



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2014 – 12:19 PM GMT

PDB ID : 1T5E
Title : The structure of MexA
Authors : Higgins, M.K.; Bokma, E.; Koronakis, E.; Hughes, C.; Koronakis, V.
Deposited on : 2004-05-04
Resolution : 3.00 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

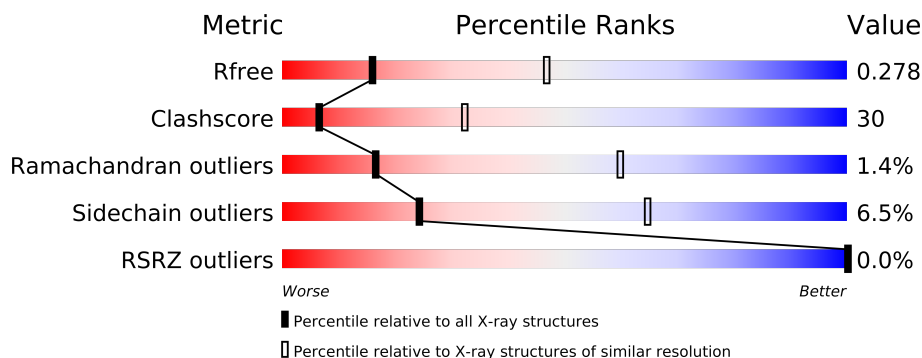
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 3.00 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}	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	360	
1	B	360	
1	C	360	
1	D	360	
1	E	360	
1	F	360	
1	G	360	
1	H	360	
1	I	360	
1	J	360	
1	K	360	
1	L	360	
1	M	360	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	3GR	E	361	-	X
2	3GR	H	361	-	X
2	3GR	K	361	-	X
2	3GR	L	361	-	X
3	GOL	J	361	-	X

2 Entry composition

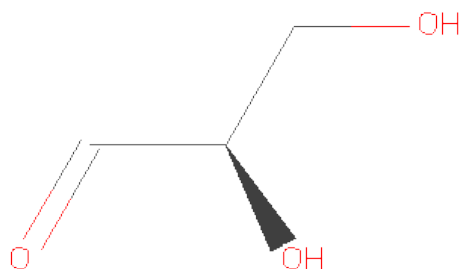
There are 3 unique types of molecules in this entry. The entry contains 23101 atoms, of which 0 are hydrogen and 0 are deuterium.

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 protein called Multidrug resistance protein mexA.

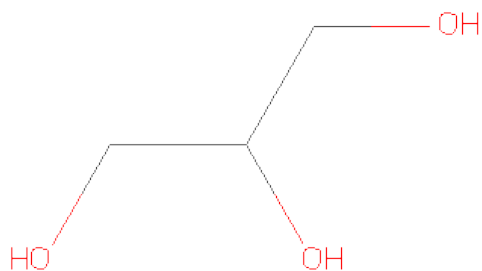
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	B	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	C	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	D	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	E	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	F	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	G	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	H	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	I	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	J	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	K	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	L	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			
1	M	231	Total	C	N	O	S	0	0	0
			1771	1101	319	349	2			

- Molecule 2 is GLYCERALDEHYDE (three-letter code: 3GR) (formula: C₃H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			6	3	3		
2	D	1	Total	C	O	0	0
			6	3	3		
2	E	1	Total	C	O	0	0
			6	3	3		
2	F	1	Total	C	O	0	0
			6	3	3		
2	G	1	Total	C	O	0	0
			6	3	3		
2	H	1	Total	C	O	0	0
			6	3	3		
2	I	1	Total	C	O	0	0
			6	3	3		
2	K	1	Total	C	O	0	0
			6	3	3		
2	L	1	Total	C	O	0	0
			6	3	3		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



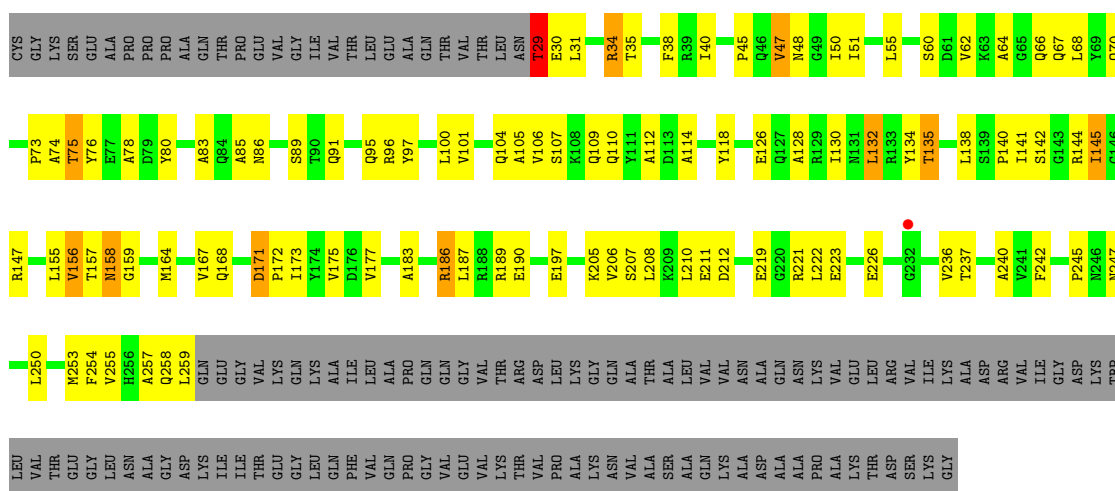
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		

3 Residue-property plots

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.

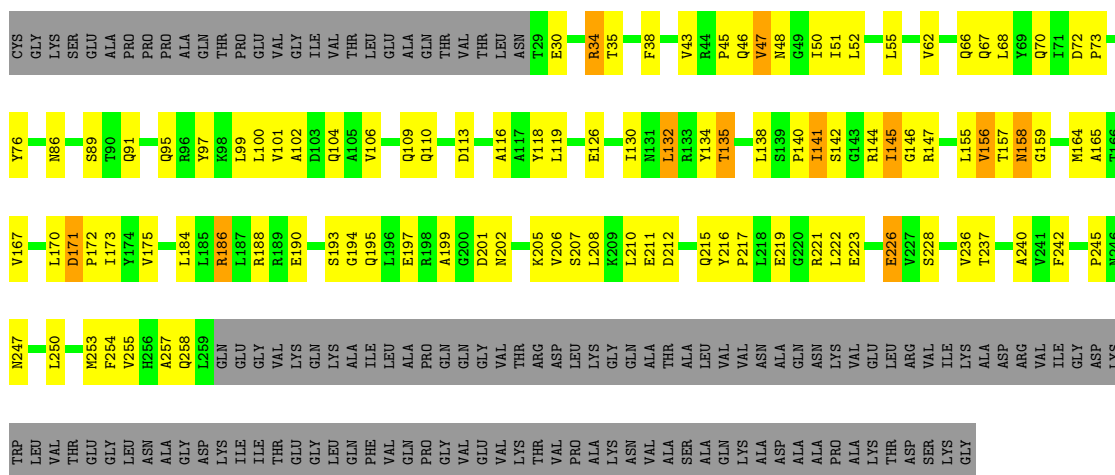
- Molecule 1: Multidrug resistance protein mexA

Chain A:



- Molecule 1: Multidrug resistance protein mexA

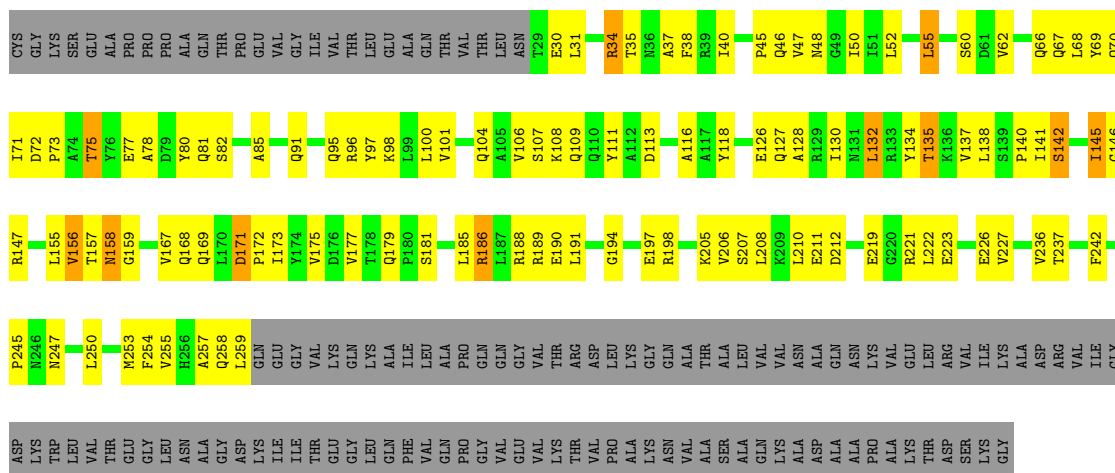
Chain B:



- Molecule 1: Multidrug resistance protein mexA

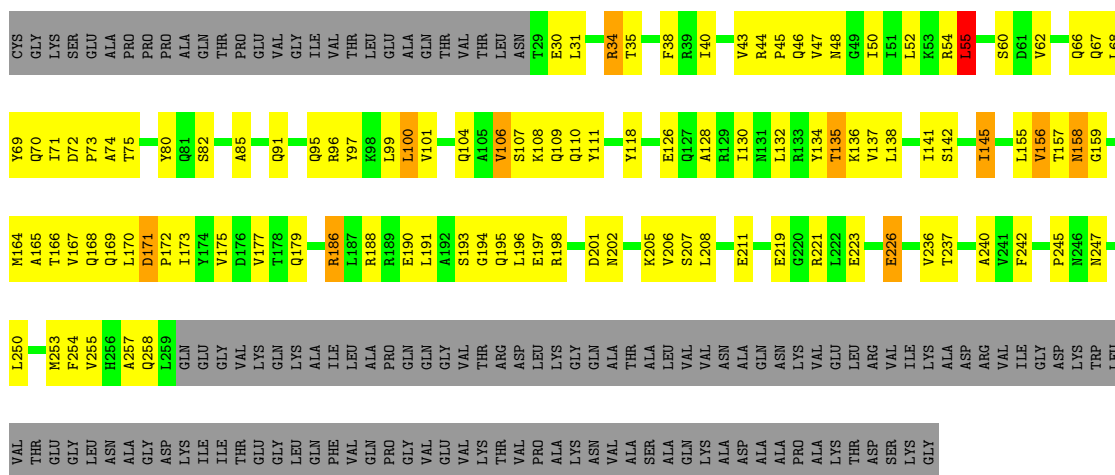
Chain C:

Chain F:



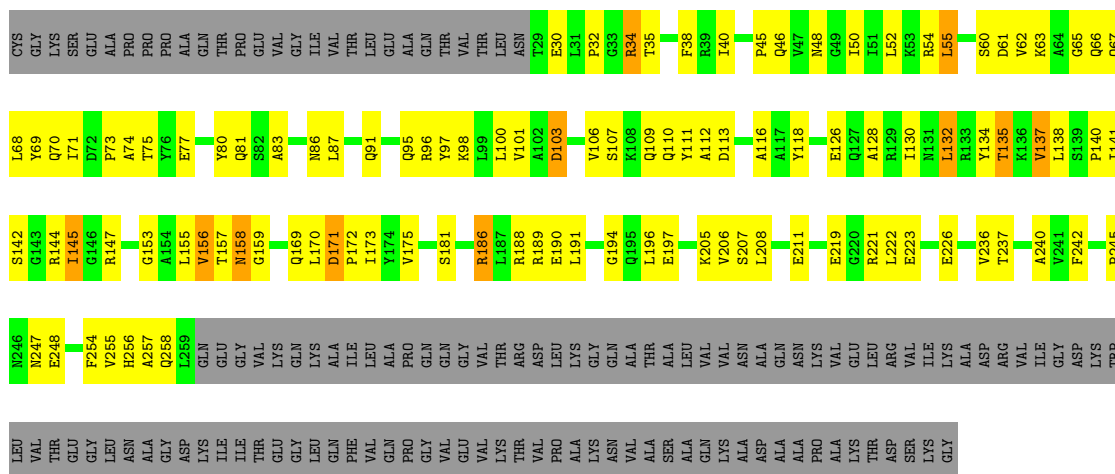
- Molecule 1: Multidrug resistance protein mexA

Chain G:



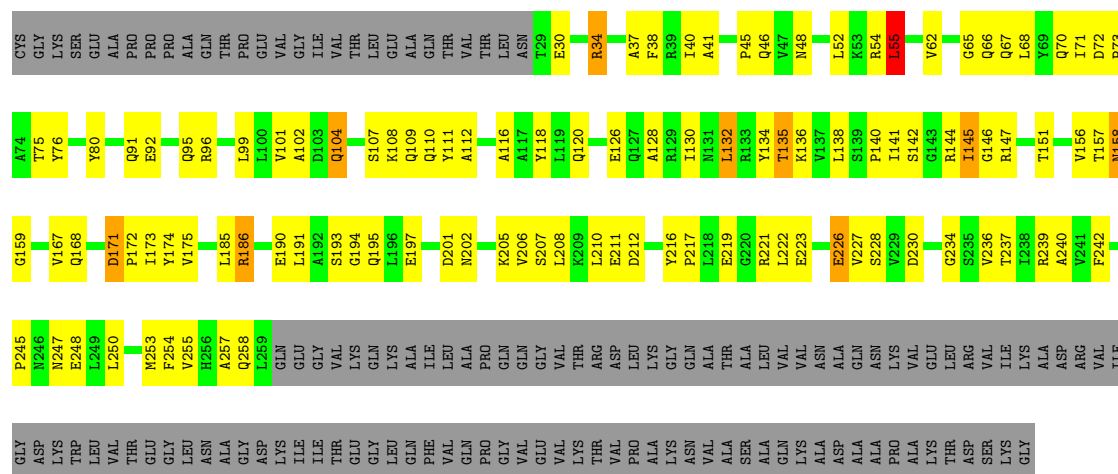
- Molecule 1: Multidrug resistance protein mexA

Chain H:



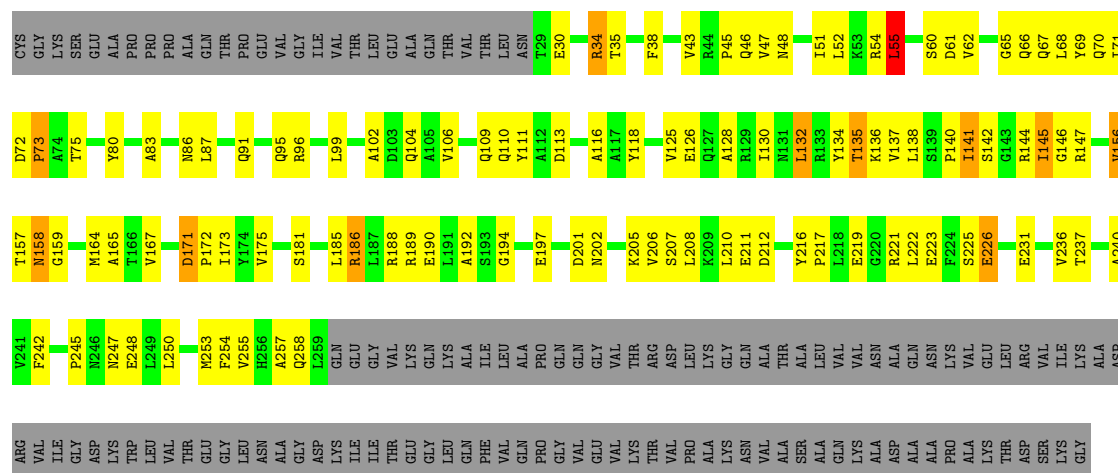
- Molecule 1: Multidrug resistance protein mexA

Chain I:



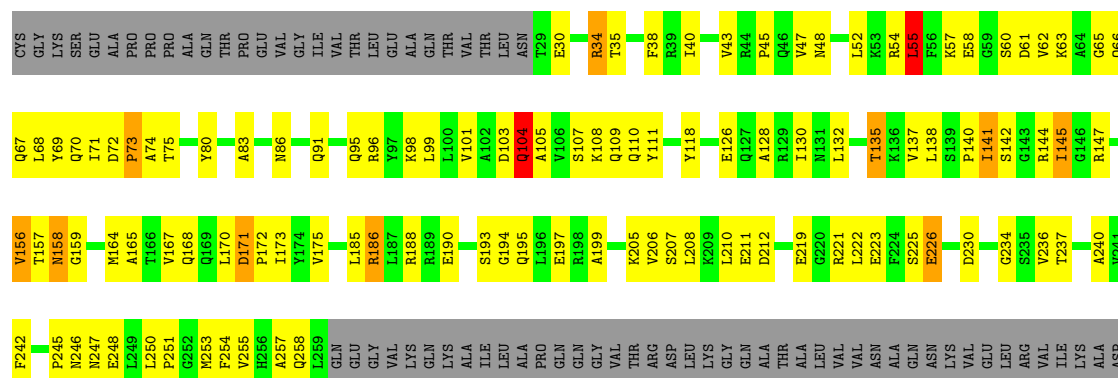
- Molecule 1: Multidrug resistance protein mexA

Chain J:



- Molecule 1: Multidrug resistance protein mexA

Chain K:



ARG VAL ILE GLY ASP LYS TRP LEU VAL THR GLN GLY LEU ASN ALA GLY ASP LYS ILE THR THR GLN GLY LEU GLN PHE VAL GLN PRO GLY VAL VAL GLN LYS THR VAL PRO ALA LYS ASN VAL VAL ALA SER ALA GLN LYS ASP ALA PRO ALA LYS THR ASP LYS GLY

• Molecule 1: Multidrug resistance protein mexA

Chain L:

CYS GLY LYS SER GLU PRO PRO PRO ALA GLN THR PRO GLU VAL GLY ILE VAL THR LEU LEU ALA GLN THR VAL THR ASN E30 R34 T35 F38 R39 I40 P45 Q46 V47 N48 L52 R53 R54 L55 S60 Q61 V62 Q66 Q67 L68 Y69 Q70 I71 D72 P73

A74 T76 E77 Y80 Q81 N86 S89 T90 Q91 Q95 R96 Y97 K98 L99 L100 V101 Q104 A105 V106 S107 K108 Q109 Q110 Y111 A112 D113 A116 A117 Y118 E126 Q127 A128 R129 I130 N131 L132 R133 T134 R136 V137 L138 S139 P140 I141 S142 V143 L144 I145 R146 R147

T151 E152 V156 T157 N158 G159 M164 Q168 Q169 L170 D171 P172 I173 Y174 V175 A183 R186 L187 R188 R189 E190 G194 E197 R198 A199 G200 D201 N202 K205 V206 S207 L208 R209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 S228 V236 T237 F242

