.69	0.46
2:H:285:LEU:HD21	2:H:512:ARG:HH12	1.81	0.46
2:H:300:ASP:OD2	2:H:302:VAL:HB	2.16	0.46
1:I:84:U:O2'	1:I:85:C:P	2.73	0.46
1:K:95:A:C2	1:K:96:C:C2	3.03	0.46
2:A:288:TYR:CE2	2:A:403:LEU:HD13	2.51	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:B:452:PHE:HE2	2:B:454:TYR:CE1	2.21	0.46
2:C:422:THR:HB	2:C:438:GLU:OE2	2.15	0.46
2:C:621:VAL:HG12	2:C:622:ASN:N	2.31	0.46
2:D:348:TYR:CD1	2:D:348:TYR:C	2.88	0.46
2:D:628:LEU:O	2:D:632:ILE:HG13	2.14	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:462:TYR:HD2	2:H:486:ASP:OD2	1.98	0.46
2:H:562:LEU:HD12	2:H:625:ILE:HD11	1.98	0.46
2:H:602:GLU:OE1	2:H:602:GLU:N	2.49	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:A:488:SER:C	2:A:490:PRO:HD2	2.36	0.46
2:A:512:ARG:NE	2:A:512:ARG:O	2.48	0.46
2:C:273:ILE:HG22	2:C:522:ILE:HD11	1.98	0.46
2:C:297:PHE:CG	2:D:362:HIS:HE1	2.34	0.46
2:D:274:PHE:O	2:D:518:MET:HE3	2.15	0.46
2:E:329:ILE:N	2:E:329:ILE:CD1	2.79	0.46
2:E:422:THR:O	2:E:423:ARG:C	2.54	0.46
2:F:397:VAL:O	2:F:401:ILE:HG12	2.15	0.46
2:G:402:ARG:NH1	2:G:402:ARG:CB	2.77	0.46
2:G:562:LEU:HD12	2:G:625:ILE:HD11	1.98	0.46
2:H:329:ILE:N	2:H:329:ILE:CD1	2.79	0.46
1:J:86:G:P	1:J:86:G:O4'	2.73	0.46
2:A:278:GLU:CB	2:A:358:PHE:HE2	2.29	0.46
2:A:462:TYR:CD1	2:A:462:TYR:N	2.84	0.46
2:A:621:VAL:HG12	2:A:622:ASN:N	2.29	0.46
2:B:280:PHE:CZ	2:B:407:MET:HG2	2.51	0.46
2:B:526:THR:HG23	2:B:533:PHE:HZ	1.81	0.46
2:B:602:GLU:OE1	2:B:602:GLU:N	2.49	0.46
2:D:347:SER:HA	2:D:498:VAL:H	1.80	0.46
2:D:548:THR:HG23	2:D:551:GLN:OE1	2.16	0.46
2:E:277:LEU:O	2:E:280:PHE:HB3	2.16	0.46
2:E:299:MET:HE1	2:E:335:PRO:HB2	1.97	0.46
2:E:386:ILE:O	2:E:509:MET:HA	2.16	0.46
2:E:550:SER:C	2:E:552:SER:H	2.18	0.46
2:E:602:GLU:OE1	2:E:602:GLU:N	2.49	0.46
2:G:298:MET:HE2	2:G:327:TYR:CD1	2.51	0.46
2:H:619:MET:HG3	2:H:624:VAL:HG12	1.98	0.46
1:I:80:U:H2'	1:I:81:C:C6	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:87:U:C2'	1:I:88:G:OP2	2.64	0.45
1:O:87:U:C2'	5:O:1519:HOH:O	2.39	0.45
1:P:87:U:H3'	5:P:1619:HOH:O	2.16	0.45
2:A:528:GLU:O	2:A:530:ALA:N	2.49	0.45
2:B:555:VAL:O	2:B:559:THR:HG23	2.16	0.45
2:B:620:ASP:HB3	2:B:623:GLU:CB	2.46	0.45
2:C:500:GLU:OE1	2:C:500:GLU:N	2.48	0.45
2:D:339:GLN:OE1	2:D:339:GLN:CA	2.64	0.45
2:D:490:PRO:HD3	2:D:509:MET:CE	2.46	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:G:585:HIS:HB2	2:G:593:MET:HE2	1.94	0.45
2:H:411:PHE:HE2	2:H:525:LEU:HD11	1.81	0.45
2:A:402:ARG:NH1	2:A:402:ARG:CB	2.78	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:D:427:ARG:HB2	2:D:434:TRP:CZ2	2.51	0.45
2:E:423:ARG:O	2:E:423:ARG:HG2	2.15	0.45
2:F:273:ILE:HG22	2:F:522:ILE:HD11	1.97	0.45
2:F:290:TYR:CZ	2:F:512:ARG:NH1	2.85	0.45
2:G:569:VAL:CG2	2:G:570:LYS:N	2.79	0.45
1:M:87:U:C3'	5:M:1319:HOH:O	2.62	0.45
1:O:97:C:C4'	1:O:98:A:OP1	2.64	0.45
2:A:294:LYS:HA	2:A:357:GLU:HG3	1.98	0.45
2:B:278:GLU:CA	2:B:358:PHE:HE2	2.29	0.45
2:B:329:ILE:N	2:B:329:ILE:CD1	2.80	0.45
2:B:545:MET:SD	2:B:582:ILE:HD13	2.56	0.45
2:C:589:ARG:O	2:C:611:ARG:HD3	2.16	0.45
2:D:300:ASP:OD2	2:D:302:VAL:HB	2.16	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:F:253:LEU:O	2:F:270:GLY:HA3	2.16	0.45
2:F:422:THR:HB	2:F:438:GLU:OE2	2.17	0.45
2:F:488:SER:C	2:F:490:PRO:HD2	2.36	0.45
2:H:298:MET:HE3	2:H:327:TYR:HB2	1.98	0.45
2:H:526:THR:O	2:H:530:ALA:N	2.49	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:C:588:ARG:C	2:C:589:ARG:HG2	2.36	0.45
2:D:536:TRP:CD1	2:D:635:ARG:HA	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:462:TYR:CE2	2:F:511:HIS:NE2	2.83	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:G:320:THR:HG22	2:G:321:SER:N	2.25	0.45
2:G:550:SER:C	2:G:552:SER:H	2.19	0.45
1:I:88:G:H1'	2:A:583:ARG:CG	2.46	0.45
1:K:85:C:C2'	2:C:577:LYS:HG2	2.46	0.45
1:K:93:U:H2'	1:K:94:C:H6	1.82	0.45
1:M:71:C:C2	1:M:72:G:C8	3.04	0.45
1:M:81:C:O2'	1:M:82:U:H5'	2.16	0.45
2:A:471:TYR:CD1	2:A:471:TYR:N	2.85	0.45
2:B:304:TRP:CE3	2:B:328:CYS:HB2	2.52	0.45
2:C:282:ARG:HD3	2:C:292:GLU:OE1	2.16	0.45
2:D:437:ALA:HA	2:D:485:LEU:HD23	1.97	0.45
2:D:519:GLU:CD	2:D:519:GLU:H	2.20	0.45
2:E:285:LEU:HD21	2:E:512:ARG:HH12	1.82	0.45
2:E:462:TYR:CE2	2:E:511:HIS:NE2	2.85	0.45
2:E:500:GLU:C	2:E:502:ASN:N	2.70	0.45
2:E:624:VAL:O	2:E:628:LEU:HG	2.17	0.45
2:F:380:THR:N	2:F:519:GLU:OE2	2.50	0.45
2:F:386:ILE:O	2:F:509:MET:HA	2.17	0.45
2:G:490:PRO:HD3	2:G:509:MET:CE	2.46	0.45
2:G:627:LYS:O	2:G:630:GLN:HB3	2.16	0.45
2:H:550:SER:C	2:H:552:SER:H	2.20	0.45
1:K:98:A:N7	2:D:345:LEU:HD13	2.31	0.45
2:A:445:LEU:HD21	2:A:466:ILE:HG12	1.98	0.45
2:B:277:LEU:O	2:B:280:PHE:HB3	2.17	0.45
2:C:411:PHE:CE2	2:C:521:PHE:HZ	2.31	0.45
2:C:551:GLN:HG2	2:C:597:GLY:C	2.37	0.45
2:C:569:VAL:HG22	2:C:570:LYS:N	2.31	0.45
2:D:421:SER:HB3	2:D:458:GLU:CB	2.35	0.45
2:E:362:HIS:HE1	2:F:297:PHE:CG	2.34	0.45
2:E:397:VAL:O	2:E:400:CYS:HB2	2.16	0.45
2:G:330:LYS:HA	2:G:331:PRO:HD3	1.63	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:A:273:ILE:HG23	2:A:537:LEU:CD2	2.46	0.45
2:A:405:TYR:HE1	2:A:416:ILE:HG21	1.82	0.45
2:B:251:LEU:HD22	2:B:588:ARG:O	2.17	0.45
2:B:300:ASP:OD2	2:B:302:VAL:HB	2.16	0.45
2:B:312:ASN:O	2:B:313:TYR:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:294:LYS:HA	2:F:357:GLU:HG3	1.98	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:A:422:THR:HB	2:A:438:GLU:OE2	2.17	0.45
2:A:482:THR:O	2:A:512:ARG:HA	2.16	0.45
2:B:551:GLN:HE21	2:B:598:ASP:N	2.14	0.45
2:C:441:LEU:O	2:C:444:ALA:HB3	2.16	0.45
2:D:332:MET:HE2	4:D:5002:TSB:HN12	1.81	0.45
2:D:609:ARG:HD3	2:D:610:THR:O	2.17	0.45
2:E:445:LEU:HD21	2:E:466:ILE:HG12	1.98	0.45
2:E:460:ALA:C	2:E:462:TYR:H	2.19	0.45
2:E:610:THR:HG22	2:E:614:LYS:O	2.17	0.45
2:F:555:VAL:O	2:F:559:THR:HG23	2.17	0.45
2:G:551:GLN:HG2	2:G:597:GLY:C	2.36	0.45
1:J:93:U:C2	1:J:94:C:C6	3.05	0.45
1:N:86:G:O6	2:F:599:LYS:CB	2.65	0.45
1:O:89:U:P	5:O:1528:HOH:O	2.75	0.45
1:P:80:U:H2'	1:P:81:C:H6	1.80	0.45
2:A:417:VAL:HG13	2:A:471:TYR:CE1	2.47	0.45
2:A:422:THR:O	2:A:458:GLU:O	2.34	0.45
2:B:427:ARG:HB2	2:B:434:TRP:CZ2	2.52	0.45
2:B:490:PRO:HD3	2:B:509:MET:CE	2.47	0.45
2:C:294:LYS:HA	2:C:294:LYS:HD2	1.84	0.45
2:C:585:HIS:HA	2:C:588:ARG:HB2	1.99	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:D:610:THR:HG22	2:D:614:LYS:O	2.17	0.45
2:E:280:PHE:CZ	2:E:407:MET:HG2	2.51	0.45
2:F:526:THR:HG23	2:F:533:PHE:CZ	2.50	0.45
2:F:562:LEU:HB3	2:F:569:VAL:HG11	1.97	0.45
2:G:383:ASP:OD2	2:G:385:HIS:HE1	2.00	0.45
2:G:567:ILE:O	2:G:569:VAL:N	2.50	0.45
1:K:90:G:C8	2:C:577:LYS:HD2	2.51	0.45
1:M:87:U:C2'	1:M:88:G:OP2	2.65	0.45
2:A:282:ARG:HD3	2:A:292:GLU:OE1	2.16	0.45
2:A:455:GLN:O	2:A:456:LEU:C	2.55	0.45
2:A:480:CYS:O	2:A:516:GLY:HA3	2.17	0.45
2:A:628:LEU:O	2:A:632:ILE:HG13	2.17	0.45
2:B:279:VAL:CG2	2:B:280:PHE:N	2.80	0.45
2:B:423:ARG:HG2	2:B:423:ARG:O	2.17	0.45
2:C:294:LYS:HA	2:C:357:GLU:HG3	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:297:PHE:CG	2:D:362:HIS:CE1	3.05	0.45
2:C:436:ARG:HG2	2:C:440:ASP:OD2	2.17	0.45
2:E:251:LEU:HD22	2:E:588:ARG:O	2.17	0.45
2:F:421:SER:CA	2:F:455:GLN:HB3	2.45	0.45
1:N:87:U:H2'	5:N:1419:HOH:O	2.16	0.44
2:B:603:SER:C	2:B:605:LYS:H	2.20	0.44
2:C:303:LEU:HD11	2:C:339:GLN:NE2	2.31	0.44
2:C:543:VAL:HG11	2:C:585:HIS:ND1	2.31	0.44
2:E:243:ASP:O	2:E:247:ILE:HG13	2.17	0.44
2:E:320:THR:HG22	2:E:321:SER:N	2.25	0.44
2:E:460:ALA:C	2:E:462:TYR:N	2.68	0.44
2:F:255:HIS:HE2	2:F:257:GLN:CG	2.30	0.44
2:F:465:LYS:HG3	2:F:484:GLN:CG	2.44	0.44
2:G:309:HIS:HB3	2:G:317:MET:HE1	1.99	0.44
2:G:397:VAL:O	2:G:401:ILE:HG12	2.17	0.44
2:H:551:GLN:HG2	2:H:597:GLY:C	2.37	0.44
2:H:569:VAL:O	2:H:570:LYS:HG2	2.17	0.44
1:I:83:U:H3	2:A:575:ASN:HD21	1.65	0.44
1:L:84:U:H4'	1:L:85:C:H5'	1.97	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:B:253:LEU:N	2:B:253:LEU:HD23	2.32	0.44
2:B:624:VAL:HG23	2:B:625:ILE:N	2.32	0.44
2:C:242:ARG:HE	2:C:246:LYS:HD3	1.82	0.44
2:C:323:GLU:O	2:C:324:ASN:O	2.35	0.44
2:C:421:SER:HB3	2:C:458:GLU:CB	2.35	0.44
2:D:329:ILE:N	2:D:329:ILE:CD1	2.80	0.44
2:F:285:LEU:HD22	2:F:290:TYR:CG	2.52	0.44
2:G:474:LEU:O	2:G:475:ASP:C	2.55	0.44
2:H:323:GLU:CD	2:H:323:GLU:H	2.19	0.44
2:H:551:GLN:HE21	2:H:598:ASP:N	2.16	0.44
1:I:86:G:H3'	5:I:109:HOH:O	2.17	0.44
1:M:84:U:H4'	1:M:85:C:H5'	1.96	0.44
1:O:84:U:C2'	2:G:548:THR:HG1	2.30	0.44
2:A:556:ASN:HD21	2:A:573:LEU:HD11	1.82	0.44
2:B:274:PHE:O	2:B:518:MET:HE3	2.17	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:C:437:ALA:HB2	2:C:487:PHE:CD2	2.52	0.44
2:D:353:LEU:HB3	2:D:387:PHE:HB2	1.98	0.44
2:D:389:THR:HG1	2:D:392:GLN:HG3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:426:LYS:HE2	2:D:426:LYS:HB3	1.84	0.44
2:D:550:SER:C	2:D:552:SER:H	2.20	0.44
2:D:585:HIS:HA	2:D:588:ARG:HB2	1.98	0.44
2:F:291:GLN:NE2	2:F:353:LEU:HD21	2.32	0.44
2:F:365:GLU:N	2:F:377:ARG:HD3	2.30	0.44
2:F:588:ARG:C	2:F:589:ARG:HG2	2.37	0.44
2:G:288:TYR:N	2:G:288:TYR:CD1	2.85	0.44
2:G:400:CYS:O	2:G:404:VAL:HG23	2.17	0.44
2:G:604:GLY:O	2:G:621:VAL:HG23	2.18	0.44
2:H:501:ASP:O	2:H:503:GLU:HG2	2.18	0.44
1:N:72:G:H2'	1:N:73:U:H6	1.82	0.44
1:P:85:C:C5	2:H:547:ILE:O	2.68	0.44
2:A:285:LEU:HD21	2:A:512:ARG:HH12	1.83	0.44
2:B:278:GLU:HA	2:B:358:PHE:HE2	1.83	0.44
2:C:254:TYR:CD2	2:C:255:HIS:N	2.85	0.44
2:C:298:MET:HG2	2:C:298:MET:O	2.16	0.44
2:C:351:LEU:HD22	2:C:387:PHE:O	2.17	0.44
2:C:362:HIS:HE1	2:D:297:PHE:CD1	2.35	0.44
2:C:590:VAL:O	2:C:611:ARG:HB3	2.17	0.44
2:D:501:ASP:O	2:D:503:GLU:HG2	2.18	0.44
2:F:411:PHE:CD2	2:F:521:PHE:HZ	2.35	0.44
2:F:455:GLN:O	2:F:456:LEU:C	2.56	0.44
2:G:251:LEU:CA	2:G:588:ARG:HH12	2.25	0.44
