Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 07:12 PM GMT

PDB ID	:	1EIY
Title	:	THE CRYSTAL STRUCTURE OF PHENYLALANYL-TRNA SYNTHETASE FROM THERMUS THERMOPHILUS COMPLEXED WITH COGNATE TRNAPHE
Authors	:	Goldgur, Y.; Mosyak, L.; Reshetnikova, L.; Ankilova, V.; Safro, M.
Deposited on	:	2000-02-29
Resolution	:	3.30 Å(reported)

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

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

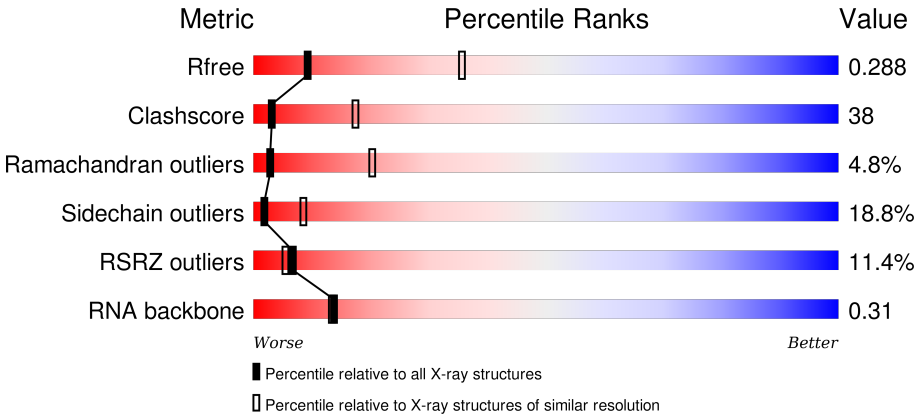
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)
RNA backbone	2183	1005 (3.82-2.78)

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

Mol	Chain	Length	Quality of chain
1	C	76	95% 7% 41% 42% 11%
2	A	350	18% 36% 48% 13% • •
3	B	785	39% 48% 12% •

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 10485 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a RNA chain called TRNA(PHE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	C	76	1623	723	291	533	76	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	49	C	G	CONFLICT	UNP Q5SGX1
C	65	G	C	CONFLICT	UNP Q5SGX1

- Molecule 2 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	345	2735	1768	477	482	8	0	0	0

- Molecule 3 is a protein called PHENYLALANYL-TRNA SYNTHETASE.

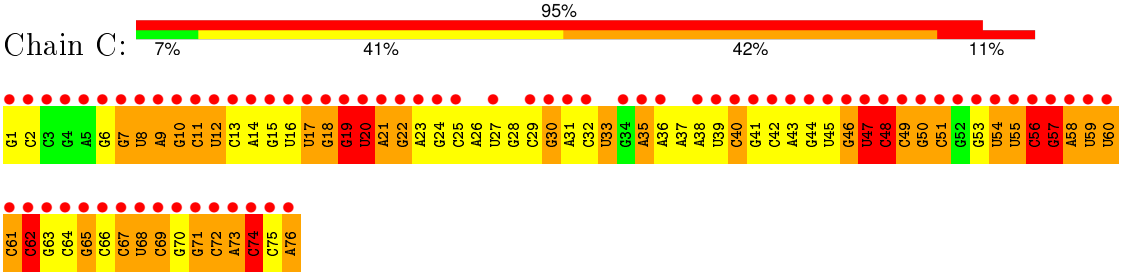
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	B	785	6127	3925	1091	1101	10	0	0	0

3 Residue-property plots (i)

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

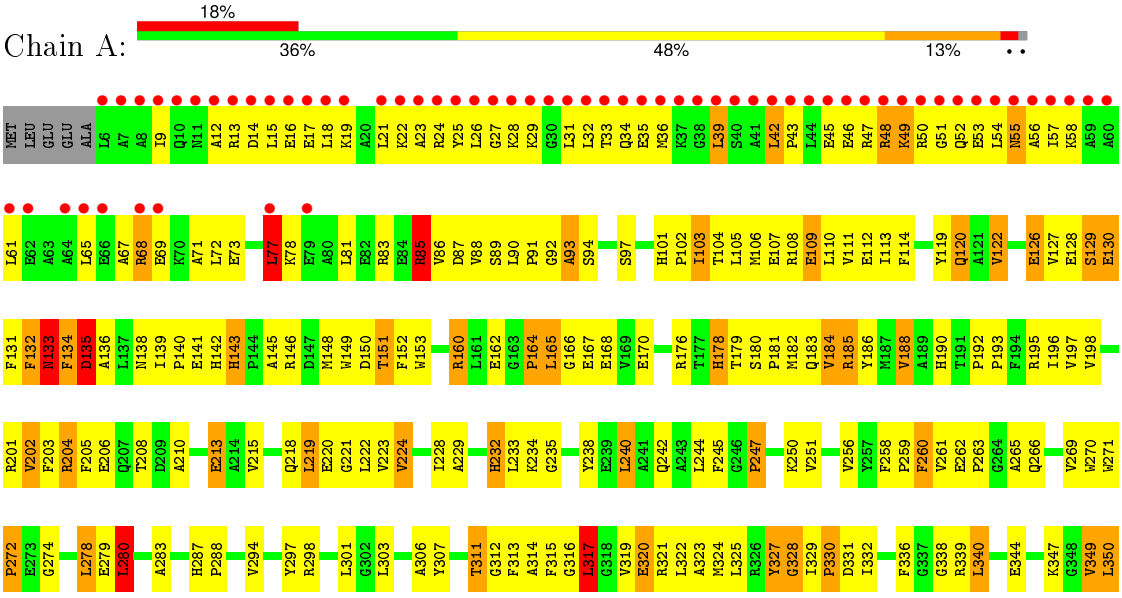
- Molecule 1: TRNA(PHE)

Chain C:



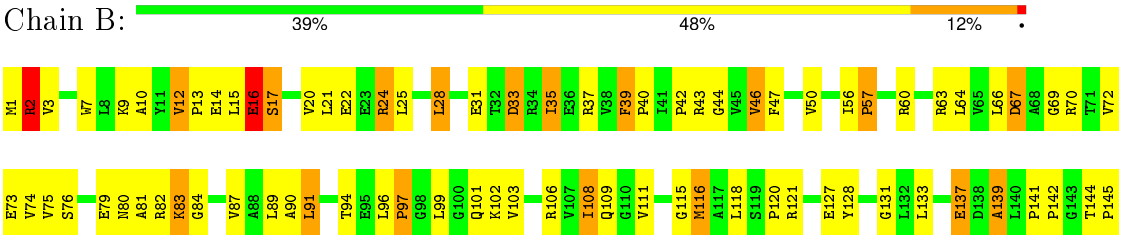
- Molecule 2: PHENYLALANYL-TRNA SYNTHETASE

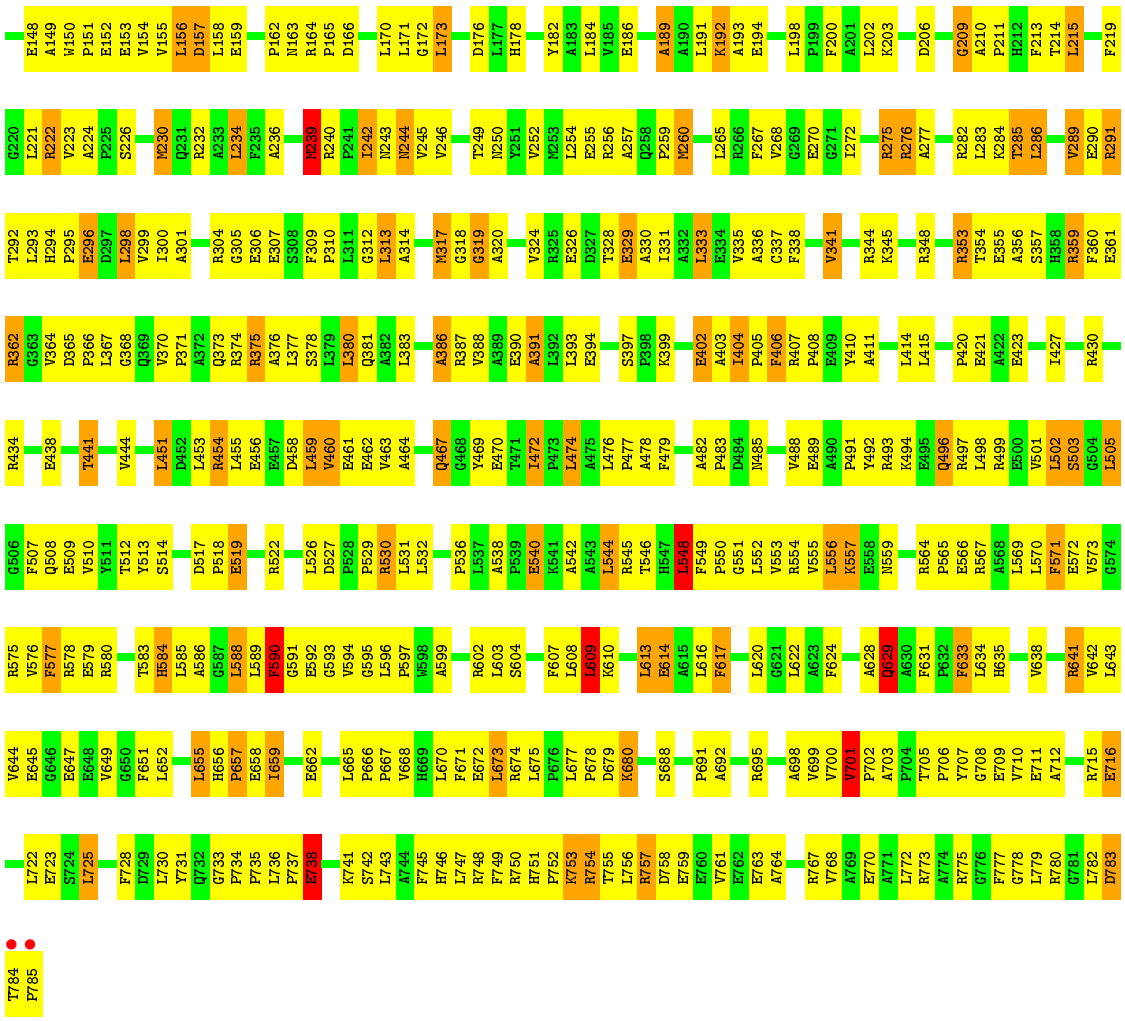
Chain A:



- Molecule 3: PHENYLALANYL-TRNA SYNTHETASE

Chain B:




E148 A149 W150 P151 E152 E153 Y154 Y155 L156 D157 L158 E159 P162 N163 R164 P165 D166 L170 L171 G172 L173 D176 L177 H178 Y182 A183 L184 Y185 E186 A189 A190 L191 K192 A193 E194 L198 P199 F200 A201 L202 K203 D206 G209 A210 P211 H212 F213 T214 L215 F219
G220 L221 R222 V223 A224 P225 S226 M230 Q231 R232 A233 L234 F235 A236 M239 R240 P241 I242 N243 N244 V245 V246 T249 N250 Y251 V252 M253 L254 E255 R256 A257 Q258 P259 M260 L265 R266 F267 V268 G269 E270 G271 I272 R275 R276 A277 R282 L283 K284 T285 L286 V289 E290 R291
T292 L293 H294 P295 E296 D297 L298 V299 I300 A301 R304 G305 E306 E307 S308 F309 P310 L311 G312 L313 A314 M317 G318 G319 A320 V324 R325 E326 D327 T328 E329 A330 I331 A332 L333 E334 V335 A336 C337 F338 V341 R344 K345 R348 R353 T354 E355 A356 S357 H358 R359 F360 E361
R362 G363 V364 D365 P366 L367 G368 Q369 V370 P371 A372 Q373 R374 R375 A376 L377 S378 I379 L380 Q381 A382 I383 A386 R387 V388 A389 E390 A391 I392 I393 E394 S397 P398 K399 E402 A403 I404 P405 F406 R407 P408 E409 Y410 A411 L414 L415 P420 E421 A422 E423 I427 R430
R434 E438 T441 V444 L451 D452 L453 R454 L455 E456 E457 D458 L459 V460 E461 E462 V463 A464 Q467 G468 Y469 E470 T471 I472 P473 L474 A475 L476 P477 A478 F479 A482 P483 D484 N485 V488 E489 A490 P491 Y492 R493 K494 E495 Q496 R497 L498 R499 E500 V501 L502 S503 G504 L505
G506 P507 Q508 E509 V510 Y511 T512 Y513 S514 D517 P518 E519 R522 L526 D527 P528 P529 R530 L531 L532 P536 L537 A538 P539 E540 K541 A542 A543 L544 R545 T546 H547 L548 P549 P550 G551 L552 V553 R554 V555 L556 K557 E558 N559 R564 P565 E566 R567 A568 L569 L570 F571 E572 V573 G574
R575 V576 F577 R578 E579 R580 T583 H584 L585 A586 G587 L588 L589 F590 G591 E592 G593 V594 G595 L596 P597 W598 A599 R602 L603 S604 F607 L608 L609 K610 L613 E614 A615 L616 F617 L620 G621 L622 A623 F624 A628 Q629 A630 F631 P632 F633 L634 H635 V638 R641 L643
V644 E645 G646 E647 E648 V649 G650 F651 L652 L655 H656 P657 E658 I659 E662 L665 P666 P667 V668 H669 L670 F671 E672 L673 R674 L675 P676 L677 P678 D679 K680 S688 P691 A692 R695 A698 V699 V700 V701 P702 A703 P704 T705 P706 Y707 G708 E709 V710 E711 A712 R715 E716
L722 E723 S724 L725 F728 D729 L730 Y731 Q732 G733 P734 P735 I736 P737 E738 K741 S742 L743 A744 F745 H746 L747 R748 F749 R750 H751 P752 K753 R754 T755 L756 R757 D758 E759 E760 V761 E762 E763 A764 R767 V768 A769 E770 A771 L772 R773 A774 R775 G776 F777 G778 L779 R780 G781 L782 D783
T784 P785

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	175.00Å 175.00Å 140.60Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	28.00 – 3.30 28.06 – 3.28	Depositor EDS
% Data completeness (in resolution range)	86.3 (28.00-3.30) 87.1 (28.06-3.28)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	4.30 (at 3.31Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.221 , 0.287 0.236 , 0.288	Depositor DCC
R_{free} test set	1652 reflections (4.98%)	DCC
Wilson B-factor (Å^2)	59.2	Xtriage
Anisotropy	0.685	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 38.0	EDS
Estimated twinning fraction	0.080 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.25$	Xtriage
Outliers	0 of 33340 reflections	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	10485	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	C	0.95	0/1813	1.09	9/2823 (0.3%)
2	A	0.89	1/2805 (0.0%)	1.07	9/3789 (0.2%)
3	B	0.82	2/6280 (0.0%)	1.07	19/8536 (0.2%)
All	All	0.86	3/10898 (0.0%)	1.08	37/15148 (0.2%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	6
3	B	0	1
All	All	0	7

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	109	GLU	CB-CG	-6.52	1.39	1.52
3	B	239	MET	SD-CE	6.10	2.12	1.77
3	B	783	ASP	CB-CG	5.08	1.62	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	39	LEU	CA-CB-CG	8.00	133.69	115.30
2	A	317	LEU	CA-CB-CG	7.52	132.59	115.30
1	C	20	U	C2'-C3'-O3'	7.50	126.00	109.50
3	B	609	LEU	CA-CB-CG	7.42	132.36	115.30
1	C	62	C	N1-C1'-C2'	-7.32	103.95	112.00
1	C	71	G	N9-C1'-C2'	-7.30	103.97	112.00
3	B	548	LEU	CA-CB-CG	7.01	131.42	115.30
2	A	350	LEU	CA-CB-CG	6.79	130.92	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2	ARG	NE-CZ-NH1	6.77	123.68	120.30
3	B	603	LEU	CA-CB-CG	6.45	130.14	115.30
1	C	68	U	N1-C1'-C2'	-6.39	104.97	112.00
2	A	185	ARG	NE-CZ-NH2	-6.19	117.20	120.30
3	B	224	ALA	C-N-CD	5.94	140.88	128.40
3	B	783	ASP	N-CA-C	5.92	126.97	111.00
3	B	333	LEU	CA-CB-CG	5.92	128.90	115.30
3	B	647	GLU	N-CA-C	5.90	126.93	111.00
3	B	643	LEU	CA-CB-CG	5.80	128.65	115.30
1	C	65	G	N9-C1'-C2'	-5.78	105.64	112.00
1	C	56	C	N1-C1'-C2'	5.74	121.46	114.00
2	A	280	LEU	N-CA-C	5.74	126.49	111.00
3	B	16	GLU	N-CA-C	5.70	126.39	111.00
1	C	47	U	N1-C1'-C2'	5.67	121.38	114.00
3	B	359	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	A	85	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	C	55	U	N1-C1'-C2'	-5.52	105.93	112.00
1	C	74	C	O4'-C4'-C3'	-5.36	98.64	104.00
3	B	380	LEU	CA-CB-CG	5.33	127.55	115.30
3	B	189	ALA	N-CA-C	-5.29	96.71	111.00
2	A	77	LEU	CA-CB-CG	5.28	127.44	115.30
2	A	151	THR	N-CA-C	5.26	125.20	111.00
3	B	28	LEU	CB-CG-CD2	-5.24	102.10	111.00
3	B	383	LEU	CA-CB-CG	5.22	127.32	115.30
3	B	472	ILE	N-CA-C	-5.21	96.94	111.00
3	B	359	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	B	230	MET	CB-CG-SD	5.18	127.94	112.40
3	B	293	LEU	N-CA-C	5.13	124.85	111.00
2	A	21	LEU	CA-CB-CG	5.05	126.91	115.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	B	617	PHE	Sidechain
1	C	19	G	Sidechain
1	C	30	G	Sidechain
1	C	48	C	Sidechain
1	C	57	G	Sidechain
1	C	60	U	Sidechain
1	C	62	C	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1623	0	822	151	0
2	A	2735	0	2725	238	0
3	B	6127	0	6180	420	0
All	All	10485	0	9727	772	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 38.