P245 N246 N247 E248 L249 L250 M253 F254 V255 H256 A257 Q258 L259 G260 G261 G262 G263 G264 G265 G266 G267 G268 G269 G270 G271 G272 G273 G274 G275 G276 G277 G278 G279 G280 G281 G282 G283 G284 G285 G286 G287 G288 G289 G290 G291 G292 G293 G294 G295 G296 G297 G298 G299 G300 G301 G302 G303 G304 G305 G306 G307 G308 G309 G310 G311 G312 G313 G314 G315 G316 G317 G318 G319 G320 G321 G322 G323 G324 G325 G326 G327 G328 G329 G330 G331 G332 G333 G334 G335 G336 G337 G338 G339 G340 G341 G342 G343 G344 G345 G346 G347 G348 G349 G350 G351 G352 G353 G354 G355 G356 G357 G358 G359 G360 G361 G362 G363 G364 G365 G366 G367 G368 G369 G370 G371 G372 G373 G374 G375 G376 G377 G378 G379 G380 G381 G382 G383 G384 G385 G386 G387 G388 G389 G390 G391 G392 G393 G394 G395 G396 G397 G398 G399 G400 G401 G402 G403 G404 G405 G406 G407 G408 G409 G410 G411 G412 G413 G414 G415 G416 G417 G418 G419 G420 G421 G422 G423 G424 G425 G426 G427 G428 G429 G430 G431 G432 G433 G434 G435 G436 G437 G438 G439 G440 G441 G442 G443 G444 G445 G446 G447 G448 G449 G450 G451 G452 G453 G454 G455 G456 G457 G458 G459 G460 G461 G462 G463 G464 G465 G466 G467 G468 G469 G470 G471 G472 G473 G474 G475 G476 G477 G478 G479 G480 G481 G482 G483 G484 G485 G486 G487 G488 G489 G490 G491 G492 G493 G494 G495 G496 G497 G498 G499 G500 G501 G502 G503 G504 G505 G506 G507 G508 G509 G510 G511 G512 G513 G514 G515 G516 G517 G518 G519 G520 G521 G522 G523 G524 G525 G526 G527 G528 G529 G530 G531 G532 G533 G534 G535 G536 G537 G538 G539 G540 G541 G542 G543 G544 G545 G546 G547 G548 G549 G550 G551 G552 G553 G554 G555 G556 G557 G558 G559 G560 G561 G562 G563 G564 G565 G566 G567 G568 G569 G570 G571 G572 G573 G574 G575 G576 G577 G578 G579 G580 G581 G582 G583 G584 G585 G586 G587 G588 G589 G590 G591 G592 G593 G594 G595 G596 G597 G598 G599 G600 G601 G602 G603 G604 G605 G606 G607 G608 G609 G610 G611 G612 G613 G614 G615 G616 G617 G618 G619 G620 G621 G622 G623 G624 G625 G626 G627 G628 G629 G630 G631 G632 G633 G634 G635 G636 G637 G638 G639 G640 G641 G642 G643 G644 G645 G646 G647 G648 G649 G650 G651 G652 G653 G654 G655 G656 G657 G658 G659 G660 G661 G662 G663 G664 G665 G666 G667 G668 G669 G670 G671 G672 G673 G674 G675 G676 G677 G678 G679 G680 G681 G682 G683 G684 G685 G686 G687 G688 G689 G690 G691 G692 G693 G694 G695 G696 G697 G698 G699 G700 G701 G702 G703 G704 G705 G706 G707 G708 G709 G710 G711 G712 G713 G714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 G725 G726 G727 G728 G729 G730 G731 G732 G733 G734 G735 G736 G737 G738 G739 G740 G741 G742 G743 G744 G745 G746 G747 G748 G749 G750 G751 G752 G753 G754 G755 G756 G757 G758 G759 G760 G761 G762 G763 G764 G765 G766 G767 G768 G769 G770 G771 G772 G773 G774 G775 G776 G777 G778 G779 G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G792 G793 G794 G795 G796 G797 G798 G799 G800 G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860 G861 G862 G863 G864 G865 G866 G867 G868 G869 G870 G871 G872 G873 G874 G875 G876 G877 G878 G879 G880 G881 G882 G883 G884 G885 G886 G887 G888 G889 G890 G891 G892 G893 G894 G895 G896 G897 G898 G899 G900 G901 G902 G903 G904 G905 G906 G907 G908 G909 G910 G911 G912 G913 G914 G915 G916 G917 G918 G919 G920 G921 G922 G923 G924 G925 G926 G927 G928 G929 G930 G931 G932 G933 G934 G935 G936 G937 G938 G939 G940 G941 G942 G943 G944 G945 G946 G947 G948 G949 G950 G951 G952 G953 G954 G955 G956 G957 G958 G959 G960 G961 G962 G963 G964 G965 G966 G967 G968 G969 G970 G971 G972 G973 G974 G975 G976 G977 G978 G979 G980 G981 G982 G983 G984 G985 G986 G987 G988 G989 G990 G991 G992 G993 G994 G995 G996 G997 G998 G999

ILE GLY ASP LYS TRP LEU VAL THR THR GLN GLY LEU LEU ALA GLN PHE VAL VAL GLN PRO GLY VAL GLY VAL VAL LYS THR ARG ASP LEU LYS K205 V206 S207 L208 R209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 S228 V236 T237 F242

ILE GLY ASP LYS TRP LEU VAL THR THR GLN GLY LEU LEU ALA GLN PHE VAL VAL GLN PRO GLY VAL GLY VAL VAL LYS THR ARG ASP LEU LYS K205 V206 S207 L208 R209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 S228 V236 T237 F242

ILE GLY ASP LYS TRP LEU VAL THR THR GLN GLY LEU LEU ALA GLN PHE VAL VAL GLN PRO GLY VAL GLY VAL VAL LYS THR ARG ASP LEU LYS K205 V206 S207 L208 R209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 S228 V236 T237 F242

• Molecule 1: Multidrug resistance protein mexA

Chain M:

CYS GLY LYS SER GLU PRO PRO PRO ALA GLN THR PRO GLU VAL GLY ILE VAL THR LEU LEU ALA GLN THR VAL THR ASN T29 R34 F38 A41 E42 V43 R44 P45 Q46 V47 N48 L49 S49 P140 I141 S142 V143 R144 A145 G146 Q147 T151 L155 V156 N157 P158 A159 T160

Y76 Y80 N86 S89 T90 Q91 Q95 R96 Y97 K98 L99 G100 V101 A102 D103 Q104 A105 V106 Q109 G110 Y111 A112 Y118 E126 Q127 A128 R129 I130 N131 L132 R133 T134 R136 V137 L138 S139 P140 I141 S142 V143 R144 A145 G146 Q147 T151 L155 V156 N157 P158 A159 T160

A165 T166 V167 L170 D171 P172 I173 Y174 V175 A183 R186 L187 E189 S193 G194 Q195 L196 R197 R198 A199 K205 V206 S207 L208 R209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 S228 V236 T237 F242

F254 V255 H256 A257 Q258 L259 G260 G261 G262 G263 G264 G265 G266 G267 G268 G269 G270 G271 G272 G273 G274 G275 G276 G277 G278 G279 G280 G281 G282 G283 G284 G285 G286 G287 G288 G289 G290 G291 G292 G293 G294 G295 G296 G297 G298 G299 G300 G301 G302 G303 G304 G305 G306 G307 G308 G309 G310 G311 G312 G313 G314 G315 G316 G317 G318 G319 G320 G321 G322 G323 G324 G325 G326 G327 G328 G329 G330 G331 G332 G333 G334 G335 G336 G337 G338 G339 G340 G341 G342 G343 G344 G345 G346 G347 G348 G349 G350 G351 G352 G353 G354 G355 G356 G357 G358 G359 G360 G361 G362 G363 G364 G365 G366 G367 G368 G369 G370 G371 G372 G373 G374 G375 G376 G377 G378 G379 G380 G381 G382 G383 G384 G385 G386 G387 G388 G389 G390 G391 G392 G393 G394 G395 G396 G397 G398 G399 G400 G401 G402 G403 G404 G405 G406 G407 G408 G409 G410 G411 G412 G413 G414 G415 G416 G417 G418 G419 G420 G421 G422 G423 G424 G425 G426 G427 G428 G429 G430 G431 G432 G433 G434 G435 G436 G437 G438 G439 G440 G441 G442 G443 G444 G445 G446 G447 G448 G449 G450 G451 G452 G453 G454 G455 G456 G457 G458 G459 G460 G461 G462 G463 G464 G465 G466 G467 G468 G469 G470 G471 G472 G473 G474 G475 G476 G477 G478 G479 G480 G481 G482 G483 G484 G485 G486 G487 G488 G489 G490 G491 G492 G493 G494 G495 G496 G497 G498 G499 G500 G501 G502 G503 G504 G505 G506 G507 G508 G509 G510 G511 G512 G513 G514 G515 G516 G517 G518 G519 G520 G521 G522 G523 G524 G525 G526 G527 G528 G529 G530 G531 G532 G533 G534 G535 G536 G537 G538 G539 G540 G541 G542 G543 G544 G545 G546 G547 G548 G549 G550 G551 G552 G553 G554 G555 G556 G557 G558 G559 G560 G561 G562 G563 G564 G565 G566 G567 G568 G569 G570 G571 G572 G573 G574 G575 G576 G577 G578 G579 G580 G581 G582 G583 G584 G585 G586 G587 G588 G589 G590 G591 G592 G593 G594 G595 G596 G597 G598 G599 G600 G601 G602 G603 G604 G605 G606 G607 G608 G609 G610 G611 G612 G613 G614 G615 G616 G617 G618 G619 G620 G621 G622 G623 G624 G625 G626 G627 G628 G629 G630 G631 G632 G633 G634 G635 G636 G637 G638 G639 G640 G641 G642 G643 G644 G645 G646 G647 G648 G649 G650 G651 G652 G653 G654 G655 G656 G657 G658 G659 G660 G661 G662 G663 G664 G665 G666 G667 G668 G669 G670 G671 G672 G673 G674 G675 G676 G677 G678 G679 G680 G681 G682 G683 G684 G685 G686 G687 G688 G689 G690 G691 G692 G693 G694 G695 G696 G697 G698 G699 G700 G701 G702 G703 G704 G705 G706 G707 G708 G709 G710 G711 G712 G713 G714 G715 G716 G717 G718 G719 G720 G721 G722 G723 G724 G725 G726 G727 G728 G729 G730 G731 G732 G733 G734 G735 G736 G737 G738 G739 G740 G741 G742 G743 G744 G745 G746 G747 G748 G749 G750 G751 G752 G753 G754 G755 G756 G757 G758 G759 G760 G761 G762 G763 G764 G765 G766 G767 G768 G769 G770 G771 G772 G773 G774 G775 G776 G777 G778 G779 G780 G781 G782 G783 G784 G785 G786 G787 G788 G789 G790 G791 G792 G793 G794 G795 G796 G797 G798 G799 G800 G801 G802 G803 G804 G805 G806 G807 G808 G809 G810 G811 G812 G813 G814 G815 G816 G817 G818 G819 G820 G821 G822 G823 G824 G825 G826 G827 G828 G829 G830 G831 G832 G833 G834 G835 G836 G837 G838 G839 G840 G841 G842 G843 G844 G845 G846 G847 G848 G849 G850 G851 G852 G853 G854 G855 G856 G857 G858 G859 G860 G861 G862 G863 G864 G865 G866 G867 G868 G869 G870 G871 G872 G873 G874 G875 G876 G877 G878 G879 G880 G881 G882 G883 G884 G885 G886 G887 G888 G889 G890 G891 G892 G893 G894 G895 G896 G897 G898 G899 G900 G901 G902 G903 G904 G905 G906 G907 G908 G909 G910 G911 G912 G913 G914 G915 G916 G917 G918 G919 G920 G921 G922 G923 G924 G925 G926 G927 G928 G929 G930 G931 G932 G933 G934 G935 G936 G937 G938 G939 G940 G941 G942 G943 G944 G945 G946 G947 G948 G949 G950 G951 G952 G953 G954 G955 G956 G957 G958 G959 G960 G961 G962 G963 G964 G965 G966 G967 G968 G969 G970 G971 G972 G973 G974 G975 G976 G977 G978 G979 G980 G981 G982 G983 G984 G985 G986 G987 G988 G989 G990 G991 G992 G993 G994 G995 G996 G997 G998 G999

GLY LEU ASN ALA GLY ASP LYS ILE THR THR GLN GLY LEU LEU ALA GLN PHE VAL GLN PRO GLY VAL GLY VAL VAL LYS THR ARG ASP LEU LYS K205 V206 S207 L208 R209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 S228 V236 T237 F242

GLY LEU ASN ALA GLY ASP LYS ILE THR THR GLN GLY LEU LEU ALA GLN PHE VAL GLN PRO GLY VAL GLY VAL VAL LYS THR ARG ASP LEU LYS K205 V206 S207 L208 R209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 S228 V236 T237 F242

GLY LEU ASN ALA GLY ASP LYS ILE THR THR GLN GLY LEU LEU ALA GLN PHE VAL GLN PRO GLY VAL GLY VAL VAL LYS THR ARG ASP LEU LYS K205 V206 S207 L208 R209 L210 E211 D212 E219 G220 R221 L222 E223 F224 S225 E226 V227 S228 V236 T237 F242

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	130.55Å 183.59Å 213.31Å 90.00° 107.38° 90.00°	Depositor
Resolution (Å)	95.00 – 3.00 83.48 – 2.99	Depositor EDS
% Data completeness (in resolution range)	97.8 (95.00-3.00) 98.3 (83.48-2.99)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.01Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.273 , 0.285 0.268 , 0.278	Depositor DCC
R_{free} test set	9310 reflections (4.91%)	DCC
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.023	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.9	EDS
Estimated twinning fraction	0.005 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 190354 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	23101	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.83% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 3GR

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	A	0.48	1/1795 (0.1%)	0.62	0/2434
1	B	0.39	0/1795	0.65	0/2434
1	C	0.40	0/1795	0.66	0/2434
1	D	0.42	0/1795	0.69	0/2434
1	E	0.47	0/1795	0.71	0/2434
1	F	0.38	0/1795	0.67	0/2434
1	G	0.37	0/1795	0.63	0/2434
1	H	0.45	0/1795	0.70	0/2434
1	I	0.49	0/1795	0.71	0/2434
1	J	0.56	0/1795	0.75	0/2434
1	K	0.52	0/1795	0.73	0/2434
1	L	0.48	0/1795	0.71	0/2434
1	M	0.39	0/1795	0.66	0/2434
All	All	0.45	1/23335 (0.0%)	0.68	0/31642

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	A	0	1
1	I	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	THR	C-N	-14.50	1.00	1.34

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	29	THR	Mainchain
1	I	111	TYR	Sidechain

5.2 Close contacts

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1771	0	1774	109	1
1	B	1771	0	1775	105	0
1	C	1771	0	1775	98	0
1	D	1771	0	1775	110	1
1	E	1771	0	1775	102	0
1	F	1771	0	1775	109	0
1	G	1771	0	1775	120	0
1	H	1771	0	1775	109	0
1	I	1771	0	1775	115	0
1	J	1771	0	1775	110	0
1	K	1771	0	1775	120	0
1	L	1771	0	1775	127	0
1	M	1771	0	1775	110	0
2	C	6	0	5	2	0
2	D	6	0	5	0	0
2	E	6	0	5	2	0
2	F	6	0	5	4	0
2	G	6	0	5	1	0
2	H	6	0	5	2	0
2	I	6	0	5	4	0
2	K	6	0	5	3	0
2	L	6	0	5	1	0
3	A	6	0	8	5	0
3	B	6	0	5	3	0
3	J	6	0	5	5	0
3	M	6	0	5	2	0
All	All	23101	0	23142	1365	1

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 30.

All (1365) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:146:GLY:HA3	2:F:361:3GR:O2	1.37	1.24
1:M:70:GLN:HE22	1:M:135:THR:HG23	1.08	1.15
1:A:70:GLN:HE22	1:A:135:THR:HG23	1.18	1.07
1:F:91:GLN:HG2	1:F:95:GLN:HE21	1.21	1.05
1:J:91:GLN:HG2	1:J:95:GLN:HE21	1.16	1.04
1:B:91:GLN:HG2	1:B:95:GLN:HE21	1.22	1.03
1:B:55:LEU:HD12	1:B:67:GLN:HG2	1.38	1.02
1:G:91:GLN:HG2	1:G:95:GLN:HE21	1.21	1.02
1:I:171:ASP:HB3	1:I:172:PRO:HD3	1.43	1.01
1:F:171:ASP:HB3	1:F:172:PRO:HD3	1.41	1.01
1:K:107:SER:HB3	1:K:110:GLN:HG3	1.42	0.99
1:K:91:GLN:HG2	1:K:95:GLN:HE21	1.22	0.99
1:C:91:GLN:HG2	1:C:95:GLN:HE21	1.27	0.99
1:K:52:LEU:HD13	1:K:72:ASP:HB2	1.44	0.98
1:I:91:GLN:HG2	1:I:95:GLN:HE21	1.25	0.98
1:E:91:GLN:HG2	1:E:95:GLN:HE21	1.25	0.98
1:L:91:GLN:HG2	1:L:95:GLN:HE21	1.26	0.98
1:A:91:GLN:HG2	1:A:95:GLN:HE21	1.26	0.97
1:D:91:GLN:HG2	1:D:95:GLN:HE21	1.26	0.97
1:C:171:ASP:HB3	1:C:172:PRO:HD3	1.44	0.97
1:G:48:ASN:ND2	1:G:158:ASN:H	1.64	0.96
3:A:361:GOL:O1	1:B:228:SER:HB3	1.65	0.96
1:M:91:GLN:HG2	1:M:95:GLN:HE21	1.30	0.95
1:D:171:ASP:HB3	1:D:172:PRO:HD3	1.46	0.95
1:G:107:SER:H	1:G:110:GLN:HE21	1.15	0.95
1:C:146:GLY:HA3	2:C:361:3GR:O1	1.65	0.94
1:G:132:LEU:O	1:G:135:THR:HB	1.68	0.94
1:A:48:ASN:ND2	1:A:158:ASN:H	1.66	0.94
1:E:171:ASP:HB3	1:E:172:PRO:HD3	1.48	0.93
1:B:132:LEU:O	1:B:135:THR:HB	1.68	0.93
1:C:132:LEU:O	1:C:135:THR:HB	1.69	0.92
1:M:48:ASN:ND2	1:M:158:ASN:H	1.68	0.92
1:G:171:ASP:HB3	1:G:172:PRO:CD	2.00	0.92
1:H:91:GLN:HG2	1:H:95:GLN:HE21	1.31	0.92
1:K:132:LEU:O	1:K:135:THR:HB	1.69	0.91
1:L:132:LEU:O	1:L:135:THR:HB	1.71	0.91
1:K:108:LYS:HD2	1:L:96:ARG:HD2	1.53	0.90
1:I:146:GLY:HA3	2:I:361:3GR:O2	1.72	0.90
1:L:48:ASN:ND2	1:L:158:ASN:H	1.70	0.90

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:171:ASP:HB3	1:K:172:PRO:CD	2.00	0.90
1:H:48:ASN:ND2	1:H:158:ASN:H	1.70	0.89
1:L:62:VAL:HG21	1:L:68:LEU:HD21	1.54	0.89
1:H:132:LEU:O	1:H:135:THR:HB	1.71	0.89
1:J:132:LEU:O	1:J:135:THR:HB	1.72	0.89
1:M:70:GLN:NE2	1:M:135:THR:HG23	1.87	0.89
1:L:171:ASP:HB3	1:L:172:PRO:CD	2.02	0.89
1:D:132:LEU:O	1:D:135:THR:HB	1.74	0.88
1:A:171:ASP:HB3	1:A:172:PRO:CD	2.03	0.88
1:G:107:SER:OG	1:G:110:GLN:HG3	1.74	0.88
1:K:48:ASN:ND2	1:K:158:ASN:H	1.72	0.88
1:B:171:ASP:HB3	1:B:172:PRO:CD	2.04	0.87
1:D:48:ASN:ND2	1:D:158:ASN:H	1.72	0.87
1:F:171:ASP:HB3	1:F:172:PRO:CD	2.05	0.87
1:I:132:LEU:O	1:I:135:THR:HB	1.75	0.86
1:M:171:ASP:HB3	1:M:172:PRO:CD	2.04	0.86
1:J:52:LEU:HD13	1:J:72:ASP:HB2	1.57	0.86
1:A:70:GLN:NE2	1:A:135:THR:HG23	1.91	0.86
1:B:145:ILE:HG23	1:B:167:VAL:HG22	1.56	0.86
1:H:62:VAL:HG23	1:H:66:GLN:CD	1.96	0.85
1:I:34:ARG:HB3	1:I:34:ARG:HH11	1.41	0.85
1:J:91:GLN:HG2	1:J:95:GLN:NE2	1.92	0.85
1:C:62:VAL:HG21	1:C:68:LEU:HD21	1.57	0.85
1:M:55:LEU:HD12	1:M:67:GLN:HG2	1.56	0.85
1:F:62:VAL:HG21	1:F:68:LEU:HD21	1.57	0.85
1:F:85:ALA:HB2	1:G:82:SER:HB2	1.57	0.85
1:G:62:VAL:HG21	1:G:68:LEU:HD21	1.58	0.85
1:B:48:ASN:ND2	1:B:158:ASN:H	1.74	0.85
1:A:62:VAL:HG21	1:A:68:LEU:HD21	1.57	0.84
1:M:132:LEU:O	1:M:135:THR:HB	1.77	0.84
1:E:62:VAL:HG21	1:E:68:LEU:HD21	1.57	0.84
1:F:146:GLY:HA3	2:F:361:3GR:HA	1.40	0.84
1:E:132:LEU:O	1:E:135:THR:HB	1.76	0.84
1:I:171:ASP:HB3	1:I:172:PRO:CD	2.07	0.84
1:E:186:ARG:HB3	1:E:186:ARG:HH11	1.41	0.84
1:B:34:ARG:HH11	1:B:34:ARG:HB3	1.41	0.83
1:L:52:LEU:HD13	1:L:72:ASP:HB2	1.57	0.83
1:C:34:ARG:HH11	1:C:34:ARG:HB3	1.42	0.83
1:B:70:GLN:HE22	1:B:135:THR:HG23	1.41	0.83
1:H:171:ASP:HB3	1:H:172:PRO:CD	2.07	0.83
1:G:34:ARG:HH11	1:G:34:ARG:HB3	1.43	0.83
1:E:55:LEU:HD12	1:E:67:GLN:HG2	1.61	0.83

