



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 08:45 AM UTC

PDB ID : 9JO9 / pdb_00009jo9
EMDB ID : EMD-61648
Title : CRP-HCAb3 complex
Authors : Li, Y.J.
Deposited on : 2024-09-24
Resolution : 3.65 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

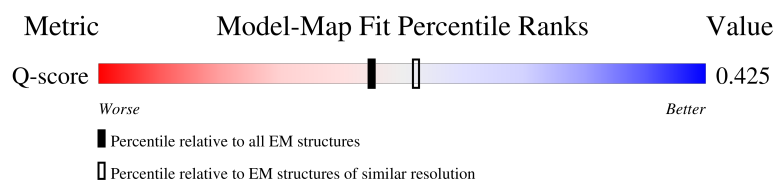
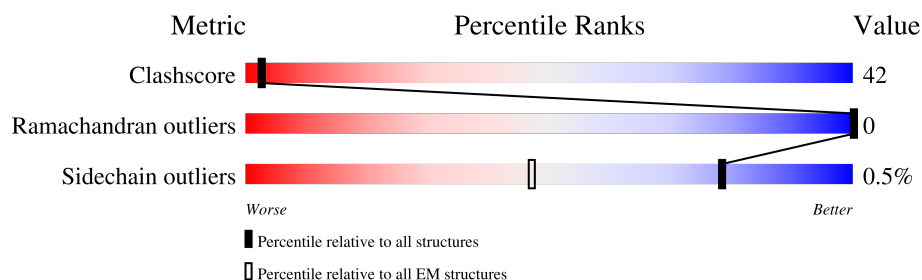
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.65 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	11564 (3.15 - 4.15)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	128	
1	C	128	
1	E	128	
1	G	128	

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Mol	Chain	Length	Quality of chain
1	I	128	
1	K	128	
1	M	128	
1	O	128	
1	P	128	
1	R	128	
2	B	206	
2	D	206	
2	F	206	
2	H	206	
2	J	206	
2	L	206	
2	N	206	
2	Q	206	
2	S	206	
2	T	206	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 42040 atoms, of which 15920 are hydrogens and 0 are deuteriums.

In the tables below, 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 CRP specific recognition heavy chain antibody 3 (HCAb3).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	O	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	A	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	C	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	E	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	G	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	I	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	K	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	M	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	P	125	Total	C	N	O	S	0	0
			980	613	171	192	4		
1	R	125	Total	C	N	O	S	0	0
			980	613	171	192	4		

- Molecule 2 is a protein called C-reactive protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	S	206	Total 3224	C 1058	H 1592	N 261	O 309	S 4	0	0
2	B	206	Total 3224	C 1058	H 1592	N 261	O 309	S 4	0	0
2	D	206	Total 3224	C 1058	H 1592	N 261	O 309	S 4	0	0
2	F	206	Total 3224	C 1058	H 1592	N 261	O 309	S 4	0	0
2	H	206	Total 3224	C 1058	H 1592	N 261	O 309	S 4	0	0

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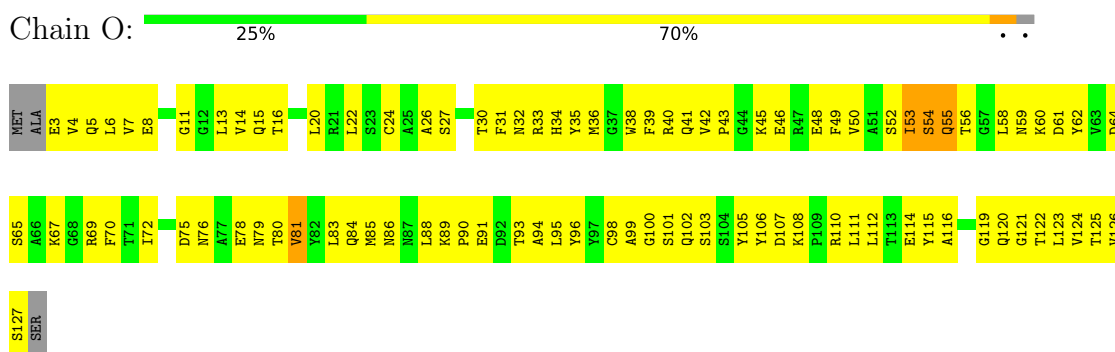
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Mol	Chain	Residues	Atoms						AltConf	Trace
2	J	206	Total	C	H	N	O	S	0	0
			3224	1058	1592	261	309	4		
2	L	206	Total	C	H	N	O	S	0	0
			3224	1058	1592	261	309	4		
2	N	206	Total	C	H	N	O	S	0	0
			3224	1058	1592	261	309	4		
2	Q	206	Total	C	H	N	O	S	0	0
			3224	1058	1592	261	309	4		
2	T	206	Total	C	H	N	O	S	0	0
			3224	1058	1592	261	309	4		

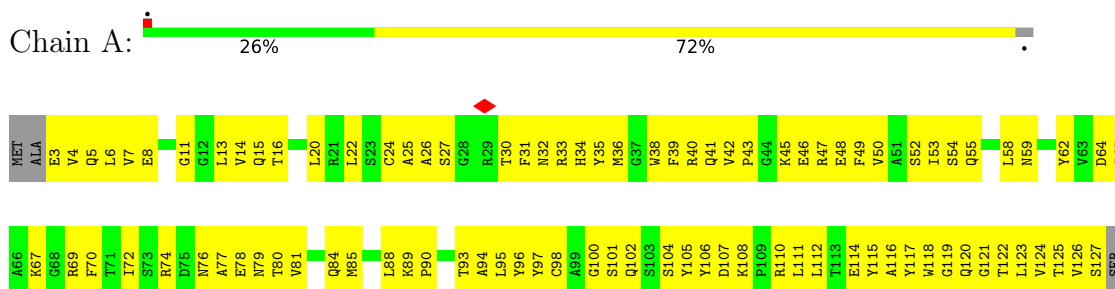
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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.

