



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:58 AM GMT

PDB ID : 3QD6  
Title : Crystal structure of the CD40 and CD154 (CD40L) complex  
Authors : Lee, J.-O.; Kim, Y.J.; Song, D.H.; Kim, H.M.; Park, B.S.  
Deposited on : 2011-01-18  
Resolution : 3.50 Å(reported)

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

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

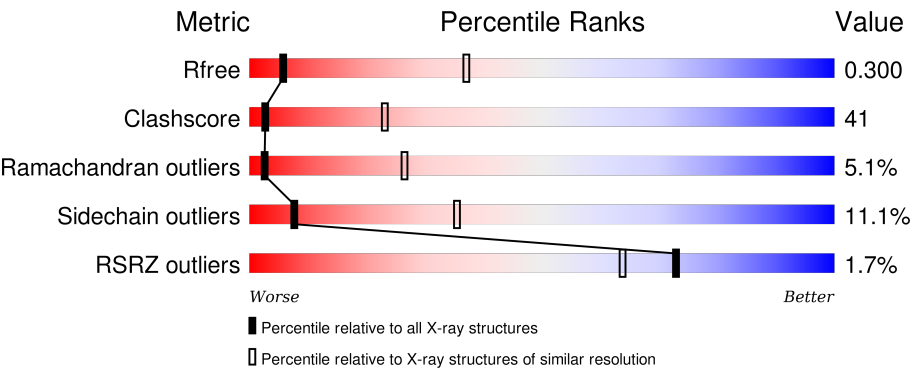
MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	91344	1051 (3.60-3.40)
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	149	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>44%36%9%•9%</div></div>
1	B	149	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>38%45%7%•9%</div></div>
1	C	149	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>40%43%7%•9%</div></div>
1	D	149	<div><div></div><div><div></div><div></div><div></div><div></div></div><div>40%42%9%•9%</div></div>
1	E	149	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>44%39%7%•9%</div></div>

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Mol	Chain	Length	Quality of chain
1	F	149	
2	R	177	
2	S	177	
2	T	177	
2	U	177	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	1411	-	-	-	X

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9896 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called CD40 ligand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	B	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	C	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	D	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	E	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			
1	F	135	Total	C	N	O	S	0	0	0
			1033	658	178	193	4			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	113	ALA	-	EXPRESSION TAG	UNP P29965
A	114	ASP	-	EXPRESSION TAG	UNP P29965
A	115	PRO	-	EXPRESSION TAG	UNP P29965
B	113	ALA	-	EXPRESSION TAG	UNP P29965
B	114	ASP	-	EXPRESSION TAG	UNP P29965
B	115	PRO	-	EXPRESSION TAG	UNP P29965
C	113	ALA	-	EXPRESSION TAG	UNP P29965
C	114	ASP	-	EXPRESSION TAG	UNP P29965
C	115	PRO	-	EXPRESSION TAG	UNP P29965
D	113	ALA	-	EXPRESSION TAG	UNP P29965
D	114	ASP	-	EXPRESSION TAG	UNP P29965
D	115	PRO	-	EXPRESSION TAG	UNP P29965
E	113	ALA	-	EXPRESSION TAG	UNP P29965
E	114	ASP	-	EXPRESSION TAG	UNP P29965
E	115	PRO	-	EXPRESSION TAG	UNP P29965
F	113	ALA	-	EXPRESSION TAG	UNP P29965
F	114	ASP	-	EXPRESSION TAG	UNP P29965

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Chain	Residue	Modelled	Actual	Comment	Reference
F	115	PRO	-	EXPRESSION TAG	UNP P29965

- Molecule 2 is a protein called Tumor necrosis factor receptor superfamily member 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	R	114	Total	C	N	O	S	0	0	0
			886	532	154	184	16			
2	S	119	Total	C	N	O	S	0	0	0
			921	554	159	192	16			
2	T	114	Total	C	N	O	S	0	0	0
			886	532	154	184	16			
2	U	119	Total	C	N	O	S	0	0	0
			921	554	159	192	16			

There are 28 discrepancies between the modelled and reference sequences:

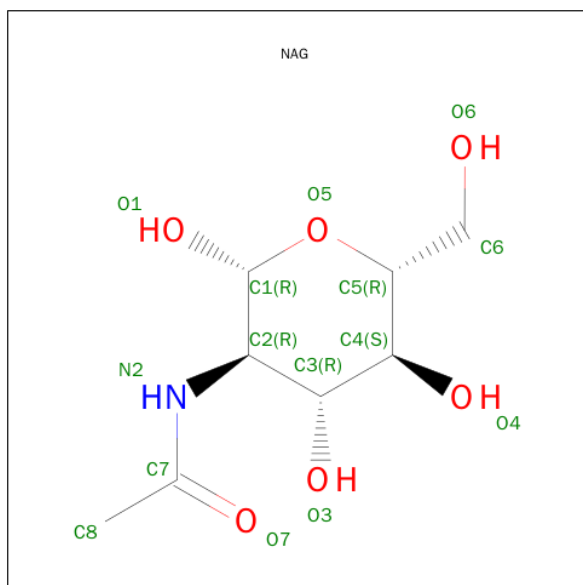
Chain	Residue	Modelled	Actual	Comment	Reference
R	191	SER	-	EXPRESSION TAG	UNP P25942
R	192	GLY	-	EXPRESSION TAG	UNP P25942
R	193	ARG	-	EXPRESSION TAG	UNP P25942
R	194	LEU	-	EXPRESSION TAG	UNP P25942
R	195	VAL	-	EXPRESSION TAG	UNP P25942
R	196	PRO	-	EXPRESSION TAG	UNP P25942
R	197	ARG	-	EXPRESSION TAG	UNP P25942
S	191	SER	-	EXPRESSION TAG	UNP P25942
S	192	GLY	-	EXPRESSION TAG	UNP P25942
S	193	ARG	-	EXPRESSION TAG	UNP P25942
S	194	LEU	-	EXPRESSION TAG	UNP P25942
S	195	VAL	-	EXPRESSION TAG	UNP P25942
S	196	PRO	-	EXPRESSION TAG	UNP P25942
S	197	ARG	-	EXPRESSION TAG	UNP P25942
T	191	SER	-	EXPRESSION TAG	UNP P25942
T	192	GLY	-	EXPRESSION TAG	UNP P25942
T	193	ARG	-	EXPRESSION TAG	UNP P25942
T	194	LEU	-	EXPRESSION TAG	UNP P25942
T	195	VAL	-	EXPRESSION TAG	UNP P25942
T	196	PRO	-	EXPRESSION TAG	UNP P25942
T	197	ARG	-	EXPRESSION TAG	UNP P25942
U	191	SER	-	EXPRESSION TAG	UNP P25942
U	192	GLY	-	EXPRESSION TAG	UNP P25942
U	193	ARG	-	EXPRESSION TAG	UNP P25942
U	194	LEU	-	EXPRESSION TAG	UNP P25942

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Chain	Residue	Modelled	Actual	Comment	Reference
U	195	VAL	-	EXPRESSION TAG	UNP P25942
U	196	PRO	-	EXPRESSION TAG	UNP P25942
U	197	ARG	-	EXPRESSION TAG	UNP P25942

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

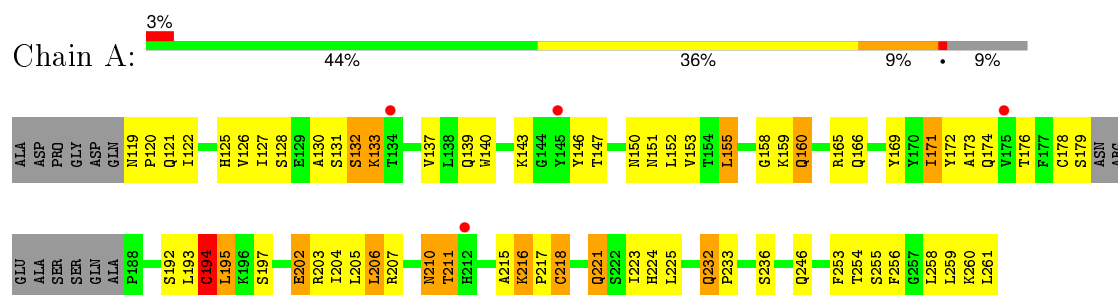


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	E	1	Total	C	N	O	0	0
			14	8	1	5		
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

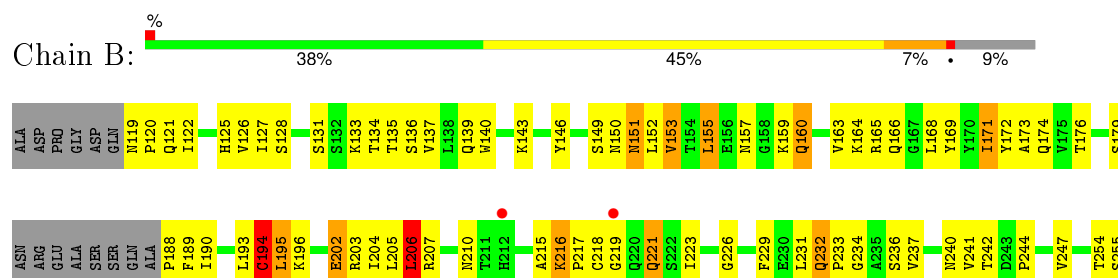
### 3 Residue-property plots [i](#)

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

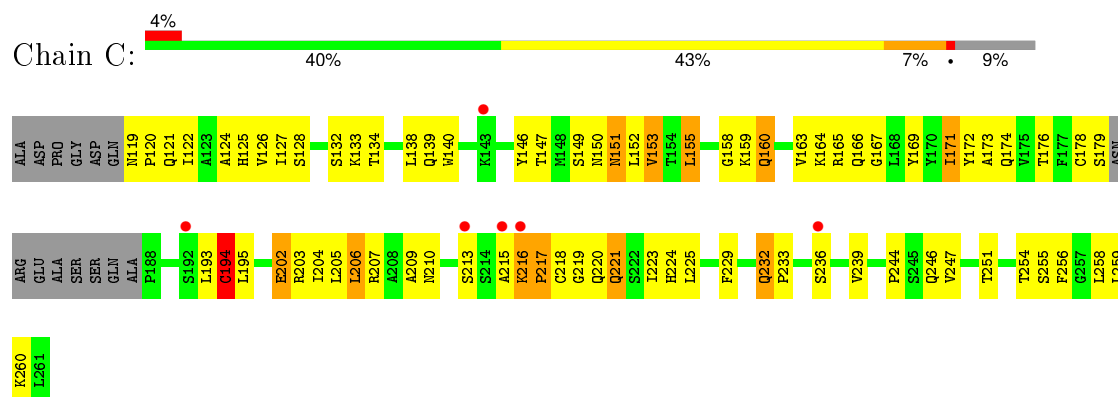
- Molecule 1: CD40 ligand



- Molecule 1: CD40 ligand



- Molecule 1: CD40 ligand



- Molecule 1: CD40 ligand

Chain D: 

ALA ASP GLN H119 H120 Q121 I122 H125 V126 I127 K133 T134 T135 S136 V137 L138 W140 K143 G144 Y145 Y146 S149 N150 N151 L152 V153 L155 E156 N157 G158 K159 Q160 L161 T162 V163 K164 R165 G167 L168 Y169 Y170 Y171 Y172 A173 Q174 S179 ASN ARG GLU

ALA SER GLN P188 F189 I190 L193 C194 L195 K196 S197 F201 R202 R203 L204 L205 L206 R207 H212 A215 R216 P217 Q218 Q219 Q220 Q221 S222 L223 L224 L225 Q226 F229 K159 Q232 Q233 S236 V241 P244 S245 Q246 G250 S255 L258 L259 R260 L261

- Molecule 1: CD40 ligand

Chain E: 

ALA ASP GLN H119 H120 Q121 I122 H125 V126 I127 S128 S131 S132 S133 T134 T135 S136 V137 L138 Q139 W140 K143 Y146 Q218 Q219 Q220 Q221 H148 L149 N150 H151 L152 V153 T154 L155 E156 N157 G158 K159 Q160 K164 R165 Q166 Y169 Y170 Y171 Y172 S179 ASN ARG GLU SER

SER GLN P188 F189 L193 L194 L195 K196 S197 E202 R203 L204 L205 A208 A209 R210 T211 H212 A215 R216 P217 Q220 Q221 F229 E230 L231 Q232 P233 S236 V237 F238 V239 P244 T254 S255 F256 G257 L258 L259 R260 L261

- Molecule 1: CD40 ligand


Chain F: 

ALA ASP GLN H119 H120 Q121 I122 H125 V126 I127 S128 S131 S132 S133 T134 Q139 W140 Y145 Y146 T147 H148 S149 N150 H151 L152 V153 T154 L155 E156 N157 G158 K159 Q160 T162 V163 K164 R165 Q166 G167 L168 Y169 Y170 Y171 Y172 A173 Q174 C178 S179 ASN

ARG GLU ALA P188 S192 L193 L194 L195 K196 S197 P198 E202 R203 L204 L205 L206 R207 N210 T211 H212 A215 R216 P217 Q220 Q221 C216 T217 P218 C219 C220 C221 S222 L223 L224 L225 V228 L231 Q232 P233 S236 V237 P244 V247 T254 S255 F256 G257 L258 L259 R260 K260