All (772) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:239:MET:SD	3:B:239:MET:CE	2.12	1.38
1:C:58:A:H4'	1:C:59:U:OP1	1.41	1.17
3:B:706:PRO:HG2	3:B:709:GLU:HB2	1.29	1.08
1:C:39:U:C2'	1:C:40:C:H5'	1.83	1.07
1:C:39:U:H2'	1:C:40:C:H5'	1.38	1.02
2:A:210:ALA:HA	2:A:331:ASP:HB2	1.38	1.02
1:C:47:U:H3'	1:C:48:C:H5'	1.38	1.01
1:C:8:U:H4'	1:C:48:C:H1'	1.42	1.01
2:A:23:ALA:HB2	2:A:65:LEU:HD21	1.40	1.01
3:B:282:ARG:HD2	3:B:292:THR:HG22	1.43	1.01
2:A:19:LYS:HD3	2:A:22:LYS:HD2	1.43	1.00
3:B:314:ALA:HB1	3:B:338:PHE:HE1	1.25	0.99
2:A:12:ALA:HA	2:A:15:LEU:HB3	1.46	0.95
3:B:221:LEU:HD23	3:B:386:ALA:HB2	1.46	0.95
3:B:12:VAL:HG22	3:B:15:LEU:HD13	1.50	0.94
1:C:61:C:H2'	1:C:62:C:C6	2.03	0.93
1:C:53:G:H2'	1:C:54:U:C6	2.05	0.90
1:C:61:C:H2'	1:C:62:C:H6	1.36	0.90
2:A:119:TYR:HD2	2:A:197:VAL:HG13	1.37	0.89
2:A:294:VAL:O	2:A:298:ARG:HG3	1.73	0.89
3:B:312:GLY:HA2	3:B:318:GLY:HA2	1.53	0.88
2:A:183:GLN:HG3	2:A:222:LEU:HD22	1.56	0.88
3:B:285:THR:HG21	3:B:291:ARG:HE	1.39	0.88
3:B:163:ASN:O	3:B:165:PRO:HD3	1.74	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:162:PRO:HA	3:B:362:ARG:HD3	1.55	0.86
1:C:8:U:C4'	1:C:48:C:H1'	2.06	0.85
1:C:55:U:C6	1:C:55:U:H3'	2.12	0.85
1:C:65:G:C2'	1:C:66:C:H5'	2.06	0.85
2:A:26:LEU:HD22	2:A:61:LEU:HD21	1.60	0.84
3:B:314:ALA:HB1	3:B:338:PHE:CE1	2.11	0.84
1:C:56:C:H2'	1:C:57:G:N7	1.93	0.83
1:C:65:G:H2'	1:C:66:C:H5'	1.58	0.83
1:C:41:G:O2'	1:C:42:C:H5'	1.77	0.83
1:C:19:G:O2'	1:C:20:U:H5'	1.78	0.83
2:A:42:LEU:H	2:A:43:PRO:HD2	1.42	0.83
3:B:609:LEU:CD1	3:B:652:LEU:HD11	2.08	0.83
2:A:287:HIS:CD2	2:A:288:PRO:HD2	2.13	0.82
2:A:179:THR:OG1	2:A:220:GLU:HG3	1.77	0.82
1:C:53:G:H2'	1:C:54:U:H6	1.43	0.82
3:B:336:ALA:HB3	3:B:338:PHE:HE2	1.40	0.82
3:B:453:LEU:HD23	3:B:458:ASP:HB3	1.60	0.82
2:A:265:ALA:HB2	3:B:469:TYR:HE1	1.43	0.81
3:B:549:PHE:O	3:B:553:VAL:HG23	1.79	0.81
3:B:734:PRO:HA	3:B:736:LEU:H	1.43	0.81
1:C:9:A:N6	1:C:23:A:H62	1.79	0.80
3:B:734:PRO:HA	3:B:736:LEU:N	1.97	0.80
1:C:19:G:O2'	1:C:20:U:C5'	2.30	0.80
3:B:609:LEU:HD13	3:B:652:LEU:HD11	1.64	0.80
3:B:505:LEU:HD12	3:B:507:PHE:HE1	1.47	0.80
3:B:249:THR:HA	3:B:260:MET:HE2	1.62	0.79
1:C:47:U:H3'	1:C:48:C:C5'	2.12	0.79
1:C:31:A:O2'	1:C:32:C:H5'	1.82	0.79
3:B:283:LEU:HD21	3:B:320:ALA:HB2	1.63	0.79
1:C:31:A:C2'	1:C:32:C:H5'	2.11	0.79
2:A:19:LYS:HG3	2:A:68:ARG:HG2	1.63	0.79
3:B:733:GLY:O	3:B:736:LEU:HB2	1.81	0.78
2:A:91:PRO:HB2	3:B:597:PRO:HG3	1.64	0.78
1:C:9:A:H4'	1:C:10:G:OP1	1.82	0.78
2:A:18:LEU:O	2:A:22:LYS:HG3	1.84	0.78
2:A:164:PRO:HB2	2:A:165:LEU:HD23	1.64	0.78
3:B:284:LYS:O	3:B:320:ALA:HA	1.82	0.78
3:B:221:LEU:CD2	3:B:386:ALA:HB2	2.14	0.78
3:B:589:LEU:CD2	3:B:609:LEU:HB2	2.13	0.77
2:A:85:ARG:HG3	2:A:85:ARG:HH11	1.46	0.77
1:C:72:C:H5"	1:C:73:A:OP2	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:589:LEU:HD22	3:B:609:LEU:HB2	1.66	0.77
1:C:63:G:H2'	1:C:64:C:C6	2.19	0.77
3:B:501:VAL:O	3:B:505:LEU:HB2	1.86	0.76
3:B:730:LEU:HD12	3:B:743:LEU:CD2	2.16	0.76
3:B:557:LYS:HG2	3:B:665:LEU:HD23	1.67	0.76
1:C:20:U:H5"	1:C:20:U:C6	2.21	0.76
1:C:9:A:N6	1:C:22:G:C5	2.53	0.75
1:C:61:C:C5	1:C:62:C:C5	2.74	0.75
1:C:47:U:H2'	1:C:50:G:OP1	1.86	0.75
1:C:75:C:OP1	3:B:159:GLU:HG3	1.87	0.75
1:C:19:G:C2'	1:C:20:U:H5'	2.16	0.74
1:C:65:G:O2'	1:C:66:C:H5'	1.87	0.74
2:A:265:ALA:HB2	3:B:469:TYR:CE1	2.21	0.74
3:B:191:LEU:HB2	3:B:381:GLN:NE2	2.01	0.74
2:A:321:ARG:O	2:A:325:LEU:HD23	1.87	0.74
1:C:14:A:H2'	1:C:15:G:H5'	1.69	0.74
2:A:51:GLY:HA2	2:A:55:ASN:ND2	2.03	0.73
3:B:312:GLY:CA	3:B:318:GLY:HA2	2.18	0.73
3:B:414:LEU:HD23	3:B:460:VAL:HG21	1.68	0.73
3:B:215:LEU:HD21	3:B:272:ILE:HG13	1.70	0.73
1:C:39:U:O2'	1:C:40:C:H5'	1.88	0.73
1:C:9:A:H62	1:C:23:A:N6	1.86	0.73
2:A:32:LEU:HA	2:A:36:MET:HG2	1.71	0.73
3:B:221:LEU:HD11	3:B:331:ILE:HG12	1.69	0.73
3:B:505:LEU:HD12	3:B:507:PHE:CE1	2.23	0.73
3:B:39:PHE:N	3:B:40:PRO:HD3	2.03	0.73
1:C:39:U:H2'	1:C:40:C:C5'	2.18	0.72
3:B:336:ALA:HB3	3:B:338:PHE:CE2	2.23	0.72
3:B:517:ASP:HB2	3:B:519:GLU:OE1	1.90	0.72
2:A:127:VAL:HG23	3:B:577:PHE:CE2	2.24	0.72
3:B:191:LEU:HB2	3:B:381:GLN:HE22	1.52	0.72
2:A:49:LYS:H	2:A:49:LYS:HD2	1.55	0.72
3:B:659:ILE:HA	3:B:662:GLU:HB3	1.72	0.71
3:B:604:SER:HA	3:B:608:LEU:HD22	1.72	0.71
3:B:715:ARG:HG3	3:B:725:LEU:HD22	1.72	0.70
2:A:109:GLU:O	2:A:113:ILE:HG13	1.91	0.70
3:B:755:THR:HG22	3:B:756:LEU:H	1.56	0.70
3:B:222:ARG:CG	3:B:222:ARG:HH11	2.03	0.70
1:C:19:G:C3'	1:C:20:U:H5'	2.22	0.70
3:B:286:LEU:HB2	3:B:319:GLY:HA3	1.73	0.70
2:A:35:GLU:O	2:A:39:LEU:HD23	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:198:LEU:HD11	3:B:391:ALA:O	1.91	0.70
1:C:61:C:C6	1:C:62:C:C5	2.80	0.70
3:B:355:GLU:O	3:B:359:ARG:HD3	1.91	0.70
2:A:107:GLU:O	2:A:111:VAL:HG23	1.92	0.69
3:B:588:LEU:HD12	3:B:668:VAL:HG11	1.71	0.69
1:C:55:U:C6	1:C:55:U:C3'	2.75	0.69
1:C:68:U:C2'	1:C:69:C:H5'	2.22	0.69
2:A:120:GLN:HB2	2:A:196:ILE:HG22	1.74	0.69
1:C:9:A:N6	1:C:23:A:N6	2.40	0.69
1:C:41:G:C2'	1:C:42:C:H5'	2.23	0.69
3:B:294:HIS:HD2	3:B:296:GLU:HB2	1.56	0.69
1:C:45:U:H3'	1:C:46:G:C5'	2.23	0.68
3:B:277:ALA:O	3:B:295:PRO:HA	1.93	0.68
3:B:96:LEU:HB2	3:B:99:LEU:HD13	1.73	0.68
3:B:536:PRO:HB3	3:B:542:ALA:HA	1.76	0.68
2:A:102:PRO:HA	2:A:105:LEU:HD12	1.74	0.68
1:C:24:G:C6	1:C:25:C:C2	2.80	0.68
2:A:13:ARG:NE	2:A:72:LEU:HD22	2.09	0.68
1:C:76:A:C8	2:A:149:TRP:CZ2	2.81	0.68
3:B:427:ILE:HG21	3:B:463:VAL:HA	1.76	0.68
1:C:33:U:H2'	1:C:35:A:OP2	1.94	0.68
3:B:624:PHE:HE2	3:B:642:VAL:HG13	1.58	0.68
3:B:13:PRO:O	3:B:14:GLU:HG2	1.94	0.68
2:A:101:HIS:CD2	2:A:103:ILE:H	2.12	0.68
2:A:129:SER:O	2:A:131:PHE:N	2.28	0.67
3:B:751:HIS:CD2	3:B:753:LYS:HB3	2.29	0.67
3:B:688:SER:HB3	3:B:752:PRO:HA	1.75	0.67
3:B:249:THR:HA	3:B:260:MET:CE	2.25	0.67
2:A:51:GLY:HA2	2:A:55:ASN:HD21	1.60	0.67
3:B:213:PHE:HE2	3:B:215:LEU:HD13	1.59	0.67
1:C:26:A:C2	1:C:27:U:C6	2.82	0.67
1:C:27:U:H2'	1:C:28:G:H8	1.59	0.67
3:B:16:GLU:O	3:B:17:SER:HB3	1.95	0.67
1:C:36:A:C2	1:C:37:A:C8	2.83	0.67
2:A:233:LEU:HD13	2:A:313:PHE:CD1	2.30	0.67
2:A:232:HIS:CD2	3:B:477:PRO:HB3	2.30	0.67
1:C:75:C:O2'	2:A:148:MET:HG2	1.95	0.67
3:B:368:GLY:O	3:B:371:PRO:HG2	1.95	0.67
3:B:701:VAL:HG23	3:B:705:THR:HG21	1.75	0.66
3:B:198:LEU:HD12	3:B:393:LEU:HD13	1.76	0.66
3:B:715:ARG:HG3	3:B:725:LEU:CD2	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:287:HIS:HD2	2:A:288:PRO:HD2	1.58	0.66
3:B:64:LEU:HD11	3:B:76:SER:HB3	1.76	0.66
1:C:54:U:H3'	1:C:58:A:H61	1.60	0.66
2:A:110:LEU:O	2:A:114:PHE:HD1	1.78	0.66
3:B:331:ILE:HD11	3:B:380:LEU:HD21	1.78	0.66
3:B:596:LEU:HB2	3:B:599:ALA:HB3	1.76	0.66
2:A:181:PRO:O	2:A:185:ARG:HG3	1.95	0.66
3:B:178:HIS:HD2	3:B:182:TYR:O	1.79	0.66
3:B:276:ARG:HH11	3:B:276:ARG:CG	2.09	0.65
1:C:65:G:H2'	1:C:66:C:C5'	2.27	0.65
3:B:282:ARG:CD	3:B:292:THR:HG22	2.25	0.65
2:A:210:ALA:CA	2:A:331:ASP:HB2	2.21	0.65
2:A:126:GLU:HG2	2:A:203:PHE:HE1	1.61	0.65
2:A:222:LEU:HD12	2:A:224:VAL:HG22	1.77	0.65
3:B:467:GLN:HE21	3:B:467:GLN:HA	1.61	0.65
3:B:376:ALA:O	3:B:380:LEU:HB2	1.97	0.65
1:C:14:A:C2'	1:C:15:G:H5'	2.27	0.65
3:B:189:ALA:HB1	3:B:378:SER:HB3	1.79	0.64
2:A:128:GLU:HG3	2:A:129:SER:H	1.62	0.64
2:A:19:LYS:HA	2:A:22:LYS:HB2	1.78	0.64
3:B:751:HIS:HB3	3:B:754:ARG:O	1.97	0.64
2:A:73:GLU:O	2:A:77:LEU:HB3	1.97	0.64
3:B:120:PRO:HD2	3:B:128:TYR:O	1.97	0.64
2:A:119:TYR:CD2	2:A:197:VAL:HG13	2.26	0.64
3:B:219:PHE:HA	3:B:330:ALA:HA	1.80	0.64
1:C:31:A:H2'	1:C:32:C:H5'	1.78	0.64
1:C:68:U:H2'	1:C:69:C:H5'	1.80	0.63
3:B:712:ALA:O	3:B:716:GLU:HG3	1.98	0.63
3:B:407:ARG:HG2	3:B:441:THR:HG23	1.79	0.63
2:A:327:TYR:N	2:A:327:TYR:CD2	2.65	0.63
2:A:43:PRO:HA	2:A:50:ARG:NH1	2.13	0.63
2:A:234:LYS:HB3	3:B:474:LEU:HD22	1.80	0.63
3:B:353:ARG:N	3:B:353:ARG:HD3	2.14	0.63
3:B:698:ALA:HB3	3:B:780:ARG:CG	2.28	0.63
3:B:624:PHE:CE2	3:B:642:VAL:HG13	2.33	0.63
3:B:404:ILE:HD13	3:B:454:ARG:O	1.99	0.63
1:C:8:U:O2'	1:C:46:G:N2	2.32	0.63
3:B:344:ARG:O	3:B:348:ARG:HG3	1.98	0.63
3:B:569:LEU:HD13	3:B:589:LEU:HD13	1.81	0.63
3:B:284:LYS:HG3	3:B:289:VAL:O	1.99	0.62
2:A:297:TYR:CE1	2:A:301:LEU:HD11	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:195:ARG:HG2	2:A:223:VAL:HG22	1.81	0.62
3:B:14:GLU:HG3	3:B:14:GLU:O	1.99	0.62
3:B:453:LEU:CD2	3:B:458:ASP:HB3	2.29	0.62
2:A:279:GLU:O	2:A:280:LEU:HB2	2.00	0.62
3:B:120:PRO:HD3	3:B:131:GLY:O	1.99	0.62
2:A:87:ASP:HB3	2:A:90:LEU:HD22	1.82	0.62