2:H:305:GLU:HA	2:H:310:TRP:HB3	1.98	0.44
2:H:542:VAL:CG1	2:H:543:VAL:N	2.80	0.44
1:K:89:U:O2'	2:C:580:PHE:CG	2.69	0.44
1:L:96:C:H2'	1:L:97:C:C6	2.52	0.44
2:A:255:HIS:HE2	2:A:257:GLN:CG	2.30	0.44
2:B:287:GLU:HB2	2:B:288:TYR:HD1	1.83	0.44
2:D:287:GLU:HB2	2:D:288:TYR:HD1	1.82	0.44
2:E:303:LEU:HD11	2:E:339:GLN:NE2	2.31	0.44
2:E:399:GLY:HA2	2:E:402:ARG:HH11	1.82	0.44
2:E:421:SER:OG	2:E:467:GLU:OE2	2.36	0.44
2:E:609:ARG:HD3	2:E:610:THR:O	2.18	0.44
2:F:471:TYR:N	2:F:471:TYR:CD1	2.86	0.44
2:H:274:PHE:C	2:H:274:PHE:CD1	2.90	0.44
2:H:323:GLU:O	2:H:324:ASN:O	2.36	0.44
1:J:88:G:H8	5:J:1023:HOH:O	1.97	0.44
1:P:72:G:H2'	1:P:73:U:H6	1.83	0.44
1:P:103:G:H5'	5:P:1625:HOH:O	2.18	0.44
2:A:273:ILE:HG23	2:A:537:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:562:LEU:HB3	2:A:569:VAL:HG11	2.00	0.44
2:B:588:ARG:C	2:B:589:ARG:HG2	2.38	0.44
2:B:619:MET:HG3	2:B:624:VAL:HG12	2.00	0.44
2:D:437:ALA:HB2	2:D:487:PHE:CD2	2.53	0.44
2:E:526:THR:O	2:E:530:ALA:HA	2.18	0.44
2:E:603:SER:C	2:E:605:LYS:H	2.19	0.44
2:F:437:ALA:HA	2:F:485:LEU:HD23	1.99	0.44
2:F:548:THR:HG23	2:F:551:GLN:OE1	2.18	0.44
2:F:569:VAL:HG22	2:F:570:LYS:N	2.33	0.44
2:G:274:PHE:CD1	2:G:274:PHE:C	2.90	0.44
2:G:365:GLU:OE1	2:G:365:GLU:HA	2.18	0.44
2:H:395:ASP:OD1	2:H:395:ASP:N	2.47	0.44
1:M:86:G:P	1:M:86:G:O4'	2.76	0.44
1:P:86:G:N9	2:H:547:ILE:HD13	2.31	0.44
2:A:285:LEU:HD22	2:A:290:TYR:CG	2.52	0.44
2:A:356:ALA:HB2	2:A:384:ALA:HB2	2.00	0.44
2:A:386:ILE:HG21	2:A:396:GLU:CG	2.48	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:D:274:PHE:CD1	2:D:274:PHE:C	2.91	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:G:287:GLU:HB2	2:G:288:TYR:HD1	1.82	0.44
2:G:288:TYR:N	2:G:288:TYR:HD1	2.15	0.44
2:H:405:TYR:HE1	2:H:416:ILE:HG21	1.83	0.44
2:H:427:ARG:HB2	2:H:434:TRP:CZ2	2.52	0.44
2:H:609:ARG:HD3	2:H:610:THR:O	2.18	0.44
1:M:98:A:H4'	5:M:1327:HOH:O	2.17	0.44
2:C:255:HIS:ND1	2:C:267:HIS:CE1	2.67	0.44
2:C:427:ARG:HA	2:C:461:PHE:O	2.18	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:E:339:GLN:OE1	2:E:339:GLN:CA	2.66	0.44
2:E:347:SER:HA	2:E:498:VAL:H	1.83	0.44
2:F:277:LEU:O	2:F:280:PHE:HB3	2.17	0.44
2:F:459:GLY:HA2	2:F:465:LYS:HE2	1.99	0.44
2:F:551:GLN:HE21	2:F:598:ASP:N	2.16	0.44
2:H:471:TYR:N	2:H:471:TYR:CD1	2.86	0.44
2:H:603:SER:C	2:H:605:LYS:N	2.71	0.44
1:J:75:U:O2'	1:J:76:G:P	2.76	0.44
1:J:83:U:H3	2:B:575:ASN:HD21	1.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:94:C:C2	1:J:95:A:C8	3.06	0.44
1:N:86:G:N3	2:F:547:ILE:CD1	2.81	0.44
2:A:313:TYR:HB3	2:A:317:MET:HE1	2.00	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:B:290:TYR:CE2	2:B:512:ARG:NH1	2.86	0.44
2:B:351:LEU:HD22	2:B:387:PHE:O	2.17	0.44
2:C:482:THR:O	2:C:512:ARG:HA	2.17	0.44
2:D:282:ARG:HD3	2:D:292:GLU:OE1	2.17	0.44
2:D:547:ILE:HG12	2:D:578:ILE:HD12	2.00	0.44
2:E:462:TYR:HE2	2:E:511:HIS:NE2	2.14	0.44
2:E:587:LEU:HD23	2:E:587:LEU:N	2.24	0.44
2:F:500:GLU:C	2:F:502:ASN:N	2.69	0.44
2:F:527:GLU:O	2:F:528:GLU:O	2.36	0.44
2:G:395:ASP:OD1	2:G:395:ASP:N	2.48	0.44
2:G:422:THR:O	2:G:423:ARG:C	2.56	0.44
2:G:462:TYR:CD2	2:G:486:ASP:OD2	2.70	0.44
2:H:600:GLU:HB3	2:H:605:LYS:O	2.17	0.44
2:H:612:ARG:HH11	2:H:612:ARG:CG	2.28	0.44
2:A:250:GLN:NE2	2:A:250:GLN:HA	2.33	0.43
2:A:557:GLU:O	2:A:560:GLN:HB3	2.18	0.43
2:B:569:VAL:O	2:B:570:LYS:HG2	2.17	0.43
2:C:278:GLU:HB3	2:C:358:PHE:CE2	2.52	0.43
2:D:298:MET:HE2	2:D:327:TYR:CD1	2.53	0.43
2:D:317:MET:HG3	2:D:331:PRO:HG3	2.00	0.43
2:D:441:LEU:O	2:D:444:ALA:HB3	2.18	0.43
2:F:300:ASP:OD2	2:F:302:VAL:HB	2.18	0.43
2:F:587:LEU:HD23	2:F:587:LEU:N	2.25	0.43
2:H:556:ASN:HD21	2:H:573:LEU:HD11	1.83	0.43
2:A:388:CYS:O	2:A:508:VAL:HG23	2.18	0.43
2:A:418:VAL:HG21	2:A:450:ILE:CG2	2.49	0.43
2:B:473:CYS:CA	5:B:221:HOH:O	2.35	0.43
2:B:480:CYS:O	2:B:516:GLY:HA3	2.18	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:C:347:SER:HA	2:C:498:VAL:H	1.83	0.43
2:D:551:GLN:HG2	2:D:597:GLY:C	2.38	0.43
2:D:555:VAL:O	2:D:559:THR: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:F:353:LEU:HB3	2:F:387:PHE:HB2	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:386:ILE:O	2:G:509:MET:HA	2.18	0.43
2:H:388:CYS:O	2:H:508:VAL:HG23	2.18	0.43
1:I:77:U:O5'	1:I:77:U:H6	2.01	0.43
1:L:72:G:H2'	1:L:73:U:H6	1.81	0.43
1:M:89:U:H2'	1:M:90:G:OP1	2.18	0.43
1:P:86:G:P	1:P:86:G:O4'	2.76	0.43
2:A:348:TYR:CE2	2:A:500:GLU:HG3	2.53	0.43
2:A:529:PHE:H	2:A:529:PHE:HD1	1.55	0.43
2:B:402:ARG:NH1	2:B:402:ARG:CB	2.79	0.43
2:C:330:LYS:HA	2:C:331:PRO:HD3	1.61	0.43
2:D:254:TYR:CD2	2:D:255:HIS:N	2.85	0.43
2:E:353:LEU:HD22	2:E:353:LEU:HA	1.82	0.43
2:E:437:ALA:HA	2:E:485:LEU:HD23	2.00	0.43
2:E:639:GLN:O	2:E:642:GLU:HG2	2.18	0.43
2:F:342:ASN:HD21	2:F:495:ALA:HA	1.83	0.43
2:F:356:ALA:HA	2:F:384:ALA:HA	2.00	0.43
2:F:604:GLY:O	2:F:621:VAL:HG23	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
1:I:72:G:H2'	1:I:73:U:C6	2.52	0.43
1:N:87:U:C2'	1:N:88:G:OP2	2.66	0.43
2:A:387:PHE:CE1	2:A:509:MET:SD	3.11	0.43
2:A:569:VAL:O	2:A:570:LYS:HG2	2.19	0.43
2:D:335:PRO:HG2	2:D:336:GLY:H	1.81	0.43
2:D:436:ARG:HG2	2:D:440:ASP:OD2	2.19	0.43
2:D:482:THR:HG21	4:D:5002:TSB:H5'2	1.99	0.43
2:D:500:GLU:C	2:D:502:ASN:N	2.70	0.43
2:E:282:ARG:HD3	2:E:292:GLU:OE1	2.19	0.43
2:F:254:TYR:HA	2:F:267:HIS:ND1	2.33	0.43
2:F:353:LEU:HD22	2:F:353:LEU:HA	1.78	0.43
2:F:417:VAL:HG13	2:F:471:TYR:CE1	2.49	0.43
2:F:482:THR:O	2:F:512:ARG:HA	2.18	0.43
2:F:585:HIS:CB	2:F:593:MET:HE3	2.47	0.43
2:G:319:THR:HG22	2:G:328:CYS:HA	1.99	0.43
2:G:348:TYR:CE2	2:G:500:GLU:HG3	2.53	0.43
2:G:436:ARG:HG2	2:G:440:ASP:OD2	2.18	0.43
2:H:610:THR:HG22	2:H:614:LYS:O	2.18	0.43
1:J:71:C:C2	1:J:72:G:C8	3.06	0.43
1:J:87:U:C2'	1:J:88:G:OP2	2.66	0.43
2:A:423:ARG:HB3	2:A:434:TRP:CE3	2.54	0.43
2:B:285:LEU:HD21	2:B:512:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:274:PHE:C	2:C:274:PHE:CD1	2.92	0.43
2:C:300:ASP:OD2	2:C:302:VAL:HB	2.19	0.43
2:C:309:HIS:HB3	2:C:317:MET:HE1	2.01	0.43
2:C:471:TYR:N	2:C:471:TYR:CD1	2.86	0.43
2:D:521:PHE:HE1	2:D:525:LEU:HD11	1.82	0.43
2:D:554:TYR:CE1	2:D:558:LEU:HD11	2.54	0.43
2:D:562:LEU:HD12	2:D:625:ILE:HD11	2.00	0.43
2:E:254:TYR:HA	2:E:267:HIS:ND1	2.34	0.43
2:E:291:GLN:NE2	2:E:353:LEU:HD21	2.32	0.43
2:F:609:ARG:HD3	2:F:610:THR:O	2.18	0.43
2:F:612:ARG:HH11	2:F:612:ARG:CG	2.32	0.43
2:G:521:PHE:HE1	2:G:525:LEU:HD11	1.84	0.43
2:G:583:ARG:O	2:G:586:THR:N	2.50	0.43
2:H:445:LEU:HD21	2:H:466:ILE:HG12	2.01	0.43
1:L:86:G:O6	2:D:599:LYS:HB2	2.18	0.43
1:N:69:G:O2'	1:N:70:G:H5'	2.18	0.43
1:N:84:U:O2'	1:N:85:C:OP2	2.30	0.43
1:P:72:G:H2'	1:P:73:U:C6	2.54	0.43
2:C:380:THR:N	2:C:519:GLU:OE2	2.50	0.43
2:C:610:THR:HG22	2:C:614:LYS:O	2.19	0.43
2:D:243:ASP:O	2:D:247:ILE:HG13	2.19	0.43
2:D:421:SER:OG	2:D:467:GLU:OE2	2.37	0.43
2:D:459:GLY:HA2	2:D:465:LYS:HE2	2.01	0.43
2:D:603:SER:C	2:D:605:LYS:H	2.21	0.43
2:E:402:ARG:NH1	2:E:402:ARG:CB	2.80	0.43
2:E:462:TYR:CD2	2:E:486:ASP:OD2	2.71	0.43
2:E:612:ARG:HH11	2:E:612:ARG:CG	2.30	0.43
2:F:320:THR:HG22	2:F:321:SER:N	2.25	0.43
2:F:423:ARG:NE	2:F:438:GLU:OE1	2.52	0.43
2:F:526:THR:O	2:F:530:ALA:HA	2.18	0.43
2:G:249:LYS:HB3	2:G:249:LYS:HZ3	1.80	0.43
2:G:609:ARG:HD3	2:G:610:THR:O	2.18	0.43
2:H:242:ARG:HE	2:H:246:LYS:HD3	1.84	0.43
1:M:95:A:H2'	1:M:96:C:O4'	2.18	0.43
1:P:87:U:O2'	1:P:88:G:P	2.77	0.43
2:A:327:TYR:CD1	2:A:327:TYR:N	2.87	0.43
2:A:465:LYS:HG3	2:A:484:GLN:CG	2.44	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:B:445:LEU:HD21	2:B:466:ILE:HG12	2.00	0.43
2:B:622:ASN:O	2:B:626:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:254:TYR:CZ	2:D:373:LEU:HD21	2.54	0.43
2:D:323:GLU:CD	2:D:323:GLU:H	2.22	0.43
2:D:423:ARG:HE	2:D:438:GLU:CD	2.22	0.43
2:E:521:PHE:HE1	2:E:525:LEU:HD11	1.84	0.43
2:F:298:MET:HE3	2:F:327:TYR:HB2	1.99	0.43
2:F:484:GLN:HE22	4:F:7002:TSB:HN8	1.67	0.43
2:H:320:THR:HG22	2:H:321:SER:N	2.29	0.43
2:H:402:ARG:NH1	2:H:402:ARG:CB	2.79	0.43
2:H:597:GLY:O	2:H:601:VAL:HG23	2.17	0.43
1:O:86:G:H1'	2:G:547:ILE:HD13	2.01	0.43
2:A:254:TYR:CE1	2:A:373:LEU:HD21	2.54	0.43
2:A:263:MET:HE2	2:B:298:MET:CG	2.40	0.43
2:A:634:SER:O	2:A:635:ARG:C	2.57	0.43
2:B:255:HIS:HE2	2:B:257:GLN:CG	2.32	0.43
2:B:544:ILE:HG22	2:B:555:VAL:HG13	2.00	0.43
2:C:520:ARG:NH1	5:C:4008:HOH:O	2.50	0.43
2:E:415:LYS:HG2	2:E:471:TYR:CD1	2.54	0.43
2:E:594:LEU:CD2	2:E:608:VAL:HG22	2.48	0.43
2:F:426:LYS:HE2	2:F:426:LYS:HB3	1.88	0.43
2:H:538:ALA:O	2:H:539:PRO:C	2.57	0.43
1:J:79:A:H1'	2:A:502:ASN:OD1	2.19	0.43
1:J:89:U:H5	2:B:583:ARG:NH2	2.16	0.43
1:K:89:U:O2	1:K:89:U:C2'	2.66	0.43
1:L:95:A:H2'	1:L:96:C:O4'	2.19	0.43
1:N:87:U:H2'	1:N:88:G:OP2	2.19	0.43
1:N:97:C:C5'	1:N:98:A:OP1	2.64	0.43
1:P:87:U:H1'	2:H:582:ILE:HG13	2.00	0.43
2:A:351:LEU:HD13	2:A:388:CYS:HA	2.00	0.43
2:A:452:PHE:CE2	2:A:454:TYR:HE1	2.24	0.43
2:B:358:PHE:N	2:B:358:PHE:CD1	2.86	0.43
2:B:622:ASN:HB3	2:H:612:ARG:O	2.19	0.43
2:C:280:PHE:CZ	2:C:407:MET:HG2	2.53	0.43
2:D:280:PHE:CZ	2:D:407:MET:HG2	2.53	0.43
2:E:242:ARG:HE	2:E:246:LYS:HD3	1.83	0.43
2:F:242:ARG:HE	2:F:246:LYS:HD3	1.83	0.43
2:F:371:HIS:O	2:F:372:GLY:C	2.56	0.43
2:G:542:VAL:CG1	2:G:543:VAL:N	2.82	0.43
2:H:243:ASP:O	2:H:247:ILE:HG13	2.19	0.43
2:H:430:SER:O	2:H:431:ASP:C	2.55	0.43
1:L:87:U:C2'	1:L:88:G:OP2	2.66	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)
2:A:567:ILE:O	2:A:569:VAL:N	2.52	0.43
2:A:630:GLN:HA	2:A:633:ARG:HH12	1.84	0.43
2:B:323:GLU:CD	2:B:323:GLU:H	2.22	0.43
2:B:353:LEU:HB3	2:B:387:PHE:HB2	2.00	0.43
2:B:410:THR:HB	2:B:411:PHE:CD1	2.53	0.43
2:E:526:THR:O	2:E:530:ALA:N	2.51	0.43
2:F:394:ARG:O	2:F:395:ASP:C	2.57	0.43