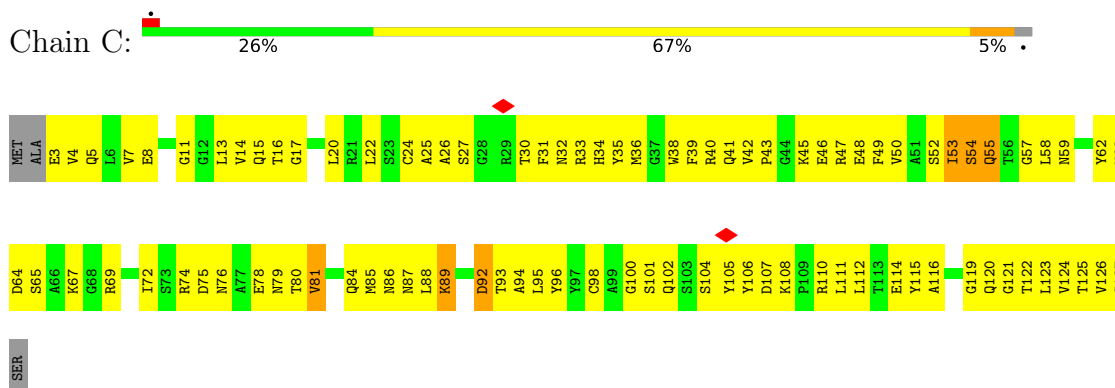
- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



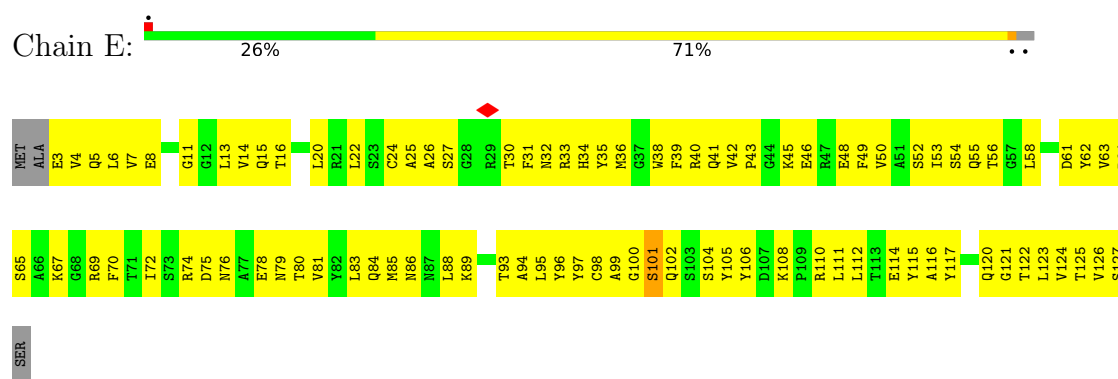
- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



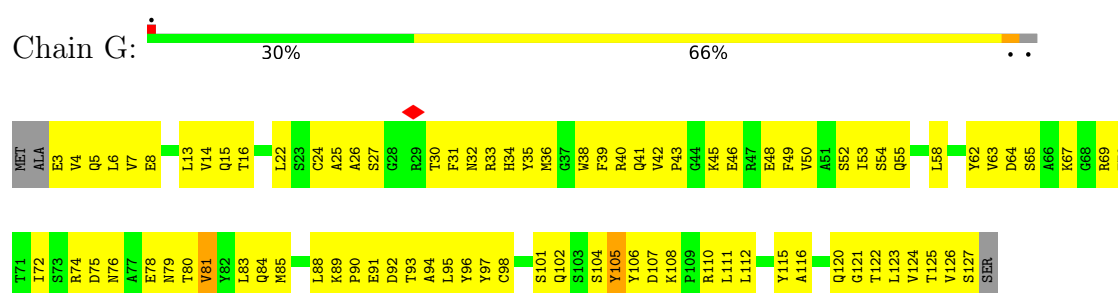
- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



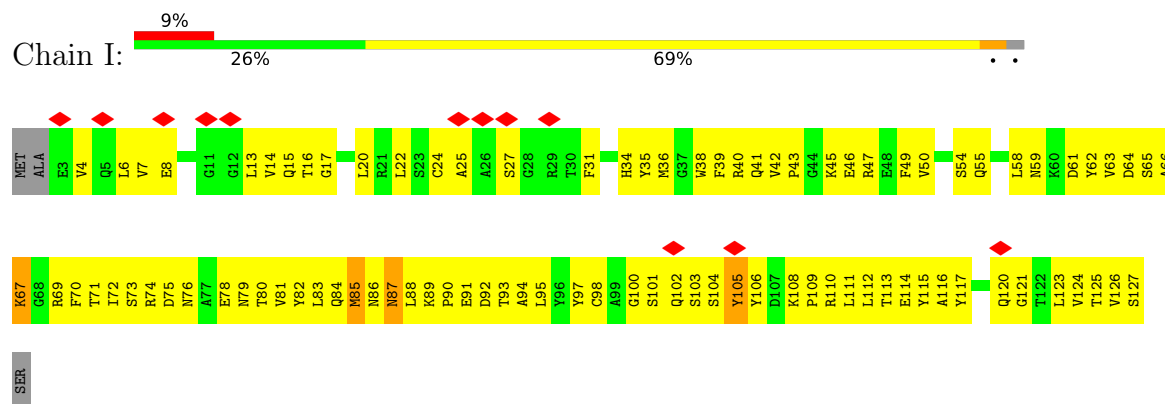
• Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



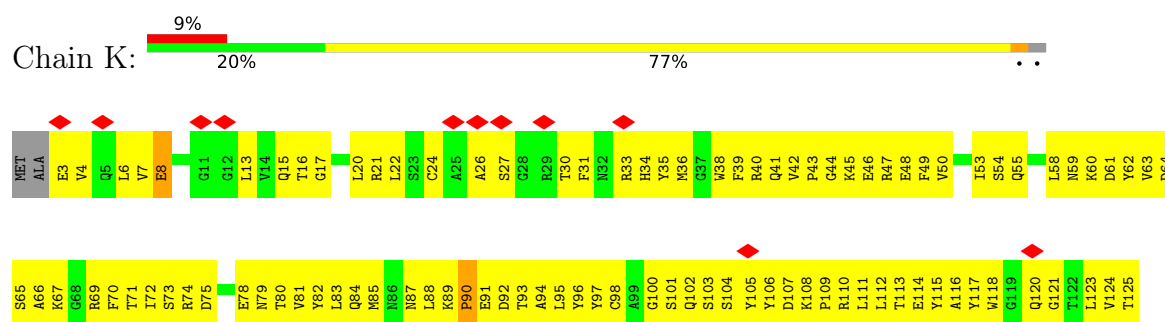
• Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



• Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



• Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)



V126
S127
SER

- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)

Chain M: 

MET ALA E3 V4 Q5 L6 V7 G11 G12 L13 V14 Q15 T16 G17 L20 L21 R21 L22 S23 C24 A25 A26 A27 G28 R29 T30 R33 H34 Y35 M36 G37 W38 F39 R40 Q41 V42 P43 G44 K45 E46 R47 E48 F49 V50 A51 S52 I53 S54 Q55 T56 G57 L58 M59 K60 D61 Y62 V63 V64

S65 A66 K67 G68 R69 F70 T71 I72 S73 R74 D75 E78 N79 T80 V81 Q84 M85 R86 L88 K89 P90 E91 D92 T93 A94 Y95 Y96 Y97 C98 A99 G100 S101 Q102 S103 S104 Y105 Y106 D107 K108 P109 R110 L111 L112 T113 E114 Y115 A116 Y117 W118 G119 Q120 L123 T124 V125 V126 S127

SER

- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)

Chain P: 

MET ALA E3 V4 Q5 L6 V7 E8 G11 G12 L13 V14 Q15 T16 G17 L20 L21 R21 L22 S23 C24 A25 A26 A27 S27 G28 R29 T30 F31 N32 R33 H34 Y35 M36 G37 W38 F39 R40 Q41 V42 P43 G44 K45 E46 R47 E48 F49 V50 I53 S54 Q55 N59 K60 D61 Y62 V63 V64 S65

A66 K67 G68 R69 I72 S73 R74 D75 N76 A77 E78 N79 T80 V81 Q84 M85 R86 L88 K89 P90 E91 D92 T93 A94 Y95 Y96 Y97 C98 A99 G100 S101 Q102 S103 S104 Y105 Y106 D107 K108 P109 R110 L111 L112 T113 E114 Y115 Q120 G121 T122 L123 V124 V125 S127 SER

- Molecule 1: CRP specific recognition heavy chain antibody 3 (HCAb3)

Chain R: 

MET ALA E3 V4 Q5 L6 V7 E8 G11 G12 L13 V14 Q15 T16 G17 L20 L21 R21 L22 S23 C24 A25 A26 A27 S27 G28 R29 T30 F31 H34 Y35 M36 G37 W38 F39 R40 Q41 V42 P43 G44 K45 E46 R47 E48 F49 V50 I53 S54 Q55 L58 M59 K60 D61 Y62 V63 V64 S65

A66 R69 F70 T71 I72 D75 N76 A77 E78 N79 T80 V81 Y82 L83 Q84 M85 R86 L88 K89 P90 E91 D92 T93 A94 Y95 Y96 Y97 C98 A99 G100 S101 Q102 S103 S104 Y105 Y106 D107 K108 P109 R110 L111 L112 T113 E114 Y115 A116 Y117 Q120 G121 T122 L123 V124 V125 S127 SER

- Molecule 2: C-reactive protein

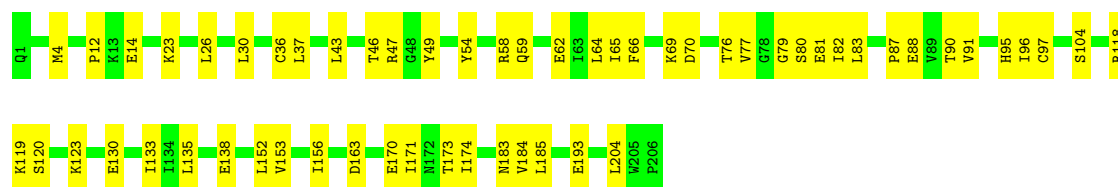
Chain S: 

Q1 K12 P13 K14 E14 S18 L22 L26 L30 V35 C36 C37 L33 L34 L35 L36 L37 L38 L39 L40 L41 L42 L43 L44 L45 L46 L47 L48 L49 L50 L51 L52 L53 L54 L55 L56 L57 L58 L59 L60 L61 L62 L63 L64 L65 L66 L67 L68 L69 L70 L71 L72 L73 L74 L75 L76 L77 L78 L79 L80 L81 L82 L83 L84 L85 L86 L87 L88 L89 L90 L91 L92 L93 L94 L95 L96 L97 L98 L99