1:C:19:G:N2	1:C:56:C:N3	2.45	0.62
3:B:779:LEU:H	3:B:783:ASP:HB2	1.64	0.62
1:C:55:U:H6	1:C:55:U:H3'	1.64	0.62
3:B:335:VAL:HB	3:B:373:GLN:HE21	1.63	0.62
2:A:164:PRO:HG2	2:A:188:VAL:HG21	1.81	0.61
3:B:458:ASP:O	3:B:462:GLU:HG2	2.00	0.61
1:C:26:A:C6	1:C:27:U:C5	2.88	0.61
1:C:8:U:H5'	1:C:48:C:O2'	1.99	0.61
3:B:736:LEU:HD11	3:B:742:SER:HB2	1.83	0.61
3:B:285:THR:HG23	3:B:317:MET:SD	2.41	0.61
3:B:635:HIS:ND1	3:B:638:VAL:HG22	2.15	0.61
1:C:56:C:H2'	1:C:57:G:C8	2.36	0.61
3:B:230:MET:O	3:B:234:LEU:HD22	2.00	0.61
2:A:54:LEU:HB3	2:A:58:LYS:NZ	2.16	0.61
2:A:85:ARG:HG3	2:A:85:ARG:NH1	2.12	0.61
2:A:134:PHE:HD1	2:A:134:PHE:O	1.84	0.61
3:B:548:LEU:HD13	3:B:576:VAL:HG23	1.83	0.60
3:B:283:LEU:HD23	3:B:284:LYS:N	2.16	0.60
1:C:24:G:H2'	1:C:25:C:O4'	2.00	0.60
2:A:307:TYR:CD1	2:A:307:TYR:N	2.66	0.60
2:A:32:LEU:CA	2:A:36:MET:HG2	2.31	0.60
2:A:101:HIS:NE2	2:A:103:ILE:HG13	2.17	0.60
2:A:120:GLN:HE21	3:B:489:GLU:HB2	1.66	0.60
3:B:17:SER:HB3	3:B:20:VAL:HB	1.83	0.60
2:A:260:PHE:HD1	2:A:261:VAL:HG13	1.66	0.60
2:A:114:PHE:CZ	2:A:240:LEU:HG	2.36	0.60
2:A:165:LEU:H	2:A:165:LEU:HD23	1.66	0.60
2:A:48:ARG:O	2:A:52:GLN:HG3	2.00	0.59
2:A:329:ILE:HG23	2:A:330:PRO:HD2	1.82	0.59
2:A:258:PHE:HB2	2:A:261:VAL:HG22	1.83	0.59
1:C:18:G:N2	1:C:55:U:O2	2.28	0.59
2:A:29:LYS:O	2:A:33:THR:HG23	2.02	0.59
3:B:655:LEU:O	3:B:657:PRO:HD3	2.02	0.59
3:B:120:PRO:HG3	3:B:133:LEU:CD2	2.32	0.59
1:C:10:G:H2'	1:C:10:G:N3	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:182:MET:HG2	2:A:198:VAL:HG11	1.84	0.59
1:C:76:A:H5"	2:A:148:MET:HB3	1.85	0.59
3:B:470:GLU:OE1	3:B:470:GLU:HA	2.02	0.59
2:A:46:GLU:O	2:A:50:ARG:HB3	2.02	0.59
3:B:651:PHE:CE2	3:B:672:GLU:HB3	2.38	0.59
3:B:666:PRO:HB2	3:B:667:PRO:HD2	1.84	0.59
2:A:250:LYS:H	2:A:270:TRP:HB3	1.68	0.59
1:C:33:U:O5'	1:C:33:U:H6	1.85	0.59
2:A:48:ARG:HB2	2:A:49:LYS:HD2	1.85	0.59
3:B:191:LEU:CD2	3:B:377:LEU:HB2	2.33	0.59
3:B:299:VAL:HG13	3:B:312:GLY:O	2.03	0.59
2:A:193:PRO:HB2	3:B:479:PHE:CE1	2.38	0.59
2:A:134:PHE:HB2	2:A:139:ILE:HB	1.84	0.58
1:C:31:A:H2'	1:C:32:C:C5'	2.33	0.58
2:A:54:LEU:HB3	2:A:58:LYS:HZ1	1.69	0.58
1:C:25:C:H2'	1:C:26:A:O4'	2.03	0.58
3:B:455:LEU:HD12	3:B:455:LEU:N	2.18	0.58
2:A:201:ARG:HD3	2:A:215:VAL:HG11	1.85	0.58
1:C:29:C:H2'	1:C:30:G:H8	1.68	0.58
3:B:589:LEU:HD21	3:B:608:LEU:HD23	1.85	0.58
2:A:133:ASN:HD21	2:A:178:HIS:CD2	2.22	0.58
3:B:259:PRO:HB3	3:B:356:ALA:HB1	1.85	0.58
2:A:103:ILE:O	2:A:107:GLU:HB2	2.03	0.58
3:B:454:ARG:HB2	3:B:455:LEU:HD12	1.85	0.58
1:C:49:C:H6	1:C:49:C:O5'	1.87	0.58
2:A:195:ARG:HG2	2:A:223:VAL:HG13	1.86	0.58
2:A:126:GLU:HG2	2:A:203:PHE:CE1	2.38	0.58
3:B:510:VAL:HG11	3:B:552:LEU:HD21	1.85	0.58
3:B:698:ALA:HB3	3:B:780:ARG:HG2	1.85	0.58
1:C:29:C:H2'	1:C:30:G:C8	2.39	0.58
2:A:150:ASP:HB3	2:A:205:PHE:HB3	1.84	0.58
3:B:747:LEU:HD23	3:B:749:PHE:CZ	2.39	0.57
3:B:590:PHE:CD1	3:B:591:GLY:N	2.73	0.57
1:C:15:G:H22	1:C:48:C:H42	1.52	0.57
3:B:546:THR:HG22	3:B:578:ARG:HB3	1.87	0.57
3:B:673:LEU:HD23	3:B:673:LEU:N	2.20	0.57
2:A:94:SER:HB3	3:B:567:ARG:HH12	1.68	0.57
3:B:631:PHE:HB2	3:B:634:LEU:HD12	1.86	0.57
2:A:238:TYR:HA	2:A:251:VAL:HG11	1.87	0.57
3:B:9:LYS:HA	3:B:12:VAL:O	2.05	0.57
3:B:695:ARG:CD	3:B:761:VAL:HG11	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:222:ARG:HG2	3:B:222:ARG:HH11	1.70	0.56
2:A:106:MET:HG2	2:A:323:ALA:HB2	1.86	0.56
3:B:149:ALA:C	3:B:151:PRO:HD3	2.25	0.56
3:B:638:VAL:HG23	3:B:638:VAL:O	2.05	0.56
1:C:45:U:C2	1:C:46:G:H5"	2.41	0.56
2:A:85:ARG:HH11	2:A:85:ARG:CG	2.17	0.56
2:A:306:ALA:HB3	2:A:307:TYR:CE1	2.40	0.56
2:A:50:ARG:O	2:A:54:LEU:HD22	2.06	0.56
3:B:42:PRO:HG2	3:B:96:LEU:HD23	1.88	0.56
3:B:99:LEU:CD2	3:B:101:GLN:HB3	2.35	0.56
3:B:353:ARG:H	3:B:353:ARG:HD3	1.69	0.56
3:B:90:ALA:HB2	3:B:118:LEU:HD21	1.87	0.56
1:C:9:A:N6	1:C:22:G:C6	2.74	0.55
3:B:33:ASP:HB2	3:B:157:ASP:HB3	1.86	0.55
3:B:298:LEU:O	3:B:313:LEU:HD23	2.06	0.55
1:C:27:U:H2'	1:C:28:G:C8	2.39	0.55
3:B:423:GLU:O	3:B:427:ILE:HG12	2.06	0.55
3:B:695:ARG:HD3	3:B:761:VAL:HG11	1.87	0.55
2:A:15:LEU:HD12	2:A:18:LEU:HD12	1.87	0.55
2:A:19:LYS:HG3	2:A:68:ARG:CG	2.36	0.55
2:A:165:LEU:CD1	2:A:303:LEU:HD11	2.36	0.55
3:B:128:TYR:CG	3:B:240:ARG:HD2	2.41	0.55
2:A:186:TYR:CZ	2:A:190:HIS:ND1	2.73	0.55
2:A:27:GLY:O	2:A:31:LEU:HD12	2.06	0.55
3:B:573:VAL:HG12	3:B:573:VAL:O	2.06	0.55
3:B:210:ALA:N	3:B:211:PRO:HD3	2.20	0.55
3:B:141:PRO:HB2	3:B:144:THR:HG23	1.88	0.55
3:B:12:VAL:HG22	3:B:15:LEU:CD1	2.30	0.55
1:C:45:U:C3'	1:C:46:G:C5'	2.84	0.55
3:B:469:TYR:HA	3:B:472:ILE:CD1	2.37	0.55
3:B:250:ASN:O	3:B:254:LEU:HG	2.07	0.55
2:A:223:VAL:HB	2:A:313:PHE:CZ	2.41	0.55
2:A:28:LYS:O	2:A:32:LEU:N	2.40	0.55
1:C:68:U:O5'	1:C:68:U:H6	1.90	0.55
2:A:263:PRO:HG3	3:B:461:GLU:HB2	1.88	0.55
2:A:42:LEU:H	2:A:43:PRO:CD	2.18	0.55
2:A:327:TYR:N	2:A:327:TYR:HD2	2.05	0.55
1:C:61:C:C5	1:C:62:C:H5	2.25	0.54
3:B:604:SER:HA	3:B:608:LEU:HB2	1.89	0.54
1:C:68:U:C6	1:C:68:U:H3'	2.43	0.54
3:B:463:VAL:O	3:B:467:GLN:HB2	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:276:ARG:HH11	3:B:276:ARG:HG3	1.71	0.54
2:A:108:ARG:O	2:A:112:GLU:HG3	2.07	0.54
2:A:49:LYS:N	2:A:49:LYS:HD2	2.20	0.54
3:B:290:GLU:HG3	3:B:290:GLU:O	2.06	0.54
1:C:33:U:O2'	1:C:35:A:N7	2.24	0.54
1:C:47:U:C3'	1:C:48:C:C5'	2.83	0.54
3:B:267:PHE:N	3:B:267:PHE:CD1	2.76	0.54
2:A:134:PHE:O	2:A:135:ASP:HB2	2.07	0.54
3:B:594:VAL:HG12	3:B:595:GLY:N	2.22	0.54
1:C:45:U:H3'	1:C:46:G:H5'	1.88	0.54
2:A:287:HIS:HD2	2:A:288:PRO:CD	2.20	0.54
2:A:262:GLU:OE2	3:B:458:ASP:HA	2.08	0.54
2:A:86:VAL:HG12	2:A:87:ASP:N	2.21	0.54
1:C:32:C:H2'	1:C:33:U:H5'	1.89	0.54
3:B:589:LEU:HD23	3:B:609:LEU:HB2	1.89	0.54
3:B:7:TRP:O	3:B:10:ALA:HB3	2.07	0.54
2:A:162:GLU:OE2	3:B:580:ARG:HD3	2.08	0.54
3:B:593:GLY:HA3	3:B:604:SER:HB3	1.89	0.54
3:B:656:HIS:CD2	3:B:658:GLU:HG3	2.43	0.54
1:C:13:C:HO2'	1:C:14:A:H8	1.56	0.54
3:B:706:PRO:CG	3:B:709:GLU:HB2	2.21	0.53
3:B:189:ALA:HB1	3:B:378:SER:CB	2.38	0.53
2:A:50:ARG:HA	2:A:54:LEU:HD13	1.89	0.53
3:B:44:GLY:HA3	3:B:94:THR:OG1	2.07	0.53
2:A:184:VAL:HG22	2:A:294:VAL:HG12	1.91	0.53
2:A:195:ARG:HG2	2:A:223:VAL:CG2	2.38	0.53
3:B:701:VAL:CG2	3:B:705:THR:HG21	2.38	0.53
3:B:731:TYR:O	3:B:741:LYS:HA	2.09	0.53
3:B:84:GLY:O	3:B:137:GLU:HB3	2.08	0.53
2:A:9:ILE:O	2:A:13:ARG:HG2	2.07	0.53
3:B:772:LEU:HD12	3:B:779:LEU:HD21	1.91	0.53
2:A:120:GLN:NE2	3:B:489:GLU:HB2	2.23	0.53
3:B:156:LEU:HD23	3:B:156:LEU:N	2.24	0.53
3:B:294:HIS:CD2	3:B:296:GLU:HB2	2.41	0.53
3:B:701:VAL:HG12	3:B:777:PHE:CD2	2.44	0.53
3:B:120:PRO:CA	3:B:133:LEU:HD21	2.39	0.52
2:A:165:LEU:N	2:A:165:LEU:HD23	2.25	0.52
3:B:491:PRO:O	3:B:494:LYS:HG2	2.08	0.52
1:C:55:U:O4	1:C:57:G:OP2	2.26	0.52
2:A:165:LEU:HD13	2:A:303:LEU:HD11	1.92	0.52
3:B:498:LEU:HG	3:B:502:LEU:HD23	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:390:GLU:O	3:B:391:ALA:HB2	2.08	0.52
2:A:202:VAL:HG21	2:A:218:GLN:HG3	1.90	0.52
1:C:9:A:N3	1:C:45:U:O4	2.43	0.52
3:B:300:ILE:HG12	3:B:314:ALA:HB2	1.90	0.52
3:B:665:LEU:HB2	3:B:666:PRO:HD2	1.92	0.52
2:A:49:LYS:O	2:A:54:LEU:HD13	2.10	0.52
1:C:63:G:H2'	1:C:64:C:H6	1.69	0.52
3:B:120:PRO:HA	3:B:133:LEU:HD21	1.91	0.52
3:B:39:PHE:H	3:B:40:PRO:HD3	1.75	0.52
3:B:404:ILE:HG22	3:B:405:PRO:HD2	1.91	0.52
1:C:19:G:HO2'	1:C:20:U:C5'	2.22	0.52
1:C:61:C:H6	1:C:61:C:H3'	1.74	0.52
3:B:566:GLU:O	3:B:591:GLY:HA3	2.09	0.52
3:B:200:PHE:HE1	3:B:215:LEU:HB3	1.75	0.52
3:B:115:GLY:O	3:B:116:MET:HB3	2.09	0.52
2:A:143:HIS:C	2:A:145:ALA:H	2.13	0.52
1:C:35:A:N1	1:C:36:A:C5	2.78	0.51
3:B:245:VAL:HG11	3:B:324:VAL:HG11	1.91	0.51
3:B:301:ALA:HB1	3:B:309:PHE:O	2.10	0.51
3:B:232:ARG:O	3:B:236:ALA:HB2	2.11	0.51
1:C:76:A:H8	2:A:149:TRP:CE2	2.27	0.51
3:B:517:ASP:HB3	3:B:540:GLU:O	2.09	0.51
1:C:50:G:H2'	1:C:51:C:O4'	2.10	0.51
1:C:43:A:O2'	1:C:44:G:H5'	2.11	0.51
2:A:88:VAL:HG23	2:A:89:SER:N	2.26	0.51
2:A:165:LEU:HD21	2:A:301:LEU:HD13	1.93	0.51
2:A:106:MET:HG3	2:A:319:VAL:HG13	1.93	0.51
2:A:140:PRO:HD2	2:A:143:HIS:HD2	1.75	0.51
2:A:181:PRO:O	2:A:184:VAL:HG12	2.10	0.51
3:B:3:VAL:HG23	3:B:156:LEU:O	2.10	0.51
3:B:193:ALA:HB3	3:B:390:GLU:HB2	1.92	0.51
1:C:19:G:C4'	1:C:20:U:H5'	2.40	0.51
1:C:19:G:H1	1:C:56:C:H42	1.58	0.51
3:B:1:MET:CG	3:B:2:ARG:H	2.22	0.51
3:B:121:ARG:HG3	3:B:121:ARG:HH11	1.76	0.51
2:A:336:PHE:HB3	3:B:513:TYR:CE1	2.46	0.51
2:A:13:ARG:HE	2:A:72:LEU:HD22	1.75	0.51