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:48:ASN:ND2	1:F:158:ASN:H	1.75	0.82
1:F:37:ALA:HB3	1:F:40:ILE:HD11	1.59	0.82
1:C:38:PHE:HB2	1:C:172:PRO:O	1.77	0.82
1:K:91:GLN:HG2	1:K:95:GLN:NE2	1.93	0.82
1:H:62:VAL:HG23	1:H:66:GLN:OE1	1.80	0.82
1:J:62:VAL:HG21	1:J:68:LEU:HD21	1.61	0.82
1:I:186:ARG:HB3	1:I:186:ARG:HH11	1.45	0.82
1:I:91:GLN:HG2	1:I:95:GLN:NE2	1.95	0.81
1:L:158:ASN:HD22	1:L:159:GLY:N	1.77	0.81
1:B:62:VAL:HG21	1:B:68:LEU:HD21	1.61	0.81
1:D:52:LEU:HD13	1:D:72:ASP:HB2	1.62	0.81
1:L:55:LEU:HD12	1:L:67:GLN:HG2	1.60	0.81
1:J:34:ARG:HH11	1:J:34:ARG:HB3	1.44	0.81
1:I:48:ASN:ND2	1:I:158:ASN:H	1.79	0.81
1:J:48:ASN:ND2	1:J:158:ASN:H	1.79	0.81
1:E:171:ASP:HB3	1:E:172:PRO:CD	2.09	0.80
1:H:158:ASN:HD22	1:H:159:GLY:N	1.79	0.80
1:H:70:GLN:HE22	1:H:135:THR:HG23	1.47	0.80
1:I:62:VAL:HG21	1:I:68:LEU:HD21	1.64	0.80
1:A:132:LEU:O	1:A:135:THR:HB	1.81	0.80
1:F:91:GLN:HG2	1:F:95:GLN:NE2	1.97	0.80
1:C:171:ASP:HB3	1:C:172:PRO:CD	2.10	0.80
1:L:34:ARG:HH11	1:L:34:ARG:HB3	1.44	0.80
1:D:62:VAL:HG21	1:D:68:LEU:HD21	1.62	0.80
1:E:48:ASN:ND2	1:E:158:ASN:H	1.78	0.80
1:J:186:ARG:HH11	1:J:186:ARG:HB3	1.47	0.79
1:B:91:GLN:HG2	1:B:95:GLN:NE2	1.97	0.79
1:D:171:ASP:HB3	1:D:172:PRO:CD	2.11	0.79
1:A:34:ARG:HH11	1:A:34:ARG:HB3	1.46	0.79
1:G:91:GLN:HG2	1:G:95:GLN:NE2	1.96	0.79
1:A:55:LEU:HD12	1:A:67:GLN:HG2	1.64	0.79
1:L:130:ILE:HD12	1:M:74:ALA:HB1	1.65	0.79
1:K:62:VAL:HG21	1:K:68:LEU:HD21	1.65	0.78
1:M:34:ARG:HB3	1:M:34:ARG:HH11	1.47	0.78
1:K:34:ARG:HB3	1:K:34:ARG:HH11	1.47	0.78
1:D:34:ARG:HH11	1:D:34:ARG:HB3	1.49	0.78
1:E:34:ARG:HH11	1:E:34:ARG:HB3	1.47	0.78
1:D:46:GLN:HB2	1:D:134:TYR:CD2	2.19	0.78
1:B:106:VAL:HG13	1:B:110:GLN:OE1	1.84	0.78
1:G:109:GLN:OE1	1:H:96:ARG:NH2	2.17	0.78
1:L:70:GLN:HE22	1:L:135:THR:HG23	1.48	0.77
1:J:171:ASP:HB3	1:J:172:PRO:CD	2.14	0.77

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:186:ARG:HH11	1:G:186:ARG:HB3	1.48	0.77
1:B:186:ARG:HB3	1:B:186:ARG:HH11	1.48	0.77
1:G:145:ILE:H	1:G:145:ILE:HD12	1.50	0.77
1:M:186:ARG:HH11	1:M:186:ARG:HB3	1.48	0.77
1:L:186:ARG:HB3	1:L:186:ARG:HH11	1.47	0.77
1:E:91:GLN:HG2	1:E:95:GLN:NE2	1.99	0.77
1:C:91:GLN:HG2	1:C:95:GLN:NE2	2.00	0.77
1:E:171:ASP:O	1:E:172:PRO:C	2.18	0.76
1:C:55:LEU:HD12	1:C:67:GLN:HG2	1.67	0.76
1:K:70:GLN:HE22	1:K:135:THR:HG23	1.50	0.76
1:D:186:ARG:HB3	1:D:186:ARG:HH11	1.48	0.76
1:G:171:ASP:O	1:G:172:PRO:C	2.22	0.76
1:F:52:LEU:HD13	1:F:72:ASP:HB2	1.68	0.76
1:H:34:ARG:HH11	1:H:34:ARG:HB3	1.51	0.75
1:E:38:PHE:HB2	1:E:172:PRO:O	1.86	0.75
1:I:206:VAL:HG11	1:I:257:ALA:HB1	1.68	0.75
1:M:62:VAL:HG23	1:M:66:GLN:OE1	1.85	0.75
1:F:145:ILE:H	1:F:145:ILE:HD12	1.49	0.75
1:A:101:VAL:HG13	1:A:106:VAL:HG23	1.69	0.75
1:H:62:VAL:HG21	1:H:68:LEU:HD21	1.68	0.74
1:M:62:VAL:HG23	1:M:66:GLN:CD	2.08	0.74
1:G:171:ASP:HB3	1:G:172:PRO:HD2	1.69	0.74
1:G:107:SER:N	1:G:110:GLN:HE21	1.84	0.74
1:C:145:ILE:HG23	1:C:167:VAL:HG22	1.70	0.74
1:D:158:ASN:HD22	1:D:159:GLY:N	1.85	0.74
1:C:48:ASN:ND2	1:C:158:ASN:H	1.85	0.74
1:D:38:PHE:HB2	1:D:172:PRO:O	1.88	0.74
1:M:38:PHE:HB2	1:M:172:PRO:O	1.87	0.74
1:M:62:VAL:HG21	1:M:68:LEU:HD21	1.68	0.74
1:D:48:ASN:HD21	1:D:158:ASN:H	1.35	0.74
1:B:38:PHE:HB2	1:B:172:PRO:O	1.88	0.74
1:F:62:VAL:HG23	1:F:66:GLN:CD	2.09	0.74
1:I:45:PRO:HG3	1:I:156:VAL:HG22	1.70	0.73
1:I:65:GLY:O	1:I:138:LEU:HD22	1.88	0.73
1:K:147:ARG:HB2	2:K:361:3GR:O3	1.88	0.73
1:G:55:LEU:HD12	1:G:67:GLN:HG2	1.69	0.73
1:A:91:GLN:HG2	1:A:95:GLN:NE2	2.03	0.73
1:B:62:VAL:HG23	1:B:66:GLN:CD	2.09	0.73
1:J:106:VAL:HG13	1:J:110:GLN:HB2	1.69	0.73
1:F:34:ARG:HH11	1:F:34:ARG:HB3	1.53	0.73
1:I:70:GLN:HE22	1:I:135:THR:HG23	1.53	0.73
1:F:101:VAL:HG21	1:F:111:TYR:HB2	1.69	0.73

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:100:LEU:HB3	1:H:106:VAL:HB	1.70	0.73
1:D:91:GLN:HG2	1:D:95:GLN:NE2	2.03	0.73
1:H:55:LEU:HD12	1:H:67:GLN:HG2	1.70	0.73
3:A:361:GOL:O1	1:B:228:SER:CB	2.36	0.73
1:B:70:GLN:NE2	1:B:135:THR:HG23	2.02	0.73
1:E:158:ASN:HD22	1:E:159:GLY:N	1.86	0.73
1:K:62:VAL:HG23	1:K:66:GLN:CD	2.08	0.73
1:H:171:ASP:O	1:H:172:PRO:C	2.21	0.72
1:D:62:VAL:HG23	1:D:66:GLN:CD	2.10	0.72
1:J:171:ASP:O	1:J:172:PRO:C	2.21	0.72
1:K:188:ARG:NH2	1:L:246:ASN:O	2.17	0.72
1:C:67:GLN:HA	1:C:138:LEU:HD23	1.71	0.72
1:A:158:ASN:HD22	1:A:159:GLY:N	1.88	0.72
1:G:62:VAL:HG23	1:G:66:GLN:CD	2.09	0.72
1:E:145:ILE:HG23	1:E:167:VAL:HG22	1.71	0.72
1:F:71:ILE:O	1:F:73:PRO:HD3	1.89	0.72
1:C:186:ARG:HH11	1:C:186:ARG:HB3	1.54	0.72
1:B:30:GLU:HG2	1:B:258:GLN:HG2	1.72	0.72
1:M:70:GLN:HE22	1:M:135:THR:CG2	1.97	0.72
1:E:62:VAL:HG23	1:E:66:GLN:CD	2.10	0.72
1:L:147:ARG:N	2:L:361:3GR:O3	2.22	0.72
1:A:186:ARG:HH11	1:A:186:ARG:HB3	1.55	0.72
1:I:147:ARG:N	2:I:361:3GR:O2	2.22	0.72
1:J:62:VAL:HG23	1:J:66:GLN:CD	2.10	0.72
1:M:158:ASN:HD22	1:M:159:GLY:N	1.88	0.71
1:E:206:VAL:HG11	1:E:257:ALA:HB1	1.72	0.71
1:H:126:GLU:O	1:H:130:ILE:HG12	1.90	0.71
1:I:171:ASP:O	1:I:172:PRO:C	2.26	0.71
1:L:101:VAL:HG11	1:L:108:LYS:HG2	1.71	0.71
1:L:38:PHE:HB2	1:L:172:PRO:O	1.88	0.71
1:L:62:VAL:HG23	1:L:66:GLN:CD	2.11	0.71
1:A:38:PHE:HB2	1:A:172:PRO:O	1.90	0.71
1:G:38:PHE:HB2	1:G:172:PRO:O	1.90	0.71
1:F:146:GLY:CA	2:F:361:3GR:O2	2.29	0.71
1:H:186:ARG:HB3	1:H:186:ARG:HH11	1.53	0.70
1:L:91:GLN:HG2	1:L:95:GLN:NE2	2.03	0.70
1:I:145:ILE:HD12	1:I:145:ILE:H	1.56	0.70
1:H:91:GLN:HG2	1:H:95:GLN:NE2	2.06	0.70
1:A:104:GLN:HG3	1:G:104:GLN:OE1	1.91	0.70
1:D:52:LEU:HD22	1:D:72:ASP:HA	1.72	0.70
1:L:100:LEU:HB3	1:L:106:VAL:HG23	1.72	0.70
1:B:62:VAL:HG23	1:B:66:GLN:OE1	1.91	0.70