2:F:405:TYR:HE1	2:F:416:ILE:HG21	1.84	0.43
2:G:313:TYR:CE1	2:G:316:ALA:HB3	2.54	0.43
2:G:417:VAL:HG11	2:G:471:TYR:CE1	2.52	0.43
2:G:480:CYS:O	2:G:516:GLY:HA3	2.19	0.43
2:G:551:GLN:HE21	2:G:598:ASP:N	2.16	0.43
2:G:628:LEU:O	2:G:632:ILE:HG13	2.19	0.43
2:H:279:VAL:CG2	2:H:280:PHE:N	2.82	0.43
2:H:383:ASP:OD2	2:H:385:HIS:CE1	2.72	0.43
1:M:84:U:O2'	1:M:85:C:OP2	2.27	0.42
2:A:299:MET:O	2:A:304:TRP:HZ3	2.02	0.42
2:A:330:LYS:HA	2:A:331:PRO:HD3	1.60	0.42
2:A:353:LEU:HB3	2:A:387:PHE:HB2	1.99	0.42
2:A:585:HIS:HA	2:A:588:ARG:HB2	2.01	0.42
2:B:397:VAL:O	2:B:400:CYS:HB2	2.19	0.42
2:C:462:TYR:CD2	2:C:486:ASP:OD2	2.71	0.42
2:C:603:SER:C	2:C:605:LYS:H	2.21	0.42
2:D:421:SER:CA	2:D:455:GLN:HB3	2.45	0.42
2:D:531:GLY:O	2:D:589:ARG:HG3	2.19	0.42
2:D:627:LYS:O	2:D:630:GLN:HB3	2.19	0.42
2:F:251:LEU:CA	2:F:588:ARG:HH12	2.25	0.42
2:F:254:TYR:CD2	2:F:255:HIS:N	2.87	0.42
2:F:273:ILE:HG23	2:F:537:LEU:HD22	2.01	0.42
2:F:529:PHE:CD2	2:F:534:PRO:HD3	2.54	0.42
2:F:585:HIS:HA	2:F:588:ARG:HB2	2.01	0.42
2:F:590:VAL:O	2:F:611:ARG:HB3	2.19	0.42
2:F:621:VAL:HG12	2:F:622:ASN:N	2.33	0.42
2:G:250:GLN:NE2	2:G:250:GLN:HA	2.34	0.42
2:G:572:ASP:OD1	2:G:574:ARG:HB2	2.18	0.42
2:H:255:HIS:HE2	2:H:257:GLN:CG	2.31	0.42
2:H:609:ARG:O	2:H:609:ARG:CG	2.67	0.42
1:L:79:A:O2'	2:C:500:GLU:O	2.35	0.42
2:B:550:SER:C	2:B:552:SER:N	2.72	0.42
2:C:249:LYS:HE2	2:C:249:LYS:HA	2.01	0.42
2:C:416:ILE:O	2:C:416:ILE:HG22	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:423:ARG:HE	2:C:438:GLU:CD	2.22	0.42
2:C:541:GLN:HE22	2:C:632:ILE:HD13	1.84	0.42
2:E:356:ALA:HA	2:E:384:ALA:HA	2.00	0.42
2:E:399:GLY:HA2	2:E:402:ARG:NH1	2.35	0.42
2:E:545:MET:SD	2:E:582:ILE:HD13	2.58	0.42
2:F:274:PHE:CD1	2:F:274:PHE:C	2.91	0.42
2:F:281:VAL:O	2:F:282:ARG:C	2.56	0.42
2:G:332:MET:HE2	4:G:8002:TSB:HN12	1.84	0.42
2:G:337:HIS:NE2	2:G:357:GLU:OE1	2.47	0.42
2:H:567:ILE:O	2:H:569:VAL:N	2.52	0.42
1:M:72:G:H2'	1:M:73:U:H6	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:A:280:PHE:CZ	2:A:407:MET:HG2	2.54	0.42
2:A:290:TYR:CZ	2:A:512:ARG:NH1	2.86	0.42
2:A:400:CYS:SG	2:A:512:ARG:HG3	2.60	0.42
2:B:386:ILE:O	2:B:509:MET:HA	2.19	0.42
2:C:627:LYS:CB	2:C:640:LEU:HD21	2.47	0.42
2:D:423:ARG:NE	2:D:438:GLU:OE1	2.52	0.42
2:F:347:SER:HA	2:F:498:VAL:H	1.84	0.42
2:F:365:GLU:OE1	2:F:365:GLU:HA	2.19	0.42
2:G:393:ILE:O	2:G:397:VAL:HG23	2.19	0.42
2:G:610:THR:HG21	2:G:614:LYS:HB3	2.00	0.42
2:H:247:ILE:HD12	2:H:526:THR:HG22	2.00	0.42
1:K:78:G:H21	2:D:502:ASN:CG	2.20	0.42
1:P:94:C:C2	1:P:95:A:C8	3.07	0.42
2:A:604:GLY:O	2:A:621:VAL:HG23	2.20	0.42
2:C:365:GLU:OE1	2:C:365:GLU:HA	2.19	0.42
2:D:422:THR:HB	2:D:438:GLU:OE2	2.19	0.42
2:D:610:THR:HG22	2:D:614:LYS:HB3	2.00	0.42
2:E:330:LYS:HA	2:E:331:PRO:HD3	1.61	0.42
2:E:417:VAL:HG13	2:E:471:TYR:CE1	2.50	0.42
2:E:490:PRO:HD3	2:E:509:MET:HE2	2.02	0.42
2:E:627:LYS:CB	2:E:640:LEU:HD21	2.47	0.42
2:F:569:VAL:O	2:F:570:LYS:HG2	2.20	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:H:347:SER:HA	2:H:498:VAL:H	1.85	0.42
2:H:529:PHE:CD2	2:H:534:PRO:HD3	2.55	0.42
1:I:86:G:C3'	5:I:109:HOH:O	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:O:78:G:P	5:O:1539:HOH:O	2.73	0.42
1:O:89:U:C2'	1:O:90:G:OP1	2.68	0.42
1:P:93:U:N3	1:P:94:C:C5	2.88	0.42
2:A:411:PHE:CD2	2:A:525:LEU:CD2	2.90	0.42
2:A:436:ARG:HG2	2:A:440:ASP:OD2	2.20	0.42
2:A:501:ASP:O	2:A:503:GLU:HG2	2.19	0.42
2:B:305:GLU:HA	2:B:310:TRP:HB3	2.01	0.42
2:C:411:PHE:CD2	2:C:521:PHE:HZ	2.37	0.42
2:C:459:GLY:HA2	2:C:465:LYS:HE2	2.01	0.42
2:C:460:ALA:C	2:C:462:TYR:N	2.72	0.42
2:C:488:SER:C	2:C:490:PRO:HD2	2.40	0.42
2:E:274:PHE:C	2:E:274:PHE:HD1	2.22	0.42
2:E:278:GLU:HG2	2:E:518:MET:HE2	2.01	0.42
2:E:317:MET:HG3	2:E:331:PRO:HG3	2.02	0.42
2:E:416:ILE:HG22	2:E:416:ILE:O	2.18	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:H:278:GLU:OE2	2:H:358:PHE:HD2	2.02	0.42
2:H:589:ARG:O	2:H:611:ARG:NH1	2.48	0.42
1:M:69:G:N7	1:P:105:C:C2	2.87	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:386:ILE:HB	2:A:510:ILE:HB	2.01	0.42
2:A:397:VAL:O	2:A:401:ILE:HG12	2.20	0.42
2:B:474:LEU:O	2:B:475:ASP:C	2.57	0.42
2:C:273:ILE:HG23	2:C:537:LEU:CD2	2.50	0.42
2:C:353:LEU:HB3	2:C:387:PHE:HB2	2.02	0.42
2:C:422:THR:O	2:C:423:ARG:C	2.57	0.42
2:D:242:ARG:HE	2:D:246:LYS:HD3	1.85	0.42
2:D:332:MET:HG2	2:D:363:ARG:NH2	2.34	0.42
2:D:400:CYS:O	2:D:404:VAL:HG23	2.19	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
2:F:602:GLU:N	2:F:602:GLU:OE1	2.53	0.42
2:G:548:THR:HG23	2:G:551:GLN:OE1	2.20	0.42
2:G:603:SER:C	2:G:605:LYS:H	2.22	0.42
2:H:459:GLY:HA2	2:H:465:LYS:HE2	2.02	0.42
1:J:87:U:H2'	1:J:88:G:OP2	2.19	0.42
1:K:70:G:C4	1:K:71:C:C5	3.07	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:69:G:N7	1:P:105:C:O2	2.52	0.42
2:C:341:PHE:O	2:C:346:LYS:NZ	2.45	0.42
2:C:365:GLU:N	2:C:377:ARG:HD3	2.33	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:D:402:ARG:NH1	2:D:402:ARG:CB	2.80	0.42
2:D:422:THR:O	2:D:423:ARG:C	2.58	0.42
2:E:297:PHE:CG	2:F:362:HIS:CE1	3.07	0.42
2:E:400:CYS:O	2:E:404:VAL:HG23	2.19	0.42
2:E:426:LYS:HE2	2:E:426:LYS:HB3	1.85	0.42
2:E:441:LEU:O	2:E:444:ALA:HB3	2.19	0.42
2:F:329:ILE:N	2:F:329:ILE:CD1	2.83	0.42
2:F:610:THR:HG22	2:F:614:LYS:O	2.19	0.42
2:G:590:VAL:O	2:G:611:ARG:HB3	2.19	0.42
2:H:543:VAL:HG11	2:H:585:HIS:CE1	2.53	0.42
2:H:604:GLY:O	2:H:621:VAL:HG23	2.20	0.42
1:I:89:U:C6	2:A:583:ARG:NH1	2.88	0.42
1:N:86:G:P	1:N:86:G:O4'	2.78	0.42
1:N:90:G:O5'	2:F:577:LYS:HD3	2.20	0.42
2:B:400:CYS:O	2:B:401:ILE:C	2.58	0.42
2:C:427:ARG:HB2	2:C:434:TRP:CZ2	2.55	0.42
2:C:550:SER:C	2:C:552:SER:H	2.23	0.42
2:C:562:LEU:HB3	2:C:569:VAL:HG11	2.01	0.42
2:C:602:GLU:N	2:C:602:GLU:OE1	2.53	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:D:452:PHE:CE2	2:D:454:TYR:HE1	2.22	0.42
2:D:542:VAL:CG1	2:D:543:VAL:N	2.82	0.42
2:E:323:GLU:CD	2:E:323:GLU:H	2.23	0.42
2:E:349:ARG:HE	2:E:349:ARG:HB2	1.61	0.42
2:G:305:GLU:HA	2:G:310:TRP:HB3	2.01	0.42
2:H:285:LEU:HD22	2:H:290:TYR:CG	2.54	0.42
2:H:462:TYR:CD2	2:H:486:ASP:OD2	2.72	0.42
2:H:531:GLY:O	2:H:589:ARG:HG3	2.20	0.42
1:K:80:U:H3'	1:K:80:U:C6	2.55	0.42
1:L:81:C:C4	1:L:82:U:C4	3.07	0.42
1:M:81:C:H2'	1:M:82:U:O4'	2.20	0.42
1:O:84:U:H3	2:G:549:ASP:CG	2.23	0.42
2:A:483:VAL:HG22	2:A:512:ARG:HB2	2.01	0.42
2:A:624:VAL:O	2:A:628:LEU:HG	2.20	0.42
2:B:252:ASP:OD1	2:B:267:HIS:CD2	2.72	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:411:PHE:HE2	2:B:521:PHE:CE1	2.27	0.42
2:B:426:LYS:HE2	2:B:426:LYS:HB3	1.87	0.42
2:C:317:MET:HG3	2:C:331:PRO:HG3	2.02	0.42
2:C:541:GLN:NE2	2:C:632:ILE:HD13	2.35	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
2:E:298:MET:CG	2:F:263:MET:HE2	2.48	0.42
2:E:441:LEU:HD23	2:E:441:LEU:HA	1.90	0.42
2:E:482:THR:O	2:E:512:ARG:HA	2.19	0.42
2:E:534:PRO:O	2:E:535:THR:C	2.58	0.42
2:E:603:SER:C	2:E:605:LYS:N	2.73	0.42
2:F:317:MET:HG3	2:F:331:PRO:HG3	2.01	0.42
2:F:327:TYR:CD1	2:F:327:TYR:N	2.87	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:F:603:SER:C	2:F:605:LYS:H	2.23	0.42
2:G:353:LEU:HB3	2:G:387:PHE:HB2	2.01	0.42
2:G:619:MET:HG3	2:G:624:VAL:HG12	2.01	0.42
2:H:394:ARG:O	2:H:397:VAL:N	2.53	0.42
2:H:621:VAL:O	2:H:622:ASN:C	2.57	0.42
1:J:84:U:H4'	1:J:85:C:H5'	2.01	0.42
1:J:95:A:H2'	1:J:96:C:O4'	2.20	0.42
2:A:610:THR:HG21	2:A:614:LYS:HB3	2.02	0.42
2:A:621:VAL:O	2:A:622:ASN:C	2.57	0.42
2:B:437:ALA:HA	2:B:485:LEU:HD23	2.02	0.42
2:B:597:GLY:O	2:B:601:VAL:HG23	2.20	0.42
2:C:421:SER:OG	2:C:467:GLU:OE2	2.37	0.42
2:C:519:GLU:CD	2:C:519:GLU:H	2.22	0.42
2:C:551:GLN:HE21	2:C:598:ASP:N	2.18	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:E:397:VAL:O	2:E:401:ILE:HG12	2.19	0.42
2:F:626:GLU:HG3	2:F:626:GLU:H	1.73	0.42
2:G:411:PHE:HE2	2:G:521:PHE:HE1	1.67	0.42
1:M:92:G:H2'	1:M:93:U:C6	2.53	0.41
2:D:583:ARG:HD3	5:D:5014:HOH:O	2.19	0.41
2:D:587:LEU:HD23	2:D:587:LEU:N	2.27	0.41
2:E:380:THR:N	2:E:519:GLU:OE2	2.52	0.41
2:E:627:LYS:O	2:E:630:GLN:HB3	2.20	0.41
2:F:287:GLU:HB2	2:F:288:TYR:CD1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:462:TYR:CD1	2:F:462:TYR:N	2.88	0.41
2:H:622:ASN:O	2:H:626:GLU:HG3	2.19	0.41
2:H:627:LYS:O	2:H:630:GLN:HB3	2.20	0.41
1:K:80:U:OP2	2:D:349:ARG:NH2	2.53	0.41
1:K:90:G:P	2:C:577:LYS:NZ	2.93	0.41
1:M:93:U:H2'	1:M:94:C:C6	2.53	0.41
1:O:77:U:O2'	1:O:98:A:N1	2.45	0.41
2:A:325:ARG:HH11	2:A:325:ARG:CG	2.24	0.41
2:A:347:SER:HA	2:A:498:VAL:H	1.84	0.41
2:B:603:SER:C	2:B:605:LYS:N	2.72	0.41
2:E:313:TYR:CE1	2:E:316:ALA:HB3	2.55	0.41
2:F:249:LYS:HB3	2:F:249:LYS:HZ3	1.84	0.41
2:F:594:LEU:CD2	2:F:608:VAL:HG22	2.50	0.41
2:H:253:LEU:O	2:H:270:GLY:HA3	2.20	0.41
2:H:460:ALA:C	2:H:462:TYR:N	2.72	0.41
2:H:500:GLU:C	2:H:502:ASN:N	2.71	0.41
1:L:83:U:H3	2:D:575:ASN:HD21	1.68	0.41
1:O:90:G:C8	2:G:577:LYS:HD3	2.55	0.41
2:A:342:ASN:HD22	2:A:342:ASN:HA	1.63	0.41
2:A:460:ALA:C	2:A:462:TYR:N	2.72	0.41
2:C:358:PHE:N	2:C:358:PHE:CD1	2.88	0.41
2:C:545:MET:SD	2:C:581:LYS:HB3	2.61	0.41
2:D:569:VAL:O	2:D:570:LYS:HG2	2.19	0.41
2:E:365:GLU:N	2:E:377:ARG:HD3	2.35	0.41
2:E:423:ARG:HE	2:E:438:GLU:CD	2.23	0.41
2:F:274:PHE:O	2:F:518:MET:HE3	2.20	0.41
2:G:473:CYS:HB2	2:G:527:GLU:OE1	2.21	0.41
2:G:562:LEU:O	2:G:565:ALA:HB3	2.20	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
1:J:74:A:C2	1:J:101:G:C2	3.09	0.41
1:K:99:C:O3'	2:C:249:LYS:NZ	2.54	0.41
1:M:76:G:N2	1:M:97:C:C2	2.89	0.41
2:A:371:HIS:O	2:A:372:GLY:C	2.57	0.41
2:C:298:MET:CG	2:D:263:MET:HE2	2.46	0.41
2:C:299:MET:HE1	2:C:335:PRO:HB2	2.03	0.41
2:D:285:LEU:HD21	2:D:512:ARG:HH12	1.85	0.41
2:D:594:LEU:CD2	2:D:608:VAL:HG22	2.51	0.41