R118 K119 S120 L121 K122 Y125 T126 V127 G128 A129 S132 I133 I134 I135 L136 L137 L138 L139 L140 L141 L142 L143 L144 L145 L146 L147 L148 L149 L150 L151 L152 L153 L154 L155 L156 L157 L158 L159 L160 L161 L162 L163 L164 L165 L166 L167 L168 L169 L170 L171 L172 L173 L174 L175 L176 L177 L178 L179 L180 L181 L182 L183 L184 L185 L186 L187 L188 L189 L190 L191 L192 L193 L194 L195 L196 L197 L198 L199 L200 L201 L202 L203 L204 L205 L206 L207 L208 L209 L210 L211 L212 L213 L214 L215 L216 L217 L218 L219 L220 L221 L222 L223 L224 L225 L226 L227 L228 L229 L230 L231 L232 L233 L234 L235 L236 L237 L238 L239 L240 L241 L242 L243 L244 L245 L246 L247 L248 L249 L250 L251 L252 L253 L254 L255 L256 L257 L258 L259 L260 L261 L262 L263 L264 L265 L266 L267 L268 L269 L270 L271 L272 L273 L274 L275 L276 L277 L278 L279 L280 L281 L282 L283 L284 L285 L286 L287 L288 L289 L290 L291 L292 L293 L294 L295 L296 L297 L298 L299 L300 L301 L302 L303 L304 L305 L306 L307 L308 L309 L310 L311 L312 L313 L314 L315 L316 L317 L318 L319 L320 L321 L322 L323 L324 L325 L326 L327 L328 L329 L330 L331 L332 L333 L334 L335 L336 L337 L338 L339 L340 L341 L342 L343 L344 L345 L346 L347 L348 L349 L350 L351 L352 L353 L354 L355 L356 L357 L358 L359 L360 L361 L362 L363 L364 L365 L366 L367 L368 L369 L370 L371 L372 L373 L374 L375 L376 L377 L378 L379 L380 L381 L382 L383 L384 L385 L386 L387 L388 L389 L390 L391 L392 L393 L394 L395 L396 L397 L398 L399 L400 L401 L402 L403 L404 L405 L406 L407 L408 L409 L410 L411 L412 L413 L414 L415 L416 L417 L418 L419 L420 L421 L422 L423 L424 L425 L426 L427 L428 L429 L430 L431 L432 L433 L434 L435 L436 L437 L438 L439 L440 L441 L442 L443 L444 L445 L446 L447 L448 L449 L450 L451 L452 L453 L454 L455 L456 L457 L458 L459 L460 L461 L462 L463 L464 L465 L466 L467 L468 L469 L470 L471 L472 L473 L474 L475 L476 L477 L478 L479 L480 L481 L482 L483 L484 L485 L486 L487 L488 L489 L490 L491 L492 L493 L494 L495 L496 L497 L498 L499 L500 L501 L502 L503 L504 L505 L506 L507 L508 L509 L510 L511 L512 L513 L514 L515 L516 L517 L518 L519 L520 L521 L522 L523 L524 L525 L526 L527 L528 L529 L530 L531 L532 L533 L534 L535 L536 L537 L538 L539 L540 L541 L542 L543 L544 L545 L546 L547 L548 L549 L550 L551 L552 L553 L554 L555 L556 L557 L558 L559 L560 L561 L562 L563 L564 L565 L566 L567 L568 L569 L570 L571 L572 L573 L574 L575 L576 L577 L578 L579 L580 L581 L582 L583 L584 L585 L586 L587 L588 L589 L590 L591 L592 L593 L594 L595 L596 L597 L598 L599 L600 L601 L602 L603 L604 L605 L606 L607 L608 L609 L610 L611 L612 L613 L614 L615 L616 L617 L618 L619 L620 L621 L622 L623 L624 L625 L626 L627 L628 L629 L630 L631 L632 L633 L634 L635 L636 L637 L638 L639 L640 L641 L642 L643 L644 L645 L646 L647 L648 L649 L650 L651 L652 L653 L654 L655 L656 L657 L658 L659 L660 L661 L662 L663 L664 L665 L666 L667 L668 L669 L670 L671 L672 L673 L674 L675 L676 L677 L678 L679 L680 L681 L682 L683 L684 L685 L686 L687 L688 L689 L690 L691 L692 L693 L694 L695 L696 L697 L698 L699 L700 L701 L702 L703 L704 L705 L706 L707 L708 L709 L710 L711 L712 L713 L714 L715 L716 L717 L718 L719 L720 L721 L722 L723 L724 L725 L726 L727 L728 L729 L730 L731 L732 L733 L734 L735 L736 L737 L738 L739 L740 L741 L742 L743 L744 L745 L746 L747 L748 L749 L750 L751 L752 L753 L754 L755 L756 L757 L758 L759 L760 L761 L762 L763 L764 L765 L766 L767 L768 L769 L770 L771 L772 L773 L774 L775 L776 L777 L778 L779 L780 L781 L782 L783 L784 L785 L786 L787 L788 L789 L790 L791 L792 L793 L794 L795 L796 L797 L798 L799 L800 L801 L802 L803 L804 L805 L806 L807 L808 L809 L810 L811 L812 L813 L814 L815 L816 L817 L818 L819 L820 L821 L822 L823 L824 L825 L826 L827 L828 L829 L830 L831 L832 L833 L834 L835 L836 L837 L838 L839 L840 L841 L842 L843 L844 L845 L846 L847 L848 L849 L850 L851 L852 L853 L854 L855 L856 L857 L858 L859 L860 L861 L862 L863 L864 L865 L866 L867 L868 L869 L870 L871 L872 L873 L874 L875 L876 L877 L878 L879 L880 L881 L882 L883 L884 L885 L886 L887 L888 L889 L890 L891 L892 L893 L894 L895 L896 L897 L898 L899 L900 L901 L902 L903 L904 L905 L906 L907 L908 L909 L910 L911 L912 L913 L914 L915 L916 L917 L918 L919 L920 L921 L922 L923 L924 L925 L926 L927 L928 L929 L930 L931 L932 L933 L934 L935 L936 L937 L938 L939 L940 L941 L942 L943 L944 L945 L946 L947 L948 L949 L950 L951 L952 L953 L954 L955 L956 L957 L958 L959 L960 L961 L962 L963 L964 L965 L966 L967 L968 L969 L970 L971 L972 L973 L974 L975 L976 L977 L978 L979 L980 L981 L982 L983 L984 L985 L986 L987 L988 L989 L990 L991 L992 L993 L994 L995 L996 L997 L998 L999