L261

- Molecule 2: Tumor necrosis factor receptor superfamily member 5

Chain R: 

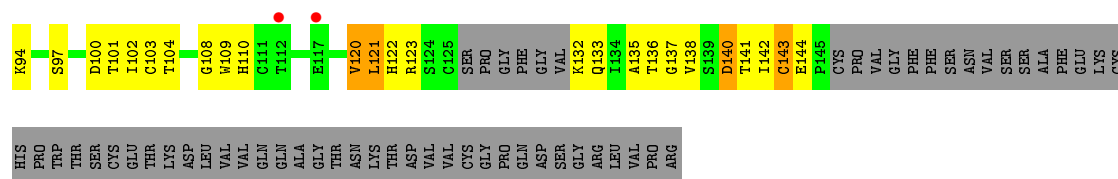
GLU PRO THR C26 R27 E28 K29 Q30 Q31 I102 L108 G108 W109 C111 S112 S113 C116 P119 V120 V121 H122 C125 S125 D125 S126 S127 S128 S129 S130 S131 S132 S133 S134 S135 S136 S137 S138 S139 S140 S141 S142 S143 S144 S145 S146 S147 S148 S149 S150 S151 S152 S153 S154 S155 S156 S157 S158 S159 S160 S161 S162 S163 S164 S165 S166 S167 S168 S169 S170 S171 S172 S173 S174 S175 S176 S177 S178 S179 S180 S181 S182 S183 S184 S185 S186 S187 S188 S189 S190 S191 S192 S193 S194 S195 S196 S197 S198 S199 S200 S201 S202 S203 S204 S205 S206 S207 S208 S209 S210 S211 S212 S213 S214 S215 S216 S217 S218 S219 S220 S221 S222 S223 S224 S225 S226 S227 S228 S229 S230 S231 S232 S233 S234 S235 S236 S237 S238 S239 S240 S241 S242 S243 S244 S245 S246 S247 S248 S249 S250 S251 S252 S253 S254 S255 S256 S257 S258 S259 S260 S261 S262 S263 S264 S265 S266 S267 S268 S269 S270 S271 S272 S273 S274 S275 S276 S277 S278 S279 S280 S281 S282 S283 S284 S285 S286 S287 S288 S289 S290 S291 S292 S293 S294 S295 S296 S297 S298 S299 S300 S301 S302 S303 S304 S305 S306 S307 S308 S309 S310 S311 S312 S313 S314 S315 S316 S317 S318 S319 S320 S321 S322 S323 S324 S325 S326 S327 S328 S329 S330 S331 S332 S333 S334 S335 S336 S337 S338 S339 S340 S341 S342 S343 S344 S345 S346 S347 S348 S349 S350 S351 S352 S353 S354 S355 S356 S357 S358 S359 S360 S361 S362 S363 S364 S365 S366 S367 S368 S369 S370 S371 S372 S373 S374 S375 S376 S377 S378 S379 S380 S381 S382 S383 S384 S385 S386 S387 S388 S389 S390 S391 S392 S393 S394 S395 S396 S397 S398 S399 S400 S401 S402 S403 S404 S405 S406 S407 S408 S409 S410 S411 S412 S413 S414 S415 S416 S417 S418 S419 S420 S421 S422 S423 S424 S425 S426 S427 S428 S429 S430 S431 S432 S433 S434 S435 S436 S437 S438 S439 S440 S441 S442 S443 S444 S445 S446 S447 S448 S449 S450 S451 S452 S453 S454 S455 S456 S457 S458 S459 S460 S461 S462 S463 S464 S465 S466 S467 S468 S469 S470 S471 S472 S473 S474 S475 S476 S477 S478 S479 S480 S481 S482 S483 S484 S485 S486 S487 S488 S489 S490 S491 S492 S493 S494 S495 S496 S497 S498 S499 S500 S501 S502 S503 S504 S505 S506 S507 S508 S509 S510 S511 S512 S513 S514 S515 S516 S517 S518 S519 S520 S521 S522 S523 S524 S525 S526 S527 S528 S529 S530 S531 S532 S533 S534 S535 S536 S537 S538 S539 S540 S541 S542 S543 S544 S545 S546 S547 S548 S549 S550 S551 S552 S553 S554 S555 S556 S557 S558 S559 S560 S561 S562 S563 S564 S565 S566 S567 S568 S569 S570 S571 S572 S573 S574 S575 S576 S577 S578 S579 S580 S581 S582 S583 S584 S585 S586 S587 S588 S589 S590 S591 S592 S593 S594 S595 S596 S597 S598 S599 S600 S601 S602 S603 S604 S605 S606 S607 S608 S609 S610 S611 S612 S613 S614 S615 S616 S617 S618 S619 S620 S621 S622 S623 S624 S625 S626 S627 S628 S629 S630 S631 S632 S633 S634 S635 S636 S637 S638 S639 S640 S641 S642 S643 S644 S645 S646 S647 S648 S649 S650 S651 S652 S653 S654 S655 S656 S657 S658 S659 S660 S661 S662 S663 S664 S665 S666 S667 S668 S669 S670 S671 S672 S673 S674 S675 S676 S677 S678 S679 S680 S681 S682 S683 S684 S685 S686 S687 S688 S689 S690 S691 S692 S693 S694 S695 S696 S697 S698 S699 S700 S701 S702 S703 S704 S705 S706 S707 S708 S709 S710 S711 S712 S713 S714 S715 S716 S717 S718 S719 S720 S721 S722 S723 S724 S725 S726 S727 S728 S729 S730 S731 S732 S733 S734 S735 S736 S737 S738 S739 S740 S741 S742 S743 S744 S745 S746 S747 S748 S749 S750 S751 S752 S753 S754 S755 S756 S757 S758 S759 S760 S761 S762 S763 S764 S765 S766 S767 S768 S769 S770 S771 S772 S773 S774 S775 S776 S777 S778 S779 S780 S781 S782 S783 S784 S785 S786 S787 S788 S789 S790 S791 S792 S793 S794 S795 S796 S797 S798 S799 S800 S801 S802 S803 S804 S805 S806 S807 S808 S809 S810 S811 S812 S813 S814 S815 S816 S817 S818 S819 S820 S821 S822 S823 S824 S825 S826 S827 S828 S829 S830 S831 S832 S833 S834 S835 S836 S837 S838 S839 S840 S841 S842 S843 S844 S845 S846 S847 S848 S849 S850 S851 S852 S853 S854 S855 S856 S857 S858 S859 S860 S861 S862 S863 S864 S865 S866 S867 S868 S869 S870 S871 S872 S873 S874 S875 S876 S877 S878 S879 S880 S881 S882 S883 S884 S885 S886 S887 S888 S889 S890 S891 S892 S893 S894 S895 S896 S897 S898 S899 S900 S901 S902 S903 S904 S905 S906 S907 S908 S909 S910 S911 S912 S913 S914 S915 S916 S917 S918 S919 S920 S921 S922 S923 S924 S925 S926 S927 S928 S929 S930 S931 S932 S933 S934 S935 S936 S937 S938 S939 S940 S941 S942 S943 S944 S945 S946 S947 S948 S949 S950 S951 S952 S953 S954 S955 S956 S957 S958 S959 S960 S961 S962 S963 S964 S965 S966 S967 S968 S969 S970 S971 S972 S973 S974 S975 S976 S977 S978 S979 S980 S981 S982 S983 S984 S985 S986 S987 S988 S989 S990 S991 S992 S993 S994 S995 S996 S997 S998 S999

- Molecule 2: Tumor necrosis factor receptor superfamily member 5

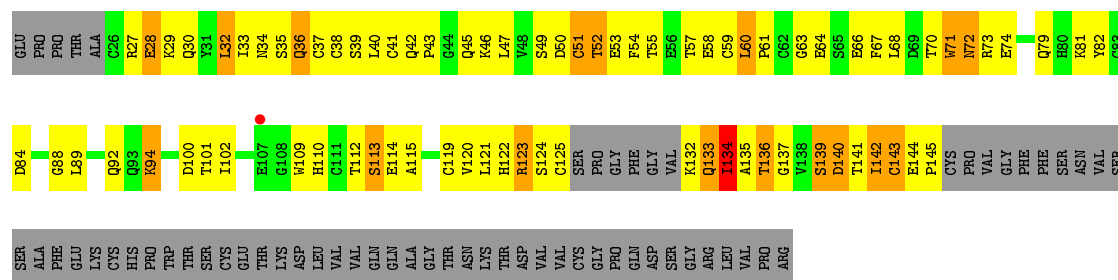
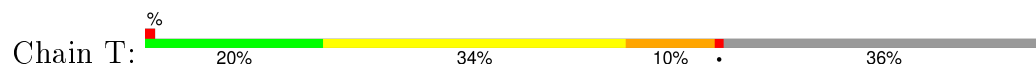
Chain S: 

E21 F22 F23 F24 A25 C26 Q30 Y31 L32 L33 L34 L35 L36 L37 L38 L39 L40 L41 L42 L43 L44 L45 L46 L47 L48 C51 T52 E53 E54 T55 E56 T57 L60 P61 B64 S65 B66 F67 L68 L69 T70 W71 W72 R73 R74 Q79 R80 R81 G88 L89 R90 R91 Q92 Q93

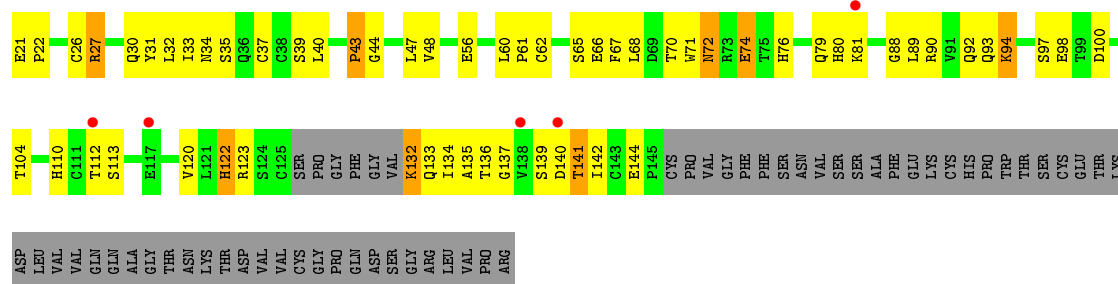




- Molecule 2: Tumor necrosis factor receptor superfamily member 5



- Molecule 2: Tumor necrosis factor receptor superfamily member 5



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	133.21Å 133.21Å 211.15Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	114.96 – 3.50 115.36 – 3.50	Depositor EDS
% Data completeness (in resolution range)	92.9 (114.96-3.50) 92.7 (115.36-3.50)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	0.10	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.07 (at 3.49Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, $R_{free}$	0.245 , 0.298 0.246 , 0.300	Depositor DCC
$R_{free}$ test set	1209 reflections (4.86%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.1	Xtriage
Anisotropy	0.002	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 58.8	EDS
Estimated twinning fraction	0.064 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.45$ , $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	1 of 24870 reflections (0.004%)	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	9896	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	68.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.58	1/1055 (0.1%)	0.73	0/1427
1	B	0.56	1/1055 (0.1%)	0.73	2/1427 (0.1%)
1	C	0.51	1/1055 (0.1%)	0.70	0/1427
1	D	0.55	1/1055 (0.1%)	0.71	1/1427 (0.1%)
1	E	0.49	0/1055	0.69	0/1427
1	F	0.51	0/1055	0.69	0/1427
2	R	0.42	0/901	0.61	0/1218
2	S	0.43	0/938	0.66	0/1271
2	T	0.43	0/901	0.67	0/1218
2	U	0.42	0/938	0.65	0/1271
All	All	0.50	4/10008 (0.0%)	0.69	3/13540 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	194	CYS	CB-SG	7.17	1.94	1.82
1	D	194	CYS	CB-SG	6.53	1.93	1.82
1	B	194	CYS	CB-SG	5.67	1.91	1.82
1	C	194	CYS	CB-SG	5.36	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	194	CYS	CA-CB-SG	6.36	125.45	114.00
1	D	194	CYS	CA-CB-SG	5.36	123.64	114.00
1	B	206	LEU	CA-CB-CG	5.16	127.18	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1033	0	1030	83	0
1	B	1033	0	1031	96	0
1	C	1033	0	1030	86	0
1	D	1033	0	1030	81	0
1	E	1033	0	1030	80	0
1	F	1033	0	1030	86	0
2	R	886	0	803	80	0
2	S	921	0	835	67	0
2	T	886	0	803	95	0
2	U	921	0	835	60	0
3	A	14	0	13	0	0
3	B	14	0	13	4	0
3	C	14	0	13	1	0
3	D	14	0	13	1	0
3	E	14	0	13	1	0
3	F	14	0	13	3	0
All	All	9896	0	9535	788	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 41.