2:E:353:LEU:HB3	2:E:387:PHE:HB2	2.01	0.41
2:F:349:ARG:HE	2:F:349:ARG:HB2	1.59	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:G:285:LEU:HD21	2:G:512:ARG:HH12	1.85	0.41
2:G:532:PHE:CZ	2:G:589:ARG:NH1	2.89	0.41
2:H:536:TRP:CE3	2:H:635:ARG:HD3	2.55	0.41
1:K:95:A:H2'	1:K:96:C:O4'	2.20	0.41
1:L:89:U:H5	2:D:583:ARG:NH2	2.18	0.41
2:A:455:GLN:O	2:A:456:LEU:O	2.38	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:B:627:LYS:CB	2:B:640:LEU:HD21	2.51	0.41
2:C:277:LEU:O	2:C:280:PHE:HB3	2.21	0.41
2:D:366:PRO:O	2:D:367:SER:C	2.59	0.41
2:E:249:LYS:HB3	2:E:249:LYS:HZ3	1.83	0.41
2:E:254:TYR:CD2	2:E:255:HIS:N	2.88	0.41
2:E:569:VAL:CG2	2:E:570:LYS:N	2.84	0.41
2:F:246:LYS:O	2:F:250:GLN:HG2	2.21	0.41
2:F:437:ALA:HB2	2:F:487:PHE:CD2	2.55	0.41
2:F:609:ARG:O	2:F:609:ARG:CG	2.69	0.41
2:G:323:GLU:O	2:G:324:ASN:O	2.38	0.41
2:G:526:THR:O	2:G:530:ALA:N	2.53	0.41
2:H:349:ARG:HE	2:H:349:ARG:HB2	1.64	0.41
2:H:465:LYS:HG3	2:H:484:GLN:CG	2.46	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:C:555:VAL:O	2:C:559:THR:HG23	2.21	0.41
2:D:482:THR:O	2:D:512:ARG:HA	2.20	0.41
2:E:253:LEU:O	2:E:270:GLY:HA3	2.20	0.41
2:E:389:THR:HG1	2:E:392:GLN:HG3	1.84	0.41
2:F:550:SER:C	2:F:552:SER:H	2.23	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:G:610:THR:HG22	2:G:614:LYS:HB3	2.02	0.41
2:H:366:PRO:O	2:H:367:SER:C	2.59	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:K:101:G:O2'	1:K:102:C:C5'	2.58	0.41
1:M:96:C:H2'	1:M:97:C:C6	2.55	0.41
1:O:70:G:O2'	1:O:71:C:H5'	2.21	0.41
2:A:274:PHE:CD1	2:A:274:PHE:C	2.94	0.41
2:A:365:GLU:N	2:A:377:ARG:HD3	2.33	0.41
2:B:514:ILE:HG22	2:B:515:LEU:HD23	2.02	0.41
2:B:609:ARG:O	2:B:609:ARG:CG	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:255:HIS:HE2	2:C:257:GLN:CG	2.34	0.41
2:C:263:MET:HE2	2:D:298:MET:CG	2.45	0.41
2:C:339:GLN:OE1	2:C:339:GLN:CA	2.67	0.41
2:D:330:LYS:HA	2:D:331:PRO:HD3	1.62	0.41
2:E:294:LYS:HA	2:E:357:GLU:HG3	2.02	0.41
2:E:298:MET:HE2	2:E:327:TYR:CD1	2.56	0.41
2:E:562:LEU:HD12	2:E:625:ILE:HD11	2.02	0.41
2:F:351:LEU:HD13	2:F:388:CYS:HA	2.02	0.41
2:F:421:SER:HB3	2:F:458:GLU:CB	2.40	0.41
2:F:554:TYR:CE1	2:F:558:LEU:HD11	2.56	0.41
2:G:371:HIS:O	2:G:372:GLY:C	2.59	0.41
2:G:543:VAL:HG21	2:G:590:VAL:HG21	2.03	0.41
2:G:584:GLU:O	2:G:588:ARG:HB2	2.20	0.41
1:O:87:U:H2'	1:O:88:G:OP2	2.20	0.41
1:P:86:G:H2'	5:P:1613:HOH:O	2.20	0.41
2:A:452:PHE:HE2	2:A:454:TYR:CE1	2.23	0.41
2:B:299:MET:O	2:B:304:TRP:HZ3	2.04	0.41
2:B:365:GLU:N	2:B:377:ARG:HD3	2.35	0.41
2:C:329:ILE:N	2:C:329:ILE:CD1	2.84	0.41
2:D:288:TYR:CZ	2:D:403:LEU:HD13	2.56	0.41
2:D:526:THR:HG23	2:D:533:PHE:CZ	2.56	0.41
2:E:323:GLU:O	2:E:324:ASN:O	2.38	0.41
2:E:421:SER:HB3	2:E:458:GLU:CB	2.32	0.41
2:F:441:LEU:HD23	2:F:441:LEU:HA	1.91	0.41
2:G:358:PHE:N	2:G:358:PHE:CD1	2.87	0.41
2:H:274:PHE:C	2:H:274:PHE:HD1	2.24	0.41
2:H:332:MET:HE2	4:H:9002:TSB:HN12	1.86	0.41
2:H:353:LEU:HB3	2:H:387:PHE:HB2	2.02	0.41
2:H:386:ILE:O	2:H:509:MET:HA	2.20	0.41
2:H:462:TYR:CE2	2:H:511:HIS:NE2	2.89	0.41
2:H:547:ILE:HG12	2:H:578:ILE:HD12	2.02	0.41
1:I:88:G:N2	5:I:111:HOH:O	2.47	0.41
1:J:93:U:N3	1:J:94:C:C5	2.89	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:O:69:G:O2'	1:O:70:G:H5'	2.21	0.41
1:O:80:U:H2'	1:O:81:C:H6	1.84	0.41
1:P:78:G:H5'	5:P:1639:HOH:O	2.21	0.41
1:P:97:C:C4'	1:P:98:A:OP1	2.69	0.41
2:A:253:LEU:O	2:A:270:GLY:HA3	2.21	0.41
2:A:300:ASP:OD2	2:A:302:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:300:ASP:HB2	2:B:259:GLU:O	2.21	0.41
2:A:459:GLY:HA2	2:A:465:LYS:HE2	2.03	0.41
2:A:501:ASP:CG	2:A:503:GLU:HB2	2.42	0.41
2:A:550:SER:C	2:A:552:SER:H	2.24	0.41
2:B:280:PHE:HE2	2:B:407:MET:HG2	1.85	0.41
2:C:452:PHE:CE2	2:C:454:TYR:HE1	2.22	0.41
2:C:480:CYS:O	2:C:516:GLY:CA	2.69	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:C:538:ALA:O	2:C:539:PRO:C	2.59	0.41
2:D:421:SER:HB3	2:D:459:GLY:N	2.35	0.41
2:E:247:ILE:HA	2:E:250:GLN:HB2	2.03	0.41
2:E:250:GLN:HA	2:E:250:GLN:NE2	2.36	0.41
2:E:348:TYR:CE2	2:E:500:GLU:HG3	2.56	0.41
2:E:455:GLN:O	2:E:456:LEU:C	2.59	0.41
2:E:528:GLU:O	2:E:530:ALA:N	2.53	0.41
2:F:348:TYR:CE2	2:F:500:GLU:HG3	2.55	0.41
2:F:358:PHE:N	2:F:358:PHE:CD1	2.88	0.41
2:F:462:TYR:HE2	2:F:511:HIS:CD2	2.39	0.41
2:F:493:LEU:N	2:F:493:LEU:HD23	2.35	0.41
2:G:298:MET:O	2:G:298:MET:HG2	2.21	0.41
2:G:377:ARG:HH11	2:G:377:ARG:HG3	1.86	0.41
2:G:517:SER:HB3	4:G:8002:TSB:H1'	2.00	0.41
2:G:594:LEU:CD2	2:G:608:VAL:HG22	2.51	0.41
2:G:602:GLU:N	2:G:602:GLU:OE1	2.54	0.41
2:H:427:ARG:HA	2:H:461:PHE:O	2.21	0.41
2:H:555:VAL:O	2:H:559:THR:HG23	2.20	0.41
1:L:72:G:H2'	1:L:73:U:C6	2.56	0.41
1:O:76:G:H21	1:O:99:C:N4	2.19	0.41
2:A:399:GLY:HA2	2:A:402:ARG:HH11	1.86	0.41
2:A:529:PHE:CD1	2:A:529:PHE:N	2.76	0.41
2:A:626:GLU:HG3	2:A:626:GLU:H	1.70	0.41
2:B:254:TYR:CD2	2:B:255:HIS:N	2.89	0.41
2:B:397:VAL:O	2:B:401:ILE:HG12	2.21	0.41
2:B:482:THR:HG21	4:B:3002:TSB:H5'2	2.02	0.41
2:C:500:GLU:C	2:C:502:ASN:N	2.72	0.41
2:C:526:THR:O	2:C:530:ALA:HA	2.20	0.41
2:D:277:LEU:O	2:D:280:PHE:HB3	2.20	0.41
2:D:320:THR:HG22	2:D:321:SER:N	2.26	0.41
2:D:390:GLU:H	2:D:390:GLU:HG2	1.71	0.41
2:D:538:ALA:O	2:D:539:PRO:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:300:ASP:HB3	2:F:259:GLU:HB2	2.03	0.41
2:E:422:THR:HB	2:E:438:GLU:OE2	2.21	0.41
2:E:427:ARG:HA	2:E:461:PHE:O	2.21	0.41
2:E:519:GLU:CD	2:E:519:GLU:H	2.22	0.41
2:F:423:ARG:HB3	2:F:434:TRP:CE3	2.56	0.41
2:G:255:HIS:HE2	2:G:257:GLN:CG	2.33	0.41
2:G:417:VAL:HG13	2:G:471:TYR:CE1	2.46	0.41
2:H:358:PHE:N	2:H:358:PHE:CD1	2.89	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:H:588:ARG:C	2:H:589:ARG:HG2	2.40	0.41
1:I:87:U:H2'	1:I:88:G:OP2	2.20	0.40
1:L:80:U:H2'	1:L:81:C:H6	1.85	0.40
1:M:69:G:P	1:P:105:C:C2'	3.09	0.40
2:A:421:SER:OG	2:A:467:GLU:OE2	2.39	0.40
2:A:441:LEU:HD23	2:A:441:LEU:HA	1.91	0.40
2:B:298:MET:CE	2:B:327:TYR:HB2	2.51	0.40
2:C:462:TYR:HE2	2:C:511:HIS:CD2	2.38	0.40
2:E:294:LYS:HA	2:E:294:LYS:HD2	1.85	0.40
2:F:424:PRO:HD2	2:F:434:TRP:CH2	2.55	0.40
2:G:294:LYS:HA	2:G:294:LYS:HD2	1.76	0.40
2:G:545:MET:CE	2:G:593:MET:HB3	2.51	0.40
2:H:426:LYS:HE2	2:H:426:LYS:HB3	1.90	0.40
2:H:562:LEU:HB3	2:H:569:VAL:HG11	2.02	0.40
1:N:89:U:O2'	2:F:580:PHE:CB	2.69	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:B:380:THR:N	2:B:519:GLU:OE2	2.54	0.40
2:B:436:ARG:HG2	2:B:440:ASP:OD2	2.21	0.40
2:C:281:VAL:O	2:C:282:ARG:C	2.60	0.40
2:C:353:LEU:HD22	2:C:353:LEU:HA	1.81	0.40
2:C:499:GLY:HA3	2:C:501:ASP:OD1	2.20	0.40
2:C:567:ILE:O	2:C:569:VAL:N	2.54	0.40
2:D:313:TYR:CE1	2:D:316:ALA:HB3	2.56	0.40
2:D:386:ILE:O	2:D:509:MET:HA	2.21	0.40
2:E:362:HIS:CD2	5:E:6011:HOH:O	2.70	0.40
2:E:430:SER:O	2:E:433:MET:HB2	2.20	0.40
2:E:437:ALA:HB2	2:E:487:PHE:CD2	2.56	0.40
2:E:501:ASP:O	2:E:503:GLU:HG2	2.22	0.40
2:G:247:ILE:HD12	2:G:526:THR:HG22	2.02	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:G:567:ILE:O	2:G:569:VAL:HG12	2.22	0.40
2:H:339:GLN:OE1	2:H:339:GLN:CA	2.69	0.40
1:P:93:U:C2	1:P:94:C:C6	3.10	0.40
2:A:423:ARG:HE	2:A:438:GLU:CD	2.23	0.40
2:A:603:SER:C	2:A:605:LYS:H	2.24	0.40
2:A:609:ARG:HD3	2:A:610:THR:O	2.22	0.40
2:C:323:GLU:CD	2:C:323:GLU:H	2.23	0.40
2:C:356:ALA:HB2	2:C:384:ALA:HB2	2.03	0.40
2:C:426:LYS:HE2	2:C:426:LYS:HB3	1.89	0.40
2:D:430:SER:O	2:D:433:MET:HB2	2.21	0.40
2:D:539:PRO:O	2:D:568:ARG:HD2	2.21	0.40
2:D:576:GLU:HG2	2:D:580:PHE:CD2	2.56	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:G:544:ILE:CG2	2:G:555:VAL:HG13	2.49	0.40
2:H:288:TYR:CZ	2:H:403:LEU:HD13	2.57	0.40
2:H:371:HIS:O	2:H:372:GLY:C	2.59	0.40
2:H:437:ALA:HA	2:H:485:LEU:HD23	2.03	0.40
1:K:79:A:OP1	2:D:349:ARG:NH2	2.54	0.40
1:M:84:U:O2'	1:M:85:C:P	2.79	0.40
1:O:92:G:H2'	1:O:93:U:C6	2.55	0.40
1:P:95:A:H2'	1:P:96:C:O4'	2.20	0.40
2:A:393:ILE:HD11	2:A:508:VAL:HG11	2.02	0.40
2:A:545:MET:SD	2:A:581:LYS:HB3	2.61	0.40
2:B:249:LYS:HE2	2:B:249:LYS:HA	2.03	0.40
2:B:356:ALA:HA	2:B:384:ALA:HA	2.04	0.40
2:B:358:PHE:N	2:B:358:PHE:HD1	2.19	0.40
2:B:551:GLN:CD	2:B:551:GLN:H	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:C:423:ARG:HG2	2:C:423:ARG:O	2.21	0.40
2:C:433:MET:HB3	2:C:433:MET:HE2	1.97	0.40
2:C:460:ALA:C	2:C:462:TYR:H	2.24	0.40
2:C:554:TYR:CE1	2:C:558:LEU:HD11	2.56	0.40
2:C:621:VAL:O	2:C:622:ASN:C	2.59	0.40
2:D:356:ALA:HA	2:D:384:ALA:CB	2.52	0.40
2:D:427:ARG:HA	2:D:461:PHE:O	2.22	0.40
2:F:323:GLU:CD	2:F:323:GLU:H	2.22	0.40
2:G:349:ARG:HE	2:G:349:ARG:HB2	1.64	0.40
2:G:554:TYR:CE1	2:G:558:LEU:HD11	2.56	0.40
2:H:251:LEU:CA	2:H:588:ARG:HH12	2.27	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:348:TYR:CE2	2:H:500:GLU:HG3	2.56	0.40
2:H:460:ALA:C	2:H:462:TYR:H	2.25	0.40
2:A:415:LYS:HG2	2:A:471:TYR:CD1	2.57	0.40
2:A:534:PRO:O	2:A:535:THR:C	2.59	0.40
2:B:501:ASP:O	2:B:502:ASN:C	2.58	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:E:490:PRO:HD3	2:E:509:MET:CE	2.51	0.40
2:E:548:THR:HG22	2:E:551:GLN:HE22	1.86	0.40
2:F:294:LYS:HA	2:F:294:LYS:HD2	1.83	0.40
2:F:356:ALA:CB	2:F:384:ALA:HB2	2.51	0.40
2:G:482:THR:O	2:G:512:ARG:HA	2.21	0.40
2:H:433:MET:HB3	2:H:433:MET:HE2	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%)	2 20
2	B	399/401 (100%)	325 (82%)	57 (14%)	17 (4%)	2 22
2	C	399/401 (100%)	327 (82%)	52 (13%)	20 (5%)	2 19
2	D	399/401 (100%)	327 (82%)	54 (14%)	18 (4%)	2 21
2	E	399/401 (100%)	327 (82%)	55 (14%)	17 (4%)	2 22
2	F	399/401 (100%)	327 (82%)	52 (13%)	20 (5%)	2 19
2	G	399/401 (100%)	323 (81%)	55 (14%)	21 (5%)	2 17
2	H	399/401 (100%)	323 (81%)	55 (14%)	21 (5%)	2 17
All	All	3192/3208 (100%)	2606 (82%)	433 (14%)	153 (5%)	2 20