3:B:214:THR:HB	3:B:335:VAL:O	2.11	0.50
3:B:764:ALA:HA	3:B:767:ARG:NH1	2.27	0.50
2:A:245:PHE:HE1	2:A:269:VAL:HG21	1.76	0.50
3:B:403:ALA:HA	3:B:444:VAL:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:698:ALA:HB3	3:B:780:ARG:HG3	1.91	0.50
1:C:1:G:H8	1:C:1:G:O5'	1.95	0.50
3:B:39:PHE:HB2	3:B:152:GLU:HA	1.92	0.50
3:B:16:GLU:O	3:B:17:SER:CB	2.59	0.50
3:B:50:VAL:HA	3:B:66:LEU:HD23	1.92	0.50
1:C:20:U:O2'	1:C:21:A:OP1	2.23	0.50
2:A:196:ILE:HD11	2:A:222:LEU:HD21	1.94	0.50
1:C:16:U:O2'	1:C:17:U:C6	2.65	0.50
2:A:119:TYR:OH	2:A:223:VAL:HG21	2.11	0.50
3:B:502:LEU:O	3:B:507:PHE:HB2	2.11	0.50
3:B:556:LEU:HG	3:B:556:LEU:O	2.10	0.50
3:B:213:PHE:CE2	3:B:215:LEU:HD13	2.43	0.50
2:A:201:ARG:HD3	2:A:215:VAL:CG1	2.42	0.50
3:B:510:VAL:CG1	3:B:552:LEU:HD21	2.41	0.50
2:A:149:TRP:CD1	2:A:204:ARG:NH1	2.80	0.50
1:C:31:A:C2'	1:C:32:C:C5'	2.88	0.50
2:A:131:PHE:O	2:A:135:ASP:HB3	2.11	0.50
2:A:196:ILE:HD11	2:A:222:LEU:CD2	2.42	0.50
3:B:286:LEU:HD23	3:B:317:MET:CE	2.41	0.50
3:B:610:LYS:O	3:B:614:GLU:HG2	2.11	0.50
3:B:674:ARG:NH1	3:B:674:ARG:HB3	2.26	0.50
3:B:284:LYS:HA	3:B:289:VAL:O	2.12	0.50
1:C:76:A:C8	2:A:149:TRP:CE2	3.00	0.50
3:B:607:PHE:HA	3:B:610:LYS:HB3	1.94	0.50
3:B:60:ARG:HH22	3:B:79:GLU:HG3	1.76	0.50
1:C:38:A:H2'	1:C:39:U:H5'	1.94	0.49
2:A:164:PRO:HD2	2:A:167:GLU:OE2	2.12	0.49
3:B:324:VAL:HG13	3:B:328:THR:HG21	1.94	0.49
3:B:551:GLY:O	3:B:555:VAL:HB	2.12	0.49
3:B:715:ARG:HH11	3:B:715:ARG:HB3	1.77	0.49
3:B:496:GLN:HA	3:B:496:GLN:HE21	1.78	0.49
3:B:285:THR:HG22	3:B:285:THR:O	2.11	0.49
3:B:656:HIS:O	3:B:659:ILE:HG13	2.12	0.49
3:B:722:LEU:HG	3:B:723:GLU:N	2.26	0.49
3:B:692:ALA:HB1	3:B:749:PHE:O	2.13	0.49
2:A:128:GLU:CG	2:A:129:SER:H	2.25	0.49
3:B:578:ARG:O	3:B:579:GLU:HB2	2.13	0.49
3:B:226:SER:HB3	3:B:244:ASN:HA	1.92	0.49
2:A:340:LEU:HB2	3:B:559:ASN:OD1	2.12	0.49
1:C:8:U:H4'	1:C:48:C:C1'	2.29	0.49
3:B:14:GLU:CG	3:B:14:GLU:O	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:233:LEU:HD13	2:A:313:PHE:HD1	1.76	0.49
3:B:364:VAL:O	3:B:366:PRO:HD3	2.13	0.49
3:B:12:VAL:CG2	3:B:15:LEU:HD13	2.31	0.49
3:B:242:ILE:HB	3:B:246:VAL:HG11	1.94	0.49
1:C:36:A:C6	1:C:37:A:N7	2.81	0.49
3:B:456:GLU:O	3:B:459:LEU:HB2	2.13	0.49
3:B:617:PHE:O	3:B:620:LEU:HB2	2.11	0.49
3:B:680:LYS:HB3	3:B:680:LYS:HE2	1.65	0.49
2:A:12:ALA:O	2:A:72:LEU:HD11	2.13	0.49
3:B:304:ARG:O	3:B:306:GLU:N	2.46	0.49
1:C:48:C:C2'	1:C:49:C:OP2	2.60	0.49
2:A:190:HIS:HB3	3:B:485:ASN:ND2	2.28	0.49
2:A:134:PHE:HB3	2:A:139:ILE:HD12	1.95	0.48
2:A:32:LEU:HA	2:A:36:MET:CG	2.41	0.48
3:B:102:LYS:HG2	3:B:103:VAL:O	2.13	0.48
3:B:666:PRO:CB	3:B:667:PRO:HD2	2.43	0.48
3:B:572:GLU:HG3	3:B:573:VAL:N	2.28	0.48
3:B:498:LEU:O	3:B:502:LEU:HD23	2.12	0.48
2:A:287:HIS:CD2	2:A:288:PRO:CD	2.91	0.48
3:B:198:LEU:HD21	3:B:391:ALA:HB3	1.96	0.48
3:B:700:VAL:HG22	3:B:778:GLY:O	2.12	0.48
1:C:8:U:O4	1:C:14:A:OP2	2.32	0.48
3:B:17:SER:CB	3:B:20:VAL:HB	2.44	0.48
2:A:130:GLU:O	2:A:135:ASP:HB2	2.14	0.48
3:B:609:LEU:CD1	3:B:652:LEU:CD1	2.88	0.48
3:B:545:ARG:NH1	3:B:548:LEU:HD12	2.28	0.48
3:B:478:ALA:O	3:B:479:PHE:HB3	2.14	0.48
2:A:297:TYR:CD1	2:A:301:LEU:HD11	2.49	0.48
3:B:530:ARG:HG2	3:B:579:GLU:H	1.79	0.48
3:B:780:ARG:HD3	3:B:785:PRO:CG	2.43	0.48
3:B:222:ARG:HG3	3:B:222:ARG:HH11	1.77	0.48
3:B:469:TYR:HA	3:B:472:ILE:HD12	1.95	0.48
3:B:556:LEU:HD23	3:B:665:LEU:HD22	1.96	0.48
3:B:355:GLU:HG3	3:B:359:ARG:NH1	2.29	0.48
3:B:564:ARG:N	3:B:565:PRO:HD3	2.29	0.48
3:B:576:VAL:HG11	3:B:584:HIS:CD2	2.48	0.48
3:B:282:ARG:HG2	3:B:292:THR:HA	1.96	0.47
3:B:592:GLU:HB2	3:B:602:ARG:HG3	1.95	0.47
3:B:149:ALA:O	3:B:151:PRO:HD3	2.14	0.47
2:A:143:HIS:CD2	2:A:145:ALA:HB3	2.49	0.47
3:B:285:THR:HB	3:B:289:VAL:HG23	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:91:PRO:HB2	3:B:597:PRO:CG	2.41	0.47
3:B:209:GLY:HA3	3:B:298:LEU:HD11	1.96	0.47
3:B:166:ASP:O	3:B:172:GLY:HA3	2.13	0.47
3:B:192:LYS:N	3:B:192:LYS:HD3	2.29	0.47
2:A:179:THR:HG1	2:A:220:GLU:HG3	1.77	0.47
2:A:152:PHE:CE1	2:A:204:ARG:O	2.68	0.47
1:C:74:C:H42	1:C:75:C:H5	1.61	0.47
3:B:215:LEU:CD2	3:B:272:ILE:HG13	2.42	0.47
2:A:234:LYS:HE2	3:B:474:LEU:CD2	2.44	0.47
2:A:140:PRO:HD2	2:A:143:HIS:CD2	2.49	0.47
3:B:674:ARG:CZ	3:B:674:ARG:HB3	2.44	0.47
3:B:102:LYS:HE3	3:B:102:LYS:HB3	1.53	0.47
2:A:72:LEU:O	2:A:72:LEU:HD23	2.15	0.47
2:A:195:ARG:HG2	2:A:223:VAL:CG1	2.43	0.47
3:B:507:PHE:CD2	3:B:569:LEU:HG	2.50	0.47
3:B:39:PHE:N	3:B:40:PRO:CD	2.75	0.47
3:B:60:ARG:O	3:B:60:ARG:HD2	2.14	0.47
3:B:556:LEU:CD2	3:B:665:LEU:HD22	2.44	0.47
3:B:695:ARG:HD3	3:B:761:VAL:CG1	2.45	0.47
2:A:16:GLU:HB3	2:A:72:LEU:HD12	1.96	0.47
1:C:41:G:H2'	1:C:42:C:H5'	1.96	0.47
3:B:193:ALA:HB2	3:B:388:VAL:HG23	1.97	0.47
2:A:32:LEU:C	2:A:36:MET:HG2	2.35	0.47
3:B:722:LEU:HD21	3:B:725:LEU:HB2	1.95	0.47
1:C:68:U:O2'	1:C:69:C:H5'	2.13	0.47
1:C:69:C:H2'	1:C:70:G:H8	1.79	0.47
2:A:143:HIS:CE1	2:A:145:ALA:HB2	2.50	0.47
3:B:566:GLU:HB3	3:B:592:GLU:OE1	2.15	0.47
2:A:122:VAL:O	2:A:198:VAL:HG13	2.15	0.47
3:B:699:VAL:HG13	3:B:772:LEU:HD13	1.97	0.47
3:B:145:PRO:HB2	3:B:148:GLU:HG2	1.97	0.47
3:B:415:LEU:O	3:B:472:ILE:HG23	2.15	0.47
3:B:257:ALA:O	3:B:259:PRO:HD3	2.15	0.47
3:B:613:LEU:O	3:B:616:LEU:HB3	2.14	0.47
2:A:192:PRO:O	3:B:482:ALA:HB2	2.15	0.47
2:A:102:PRO:HA	2:A:105:LEU:CD1	2.43	0.47
2:A:234:LYS:HB3	3:B:474:LEU:CD2	2.43	0.47
2:A:97:SER:HB3	2:A:347:LYS:NZ	2.30	0.47
3:B:518:PRO:HD3	3:B:542:ALA:HB3	1.97	0.46
1:C:27:U:H5'	3:B:564:ARG:NH2	2.30	0.46
3:B:672:GLU:C	3:B:673:LEU:HD23	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:71:G:H3'	1:C:71:G:C8	2.50	0.46
3:B:75:VAL:HG22	3:B:108:ILE:HD12	1.96	0.46
1:C:21:A:C2	1:C:48:C:C5	3.04	0.46
2:A:132:PHE:HE1	2:A:164:PRO:HD3	1.80	0.46
3:B:641:ARG:HA	3:B:651:PHE:HA	1.97	0.46
2:A:263:PRO:CB	3:B:461:GLU:HB2	2.45	0.46
2:A:229:ALA:O	2:A:232:HIS:HB2	2.15	0.46
2:A:235:GLY:O	2:A:238:TYR:HB3	2.16	0.46
3:B:255:GLU:OE1	3:B:375:ARG:NH1	2.48	0.46
3:B:699:VAL:O	3:B:742:SER:HA	2.16	0.46
3:B:736:LEU:O	3:B:738:GLU:N	2.46	0.46
3:B:193:ALA:HB1	3:B:390:GLU:N	2.31	0.46
2:A:240:LEU:HD11	2:A:317:LEU:HD11	1.98	0.46
3:B:589:LEU:HD12	3:B:590:PHE:H	1.81	0.46
3:B:252:VAL:HG12	3:B:252:VAL:O	2.15	0.46
3:B:509:GLU:HB2	3:B:571:PHE:HE2	1.81	0.46
1:C:76:A:H8	2:A:149:TRP:CZ2	2.33	0.46
3:B:585:LEU:HB2	3:B:675:LEU:HD11	1.96	0.46
1:C:47:U:O2	1:C:50:G:H5"	2.16	0.46
1:C:19:G:H1	1:C:56:C:N4	2.14	0.46
2:A:148:MET:HB2	2:A:149:TRP:CE3	2.51	0.46
2:A:263:PRO:HB3	3:B:461:GLU:HB2	1.96	0.46
3:B:341:VAL:HA	3:B:344:ARG:HB3	1.97	0.46
3:B:496:GLN:CA	3:B:496:GLN:HE21	2.29	0.46
2:A:142:HIS:CE1	3:B:345:LYS:HD2	2.51	0.46
3:B:773:ARG:HH21	3:B:782:LEU:CD1	2.28	0.46
1:C:35:A:C2	1:C:36:A:C8	3.04	0.46
3:B:485:ASN:O	3:B:488:VAL:HG22	2.16	0.46
3:B:35:ILE:HD11	3:B:156:LEU:HD13	1.97	0.46
2:A:269:VAL:HG23	2:A:269:VAL:O	2.15	0.46
3:B:275:ARG:HG2	3:B:275:ARG:HH11	1.81	0.46
2:A:195:ARG:CG	2:A:223:VAL:HG13	2.45	0.45
3:B:780:ARG:HD3	3:B:785:PRO:HG2	1.97	0.45
1:C:68:U:C6	1:C:68:U:C3'	2.99	0.45
2:A:141:GLU:HG2	2:A:146:ARG:CZ	2.45	0.45
3:B:345:LYS:HE2	3:B:345:LYS:HA	1.99	0.45
1:C:55:U:H6	1:C:55:U:O5'	2.00	0.45
1:C:75:C:H2'	1:C:75:C:O2	2.16	0.45
2:A:110:LEU:HD11	2:A:322:LEU:HD12	1.99	0.45
2:A:53:GLU:HA	2:A:57:ILE:HD12	1.99	0.45
3:B:46:VAL:CG2	3:B:47:PHE:N	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:344:GLU:O	2:A:347:LYS:HG2	2.15	0.45
1:C:58:A:C4'	1:C:59:U:OP1	2.33	0.45
1:C:24:G:O6	1:C:25:C:N3	2.50	0.45
3:B:751:HIS:HD2	3:B:753:LYS:HB3	1.80	0.45
3:B:631:PHE:CZ	3:B:641:ARG:HB3	2.52	0.45
3:B:242:ILE:HB	3:B:246:VAL:CG1	2.47	0.45
2:A:271:TRP:CE3	2:A:274:GLY:HA3	2.52	0.45
1:C:27:U:C2	1:C:28:G:N7	2.85	0.45
3:B:1:MET:HG2	3:B:2:ARG:H	1.81	0.45
3:B:707:TYR:O	3:B:709:GLU:N	2.50	0.45
1:C:56:C:H6	1:C:56:C:OP1	1.99	0.45
2:A:298:ARG:HH12	2:A:306:ALA:HB2	1.82	0.45
3:B:780:ARG:CD	3:B:785:PRO:HG2	2.47	0.45
3:B:173:LEU:HA	3:B:173:LEU:HD13	1.66	0.45
3:B:82:ARG:HG3	3:B:83:LYS:O	2.17	0.45
2:A:132:PHE:HA	2:A:132:PHE:HD2	1.63	0.45
2:A:180:SER:N	2:A:181:PRO:HD2	2.32	0.45
3:B:430:ARG:CB	3:B:430:ARG:HH11	2.30	0.45
3:B:459:LEU:O	3:B:462:GLU:HB2	2.16	0.45
3:B:430:ARG:NH1	3:B:430:ARG:HB3	2.32	0.45
1:C:47:U:H5'	1:C:48:C:OP2	2.17	0.44
3:B:286:LEU:HD23	3:B:317:MET:HE1	1.99	0.44
3:B:604:SER:CA	3:B:608:LEU:HD22	2.43	0.44
3:B:464:ALA:O	3:B:469:TYR:CE2	2.70	0.44
3:B:512:THR:HG22	3:B:555:VAL:HG21	1.99	0.44