All (788) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:136:THR:HG22	2:T:139:SER:HB2	1.25	1.16
1:D:259:LEU:HD22	1:E:261:LEU:HD21	1.27	1.15
1:B:171:ILE:HD11	1:B:193:LEU:HD11	1.32	1.11
1:E:166:GLN:HB2	1:E:233:PRO:HD3	1.32	1.11
1:E:216:LYS:HB2	1:E:217:PRO:HD3	1.28	1.08
1:A:216:LYS:HB2	1:A:217:PRO:HD3	1.27	1.08
1:F:216:LYS:HB2	1:F:217:PRO:HD3	1.35	1.08
1:C:171:ILE:HD11	1:C:193:LEU:HD11	1.35	1.07
1:A:261:LEU:HD21	1:C:259:LEU:HD22	1.34	1.06
2:T:49:SER:HB2	2:T:58:GLU:HB2	1.38	1.05
1:E:119:ASN:HD22	1:E:121:GLN:HG2	1.19	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:194:CYS:SG	3:F:1411:NAG:O6	2.12	1.04
1:E:119:ASN:ND2	1:E:121:GLN:HG2	1.71	1.04
1:F:166:GLN:HB2	1:F:233:PRO:HD3	1.36	1.04
2:S:39:SER:O	2:S:57:THR:HG21	1.59	1.03
1:D:216:LYS:HB2	1:D:217:PRO:HD3	1.41	1.02
1:C:216:LYS:HB2	1:C:217:PRO:HD3	1.39	1.02
1:A:166:GLN:HB2	1:A:233:PRO:HD3	1.39	1.01
1:A:171:ILE:HD11	1:A:193:LEU:HD11	1.44	1.00
1:C:119:ASN:HD22	1:C:121:GLN:HG2	1.29	0.98
1:C:204:ILE:HD13	1:C:207:ARG:HD2	1.46	0.97
1:D:171:ILE:HD11	1:D:193:LEU:HD11	1.47	0.96
1:B:194:CYS:SG	1:B:203:ARG:O	2.24	0.96
2:T:132:LYS:HB3	2:T:142:ILE:HD11	1.48	0.95
1:F:171:ILE:HD11	1:F:193:LEU:HD11	1.49	0.95
2:R:48:VAL:HG21	2:R:60:LEU:HD13	1.49	0.95
1:B:119:ASN:HD21	1:B:121:GLN:HG2	1.29	0.94
1:E:194:CYS:SG	3:E:1411:NAG:O6	2.25	0.94
1:E:259:LEU:HD22	1:F:261:LEU:HD21	1.49	0.94
2:T:136:THR:HG22	2:T:139:SER:CB	1.98	0.93
1:D:171:ILE:HD11	1:D:193:LEU:HD21	1.51	0.93
1:E:216:LYS:HB2	1:E:217:PRO:CD	1.98	0.93
1:A:216:LYS:HB2	1:A:217:PRO:CD	1.99	0.92
2:T:136:THR:N	2:T:139:SER:HB3	1.86	0.91
2:S:110:HIS:CE1	2:S:120:VAL:HB	2.05	0.91
1:D:166:GLN:HB2	1:D:233:PRO:HD3	1.51	0.91
1:A:204:ILE:HD13	1:A:207:ARG:HD2	1.53	0.90
2:S:21:GLU:HG3	2:S:22:PRO:HD2	1.52	0.89
2:R:132:LYS:HB3	2:R:142:ILE:HG23	1.55	0.89
2:S:44:GLY:HA2	2:S:97:SER:O	1.72	0.88
1:C:166:GLN:HB2	1:C:233:PRO:HD3	1.53	0.88
1:A:179:SER:HB3	1:A:246:GLN:NE2	1.88	0.88
2:T:39:SER:O	2:T:57:THR:HG21	1.74	0.88
2:R:46:LYS:O	2:R:59:CYS:HB3	1.74	0.87
1:B:204:ILE:HD13	1:B:207:ARG:HD2	1.57	0.87
1:B:133:LYS:HG3	1:B:134:THR:H	1.39	0.86
1:B:216:LYS:HB2	1:B:217:PRO:HD3	1.58	0.86
2:R:30:GLN:HA	2:R:39:SER:HA	1.57	0.86
2:R:51:CYS:HB2	2:R:56:GLU:HA	1.58	0.86
1:F:119:ASN:HD21	1:F:121:GLN:HG2	1.39	0.85
1:B:166:GLN:HB2	1:B:233:PRO:HD3	1.58	0.85
2:T:135:ALA:HB2	2:T:141:THR:N	1.91	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:204:ILE:HD13	1:D:207:ARG:HD2	1.60	0.84
1:E:171:ILE:HD11	1:E:193:LEU:HD11	1.58	0.83
1:D:216:LYS:CB	1:D:217:PRO:HD3	2.08	0.83
1:B:234:GLY:O	2:T:94:LYS:HE2	1.77	0.83
1:F:194:CYS:SG	1:F:203:ARG:O	2.37	0.83
1:B:119:ASN:HD21	1:B:121:GLN:CG	1.91	0.83
2:T:136:THR:H	2:T:139:SER:HB3	1.44	0.82
2:U:135:ALA:HB2	2:U:141:THR:HG23	1.61	0.82
1:F:166:GLN:HB2	1:F:233:PRO:CD	2.10	0.81
2:U:133:GLN:HB3	2:U:142:ILE:CG2	2.10	0.81
1:E:219:GLY:HA2	1:F:211:THR:HG21	1.63	0.80
1:B:136:SER:HA	1:B:244:PRO:HG3	1.62	0.80
1:B:171:ILE:HD11	1:B:193:LEU:CD1	2.11	0.80
2:T:135:ALA:HB2	2:T:141:THR:H	1.44	0.80
1:C:178:CYS:HB3	1:C:220:GLN:HA	1.60	0.80
1:E:194:CYS:SG	1:E:203:ARG:O	2.40	0.80
2:T:123:ARG:HB2	2:T:123:ARG:HH11	1.46	0.80
1:E:166:GLN:HB2	1:E:233:PRO:CD	2.10	0.80
1:B:216:LYS:CB	1:B:217:PRO:HD3	2.12	0.80
1:D:171:ILE:CD1	1:D:193:LEU:HD21	2.12	0.79
2:T:133:GLN:H	2:T:142:ILE:HD11	1.46	0.79
1:F:216:LYS:HB2	1:F:217:PRO:CD	2.13	0.79
1:A:194:CYS:SG	1:A:203:ARG:O	2.40	0.79
2:U:21:GLU:HG2	2:U:22:PRO:CD	2.13	0.79
1:B:210:ASN:HD21	1:B:221:GLN:HG2	1.48	0.79
2:S:68:LEU:HD13	2:S:72:ASN:OD1	1.82	0.78
1:C:119:ASN:ND2	1:C:121:GLN:HG2	1.98	0.78
1:C:194:CYS:SG	1:C:203:ARG:O	2.42	0.78
2:U:68:LEU:HD13	2:U:72:ASN:OD1	1.83	0.77
2:S:60:LEU:HD23	2:S:61:PRO:HD2	1.65	0.77
1:A:210:ASN:HB2	1:A:223:ILE:HD11	1.65	0.77
1:D:216:LYS:HB2	1:D:217:PRO:CD	2.12	0.77
1:B:133:LYS:HG3	1:B:134:THR:N	1.99	0.77
1:C:171:ILE:HD11	1:C:193:LEU:CD1	2.15	0.76
1:E:204:ILE:HD13	1:E:207:ARG:HD2	1.65	0.76
2:T:49:SER:CB	2:T:58:GLU:HB2	2.15	0.75
1:B:216:LYS:HB2	1:B:217:PRO:CD	2.16	0.75
2:U:132:LYS:HD2	2:U:133:GLN:N	2.02	0.75
2:U:62:CYS:HB3	2:U:66:GLU:HB2	1.69	0.74
1:B:166:GLN:HG2	1:B:232:GLN:HA	1.69	0.74
1:A:119:ASN:HD21	1:A:121:GLN:CG	2.00	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:1411:NAG:O3	3:B:1411:NAG:H83	1.86	0.74
2:S:21:GLU:CG	2:S:22:PRO:HD2	2.18	0.74
2:U:72:ASN:HD22	2:U:72:ASN:H	1.36	0.74
1:F:210:ASN:OD1	1:F:221:GLN:HG2	1.87	0.74
1:F:232:GLN:CD	1:F:232:GLN:H	1.91	0.73
2:T:123:ARG:HB2	2:T:123:ARG:NH1	2.01	0.73
2:T:124:SER:HA	2:T:143:CYS:HB2	1.70	0.73
1:E:171:ILE:HD11	1:E:193:LEU:HD21	1.70	0.73
1:D:136:SER:HB2	1:D:241:VAL:O	1.87	0.73
2:S:47:LEU:HD23	2:S:48:VAL:N	2.03	0.73
1:F:204:ILE:HD13	1:F:207:ARG:HD2	1.69	0.73
1:B:196:LYS:HG3	2:T:94:LYS:NZ	2.04	0.73
1:E:232:GLN:CD	1:E:232:GLN:H	1.91	0.73
1:E:216:LYS:HD2	1:E:216:LYS:H	1.53	0.73
2:S:30:GLN:NE2	2:S:37:CYS:HB3	2.04	0.73
2:T:136:THR:CG2	2:T:139:SER:HB2	2.14	0.73
1:A:259:LEU:HD22	1:B:261:LEU:HD21	1.69	0.72
1:C:194:CYS:SG	3:C:1411:NAG:O6	2.48	0.72
1:D:194:CYS:SG	1:D:203:ARG:O	2.48	0.72
2:T:135:ALA:CB	2:T:141:THR:HG23	2.19	0.72
1:A:166:GLN:HG2	1:A:232:GLN:HA	1.71	0.72
1:A:166:GLN:HB2	1:A:233:PRO:CD	2.17	0.72
1:D:171:ILE:HD11	1:D:193:LEU:CD1	2.18	0.71
1:E:219:GLY:CA	1:F:211:THR:HG21	2.19	0.71
1:D:122:ILE:HD12	1:D:122:ILE:N	2.05	0.71
1:F:122:ILE:N	1:F:122:ILE:HD12	2.04	0.71
1:F:166:GLN:CG	1:F:232:GLN:HA	2.20	0.71
2:T:132:LYS:HB3	2:T:142:ILE:CD1	2.21	0.71
2:S:60:LEU:HD23	2:S:61:PRO:CD	2.20	0.71
1:E:166:GLN:CG	1:E:232:GLN:HA	2.20	0.71
1:A:166:GLN:CB	1:A:233:PRO:HD3	2.18	0.71
1:B:160:GLN:HG3	1:B:236:SER:HB3	1.73	0.71
1:C:119:ASN:CG	1:C:120:PRO:HD2	2.12	0.70
1:D:171:ILE:HD11	1:D:193:LEU:CD2	2.21	0.70
1:B:171:ILE:CD1	1:B:193:LEU:HD11	2.18	0.70
2:T:135:ALA:HB2	2:T:141:THR:HG23	1.74	0.70
2:U:134:ILE:HG22	2:U:135:ALA:H	1.56	0.70
1:B:210:ASN:ND2	1:B:221:GLN:HG2	2.05	0.70
2:R:51:CYS:CB	2:R:56:GLU:HA	2.21	0.70
2:R:40:LEU:HD13	2:R:71:TRP:O	1.92	0.70
2:T:63:GLY:H	2:T:66:GLU:HB2	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:U:21:GLU:HG2	2:U:22:PRO:HD2	1.72	0.70
1:A:119:ASN:OD1	1:A:120:PRO:HD2	1.90	0.70
2:T:139:SER:O	2:T:140:ASP:HB2	1.91	0.70
2:S:47:LEU:C	2:S:47:LEU:HD23	2.12	0.69
1:B:171:ILE:HD11	1:B:193:LEU:HD21	1.74	0.69
2:T:51:CYS:HB2	2:T:55:THR:O	1.92	0.69
1:A:139:GLN:HE22	1:A:159:LYS:HE3	1.57	0.69
2:T:30:GLN:OE1	2:T:37:CYS:HB3	1.93	0.69
2:R:134:ILE:HG13	2:R:135:ALA:N	2.06	0.69
2:T:60:LEU:HD13	2:T:61:PRO:HD2	1.75	0.69
1:C:166:GLN:HG2	1:C:232:GLN:HA	1.75	0.68
2:S:36:GLN:OE1	2:S:53:GLU:HA	1.92	0.68
2:T:39:SER:HB2	2:T:57:THR:HG22	1.74	0.68
1:F:171:ILE:HD11	1:F:193:LEU:HD21	1.76	0.68
1:D:166:GLN:CB	1:D:233:PRO:HD3	2.24	0.68
1:D:261:LEU:HD21	1:F:259:LEU:HD22	1.75	0.68
2:T:122:HIS:CE1	2:T:135:ALA:HB1	2.29	0.68
1:B:127:ILE:HG21	2:R:79:GLN:OE1	1.94	0.68
2:S:135:ALA:H	2:S:141:THR:HG22	1.59	0.68
1:B:119:ASN:ND2	1:B:121:GLN:HG2	2.07	0.68
2:U:32:LEU:HD12	2:U:33:ILE:N	2.08	0.68
2:S:135:ALA:HB2	2:S:141:THR:HG23	1.76	0.67
1:A:261:LEU:CD2	1:C:259:LEU:HD22	2.20	0.67
1:D:166:GLN:HG2	1:D:232:GLN:HA	1.76	0.67
1:E:139:GLN:HE22	1:E:159:LYS:HE3	1.60	0.67
1:F:194:CYS:SG	3:F:1411:NAG:C6	2.83	0.67
2:T:125:CYS:N	2:T:143:CYS:SG	2.67	0.67
1:A:132:SER:O	1:A:133:LYS:HB2	1.93	0.67
1:D:166:GLN:HB2	1:D:233:PRO:CD	2.24	0.67
1:C:125:HIS:CE1	1:C:255:SER:HB2	2.30	0.67
1:F:166:GLN:CB	1:F:233:PRO:HD3	2.19	0.67
2:U:133:GLN:HB3	2:U:142:ILE:HG22	1.75	0.67
2:S:26:CYS:HB3	2:S:30:GLN:HE21	1.60	0.66
1:C:232:GLN:CD	1:C:232:GLN:H	1.98	0.66
1:C:194:CYS:SG	1:C:202:GLU:OE1	2.53	0.66
2:U:44:GLY:HA2	2:U:97:SER:O	1.96	0.66
1:C:178:CYS:CB	1:C:220:GLN:HA	2.25	0.66
2:U:110:HIS:CE1	2:U:120:VAL:HB	2.31	0.66
1:A:166:GLN:CG	1:A:232:GLN:HA	2.25	0.65
1:B:125:HIS:CE1	1:B:255:SER:HB2	2.31	0.65
1:A:171:ILE:HD11	1:A:193:LEU:CD1	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:166:GLN:CB	1:E:233:PRO:HD3	2.19	0.65
2:T:67:PHE:CZ	2:T:100:ASP:HB2	2.31	0.65
1:C:216:LYS:CB	1:C:217:PRO:HD3	2.22	0.65
2:S:42:GLN:HG2	2:S:45:GLN:OE1	1.97	0.65
1:B:171:ILE:CD1	1:B:193:LEU:HD21	2.27	0.65
2:T:81:LYS:HB2	2:T:100:ASP:OD2	1.96	0.64
1:A:232:GLN:CD	1:A:232:GLN:H	1.99	0.64
1:E:160:GLN:HG3	1:E:236:SER:HB3	1.80	0.64
1:C:119:ASN:HD22	1:C:121:GLN:CG	2.06	0.64
1:C:179:SER:HB2	1:C:246:GLN:NE2	2.12	0.64
1:E:166:GLN:HG2	1:E:232:GLN:HA	1.77	0.64
1:D:126:VAL:HG11	1:D:155:LEU:HD11	1.78	0.64
1:B:196:LYS:HG3	2:T:94:LYS:HZ2	1.62	0.64
1:E:131:SER:HB2	1:E:139:GLN:HG3	1.80	0.64
2:U:81:LYS:HB2	2:U:100:ASP:OD2	1.97	0.64
2:S:133:GLN:O	2:S:141:THR:HA	1.96	0.64
2:S:31:TYR:CE2	2:S:38:CYS:HB2	2.32	0.64
2:T:113:SER:C	2:T:115:ALA:H	2.01	0.64