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 (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	356/356 (100%)	317 (89%)	39 (11%)	6 29
2	B	356/356 (100%)	318 (89%)	38 (11%)	6 30
2	C	356/356 (100%)	321 (90%)	35 (10%)	8 33

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	356/356 (100%)	321 (90%)	35 (10%)	8	33
2	E	356/356 (100%)	319 (90%)	37 (10%)	7	31
2	F	356/356 (100%)	320 (90%)	36 (10%)	7	32
2	G	356/356 (100%)	315 (88%)	41 (12%)	5	26
2	H	356/356 (100%)	320 (90%)	36 (10%)	7	32
All	All	2848/2848 (100%)	2551 (90%)	297 (10%)	7	31

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

Sometimes 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 (i)

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 monosaccharides 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	D	5002	3	29,32,32	2.51	4 (13%)	33,48,48	0.97	2 (6%)
4	TSB	G	8002	3	29,32,32	2.47	5 (17%)	33,48,48	1.44	4 (12%)
4	TSB	A	2002	3	29,32,32	1.93	4 (13%)	33,48,48	1.16	4 (12%)
4	TSB	F	7002	3	29,32,32	2.00	3 (10%)	33,48,48	1.15	5 (15%)
4	TSB	B	3002	3	29,32,32	2.91	4 (13%)	33,48,48	1.04	3 (9%)
4	TSB	H	9002	3	29,32,32	2.24	4 (13%)	33,48,48	1.20	4 (12%)
4	TSB	E	6002	3	29,32,32	2.65	4 (13%)	33,48,48	1.09	2 (6%)
4	TSB	C	4002	3	29,32,32	2.24	4 (13%)	33,48,48	1.10	3 (9%)

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	D	5002	3	-	4/18/39/39	0/3/3/3
4	TSB	G	8002	3	-	3/18/39/39	0/3/3/3
4	TSB	A	2002	3	-	5/18/39/39	0/3/3/3
4	TSB	F	7002	3	-	4/18/39/39	0/3/3/3
4	TSB	B	3002	3	-	5/18/39/39	0/3/3/3
4	TSB	H	9002	3	-	4/18/39/39	0/3/3/3
4	TSB	E	6002	3	-	5/18/39/39	0/3/3/3
4	TSB	C	4002	3	-	4/18/39/39	0/3/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	3002	TSB	O1S-S1	11.28	1.52	1.42
4	E	6002	TSB	O1S-S1	10.21	1.51	1.42
4	G	8002	TSB	O2S-S1	9.74	1.50	1.42
4	B	3002	TSB	O2S-S1	9.46	1.50	1.42
4	D	5002	TSB	O1S-S1	9.22	1.50	1.42
4	E	6002	TSB	O2S-S1	8.77	1.49	1.42
4	H	9002	TSB	O2S-S1	8.50	1.49	1.42
4	C	4002	TSB	O2S-S1	8.37	1.49	1.42
4	D	5002	TSB	O2S-S1	8.01	1.49	1.42
4	F	7002	TSB	O2S-S1	7.46	1.48	1.42
4	A	2002	TSB	O2S-S1	7.08	1.48	1.42
4	H	9002	TSB	O1S-S1	6.92	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	4002	TSB	O1S-S1	6.80	1.48	1.42
4	G	8002	TSB	O1S-S1	6.77	1.48	1.42
4	F	7002	TSB	O1S-S1	6.25	1.47	1.42
4	A	2002	TSB	O1S-S1	5.65	1.47	1.42
4	C	4002	TSB	S1-N8	3.94	1.66	1.59
4	B	3002	TSB	S1-N8	3.42	1.65	1.59
4	D	5002	TSB	CA-C	3.38	1.56	1.53
4	F	7002	TSB	S1-N8	3.28	1.65	1.59
4	D	5002	TSB	S1-N8	3.23	1.65	1.59
4	A	2002	TSB	S1-N8	2.98	1.65	1.59
4	G	8002	TSB	C2-N3	2.97	1.36	1.32
4	H	9002	TSB	S1-N8	2.88	1.65	1.59
4	G	8002	TSB	S1-N8	2.80	1.64	1.59
4	B	3002	TSB	CA-C	2.29	1.55	1.53
4	G	8002	TSB	C4-N3	-2.21	1.32	1.35
4	E	6002	TSB	CA-C	2.18	1.55	1.53
4	E	6002	TSB	S1-N8	2.09	1.63	1.59
4	H	9002	TSB	C2-N3	2.02	1.35	1.32
4	C	4002	TSB	CA-C	2.01	1.55	1.53
4	A	2002	TSB	C-N8	-2.01	1.33	1.37

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	8002	TSB	O-C-CA	-4.75	116.99	120.73
4	G	8002	TSB	C-CA-N	-3.96	104.23	110.28
4	E	6002	TSB	C-CA-N	-3.85	104.40	110.28
4	H	9002	TSB	O-C-CA	-3.79	117.75	120.73
4	F	7002	TSB	O-C-CA	-3.22	118.20	120.73
4	B	3002	TSB	C-CA-N	-3.16	105.45	110.28
4	A	2002	TSB	O-C-CA	-3.11	118.28	120.73
4	A	2002	TSB	C-CA-N	-3.02	105.66	110.28
4	C	4002	TSB	O-C-CA	-3.02	118.35	120.73
4	G	8002	TSB	CA-C-N8	2.68	120.68	114.23
4	C	4002	TSB	C-CA-N	-2.54	106.41	110.28
4	D	5002	TSB	C-CA-N	-2.53	106.41	110.28
4	B	3002	TSB	O-C-CA	-2.51	118.76	120.73
4	H	9002	TSB	C-CA-N	-2.51	106.45	110.28
4	G	8002	TSB	C5-C6-N6	2.32	123.87	120.35
4	H	9002	TSB	CA-C-N8	2.22	119.59	114.23
4	A	2002	TSB	CA-C-N8	2.16	119.43	114.23
4	A	2002	TSB	C5-C6-N6	2.16	123.63	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	7002	TSB	O5'-C5'-C4'	2.15	111.64	107.62
4	E	6002	TSB	O-C-CA	-2.12	119.06	120.73
4	F	7002	TSB	C5'-O5'-S1	2.11	121.74	117.37
4	B	3002	TSB	CA-C-N8	2.11	119.31	114.23
4	F	7002	TSB	C-CA-N	-2.08	107.10	110.28
4	H	9002	TSB	C5-C6-N6	2.06	123.48	120.35
4	F	7002	TSB	CA-C-N8	2.05	119.16	114.23
4	C	4002	TSB	C5-C6-N6	2.04	123.45	120.35
4	D	5002	TSB	C5-C6-N6	2.03	123.44	120.35

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2002	TSB	C-N8-S1-O1S
4	A	2002	TSB	C-N8-S1-O2S
4	A	2002	TSB	C5'-O5'-S1-N8
4	B	3002	TSB	C-N8-S1-O1S
4	B	3002	TSB	C-N8-S1-O2S
4	B	3002	TSB	C5'-O5'-S1-N8
4	C	4002	TSB	C5'-O5'-S1-N8
4	D	5002	TSB	C-N8-S1-O2S
4	D	5002	TSB	C5'-O5'-S1-N8
4	E	6002	TSB	C-N8-S1-O1S
4	E	6002	TSB	C-N8-S1-O2S
4	E	6002	TSB	C5'-O5'-S1-N8
4	F	7002	TSB	C5'-O5'-S1-N8
4	G	8002	TSB	C-N8-S1-O2S
4	G	8002	TSB	C5'-O5'-S1-N8
4	H	9002	TSB	C-N8-S1-O2S
4	H	9002	TSB	C5'-O5'-S1-N8
4	A	2002	TSB	C5'-O5'-S1-O1S
4	B	3002	TSB	C5'-O5'-S1-O1S
4	C	4002	TSB	C5'-O5'-S1-O1S
4	D	5002	TSB	C5'-O5'-S1-O1S
4	E	6002	TSB	C5'-O5'-S1-O1S
4	F	7002	TSB	C5'-O5'-S1-O1S
4	H	9002	TSB	C5'-O5'-S1-O1S
4	C	4002	TSB	C-N8-S1-O2S
4	F	7002	TSB	C-N8-S1-O2S
4	F	7002	TSB	C5'-O5'-S1-O2S
4	G	8002	TSB	C5'-O5'-S1-O1S

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Mol	Chain	Res	Type	Atoms
4	A	2002	TSB	C5'-O5'-S1-O2S
4	B	3002	TSB	C5'-O5'-S1-O2S
4	C	4002	TSB	C5'-O5'-S1-O2S
4	D	5002	TSB	C5'-O5'-S1-O2S
4	E	6002	TSB	C5'-O5'-S1-O2S
4	H	9002	TSB	C5'-O5'-S1-O2S

There are no ring outliers.