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:186:ARG:HB3	1:K:186:ARG:HH11	1.56	0.70
1:M:170:LEU:HD21	1:M:251:PRO:HD3	1.74	0.70
1:I:62:VAL:HG23	1:I:66:GLN:CD	2.12	0.70
1:M:145:ILE:HG23	1:M:167:VAL:HG22	1.72	0.70
1:J:55:LEU:HD12	1:J:67:GLN:HG2	1.73	0.70
1:E:45:PRO:HG3	1:E:156:VAL:HG22	1.73	0.70
1:L:101:VAL:HG21	1:L:111:TYR:HB2	1.73	0.70
1:J:206:VAL:HG11	1:J:257:ALA:HB1	1.71	0.70
1:C:70:GLN:HE22	1:C:135:THR:HG23	1.54	0.69
1:E:70:GLN:HE22	1:E:135:THR:HG23	1.57	0.69
1:H:45:PRO:HG3	1:H:156:VAL:HG22	1.72	0.69
1:D:126:GLU:O	1:D:130:ILE:HG12	1.92	0.69
1:F:206:VAL:HG11	1:F:257:ALA:HB1	1.74	0.69
1:L:171:ASP:O	1:L:172:PRO:C	2.30	0.69
1:M:67:GLN:HA	1:M:138:LEU:HD23	1.75	0.69
1:C:45:PRO:HG3	1:C:156:VAL:HG22	1.75	0.69
1:K:158:ASN:HD22	1:K:159:GLY:N	1.90	0.69
1:F:197:GLU:OE2	1:F:205:LYS:HD2	1.93	0.69
1:K:171:ASP:O	1:K:172:PRO:C	2.28	0.69
1:K:62:VAL:HG23	1:K:66:GLN:OE1	1.93	0.69
1:H:206:VAL:HG11	1:H:257:ALA:HB1	1.75	0.69
1:A:48:ASN:HD21	1:A:158:ASN:H	1.37	0.69
1:B:70:GLN:HE22	1:B:135:THR:CG2	2.05	0.69
1:G:67:GLN:HA	1:G:138:LEU:HD23	1.74	0.69
1:E:104:GLN:HG2	1:K:108:LYS:HB2	1.74	0.69
1:B:206:VAL:HG11	1:B:257:ALA:HB1	1.75	0.69
1:F:186:ARG:HH11	1:F:186:ARG:HB3	1.57	0.69
1:A:45:PRO:HG3	1:A:156:VAL:HG22	1.73	0.69
1:F:132:LEU:O	1:F:135:THR:HB	1.92	0.69
1:B:67:GLN:HA	1:B:138:LEU:HD23	1.75	0.69
1:K:52:LEU:HD22	1:K:72:ASP:HA	1.76	0.68
1:G:107:SER:H	1:G:110:GLN:NE2	1.90	0.68
1:D:100:LEU:HB3	1:D:106:VAL:HG23	1.75	0.68
1:J:45:PRO:HG3	1:J:156:VAL:HG22	1.74	0.68
1:D:110:GLN:C	1:D:112:ALA:H	1.96	0.68
1:I:109:GLN:NE2	1:J:96:ARG:HH21	1.91	0.68
1:B:146:GLY:HA3	3:B:361:GOL:H12	1.75	0.68
1:H:145:ILE:H	1:H:145:ILE:HD12	1.58	0.68
1:J:67:GLN:OE1	1:J:136:LYS:HD3	1.92	0.68
1:E:52:LEU:HD13	1:E:72:ASP:HB2	1.76	0.68
1:F:171:ASP:O	1:F:172:PRO:C	2.27	0.68
1:C:62:VAL:HG23	1:C:66:GLN:CD	2.14	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:45:PRO:HG3	1:L:156:VAL:HG22	1.74	0.68
1:K:206:VAL:HG11	1:K:257:ALA:HB1	1.76	0.68
1:M:91:GLN:HG2	1:M:95:GLN:NE2	2.06	0.68
1:B:171:ASP:O	1:B:172:PRO:C	2.28	0.68
1:D:103:ASP:C	1:D:105:ALA:H	1.97	0.68
1:E:99:LEU:O	1:E:102:ALA:HB3	1.94	0.67
1:F:145:ILE:HG23	1:F:167:VAL:HG22	1.75	0.67
1:A:206:VAL:HG11	1:A:257:ALA:HB1	1.77	0.67
1:F:38:PHE:HB2	1:F:172:PRO:O	1.95	0.67
1:J:38:PHE:HB2	1:J:172:PRO:O	1.95	0.67
1:A:107:SER:OG	1:A:110:GLN:HG3	1.94	0.67
1:H:46:GLN:HB2	1:H:134:TYR:CD2	2.30	0.67
1:H:147:ARG:N	2:H:361:3GR:O2	2.26	0.66
1:K:55:LEU:HD12	1:K:67:GLN:HG2	1.77	0.66
1:L:70:GLN:NE2	1:L:135:THR:HG23	2.10	0.66
1:B:45:PRO:HG3	1:B:156:VAL:HG22	1.77	0.66
1:K:70:GLN:NE2	1:K:135:THR:HG23	2.09	0.66
1:A:171:ASP:HB3	1:A:172:PRO:HD2	1.76	0.66
1:I:158:ASN:HD22	1:I:159:GLY:N	1.93	0.66
1:B:126:GLU:O	1:B:130:ILE:HG12	1.95	0.66
1:F:67:GLN:HA	1:F:138:LEU:HD23	1.78	0.66
1:M:147:ARG:HD2	3:M:361:GOL:H12	1.76	0.66
1:D:97:TYR:O	1:D:101:VAL:HG23	1.96	0.66
1:G:226:GLU:HG3	1:H:144:ARG:HE	1.61	0.66
1:I:38:PHE:HB2	1:I:172:PRO:O	1.95	0.66
1:G:48:ASN:HD22	1:G:158:ASN:H	1.44	0.66
1:M:100:LEU:HB3	1:M:106:VAL:HG23	1.77	0.66
1:K:107:SER:HB3	1:K:110:GLN:CG	2.21	0.65
1:D:45:PRO:HG3	1:D:156:VAL:HG22	1.77	0.65
1:J:245:PRO:C	1:J:247:ASN:H	2.00	0.65
1:K:48:ASN:HD21	1:K:158:ASN:H	1.44	0.65
1:A:40:ILE:HG12	1:A:168:GLN:HG2	1.76	0.65
1:H:97:TYR:O	1:H:101:VAL:HG23	1.96	0.65
1:C:106:VAL:HG22	1:C:110:GLN:HB2	1.78	0.65
1:H:35:THR:HG22	1:H:175:VAL:HG22	1.79	0.65
1:F:126:GLU:O	1:F:130:ILE:HG12	1.96	0.65
1:A:145:ILE:HG23	1:A:167:VAL:HG22	1.79	0.65
1:J:145:ILE:HG23	1:J:167:VAL:HG22	1.77	0.65
1:M:245:PRO:C	1:M:247:ASN:H	2.00	0.65
1:L:188:ARG:HH21	1:M:248:GLU:HA	1.61	0.65
1:G:101:VAL:HG21	1:G:111:TYR:HB2	1.79	0.65
1:E:38:PHE:CD2	1:E:169:GLN:NE2	2.65	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:48:ASN:ND2	1:C:157:THR:HA	2.12	0.65
1:A:62:VAL:HG23	1:A:66:GLN:CD	2.16	0.65
1:D:97:TYR:HA	1:D:106:VAL:HG21	1.79	0.65
1:A:70:GLN:HE22	1:A:135:THR:CG2	2.04	0.65
1:E:248:GLU:HB3	1:F:185:LEU:HD21	1.79	0.65
1:H:48:ASN:HD21	1:H:158:ASN:H	1.45	0.64
1:L:206:VAL:HG11	1:L:257:ALA:HB1	1.79	0.64
1:F:245:PRO:C	1:F:247:ASN:H	2.00	0.64
1:E:186:ARG:O	1:E:190:GLU:HG3	1.97	0.64
1:L:126:GLU:O	1:L:130:ILE:HG12	1.97	0.64
1:B:245:PRO:C	1:B:247:ASN:H	2.01	0.64
1:E:38:PHE:HD2	1:E:169:GLN:NE2	1.94	0.64
1:G:145:ILE:HG23	1:G:167:VAL:HG22	1.78	0.64
1:K:186:ARG:HD3	1:K:190:GLU:OE2	1.97	0.64
1:L:35:THR:HG22	1:L:175:VAL:HG22	1.79	0.64
1:A:126:GLU:O	1:A:130:ILE:HG12	1.97	0.64
1:C:52:LEU:HD13	1:C:72:ASP:HB2	1.77	0.64
1:C:145:ILE:H	1:C:145:ILE:HD12	1.63	0.64
1:G:245:PRO:C	1:G:247:ASN:H	2.02	0.64
1:J:144:ARG:HG3	1:J:144:ARG:HH11	1.63	0.64
1:L:189:ARG:NH2	1:M:212:ASP:OD1	2.28	0.64
1:D:71:ILE:O	1:D:73:PRO:HD3	1.97	0.64
1:C:197:GLU:OE2	1:C:205:LYS:HD2	1.98	0.64
1:I:245:PRO:C	1:I:247:ASN:H	2.00	0.64
1:G:206:VAL:HG11	1:G:257:ALA:HB1	1.79	0.64
1:I:52:LEU:HD13	1:I:72:ASP:HB2	1.80	0.64
1:L:38:PHE:HD2	1:L:169:GLN:NE2	1.95	0.63
1:E:186:ARG:HH11	1:E:186:ARG:CB	2.11	0.63
1:H:30:GLU:HG2	1:H:258:GLN:HG2	1.79	0.63
1:D:171:ASP:O	1:D:172:PRO:C	2.34	0.63
1:G:186:ARG:HD3	1:G:190:GLU:OE2	1.98	0.63
1:K:67:GLN:HA	1:K:138:LEU:HD23	1.80	0.63
1:M:206:VAL:HG11	1:M:257:ALA:HB1	1.81	0.63
1:C:245:PRO:C	1:C:247:ASN:H	2.02	0.63
1:G:40:ILE:HG12	1:G:168:GLN:HG2	1.81	0.63
1:M:197:GLU:OE2	1:M:205:LYS:HD2	1.98	0.63
1:B:186:ARG:O	1:B:190:GLU:HG3	1.98	0.63
1:F:70:GLN:HE22	1:F:135:THR:HG23	1.64	0.63
1:K:54:ARG:HD2	1:K:54:ARG:O	1.99	0.63
1:H:70:GLN:NE2	1:H:135:THR:HG23	2.13	0.63
1:J:52:LEU:HD22	1:J:72:ASP:HA	1.81	0.63
1:M:186:ARG:CB	1:M:186:ARG:HH11	2.12	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:206:VAL:HG11	1:D:257:ALA:HB1	1.80	0.63
1:B:48:ASN:ND2	1:B:157:THR:HA	2.13	0.62
1:C:206:VAL:HG11	1:C:257:ALA:HB1	1.80	0.62
1:E:126:GLU:O	1:E:130:ILE:HG12	2.00	0.62
1:C:107:SER:OG	1:C:110:GLN:HG3	1.98	0.62
1:G:31:LEU:HB3	1:G:177:VAL:CG1	2.29	0.62
1:K:126:GLU:O	1:K:130:ILE:HG12	1.99	0.62
1:M:171:ASP:HB3	1:M:172:PRO:HD2	1.81	0.62
1:K:38:PHE:HB2	1:K:172:PRO:O	1.99	0.62
1:F:145:ILE:N	1:F:145:ILE:HD12	2.15	0.62
1:E:106:VAL:HG13	1:E:110:GLN:HB2	1.79	0.62
1:E:62:VAL:HG23	1:E:66:GLN:OE1	2.00	0.62
1:A:30:GLU:HG2	1:A:258:GLN:HG2	1.80	0.62
1:A:245:PRO:C	1:A:247:ASN:H	2.01	0.62
1:L:38:PHE:CD2	1:L:169:GLN:NE2	2.68	0.62
1:I:96:ARG:O	1:I:99:LEU:HB3	1.98	0.62
1:D:221:ARG:HD3	1:D:223:GLU:OE2	2.00	0.62
1:F:186:ARG:HD3	1:F:190:GLU:OE2	1.99	0.62
1:E:48:ASN:HD21	1:E:158:ASN:H	1.47	0.62
1:E:30:GLU:HG2	1:E:258:GLN:HG2	1.82	0.62
1:B:51:ILE:HD11	1:B:164:MET:HE3	1.81	0.62
1:G:48:ASN:ND2	1:G:158:ASN:N	2.44	0.61
1:F:45:PRO:HG3	1:F:156:VAL:HG22	1.82	0.61
1:F:158:ASN:HD22	1:F:159:GLY:N	1.98	0.61
1:K:43:VAL:HG23	1:K:165:ALA:O	2.00	0.61
1:I:228:SER:HB3	3:J:361:GOL:H2	1.82	0.61
1:G:145:ILE:N	1:G:145:ILE:HD12	2.15	0.61
1:C:208:LEU:HB2	1:C:242:PHE:CE2	2.36	0.61
1:L:95:GLN:O	1:L:99:LEU:HD13	2.00	0.61
1:A:186:ARG:O	1:A:190:GLU:HG3	2.01	0.61
1:J:186:ARG:O	1:J:190:GLU:HG3	2.00	0.61
1:H:67:GLN:HA	1:H:138:LEU:HD23	1.81	0.61
1:C:186:ARG:HD3	1:C:190:GLU:OE2	1.99	0.61
1:L:245:PRO:C	1:L:247:ASN:H	2.04	0.61
1:M:48:ASN:HD21	1:M:158:ASN:H	1.43	0.61
1:I:145:ILE:N	1:I:145:ILE:HD12	2.15	0.61
1:H:188:ARG:HH21	1:I:248:GLU:HA	1.66	0.61
1:H:112:ALA:HB1	1:I:92:GLU:HG3	1.83	0.61
1:L:208:LEU:HB2	1:L:242:PHE:CE2	2.36	0.61
1:F:48:ASN:HD21	1:F:158:ASN:H	1.49	0.61
1:I:109:GLN:NE2	1:J:96:ARG:NH2	2.48	0.61
1:A:47:VAL:HG22	1:A:76:TYR:CZ	2.36	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:188:ARG:NH2	1:K:246:ASN:O	2.34	0.61
1:I:197:GLU:OE2	1:I:205:LYS:HD2	2.01	0.61
1:L:40:ILE:O	1:M:151:THR:HB	2.01	0.60
1:B:158:ASN:HD22	1:B:159:GLY:N	1.99	0.60
1:L:145:ILE:H	1:L:145:ILE:HD12	1.66	0.60
1:K:186:ARG:O	1:K:190:GLU:HG3	2.00	0.60
1:J:144:ARG:HG3	1:J:144:ARG:NH1	2.16	0.60
1:M:45:PRO:HG3	1:M:156:VAL:HG22	1.83	0.60
1:E:221:ARG:HD3	1:E:223:GLU:OE2	2.01	0.60
1:C:171:ASP:O	1:C:172:PRO:C	2.37	0.60
1:I:185:LEU:HD21	1:J:248:GLU:HB3	1.83	0.60
1:M:91:GLN:HG3	1:M:118:TYR:CE1	2.37	0.60
1:G:71:ILE:O	1:G:73:PRO:HD3	2.02	0.60
1:J:146:GLY:HA3	3:J:361:GOL:H12	1.83	0.60
1:F:82:SER:HA	1:G:82:SER:OG	2.01	0.60
1:G:145:ILE:HG23	1:G:167:VAL:CG2	2.32	0.60
1:B:186:ARG:HD3	1:B:190:GLU:OE2	2.02	0.60
1:D:110:GLN:C	1:D:112:ALA:N	2.55	0.60
1:I:186:ARG:HH11	1:I:186:ARG:CB	2.13	0.60
1:B:100:LEU:HB3	1:B:106:VAL:HG23	1.83	0.60
1:D:245:PRO:C	1:D:247:ASN:H	2.05	0.60
1:G:158:ASN:HD22	1:G:159:GLY:N	2.00	0.60
1:L:171:ASP:HB3	1:L:172:PRO:HD2	1.83	0.60
1:I:55:LEU:N	1:I:55:LEU:HD23	2.17	0.60
1:G:62:VAL:HG23	1:G:66:GLN:OE1	2.01	0.59
1:L:101:VAL:CG2	1:L:111:TYR:HB2	2.31	0.59
1:H:107:SER:OG	1:H:110:GLN:HG3	2.02	0.59
1:G:48:ASN:HD21	1:G:158:ASN:H	1.45	0.59
1:D:100:LEU:HD21	1:K:103:ASP:HB3	1.84	0.59
1:M:211:GLU:HB3	1:M:254:PHE:O	2.01	0.59
1:D:186:ARG:O	1:D:190:GLU:HG3	2.03	0.59
1:C:186:ARG:O	1:C:190:GLU:HG3	2.01	0.59
1:I:146:GLY:CA	2:I:361:3GR:O2	2.50	0.59
1:L:48:ASN:HD21	1:L:158:ASN:H	1.44	0.59
1:D:55:LEU:HD12	1:D:67:GLN:HG2	1.84	0.59
1:A:208:LEU:HD11	1:A:255:VAL:HG21	1.85	0.59
1:G:126:GLU:O	1:G:130:ILE:HG12	2.03	0.59
1:J:231:GLU:HG2	1:K:251:PRO:HB2	1.84	0.59
1:L:186:ARG:O	1:L:190:GLU:HG3	2.01	0.59
1:A:29:THR:HG22	1:A:30:GLU:N	2.17	0.59
1:H:140:PRO:O	1:H:141:ILE:HD12	2.03	0.59
1:J:62:VAL:HG23	1:J:66:GLN:OE1	2.01	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:186:ARG:O	1:M:190:GLU:HG3	2.03	0.59
1:C:206:VAL:HG13	1:C:258:GLN:O	2.02	0.59
1:M:101:VAL:CG2	1:M:111:TYR:HB2	2.33	0.59
1:G:197:GLU:OE2	1:G:205:LYS:HD2	2.03	0.59
1:L:226:GLU:HG3	1:M:144:ARG:HE	1.68	0.59
1:I:228:SER:CB	3:J:361:GOL:H2	2.33	0.58
1:I:70:GLN:NE2	1:I:135:THR:HG23	2.18	0.58
1:A:145:ILE:H	1:A:145:ILE:HD12	1.66	0.58
1:E:158:ASN:HD22	1:E:159:GLY:H	1.49	0.58
1:M:101:VAL:HG21	1:M:111:TYR:HB2	1.85	0.58
1:H:189:ARG:NH2	1:I:212:ASP:OD1	2.32	0.58
1:J:126:GLU:O	1:J:130:ILE:HG12	2.02	0.58
1:C:54:ARG:O	1:C:54:ARG:HG2	2.03	0.58
1:L:91:GLN:HG3	1:L:118:TYR:CE1	2.38	0.58
1:C:170:LEU:HD11	1:C:251:PRO:HD3	1.85	0.58
1:A:144:ARG:NE	1:B:226:GLU:OE2	2.36	0.58
1:A:211:GLU:HB3	1:A:254:PHE:O	2.03	0.58
1:B:208:LEU:HB2	1:B:242:PHE:CE2	2.39	0.58
1:J:185:LEU:HD21	1:K:248:GLU:HB3	1.86	0.58
1:F:147:ARG:HD2	2:F:361:3GR:O3	2.03	0.58
1:E:95:GLN:O	1:E:99:LEU:HD13	2.02	0.58
1:B:221:ARG:HD3	1:B:223:GLU:OE2	2.02	0.58
1:L:62:VAL:HG23	1:L:66:GLN:NE2	2.18	0.58
1:D:158:ASN:HD22	1:D:159:GLY:H	1.49	0.58
1:D:96:ARG:HG2	1:D:100:LEU:HD12	1.84	0.58
1:D:208:LEU:HD11	1:D:255:VAL:HG21	1.85	0.58
1:F:62:VAL:HG23	1:F:66:GLN:NE2	2.18	0.58
1:I:62:VAL:HG23	1:I:66:GLN:OE1	2.03	0.58
1:H:186:ARG:HD3	1:H:190:GLU:OE2	2.04	0.58
1:F:30:GLU:HG2	1:F:258:GLN:HG2	1.84	0.58
1:J:109:GLN:OE1	1:K:96:ARG:NH2	2.37	0.58
1:M:208:LEU:HB2	1:M:242:PHE:CE2	2.38	0.58
1:G:206:VAL:HG13	1:G:258:GLN:O	2.04	0.58
1:I:71:ILE:O	1:I:73:PRO:HD3	2.03	0.58
1:H:100:LEU:CB	1:H:106:VAL:HB	2.33	0.58
1:E:147:ARG:N	2:E:361:3GR:O2	2.34	0.58
1:C:104:GLN:HB2	1:I:108:LYS:HE3	1.85	0.58
1:M:48:ASN:O	1:M:76:TYR:OH	2.07	0.58
1:D:104:GLN:HE22	1:J:104:GLN:HE22	1.50	0.58
1:F:35:THR:HG22	1:F:175:VAL:HG22	1.86	0.58
1:D:62:VAL:CG1	1:D:145:ILE:HG13	2.33	0.58
1:F:186:ARG:O	1:F:190:GLU:HG3	2.02	0.58