1:D:139:GLN:HE22	1:D:159:LYS:HE3	1.62	0.64
1:E:119:ASN:HD22	1:E:121:GLN:CG	2.04	0.63
2:R:27:ARG:O	2:R:30:GLN:HG2	1.98	0.63
2:S:60:LEU:HD23	2:S:61:PRO:N	2.14	0.63
1:B:232:GLN:H	1:B:232:GLN:CD	2.01	0.63
1:B:173:ALA:HB2	1:B:256:PHE:HD1	1.63	0.63
1:B:122:ILE:HD12	1:B:122:ILE:N	2.12	0.63
1:E:122:ILE:HD12	1:E:122:ILE:N	2.14	0.63
1:F:166:GLN:HG2	1:F:232:GLN:HA	1.78	0.63
1:D:193:LEU:O	1:D:193:LEU:HG	1.99	0.63
1:C:166:GLN:HB2	1:C:233:PRO:CD	2.27	0.63
1:E:119:ASN:CG	1:E:120:PRO:HD2	2.19	0.63
2:R:135:ALA:HB2	2:R:141:THR:HG23	1.80	0.63
2:T:113:SER:O	2:T:115:ALA:N	2.32	0.63
2:T:122:HIS:ND1	2:T:135:ALA:HB1	2.14	0.63
1:F:171:ILE:HD11	1:F:193:LEU:CD1	2.27	0.62
2:S:110:HIS:HA	2:S:137:GLY:HA2	1.81	0.62
1:E:139:GLN:HE22	1:E:159:LYS:CE	2.12	0.62
1:E:125:HIS:CE1	1:E:255:SER:HB2	2.34	0.62
1:E:216:LYS:CB	1:E:217:PRO:HD3	2.18	0.62
1:E:119:ASN:ND2	1:E:121:GLN:CG	2.56	0.62
1:A:194:CYS:SG	1:A:202:GLU:OE1	2.58	0.62
2:R:44:GLY:HA2	2:R:97:SER:O	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:LEU:O	1:B:206:LEU:HD13	1.99	0.62
1:D:171:ILE:CD1	1:D:193:LEU:HD11	2.26	0.61
2:R:47:LEU:HD23	2:R:48:VAL:N	2.15	0.61
2:U:30:GLN:NE2	2:U:37:CYS:HB3	2.15	0.61
2:T:33:ILE:HG21	2:T:38:CYS:SG	2.40	0.61
1:B:136:SER:HB2	1:B:241:VAL:O	2.01	0.61
1:C:171:ILE:HD11	1:C:193:LEU:HD21	1.81	0.61
2:S:135:ALA:N	2:S:141:THR:HG22	2.16	0.61
1:D:135:THR:HG23	1:D:137:VAL:H	1.64	0.61
1:D:205:LEU:O	1:D:206:LEU:HD13	2.01	0.61
1:F:119:ASN:HD22	1:F:120:PRO:HD2	1.64	0.61
1:C:139:GLN:HE22	1:C:159:LYS:HE3	1.64	0.61
2:S:109:TRP:CE3	2:S:120:VAL:O	2.53	0.61
1:A:119:ASN:HD21	1:A:121:GLN:HG2	1.64	0.61
1:F:125:HIS:CE1	1:F:255:SER:HB2	2.36	0.60
1:B:216:LYS:CB	1:B:217:PRO:CD	2.77	0.60
1:A:119:ASN:HD21	1:A:121:GLN:HG3	1.65	0.60
2:S:67:PHE:CZ	2:S:100:ASP:HB2	2.36	0.60
1:C:122:ILE:N	1:C:122:ILE:HD12	2.16	0.60
1:B:166:GLN:CG	1:B:232:GLN:HA	2.31	0.60
2:R:27:ARG:O	2:R:30:GLN:CG	2.50	0.60
2:U:134:ILE:HG22	2:U:135:ALA:N	2.16	0.60
1:B:242:THR:HG22	3:B:1411:NAG:H81	1.84	0.60
2:R:121:LEU:H	2:R:121:LEU:HD12	1.66	0.60
1:F:216:LYS:CB	1:F:217:PRO:HD3	2.23	0.60
2:R:30:GLN:CA	2:R:39:SER:HA	2.29	0.60
1:D:150:ASN:OD1	1:D:152:LEU:HB2	2.02	0.60
1:A:122:ILE:N	1:A:122:ILE:HD12	2.16	0.60
1:F:122:ILE:H	1:F:122:ILE:HD12	1.65	0.60
2:R:135:ALA:HB1	2:R:139:SER:O	2.02	0.60
1:A:125:HIS:CE1	1:A:255:SER:HB2	2.37	0.60
1:D:194:CYS:SG	1:D:202:GLU:OE1	2.59	0.59
2:T:51:CYS:HB3	2:T:57:THR:N	2.17	0.59
1:F:139:GLN:HE22	1:F:159:LYS:HE3	1.68	0.59
2:U:32:LEU:HD12	2:U:33:ILE:H	1.65	0.59
2:R:108:GLY:HA2	2:R:122:HIS:ND1	2.18	0.59
2:T:36:GLN:OE1	2:T:53:GLU:HA	2.01	0.59
1:A:210:ASN:HD22	1:A:211:THR:H	1.50	0.59
1:B:166:GLN:HB2	1:B:233:PRO:CD	2.30	0.59
1:C:127:ILE:HG21	2:S:79:GLN:OE1	2.03	0.59
1:F:258:LEU:C	1:F:258:LEU:HD12	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:111:CYS:SG	2:R:138:VAL:HG12	2.43	0.59
1:D:125:HIS:CE1	1:D:255:SER:HB2	2.38	0.59
2:R:135:ALA:CB	2:R:141:THR:HG23	2.33	0.58
2:U:110:HIS:HD2	2:U:122:HIS:HD2	1.51	0.58
1:C:166:GLN:CG	1:C:232:GLN:HA	2.33	0.58
1:A:171:ILE:HD11	1:A:193:LEU:HD21	1.85	0.58
1:F:193:LEU:HG	1:F:193:LEU:O	2.03	0.58
2:S:24:THR:O	2:S:24:THR:OG1	2.19	0.58
1:C:216:LYS:N	1:C:216:LYS:HD2	2.18	0.58
2:U:72:ASN:N	2:U:72:ASN:HD22	2.00	0.58
1:B:139:GLN:HE22	1:B:159:LYS:HG2	1.67	0.58
1:F:194:CYS:SG	1:F:202:GLU:OE1	2.62	0.58
2:T:40:LEU:HD12	2:T:73:ARG:HB3	1.86	0.58
2:U:31:TYR:HB3	2:U:40:LEU:HD21	1.86	0.58
1:C:216:LYS:HB2	1:C:217:PRO:CD	2.26	0.58
2:T:27:ARG:O	2:T:30:GLN:HB3	2.04	0.58
1:C:171:ILE:CD1	1:C:193:LEU:HD21	2.33	0.58
1:A:211:THR:HB	1:C:221:GLN:OE1	2.04	0.58
1:E:171:ILE:CD1	1:E:193:LEU:HD21	2.34	0.57
1:F:119:ASN:OD1	1:F:149:SER:HB2	2.05	0.57
2:S:81:LYS:HB2	2:S:100:ASP:OD2	2.04	0.57
1:F:205:LEU:O	1:F:206:LEU:HD13	2.03	0.57
1:C:171:ILE:CD1	1:C:193:LEU:HD11	2.22	0.57
1:F:171:ILE:CD1	1:F:193:LEU:HD21	2.34	0.57
2:U:135:ALA:CB	2:U:141:THR:HG23	2.33	0.57
1:C:171:ILE:CG1	1:C:193:LEU:HD21	2.34	0.56
1:E:139:GLN:NE2	1:E:159:LYS:HE3	2.19	0.56
1:B:166:GLN:CB	1:B:233:PRO:HD3	2.34	0.56
2:S:123:ARG:NH2	2:S:140:ASP:OD2	2.39	0.56
2:R:67:PHE:CZ	2:R:100:ASP:HB2	2.40	0.56
1:C:133:LYS:O	1:C:134:THR:C	2.43	0.56
1:E:166:GLN:HG2	1:E:231:LEU:O	2.05	0.56
1:C:171:ILE:HG12	1:C:193:LEU:HD21	1.86	0.56
1:E:193:LEU:O	1:E:193:LEU:HG	2.05	0.56
2:S:110:HIS:HD2	2:S:122:HIS:HA	1.70	0.56
1:E:133:LYS:HE2	1:E:134:THR:O	2.06	0.56
1:D:215:ALA:HB3	1:D:219:GLY:N	2.20	0.56
2:R:135:ALA:HB2	2:R:141:THR:N	2.20	0.56
1:C:139:GLN:HE22	1:C:159:LYS:CE	2.17	0.56
1:F:139:GLN:HE22	1:F:159:LYS:CE	2.18	0.56
2:S:64:GLU:O	2:S:65:SER:CB	2.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:ASN:OD1	1:A:152:LEU:HB2	2.06	0.56
2:R:112:THR:HG22	2:R:112:THR:O	2.07	0.55
2:U:48:VAL:HG21	2:U:60:LEU:HG	1.88	0.55
1:F:119:ASN:HD21	1:F:121:GLN:CG	2.16	0.55
2:R:33:ILE:HG22	2:R:34:ASN:N	2.22	0.55
1:E:205:LEU:HD13	1:E:229:PHE:CD2	2.42	0.55
3:D:1411:NAG:H83	3:D:1411:NAG:H3	1.89	0.55
1:F:119:ASN:HD22	1:F:120:PRO:CD	2.20	0.55
1:A:160:GLN:HG3	1:A:236:SER:HB3	1.87	0.55
1:D:188:PRO:O	1:D:190:ILE:HG13	2.07	0.55
2:R:51:CYS:HB3	2:R:57:THR:N	2.22	0.55
1:B:169:TYR:CE2	1:B:260:LYS:HB2	2.42	0.55
2:R:52:THR:HG23	2:R:54:PHE:H	1.72	0.55
2:U:123:ARG:NE	2:U:140:ASP:OD2	2.40	0.55
1:A:258:LEU:C	1:A:258:LEU:HD12	2.27	0.55
1:C:160:GLN:HG3	1:C:236:SER:HB3	1.88	0.55
1:C:166:GLN:CB	1:C:233:PRO:HD3	2.32	0.55
1:B:139:GLN:HE22	1:B:159:LYS:HE3	1.71	0.55
2:T:32:LEU:C	2:T:32:LEU:HD22	2.27	0.55
2:T:133:GLN:HA	2:T:133:GLN:OE1	2.06	0.54
2:U:110:HIS:HA	2:U:137:GLY:O	2.07	0.54
1:B:194:CYS:SG	1:B:202:GLU:OE1	2.65	0.54
2:R:72:ASN:HD22	2:R:72:ASN:H	1.53	0.54
2:S:52:THR:OG1	2:S:55:THR:HG23	2.06	0.54
1:E:171:ILE:HD11	1:E:193:LEU:CD1	2.35	0.54
1:E:149:SER:O	1:E:150:ASN:HB3	2.07	0.54
1:A:179:SER:HB3	1:A:246:GLN:HE22	1.68	0.54
2:S:32:LEU:HD23	2:S:32:LEU:C	2.27	0.54
1:A:139:GLN:HE22	1:A:159:LYS:CE	2.20	0.54
1:F:178:CYS:O	1:F:178:CYS:SG	2.65	0.54
2:U:135:ALA:HA	2:U:140:ASP:O	2.06	0.54
1:B:139:GLN:NE2	1:B:159:LYS:HG2	2.22	0.54
1:B:126:VAL:HG11	1:B:155:LEU:HD11	1.87	0.54
2:T:110:HIS:O	2:T:119:CYS:HA	2.08	0.54
1:D:139:GLN:HE22	1:D:159:LYS:CE	2.21	0.54
1:E:136:SER:HA	1:E:244:PRO:HG3	1.89	0.54
2:T:30:GLN:HG3	2:T:38:CYS:O	2.08	0.54
1:F:169:TYR:CE2	1:F:260:LYS:HB2	2.43	0.54
1:F:149:SER:O	1:F:150:ASN:HB3	2.07	0.54
1:B:173:ALA:HB2	1:B:256:PHE:CD1	2.42	0.54
1:E:210:ASN:OD1	1:E:221:GLN:HG2	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:LEU:HD12	1:D:258:LEU:C	2.29	0.53
1:C:259:LEU:HD12	1:C:259:LEU:O	2.08	0.53
1:F:150:ASN:OD1	1:F:152:LEU:HB2	2.08	0.53
2:R:136:THR:N	2:R:139:SER:HB3	2.23	0.53
1:A:132:SER:O	1:A:133:LYS:CB	2.56	0.53
1:D:127:ILE:HG21	2:T:79:GLN:OE1	2.08	0.53
1:B:119:ASN:OD1	1:B:120:PRO:HD2	2.08	0.53
2:R:136:THR:OG1	2:R:139:SER:HB3	2.08	0.53
2:U:136:THR:HG1	2:U:139:SER:CB	2.21	0.53
2:R:31:TYR:HE1	2:R:33:ILE:HG12	1.74	0.53
2:S:133:GLN:HB3	2:S:142:ILE:HG12	1.89	0.53
1:E:135:THR:O	1:E:136:SER:HB2	2.08	0.53
2:R:32:LEU:C	2:R:32:LEU:HD22	2.28	0.53
1:E:143:LYS:HD2	2:U:65:SER:HB2	1.91	0.53
1:D:166:GLN:CG	1:D:232:GLN:HA	2.39	0.53
1:E:127:ILE:HG21	2:U:79:GLN:OE1	2.08	0.53
1:F:215:ALA:O	1:F:216:LYS:C	2.47	0.53
2:S:108:GLY:O	2:S:121:LEU:HD13	2.09	0.53
2:U:26:CYS:HB3	2:U:30:GLN:HE21	1.72	0.53
2:T:88:GLY:C	2:T:89:LEU:HD12	2.30	0.53
1:A:139:GLN:NE2	1:A:159:LYS:HE3	2.23	0.53
2:T:46:LYS:HG2	2:T:60:LEU:O	2.09	0.53
2:S:135:ALA:CB	2:S:141:THR:HG23	2.38	0.53
2:T:40:LEU:HD21	2:T:71:TRP:O	2.09	0.53
1:A:179:SER:CB	1:A:246:GLN:NE2	2.68	0.52
1:D:201:PHE:CE1	2:R:55:THR:HG22	2.44	0.52
2:T:112:THR:HG22	2:T:112:THR:O	2.09	0.52
1:B:160:GLN:HB2	1:B:237:VAL:O	2.08	0.52
1:F:166:GLN:HG2	1:F:231:LEU:O	2.09	0.52
2:U:44:GLY:O	2:U:61:PRO:HA	2.10	0.52
2:U:110:HIS:CD2	2:U:122:HIS:HD2	2.27	0.52
2:T:139:SER:O	2:T:140:ASP:CB	2.57	0.52
1:B:171:ILE:HD11	1:B:193:LEU:CD2	2.39	0.52
1:C:169:TYR:CE2	1:C:260:LYS:HB2	2.45	0.52
2:T:27:ARG:O	2:T:28:GLU:O	2.27	0.52
1:F:139:GLN:NE2	1:F:159:LYS:HE3	2.25	0.52
2:R:30:GLN:CB	2:R:39:SER:HA	2.40	0.52
2:R:81:LYS:HB2	2:R:100:ASP:OD2	2.10	0.52
1:B:171:ILE:HG13	1:B:172:TYR:N	2.25	0.52
1:D:171:ILE:CG1	1:D:193:LEU:HD21	2.40	0.52
1:F:192:SER:CB	1:F:207:ARG:HG2	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ILE:H	1:C:122:ILE:HD12	1.74	0.52
1:A:171:ILE:CD1	1:A:193:LEU:HD21	2.41	0.51
2:S:21:GLU:OE1	2:S:24:THR:HG21	2.10	0.51
1:A:179:SER:CB	1:A:246:GLN:HE22	2.23	0.51
1:C:179:SER:CB	1:C:246:GLN:NE2	2.73	0.51
2:T:36:GLN:HE22	2:T:53:GLU:HA	1.75	0.51
1:E:126:VAL:HG12	1:E:127:ILE:N	2.25	0.51
1:F:160:GLN:HG3	1:F:236:SER:HB3	1.93	0.51
1:D:160:GLN:HG3	1:D:236:SER:HB3	1.92	0.51
2:R:109:TRP:HA	2:R:120:VAL:O	2.11	0.51