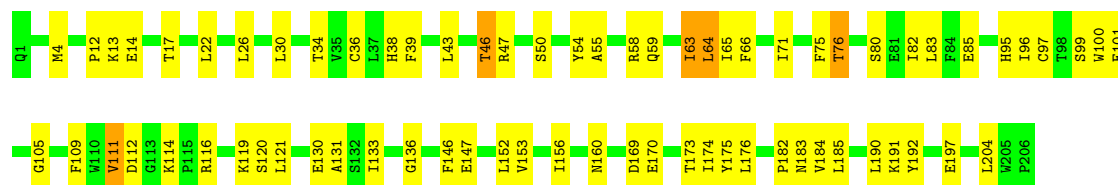
- Molecule 2: C-reactive protein

Chain B:  72% 28%



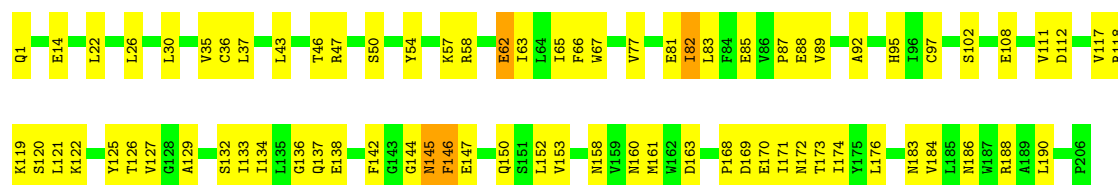
• Molecule 2: C-reactive protein

Chain D:  66% 32% •



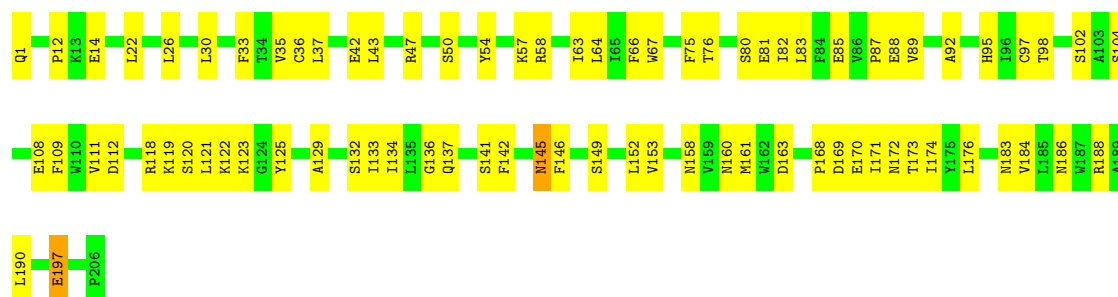
• Molecule 2: C-reactive protein

Chain F:  63% 35% •



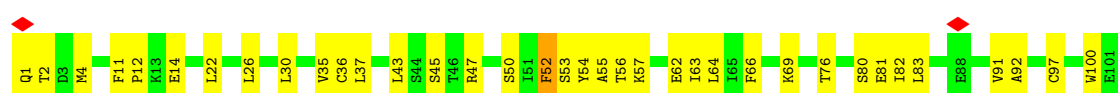
• Molecule 2: C-reactive protein

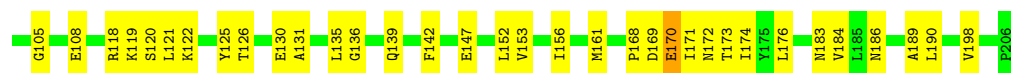
Chain H:  62% 37% •



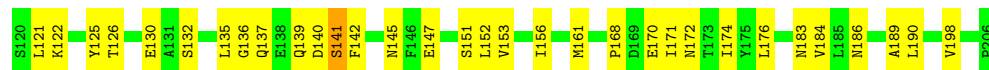
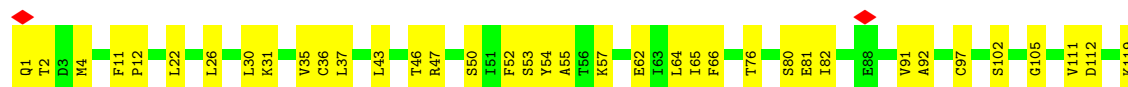
• Molecule 2: C-reactive protein

Chain J:  66% 33% •

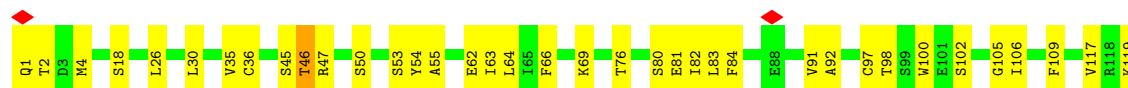




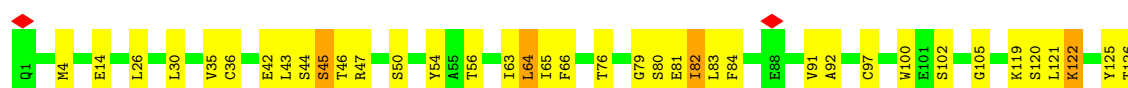
• Molecule 2: C-reactive protein



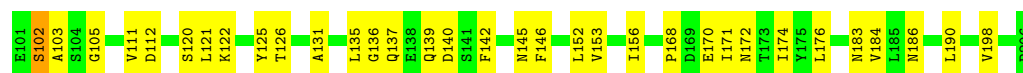
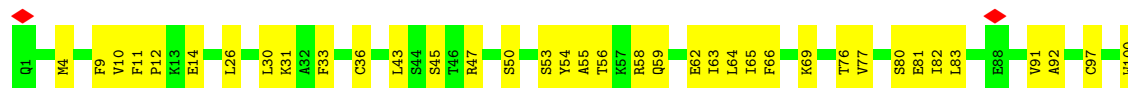
• Molecule 2: C-reactive protein



• Molecule 2: C-reactive protein



• Molecule 2: C-reactive protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	249262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.610	Depositor
Minimum map value	-0.226	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.0959	Depositor
Map size (Å)	218.88, 218.88, 218.88	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.30	0/1000	0.50	0/1352
1	C	0.33	1/1000 (0.1%)	0.60	2/1352 (0.1%)
1	E	0.32	1/1000 (0.1%)	0.43	0/1352
1	G	0.34	0/1000	0.56	1/1352 (0.1%)
1	I	0.39	1/1000 (0.1%)	0.59	3/1352 (0.2%)
1	K	0.44	3/1000 (0.3%)	0.48	0/1352
1	M	0.44	1/1000 (0.1%)	0.65	3/1352 (0.2%)
1	O	0.32	0/1000	0.52	3/1352 (0.2%)
1	P	0.50	5/1000 (0.5%)	0.63	1/1352 (0.1%)
1	R	0.48	2/1000 (0.2%)	0.55	1/1352 (0.1%)
2	B	0.34	1/1678 (0.1%)	0.67	1/2279 (0.0%)
2	D	0.51	7/1678 (0.4%)	0.76	7/2279 (0.3%)
2	F	0.46	4/1678 (0.2%)	0.79	7/2279 (0.3%)
2	H	0.28	0/1678	0.76	4/2279 (0.2%)
2	J	0.48	3/1678 (0.2%)	0.77	6/2279 (0.3%)
2	L	0.41	1/1678 (0.1%)	0.74	6/2279 (0.3%)
2	N	0.44	1/1678 (0.1%)	0.77	5/2279 (0.2%)
2	Q	0.51	6/1678 (0.4%)	0.81	3/2279 (0.1%)
2	S	0.33	1/1678 (0.1%)	0.76	2/2279 (0.1%)
2	T	0.42	2/1678 (0.1%)	0.76	4/2279 (0.2%)
All	All	0.41	40/26780 (0.1%)	0.69	59/36310 (0.2%)