3:B:202:LEU:HB2	3:B:215:LEU:HD23	2.00	0.44
2:A:240:LEU:O	2:A:244:LEU:HB2	2.17	0.44
1:C:14:A:H2'	1:C:15:G:C5'	2.44	0.44
2:A:12:ALA:O	2:A:16:GLU:N	2.50	0.44
2:A:233:LEU:CD1	2:A:313:PHE:CD1	3.00	0.44
3:B:28:LEU:HA	3:B:28:LEU:HD23	1.68	0.44
2:A:263:PRO:CG	3:B:461:GLU:HB2	2.47	0.44
3:B:628:ALA:O	3:B:629:GLN:HB2	2.17	0.44
2:A:208:THR:HG22	2:A:208:THR:O	2.16	0.44
2:A:213:GLU:HG3	2:A:332:ILE:HG23	1.99	0.44
1:C:10:G:C2	1:C:11:C:C5	3.05	0.44
3:B:56:ILE:HD11	3:B:63:ARG:HB2	1.99	0.44
2:A:324:MET:O	2:A:328:GLY:HA2	2.17	0.44
1:C:19:G:H4'	1:C:20:U:H5'	1.99	0.44
3:B:213:PHE:HE2	3:B:215:LEU:CD1	2.28	0.44
1:C:24:G:N7	1:C:25:C:C6	2.86	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:U:C2	1:C:28:G:C8	3.06	0.44
2:A:143:HIS:C	2:A:145:ALA:N	2.71	0.44
3:B:25:LEU:HD13	3:B:158:LEU:HD21	2.00	0.44
3:B:707:TYR:HE1	3:B:745:PHE:HZ	1.65	0.44
2:A:52:GLN:O	2:A:56:ALA:HB3	2.17	0.44
2:A:28:LYS:O	2:A:32:LEU:HG	2.17	0.44
2:A:78:LYS:HA	2:A:81:LEU:HD12	1.98	0.44
2:A:228:ILE:N	2:A:228:ILE:CD1	2.80	0.44
3:B:120:PRO:HG3	3:B:133:LEU:HD21	1.99	0.44
3:B:2:ARG:HG3	3:B:155:VAL:CG1	2.47	0.44
2:A:67:ALA:O	2:A:71:ALA:HB3	2.18	0.44
2:A:133:ASN:ND2	2:A:178:HIS:CD2	2.86	0.44
3:B:710:VAL:HG21	3:B:743:LEU:HD12	1.99	0.44
3:B:461:GLU:O	3:B:461:GLU:HG2	2.17	0.44
3:B:703:ALA:O	3:B:741:LYS:HD3	2.18	0.44
2:A:65:LEU:O	2:A:69:GLU:HB3	2.18	0.44
2:A:183:GLN:CG	2:A:222:LEU:HD22	2.39	0.44
3:B:701:VAL:HB	3:B:777:PHE:CE2	2.53	0.44
3:B:761:VAL:O	3:B:764:ALA:HB3	2.18	0.44
3:B:430:ARG:NH1	3:B:430:ARG:CB	2.80	0.44
3:B:666:PRO:HB2	3:B:667:PRO:CD	2.48	0.43
2:A:329:ILE:HG23	2:A:330:PRO:CD	2.48	0.43
3:B:644:VAL:HG23	3:B:649:VAL:CG2	2.48	0.43
3:B:730:LEU:CD1	3:B:743:LEU:CD2	2.91	0.43
3:B:128:TYR:CB	3:B:240:ARG:HD2	2.48	0.43
2:A:283:ALA:CB	2:A:315:PHE:HA	2.48	0.43
1:C:20:U:H6	1:C:20:U:H3'	1.82	0.43
1:C:26:A:C5	1:C:27:U:C5	3.06	0.43
2:A:266:GLN:HG3	2:A:266:GLN:O	2.18	0.43
2:A:134:PHE:CD1	2:A:134:PHE:O	2.68	0.43
2:A:224:VAL:HG13	2:A:312:GLY:HA3	2.00	0.43
2:A:182:MET:CG	2:A:198:VAL:HG11	2.48	0.43
2:A:198:VAL:N	2:A:220:GLU:O	2.45	0.43
3:B:47:PHE:CZ	3:B:139:ALA:HB3	2.54	0.43
2:A:221:GLY:O	2:A:314:ALA:HA	2.18	0.43
2:A:242:GLN:HE22	2:A:247:PRO:HA	1.83	0.43
2:A:197:VAL:HB	2:A:219:LEU:HD11	2.00	0.43
2:A:12:ALA:C	2:A:72:LEU:HD11	2.38	0.43
3:B:555:VAL:HG12	3:B:556:LEU:N	2.34	0.43
3:B:407:ARG:NH2	3:B:410:TYR:CG	2.87	0.43
2:A:340:LEU:O	2:A:344:GLU:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:357:SER:O	3:B:360:PHE:N	2.51	0.43
3:B:677:LEU:HB3	3:B:678:PRO:HD2	2.01	0.43
3:B:165:PRO:HG2	3:B:451:LEU:HD23	2.00	0.43
3:B:164:ARG:HA	3:B:164:ARG:HD2	1.36	0.43
3:B:408:PRO:O	3:B:411:ALA:HB3	2.18	0.43
3:B:707:TYR:HE1	3:B:745:PHE:CZ	2.36	0.43
2:A:232:HIS:HD2	3:B:477:PRO:HB3	1.83	0.43
3:B:596:LEU:HB2	3:B:599:ALA:CB	2.48	0.43
2:A:271:TRP:HB2	2:A:278:LEU:HD22	1.99	0.43
3:B:283:LEU:CD2	3:B:320:ALA:HB2	2.42	0.43
3:B:260:MET:HB3	3:B:335:VAL:HG22	2.01	0.43
3:B:259:PRO:HB3	3:B:356:ALA:CB	2.48	0.43
3:B:306:GLU:HA	3:B:306:GLU:OE2	2.19	0.43
3:B:531:LEU:HB2	3:B:544:LEU:HD12	2.00	0.43
3:B:67:ASP:C	3:B:69:GLY:H	2.22	0.43
2:A:16:GLU:HB3	2:A:72:LEU:CD1	2.49	0.42
2:A:195:ARG:HA	2:A:223:VAL:HG22	2.01	0.42
2:A:128:GLU:HG2	2:A:181:PRO:HB3	2.00	0.42
3:B:469:TYR:HA	3:B:472:ILE:HD11	2.01	0.42
3:B:377:LEU:HB3	3:B:388:VAL:HG11	2.00	0.42
3:B:206:ASP:OD2	3:B:276:ARG:NH1	2.51	0.42
3:B:573:VAL:HA	3:B:584:HIS:O	2.19	0.42
3:B:194:GLU:OE2	3:B:387:ARG:NH2	2.52	0.42
1:C:20:U:H3'	1:C:20:U:C6	2.54	0.42
3:B:1:MET:N	3:B:158:LEU:O	2.52	0.42
1:C:6:G:C2'	1:C:7:G:O5'	2.67	0.42
2:A:140:PRO:O	2:A:143:HIS:HB2	2.19	0.42
2:A:271:TRP:O	2:A:272:PRO:C	2.58	0.42
1:C:45:U:H2'	1:C:46:G:O5'	2.18	0.42
1:C:8:U:O4	1:C:13:C:H2'	2.19	0.42
3:B:406:PHE:HA	3:B:456:GLU:HG3	2.02	0.42
3:B:128:TYR:CD2	3:B:240:ARG:HD2	2.54	0.42
3:B:430:ARG:HB2	3:B:430:ARG:HH11	1.83	0.42
1:C:20:U:C3'	1:C:20:U:C6	3.02	0.42
3:B:99:LEU:HD23	3:B:101:GLN:HB3	1.99	0.42
2:A:105:LEU:HD13	2:A:349:VAL:HG21	2.02	0.42
3:B:507:PHE:CE2	3:B:569:LEU:HG	2.55	0.42
3:B:223:VAL:HG13	3:B:243:ASN:HB2	2.01	0.42
3:B:80:ASN:O	3:B:82:ARG:NH1	2.52	0.42
3:B:779:LEU:HB3	3:B:780:ARG:H	1.63	0.42
2:A:234:LYS:HE2	2:A:234:LYS:HB3	1.79	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:150:TRP:CZ2	3:B:232:ARG:HA	2.55	0.42
3:B:644:VAL:O	3:B:645:GLU:C	2.58	0.42
3:B:514:SER:O	3:B:545:ARG:HG2	2.20	0.42
3:B:91:LEU:HA	3:B:91:LEU:HD23	1.89	0.42
3:B:309:PHE:HA	3:B:310:PRO:HD3	1.68	0.42
2:A:220:GLU:HA	2:A:316:GLY:HA2	2.02	0.42
3:B:734:PRO:CA	3:B:736:LEU:H	2.23	0.42
3:B:491:PRO:HG2	3:B:492:TYR:H	1.85	0.42
3:B:496:GLN:NE2	3:B:496:GLN:HA	2.35	0.42
2:A:178:HIS:CD2	2:A:178:HIS:H	2.38	0.42
3:B:701:VAL:HA	3:B:702:PRO:HD2	1.82	0.42
1:C:76:A:C8	2:A:149:TRP:NE1	2.88	0.42
3:B:467:GLN:NE2	3:B:467:GLN:HA	2.33	0.42
2:A:110:LEU:HD12	2:A:319:VAL:HG22	2.02	0.42
1:C:49:C:O5'	1:C:49:C:C6	2.69	0.41
2:A:228:ILE:O	2:A:311:THR:HG21	2.19	0.41
3:B:265:LEU:HD23	3:B:265:LEU:HA	1.79	0.41
1:C:37:A:C6	1:C:38:A:C8	3.08	0.41
1:C:39:U:C2'	1:C:40:C:C5'	2.75	0.41
1:C:45:U:H2'	1:C:46:G:H5"	2.02	0.41
1:C:61:C:C4	1:C:62:C:C4	3.08	0.41
3:B:96:LEU:HA	3:B:97:PRO:HD3	1.60	0.41
3:B:21:LEU:O	3:B:24:ARG:N	2.53	0.41
1:C:65:G:C2'	1:C:66:C:C5'	2.88	0.41
3:B:772:LEU:HB3	3:B:777:PHE:O	2.20	0.41
3:B:538:ALA:HB1	3:B:540:GLU:OE2	2.20	0.41
3:B:633:PHE:O	3:B:656:HIS:HB2	2.21	0.41
3:B:243:ASN:O	3:B:245:VAL:N	2.53	0.41
3:B:245:VAL:CG1	3:B:324:VAL:HG11	2.50	0.41
3:B:715:ARG:CG	3:B:725:LEU:HD22	2.46	0.41
3:B:90:ALA:CB	3:B:118:LEU:HD21	2.50	0.41
3:B:364:VAL:HG12	3:B:365:ASP:N	2.35	0.41
1:C:11:C:C2	1:C:12:U:C5	3.09	0.41
2:A:135:ASP:HB3	2:A:136:ALA:H	1.74	0.41
2:A:160:ARG:NE	3:B:580:ARG:HH21	2.19	0.41
3:B:614:GLU:HG2	3:B:614:GLU:H	1.65	0.41
3:B:728:PHE:CG	3:B:746:HIS:CD2	3.08	0.41
1:C:47:U:H6	1:C:47:U:O5'	2.04	0.41
2:A:49:LYS:H	2:A:49:LYS:CD	2.29	0.41
3:B:692:ALA:HB2	3:B:750:ARG:HD2	2.03	0.41
3:B:211:PRO:HD2	3:B:337:CYS:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:254:LEU:HD23	3:B:254:LEU:HA	1.77	0.41
2:A:132:PHE:C	2:A:133:ASN:O	2.59	0.41
2:A:132:PHE:CE1	2:A:164:PRO:HD3	2.55	0.41
1:C:36:A:N1	1:C:37:A:C8	2.88	0.41
2:A:23:ALA:O	2:A:27:GLY:N	2.51	0.41
3:B:243:ASN:H	3:B:246:VAL:HG12	1.85	0.41
3:B:153:GLU:HG3	3:B:154:VAL:N	2.35	0.41
3:B:171:LEU:HD21	3:B:186:GLU:HG3	2.03	0.41
2:A:184:VAL:O	2:A:188:VAL:HG22	2.21	0.41
3:B:289:VAL:HG21	3:B:291:ARG:CZ	2.51	0.41
1:C:26:A:H2'	1:C:26:A:N3	2.35	0.41
3:B:420:PRO:HD2	3:B:423:GLU:OE2	2.21	0.41
3:B:178:HIS:CD2	3:B:182:TYR:O	2.67	0.41
3:B:576:VAL:HG11	3:B:584:HIS:NE2	2.36	0.41
3:B:90:ALA:O	3:B:91:LEU:O	2.38	0.41
3:B:594:VAL:CG1	3:B:595:GLY:N	2.83	0.41
3:B:482:ALA:HA	3:B:483:PRO:HD3	1.93	0.41
2:A:141:GLU:HG3	2:A:141:GLU:H	1.71	0.41
3:B:586:ALA:HA	3:B:671:PHE:O	2.20	0.41
3:B:73:GLU:O	3:B:74:VAL:HG23	2.21	0.41
1:C:61:C:H3'	1:C:61:C:C6	2.55	0.41
2:A:298:ARG:NH1	2:A:306:ALA:HB2	2.36	0.41
3:B:370:VAL:O	3:B:373:GLN:HB2	2.21	0.41
1:C:76:A:N7	2:A:149:TRP:HZ2	2.18	0.41
3:B:243:ASN:O	3:B:244:ASN:C	2.58	0.41
1:C:9:A:N6	1:C:22:G:N7	2.68	0.40
3:B:286:LEU:HD23	3:B:317:MET:HE2	2.03	0.40
2:A:50:ARG:HA	2:A:54:LEU:CD1	2.50	0.40
3:B:414:LEU:CD2	3:B:460:VAL:HG21	2.47	0.40
3:B:96:LEU:HB2	3:B:99:LEU:CD1	2.46	0.40
2:A:86:VAL:CG1	2:A:87:ASP:N	2.83	0.40
1:C:45:U:H2'	1:C:46:G:C5'	2.50	0.40
3:B:489:GLU:HG2	3:B:493:ARG:HG3	2.03	0.40
3:B:329:GLU:CD	3:B:329:GLU:N	2.75	0.40
2:A:92:GLY:O	2:A:93:ALA:C	2.60	0.40
2:A:14:ASP:O	2:A:17:GLU:HB3	2.19	0.40
2:A:197:VAL:HB	2:A:219:LEU:CD1	2.51	0.40
3:B:589:LEU:O	3:B:590:PHE:CB	2.68	0.40
3:B:353:ARG:CD	3:B:353:ARG:H	2.33	0.40
3:B:622:LEU:HA	3:B:645:GLU:OE1	2.21	0.40
3:B:402:GLU:OE2	3:B:402:GLU:HA	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:27:GLY:O	2:A:31:LEU:HB2	2.22	0.40
3:B:768:VAL:O	3:B:772:LEU:HG	2.22	0.40
3:B:455:LEU:N	3:B:455:LEU:CD1	2.84	0.40
3:B:499:ARG:O	3:B:503:SER:HB2	2.21	0.40
3:B:757:ARG:O	3:B:759:GLU:N	2.54	0.40
2:A:65:LEU:HD23	2:A:65:LEU:HA	1.89	0.40
2:A:139:ILE:HG12	2:A:259:PRO:HG3	2.03	0.40
2:A:126:GLU:OE2	3:B:575:ARG:HB2	2.22	0.40
3:B:56:ILE:HA	3:B:57:PRO:HD3	1.86	0.40
1:C:67:C:OP2	1:C:67:C:C5	2.74	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	343/350 (98%)	286 (83%)	42 (12%)	15 (4%)	3	22
3	B	783/785 (100%)	647 (83%)	97 (12%)	39 (5%)	3	19
All	All	1126/1135 (99%)	933 (83%)	139 (12%)	54 (5%)	3	20