2:T:32:LEU:O	2:T:32:LEU:HD13	2.10	0.51
1:F:165:ARG:HB2	1:F:165:ARG:HH11	1.75	0.51
1:F:232:GLN:CD	1:F:232:GLN:N	2.63	0.51
1:B:122:ILE:HD12	1:B:122:ILE:H	1.75	0.51
1:D:169:TYR:CE2	1:D:260:LYS:HB2	2.46	0.51
1:B:237:VAL:HG23	1:B:256:PHE:HZ	1.75	0.51
2:T:47:LEU:HD23	2:T:73:ARG:O	2.10	0.51
2:T:89:LEU:N	2:T:89:LEU:HD12	2.25	0.51
1:F:160:GLN:HB2	1:F:237:VAL:O	2.10	0.51
1:A:122:ILE:H	1:A:122:ILE:HD12	1.75	0.51
1:C:149:SER:O	1:C:150:ASN:HB3	2.11	0.51
2:T:122:HIS:ND1	2:T:135:ALA:CB	2.74	0.50
1:F:119:ASN:ND2	1:F:121:GLN:HG2	2.19	0.50
2:R:134:ILE:HA	2:R:141:THR:HG22	1.94	0.50
1:A:131:SER:O	1:A:133:LYS:N	2.43	0.50
1:E:150:ASN:OD1	1:E:152:LEU:HB2	2.10	0.50
1:A:155:LEU:HD22	1:A:158:GLY:HA2	1.92	0.50
2:T:133:GLN:H	2:T:142:ILE:CD1	2.20	0.50
1:E:258:LEU:C	1:E:258:LEU:HD12	2.31	0.50
1:A:210:ASN:HD22	1:A:211:THR:N	2.09	0.50
2:S:70:THR:O	2:S:72:ASN:N	2.44	0.50
1:D:139:GLN:NE2	1:D:159:LYS:HE3	2.26	0.50
2:S:65:SER:O	2:S:80:HIS:N	2.31	0.50
1:B:258:LEU:HD12	1:B:258:LEU:C	2.32	0.50
1:D:126:VAL:HG21	1:D:161:LEU:HD21	1.94	0.50
1:B:128:SER:HB3	1:B:254:THR:HG22	1.94	0.50
2:T:52:THR:HG23	2:T:55:THR:HB	1.92	0.50
1:F:232:GLN:N	1:F:232:GLN:NE2	2.60	0.50
1:C:151:ASN:O	1:C:164:LYS:HD2	2.12	0.50
1:E:122:ILE:HD12	1:E:122:ILE:H	1.73	0.50
2:S:64:GLU:O	2:S:65:SER:HB2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:136:THR:O	2:S:138:VAL:N	2.39	0.50
2:R:68:LEU:HD13	2:R:72:ASN:OD1	2.12	0.50
1:C:153:VAL:HG12	1:C:163:VAL:HG12	1.94	0.50
1:F:202:GLU:OE1	3:F:1411:NAG:H61	2.12	0.50
1:C:139:GLN:NE2	1:C:159:LYS:HE3	2.26	0.50
1:A:205:LEU:O	1:A:206:LEU:HD13	2.10	0.50
2:T:135:ALA:HB3	2:T:141:THR:HG23	1.92	0.49
2:T:134:ILE:HG12	2:T:135:ALA:N	2.27	0.49
2:U:70:THR:O	2:U:72:ASN:N	2.45	0.49
1:A:171:ILE:HG13	1:A:172:TYR:N	2.25	0.49
2:R:132:LYS:HE2	2:R:144:GLU:HG2	1.94	0.49
2:U:132:LYS:C	2:U:132:LYS:HD2	2.32	0.49
2:U:31:TYR:HB3	2:U:40:LEU:CD2	2.42	0.49
1:B:188:PRO:O	1:B:190:ILE:HG13	2.12	0.49
1:E:164:LYS:O	1:E:233:PRO:HB3	2.13	0.49
2:R:33:ILE:HD11	2:R:38:CYS:SG	2.52	0.49
1:F:155:LEU:HD22	1:F:158:GLY:HA2	1.93	0.49
2:R:110:HIS:O	2:R:119:CYS:HA	2.12	0.49
1:C:244:PRO:O	1:C:247:VAL:HG12	2.12	0.49
1:B:135:THR:HG22	1:B:137:VAL:HG23	1.94	0.49
1:A:195:LEU:HD12	1:A:236:SER:O	2.13	0.49
1:A:205:LEU:C	1:A:206:LEU:HD13	2.33	0.49
1:F:171:ILE:CD1	1:F:193:LEU:HD11	2.34	0.49
1:B:210:ASN:HB2	1:B:223:ILE:HD11	1.92	0.49
1:C:128:SER:HA	1:C:140:TRP:CE3	2.48	0.49
1:E:232:GLN:NE2	1:E:232:GLN:N	2.61	0.49
2:U:137:GLY:C	2:U:139:SER:H	2.15	0.49
1:E:155:LEU:HD23	1:E:160:GLN:O	2.13	0.49
1:E:189:PHE:HB2	1:E:212:HIS:CE1	2.48	0.49
1:C:232:GLN:CD	1:C:232:GLN:N	2.66	0.49
2:T:113:SER:C	2:T:115:ALA:N	2.66	0.49
1:A:122:ILE:HD13	1:A:260:LYS:HD3	1.95	0.49
1:A:126:VAL:HG12	1:A:127:ILE:N	2.28	0.49
2:R:47:LEU:C	2:R:47:LEU:HD23	2.33	0.49
1:D:150:ASN:OD1	1:D:152:LEU:CB	2.60	0.49
1:F:205:LEU:C	1:F:206:LEU:HD13	2.33	0.49
1:D:122:ILE:HD12	1:D:122:ILE:H	1.75	0.49
2:R:43:PRO:O	2:R:98:GLU:HB3	2.13	0.49
2:S:142:ILE:HG22	2:S:143:CYS:N	2.28	0.49
1:D:149:SER:O	1:D:150:ASN:HB3	2.12	0.49
2:T:29:LYS:HE2	2:T:71:TRP:CZ2	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:LEU:O	1:A:193:LEU:HG	2.13	0.48
2:R:51:CYS:HB3	2:R:57:THR:H	1.76	0.48
2:R:143:CYS:O	2:R:144:GLU:HB3	2.13	0.48
2:R:70:THR:O	2:R:72:ASN:N	2.46	0.48
1:B:232:GLN:N	1:B:232:GLN:CD	2.66	0.48
2:U:67:PHE:CZ	2:U:100:ASP:HB2	2.48	0.48
1:F:126:VAL:HG11	1:F:155:LEU:HD11	1.95	0.48
1:A:119:ASN:ND2	1:A:121:GLN:HG2	2.27	0.48
2:S:41:CYS:O	2:S:71:TRP:HA	2.13	0.48
1:C:205:LEU:O	1:C:206:LEU:HD13	2.14	0.48
1:B:136:SER:HA	1:B:244:PRO:CG	2.39	0.48
1:A:224:HIS:C	1:A:225:LEU:HD12	2.33	0.48
1:E:151:ASN:O	1:E:164:LYS:HD2	2.13	0.48
2:R:65:SER:HA	2:R:80:HIS:HD2	1.79	0.48
1:B:244:PRO:O	1:B:247:VAL:HG12	2.14	0.48
1:B:240:ASN:OD1	3:B:1411:NAG:H2	2.14	0.48
1:E:237:VAL:HG23	1:E:256:PHE:HZ	1.78	0.48
1:F:129:GLU:O	1:F:131:SER:N	2.47	0.48
2:U:66:GLU:O	2:U:67:PHE:HB3	2.13	0.48
1:D:205:LEU:HD13	1:D:229:PHE:CD2	2.48	0.48
1:B:139:GLN:HE22	1:B:159:LYS:CE	2.26	0.48
1:F:232:GLN:H	1:F:232:GLN:NE2	2.11	0.48
1:C:119:ASN:OD1	1:C:120:PRO:HD2	2.14	0.48
2:U:142:ILE:O	2:U:142:ILE:HG23	2.12	0.48
1:B:193:LEU:HG	1:B:193:LEU:O	2.13	0.48
1:A:210:ASN:OD1	1:A:221:GLN:HG2	2.14	0.48
1:E:209:ALA:O	1:E:210:ASN:HB2	2.14	0.48
1:A:210:ASN:CB	1:A:223:ILE:HD11	2.38	0.47
1:B:131:SER:HB2	1:B:139:GLN:HG3	1.97	0.47
1:D:165:ARG:O	1:D:169:TYR:OH	2.27	0.47
1:B:215:ALA:O	1:B:216:LYS:O	2.32	0.47
1:F:155:LEU:HD23	1:F:160:GLN:O	2.15	0.47
1:B:165:ARG:HH11	1:B:165:ARG:HB2	1.78	0.47
1:A:216:LYS:CB	1:A:217:PRO:HD3	2.20	0.47
1:C:258:LEU:C	1:C:258:LEU:HD12	2.34	0.47
1:A:211:THR:HG21	1:C:213:SER:CB	2.43	0.47
1:A:169:TYR:CE2	1:A:260:LYS:HB2	2.49	0.47
1:E:143:LYS:O	1:E:146:TYR:HB3	2.14	0.47
2:S:90:ARG:HG2	2:S:104:THR:O	2.14	0.47
1:F:128:SER:HB3	1:F:254:THR:O	2.15	0.47
1:E:194:CYS:SG	1:E:202:GLU:OE1	2.72	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:111:CYS:HB3	2:R:116:CYS:HA	1.97	0.47
1:D:165:ARG:HH11	1:D:165:ARG:HB2	1.80	0.47
1:A:176:THR:HG21	1:A:253:PHE:CD1	2.50	0.47
1:E:165:ARG:HH11	1:E:165:ARG:HB2	1.79	0.47
1:F:166:GLN:HB2	1:F:233:PRO:CG	2.44	0.47
2:U:112:THR:HG22	2:U:112:THR:O	2.14	0.47
2:T:42:GLN:HG3	2:T:45:GLN:HG3	1.96	0.47
1:C:150:ASN:OD1	1:C:152:LEU:HB2	2.15	0.47
1:B:149:SER:O	1:B:150:ASN:HB3	2.15	0.47
1:D:136:SER:HA	1:D:244:PRO:HG3	1.97	0.47
2:R:40:LEU:HD13	2:R:71:TRP:HB3	1.97	0.47
1:D:232:GLN:CD	1:D:232:GLN:H	2.19	0.47
1:C:178:CYS:HB2	1:C:219:GLY:C	2.35	0.47
1:F:179:SER:HA	1:F:212:HIS:ND1	2.29	0.47
3:B:1411:NAG:C8	3:B:1411:NAG:O3	2.60	0.47
2:R:52:THR:HG23	2:R:53:GLU:N	2.30	0.47
1:B:171:ILE:O	1:B:226:GLY:HA2	2.15	0.46
1:E:171:ILE:CG1	1:E:193:LEU:HD21	2.45	0.46
1:E:160:GLN:HB3	1:E:160:GLN:HE21	1.57	0.46
1:A:165:ARG:HB2	1:A:165:ARG:HH11	1.80	0.46
1:D:216:LYS:CB	1:D:217:PRO:CD	2.79	0.46
2:R:134:ILE:C	2:R:141:THR:HG22	2.35	0.46
1:B:131:SER:HB2	1:B:139:GLN:CG	2.46	0.46
1:A:215:ALA:HB3	1:A:218:CYS:C	2.36	0.46
2:S:33:ILE:O	2:S:34:ASN:HB2	2.15	0.46
1:B:195:LEU:HD12	1:B:236:SER:O	2.15	0.46
1:E:138:LEU:HD12	1:E:239:VAL:CG1	2.46	0.46
1:E:232:GLN:CD	1:E:232:GLN:N	2.63	0.46
2:T:132:LYS:CB	2:T:142:ILE:HD11	2.32	0.46
2:S:135:ALA:H	2:S:141:THR:CG2	2.28	0.46
2:S:136:THR:C	2:S:138:VAL:H	2.19	0.46
1:C:140:TRP:CZ3	1:C:254:THR:HG22	2.50	0.46
1:C:164:LYS:O	1:C:233:PRO:HB3	2.16	0.46
1:B:122:ILE:HD13	1:B:260:LYS:HD3	1.98	0.46
2:S:64:GLU:OE1	2:S:65:SER:N	2.48	0.46
1:C:155:LEU:HD23	1:C:160:GLN:O	2.16	0.46
2:S:51:CYS:HB2	2:S:56:GLU:C	2.36	0.46
1:A:128:SER:HB3	1:A:254:THR:O	2.15	0.46
2:U:137:GLY:C	2:U:139:SER:N	2.69	0.46
2:T:40:LEU:CD1	2:T:73:ARG:HB3	2.46	0.46
1:D:168:LEU:HD11	1:F:147:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:R:69:ASP:O	2:R:70:THR:HB	2.16	0.46
1:D:155:LEU:HD22	1:D:158:GLY:HA2	1.97	0.46
1:D:150:ASN:C	1:D:152:LEU:H	2.19	0.46
1:D:153:VAL:HG12	1:D:163:VAL:HG12	1.98	0.46
1:F:225:LEU:HD12	1:F:225:LEU:N	2.31	0.46
1:D:179:SER:OG	1:D:212:HIS:HB3	2.15	0.46
2:T:49:SER:HB2	2:T:58:GLU:CB	2.27	0.46
2:T:51:CYS:CB	2:T:57:THR:N	2.78	0.46
1:A:173:ALA:HB2	1:A:256:PHE:HD1	1.81	0.46
2:T:68:LEU:HD13	2:T:72:ASN:OD1	2.16	0.46
2:T:49:SER:O	2:T:57:THR:HA	2.16	0.46
1:F:171:ILE:HG13	1:F:172:TYR:N	2.29	0.46
1:E:171:ILE:HG13	1:E:172:TYR:N	2.30	0.45
2:U:43:PRO:HG3	2:U:70:THR:CA	2.47	0.45
1:A:173:ALA:HB2	1:A:256:PHE:CD1	2.50	0.45
2:U:144:GLU:HG3	2:U:144:GLU:O	2.15	0.45
2:S:88:GLY:C	2:S:89:LEU:HD12	2.37	0.45
1:A:232:GLN:N	1:A:232:GLN:CD	2.68	0.45
1:F:171:ILE:HD11	1:F:193:LEU:CD2	2.45	0.45
1:A:179:SER:CA	1:A:218:CYS:HB2	2.47	0.45
1:D:140:TRP:CZ3	1:D:254:THR:HG22	2.51	0.45
1:F:228:VAL:HG13	1:F:261:LEU:HD11	1.98	0.45
2:S:110:HIS:CD2	2:S:122:HIS:HA	2.49	0.45
2:S:26:CYS:HB3	2:S:30:GLN:NE2	2.30	0.45
1:C:218:CYS:SG	1:C:219:GLY:N	2.90	0.45
2:R:135:ALA:N	2:R:141:THR:HG22	2.32	0.45
1:B:169:TYR:CD1	1:B:231:LEU:HD12	2.51	0.45
2:R:133:GLN:HB3	2:R:142:ILE:HG22	1.98	0.45
2:T:122:HIS:CE1	2:T:135:ALA:CB	2.98	0.45
1:A:204:ILE:HD13	1:A:207:ARG:CD	2.36	0.45
2:R:33:ILE:CD1	2:R:50:ASP:HB3	2.47	0.45
1:F:244:PRO:O	1:F:247:VAL:HG12	2.17	0.45
1:D:166:GLN:HB2	1:D:233:PRO:CG	2.47	0.45
2:R:30:GLN:HA	2:R:39:SER:CA	2.38	0.45
2:S:72:ASN:HD22	2:S:72:ASN:N	2.15	0.45
2:R:43:PRO:HG3	2:R:71:TRP:N	2.32	0.45
1:B:205:LEU:HD13	1:B:229:PHE:CD2	2.52	0.45
2:U:26:CYS:O	2:U:27:ARG:O	2.34	0.45
1:B:125:HIS:CE1	1:B:255:SER:CB	3.00	0.45
1:C:165:ARG:O	1:C:169:TYR:OH	2.29	0.45
2:T:36:GLN:NE2	2:T:53:GLU:HA	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:188:PRO:O	1:D:189:PHE:C	2.55	0.44
1:D:195:LEU:HD12	1:D:236:SER:O	2.17	0.44
1:E:216:LYS:CB	1:E:217:PRO:CD	2.83	0.44
1:E:171:ILE:HD11	1:E:193:LEU:CD2	2.44	0.44