8 monomers are involved in 31 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

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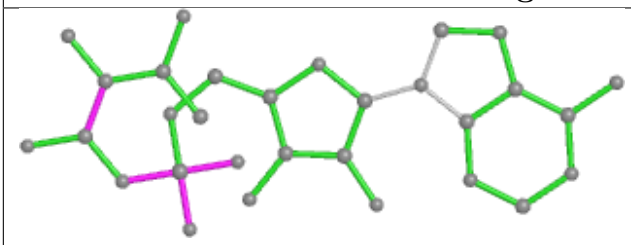
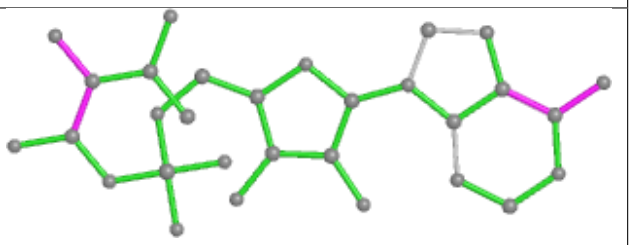
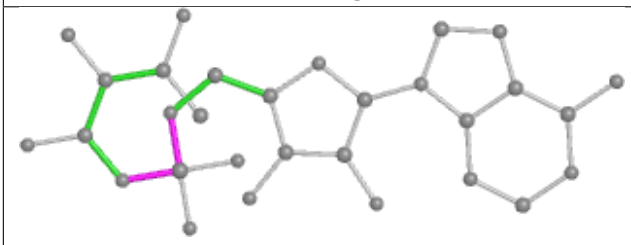
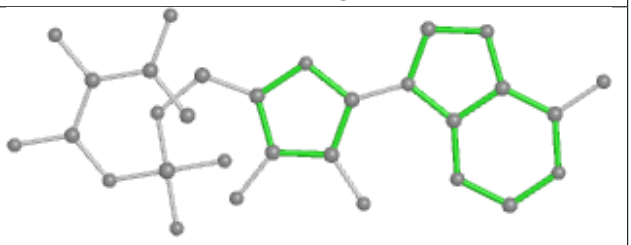
 Bond lengths	 Bond angles
 Torsions	 Rings

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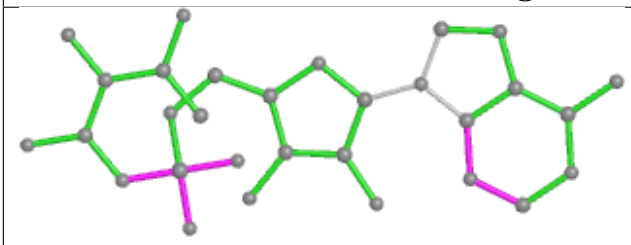
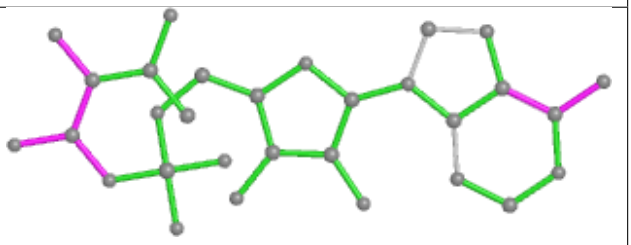
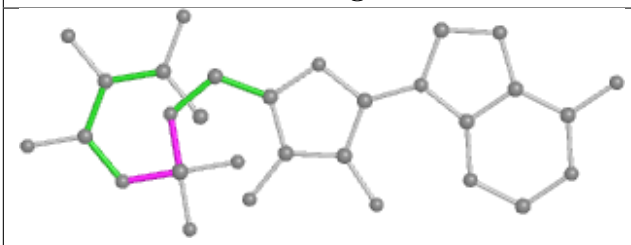
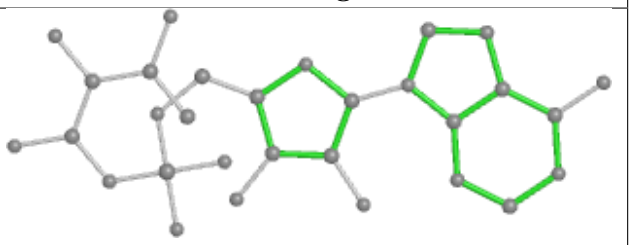
 Bond lengths	 Bond angles
 Torsions	 Rings

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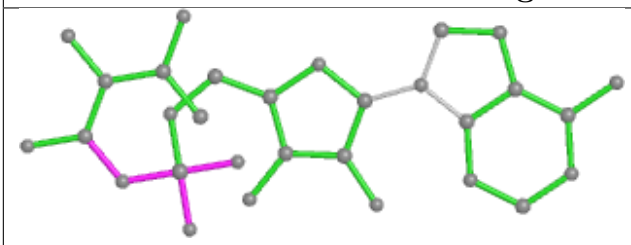
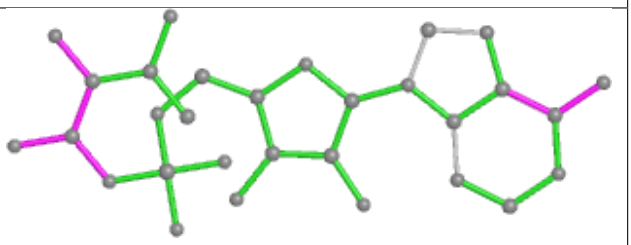
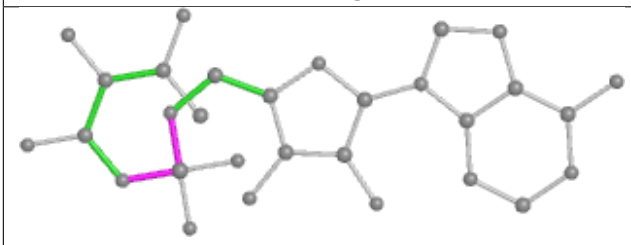
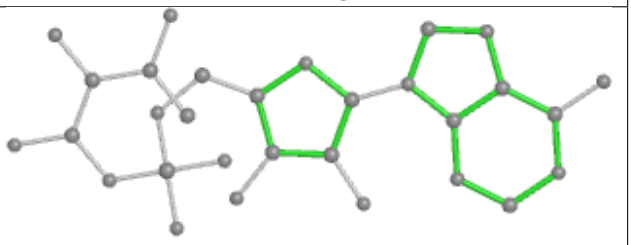
 Bond lengths	 Bond angles
 Torsions	 Rings

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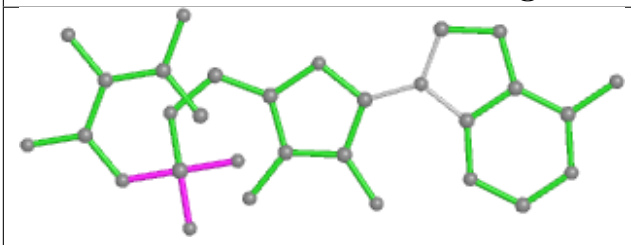
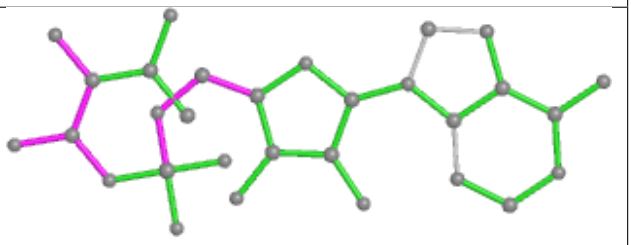
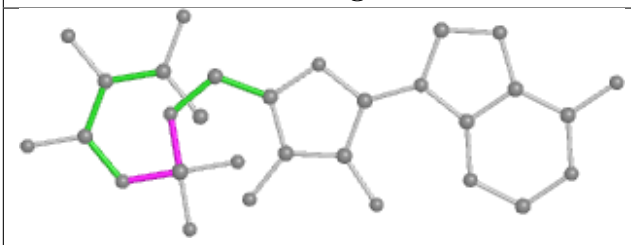
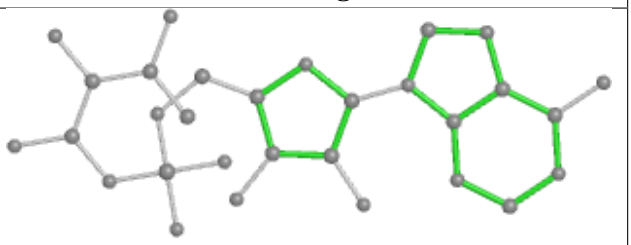
 Bond lengths	 Bond angles
 Torsions	 Rings