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	48	ARG
2	A	130	GLU
2	A	135	ASP
3	B	16	GLU
3	B	39	PHE
3	B	286	LEU
3	B	326	GLU
3	B	386	ALA

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Mol	Chain	Res	Type
3	B	391	ALA
3	B	406	PHE
3	B	629	GLN
3	B	691	PRO
3	B	701	VAL
3	B	738	GLU
2	A	133	ASN
2	A	247	PRO
2	A	280	LEU
2	A	320	GLU
2	A	328	GLY
2	A	338	GLY
3	B	97	PRO
3	B	139	ALA
3	B	244	ASN
3	B	305	GLY
3	B	725	LEU
3	B	757	ARG
2	A	272	PRO
3	B	17	SER
3	B	256	ARG
3	B	367	LEU
3	B	590	PHE
3	B	737	PRO
3	B	753	LYS
2	A	330	PRO
3	B	291	ARG
2	A	166	GLY
3	B	57	PRO
3	B	81	ALA
3	B	91	LEU
3	B	116	MET
3	B	127	GLU
3	B	319	GLY
3	B	421	GLU
3	B	748	ARG
3	B	758	ASP
3	B	784	THR
2	A	42	LEU
2	A	93	ALA
2	A	164	PRO
3	B	657	PRO

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Mol	Chain	Res	Type
3	B	142	PRO
3	B	209	GLY
3	B	708	GLY
3	B	735	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	A	272/277 (98%)	220 (81%)	52 (19%)	2 8
3	B	630/630 (100%)	512 (81%)	118 (19%)	2 9
All	All	902/907 (99%)	732 (81%)	170 (19%)	2 8