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	46	THR	C-N	8.34	1.45	1.33
1	M	12	GLY	C-N	8.20	1.44	1.33
2	L	53	SER	C-N	-8.10	1.22	1.33
2	D	63	ILE	C-N	8.03	1.44	1.33
2	B	65	ILE	C-N	-7.94	1.23	1.33
2	D	100	TRP	C-N	7.89	1.44	1.33
2	F	144	GLY	C-N	7.68	1.44	1.33
1	E	101	SER	C-N	-7.59	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Q	46	THR	C-N	7.58	1.43	1.33
2	J	53	SER	C-N	-7.20	1.24	1.33
1	P	8	GLU	C-N	-7.17	1.24	1.33
2	D	75	PHE	C-N	6.60	1.42	1.33
1	R	12	GLY	C-N	6.57	1.42	1.33
2	T	10	VAL	C-N	-6.52	1.25	1.33
2	D	64	LEU	C-N	6.51	1.41	1.33
1	P	23	SER	C-N	6.42	1.41	1.33
1	K	82	TYR	C-N	-6.39	1.25	1.33
2	J	52	PHE	C-N	-6.34	1.25	1.33
2	T	9	PHE	C-N	-6.27	1.25	1.33
2	F	65	ILE	C-N	-6.27	1.23	1.33
2	F	82	ILE	C-N	6.14	1.41	1.33
2	D	101	GLU	C-N	6.11	1.42	1.33
2	F	146	PHE	C-N	5.90	1.42	1.33
1	K	90	PRO	C-N	-5.86	1.26	1.33
2	J	170	GLU	C-O	-5.85	1.17	1.24
2	D	76	THR	C-N	5.73	1.41	1.33
2	Q	64	LEU	C-N	-5.72	1.26	1.33
2	D	111	VAL	C-O	-5.62	1.18	1.24
2	Q	189	ALA	C-N	-5.59	1.25	1.33
1	P	20	LEU	C-N	5.57	1.41	1.33
2	Q	65	ILE	C-N	-5.53	1.25	1.33
2	Q	45	SER	C-N	-5.52	1.25	1.33
1	I	87	ASN	C-N	-5.51	1.25	1.33
1	P	107	ASP	C-N	5.50	1.42	1.33
2	S	65	ILE	C-N	-5.47	1.25	1.33
1	R	15	GLN	C-N	5.44	1.40	1.33
2	Q	82	ILE	C-N	5.32	1.40	1.33
1	C	92	ASP	C-N	-5.29	1.26	1.33
1	P	24	CYS	C-N	5.08	1.40	1.33
1	K	8	GLU	C-N	-5.01	1.27	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	105	TYR	N-CA-C	7.75	121.54	109.07
2	J	53	SER	CA-C-N	7.67	133.58	123.00
2	J	53	SER	C-N-CA	7.67	133.58	123.00
2	H	145	ASN	N-CA-C	7.33	121.74	111.92
1	P	106	TYR	N-CA-C	7.20	117.37	107.73
1	C	55	GLN	N-CA-C	-7.05	103.53	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	97	TYR	N-CA-C	6.83	119.66	108.52
1	M	103	SER	N-CA-C	-6.69	104.69	112.92
2	L	53	SER	CA-C-N	6.54	132.02	123.00
2	L	53	SER	C-N-CA	6.54	132.02	123.00
2	N	46	THR	O-C-N	6.48	129.21	121.76
2	F	145	ASN	N-CA-C	6.35	120.64	111.56
2	S	92	ALA	N-CA-C	6.35	113.94	108.22
2	F	92	ALA	N-CA-C	6.33	113.92	108.22
2	H	92	ALA	N-CA-C	6.11	113.72	108.22
1	O	54	SER	N-CA-C	6.11	118.86	110.24
2	N	92	ALA	N-CA-C	5.91	113.54	108.22
2	N	46	THR	OG1-CB-CG2	5.88	121.06	109.30
2	Q	92	ALA	N-CA-C	5.88	113.51	108.22
2	J	62	GLU	N-CA-C	-5.85	104.82	111.14
1	C	54	SER	N-CA-C	5.84	118.70	110.23
2	D	63	ILE	O-C-N	5.73	129.74	122.57
1	M	12	GLY	O-C-N	5.68	130.51	124.15
2	Q	65	ILE	N-CA-C	-5.66	99.59	107.80
2	D	111	VAL	CA-C-O	-5.66	114.05	120.67
2	L	92	ALA	N-CA-C	5.63	113.29	108.22
2	L	141	SER	N-CA-C	-5.63	100.92	108.86
2	T	92	ALA	N-CA-C	5.62	113.27	108.22
1	R	78	GLU	N-CA-C	-5.61	106.20	113.16
2	T	65	ILE	N-CA-C	-5.61	99.67	107.80
2	L	62	GLU	N-CA-C	-5.56	104.86	111.03
2	D	111	VAL	N-CA-C	-5.54	100.50	108.48
2	J	92	ALA	N-CA-C	5.51	113.18	108.22
2	F	65	ILE	N-CA-C	-5.44	99.92	107.80
2	N	62	GLU	N-CA-C	-5.42	105.01	111.03
1	O	55	GLN	N-CA-C	-5.38	104.46	111.02
2	F	144	GLY	O-C-N	5.36	129.06	123.92
2	D	111	VAL	CA-C-N	5.34	129.99	122.46
2	D	111	VAL	C-N-CA	5.34	129.99	122.46
1	I	105	TYR	N-CA-CB	-5.31	102.24	110.57
2	B	65	ILE	N-CA-C	-5.28	100.85	108.87
2	F	62	GLU	N-CA-C	-5.27	106.70	113.23
1	I	106	TYR	N-CA-C	5.25	115.17	108.24
2	N	190	LEU	N-CA-C	5.25	117.64	110.55
2	L	65	ILE	N-CA-C	-5.22	100.22	107.80
2	F	65	ILE	CA-C-N	5.21	131.17	122.73
2	F	65	ILE	C-N-CA	5.21	131.17	122.73
2	D	46	THR	OG1-CB-CG2	5.16	119.61	109.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	53	ILE	N-CA-C	5.13	115.66	108.17
2	S	65	ILE	N-CA-C	-5.11	100.39	107.80
2	J	62	GLU	CA-C-N	-5.10	115.90	122.99
2	J	62	GLU	C-N-CA	-5.10	115.90	122.99
2	H	122	LYS	CA-C-N	-5.09	114.22	121.50
2	H	122	LYS	C-N-CA	-5.09	114.22	121.50
2	T	102	SER	CA-C-N	-5.08	112.96	120.38
2	T	102	SER	C-N-CA	-5.08	112.96	120.38
1	G	105	TYR	N-CA-C	5.08	117.51	109.24
2	D	46	THR	CA-CB-CG2	5.02	119.03	110.50
2	Q	122	LYS	CB-CA-C	-5.02	104.36	112.09