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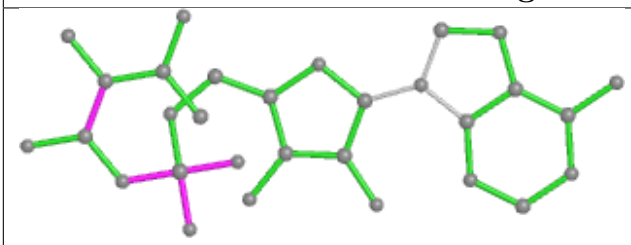
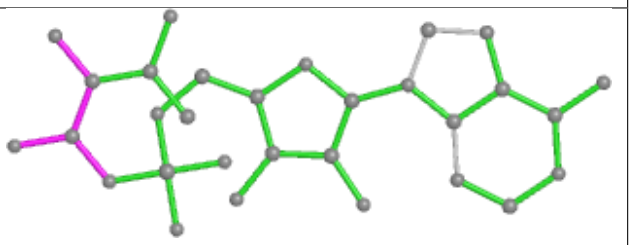
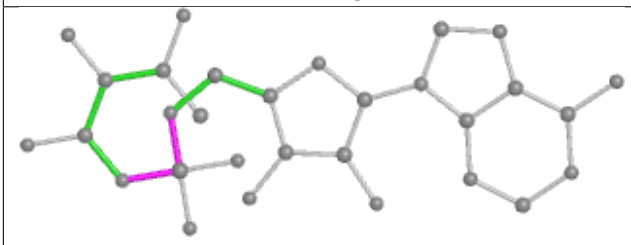
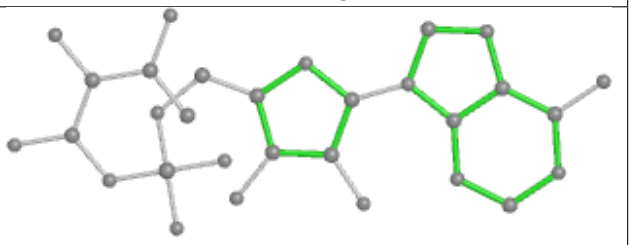
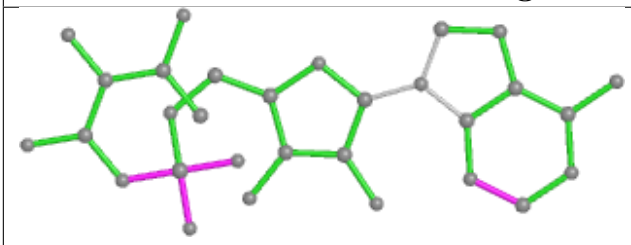
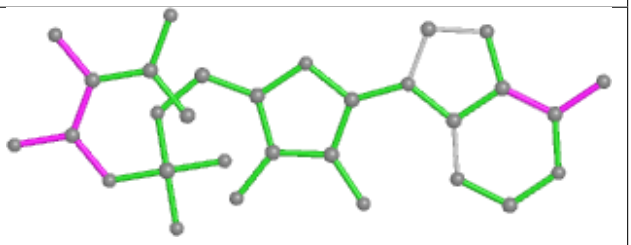
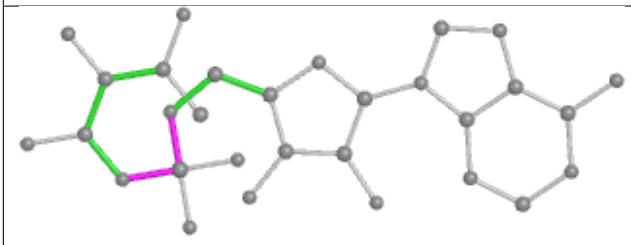
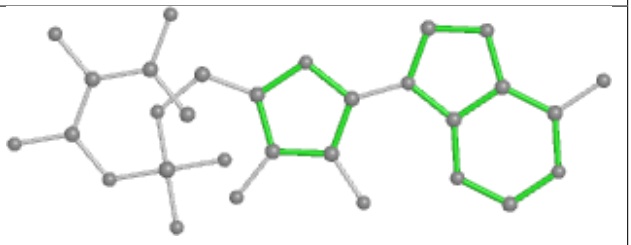
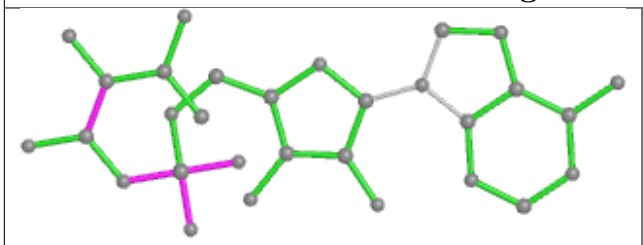
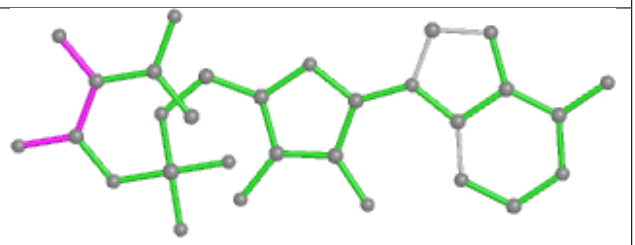
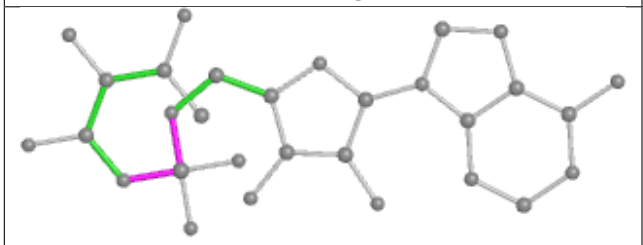
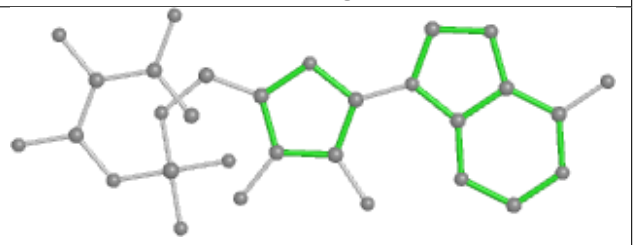
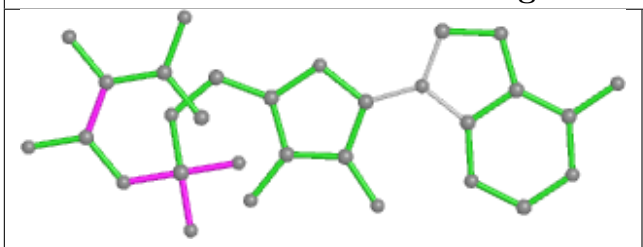
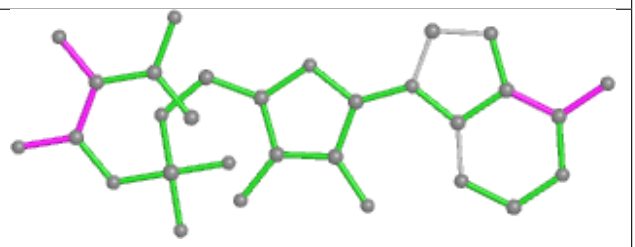
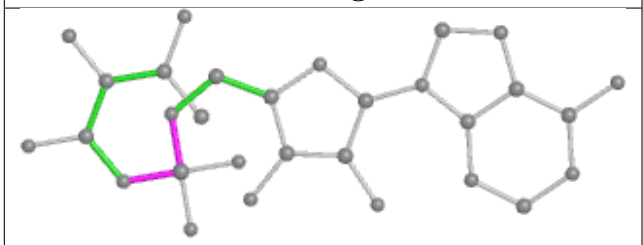
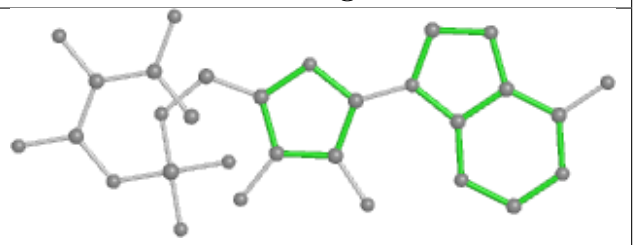
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TSB H 9002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TSB E 6002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand TSB C 4002	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	I	37/37 (100%)	1.49	12 (32%)	0	0	82, 115, 150, 153	0
1	J	37/37 (100%)	0.91	6 (16%)	1	2	55, 88, 135, 152	0
1	K	37/37 (100%)	2.68	24 (64%)	0	0	119, 148, 168, 184	0
1	L	37/37 (100%)	1.61	13 (35%)	0	0	110, 134, 170, 180	0
1	M	37/37 (100%)	1.05	6 (16%)	1	2	60, 86, 153, 166	0
1	N	37/37 (100%)	3.69	34 (91%)	0	0	140, 163, 181, 184	0
1	O	37/37 (100%)	0.42	1 (2%)	54	48	45, 67, 115, 124	0
1	P	37/37 (100%)	1.21	9 (24%)	0	0	46, 104, 155, 159	0
2	A	401/401 (100%)	-0.23	3 (0%)	87	83	15, 68, 109, 136	0
2	B	401/401 (100%)	-0.14	4 (0%)	82	77	17, 62, 105, 137	0
2	C	401/401 (100%)	0.26	19 (4%)	31	28	55, 101, 146, 160	0
2	D	401/401 (100%)	0.53	42 (10%)	6	7	80, 123, 147, 158	0
2	E	401/401 (100%)	0.66	49 (12%)	4	5	75, 126, 150, 168	0
2	F	401/401 (100%)	0.43	33 (8%)	11	12	47, 105, 148, 168	0
2	G	401/401 (100%)	-0.29	0	100	100	7, 48, 98, 132	0
2	H	401/401 (100%)	-0.21	3 (0%)	87	83	14, 68, 105, 135	0
All	All	3504/3504 (100%)	0.25	258 (7%)	14	14	7, 91, 147, 184	0

All (258) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	546	ASN	8.1
2	C	546	ASN	7.9
1	N	97	C	7.6
2	C	596	CYS	7.1
1	N	85	C	6.6

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Mol	Chain	Res	Type	RSRZ
1	N	94	C	6.6
2	F	571	ALA	6.6
1	N	84	U	6.5
1	N	83	U	6.3
1	K	74	A	6.3
1	K	72	G	6.1
1	N	80	U	5.6
2	F	596	CYS	5.6
2	D	642	GLU	5.5
2	E	498	VAL	5.4
2	D	427	ARG	5.4
2	F	260	ALA	5.1
1	K	85	C	5.0
1	K	84	U	4.9
2	D	641	GLU	4.9
1	L	85	C	4.8
1	K	73	U	4.7
1	K	71	C	4.7
1	M	69	G	4.7
1	N	87	U	4.6
2	D	482	THR	4.6
1	K	76	G	4.5
1	I	70	G	4.5
1	N	79	A	4.4
2	D	484	GLN	4.4
1	M	85	C	4.4
1	N	78	G	4.3
1	I	85	C	4.3
1	K	80	U	4.2
2	C	551	GLN	4.2
1	N	70	G	4.2
1	M	105	C	4.0
2	E	356	ALA	4.0
1	L	78	G	3.9
1	N	75	U	3.8
1	N	96	C	3.7
1	N	102	C	3.7
2	E	504	ARG	3.7
2	E	317	MET	3.6
1	J	85	C	3.6
2	E	547	ILE	3.6
1	K	82	U	3.6

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Mol	Chain	Res	Type	RSRZ
1	K	70	G	3.6
2	B	360	SER	3.5
2	E	316	ALA	3.5
1	N	81	C	3.5
1	N	82	U	3.5
1	I	69	G	3.5
1	N	86	G	3.5
2	D	481	GLY	3.5
1	K	101	G	3.5
2	E	371	HIS	3.5
1	N	98	A	3.5
1	K	94	C	3.4
1	K	97	C	3.4
1	N	101	G	3.4
1	N	103	G	3.4
1	N	91	G	3.4
1	L	70	G	3.4
2	F	364	ASN	3.3
1	I	103	G	3.3
2	E	427	ARG	3.3
2	D	472	ASP	3.3
2	E	384	ALA	3.3
2	F	259	GLU	3.3
2	D	640	LEU	3.3
2	D	348	TYR	3.3
1	K	75	U	3.2
2	E	499	GLY	3.2
1	N	99	C	3.2
2	E	377	ARG	3.2
2	F	484	GLN	3.2
1	I	71	C	3.2
1	N	92	G	3.2
2	D	415	LYS	3.2
2	D	474	LEU	3.1
1	J	84	U	3.1
2	D	503	GLU	3.1
1	I	101	G	3.1
1	N	90	G	3.1
1	I	102	C	3.0
1	K	103	G	3.0
2	F	575	ASN	3.0
1	N	105	C	3.0

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Mol	Chain	Res	Type	RSRZ
1	N	73	U	3.0
1	K	83	U	3.0
2	D	596	CYS	2.9
2	D	501	ASP	2.9
1	N	95	A	2.9
1	N	93	U	2.9
1	K	104	C	2.9
2	E	383	ASP	2.8
2	F	482	THR	2.8
1	N	104	C	2.8
2	E	366	PRO	2.8
2	C	259	GLU	2.8
2	E	291	GLN	2.8
2	D	498	VAL	2.8
2	D	511	HIS	2.8
2	D	504	ARG	2.8
2	D	356	ALA	2.8
2	D	499	GLY	2.8
2	F	545	MET	2.8
2	F	377	ARG	2.7
2	F	261	PRO	2.7
2	C	327	TYR	2.7
2	E	374	MET	2.7
1	N	71	C	2.7
1	N	74	A	2.7
2	D	516	GLY	2.7
1	P	76	G	2.7
2	E	497	TYR	2.7
2	C	548	THR	2.7
2	F	242	ARG	2.7
2	D	286	LYS	2.7
2	C	579	GLY	2.7
2	C	642	GLU	2.7
2	C	482	THR	2.6
2	E	333	ASN	2.6
1	N	72	G	2.6
1	L	84	U	2.6
1	I	74	A	2.6
1	K	102	C	2.6
2	D	502	ASN	2.6
2	E	482	THR	2.6
2	E	288	TYR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	372	GLY	2.6
1	N	100	U	2.6
2	F	549	ASP	2.6
2	F	481	GLY	2.6
1	P	70	G	2.6
2	E	423	ARG	2.6
2	B	499	GLY	2.6
2	D	476	ARG	2.6
1	O	69	G	2.6
2	E	355	MET	2.6
2	C	550	SER	2.6
2	D	333	ASN	2.5
1	I	105	C	2.5
1	L	87	U	2.5
1	L	101	G	2.5
2	B	502	ASN	2.5
2	D	383	ASP	2.5
1	J	105	C	2.5
1	K	81	C	2.5
2	F	513	ALA	2.5
2	D	513	ALA	2.5
2	E	481	GLY	2.5
2	D	505	LYS	2.5
2	F	574	ARG	2.5
2	E	385	HIS	2.5
1	L	69	G	2.4
1	K	105	C	2.4
1	P	97	C	2.4
2	E	419	LYS	2.4
1	J	103	G	2.4
2	H	500	GLU	2.4
2	D	475	ASP	2.4
2	F	543	VAL	2.4
1	J	104	C	2.4
2	E	516	GLY	2.4
2	C	478	TRP	2.4
2	E	641	GLU	2.4
2	E	398	ASN	2.4
2	D	392	GLN	2.4
2	D	378	GLY	2.4
2	D	480	CYS	2.4
2	E	417	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	69	G	2.4
2	F	372	GLY	2.4
2	F	548	THR	2.4
2	E	596	CYS	2.4
1	P	105	C	2.4
2	E	496	SER	2.4
2	E	513	ALA	2.4
2	F	376	VAL	2.4
1	M	104	C	2.4
1	P	101	G	2.4
2	E	388	CYS	2.4
1	M	84	U	2.3
2	D	317	MET	2.3
2	D	500	GLU	2.3
2	F	244	HIS	2.3
1	L	100	U	2.3
2	C	374	MET	2.3
1	L	86	G	2.3
2	E	354	ARG	2.3
2	F	547	ILE	2.3
2	E	378	GLY	2.3
2	F	307	THR	2.3
2	F	367	SER	2.3
1	L	105	C	2.3
2	H	499	GLY	2.3
2	D	473	CYS	2.3
1	P	72	G	2.3
2	C	578	ILE	2.3
2	E	474	LEU	2.3
1	L	81	C	2.2
2	D	517	SER	2.2
2	D	547	ILE	2.2
2	F	582	ILE	2.2
2	F	455	GLN	2.2
1	P	73	U	2.2
2	F	552	SER	2.2
1	N	88	G	2.2
2	C	325	ARG	2.2
2	E	422	THR	2.2
2	E	456	LEU	2.2
2	C	586	THR	2.2
2	F	486	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	K	99	C	2.2
2	C	556	ASN	2.2
2	E	614	LYS	2.2
2	A	500	GLU	2.2
2	C	558	LEU	2.2
2	A	499	GLY	2.2
2	E	502	ASN	2.2
2	A	642	GLU	2.2
2	D	497	TYR	2.2
1	K	93	U	2.2
1	K	95	A	2.1
2	E	332	MET	2.1
2	B	361	CYS	2.1
2	D	373	LEU	2.1
2	E	348	TYR	2.1
1	M	70	G	2.1
2	F	323	GLU	2.1
1	I	84	U	2.1
2	F	604	GLY	2.1
2	E	503	GLU	2.1
2	C	641	GLU	2.1
2	E	517	SER	2.1
1	I	97	C	2.1
1	P	102	C	2.1
1	I	79	A	2.1
1	K	98	A	2.1
2	F	262	GLY	2.1
1	L	75	U	2.1
1	P	84	U	2.1
2	H	479	GLN	2.1
2	E	467	GLU	2.1
2	D	479	GLN	2.0
1	J	69	G	2.0
2	E	363	ARG	2.0
2	F	603	SER	2.0
2	E	500	GLU	2.0
2	C	547	ILE	2.0
2	D	384	ALA	2.0
2	D	432	GLU	2.0
2	E	284	LYS	2.0
1	L	104	C	2.0
2	E	311	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
2	E	301	ARG	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