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	24	ARG
2	A	25	TYR
2	A	34	GLN
2	A	45	GLU
2	A	47	ARG
2	A	49	LYS
2	A	55	ASN
2	A	68	ARG
2	A	77	LEU
2	A	83	ARG
2	A	85	ARG
2	A	103	ILE
2	A	104	THR
2	A	120	GLN
2	A	122	VAL
2	A	126	GLU
2	A	129	SER
2	A	132	PHE
2	A	133	ASN

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Mol	Chain	Res	Type
2	A	134	PHE
2	A	135	ASP
2	A	138	ASN
2	A	143	HIS
2	A	151	THR
2	A	153	TRP
2	A	160	ARG
2	A	165	LEU
2	A	168	GLU
2	A	170	GLU
2	A	176	ARG
2	A	178	HIS
2	A	184	VAL
2	A	188	VAL
2	A	202	VAL
2	A	204	ARG
2	A	206	GLU
2	A	213	GLU
2	A	219	LEU
2	A	224	VAL
2	A	232	HIS
2	A	240	LEU
2	A	256	VAL
2	A	260	PHE
2	A	278	LEU
2	A	311	THR
2	A	317	LEU
2	A	320	GLU
2	A	327	TYR
2	A	339	ARG
2	A	340	LEU
2	A	349	VAL
2	A	350	LEU
3	B	2	ARG
3	B	12	VAL
3	B	16	GLU
3	B	22	GLU
3	B	24	ARG
3	B	31	GLU
3	B	33	ASP
3	B	35	ILE
3	B	37	ARG

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Mol	Chain	Res	Type
3	B	43	ARG
3	B	46	VAL
3	B	67	ASP
3	B	70	ARG
3	B	72	VAL
3	B	83	LYS
3	B	87	VAL
3	B	89	LEU
3	B	106	ARG
3	B	108	ILE
3	B	109	GLN
3	B	111	VAL
3	B	137	GLU
3	B	156	LEU
3	B	157	ASP
3	B	170	LEU
3	B	173	LEU
3	B	176	ASP
3	B	184	LEU
3	B	192	LYS
3	B	203	LYS
3	B	215	LEU
3	B	222	ARG
3	B	234	LEU
3	B	239	MET
3	B	242	ILE
3	B	260	MET
3	B	268	VAL
3	B	270	GLU
3	B	275	ARG
3	B	276	ARG
3	B	285	THR
3	B	289	VAL
3	B	296	GLU
3	B	298	LEU
3	B	307	GLU
3	B	313	LEU
3	B	317	MET
3	B	329	GLU
3	B	333	LEU
3	B	341	VAL
3	B	353	ARG

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Mol	Chain	Res	Type
3	B	354	THR
3	B	361	GLU
3	B	362	ARG
3	B	374	ARG
3	B	375	ARG
3	B	394	GLU
3	B	397	SER
3	B	399	LYS
3	B	402	GLU
3	B	404	ILE
3	B	434	ARG
3	B	438	GLU
3	B	441	THR
3	B	451	LEU
3	B	454	ARG
3	B	459	LEU
3	B	460	VAL
3	B	467	GLN
3	B	474	LEU
3	B	476	LEU
3	B	496	GLN
3	B	497	ARG
3	B	502	LEU
3	B	503	SER
3	B	505	LEU
3	B	508	GLN
3	B	519	GLU
3	B	522	ARG
3	B	526	LEU
3	B	527	ASP
3	B	529	PRO
3	B	530	ARG
3	B	532	LEU
3	B	540	GLU
3	B	544	LEU
3	B	548	LEU
3	B	550	PRO
3	B	554	ARG
3	B	556	LEU
3	B	557	LYS
3	B	570	LEU
3	B	571	PHE

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Mol	Chain	Res	Type
3	B	577	PHE
3	B	583	THR
3	B	584	HIS
3	B	588	LEU
3	B	590	PHE
3	B	609	LEU
3	B	613	LEU
3	B	614	GLU
3	B	629	GLN
3	B	633	PHE
3	B	641	ARG
3	B	655	LEU
3	B	659	ILE
3	B	670	LEU
3	B	673	LEU
3	B	679	ASP
3	B	680	LYS
3	B	701	VAL
3	B	711	GLU
3	B	716	GLU
3	B	738	GLU
3	B	754	ARG
3	B	763	GLU
3	B	770	GLU
3	B	775	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	34	GLN
2	A	52	GLN
2	A	120	GLN
2	A	133	ASN
2	A	138	ASN
2	A	143	HIS
2	A	178	HIS
2	A	207	GLN
2	A	232	HIS
2	A	242	GLN
2	A	287	HIS
2	A	292	GLN
3	B	178	HIS

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Mol	Chain	Res	Type
3	B	258	GLN
3	B	294	HIS
3	B	373	GLN
3	B	381	GLN
3	B	467	GLN
3	B	485	ASN
3	B	496	GLN
3	B	690	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	75/76 (98%)	33 (44%)	8 (10%)

All (33) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	C
1	C	7	G
1	C	8	U
1	C	10	G
1	C	11	C
1	C	12	U
1	C	17	U
1	C	18	G
1	C	20	U
1	C	21	A
1	C	22	G
1	C	33	U
1	C	35	A
1	C	40	C
1	C	46	G
1	C	47	U
1	C	48	C
1	C	49	C
1	C	50	G
1	C	51	C
1	C	54	U
1	C	56	C
1	C	57	G
1	C	58	A

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Mol	Chain	Res	Type
1	C	59	U
1	C	60	U
1	C	61	C
1	C	67	C
1	C	69	C
1	C	72	C
1	C	73	A
1	C	74	C
1	C	76	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	7	G
1	C	9	A
1	C	19	G
1	C	20	U
1	C	47	U
1	C	56	C
1	C	57	G
1	C	58	A

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	C	76/76 (100%)	5.06	72 (94%) 0 0	80, 80, 80, 80	76 (100%)
2	A	345/350 (98%)	0.97	63 (18%) 2 1	17, 59, 95, 138	71 (20%)
3	B	785/785 (100%)	-0.13	2 (0%) 94 94	9, 62, 98, 140	0
All	All	1206/1211 (99%)	0.51	137 (11%) 7 5	9, 64, 98, 140	147 (12%)

All (137) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	56	C	17.2
1	C	19	G	14.3
1	C	20	U	14.2
1	C	57	G	12.8
1	C	18	G	12.0
1	C	63	G	10.2
2	A	11	ASN	10.1
2	A	10	GLN	10.0
2	A	33	THR	9.6
1	C	64	C	9.4
2	A	50	ARG	9.0
2	A	34	GLN	8.8
1	C	51	C	8.8
2	A	9	ILE	8.1
1	C	55	U	8.0
2	A	35	GLU	8.0
2	A	25	TYR	7.9
2	A	8	ALA	7.9
2	A	39	LEU	7.7
2	A	12	ALA	7.6
1	C	21	A	7.2
1	C	4	G	7.2
2	A	49	LYS	7.0

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Mol	Chain	Res	Type	RSRZ
2	A	26	LEU	7.0
1	C	5	A	6.9
2	A	38	GLY	6.9
2	A	52	GLN	6.8
1	C	53	G	6.7
1	C	17	U	6.6
1	C	70	G	6.5
2	A	32	LEU	6.5
1	C	73	A	6.5
2	A	14	ASP	6.5
1	C	52	G	6.3
2	A	54	LEU	6.2
2	A	30	GLY	6.2
1	C	48	C	6.1
2	A	40	SER	6.1
1	C	58	A	6.0
1	C	50	G	6.0
2	A	21	LEU	6.0
2	A	57	ILE	6.0
2	A	36	MET	5.9
2	A	43	PRO	5.9
2	A	46	GLU	5.8
2	A	65	LEU	5.8
2	A	31	LEU	5.7
2	A	42	LEU	5.7
2	A	51	GLY	5.7
1	C	44	G	5.7
2	A	23	ALA	5.7
2	A	18	LEU	5.6
1	C	68	U	5.6
1	C	6	G	5.5
1	C	71	G	5.5
2	A	53	GLU	5.4
1	C	2	C	5.4
1	C	62	C	5.4
1	C	16	U	5.4
1	C	10	G	5.3
2	A	16	GLU	5.3
1	C	54	U	5.2
1	C	1	G	5.2
1	C	65	G	5.1
2	A	61	LEU	5.0

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Mol	Chain	Res	Type	RSRZ
2	A	37	LYS	4.9
2	A	47	ARG	4.9
2	A	19	LYS	4.9
1	C	75	C	4.8
1	C	22	G	4.8
1	C	24	G	4.8
1	C	72	C	4.7
1	C	9	A	4.7
2	A	13	ARG	4.7
1	C	15	G	4.6
1	C	3	C	4.6
1	C	76	A	4.6
2	A	64	ALA	4.5
2	A	27	GLY	4.5
2	A	55	ASN	4.5
2	A	41	ALA	4.4
2	A	7	ALA	4.3
2	A	22	LYS	4.3
1	C	11	C	4.3
1	C	23	A	4.2
1	C	46	G	4.1
2	A	60	ALA	4.1
1	C	8	U	4.1
2	A	58	LYS	4.1
2	A	56	ALA	4.1
1	C	61	C	4.1
2	A	24	ARG	4.0
2	A	29	LYS	4.0
2	A	28	LYS	3.9
1	C	66	C	3.8
1	C	25	C	3.6
1	C	60	U	3.6
1	C	42	C	3.5
2	A	48	ARG	3.5
1	C	74	C	3.5
1	C	67	C	3.4
1	C	41	G	3.4
1	C	40	C	3.3
2	A	68	ARG	3.3
1	C	59	U	3.3
1	C	12	U	3.3
1	C	69	C	3.3

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Mol	Chain	Res	Type	RSRZ
2	A	69	GLU	3.3
1	C	14	A	3.3
1	C	43	A	3.3
1	C	35	A	3.2
1	C	30	G	3.1
1	C	49	C	3.1
2	A	66	GLU	3.0
1	C	29	C	2.9
2	A	6	LEU	2.9
2	A	15	LEU	2.8
2	A	59	ALA	2.8
2	A	77	LEU	2.8
3	B	784	THR	2.8
2	A	45	GLU	2.8
2	A	44	LEU	2.7
1	C	32	C	2.6
1	C	31	A	2.6
1	C	45	U	2.5
1	C	7	G	2.4
1	C	39	U	2.4
1	C	34	G	2.4
2	A	79	GLU	2.4
1	C	38	A	2.3
3	B	785	PRO	2.3
1	C	47	U	2.3
2	A	17	GLU	2.3
1	C	36	A	2.2
1	C	27	U	2.1
2	A	62	GLU	2.1
1	C	13	C	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.