2:U:132:LYS:N	2:U:142:ILE:O	2.50	0.44
1:C:176:THR:HA	1:C:221:GLN:O	2.16	0.44
2:S:31:TYR:HB3	2:S:40:LEU:HD21	1.99	0.44
1:D:201:PHE:HE1	2:R:55:THR:HG22	1.81	0.44
2:T:34:ASN:HB3	2:T:35:SER:H	1.39	0.44
1:C:174:GLN:HA	1:C:223:ILE:O	2.16	0.44
1:D:171:ILE:HG13	1:D:172:TYR:N	2.30	0.44
2:S:109:TRP:HA	2:S:121:LEU:HA	1.99	0.44
2:U:72:ASN:ND2	2:U:72:ASN:H	2.08	0.44
1:A:131:SER:O	1:A:132:SER:C	2.55	0.44
1:B:165:ARG:HH11	1:B:165:ARG:CB	2.31	0.44
1:F:140:TRP:CZ3	1:F:254:THR:HG22	2.52	0.44
1:B:171:ILE:CG1	1:B:193:LEU:HD21	2.47	0.44
2:T:123:ARG:HG3	2:T:123:ARG:H	1.64	0.44
2:S:72:ASN:C	2:S:72:ASN:ND2	2.70	0.44
2:R:132:LYS:HB2	2:R:144:GLU:HG2	1.99	0.44
1:B:205:LEU:C	1:B:206:LEU:HD13	2.38	0.44
2:R:108:GLY:HA2	2:R:122:HIS:CE1	2.52	0.44
1:A:160:GLN:HB3	1:A:160:GLN:HE21	1.61	0.44
1:F:124:ALA:HA	1:F:147:THR:O	2.18	0.44
1:B:237:VAL:HG23	1:B:256:PHE:CZ	2.52	0.44
2:T:40:LEU:O	2:T:41:CYS:C	2.56	0.44
1:A:140:TRP:CZ3	1:A:254:THR:HG22	2.52	0.44
1:C:173:ALA:HB2	1:C:256:PHE:HD1	1.83	0.44
2:T:101:THR:HG22	2:T:102:ILE:N	2.31	0.44
1:A:232:GLN:N	1:A:232:GLN:NE2	2.66	0.44
2:R:136:THR:H	2:R:139:SER:HB3	1.82	0.44
2:U:110:HIS:CD2	2:U:122:HIS:HA	2.53	0.44
2:U:112:THR:OG1	2:U:120:VAL:HG23	2.18	0.44
1:E:197:SER:HB2	1:E:232:GLN:OE1	2.18	0.44
2:R:132:LYS:HE2	2:R:144:GLU:CG	2.48	0.44
2:T:53:GLU:OE1	2:T:54:PHE:HE1	2.01	0.44
2:R:88:GLY:C	2:R:89:LEU:HD12	2.38	0.44
1:A:192:SER:CB	1:A:207:ARG:HG2	2.47	0.44
1:C:232:GLN:NE2	1:C:232:GLN:N	2.66	0.44
2:T:60:LEU:HD13	2:T:61:PRO:CD	2.45	0.44
1:D:205:LEU:C	1:D:206:LEU:HD13	2.37	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:140:TRP:CZ3	1:E:254:THR:HG22	2.53	0.44
2:U:88:GLY:C	2:U:89:LEU:HD12	2.38	0.44
1:F:197:SER:OG	1:F:198:PRO:HD2	2.18	0.43
1:F:119:ASN:HD22	1:F:120:PRO:N	2.16	0.43
2:U:110:HIS:CB	2:U:137:GLY:O	2.66	0.43
1:D:151:ASN:O	1:D:164:LYS:HD2	2.18	0.43
1:E:232:GLN:NE2	1:E:232:GLN:H	2.14	0.43
1:D:171:ILE:O	1:D:226:GLY:HA2	2.18	0.43
2:S:72:ASN:HD22	2:S:72:ASN:H	1.66	0.43
1:B:139:GLN:NE2	1:B:159:LYS:HE3	2.34	0.43
2:T:72:ASN:C	2:T:72:ASN:ND2	2.70	0.43
2:R:132:LYS:HE2	2:R:144:GLU:CB	2.48	0.43
2:R:29:LYS:O	2:R:30:GLN:HB3	2.19	0.43
1:E:237:VAL:HG23	1:E:256:PHE:CZ	2.53	0.43
1:F:195:LEU:HD12	1:F:236:SER:O	2.18	0.43
1:A:210:ASN:HB2	1:A:223:ILE:CD1	2.41	0.43
1:C:209:ALA:O	1:C:210:ASN:HB2	2.18	0.43
2:T:110:HIS:NE2	2:T:140:ASP:OD1	2.52	0.43
1:F:237:VAL:HG23	1:F:256:PHE:HZ	1.81	0.43
1:A:171:ILE:HG12	1:A:193:LEU:HD21	2.01	0.43
1:B:121:GLN:HG2	1:B:121:GLN:H	1.67	0.43
1:B:216:LYS:HB3	1:B:217:PRO:HD3	1.95	0.43
1:E:125:HIS:CE1	1:E:255:SER:CB	3.01	0.43
1:A:150:ASN:C	1:A:152:LEU:H	2.22	0.43
1:E:205:LEU:O	1:E:206:LEU:HD13	2.18	0.43
2:R:27:ARG:O	2:R:30:GLN:HG3	2.18	0.43
1:A:174:GLN:HA	1:A:223:ILE:O	2.19	0.43
1:D:133:LYS:HG2	1:D:245:SER:HB3	2.00	0.43
1:B:157:ASN:ND2	1:B:157:ASN:O	2.52	0.43
2:T:67:PHE:CE2	2:T:100:ASP:OD1	2.72	0.43
1:B:179:SER:C	1:B:218:CYS:HB2	2.38	0.43
1:B:171:ILE:HG12	1:B:193:LEU:HD21	2.00	0.43
2:S:32:LEU:HD23	2:S:33:ILE:N	2.34	0.43
1:E:160:GLN:HB2	1:E:237:VAL:O	2.19	0.43
1:C:124:ALA:HA	1:C:147:THR:O	2.18	0.43
1:F:156:GLU:HG3	1:F:162:THR:OG1	2.19	0.43
2:U:90:ARG:HG2	2:U:104:THR:O	2.17	0.43
1:D:218:CYS:O	1:D:219:GLY:O	2.36	0.43
1:E:128:SER:HB3	1:E:254:THR:O	2.19	0.43
1:F:171:ILE:CG1	1:F:193:LEU:HD21	2.49	0.42
2:T:133:GLN:N	2:T:142:ILE:HD11	2.24	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:126:VAL:HG12	1:C:127:ILE:N	2.34	0.42
2:S:103:CYS:O	2:S:104:THR:HG23	2.19	0.42
1:C:173:ALA:HB2	1:C:256:PHE:CD1	2.53	0.42
2:R:46:LYS:HB3	2:R:77:CYS:SG	2.60	0.42
2:U:43:PRO:HG3	2:U:70:THR:C	2.40	0.42
2:S:66:GLU:O	2:S:67:PHE:HB3	2.19	0.42
1:B:140:TRP:CZ3	1:B:254:THR:HG22	2.54	0.42
2:T:70:THR:O	2:T:72:ASN:N	2.52	0.42
1:A:143:LYS:O	1:A:146:TYR:HB3	2.19	0.42
1:D:197:SER:HB2	1:D:232:GLN:OE1	2.18	0.42
1:C:206:LEU:CD1	1:C:229:PHE:HZ	2.33	0.42
1:B:165:ARG:CB	1:B:165:ARG:NH1	2.83	0.42
1:C:193:LEU:O	1:C:193:LEU:HG	2.19	0.42
2:R:134:ILE:CA	2:R:141:THR:HG22	2.49	0.42
1:C:139:GLN:HE22	1:C:159:LYS:HG2	1.85	0.42
2:U:93:GLN:O	2:U:94:LYS:O	2.38	0.42
1:C:171:ILE:HD11	1:C:193:LEU:CD2	2.47	0.42
1:E:220:GLN:O	1:F:211:THR:HG23	2.19	0.42
1:D:126:VAL:HG12	1:D:127:ILE:N	2.34	0.42
2:U:65:SER:HA	2:U:80:HIS:HD2	1.84	0.42
1:A:197:SER:HB2	1:A:232:GLN:OE1	2.20	0.42
1:C:125:HIS:CE1	1:C:255:SER:CB	3.01	0.42
1:E:143:LYS:CD	2:U:65:SER:HB2	2.49	0.42
2:R:109:TRP:HB3	2:R:119:CYS:HB3	2.01	0.42
1:F:224:HIS:C	1:F:225:LEU:HD12	2.40	0.42
2:S:89:LEU:HD12	2:S:89:LEU:N	2.34	0.42
2:S:101:THR:HG22	2:S:102:ILE:N	2.35	0.42
1:D:156:GLU:CG	1:D:162:THR:OG1	2.68	0.42
1:D:174:GLN:HA	1:D:223:ILE:O	2.19	0.42
1:B:153:VAL:HG12	1:B:163:VAL:HG12	2.01	0.42
2:U:110:HIS:CA	2:U:137:GLY:O	2.68	0.42
1:D:160:GLN:HE21	1:D:160:GLN:HB3	1.50	0.42
1:F:174:GLN:HA	1:F:223:ILE:O	2.20	0.42
1:C:224:HIS:C	1:C:225:LEU:HD12	2.40	0.42
1:E:166:GLN:HB2	1:E:233:PRO:CG	2.50	0.42
1:A:171:ILE:CG1	1:A:193:LEU:HD21	2.50	0.42
1:D:171:ILE:HD11	1:D:193:LEU:CG	2.49	0.42
1:A:179:SER:N	1:A:218:CYS:HB2	2.35	0.42
1:C:165:ARG:HB2	1:C:165:ARG:HH11	1.85	0.42
1:A:147:THR:HG21	1:B:168:LEU:HD11	2.01	0.42
1:C:215:ALA:C	1:C:216:LYS:HD2	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:164:LYS:O	1:B:233:PRO:HB3	2.20	0.42
2:T:42:GLN:HB3	2:T:71:TRP:CZ3	2.55	0.42
2:U:74:GLU:HG2	2:U:76:HIS:O	2.19	0.42
2:R:132:LYS:HE2	2:R:144:GLU:HB3	2.02	0.41
1:C:178:CYS:O	1:C:179:SER:HB2	2.20	0.41
1:C:125:HIS:HE1	1:C:255:SER:HB2	1.82	0.41
1:B:143:LYS:O	1:B:146:TYR:HB3	2.19	0.41
1:C:259:LEU:C	1:C:259:LEU:HD12	2.41	0.41
1:C:166:GLN:OE1	1:C:167:GLY:N	2.53	0.41
1:B:151:ASN:O	1:B:164:LYS:HD2	2.20	0.41
1:A:165:ARG:O	1:A:169:TYR:OH	2.32	0.41
1:B:150:ASN:C	1:B:152:LEU:H	2.23	0.41
2:R:101:THR:HG22	2:R:102:ILE:N	2.35	0.41
1:C:171:ILE:HG13	1:C:172:TYR:N	2.27	0.41
2:R:33:ILE:CG2	2:R:34:ASN:H	2.30	0.41
2:U:112:THR:O	2:U:113:SER:HB2	2.20	0.41
1:B:171:ILE:HD11	1:B:193:LEU:CG	2.49	0.41
2:T:39:SER:O	2:T:57:THR:CG2	2.58	0.41
1:B:215:ALA:O	1:B:216:LYS:C	2.58	0.41
1:C:205:LEU:C	1:C:206:LEU:HD13	2.40	0.41
1:D:121:GLN:H	1:D:121:GLN:HG2	1.63	0.41
2:T:120:VAL:HG12	2:T:121:LEU:HD23	2.02	0.41
2:R:40:LEU:HD22	2:R:72:ASN:C	2.40	0.41
1:D:261:LEU:CD2	1:F:259:LEU:HD22	2.48	0.41
2:S:67:PHE:CE2	2:S:100:ASP:OD1	2.73	0.41
2:T:89:LEU:N	2:T:89:LEU:CD1	2.83	0.41
1:D:156:GLU:HG3	1:D:162:THR:OG1	2.21	0.41
1:D:224:HIS:C	1:D:225:LEU:HD12	2.41	0.41
1:E:169:TYR:CE2	1:E:260:LYS:HB2	2.55	0.41
2:T:133:GLN:HE22	2:T:134:ILE:CD1	2.33	0.41
2:R:33:ILE:HG22	2:R:34:ASN:H	1.82	0.41
1:E:215:ALA:HB3	1:E:219:GLY:HA3	2.03	0.41
2:U:110:HIS:HD2	2:U:122:HIS:HA	1.85	0.41
1:D:135:THR:HG23	1:D:137:VAL:N	2.34	0.41
1:B:150:ASN:OD1	1:B:152:LEU:HB2	2.20	0.41
2:R:133:GLN:H	2:R:142:ILE:HG23	1.85	0.41
2:R:135:ALA:HB2	2:R:140:ASP:C	2.41	0.41
2:S:42:GLN:CG	2:S:45:GLN:OE1	2.65	0.41
1:D:150:ASN:OD1	1:D:152:LEU:HG	2.20	0.41
1:A:125:HIS:HE1	1:A:255:SER:HB2	1.85	0.41
2:R:112:THR:O	2:R:113:SER:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:LEU:N	1:A:225:LEU:HD12	2.35	0.41
1:B:174:GLN:HA	1:B:223:ILE:O	2.20	0.41
2:T:46:LYS:HE3	2:T:60:LEU:HB3	2.02	0.41
1:D:143:LYS:O	1:D:146:TYR:HB3	2.21	0.41
1:F:153:VAL:HG12	1:F:163:VAL:HG12	2.02	0.41
2:T:136:THR:O	2:T:139:SER:N	2.54	0.41
1:F:197:SER:HB2	1:F:232:GLN:OE1	2.21	0.41
2:S:110:HIS:CD2	2:S:122:HIS:N	2.89	0.41
1:C:166:GLN:C	1:C:166:GLN:OE1	2.58	0.41
2:S:26:CYS:SG	2:S:32:LEU:HB2	2.60	0.41
1:E:131:SER:C	1:E:133:LYS:H	2.24	0.41
2:U:30:GLN:HE21	2:U:37:CYS:HB3	1.83	0.41
2:T:42:GLN:HB2	2:T:43:PRO:HD2	2.03	0.41
1:C:138:LEU:HD12	1:C:239:VAL:CG1	2.51	0.41
1:E:259:LEU:HD22	1:F:261:LEU:CD2	2.34	0.41
2:S:40:LEU:HD13	2:S:71:TRP:O	2.21	0.41
2:T:45:GLN:HB3	2:T:59:CYS:HB3	2.03	0.41
1:D:215:ALA:CB	1:D:219:GLY:HA3	2.51	0.41
1:F:171:ILE:HG12	1:F:193:LEU:HD21	2.03	0.40
2:S:22:PRO:O	2:S:24:THR:N	2.54	0.40
2:R:50:ASP:HA	2:R:57:THR:CG2	2.50	0.40
2:T:30:GLN:CG	2:T:38:CYS:O	2.69	0.40
2:R:136:THR:OG1	2:R:139:SER:CB	2.69	0.40
1:F:160:GLN:HE21	1:F:160:GLN:HB3	1.52	0.40
2:T:109:TRP:CD1	2:T:109:TRP:N	2.88	0.40
2:T:144:GLU:HA	2:T:145:PRO:HD3	1.82	0.40
1:B:176:THR:HA	1:B:221:GLN:O	2.20	0.40
2:R:67:PHE:CE2	2:R:100:ASP:OD1	2.75	0.40
1:C:155:LEU:HD22	1:C:158:GLY:HA2	2.03	0.40
1:F:165:ARG:CB	1:F:165:ARG:NH1	2.85	0.40
2:R:33:ILE:CD1	2:R:38:CYS:SG	3.10	0.40
2:U:43:PRO:O	2:U:98:GLU:HB3	2.22	0.40
1:B:205:LEU:HD23	1:B:205:LEU:HA	1.89	0.40
1:D:250:GLY:HA2	2:T:82:TYR:HB3	2.03	0.40
1:D:205:LEU:HA	1:D:205:LEU:HD23	1.92	0.40
1:C:251:THR:HA	2:S:79:GLN:NE2	2.36	0.40
1:D:215:ALA:HB3	1:D:219:GLY:HA3	2.03	0.40
2:T:82:TYR:CE2	2:T:84:ASP:HA	2.56	0.40
1:E:147:THR:HG21	1:F:168:LEU:HD11	2.04	0.40