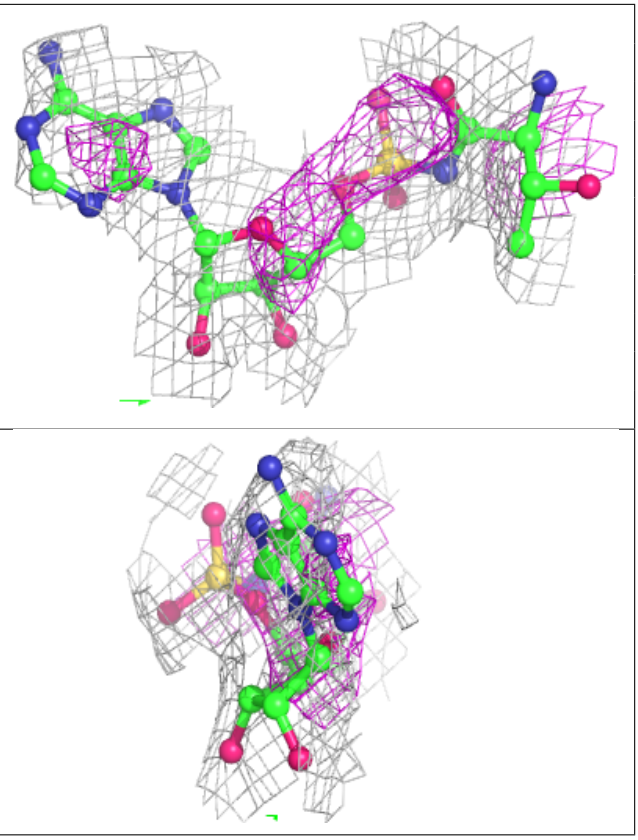
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TSB	E	6002	30/30	0.65	0.51	86,122,126,127	0
3	ZN	E	1	1/1	0.73	0.26	185,185,185,185	0
4	TSB	D	5002	30/30	0.75	0.58	94,112,119,120	0
3	ZN	D	1	1/1	0.77	0.30	135,135,135,135	0
3	ZN	F	1	1/1	0.81	0.26	101,101,101,101	0
4	TSB	F	7002	30/30	0.81	0.43	89,103,111,112	0
4	TSB	C	4002	30/30	0.87	0.36	73,88,100,102	0
4	TSB	H	9002	30/30	0.91	0.40	30,48,71,72	0
4	TSB	G	8002	30/30	0.94	0.31	0,18,49,50	0
3	ZN	C	1	1/1	0.95	0.27	95,95,95,95	0
3	ZN	G	1	1/1	0.95	0.24	27,27,27,27	0
4	TSB	B	3002	30/30	0.95	0.38	32,50,57,58	0
4	TSB	A	2002	30/30	0.96	0.29	31,44,58,65	0
3	ZN	H	1	1/1	0.98	0.27	54,54,54,54	0
3	ZN	A	1	1/1	0.99	0.23	42,42,42,42	0
3	ZN	B	1	1/1	0.99	0.32	52,52,52,52	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

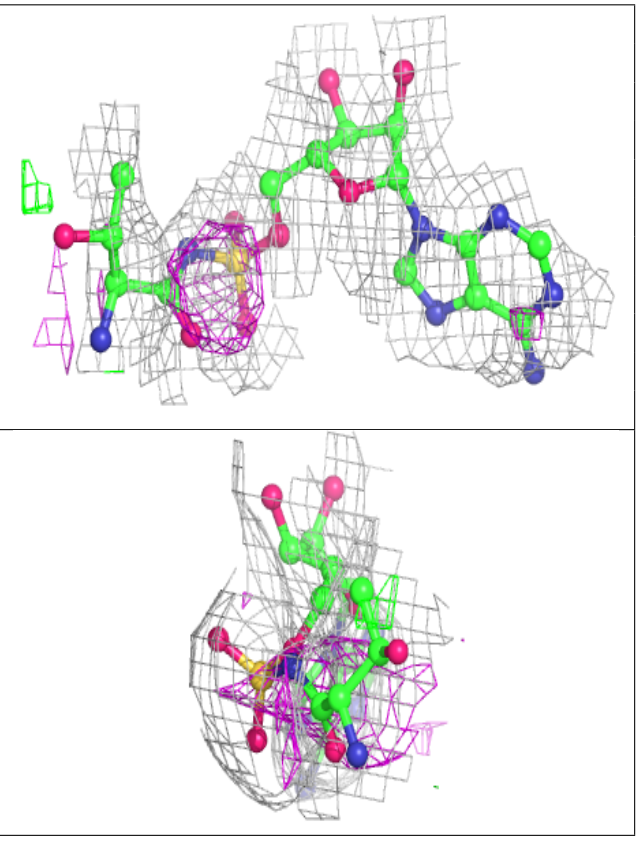
Electron density around TSB E 6002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



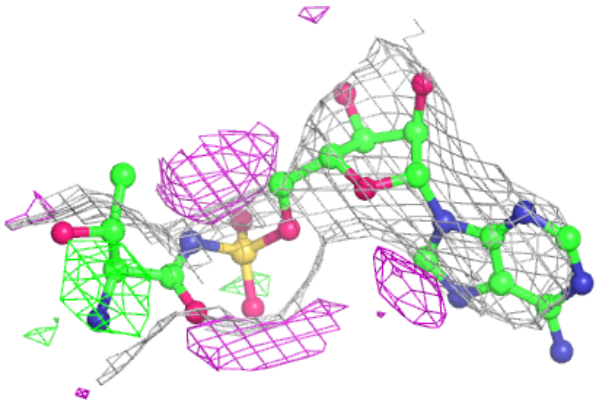
Electron density around TSB D 5002:

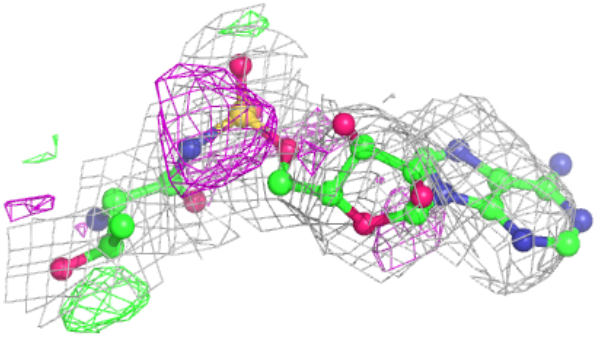
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

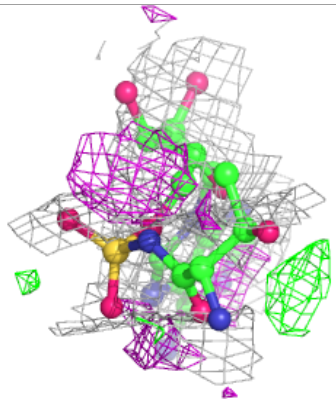


Electron density around TSB F 7002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

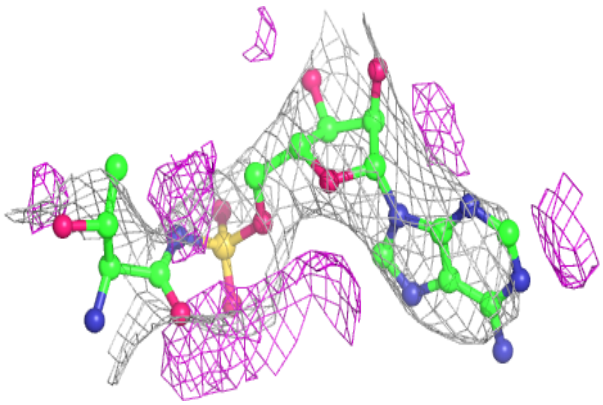


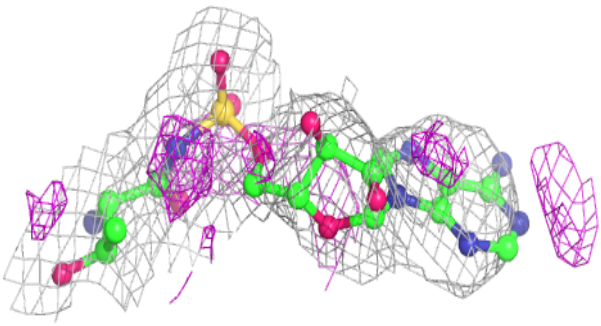


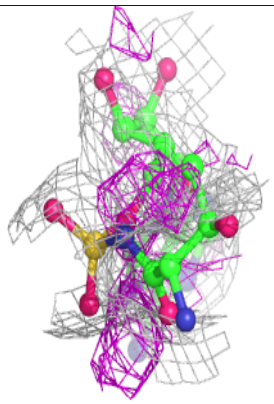


Electron density around TSB C 4002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

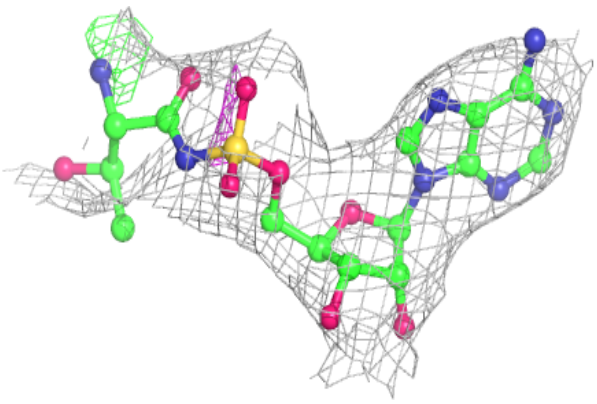


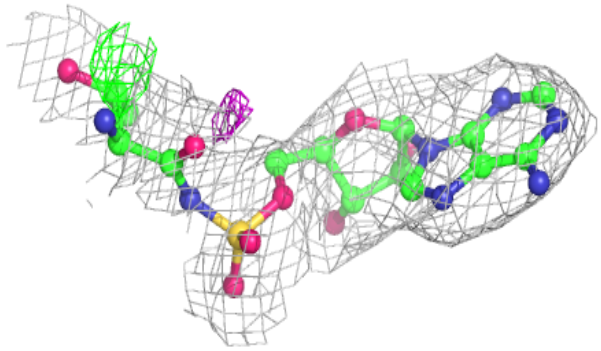


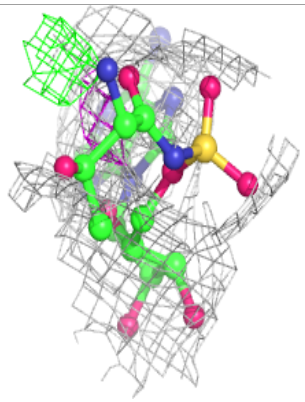


Electron density around TSB H 9002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

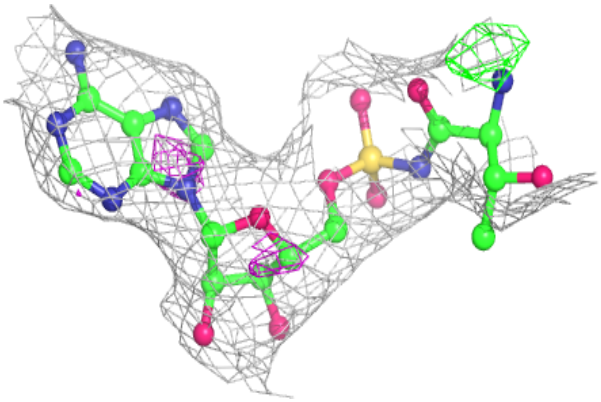


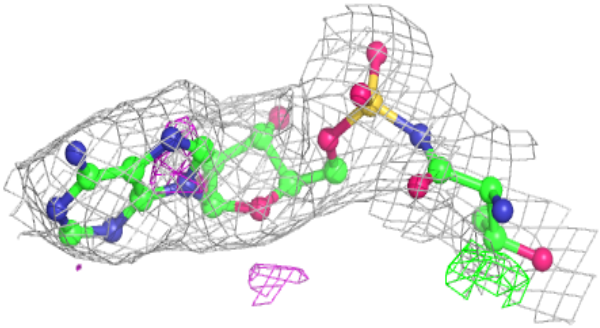


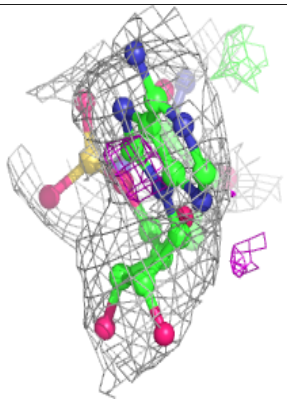


Electron density around TSB G 8002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

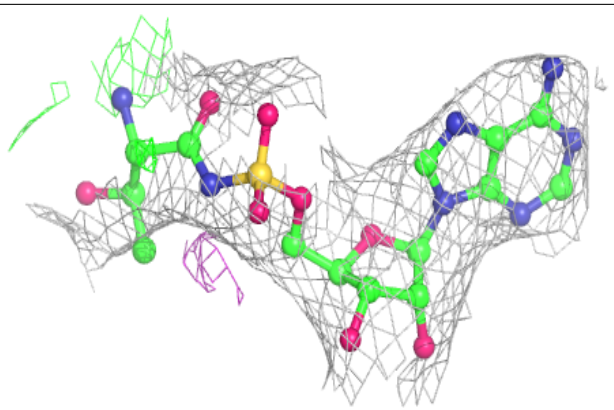


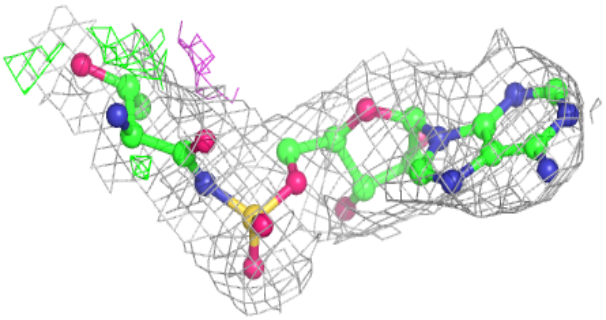


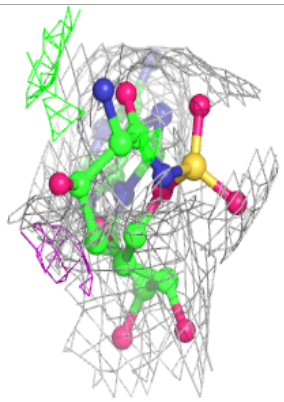


Electron density around TSB B 3002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

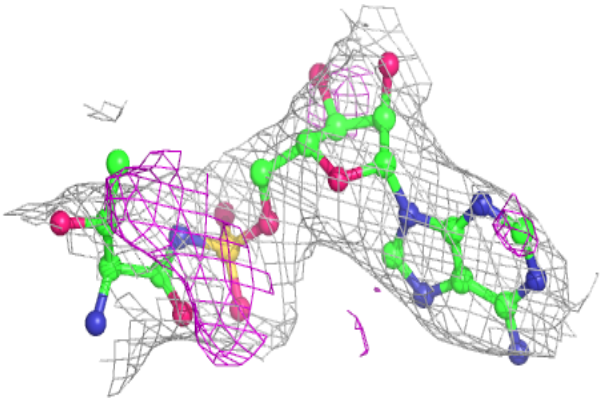


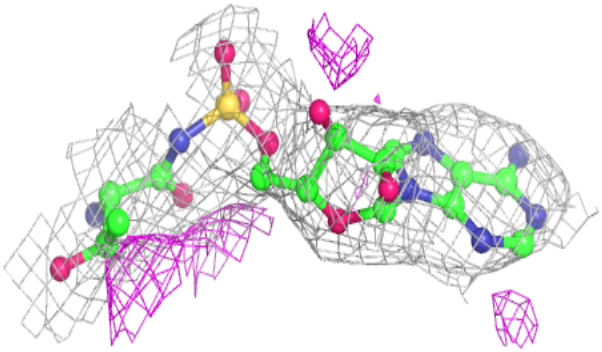


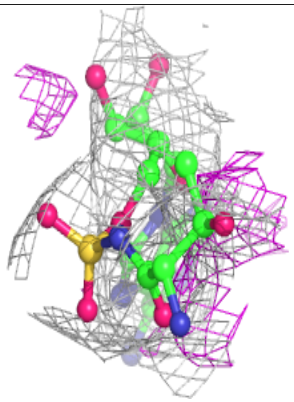


Electron density around TSB A 2002:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)







6.5 Other polymers (i)

There are no such residues in this entry.