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:206:VAL:HG12	1:L:207:SER:N	2.19	0.58
1:G:50:ILE:HD13	1:G:155:LEU:HA	1.85	0.58
1:A:171:ASP:O	1:A:172:PRO:C	2.39	0.57
1:E:145:ILE:H	1:E:145:ILE:HD12	1.69	0.57
1:L:186:ARG:HD3	1:L:190:GLU:OE2	2.04	0.57
1:G:52:LEU:HD13	1:G:72:ASP:HB2	1.85	0.57
1:G:31:LEU:HB3	1:G:177:VAL:HG11	1.84	0.57
1:L:197:GLU:OE2	1:L:205:LYS:HD2	2.04	0.57
1:C:70:GLN:NE2	1:C:135:THR:HG23	2.19	0.57
1:J:67:GLN:HA	1:J:138:LEU:HD23	1.84	0.57
1:L:206:VAL:HG13	1:L:258:GLN:O	2.05	0.57
1:M:98:LYS:HA	1:M:111:TYR:CE1	2.39	0.57
1:H:211:GLU:HB3	1:H:254:PHE:O	2.04	0.57
1:K:245:PRO:C	1:K:247:ASN:H	2.06	0.57
1:I:107:SER:OG	1:I:110:GLN:HG3	2.04	0.57
1:A:91:GLN:HG3	1:A:118:TYR:CE1	2.39	0.57
1:K:171:ASP:HB3	1:K:172:PRO:HD3	1.82	0.57
1:A:62:VAL:CG1	1:A:145:ILE:HG13	2.35	0.57
1:H:171:ASP:HB3	1:H:172:PRO:HD2	1.85	0.57
1:I:55:LEU:HD12	1:I:67:GLN:HG2	1.87	0.57
1:H:197:GLU:OE2	1:H:205:LYS:HD2	2.04	0.57
1:E:67:GLN:HA	1:E:138:LEU:HD23	1.87	0.57
1:G:186:ARG:HH11	1:G:186:ARG:CB	2.18	0.57
1:M:101:VAL:HG21	1:M:111:TYR:CG	2.39	0.57
1:G:141:ILE:HG23	1:G:142:SER:N	2.20	0.57
1:J:186:ARG:HH11	1:J:186:ARG:CB	2.17	0.57
1:E:206:VAL:HG21	1:E:222:LEU:HB2	1.86	0.57
1:F:108:LYS:HE3	1:L:104:GLN:NE2	2.20	0.57
1:I:54:ARG:O	1:I:54:ARG:HD2	2.05	0.57
1:H:91:GLN:HG3	1:H:118:TYR:CE1	2.40	0.57
1:B:48:ASN:HD21	1:B:158:ASN:H	1.49	0.57
1:L:186:ARG:CB	1:L:186:ARG:HH11	2.18	0.57
1:L:101:VAL:HG21	1:L:111:TYR:CB	2.33	0.57
1:H:245:PRO:C	1:H:247:ASN:H	2.05	0.57
1:C:126:GLU:O	1:C:130:ILE:HG12	2.03	0.57
1:C:211:GLU:HB3	1:C:254:PHE:O	2.04	0.57
1:L:158:ASN:HD22	1:L:158:ASN:C	2.04	0.57
1:J:145:ILE:HD12	1:J:145:ILE:H	1.69	0.57
1:I:48:ASN:HD21	1:I:157:THR:HG23	1.70	0.57
1:D:67:GLN:HA	1:D:138:LEU:HD23	1.85	0.57
1:J:208:LEU:HD11	1:J:255:VAL:HG21	1.87	0.57
1:A:221:ARG:HD3	1:A:223:GLU:OE2	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:H:71:ILE:O	1:H:73:PRO:HD3	2.04	0.57
1:K:108:LYS:CD	1:L:96:ARG:HD2	2.30	0.57
1:A:67:GLN:HA	1:A:138:LEU:HD23	1.87	0.57
1:B:197:GLU:OE2	1:B:205:LYS:HD2	2.04	0.57
1:K:171:ASP:HB3	1:K:172:PRO:HD2	1.87	0.56
1:K:221:ARG:HD3	1:K:223:GLU:OE2	2.04	0.56
1:I:186:ARG:O	1:I:190:GLU:HG3	2.04	0.56
1:H:109:GLN:NE2	1:H:110:GLN:HG3	2.20	0.56
1:C:158:ASN:HD22	1:C:159:GLY:N	2.04	0.56
1:E:147:ARG:HG3	1:F:227:VAL:HG12	1.87	0.56
1:L:86:ASN:O	1:L:89:SER:HB3	2.06	0.56
1:B:171:ASP:HB3	1:B:172:PRO:HD2	1.83	0.56
1:D:145:ILE:HG23	1:D:167:VAL:HG22	1.87	0.56
1:C:71:ILE:O	1:C:73:PRO:HD3	2.05	0.56
1:I:37:ALA:HB3	1:I:40:ILE:HD11	1.86	0.56
1:F:78:ALA:HA	1:G:85:ALA:HB1	1.88	0.56
1:G:97:TYR:HD2	1:G:106:VAL:HG11	1.70	0.56
1:I:186:ARG:HD3	1:I:190:GLU:OE2	2.06	0.56
1:D:62:VAL:HG23	1:D:66:GLN:OE1	2.05	0.56
1:M:126:GLU:O	1:M:130:ILE:HG12	2.06	0.56
1:L:211:GLU:HB3	1:L:254:PHE:O	2.06	0.56
1:E:91:GLN:HG3	1:E:118:TYR:CE1	2.41	0.56
1:K:147:ARG:CB	2:K:361:3GR:O3	2.54	0.56
1:A:47:VAL:HG22	1:A:76:TYR:OH	2.06	0.56
1:B:211:GLU:HB3	1:B:254:PHE:O	2.05	0.56
1:G:208:LEU:HD11	1:G:255:VAL:HG21	1.88	0.56
1:C:48:ASN:HD22	1:C:157:THR:HA	1.70	0.56
1:D:208:LEU:HB2	1:D:242:PHE:CE2	2.41	0.56
1:B:144:ARG:HH11	1:B:144:ARG:HG3	1.71	0.56
1:E:35:THR:HG22	1:E:175:VAL:HG22	1.87	0.56
1:J:206:VAL:HG21	1:J:222:LEU:HB2	1.87	0.56
1:I:141:ILE:HG23	1:I:142:SER:N	2.21	0.56
1:F:211:GLU:HB3	1:F:254:PHE:O	2.06	0.56
1:M:109:GLN:O	1:M:112:ALA:HB3	2.05	0.56
1:J:30:GLU:HG2	1:J:258:GLN:HG2	1.88	0.56
1:G:208:LEU:HB2	1:G:242:PHE:CE2	2.41	0.56
1:E:245:PRO:C	1:E:247:ASN:H	2.08	0.56
1:C:52:LEU:HD22	1:C:72:ASP:HA	1.88	0.55
1:M:141:ILE:CG2	1:M:142:SER:N	2.70	0.55
1:J:158:ASN:HD22	1:J:159:GLY:N	2.03	0.55
1:G:186:ARG:O	1:G:190:GLU:HG3	2.06	0.55
1:L:221:ARG:HD3	1:L:223:GLU:OE2	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:250:LEU:O	1:M:253:MET:HG3	2.06	0.55
1:D:250:LEU:O	1:D:253:MET:HG3	2.07	0.55
1:B:55:LEU:CD1	1:B:67:GLN:HG2	2.27	0.55
1:E:48:ASN:ND2	1:E:157:THR:HA	2.21	0.55
1:B:206:VAL:HG13	1:B:258:GLN:O	2.06	0.55
1:H:145:ILE:N	1:H:145:ILE:HD12	2.21	0.55
1:G:45:PRO:HG3	1:G:156:VAL:HG22	1.87	0.55
1:C:35:THR:HG22	1:C:175:VAL:HG22	1.87	0.55
1:K:45:PRO:HG3	1:K:156:VAL:HG22	1.88	0.55
1:J:48:ASN:HD21	1:J:158:ASN:H	1.53	0.55
1:J:171:ASP:HB3	1:J:172:PRO:HD3	1.88	0.55
1:L:71:ILE:O	1:L:73:PRO:HD3	2.06	0.55
1:C:62:VAL:HG23	1:C:66:GLN:OE1	2.06	0.55
1:D:211:GLU:HB3	1:D:254:PHE:O	2.06	0.55
1:J:70:GLN:HE22	1:J:135:THR:HG23	1.72	0.55
1:M:171:ASP:O	1:M:172:PRO:C	2.41	0.55
1:F:48:ASN:ND2	1:F:157:THR:HA	2.22	0.55
1:K:145:ILE:HD12	1:K:145:ILE:H	1.72	0.55
1:C:106:VAL:HG23	1:C:110:GLN:CD	2.27	0.55
1:A:208:LEU:HD11	1:A:255:VAL:CG2	2.36	0.55
1:C:147:ARG:HG3	1:D:227:VAL:HG12	1.87	0.55
1:J:62:VAL:CG1	1:J:145:ILE:HG13	2.37	0.55
1:J:34:ARG:HH11	1:J:34:ARG:CB	2.18	0.55
1:F:206:VAL:HG12	1:F:207:SER:N	2.20	0.55
1:H:137:VAL:HG12	1:H:137:VAL:O	2.07	0.55
1:D:103:ASP:C	1:D:105:ALA:N	2.58	0.55
1:A:96:ARG:NH2	1:B:109:GLN:NE2	2.55	0.55
1:K:103:ASP:C	1:K:105:ALA:H	2.10	0.54
1:K:55:LEU:HD23	1:K:55:LEU:N	2.22	0.54
1:H:208:LEU:HD11	1:H:255:VAL:HG21	1.88	0.54
1:D:206:VAL:HG13	1:D:258:GLN:O	2.07	0.54
1:K:98:LYS:O	1:K:101:VAL:HG12	2.07	0.54
1:E:211:GLU:HB3	1:E:254:PHE:O	2.07	0.54
1:B:186:ARG:CB	1:B:186:ARG:HH11	2.19	0.54
1:L:40:ILE:HG12	1:L:168:GLN:HG2	1.90	0.54
1:L:70:GLN:HE22	1:L:135:THR:CG2	2.17	0.54
1:I:34:ARG:CB	1:I:34:ARG:HH11	2.15	0.54
1:A:101:VAL:CG1	1:A:106:VAL:HG23	2.37	0.54
1:B:35:THR:HG22	1:B:175:VAL:HG22	1.89	0.54
1:L:99:LEU:N	1:L:99:LEU:HD12	2.23	0.54
1:F:60:SER:O	1:F:145:ILE:HD12	2.07	0.54
1:I:48:ASN:HD22	1:I:157:THR:HA	1.73	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:197:GLU:OE2	1:A:205:LYS:HD2	2.07	0.54
1:E:170:LEU:O	1:E:171:ASP:O	2.26	0.54
1:E:171:ASP:O	1:E:173:ILE:N	2.40	0.54
1:B:48:ASN:HD22	1:B:157:THR:HA	1.73	0.54
1:I:48:ASN:ND2	1:I:157:THR:HG23	2.22	0.54
1:G:101:VAL:CG2	1:G:111:TYR:HB2	2.38	0.54
1:D:208:LEU:HD11	1:D:255:VAL:CG2	2.38	0.54
1:M:141:ILE:HG23	1:M:142:SER:N	2.22	0.54
1:D:197:GLU:OE2	1:D:205:LYS:HD2	2.07	0.54
1:K:71:ILE:O	1:K:73:PRO:HD3	2.08	0.54
1:M:62:VAL:CG1	1:M:145:ILE:HG13	2.38	0.54
1:M:206:VAL:HG12	1:M:207:SER:N	2.23	0.54
1:K:99:LEU:N	1:K:99:LEU:HD12	2.23	0.54
1:D:145:ILE:H	1:D:145:ILE:HD12	1.72	0.54
1:D:186:ARG:HD3	1:D:190:GLU:OE2	2.07	0.54
1:F:206:VAL:O	1:F:219:GLU:HB2	2.08	0.54
1:D:30:GLU:HG2	1:D:258:GLN:HG2	1.90	0.54
1:C:208:LEU:HD11	1:C:255:VAL:HG21	1.90	0.54
1:M:144:ARG:HG3	1:M:144:ARG:HH11	1.73	0.54
1:J:221:ARG:HD3	1:J:223:GLU:OE2	2.08	0.54
1:A:109:GLN:O	1:A:112:ALA:HB3	2.08	0.54
1:C:108:LYS:HG3	1:I:104:GLN:HB3	1.89	0.54
1:A:186:ARG:HD3	1:A:190:GLU:OE2	2.07	0.54
1:L:206:VAL:HG21	1:L:222:LEU:HB2	1.90	0.54
1:M:97:TYR:O	1:M:101:VAL:HG23	2.07	0.54
1:K:70:GLN:HE22	1:K:135:THR:CG2	2.17	0.53
1:D:186:ARG:CB	1:D:186:ARG:HH11	2.20	0.53
1:A:141:ILE:HG23	1:A:142:SER:N	2.23	0.53
1:C:221:ARG:HD3	1:C:223:GLU:OE2	2.08	0.53
1:D:236:VAL:HG12	1:D:237:THR:N	2.24	0.53
1:B:140:PRO:O	1:B:141:ILE:HD12	2.09	0.53
1:A:48:ASN:HD22	1:A:158:ASN:H	1.53	0.53
1:A:206:VAL:HG13	1:A:258:GLN:O	2.07	0.53
1:G:236:VAL:HG12	1:G:237:THR:N	2.23	0.53
1:M:101:VAL:HG21	1:M:111:TYR:CB	2.38	0.53
1:G:221:ARG:HD3	1:G:223:GLU:OE2	2.09	0.53
1:I:208:LEU:HD11	1:I:255:VAL:HG21	1.89	0.53
1:K:35:THR:HG22	1:K:175:VAL:HG22	1.91	0.53
1:F:62:VAL:CG1	1:F:145:ILE:HG13	2.39	0.53
1:I:206:VAL:HG12	1:I:207:SER:N	2.24	0.53
1:F:96:ARG:O	1:F:100:LEU:HG	2.09	0.53
1:K:206:VAL:HG12	1:K:207:SER:N	2.24	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:96:ARG:O	1:M:100:LEU:HD13	2.09	0.53
1:I:70:GLN:HE21	1:I:73:PRO:HD3	1.73	0.53
1:J:48:ASN:ND2	1:J:157:THR:HA	2.24	0.53
1:F:98:LYS:HG3	1:F:111:TYR:OH	2.08	0.53
1:E:206:VAL:HG13	1:E:258:GLN:O	2.09	0.53
1:J:186:ARG:HD3	1:J:190:GLU:OE2	2.09	0.52
1:I:206:VAL:HG13	1:I:258:GLN:O	2.08	0.52
1:E:197:GLU:OE2	1:E:205:LYS:HD2	2.10	0.52
1:L:210:LEU:C	1:L:212:ASP:H	2.12	0.52
1:E:144:ARG:HH11	1:E:144:ARG:HG3	1.74	0.52
1:A:147:ARG:HD2	3:A:361:GOL:C1	2.39	0.52
1:D:110:GLN:OE1	1:D:110:GLN:HA	2.09	0.52
1:G:211:GLU:HB3	1:G:254:PHE:O	2.09	0.52
1:H:221:ARG:HD3	1:H:223:GLU:OE2	2.09	0.52
1:M:236:VAL:HG12	1:M:237:THR:N	2.24	0.52
1:A:29:THR:CG2	1:A:30:GLU:N	2.71	0.52
1:F:141:ILE:HG23	1:F:142:SER:N	2.25	0.52
1:D:40:ILE:HG12	1:D:168:GLN:HG2	1.92	0.52
1:F:50:ILE:HD13	1:F:155:LEU:HA	1.91	0.52
1:C:48:ASN:HD21	1:C:157:THR:CG2	2.21	0.52
1:H:145:ILE:H	1:H:145:ILE:CD1	2.18	0.52
1:F:80:TYR:HA	1:F:128:ALA:HB1	1.91	0.52
1:F:38:PHE:HD2	1:F:169:GLN:OE1	1.93	0.52
1:L:48:ASN:ND2	1:L:158:ASN:N	2.50	0.52
1:B:48:ASN:ND2	1:B:158:ASN:N	2.52	0.52
1:B:206:VAL:HG12	1:B:207:SER:N	2.25	0.52
1:G:208:LEU:HD11	1:G:255:VAL:CG2	2.40	0.52
1:C:141:ILE:CG2	1:C:142:SER:N	2.72	0.52
1:C:70:GLN:HE22	1:C:135:THR:CG2	2.22	0.52
1:E:104:GLN:HE22	1:K:104:GLN:HA	1.75	0.52
1:L:62:VAL:CG1	1:L:145:ILE:HG13	2.40	0.52
1:A:104:GLN:HB2	1:G:108:LYS:CD	2.39	0.52
1:J:206:VAL:HG13	1:J:258:GLN:O	2.09	0.52
1:A:147:ARG:HD2	3:A:361:GOL:H12	1.92	0.52
1:G:145:ILE:CD1	1:G:145:ILE:H	2.13	0.52
1:F:206:VAL:HG13	1:F:258:GLN:O	2.08	0.52
1:L:45:PRO:HD3	1:L:164:MET:SD	2.48	0.52
1:A:208:LEU:HB2	1:A:242:PHE:CE2	2.45	0.52
1:M:221:ARG:HD3	1:M:223:GLU:OE2	2.10	0.52
1:G:69:TYR:CD1	1:G:164:MET:HE2	2.45	0.52
1:M:48:ASN:HD22	1:M:158:ASN:H	1.50	0.52
1:E:46:GLN:HB2	1:E:134:TYR:CD2	2.44	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:52:LEU:HD22	1:E:72:ASP:HA	1.91	0.52
1:A:206:VAL:HG12	1:A:207:SER:N	2.25	0.52
1:B:208:LEU:HD11	1:B:255:VAL:HG21	1.91	0.52
1:K:83:ALA:O	1:K:86:ASN:N	2.43	0.52
1:F:221:ARG:HD3	1:F:223:GLU:OE2	2.10	0.52
1:C:146:GLY:CA	2:C:361:3GR:O1	2.49	0.52
1:L:67:GLN:HE22	1:L:136:LYS:HD3	1.74	0.52
1:C:206:VAL:HG12	1:C:207:SER:N	2.25	0.52
1:I:208:LEU:HB2	1:I:242:PHE:CE2	2.44	0.52
1:E:144:ARG:NH1	1:E:144:ARG:HG3	2.25	0.52
1:K:208:LEU:HD11	1:K:255:VAL:HG21	1.90	0.52
1:G:106:VAL:HG13	1:G:110:GLN:HB2	1.92	0.52
1:L:48:ASN:ND2	1:L:157:THR:HA	2.24	0.52
1:I:48:ASN:ND2	1:I:157:THR:HA	2.25	0.52
1:I:62:VAL:CG1	1:I:145:ILE:HG13	2.40	0.52
1:I:211:GLU:HB3	1:I:254:PHE:O	2.10	0.52
1:B:144:ARG:NH1	1:B:144:ARG:HG3	2.24	0.51
1:D:141:ILE:HG23	1:D:142:SER:N	2.25	0.51
1:D:95:GLN:O	1:D:99:LEU:HD13	2.11	0.51
1:A:147:ARG:HD2	3:A:361:GOL:O1	2.09	0.51
1:L:130:ILE:CG2	1:L:134:TYR:HE1	2.23	0.51
1:M:206:VAL:HG21	1:M:222:LEU:HB2	1.91	0.51
1:M:47:VAL:HG22	1:M:76:TYR:CZ	2.44	0.51
1:I:141:ILE:CG2	1:I:142:SER:N	2.73	0.51
1:L:250:LEU:O	1:L:253:MET:HG3	2.09	0.51
1:A:175:VAL:HB	1:A:240:ALA:HB3	1.92	0.51
1:J:140:PRO:O	1:J:141:ILE:HD12	2.11	0.51
1:E:208:LEU:HD11	1:E:255:VAL:HG21	1.93	0.51
1:D:34:ARG:CB	1:D:34:ARG:HH11	2.22	0.51
1:C:145:ILE:HD12	1:C:145:ILE:N	2.23	0.51
1:C:48:ASN:ND2	1:C:157:THR:HG23	2.26	0.51
1:A:104:GLN:CB	1:G:108:LYS:HD2	2.41	0.51
1:D:97:TYR:HB3	1:D:106:VAL:HG11	1.92	0.51
1:A:35:THR:HG22	1:A:175:VAL:HG22	1.92	0.51
1:J:80:TYR:HA	1:J:128:ALA:HB1	1.93	0.51
1:L:158:ASN:C	1:L:158:ASN:ND2	2.63	0.51
1:H:70:GLN:HE22	1:H:135:THR:CG2	2.20	0.51
1:G:206:VAL:HG12	1:G:207:SER:N	2.25	0.51
1:D:55:LEU:HD23	1:D:55:LEU:N	2.25	0.51
1:I:208:LEU:HD11	1:I:255:VAL:CG2	2.41	0.51
1:C:250:LEU:O	1:C:253:MET:HG3	2.10	0.51
1:D:158:ASN:ND2	1:D:159:GLY:N	2.57	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:145:ILE:HD12	1:B:145:ILE:H	1.74	0.51
1:F:97:TYR:O	1:F:101:VAL:HG23	2.10	0.51
1:I:70:GLN:NE2	1:I:73:PRO:HD3	2.26	0.51
1:M:62:VAL:HG12	1:M:145:ILE:HG13	1.93	0.51
1:E:206:VAL:HG12	1:E:207:SER:N	2.24	0.51
1:L:206:VAL:O	1:L:219:GLU:HB2	2.10	0.51
1:B:102:ALA:C	1:B:104:GLN:H	2.14	0.51
1:L:140:PRO:O	1:L:141:ILE:HD12	2.10	0.51
1:E:246:ASN:O	1:F:188:ARG:NH2	2.37	0.51
1:H:69:TYR:HB2	1:H:137:VAL:HB	1.91	0.51
1:A:236:VAL:HG12	1:A:237:THR:N	2.25	0.51
1:C:183:ALA:O	1:C:187:LEU:HG	2.11	0.51
1:K:107:SER:CB	1:K:110:GLN:HG3	2.29	0.51
1:E:151:THR:HB	1:F:40:ILE:O	2.10	0.51
1:D:62:VAL:HG12	1:D:145:ILE:HG13	1.92	0.51
1:E:34:ARG:CB	1:E:34:ARG:HH11	2.19	0.51
1:F:71:ILE:O	1:F:73:PRO:CD	2.59	0.51
1:M:210:LEU:C	1:M:212:ASP:H	2.14	0.51
1:M:144:ARG:HG3	1:M:144:ARG:NH1	2.26	0.51
1:A:210:LEU:C	1:A:212:ASP:H	2.14	0.51
1:K:69:TYR:CD1	1:K:164:MET:HE2	2.46	0.51
1:F:208:LEU:HB2	1:F:242:PHE:CE2	2.45	0.51
1:A:48:ASN:ND2	1:A:158:ASN:N	2.48	0.51
1:L:171:ASP:HB3	1:L:172:PRO:HD3	1.87	0.51
1:I:126:GLU:O	1:I:130:ILE:HG12	2.10	0.51
1:E:236:VAL:HG12	1:E:237:THR:N	2.25	0.51
1:I:146:GLY:HA3	2:I:361:3GR:HA	1.75	0.50
1:I:145:ILE:CD1	1:I:145:ILE:H	2.17	0.50
1:C:48:ASN:HD21	1:C:157:THR:HG23	1.74	0.50
1:D:100:LEU:CD2	1:K:103:ASP:HB3	2.42	0.50
1:D:96:ARG:NH2	1:E:109:GLN:OE1	2.45	0.50
1:M:64:ALA:HB2	1:M:141:ILE:C	2.32	0.50
1:B:141:ILE:HG23	1:B:142:SER:N	2.26	0.50
1:D:113:ASP:O	1:D:116:ALA:HB3	2.11	0.50
1:K:197:GLU:OE2	1:K:205:LYS:HD2	2.11	0.50
1:F:145:ILE:H	1:F:145:ILE:CD1	2.13	0.50
1:E:158:ASN:ND2	1:E:159:GLY:N	2.58	0.50
1:J:171:ASP:O	1:J:173:ILE:N	2.43	0.50
1:M:145:ILE:H	1:M:145:ILE:HD12	1.76	0.50
1:M:134:TYR:C	1:M:136:LYS:N	2.65	0.50
1:K:185:LEU:HD21	1:L:248:GLU:HB3	1.93	0.50
1:M:183:ALA:O	1:M:187:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:101:VAL:CG2	1:F:111:TYR:HB2	2.39	0.50
1:K:158:ASN:HD22	1:K:159:GLY:H	1.57	0.50
1:E:186:ARG:HD3	1:E:190:GLU:OE2	2.10	0.50
1:B:215:GLN:HE22	1:B:258:GLN:HE22	1.58	0.50
1:K:40:ILE:O	1:L:151:THR:HB	2.12	0.50
1:D:206:VAL:HG12	1:D:207:SER:N	2.26	0.50
1:C:43:VAL:HG23	1:C:165:ALA:O	2.11	0.50
1:J:145:ILE:HD12	1:J:145:ILE:N	2.26	0.50
1:H:208:LEU:HD11	1:H:255:VAL:CG2	2.42	0.50
1:I:116:ALA:O	1:I:120:GLN:HG3	2.11	0.50
1:H:158:ASN:HD22	1:H:158:ASN:C	2.10	0.50