There are no symmetry-related clashes.

## 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	131/149 (88%)	107 (82%)	18 (14%)	6 (5%)	3	29
1	B	131/149 (88%)	106 (81%)	21 (16%)	4 (3%)	5	41
1	C	131/149 (88%)	106 (81%)	22 (17%)	3 (2%)	8	48
1	D	131/149 (88%)	109 (83%)	16 (12%)	6 (5%)	3	29
1	E	131/149 (88%)	111 (85%)	16 (12%)	4 (3%)	5	41
1	F	131/149 (88%)	109 (83%)	13 (10%)	9 (7%)	1	18
2	R	110/177 (62%)	82 (74%)	16 (14%)	12 (11%)	0	8
2	S	115/177 (65%)	78 (68%)	34 (30%)	3 (3%)	7	45
2	T	110/177 (62%)	80 (73%)	20 (18%)	10 (9%)	1	11
2	U	115/177 (65%)	86 (75%)	23 (20%)	6 (5%)	2	25
All	All	1236/1602 (77%)	974 (79%)	199 (16%)	63 (5%)	2	26

All (63) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	133	LYS
1	A	216	LYS
1	B	216	LYS
1	D	216	LYS
1	D	219	GLY
1	E	216	LYS
1	F	130	ALA
1	F	212	HIS
2	T	28	GLU
2	T	114	GLU
2	T	139	SER
2	T	140	ASP
2	U	27	ARG