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	980	0	941	160	0
1	C	980	0	939	185	0
1	E	980	0	939	153	0
1	G	980	0	939	160	0
1	I	980	0	941	128	0
1	K	980	0	941	184	0
1	M	980	0	941	164	0
1	O	980	0	941	192	0
1	P	980	0	941	131	0
1	R	980	0	941	145	0
2	B	1632	1592	1595	62	0
2	D	1632	1592	1595	65	0
2	F	1632	1592	1595	75	0
2	H	1632	1592	1595	70	0
2	J	1632	1592	1595	66	0
2	L	1632	1592	1595	64	0
2	N	1632	1592	1595	60	0
2	Q	1632	1592	1595	50	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	S	1632	1592	1595	81	0
2	T	1632	1592	1595	60	0
All	All	26120	15920	25354	2134	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 42.

All (2134) 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)
1:O:105:TYR:O	1:O:106:TYR:CD2	1.84	1.31
1:A:35:TYR:CE2	1:A:102:GLN:HB2	1.65	1.29
1:O:95:LEU:CD1	1:P:13:LEU:HD21	1.61	1.27
1:C:95:LEU:CD1	1:K:13:LEU:HD21	1.63	1.26
1:C:13:LEU:HD21	1:K:95:LEU:CD1	1.68	1.22
1:C:123:LEU:HD13	1:K:13:LEU:HD23	1.18	1.18
1:I:24:CYS:O	1:I:80:THR:HG23	1.34	1.18
1:C:105:TYR:O	1:C:106:TYR:CD2	1.97	1.17
1:G:102:GLN:HG3	1:G:104:SER:O	1.42	1.16
1:E:105:TYR:O	1:E:106:TYR:CD2	1.98	1.15
1:K:104:SER:HB3	1:K:106:TYR:CE2	1.84	1.12
1:C:8:GLU:HG3	1:C:98:CYS:SG	1.90	1.11
1:K:104:SER:HB3	1:K:106:TYR:HE2	0.98	1.11
1:O:95:LEU:HD12	1:P:13:LEU:CD2	1.82	1.10
1:C:95:LEU:HD12	1:K:13:LEU:CD2	1.82	1.10
1:O:8:GLU:HG3	1:O:98:CYS:SG	1.90	1.09
1:K:24:CYS:O	1:K:80:THR:HG23	1.51	1.09
1:O:123:LEU:HD13	1:P:13:LEU:HD23	1.20	1.09
2:Q:82:ILE:HD12	2:Q:121:LEU:HD22	1.31	1.09
1:E:93:THR:HG23	1:E:125:THR:HA	1.32	1.07
1:G:93:THR:OG1	1:G:125:THR:HA	1.54	1.07
2:F:82:ILE:CD1	2:F:121:LEU:HD12	1.84	1.06
1:K:71:THR:O	1:K:83:LEU:HD12	1.53	1.06
2:T:82:ILE:HD12	2:T:121:LEU:HD22	1.34	1.06
1:O:123:LEU:CD1	1:P:13:LEU:HD23	1.86	1.05
1:M:35:TYR:HB2	1:M:108:LYS:HE3	1.38	1.05
1:P:41:GLN:HB2	1:P:47:ARG:HG2	1.33	1.05
2:F:50:SER:O	2:F:152:LEU:HD23	1.55	1.05
2:N:82:ILE:HD12	2:N:121:LEU:HD22	1.32	1.05
2:J:82:ILE:HD12	2:J:121:LEU:HD22	1.35	1.05
2:L:82:ILE:HD12	2:L:121:LEU:HD22	1.35	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:95:LEU:HD12	1:P:13:LEU:HD21	1.08	1.04
1:C:123:LEU:CD1	1:K:13:LEU:HD23	1.86	1.04
1:C:13:LEU:CD2	1:K:95:LEU:CD1	2.36	1.03
2:S:50:SER:O	2:S:152:LEU:HD23	1.56	1.03
1:C:95:LEU:HD12	1:K:13:LEU:HD21	1.08	1.02
1:A:105:TYR:O	1:A:106:TYR:CD1	2.11	1.02
1:R:25:ALA:HA	1:R:80:THR:HG22	1.40	1.02
2:T:64:LEU:HD21	2:T:66:PHE:HB2	1.42	1.01
1:O:105:TYR:O	1:O:106:TYR:CG	2.12	1.00
1:A:4:VAL:HG11	1:A:26:ALA:HB1	1.44	1.00
1:A:89:LYS:HE3	1:A:89:LYS:HA	1.42	1.00
1:E:64:ASP:HA	1:E:67:LYS:NZ	1.76	1.00
1:O:36:MET:HG3	1:O:81:VAL:HG11	1.43	0.99
1:A:35:TYR:CE2	1:A:102:GLN:CB	2.44	0.99
1:I:36:MET:HG3	1:I:81:VAL:HG21	1.40	0.99
1:O:13:LEU:HD23	1:P:123:LEU:HD13	1.44	0.99
2:F:82:ILE:HD12	2:F:121:LEU:HD12	1.39	0.99
1:G:83:LEU:HD22	1:G:85:MET:HE2	1.42	0.99
1:O:4:VAL:HG11	1:O:26:ALA:HB1	1.43	0.98
1:O:54:SER:HA	1:O:108:LYS:HZ3	1.28	0.97
1:C:95:LEU:CD1	1:K:13:LEU:CD2	2.42	0.97
1:E:24:CYS:HB3	1:E:81:VAL:HG22	1.41	0.97
1:E:105:TYR:O	1:E:106:TYR:CG	2.17	0.97
2:B:14:GLU:HG3	2:B:47:ARG:NH2	1.80	0.97
1:E:36:MET:HG3	1:E:81:VAL:HG11	1.46	0.97
1:C:13:LEU:HD21	1:K:95:LEU:HD12	1.47	0.96