1:H:62:VAL:HG23	1:H:66:GLN:NE2	2.27	0.50
1:F:186:ARG:HH11	1:F:186:ARG:CB	2.24	0.50
1:E:101:VAL:HG23	1:E:106:VAL:O	2.12	0.50
1:H:38:PHE:HB2	1:H:172:PRO:O	2.12	0.50
1:C:208:LEU:HD11	1:C:255:VAL:CG2	2.41	0.50
1:F:236:VAL:HG12	1:F:237:THR:N	2.27	0.50
1:K:210:LEU:C	1:K:212:ASP:H	2.14	0.50
1:A:51:ILE:HD11	1:A:164:MET:HE3	1.93	0.50
1:J:35:THR:HG22	1:J:175:VAL:HG22	1.93	0.50
1:B:91:GLN:HG3	1:B:118:TYR:CE1	2.47	0.49
1:L:158:ASN:HD22	1:L:159:GLY:H	1.60	0.49
1:H:186:ARG:O	1:H:190:GLU:HG3	2.12	0.49
1:I:245:PRO:C	1:I:247:ASN:N	2.65	0.49
1:H:141:ILE:HG23	1:H:142:SER:N	2.27	0.49
1:M:208:LEU:HD11	1:M:255:VAL:HG21	1.94	0.49
1:J:208:LEU:HD11	1:J:255:VAL:CG2	2.41	0.49
1:F:55:LEU:HD23	1:F:55:LEU:N	2.27	0.49
1:M:80:TYR:HA	1:M:128:ALA:HB1	1.94	0.49
1:L:170:LEU:O	1:L:171:ASP:O	2.30	0.49
1:F:101:VAL:HG21	1:F:111:TYR:CB	2.40	0.49
1:M:170:LEU:HD21	1:M:251:PRO:CD	2.42	0.49
1:B:147:ARG:HB2	3:B:361:GOL:O2	2.12	0.49
1:K:140:PRO:O	1:K:141:ILE:HD12	2.12	0.49
1:L:48:ASN:HD22	1:L:157:THR:HA	1.76	0.49
1:A:62:VAL:HG23	1:A:66:GLN:OE1	2.12	0.49
1:L:34:ARG:CB	1:L:34:ARG:HH11	2.19	0.49
1:F:208:LEU:HD11	1:F:255:VAL:HG21	1.94	0.49
1:C:210:LEU:C	1:C:212:ASP:H	2.15	0.49
1:B:236:VAL:HG12	1:B:237:THR:N	2.28	0.49
1:L:201:ASP:O	1:L:202:ASN:HB2	2.13	0.49
1:J:55:LEU:N	1:J:55:LEU:HD23	2.27	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:206:VAL:HG21	1:K:222:LEU:HB2	1.94	0.49
1:J:208:LEU:HB2	1:J:242:PHE:CE2	2.47	0.49
1:C:141:ILE:HG23	1:C:142:SER:N	2.27	0.49
1:K:211:GLU:HB3	1:K:254:PHE:O	2.12	0.49
1:G:91:GLN:HG3	1:G:118:TYR:CE1	2.47	0.49
1:D:110:GLN:O	1:D:112:ALA:N	2.46	0.49
1:G:48:ASN:ND2	1:G:157:THR:HG23	2.27	0.49
1:G:206:VAL:O	1:G:219:GLU:HB2	2.13	0.49
1:K:62:VAL:CG1	1:K:145:ILE:HG13	2.43	0.49
1:K:208:LEU:HD11	1:K:255:VAL:CG2	2.43	0.49
1:H:83:ALA:O	1:H:86:ASN:N	2.46	0.49
1:J:236:VAL:HG21	1:K:250:LEU:HD12	1.94	0.49
1:J:197:GLU:OE2	1:J:205:LYS:HD2	2.12	0.49
1:H:158:ASN:ND2	1:H:159:GLY:N	2.56	0.49
1:B:171:ASP:O	1:B:173:ILE:N	2.45	0.49
1:G:62:VAL:CG1	1:G:145:ILE:HG13	2.43	0.49
1:H:206:VAL:HG21	1:H:222:LEU:HB2	1.95	0.49
1:D:103:ASP:O	1:D:104:GLN:HB3	2.12	0.49
1:I:226:GLU:HG3	1:J:144:ARG:HE	1.78	0.49
1:C:170:LEU:CD1	1:C:173:ILE:HD12	2.42	0.48
1:H:206:VAL:HG13	1:H:258:GLN:O	2.13	0.48
1:L:30:GLU:HG2	1:L:258:GLN:HG2	1.94	0.48
1:G:141:ILE:CG2	1:G:142:SER:N	2.76	0.48
1:B:50:ILE:HD13	1:B:155:LEU:HA	1.94	0.48
1:E:80:TYR:HA	1:E:128:ALA:HB1	1.93	0.48
1:C:91:GLN:HG3	1:C:118:TYR:CE1	2.47	0.48
1:E:70:GLN:NE2	1:E:135:THR:HG23	2.25	0.48
1:L:46:GLN:HB2	1:L:134:TYR:CD2	2.48	0.48
1:A:206:VAL:O	1:A:219:GLU:HB2	2.13	0.48
1:M:140:PRO:O	1:M:141:ILE:HD12	2.13	0.48
1:K:111:TYR:C	1:K:111:TYR:CD2	2.86	0.48
1:E:65:GLY:O	1:E:138:LEU:HD22	2.13	0.48
1:M:245:PRO:C	1:M:247:ASN:N	2.66	0.48
1:B:245:PRO:C	1:B:247:ASN:N	2.66	0.48
1:C:245:PRO:C	1:C:247:ASN:N	2.66	0.48
1:K:99:LEU:N	1:K:99:LEU:CD1	2.77	0.48
1:K:145:ILE:N	1:K:145:ILE:HD12	2.28	0.48
1:M:186:ARG:HD3	1:M:190:GLU:OE2	2.13	0.48
1:A:141:ILE:CG2	1:A:142:SER:N	2.76	0.48
1:G:69:TYR:HB2	1:G:137:VAL:HB	1.95	0.48
1:D:77:GLU:OE2	1:D:81:GLN:NE2	2.47	0.48
1:F:69:TYR:HB2	1:F:137:VAL:HB	1.95	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:158:ASN:HD22	1:A:158:ASN:C	2.15	0.48
1:D:70:GLN:NE2	1:D:135:THR:HG23	2.28	0.48
1:J:236:VAL:CG2	1:K:250:LEU:HD12	2.43	0.48
1:B:97:TYR:O	1:B:101:VAL:HG23	2.14	0.48
1:D:91:GLN:HG3	1:D:118:TYR:CE1	2.49	0.48
1:H:158:ASN:HD22	1:H:159:GLY:H	1.58	0.48
1:F:37:ALA:HB3	1:F:40:ILE:CD1	2.36	0.48
1:J:60:SER:O	1:J:145:ILE:HD12	2.14	0.48
1:L:67:GLN:HA	1:L:138:LEU:HD23	1.95	0.48
1:E:147:ARG:H	2:E:361:3GR:HA	1.57	0.48
1:G:188:ARG:HH21	1:H:248:GLU:HA	1.78	0.48
1:E:96:ARG:NH2	1:F:109:GLN:OE1	2.46	0.48
1:L:110:GLN:C	1:L:112:ALA:N	2.63	0.48
1:H:87:LEU:HD12	1:H:87:LEU:O	2.14	0.48
1:D:74:ALA:HB1	1:E:130:ILE:HD12	1.96	0.48
1:H:141:ILE:CG2	1:H:142:SER:N	2.77	0.48
1:K:145:ILE:HG23	1:K:167:VAL:HG22	1.95	0.48
1:K:69:TYR:HB2	1:K:137:VAL:HB	1.96	0.48
1:L:52:LEU:HD22	1:L:72:ASP:HA	1.96	0.48
1:A:186:ARG:HH11	1:A:186:ARG:CB	2.25	0.48
1:J:245:PRO:O	1:J:247:ASN:N	2.46	0.48
1:K:141:ILE:HG23	1:K:142:SER:N	2.28	0.48
1:C:116:ALA:O	1:C:120:GLN:HG3	2.13	0.48
1:K:230:ASP:O	1:K:234:GLY:N	2.45	0.48
1:L:145:ILE:HD12	1:L:145:ILE:N	2.29	0.47
1:G:60:SER:O	1:G:145:ILE:HD12	2.13	0.47
1:B:158:ASN:HD22	1:B:159:GLY:H	1.61	0.47
1:H:171:ASP:HB3	1:H:172:PRO:HD3	1.94	0.47
1:K:103:ASP:C	1:K:105:ALA:N	2.68	0.47
1:M:206:VAL:O	1:M:219:GLU:HB2	2.14	0.47
1:L:245:PRO:C	1:L:247:ASN:N	2.67	0.47
1:H:236:VAL:HG12	1:H:237:THR:N	2.29	0.47
1:E:48:ASN:HD22	1:E:157:THR:HA	1.79	0.47
1:K:250:LEU:O	1:K:253:MET:HG3	2.14	0.47
1:M:103:ASP:O	1:M:105:ALA:N	2.47	0.47
1:I:236:VAL:HG12	1:I:237:THR:N	2.29	0.47
1:C:34:ARG:HH11	1:C:34:ARG:CB	2.20	0.47
1:J:145:ILE:CD1	1:J:145:ILE:H	2.25	0.47
1:J:206:VAL:HG12	1:J:207:SER:N	2.28	0.47
1:C:206:VAL:O	1:C:219:GLU:HB2	2.13	0.47
1:L:69:TYR:HB2	1:L:137:VAL:HB	1.97	0.47
1:G:70:GLN:HE21	1:G:73:PRO:HD3	1.80	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:L:48:ASN:ND2	1:L:157:THR:HG23	2.30	0.47
1:L:110:GLN:O	1:L:113:ASP:N	2.48	0.47
1:F:31:LEU:HB3	1:F:177:VAL:CG1	2.45	0.47
1:H:98:LYS:HB2	1:H:111:TYR:CE1	2.49	0.47
1:J:226:GLU:OE2	1:K:144:ARG:NE	2.48	0.47
1:A:31:LEU:HB3	1:A:177:VAL:HG11	1.96	0.47
1:D:70:GLN:HE21	1:D:73:PRO:HD3	1.79	0.47
1:K:186:ARG:HH11	1:K:186:ARG:CB	2.25	0.47
1:A:96:ARG:NH2	1:B:109:GLN:CD	2.67	0.47
1:D:141:ILE:CG2	1:D:142:SER:N	2.77	0.47
1:B:210:LEU:C	1:B:212:ASP:H	2.17	0.47
1:A:100:LEU:HB3	1:A:105:ALA:HB3	1.97	0.47
1:K:95:GLN:O	1:K:99:LEU:HD13	2.13	0.47
1:A:171:ASP:HB3	1:A:172:PRO:HD3	1.94	0.47
1:E:145:ILE:HD12	1:E:145:ILE:N	2.29	0.47
1:K:62:VAL:HG12	1:K:145:ILE:HG13	1.97	0.47
1:I:206:VAL:HG21	1:I:222:LEU:HB2	1.96	0.47
1:C:80:TYR:HA	1:C:128:ALA:HB1	1.97	0.47
1:D:210:LEU:C	1:D:212:ASP:H	2.16	0.47
1:F:77:GLU:OE2	1:F:81:GLN:NE2	2.47	0.47
1:L:60:SER:O	1:L:145:ILE:HD12	2.15	0.47
1:F:85:ALA:HB2	1:G:82:SER:CB	2.36	0.47
1:I:30:GLU:HG2	1:I:258:GLN:HG2	1.96	0.47
1:B:206:VAL:O	1:B:219:GLU:HB2	2.15	0.47
1:H:206:VAL:HG12	1:H:207:SER:N	2.30	0.47
1:F:70:GLN:NE2	1:F:135:THR:HG23	2.28	0.47
1:L:245:PRO:O	1:L:247:ASN:N	2.48	0.47
1:J:130:ILE:HG22	1:J:134:TYR:CE1	2.50	0.47
1:M:208:LEU:HD11	1:M:255:VAL:CG2	2.45	0.47
1:A:210:LEU:C	1:A:212:ASP:N	2.68	0.47
1:G:166:THR:HB	2:G:361:3GR:O1	2.15	0.47
1:I:221:ARG:HD3	1:I:223:GLU:OE2	2.14	0.47
1:I:171:ASP:O	1:I:173:ILE:N	2.47	0.47
1:G:48:ASN:ND2	1:G:157:THR:HA	2.29	0.47
1:J:62:VAL:HG23	1:J:66:GLN:NE2	2.30	0.47
1:L:67:GLN:NE2	1:L:136:LYS:HD3	2.30	0.47
1:H:144:ARG:HG3	1:H:144:ARG:NH1	2.30	0.47
1:L:206:VAL:CG1	1:L:207:SER:N	2.78	0.47
1:C:147:ARG:NH2	1:D:237:THR:HG21	2.29	0.47
1:E:145:ILE:CD1	1:E:145:ILE:H	2.25	0.47
1:H:171:ASP:O	1:H:173:ILE:N	2.47	0.47
1:G:34:ARG:HH11	1:G:34:ARG:CB	2.19	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:65:GLY:O	1:K:138:LEU:HD22	2.14	0.47
1:F:208:LEU:HD11	1:F:255:VAL:CG2	2.43	0.47
1:L:236:VAL:HG12	1:L:237:THR:N	2.30	0.47
1:K:236:VAL:HG12	1:K:237:THR:N	2.30	0.47
1:E:43:VAL:HG23	1:E:165:ALA:O	2.15	0.47
1:E:140:PRO:O	1:E:141:ILE:HD12	2.15	0.47
1:J:211:GLU:HB3	1:J:254:PHE:O	2.14	0.47
1:I:48:ASN:HD21	1:I:158:ASN:H	1.58	0.46
1:F:245:PRO:C	1:F:247:ASN:N	2.65	0.46
1:I:245:PRO:O	1:I:247:ASN:N	2.48	0.46
1:B:175:VAL:HB	1:B:240:ALA:HB3	1.97	0.46
1:A:97:TYR:CD1	1:A:114:ALA:HB2	2.50	0.46
1:L:54:ARG:O	1:L:54:ARG:HD2	2.15	0.46
1:G:48:ASN:HD21	1:G:158:ASN:N	2.09	0.46
1:H:171:ASP:CB	1:H:172:PRO:CD	2.89	0.46
1:G:245:PRO:C	1:G:247:ASN:N	2.67	0.46
1:B:208:LEU:HD11	1:B:255:VAL:CG2	2.45	0.46
1:K:210:LEU:C	1:K:212:ASP:N	2.68	0.46
1:I:80:TYR:HA	1:I:128:ALA:HB1	1.96	0.46
1:D:54:ARG:HD2	1:D:54:ARG:O	2.15	0.46
1:G:38:PHE:HD2	1:G:169:GLN:NE2	2.13	0.46
1:H:48:ASN:ND2	1:H:157:THR:HA	2.30	0.46
1:I:48:ASN:ND2	1:I:158:ASN:N	2.58	0.46
1:B:147:ARG:HG3	1:C:227:VAL:HG12	1.96	0.46
1:K:175:VAL:HB	1:K:240:ALA:HB3	1.97	0.46
1:G:250:LEU:O	1:G:253:MET:HG3	2.15	0.46
1:M:175:VAL:HB	1:M:240:ALA:HB3	1.96	0.46
1:J:54:ARG:HD2	1:J:54:ARG:O	2.15	0.46
1:A:171:ASP:O	1:A:173:ILE:N	2.49	0.46
1:A:104:GLN:HB2	1:G:108:LYS:HD2	1.97	0.46
1:C:107:SER:H	1:C:110:GLN:HE21	1.63	0.46
1:L:208:LEU:HD11	1:L:255:VAL:HG21	1.97	0.46
1:M:130:ILE:CG2	1:M:134:TYR:HE1	2.28	0.46
1:L:210:LEU:C	1:L:212:ASP:N	2.68	0.46
1:M:158:ASN:ND2	1:M:159:GLY:N	2.62	0.46
1:F:106:VAL:HG12	1:F:107:SER:N	2.30	0.46
1:D:147:ARG:NH2	1:E:237:THR:HG21	2.29	0.46
1:E:210:LEU:C	1:E:212:ASP:H	2.18	0.46
1:M:210:LEU:C	1:M:212:ASP:N	2.69	0.46
1:L:226:GLU:OE2	1:M:144:ARG:HD3	2.15	0.46
1:I:210:LEU:C	1:I:212:ASP:H	2.18	0.46
1:F:141:ILE:CG2	1:F:142:SER:N	2.78	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:69:TYR:HB2	1:C:137:VAL:HB	1.97	0.46
1:M:171:ASP:O	1:M:173:ILE:N	2.49	0.46
1:F:167:VAL:HG12	1:F:168:GLN:N	2.31	0.46
1:F:62:VAL:HG23	1:F:66:GLN:OE1	2.15	0.46
1:D:69:TYR:HB2	1:D:137:VAL:HB	1.96	0.46
1:I:67:GLN:HA	1:I:138:LEU:HD23	1.98	0.46
1:F:206:VAL:CG1	1:F:207:SER:N	2.79	0.46
1:A:245:PRO:C	1:A:247:ASN:N	2.67	0.46
1:I:41:ALA:HB1	1:I:140:PRO:CG	2.46	0.46
1:D:70:GLN:HE22	1:D:135:THR:HG23	1.80	0.46
1:A:62:VAL:HG12	1:A:145:ILE:HG13	1.96	0.46
1:L:130:ILE:HG22	1:L:134:TYR:CE1	2.50	0.46
1:M:73:PRO:O	1:M:74:ALA:C	2.54	0.46
1:J:46:GLN:OE1	1:J:134:TYR:CE2	2.69	0.46
1:M:43:VAL:HG23	1:M:165:ALA:O	2.16	0.46
1:A:80:TYR:HA	1:A:128:ALA:HB1	1.97	0.46
1:K:48:ASN:HD22	1:K:158:ASN:H	1.56	0.46
1:D:145:ILE:H	1:D:145:ILE:CD1	2.27	0.46
1:D:145:ILE:N	1:D:145:ILE:HD12	2.30	0.46
1:L:46:GLN:CD	1:L:134:TYR:CE2	2.90	0.46
1:A:104:GLN:HB2	1:G:108:LYS:HD3	1.98	0.46
1:K:206:VAL:O	1:K:219:GLU:HB2	2.16	0.46
1:M:100:LEU:HD12	1:M:100:LEU:N	2.31	0.46
1:H:245:PRO:C	1:H:247:ASN:N	2.69	0.46
1:G:46:GLN:OE1	1:G:134:TYR:CE2	2.69	0.46
1:G:135:THR:HG22	1:G:136:LYS:HG3	1.96	0.45
1:M:48:ASN:HD21	1:M:158:ASN:N	2.12	0.45
1:L:171:ASP:O	1:L:173:ILE:N	2.49	0.45
1:C:186:ARG:HH11	1:C:186:ARG:CB	2.25	0.45
1:K:208:LEU:HB2	1:K:242:PHE:CE2	2.50	0.45
1:M:158:ASN:HD22	1:M:159:GLY:H	1.63	0.45
1:H:158:ASN:C	1:H:158:ASN:ND2	2.68	0.45
1:L:62:VAL:HG23	1:L:66:GLN:OE1	2.16	0.45
1:A:73:PRO:O	1:A:74:ALA:C	2.53	0.45
1:J:91:GLN:HG3	1:J:118:TYR:CE1	2.51	0.45
1:K:109:GLN:OE1	1:L:96:ARG:NH2	2.50	0.45
1:C:107:SER:H	1:C:110:GLN:NE2	2.14	0.45
1:C:206:VAL:HG21	1:C:222:LEU:HB2	1.98	0.45
1:E:141:ILE:HG23	1:E:142:SER:N	2.32	0.45
1:D:80:TYR:HA	1:D:128:ALA:HB1	1.98	0.45
1:G:193:SER:C	1:G:195:GLN:H	2.20	0.45
1:G:193:SER:O	1:G:195:GLN:N	2.49	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:206:VAL:HG21	1:D:222:LEU:HB2	1.97	0.45
1:D:206:VAL:O	1:D:219:GLU:HB2	2.17	0.45
1:B:141:ILE:CG2	1:B:142:SER:N	2.79	0.45
1:J:210:LEU:C	1:J:212:ASP:H	2.18	0.45
1:B:250:LEU:O	1:B:253:MET:HG3	2.17	0.45
1:L:158:ASN:ND2	1:L:159:GLY:N	2.55	0.45
1:F:48:ASN:HD22	1:F:158:ASN:H	1.62	0.45
1:G:236:VAL:HG12	1:G:237:THR:H	1.82	0.45
1:J:113:ASP:O	1:J:116:ALA:HB3	2.16	0.45
1:M:86:ASN:O	1:M:89:SER:HB3	2.15	0.45
1:G:38:PHE:CD2	1:G:169:GLN:NE2	2.85	0.45
1:G:171:ASP:O	1:G:173:ILE:N	2.49	0.45
1:K:145:ILE:CD1	1:K:145:ILE:H	2.26	0.45
1:B:109:GLN:O	1:B:113:ASP:OD2	2.35	0.45
1:E:130:ILE:CG2	1:E:134:TYR:HE1	2.30	0.45
1:J:245:PRO:C	1:J:247:ASN:N	2.65	0.45
1:K:141:ILE:CG2	1:K:142:SER:N	2.80	0.45
1:A:85:ALA:HB1	1:B:119:LEU:HB3	1.98	0.45
1:E:62:VAL:HG23	1:E:66:GLN:NE2	2.32	0.45
1:K:206:VAL:HG13	1:K:258:GLN:O	2.17	0.45
1:M:245:PRO:O	1:M:247:ASN:N	2.49	0.45
1:C:210:LEU:C	1:C:212:ASP:N	2.69	0.45
1:F:210:LEU:C	1:F:212:ASP:H	2.20	0.45
1:D:73:PRO:O	1:D:74:ALA:C	2.52	0.45
1:I:206:VAL:O	1:I:219:GLU:HB2	2.17	0.45
1:I:46:GLN:HB2	1:I:134:TYR:CD2	2.51	0.45
1:C:31:LEU:HB3	1:C:177:VAL:HG11	1.99	0.45
1:K:171:ASP:O	1:K:173:ILE:N	2.49	0.45
1:B:171:ASP:HB3	1:B:172:PRO:HD3	1.91	0.45
1:H:38:PHE:CD2	1:H:169:GLN:NE2	2.84	0.45
1:K:60:SER:O	1:K:145:ILE:HD12	2.16	0.45
1:B:100:LEU:O	1:B:106:VAL:N	2.46	0.45
1:I:140:PRO:O	1:I:141:ILE:HD12	2.16	0.45
1:L:48:ASN:HD21	1:L:158:ASN:N	2.14	0.44
1:H:48:ASN:HD21	1:H:158:ASN:N	2.15	0.44
1:D:100:LEU:O	1:D:106:VAL:HB	2.16	0.44
1:D:210:LEU:C	1:D:212:ASP:N	2.71	0.44
1:A:250:LEU:O	1:A:253:MET:HG3	2.17	0.44
1:G:54:ARG:O	1:G:54:ARG:HD2	2.16	0.44
1:H:48:ASN:HD22	1:H:158:ASN:H	1.56	0.44
1:F:48:ASN:HD22	1:F:157:THR:HA	1.81	0.44
1:H:34:ARG:CB	1:H:34:ARG:HH11	2.24	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:100:LEU:HB2	1:D:106:VAL:HG21	1.99	0.44
1:H:245:PRO:O	1:H:247:ASN:N	2.51	0.44
1:C:175:VAL:HB	1:C:240:ALA:HB3	1.99	0.44
1:F:250:LEU:O	1:F:253:MET:HG3	2.17	0.44
1:H:40:ILE:O	1:I:151:THR:HB	2.17	0.44
1:E:68:LEU:HD11	1:E:139:SER:HB2	2.00	0.44
1:H:80:TYR:HA	1:H:128:ALA:HB1	1.98	0.44
1:I:195:GLN:HG2	1:I:195:GLN:O	2.17	0.44
1:J:201:ASP:O	1:J:202:ASN:HB2	2.16	0.44
1:K:73:PRO:O	1:K:74:ALA:C	2.55	0.44
1:M:158:ASN:HD22	1:M:158:ASN:C	2.18	0.44
1:M:34:ARG:HH11	1:M:34:ARG:CB	2.25	0.44
1:F:98:LYS:HG3	1:F:111:TYR:CZ	2.52	0.44
1:D:97:TYR:CB	1:D:106:VAL:HG11	2.47	0.44
1:A:245:PRO:O	1:A:247:ASN:N	2.50	0.44
1:M:134:TYR:C	1:M:136:LYS:H	2.20	0.44
1:E:245:PRO:O	1:E:247:ASN:N	2.50	0.44
1:F:100:LEU:HB3	1:F:106:VAL:HG23	1.99	0.44
1:K:80:TYR:HA	1:K:128:ALA:HB1	1.99	0.44
1:G:80:TYR:HA	1:G:128:ALA:HB1	1.99	0.44
1:G:35:THR:HG22	1:G:175:VAL:HG22	1.98	0.44
1:K:71:ILE:O	1:K:72:ASP:C	2.55	0.44
1:A:145:ILE:HG23	1:A:167:VAL:CG2	2.47	0.44
1:K:34:ARG:HH11	1:K:34:ARG:CB	2.22	0.44
1:I:109:GLN:O	1:I:112:ALA:HB3	2.17	0.44
1:J:236:VAL:HG12	1:J:237:THR:N	2.33	0.44
1:B:250:LEU:HD12	1:C:236:VAL:HG21	1.98	0.44
1:A:86:ASN:O	1:A:89:SER:HB3	2.18	0.44