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Mol	Chain	Res	Type
2	U	94	LYS
1	A	130	ALA
1	A	218	CYS
1	B	219	GLY
1	D	189	PHE
1	D	218	CYS
1	F	131	SER
1	F	210	ASN
1	F	219	GLY
2	R	30	GLN
2	R	35	SER
2	R	63	GLY
2	R	65	SER
2	R	71	TRP
2	R	94	LYS
2	S	71	TRP
2	S	94	LYS
2	U	71	TRP
1	C	216	LYS
1	F	149	SER
1	F	217	PRO
2	R	40	LEU
2	T	71	TRP
2	T	113	SER
1	A	151	ASN
1	B	151	ASN
1	C	151	ASN
1	D	151	ASN
1	D	220	GLN
1	E	210	ASN
1	F	151	ASN
1	F	218	CYS
2	R	33	ILE
2	R	122	HIS
2	R	134	ILE
2	T	137	GLY
2	U	34	ASN
2	U	43	PRO
1	B	189	PHE
1	C	217	PRO
2	R	113	SER
2	S	120	VAL

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Mol	Chain	Res	Type
2	U	122	HIS
1	E	151	ASN
1	E	219	GLY
2	T	94	LYS
2	T	134	ILE
2	T	142	ILE
2	R	43	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	114/124 (92%)	100 (88%)	14 (12%)	6	29
1	B	114/124 (92%)	104 (91%)	10 (9%)	12	48
1	C	114/124 (92%)	102 (90%)	12 (10%)	8	38
1	D	114/124 (92%)	103 (90%)	11 (10%)	10	43
1	E	114/124 (92%)	101 (89%)	13 (11%)	7	33
1	F	114/124 (92%)	100 (88%)	14 (12%)	6	29
2	R	106/160 (66%)	97 (92%)	9 (8%)	13	49
2	S	110/160 (69%)	93 (84%)	17 (16%)	3	20
2	T	106/160 (66%)	91 (86%)	15 (14%)	4	24
2	U	110/160 (69%)	101 (92%)	9 (8%)	14	51
All	All	1116/1384 (81%)	992 (89%)	124 (11%)	8	35

All (124) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	VAL
1	A	153	VAL
1	A	155	LEU
1	A	160	GLN
1	A	171	ILE
1	A	178	CYS

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Mol	Chain	Res	Type
1	A	194	CYS
1	A	195	LEU
1	A	202	GLU
1	A	206	LEU
1	A	210	ASN
1	A	211	THR
1	A	221	GLN
1	A	232	GLN
1	B	153	VAL
1	B	155	LEU
1	B	160	GLN
1	B	171	ILE
1	B	194	CYS
1	B	195	LEU
1	B	202	GLU
1	B	206	LEU
1	B	221	GLN
1	B	232	GLN
1	C	132	SER
1	C	146	TYR
1	C	153	VAL
1	C	155	LEU
1	C	160	GLN
1	C	171	ILE
1	C	194	CYS
1	C	195	LEU
1	C	202	GLU
1	C	206	LEU
1	C	221	GLN
1	C	232	GLN
1	D	145	TYR
1	D	153	VAL
1	D	155	LEU
1	D	160	GLN
1	D	171	ILE
1	D	194	CYS
1	D	195	LEU
1	D	202	GLU
1	D	206	LEU
1	D	221	GLN
1	D	232	GLN
1	E	132	SER

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Mol	Chain	Res	Type
1	E	133	LYS
1	E	153	VAL
1	E	155	LEU
1	E	157	ASN
1	E	160	GLN
1	E	171	ILE
1	E	195	LEU
1	E	202	GLU
1	E	206	LEU
1	E	210	ASN
1	E	221	GLN
1	E	232	GLN
1	F	119	ASN
1	F	133	LYS
1	F	134	THR
1	F	145	TYR
1	F	153	VAL
1	F	155	LEU
1	F	160	GLN
1	F	171	ILE
1	F	178	CYS
1	F	195	LEU
1	F	202	GLU
1	F	206	LEU
1	F	221	GLN
1	F	232	GLN
2	R	32	LEU
2	R	53	GLU
2	R	54	PHE
2	R	57	THR
2	R	59	CYS
2	R	72	ASN
2	R	74	GLU
2	R	92	GLN
2	R	125	CYS
2	S	24	THR
2	S	33	ILE
2	S	39	SER
2	S	51	CYS
2	S	55	THR
2	S	57	THR
2	S	60	LEU

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Mol	Chain	Res	Type
2	S	61	PRO
2	S	64	GLU
2	S	72	ASN
2	S	74	GLU
2	S	92	GLN
2	S	121	LEU
2	S	132	LYS
2	S	140	ASP
2	S	143	CYS
2	S	144	GLU
2	T	32	LEU
2	T	36	GLN
2	T	50	ASP
2	T	51	CYS
2	T	52	THR
2	T	60	LEU
2	T	64	GLU
2	T	72	ASN
2	T	74	GLU
2	T	92	GLN
2	T	123	ARG
2	T	133	GLN
2	T	134	ILE
2	T	136	THR
2	T	143	CYS
2	U	35	SER
2	U	39	SER
2	U	47	LEU
2	U	56	GLU
2	U	72	ASN
2	U	74	GLU
2	U	92	GLN
2	U	132	LYS
2	U	141	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	121	GLN
1	A	139	GLN
1	A	157	ASN

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Mol	Chain	Res	Type
1	A	160	GLN
1	A	210	ASN
1	A	246	GLN
1	B	119	ASN
1	B	139	GLN
1	B	157	ASN
1	B	160	GLN
1	C	119	ASN
1	C	121	GLN
1	C	139	GLN
1	C	157	ASN
1	C	160	GLN
1	C	212	HIS
1	C	220	GLN
1	C	246	GLN
1	D	121	GLN
1	D	139	GLN
1	D	157	ASN
1	D	160	GLN
1	E	119	ASN
1	E	121	GLN
1	E	139	GLN
1	E	157	ASN
1	E	160	GLN
1	E	210	ASN
1	F	119	ASN
1	F	139	GLN
1	F	157	ASN
1	F	160	GLN
1	F	221	GLN
2	R	80	HIS
2	S	30	GLN
2	S	80	HIS
2	S	110	HIS
2	S	133	GLN
2	T	45	GLN
2	T	80	HIS
2	U	30	GLN
2	U	34	ASN
2	U	72	ASN
2	U	80	HIS
2	U	110	HIS

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Mol	Chain	Res	Type
2	U	122	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

6 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	NAG	A	1411	1	14,14,15	0.76	1 (7%)	15,19,21	1.04	1 (6%)
3	NAG	B	1411	1	14,14,15	0.79	1 (7%)	15,19,21	0.79	0
3	NAG	C	1411	1	14,14,15	0.74	0	15,19,21	0.92	2 (13%)
3	NAG	D	1411	1	14,14,15	0.88	1 (7%)	15,19,21	0.83	1 (6%)
3	NAG	E	1411	1	14,14,15	0.88	1 (7%)	15,19,21	1.49	3 (20%)
3	NAG	F	1411	1	14,14,15	1.03	1 (7%)	15,19,21	0.88	1 (6%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	A	1411	1	-	2/6/23/26	0/1/1/1
3	NAG	B	1411	1	-	2/6/23/26	0/1/1/1
3	NAG	C	1411	1	-	0/6/23/26	0/1/1/1
3	NAG	D	1411	1	-	0/6/23/26	0/1/1/1
3	NAG	E	1411	1	-	0/6/23/26	0/1/1/1
3	NAG	F	1411	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1411	NAG	C4-C5	2.08	1.57	1.53
3	D	1411	NAG	C1-C2	2.09	1.55	1.52
3	B	1411	NAG	C1-C2	2.11	1.55	1.52
3	A	1411	NAG	C1-C2	2.24	1.55	1.52
3	F	1411	NAG	C1-C2	2.43	1.55	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	1411	NAG	C2-N2-C7	-3.14	119.01	123.04
3	E	1411	NAG	C4-C3-C2	-2.69	107.04	111.23
3	F	1411	NAG	C2-N2-C7	-2.28	120.11	123.04
3	A	1411	NAG	C3-C4-C5	-2.25	106.28	110.20
3	D	1411	NAG	C2-N2-C7	-2.24	120.16	123.04
3	C	1411	NAG	C2-N2-C7	-2.11	120.33	123.04
3	C	1411	NAG	C3-C4-C5	2.24	114.10	110.20
3	E	1411	NAG	C1-O5-C5	2.73	115.71	112.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1411	NAG	C8-C7-N2-C2
3	B	1411	NAG	C8-C7-N2-C2
3	B	1411	NAG	O7-C7-N2-C2
3	A	1411	NAG	O7-C7-N2-C2

There are no ring outliers.

5 monomers are involved in 10 short contacts:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1411	NAG	4	0
3	C	1411	NAG	1	0
3	D	1411	NAG	1	0
3	E	1411	NAG	1	0
3	F	1411	NAG	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q < 0.9
1	A	135/149 (90%)	0.27	4 (2%) 54 43	29, 58, 89, 97	0
1	B	135/149 (90%)	0.23	2 (1%) 76 67	29, 58, 84, 88	0
1	C	135/149 (90%)	0.39	6 (4%) 38 29	29, 59, 91, 99	0
1	D	135/149 (90%)	0.19	0 100 100	27, 56, 79, 94	0
1	E	135/149 (90%)	0.33	1 (0%) 89 82	29, 59, 89, 98	0
1	F	135/149 (90%)	0.28	0 100 100	29, 59, 91, 96	0
2	R	114/177 (64%)	-0.07	0 100 100	60, 88, 106, 112	0
2	S	119/177 (67%)	0.32	3 (2%) 61 50	41, 71, 110, 115	0
2	T	114/177 (64%)	0.13	1 (0%) 85 78	58, 79, 112, 119	0
2	U	119/177 (67%)	0.23	5 (4%) 40 31	43, 75, 101, 105	0
All	All	1276/1602 (79%)	0.24	22 (1%) 73 64	27, 65, 101, 119	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	213	SER	3.8
2	U	117	GLU	3.1
2	S	112	THR	3.0
2	U	112	THR	2.9
1	A	134	THR	2.8
1	B	212	HIS	2.6
2	U	81	LYS	2.6
1	E	143	LYS	2.5
1	C	236	SER	2.4
1	C	216	LYS	2.4
1	C	215	ALA	2.3
1	C	192	SER	2.2
1	A	145	TYR	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	143	LYS	2.2
2	S	117	GLU	2.1
1	A	175	VAL	2.1
1	B	219	GLY	2.1
2	U	140	ASP	2.1
2	T	107	GLU	2.0
1	A	212	HIS	2.0
2	U	138	VAL	2.0
2	S	81	LYS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	NAG	C	1411	14/15	0.73	0.49	1.13	88,94,97,97	0
3	NAG	F	1411	14/15	0.76	0.33	0.09	75,81,82,83	0
3	NAG	E	1411	14/15	0.77	0.34	-0.00	74,79,81,81	0
3	NAG	A	1411	14/15	0.89	0.23	-0.50	78,82,86,87	0
3	NAG	B	1411	14/15	0.88	0.17	-1.21	81,84,86,86	0
3	NAG	D	1411	14/15	0.83	0.23	-1.64	84,89,92,92	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.