1:K:52:LEU:HA	1:K:52:LEU:HD12	1.82	0.44
1:A:145:ILE:N	1:A:145:ILE:HD12	2.32	0.44
1:B:206:VAL:HG21	1:B:222:LEU:HB2	1.99	0.44
1:F:206:VAL:HG22	1:F:259:LEU:CD2	2.48	0.44
1:C:140:PRO:O	1:C:141:ILE:HD12	2.17	0.44
1:G:158:ASN:ND2	1:G:159:GLY:N	2.66	0.44
1:I:158:ASN:ND2	1:I:159:GLY:N	2.64	0.44
1:C:48:ASN:HD21	1:C:158:ASN:H	1.59	0.44
1:D:97:TYR:O	1:D:106:VAL:HG11	2.18	0.44
1:C:206:VAL:HG22	1:C:259:LEU:CD2	2.48	0.44
1:J:210:LEU:C	1:J:212:ASP:N	2.71	0.44
1:D:35:THR:HG22	1:D:175:VAL:HG22	2.00	0.44
1:I:91:GLN:HG3	1:I:118:TYR:CE1	2.53	0.44
1:H:62:VAL:CG2	1:H:66:GLN:OE1	2.59	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:J:48:ASN:HD22	1:J:157:THR:HA	1.83	0.44
1:D:101:VAL:C	1:D:103:ASP:H	2.21	0.44
1:H:144:ARG:HG3	1:H:144:ARG:HH11	1.83	0.44
1:J:175:VAL:HB	1:J:240:ALA:HB3	1.99	0.44
1:C:236:VAL:HG12	1:C:237:THR:N	2.33	0.44
1:G:191:LEU:C	1:G:191:LEU:HD13	2.38	0.44
1:F:91:GLN:HG3	1:F:118:TYR:CE1	2.53	0.43
1:H:48:ASN:ND2	1:H:158:ASN:N	2.52	0.43
1:H:62:VAL:HG22	1:H:63:LYS:N	2.33	0.43
1:C:145:ILE:H	1:C:145:ILE:CD1	2.22	0.43
1:D:101:VAL:HA	1:D:106:VAL:O	2.17	0.43
1:A:206:VAL:HG21	1:A:222:LEU:HB2	1.99	0.43
1:E:208:LEU:HB2	1:E:242:PHE:CE2	2.53	0.43
1:K:40:ILE:HG12	1:K:168:GLN:HG2	1.99	0.43
1:I:236:VAL:HG21	1:J:250:LEU:HD12	1.99	0.43
1:F:31:LEU:HB3	1:F:177:VAL:HG11	2.00	0.43
1:B:216:TYR:HA	1:B:217:PRO:HD2	1.85	0.43
1:D:86:ASN:O	1:D:89:SER:HB3	2.18	0.43
1:F:46:GLN:HB2	1:F:134:TYR:CD2	2.52	0.43
1:A:101:VAL:HG13	1:A:106:VAL:CG2	2.45	0.43
1:A:144:ARG:HE	1:B:226:GLU:HG3	1.83	0.43
1:K:245:PRO:C	1:K:247:ASN:N	2.70	0.43
1:K:57:LYS:O	1:K:58:GLU:C	2.55	0.43
1:L:77:GLU:OE2	1:L:81:GLN:NE2	2.51	0.43
1:B:146:GLY:HA3	3:B:361:GOL:C1	2.46	0.43
1:B:245:PRO:O	1:B:247:ASN:N	2.51	0.43
1:J:83:ALA:O	1:J:86:ASN:N	2.51	0.43
1:E:69:TYR:HB2	1:E:137:VAL:HB	2.00	0.43
1:H:77:GLU:OE2	1:H:81:GLN:NE2	2.51	0.43
1:M:48:ASN:ND2	1:M:157:THR:HA	2.33	0.43
1:B:48:ASN:HD22	1:B:158:ASN:H	1.63	0.43
1:J:46:GLN:HB2	1:J:134:TYR:CD2	2.53	0.43
1:M:41:ALA:HB1	1:M:140:PRO:HG2	2.01	0.43
1:M:206:VAL:CG1	1:M:207:SER:N	2.82	0.43
1:H:73:PRO:O	1:H:74:ALA:C	2.56	0.43
1:F:140:PRO:O	1:F:141:ILE:HD12	2.18	0.43
1:C:69:TYR:CD1	1:C:164:MET:HE1	2.53	0.43
1:C:47:VAL:HG22	1:C:76:TYR:CZ	2.53	0.43
1:K:193:SER:O	1:K:195:GLN:N	2.52	0.43
1:I:250:LEU:O	1:I:253:MET:HG3	2.19	0.43
1:E:75:THR:HG23	1:F:127:GLN:HE22	1.83	0.43
1:H:191:LEU:C	1:H:191:LEU:HD13	2.39	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:171:ASP:O	1:D:173:ILE:N	2.52	0.43
1:F:104:GLN:HE22	1:L:108:LYS:HB2	1.84	0.43
1:D:104:GLN:NE2	1:J:104:GLN:HE22	2.13	0.43
1:C:106:VAL:CG2	1:C:110:GLN:HB2	2.47	0.43
1:H:107:SER:OG	1:H:109:GLN:NE2	2.51	0.43
1:E:184:LEU:HD13	1:E:188:ARG:HG3	2.00	0.43
1:G:44:ARG:HD2	1:H:153:GLY:O	2.18	0.43
1:B:99:LEU:N	1:B:99:LEU:HD22	2.34	0.43
1:E:104:GLN:NE2	1:K:104:GLN:HA	2.33	0.43
1:H:208:LEU:HB2	1:H:242:PHE:CE2	2.54	0.43
1:J:250:LEU:O	1:J:253:MET:HG3	2.19	0.43
1:G:175:VAL:HB	1:G:240:ALA:HB3	2.00	0.43
1:D:175:VAL:HB	1:D:240:ALA:HB3	2.01	0.43
1:B:43:VAL:HG23	1:B:165:ALA:O	2.18	0.43
1:K:99:LEU:H	1:K:99:LEU:CD1	2.32	0.43
1:G:171:ASP:HB3	1:G:172:PRO:HD3	1.96	0.43
1:I:145:ILE:HG23	1:I:167:VAL:HG22	2.01	0.43
1:E:71:ILE:O	1:E:72:ASP:C	2.57	0.43
1:G:245:PRO:O	1:G:247:ASN:N	2.52	0.43
1:I:41:ALA:HB1	1:I:140:PRO:HG2	2.00	0.43
1:A:96:ARG:HH22	1:B:109:GLN:NE2	2.17	0.43
1:E:208:LEU:HD11	1:E:255:VAL:CG2	2.48	0.43
1:B:210:LEU:C	1:B:212:ASP:N	2.71	0.43
1:K:226:GLU:HG3	1:L:144:ARG:HE	1.84	0.43
1:L:144:ARG:HG3	1:L:144:ARG:HH11	1.83	0.43
1:A:158:ASN:ND2	1:A:158:ASN:C	2.72	0.43
1:E:210:LEU:C	1:E:212:ASP:N	2.72	0.43
1:G:191:LEU:HD11	1:G:198:ARG:NH1	2.34	0.43
1:I:230:ASP:O	1:I:234:GLY:N	2.48	0.43
1:B:184:LEU:HD13	1:B:188:ARG:HG3	2.00	0.43
1:B:158:ASN:ND2	1:B:159:GLY:N	2.65	0.43
1:E:60:SER:O	1:E:145:ILE:HD12	2.19	0.43
1:I:158:ASN:HD22	1:I:159:GLY:H	1.65	0.43
1:L:130:ILE:HG22	1:L:134:TYR:HE1	1.84	0.43
1:L:113:ASP:O	1:L:116:ALA:HB3	2.19	0.43
1:I:175:VAL:HB	1:I:240:ALA:HB3	1.99	0.43
1:B:170:LEU:O	1:B:171:ASP:O	2.37	0.42
1:K:103:ASP:O	1:K:105:ALA:N	2.52	0.42
1:F:245:PRO:O	1:F:247:ASN:N	2.51	0.42
1:G:206:VAL:CG1	1:G:207:SER:N	2.82	0.42
1:I:52:LEU:HD12	1:I:52:LEU:HA	1.92	0.42
1:C:31:LEU:HD22	1:C:179:GLN:CD	2.39	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:47:VAL:HG22	1:B:76:TYR:CZ	2.54	0.42
1:K:91:GLN:HG3	1:K:118:TYR:CE1	2.53	0.42
1:D:71:ILE:O	1:D:72:ASP:C	2.57	0.42
1:B:46:GLN:HB2	1:B:134:TYR:CD2	2.53	0.42
1:L:73:PRO:O	1:L:74:ALA:C	2.54	0.42
1:B:51:ILE:CD1	1:B:164:MET:HE3	2.48	0.42
1:K:170:LEU:HD21	1:K:251:PRO:CG	2.49	0.42
1:F:113:ASP:O	1:F:116:ALA:HB3	2.19	0.42
1:A:158:ASN:ND2	1:A:159:GLY:N	2.63	0.42
1:F:62:VAL:HG12	1:F:145:ILE:HG13	2.00	0.42
1:H:38:PHE:HD2	1:H:169:GLN:NE2	2.16	0.42
1:J:62:VAL:HG12	1:J:145:ILE:HG13	2.01	0.42
1:H:101:VAL:HA	1:H:106:VAL:O	2.18	0.42
1:H:55:LEU:HD23	1:H:55:LEU:N	2.33	0.42
1:E:206:VAL:O	1:E:219:GLU:HB2	2.19	0.42
1:D:104:GLN:C	1:D:106:VAL:N	2.72	0.42
1:K:206:VAL:CG1	1:K:207:SER:N	2.83	0.42
1:C:245:PRO:O	1:C:247:ASN:N	2.52	0.42
1:K:193:SER:C	1:K:195:GLN:H	2.23	0.42
1:B:52:LEU:HA	1:B:52:LEU:HD12	1.80	0.42
1:I:227:VAL:HG12	1:J:147:ARG:HG3	2.01	0.42
1:D:46:GLN:OE1	1:D:134:TYR:CE2	2.73	0.42
1:M:145:ILE:H	1:M:145:ILE:CD1	2.33	0.42
1:J:106:VAL:HG13	1:J:110:GLN:CB	2.45	0.42
1:L:97:TYR:O	1:L:101:VAL:HG23	2.20	0.42
1:F:206:VAL:CG1	1:F:258:GLN:H	2.33	0.42
1:H:206:VAL:O	1:H:219:GLU:HB2	2.19	0.42
1:I:191:LEU:C	1:I:191:LEU:HD13	2.39	0.42
1:A:48:ASN:HD21	1:A:158:ASN:N	2.09	0.42
1:E:62:VAL:CG2	1:E:68:LEU:HD21	2.41	0.42
1:I:48:ASN:O	1:I:76:TYR:OH	2.25	0.42
1:J:206:VAL:O	1:J:219:GLU:HB2	2.19	0.42
1:E:71:ILE:O	1:E:73:PRO:HD3	2.20	0.42
1:H:147:ARG:N	2:H:361:3GR:HA	2.18	0.42
1:A:130:ILE:CG2	1:A:134:TYR:HE1	2.32	0.42
1:C:130:ILE:HG22	1:C:134:TYR:CE1	2.55	0.42
1:A:50:ILE:HD13	1:A:155:LEU:HA	2.01	0.42
1:I:144:ARG:NH1	1:I:144:ARG:HG3	2.35	0.42
1:I:62:VAL:HG12	1:I:145:ILE:HG13	2.01	0.42
1:G:101:VAL:HG21	1:G:111:TYR:CB	2.47	0.42
1:I:210:LEU:C	1:I:212:ASP:N	2.73	0.42
1:E:245:PRO:O	1:E:246:ASN:HB2	2.20	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:216:TYR:HA	1:D:217:PRO:HD2	1.87	0.42
1:H:54:ARG:O	1:H:54:ARG:HD2	2.19	0.42
1:G:96:ARG:O	1:G:99:LEU:HB2	2.18	0.42
1:B:145:ILE:HD12	1:B:145:ILE:N	2.35	0.42
1:L:101:VAL:HG13	1:L:106:VAL:O	2.20	0.42
1:I:52:LEU:HD22	1:I:72:ASP:HA	2.00	0.42
1:J:111:TYR:CD2	1:J:111:TYR:C	2.92	0.42
1:L:99:LEU:N	1:L:99:LEU:CD1	2.82	0.42
1:C:171:ASP:O	1:C:173:ILE:N	2.53	0.42
1:M:158:ASN:ND2	1:M:158:ASN:C	2.72	0.42
1:G:171:ASP:CB	1:G:172:PRO:CD	2.84	0.42
1:A:60:SER:O	1:A:145:ILE:HD12	2.20	0.42
1:A:34:ARG:HH11	1:A:34:ARG:CB	2.25	0.42
1:F:206:VAL:HG21	1:F:222:LEU:HB2	2.02	0.42
1:H:60:SER:O	1:H:145:ILE:HD12	2.19	0.42
1:H:175:VAL:HB	1:H:240:ALA:HB3	2.02	0.42
1:B:199:ALA:HB2	1:B:205:LYS:N	2.35	0.42
1:A:31:LEU:HB3	1:A:177:VAL:CG1	2.50	0.42
1:H:103:ASP:N	1:H:103:ASP:OD1	2.53	0.42
1:G:190:GLU:CB	1:G:196:LEU:HD13	2.50	0.42
1:M:206:VAL:HG13	1:M:258:GLN:O	2.19	0.42
1:B:113:ASP:O	1:B:116:ALA:HB3	2.19	0.42
1:E:77:GLU:OE2	1:E:81:GLN:NE2	2.53	0.42
1:G:70:GLN:HE22	1:G:135:THR:HG23	1.85	0.42
1:M:100:LEU:CB	1:M:106:VAL:HG23	2.47	0.42
1:M:101:VAL:HG21	1:M:111:TYR:CD1	2.55	0.42
1:I:201:ASP:O	1:I:202:ASN:HB2	2.19	0.42
1:L:145:ILE:H	1:L:145:ILE:CD1	2.25	0.41
1:J:70:GLN:NE2	1:J:135:THR:HG23	2.35	0.41
1:C:60:SER:O	1:C:145:ILE:HD12	2.19	0.41
1:A:104:GLN:HG2	1:G:104:GLN:HE22	1.84	0.41
1:C:130:ILE:CG2	1:C:134:TYR:HE1	2.33	0.41
1:A:183:ALA:O	1:A:187:LEU:HG	2.20	0.41
1:J:91:GLN:CG	1:J:95:GLN:HE21	2.07	0.41
1:J:146:GLY:HA3	3:J:361:GOL:C1	2.49	0.41
1:M:48:ASN:ND2	1:M:158:ASN:N	2.50	0.41
1:E:130:ILE:HG22	1:E:134:TYR:CE1	2.55	0.41
1:E:206:VAL:CG1	1:E:207:SER:N	2.83	0.41
1:J:67:GLN:CD	1:J:136:LYS:HD3	2.40	0.41
1:K:30:GLU:HG2	1:K:258:GLN:HG2	2.02	0.41
1:G:226:GLU:CG	1:H:144:ARG:HE	2.29	0.41
1:G:31:LEU:HD22	1:G:179:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:75:THR:O	1:F:78:ALA:N	2.53	0.41
1:J:99:LEU:O	1:J:102:ALA:HB3	2.20	0.41
1:B:193:SER:O	1:B:195:GLN:N	2.53	0.41
1:J:146:GLY:HA3	3:J:361:GOL:O2	2.21	0.41
1:J:70:GLN:HE21	1:J:73:PRO:HD3	1.85	0.41
1:K:48:ASN:ND2	1:K:157:THR:HG23	2.35	0.41
1:B:206:VAL:CG1	1:B:207:SER:N	2.83	0.41
1:M:199:ALA:HB2	1:M:205:LYS:N	2.36	0.41
1:E:245:PRO:C	1:E:247:ASN:N	2.73	0.41
1:C:31:LEU:HB3	1:C:177:VAL:CG1	2.49	0.41
1:I:216:TYR:HA	1:I:217:PRO:HD2	1.85	0.41
1:F:191:LEU:HD11	1:F:198:ARG:NH1	2.35	0.41
1:A:75:THR:O	1:A:78:ALA:N	2.54	0.41
1:L:48:ASN:HD22	1:L:158:ASN:H	1.59	0.41
1:B:48:ASN:HD21	1:B:158:ASN:N	2.14	0.41
1:K:62:VAL:HG22	1:K:63:LYS:N	2.35	0.41
1:E:92:GLU:OE1	1:E:96:ARG:NH1	2.53	0.41
1:F:210:LEU:C	1:F:212:ASP:N	2.73	0.41
1:H:50:ILE:HD13	1:H:155:LEU:HA	2.02	0.41
1:J:43:VAL:HG23	1:J:165:ALA:O	2.21	0.41
1:A:48:ASN:ND2	1:A:157:THR:HA	2.34	0.41
1:I:135:THR:HG22	1:I:136:LYS:HG3	2.02	0.41
1:D:100:LEU:CB	1:D:106:VAL:CG2	2.99	0.41
1:D:100:LEU:O	1:D:106:VAL:N	2.54	0.41
1:G:30:GLU:HA	1:G:257:ALA:O	2.20	0.41
1:F:31:LEU:HD22	1:F:179:GLN:CD	2.41	0.41
1:C:201:ASP:O	1:C:202:ASN:HB2	2.20	0.41
1:L:183:ALA:O	1:L:187:LEU:HG	2.21	0.41
1:C:86:ASN:O	1:C:89:SER:HB3	2.21	0.41
1:G:73:PRO:O	1:G:74:ALA:C	2.59	0.41
1:J:71:ILE:O	1:J:73:PRO:HD3	2.21	0.41
1:J:65:GLY:O	1:J:138:LEU:HD22	2.20	0.41
1:A:206:VAL:CG1	1:A:207:SER:N	2.82	0.41
1:L:80:TYR:HA	1:L:128:ALA:HB1	2.03	0.41
1:L:130:ILE:CG2	1:L:134:TYR:CE1	3.04	0.41
1:A:140:PRO:O	1:A:141:ILE:HD12	2.20	0.41
1:A:83:ALA:O	1:A:86:ASN:N	2.54	0.41
1:J:51:ILE:HD11	1:J:164:MET:HE3	2.03	0.41
1:D:184:LEU:HD13	1:D:188:ARG:HG3	2.03	0.41
1:M:47:VAL:HG22	1:M:76:TYR:OH	2.20	0.41
1:G:62:VAL:HG23	1:G:66:GLN:NE2	2.34	0.41
1:M:145:ILE:HD12	1:M:145:ILE:N	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:K:130:ILE:HD12	1:L:74:ALA:HB1	2.03	0.41
1:G:134:TYR:OH	1:H:74:ALA:HB3	2.20	0.41
1:F:109:GLN:HE21	1:F:113:ASP:CG	2.24	0.41
1:I:46:GLN:OE1	1:I:134:TYR:CE2	2.73	0.41
1:B:52:LEU:HD22	1:B:72:ASP:HA	2.02	0.41
1:M:69:TYR:HB2	1:M:137:VAL:HB	2.03	0.41
1:G:170:LEU:O	1:G:171:ASP:O	2.39	0.41
1:H:48:ASN:HD22	1:H:157:THR:HA	1.84	0.41
1:E:62:VAL:CG1	1:E:145:ILE:HG13	2.51	0.41
1:E:62:VAL:CG2	1:E:66:GLN:OE1	2.68	0.41
1:F:48:ASN:ND2	1:F:157:THR:HG23	2.35	0.41
1:J:48:ASN:HD21	1:J:157:THR:HG23	1.85	0.41
1:I:206:VAL:CG1	1:I:207:SER:N	2.83	0.41
1:A:206:VAL:HG22	1:A:259:LEU:HD21	2.01	0.41
1:C:206:VAL:CG1	1:C:207:SER:N	2.83	0.41
1:J:46:GLN:OE1	1:J:134:TYR:HE2	2.02	0.41
1:L:199:ALA:HB2	1:L:205:LYS:N	2.36	0.41
1:M:41:ALA:HB1	1:M:140:PRO:CG	2.51	0.41
1:L:141:ILE:CG2	1:L:142:SER:N	2.83	0.41
1:I:193:SER:C	1:I:195:GLN:H	2.23	0.41
1:M:50:ILE:HD13	1:M:155:LEU:HA	2.03	0.41
1:J:87:LEU:CD2	1:J:125:VAL:HG21	2.51	0.41
1:J:87:LEU:HD23	1:J:125:VAL:HG21	2.03	0.41
1:J:189:ARG:O	1:J:192:ALA:N	2.54	0.41
1:L:228:SER:HB3	3:M:361:GOL:H11	2.03	0.41
1:H:170:LEU:O	1:H:171:ASP:O	2.38	0.41
1:D:46:GLN:CD	1:D:134:TYR:CE2	2.94	0.41
1:I:40:ILE:HD12	1:I:168:GLN:HG2	2.02	0.41
1:I:193:SER:O	1:I:195:GLN:N	2.53	0.41
1:C:193:SER:C	1:C:195:GLN:H	2.25	0.41
1:H:52:LEU:HA	1:H:52:LEU:HD12	1.81	0.41
1:G:107:SER:N	1:G:110:GLN:NE2	2.58	0.40
1:L:227:VAL:HG12	1:M:147:ARG:HG3	2.03	0.40
1:D:206:VAL:CG1	1:D:207:SER:N	2.83	0.40
1:D:245:PRO:C	1:D:247:ASN:N	2.68	0.40
1:I:40:ILE:HG22	1:I:41:ALA:N	2.36	0.40
1:E:199:ALA:HB2	1:E:205:LYS:N	2.36	0.40
1:J:141:ILE:HG23	1:J:142:SER:N	2.36	0.40
1:B:86:ASN:O	1:B:89:SER:HB3	2.22	0.40
1:J:216:TYR:HA	1:J:217:PRO:HD2	1.87	0.40
1:H:32:PRO:HB3	1:H:256:HIS:CE1	2.56	0.40
1:G:48:ASN:HD22	1:G:157:THR:HA	1.86	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:52:LEU:HA	1:G:52:LEU:HD12	1.84	0.40
1:K:199:ALA:HB2	1:K:205:LYS:N	2.36	0.40
1:I:174:TYR:CD2	1:I:239:ARG:HD3	2.57	0.40
1:M:193:SER:O	1:M:195:GLN:N	2.54	0.40
1:G:43:VAL:HG23	1:G:165:ALA:O	2.21	0.40
1:M:171:ASP:HB3	1:M:172:PRO:HD3	1.92	0.40
1:B:130:ILE:CG2	1:B:134:TYR:HE1	2.35	0.40
1:D:193:SER:O	1:D:195:GLN:N	2.54	0.40
1:B:201:ASP:O	1:B:202:ASN:HB2	2.21	0.40
1:F:171:ASP:O	1:F:173:ILE:N	2.54	0.40
1:A:145:ILE:H	1:A:145:ILE:CD1	2.26	0.40
1:K:147:ARG:N	2:K:361:3GR:O3	2.53	0.40
1:H:65:GLY:O	1:H:138:LEU:HD22	2.21	0.40
1:L:101:VAL:HG11	1:L:108:LYS:CG	2.47	0.40
1:L:109:GLN:HB3	1:M:96:ARG:CD	2.52	0.40
1:A:64:ALA:HB2	1:A:141:ILE:C	2.41	0.40
1:B:47:VAL:HG22	1:B:76:TYR:OH	2.22	0.40
1:G:100:LEU:HA	1:G:100:LEU:HD12	1.85	0.40
1:F:48:ASN:ND2	1:F:158:ASN:N	2.55	0.40
1:D:199:ALA:HB2	1:D:205:LYS:N	2.36	0.40
1:J:69:TYR:HB2	1:J:137:VAL:HB	2.03	0.40
1:G:201:ASP:O	1:G:202:ASN:HB2	2.22	0.40
1:H:113:ASP:O	1:H:116:ALA:HB3	2.20	0.40
1:I:101:VAL:CG1	1:I:102:ALA:N	2.84	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:189:ARG:NH2	1:D:194:GLY:O[2_656]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	
1	A	229/360 (64%)	207 (90%)	21 (9%)	1 (0%)	43	87
1	B	229/360 (64%)	203 (89%)	24 (10%)	2 (1%)	25	73
1	C	229/360 (64%)	209 (91%)	18 (8%)	2 (1%)	25	73
1	D	229/360 (64%)	200 (87%)	24 (10%)	5 (2%)	10	45
1	E	229/360 (64%)	211 (92%)	15 (7%)	3 (1%)	18	62
1	F	229/360 (64%)	209 (91%)	17 (7%)	3 (1%)	18	62
1	G	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	14	54
1	H	229/360 (64%)	205 (90%)	19 (8%)	5 (2%)	10	45
1	I	229/360 (64%)	210 (92%)	16 (7%)	3 (1%)	18	62
1	J	229/360 (64%)	208 (91%)	17 (7%)	4 (2%)	14	54
1	K	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	14	54
1	L	229/360 (64%)	205 (90%)	20 (9%)	4 (2%)	14	54
1	M	229/360 (64%)	204 (89%)	22 (10%)	3 (1%)	18	62
All	All	2977/4680 (64%)	2681 (90%)	253 (8%)	43 (1%)	16	60

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	171	ASP
1	B	171	ASP
1	C	171	ASP
1	D	171	ASP
1	E	171	ASP
1	F	171	ASP
1	G	171	ASP
1	H	171	ASP
1	I	171	ASP
1	J	171	ASP
1	K	171	ASP
1	L	171	ASP
1	M	104	GLN
1	M	171	ASP
1	G	194	GLY
1	I	194	GLY
1	K	55	LEU
1	K	194	GLY
1	D	55	LEU
1	D	102	ALA

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Mol	Chain	Res	Type
1	F	194	GLY
1	G	55	LEU
1	J	181	SER
1	J	194	GLY
1	L	55	LEU
1	B	194	GLY
1	C	194	GLY
1	D	111	TYR
1	F	181	SER
1	H	137	VAL
1	I	55	LEU
1	J	55	LEU
1	L	104	GLN
1	L	194	GLY
1	M	194	GLY
1	E	194	GLY
1	H	55	LEU
1	H	181	SER
1	D	194	GLY
1	E	181	SER
1	G	106	VAL
1	K	104	GLN
1	H	194	GLY

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	
1	A	186/287 (65%)	176 (95%)	10 (5%)	31	74
1	B	186/287 (65%)	175 (94%)	11 (6%)	28	70
1	C	186/287 (65%)	176 (95%)	10 (5%)	31	74
1	D	186/287 (65%)	173 (93%)	13 (7%)	21	62
1	E	186/287 (65%)	170 (91%)	16 (9%)	15	50
1	F	186/287 (65%)	173 (93%)	13 (7%)	21	62
1	G	186/287 (65%)	175 (94%)	11 (6%)	28	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	186/287 (65%)	174 (94%)	12 (6%)	24	65
1	I	186/287 (65%)	176 (95%)	10 (5%)	31	74
1	J	186/287 (65%)	171 (92%)	15 (8%)	17	53
1	K	186/287 (65%)	171 (92%)	15 (8%)	17	53
1	L	186/287 (65%)	174 (94%)	12 (6%)	24	65
1	M	186/287 (65%)	177 (95%)	9 (5%)	35	79
All	All	2418/3731 (65%)	2261 (94%)	157 (6%)	24	65

All (157) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ARG
1	A	47	VAL
1	A	75	THR
1	A	132	LEU
1	A	135	THR
1	A	145	ILE
1	A	156	VAL
1	A	158	ASN
1	A	186	ARG
1	A	226	GLU
1	B	34	ARG
1	B	47	VAL
1	B	73	PRO
1	B	132	LEU
1	B	135	THR
1	B	141	ILE
1	B	145	ILE
1	B	156	VAL
1	B	158	ASN
1	B	186	ARG
1	B	226	GLU
1	C	34	ARG
1	C	75	THR
1	C	132	LEU
1	C	135	THR
1	C	145	ILE
1	C	156	VAL
1	C	158	ASN
1	C	170	LEU

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Mol	Chain	Res	Type
1	C	186	ARG
1	C	226	GLU
1	D	34	ARG
1	D	55	LEU
1	D	75	THR
1	D	104	GLN
1	D	132	LEU
1	D	135	THR
1	D	145	ILE
1	D	156	VAL
1	D	158	ASN
1	D	186	ARG
1	D	189	ARG
1	D	225	SER
1	D	226	GLU
1	E	34	ARG
1	E	47	VAL
1	E	61	ASP
1	E	73	PRO
1	E	75	THR
1	E	132	LEU
1	E	135	THR
1	E	141	ILE
1	E	145	ILE
1	E	156	VAL
1	E	158	ASN
1	E	186	ARG
1	E	189	ARG
1	E	196	LEU
1	E	225	SER
1	E	226	GLU
1	F	34	ARG
1	F	47	VAL
1	F	55	LEU
1	F	75	THR
1	F	132	LEU
1	F	135	THR
1	F	142	SER
1	F	145	ILE
1	F	156	VAL
1	F	158	ASN
1	F	186	ARG

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Mol	Chain	Res	Type
1	F	189	ARG
1	F	226	GLU
1	G	34	ARG
1	G	47	VAL
1	G	55	LEU
1	G	75	THR
1	G	100	LEU
1	G	135	THR
1	G	145	ILE
1	G	156	VAL
1	G	158	ASN
1	G	186	ARG
1	G	226	GLU
1	H	34	ARG
1	H	61	ASP
1	H	75	THR
1	H	103	ASP
1	H	132	LEU
1	H	135	THR
1	H	145	ILE
1	H	156	VAL
1	H	158	ASN
1	H	186	ARG
1	H	196	LEU
1	H	226	GLU
1	I	34	ARG
1	I	55	LEU
1	I	75	THR
1	I	104	GLN
1	I	132	LEU
1	I	135	THR
1	I	145	ILE
1	I	158	ASN
1	I	186	ARG
1	I	226	GLU
1	J	34	ARG
1	J	47	VAL
1	J	55	LEU
1	J	61	ASP
1	J	73	PRO
1	J	75	THR
1	J	132	LEU

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Mol	Chain	Res	Type
1	J	135	THR
1	J	141	ILE
1	J	145	ILE
1	J	156	VAL
1	J	158	ASN
1	J	186	ARG
1	J	225	SER
1	J	226	GLU
1	K	34	ARG
1	K	47	VAL
1	K	55	LEU
1	K	61	ASP
1	K	73	PRO
1	K	75	THR
1	K	104	GLN
1	K	135	THR
1	K	141	ILE
1	K	145	ILE
1	K	156	VAL
1	K	158	ASN
1	K	186	ARG
1	K	225	SER
1	K	226	GLU
1	L	34	ARG
1	L	47	VAL
1	L	75	THR
1	L	132	LEU
1	L	135	THR
1	L	145	ILE
1	L	152	GLU
1	L	156	VAL
1	L	158	ASN
1	L	186	ARG
1	L	225	SER
1	L	226	GLU
1	M	34	ARG
1	M	132	LEU
1	M	135	THR
1	M	145	ILE
1	M	156	VAL
1	M	158	ASN
1	M	186	ARG

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Mol	Chain	Res	Type
1	M	196	LEU
1	M	226	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	70	GLN
1	A	84	GLN
1	A	95	GLN
1	A	158	ASN
1	A	169	GLN
1	A	215	GLN
1	B	36	ASN
1	B	48	ASN
1	B	70	GLN
1	B	95	GLN
1	B	158	ASN
1	B	215	GLN
1	C	48	ASN
1	C	84	GLN
1	C	95	GLN
1	C	110	GLN
1	C	158	ASN
1	C	169	GLN
1	C	215	GLN
1	D	36	ASN
1	D	48	ASN
1	D	84	GLN
1	D	95	GLN
1	D	104	GLN
1	D	127	GLN
1	D	158	ASN
1	D	169	GLN
1	D	215	GLN
1	E	48	ASN
1	E	84	GLN
1	E	95	GLN
1	E	104	GLN
1	E	158	ASN
1	E	169	GLN
1	E	215	GLN

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Mol	Chain	Res	Type
1	F	48	ASN
1	F	84	GLN
1	F	95	GLN
1	F	104	GLN
1	F	127	GLN
1	F	158	ASN
1	G	48	ASN
1	G	84	GLN
1	G	95	GLN
1	G	110	GLN
1	G	158	ASN
1	G	162	ASN
1	G	168	GLN
1	G	169	GLN
1	G	215	GLN
1	H	36	ASN
1	H	48	ASN
1	H	84	GLN
1	H	95	GLN
1	H	109	GLN
1	H	158	ASN
1	H	169	GLN
1	H	215	GLN
1	I	36	ASN
1	I	48	ASN
1	I	84	GLN
1	I	95	GLN
1	I	109	GLN
1	I	115	ASN
1	I	158	ASN
1	I	169	GLN
1	I	215	GLN
1	J	36	ASN
1	J	48	ASN
1	J	91	GLN
1	J	95	GLN
1	J	158	ASN
1	J	215	GLN
1	K	36	ASN
1	K	48	ASN
1	K	95	GLN
1	K	104	GLN

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Mol	Chain	Res	Type
1	K	158	ASN
1	K	215	GLN
1	L	48	ASN
1	L	70	GLN
1	L	95	GLN
1	L	104	GLN
1	L	158	ASN
1	L	169	GLN
1	L	215	GLN
1	M	36	ASN
1	M	48	ASN
1	M	70	GLN
1	M	84	GLN
1	M	95	GLN
1	M	109	GLN
1	M	110	GLN
1	M	158	ASN
1	M	168	GLN
1	M	215	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

13 ligands are modelled in this entry.

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	$\# Z > 2$
3	GOL	A	361	-	5,5,5	0.19	0	5,5,5	0.49	0
3	GOL	B	361	-	5,5,5	4.61	1 (20%)	5,5,5	4.19	1 (20%)
2	3GR	C	361	-	5,5,5	2.08	1 (20%)	5,5,5	5.35	1 (20%)
2	3GR	D	361	-	5,5,5	2.08	1 (20%)	5,5,5	5.35	1 (20%)
2	3GR	E	361	-	5,5,5	2.09	1 (20%)	5,5,5	5.34	1 (20%)
2	3GR	F	361	-	5,5,5	2.08	1 (20%)	5,5,5	5.34	1 (20%)
2	3GR	G	361	-	5,5,5	2.09	1 (20%)	5,5,5	5.34	1 (20%)
2	3GR	H	361	-	5,5,5	2.08	1 (20%)	5,5,5	5.35	1 (20%)
2	3GR	I	361	-	5,5,5	2.09	1 (20%)	5,5,5	5.34	1 (20%)
3	GOL	J	361	1	5,5,5	4.61	1 (20%)	5,5,5	4.19	1 (20%)
2	3GR	K	361	-	5,5,5	2.08	1 (20%)	5,5,5	5.35	1 (20%)
2	3GR	L	361	-	5,5,5	2.08	1 (20%)	5,5,5	5.35	1 (20%)
3	GOL	M	361	1	5,5,5	4.61	1 (20%)	5,5,5	4.20	1 (20%)

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
3	GOL	A	361	-	-	0/4/4/4	0/0/0/0
3	GOL	B	361	-	-	0/4/4/4	0/0/0/0
2	3GR	C	361	-	1/1/1/2	0/3/4/4	0/0/0/0
2	3GR	D	361	-	1/1/1/2	0/3/4/4	0/0/0/0
2	3GR	E	361	-	1/1/1/2	0/3/4/4	0/0/0/0
2	3GR	F	361	-	1/1/1/2	0/3/4/4	0/0/0/0
2	3GR	G	361	-	1/1/1/2	0/3/4/4	0/0/0/0
2	3GR	H	361	-	1/1/1/2	0/3/4/4	0/0/0/0
2	3GR	I	361	-	1/1/1/2	0/3/4/4	0/0/0/0
3	GOL	J	361	1	-	0/4/4/4	0/0/0/0
2	3GR	K	361	-	1/1/1/2	0/3/4/4	0/0/0/0
2	3GR	L	361	-	1/1/1/2	0/3/4/4	0/0/0/0
3	GOL	M	361	1	-	0/4/4/4	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	361	GOL	O3-C3	-10.26	0.97	1.42
3	B	361	GOL	O3-C3	-10.25	0.97	1.42
3	J	361	GOL	O3-C3	-10.25	0.97	1.42
2	G	361	3GR	O3-C3	-4.44	0.97	1.19
2	I	361	3GR	O3-C3	-4.44	0.97	1.19
2	H	361	3GR	O3-C3	-4.43	0.97	1.19
2	L	361	3GR	O3-C3	-4.43	0.97	1.19
2	E	361	3GR	O3-C3	-4.43	0.97	1.19
2	C	361	3GR	O3-C3	-4.42	0.97	1.19
2	D	361	3GR	O3-C3	-4.42	0.97	1.19
2	K	361	3GR	O3-C3	-4.42	0.97	1.19
2	F	361	3GR	O3-C3	-4.42	0.97	1.19

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	361	3GR	O3-C3-C2	11.90	155.34	125.34
2	D	361	3GR	O3-C3-C2	11.89	155.32	125.34
2	K	361	3GR	O3-C3-C2	11.90	155.32	125.34
2	H	361	3GR	O3-C3-C2	11.89	155.32	125.34
2	L	361	3GR	O3-C3-C2	11.89	155.31	125.34
2	G	361	3GR	O3-C3-C2	11.88	155.29	125.34
2	E	361	3GR	O3-C3-C2	11.88	155.29	125.34
2	F	361	3GR	O3-C3-C2	11.88	155.28	125.34
2	I	361	3GR	O3-C3-C2	11.88	155.28	125.34
3	M	361	GOL	O3-C3-C2	9.36	155.36	109.71
3	J	361	GOL	O3-C3-C2	9.35	155.34	109.71
3	B	361	GOL	O3-C3-C2	9.35	155.32	109.71

All (9) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	E	361	3GR	C2
2	I	361	3GR	C2
2	C	361	3GR	C2
2	G	361	3GR	C2
2	H	361	3GR	C2
2	L	361	3GR	C2
2	D	361	3GR	C2
2	F	361	3GR	C2
2	K	361	3GR	C2

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	A	231/360 (64%)	0.15	1 (0%)	90	41	56, 93, 132, 143	2 (0%)
1	B	231/360 (64%)	-0.04	0	100	100	37, 80, 110, 123	2 (0%)
1	C	231/360 (64%)	-0.06	0	100	100	39, 77, 111, 116	2 (0%)
1	D	231/360 (64%)	-0.03	0	100	100	30, 82, 109, 123	2 (0%)
1	E	231/360 (64%)	-0.07	0	100	100	22, 61, 95, 111	2 (0%)
1	F	231/360 (64%)	-0.05	0	100	100	53, 80, 106, 111	2 (0%)
1	G	231/360 (64%)	0.01	0	100	100	51, 86, 118, 126	2 (0%)
1	H	231/360 (64%)	-0.02	0	100	100	28, 64, 98, 109	2 (0%)
1	I	231/360 (64%)	0.01	0	100	100	24, 62, 96, 109	2 (0%)
1	J	231/360 (64%)	-0.05	0	100	100	15, 48, 84, 100	2 (0%)
1	K	231/360 (64%)	-0.07	0	100	100	20, 59, 92, 107	2 (0%)
1	L	231/360 (64%)	-0.07	0	100	100	25, 63, 102, 115	2 (0%)
1	M	231/360 (64%)	0.02	0	100	100	40, 93, 117, 130	2 (0%)
All	All	3003/4680 (64%)	-0.02	1 (0%)	100	100	15, 75, 114, 143	26 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	GLY	2.2

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	3GR	E	361	6/6	0.36	8.17	93,95,98,102	0
3	GOL	J	361	6/6	0.40	6.63	92,94,94,96	0
2	3GR	K	361	6/6	0.35	4.35	79,80,83,84	0
2	3GR	L	361	6/6	0.33	2.69	81,82,83,86	0
2	3GR	H	361	6/6	0.32	2.28	87,88,89,90	0
2	3GR	D	361	6/6	0.32	1.85	93,93,94,95	0
2	3GR	C	361	6/6	0.28	1.85	100,100,101,102	0
3	GOL	A	361	6/6	0.30	1.53	97,98,99,102	0
3	GOL	M	361	6/6	0.26	1.43	99,100,101,101	0
2	3GR	I	361	6/6	0.28	0.98	87,87,88,88	0
3	GOL	B	361	6/6	0.29	0.82	95,96,96,96	0
2	3GR	F	361	6/6	0.25	0.31	99,100,101,103	0
2	3GR	G	361	6/6	0.20	-0.54	103,104,105,106	0

6.5 Other polymers ⓘ

There are no such residues in this entry.