2:H:50:SER:O	2:H:152:LEU:HD23	1.65	0.96
1:C:53:ILE:HB	1:C:72:ILE:HD13	1.47	0.96
1:O:54:SER:HA	1:O:108:LYS:CE	1.95	0.96
1:C:4:VAL:HG11	1:C:26:ALA:HB1	1.46	0.96
1:C:64:ASP:HA	1:C:67:LYS:NZ	1.81	0.96
1:M:53:ILE:HB	1:M:72:ILE:HD11	1.48	0.96
2:S:38:HIS:CE1	2:S:205:TRP:CD2	2.54	0.95
2:T:64:LEU:CD2	2:T:66:PHE:HB2	1.96	0.95
1:C:54:SER:HA	1:C:108:LYS:NZ	1.82	0.95
1:C:55:GLN:HA	1:C:74:ARG:NH1	1.79	0.95
1:O:24:CYS:HB3	1:O:81:VAL:HG22	1.49	0.95
1:A:64:ASP:HA	1:A:67:LYS:NZ	1.80	0.95
1:A:35:TYR:HE2	1:A:102:GLN:HB2	0.98	0.95
1:C:54:SER:HA	1:C:108:LYS:CE	1.96	0.95
1:O:24:CYS:HG	1:O:98:CYS:HG	0.99	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:13:LEU:CD2	1:K:95:LEU:HD12	1.94	0.94
1:C:105:TYR:O	1:C:106:TYR:CG	2.19	0.94
1:O:95:LEU:CD1	1:P:13:LEU:CD2	2.40	0.94
1:E:105:TYR:HB3	2:F:83:LEU:HG	1.50	0.94
1:O:54:SER:HA	1:O:108:LYS:NZ	1.82	0.93
1:G:36:MET:HB2	1:G:53:ILE:HG22	1.47	0.93
1:A:24:CYS:HB3	1:A:81:VAL:HG22	1.50	0.93
1:O:107:ASP:HB3	2:S:80:SER:OG	1.69	0.92
2:S:38:HIS:CE1	2:S:205:TRP:CG	2.56	0.92
1:G:42:VAL:HB	1:G:45:LYS:HE3	1.52	0.92
1:G:24:CYS:HB3	1:G:81:VAL:HG22	1.51	0.92
2:B:37:LEU:HD21	2:B:96:ILE:HD11	1.50	0.92
1:K:54:SER:HB3	1:K:108:LYS:HE2	1.51	0.92
1:E:42:VAL:HB	1:E:45:LYS:HE3	1.53	0.91
1:E:64:ASP:HA	1:E:67:LYS:HZ3	1.31	0.91
2:Q:50:SER:O	2:Q:152:LEU:HD23	1.70	0.91
1:K:44:GLY:O	1:K:45:LYS:HG3	1.71	0.91
1:M:89:LYS:HE2	1:M:91:GLU:OE1	1.71	0.91
1:E:4:VAL:HG11	1:E:26:ALA:HB1	1.53	0.91
1:A:36:MET:HB2	1:A:53:ILE:HG22	1.50	0.90
2:J:100:TRP:CH2	2:J:102:SER:HB2	2.06	0.90
1:O:91:GLU:OE1	1:O:91:GLU:N	2.03	0.90
1:A:42:VAL:HB	1:A:45:LYS:HE3	1.52	0.90
2:N:100:TRP:CH2	2:N:102:SER:HB2	2.06	0.90
1:M:53:ILE:HB	1:M:72:ILE:CD1	2.01	0.90
1:I:54:SER:HB3	1:I:108:LYS:HE2	1.52	0.90
1:R:101:SER:HB3	1:R:116:ALA:H	1.36	0.90
1:C:24:CYS:HB3	1:C:81:VAL:HG22	1.53	0.89
1:G:36:MET:HB2	1:G:53:ILE:CG2	2.02	0.89
2:H:64:LEU:CD2	2:H:66:PHE:HB2	2.02	0.89
1:I:120:GLN:OE1	1:I:120:GLN:N	2.04	0.89
1:C:62:TYR:HB2	1:C:67:LYS:HG2	1.52	0.89
1:G:64:ASP:HA	1:G:67:LYS:NZ	1.88	0.89
1:P:120:GLN:OE1	1:P:120:GLN:N	2.04	0.89
1:A:36:MET:HG3	1:A:81:VAL:HG11	1.54	0.89
2:B:14:GLU:HG3	2:B:47:ARG:HH22	1.37	0.89
1:E:55:GLN:HE21	2:F:83:LEU:HD23	1.36	0.89
1:G:13:LEU:HD21	1:R:95:LEU:CD1	2.03	0.89
1:I:101:SER:HB3	1:I:116:ALA:H	1.36	0.89
1:P:40:ARG:HH12	1:P:92:ASP:HA	1.38	0.89
2:J:136:GLY:HA2	2:J:152:LEU:HG	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:136:GLY:HA2	2:N:152:LEU:HG	1.53	0.88
1:O:8:GLU:CG	1:O:98:CYS:SG	2.62	0.88
1:A:36:MET:HB2	1:A:53:ILE:CG2	2.03	0.88
2:J:50:SER:O	2:J:152:LEU:HD23	1.74	0.88
1:K:104:SER:CB	1:K:106:TYR:HE2	1.84	0.88
1:G:36:MET:HG3	1:G:81:VAL:HG11	1.54	0.88
1:R:88:LEU:HB3	1:R:126:VAL:HG21	1.56	0.88
1:R:93:THR:HG23	1:R:125:THR:HA	1.55	0.88
1:M:36:MET:HB2	1:M:53:ILE:CG2	2.04	0.87
2:T:50:SER:O	2:T:152:LEU:HD23	1.74	0.87
2:L:136:GLY:HA2	2:L:152:LEU:HG	1.54	0.87
1:G:54:SER:HA	1:G:108:LYS:CE	2.05	0.87
1:A:64:ASP:HA	1:A:67:LYS:HZ3	1.38	0.87
1:K:60:LYS:HD2	1:K:72:ILE:HG23	1.55	0.87
1:R:105:TYR:O	1:R:106:TYR:CD2	2.27	0.87
2:H:64:LEU:HD21	2:H:66:PHE:HB2	1.55	0.86
1:K:8:GLU:OE2	1:K:121:GLY:CA	2.23	0.86
2:S:140:ASP:HB2	2:S:145:ASN:CG	1.99	0.86
1:A:13:LEU:HD23	1:M:123:LEU:HD13	1.58	0.86
2:Q:136:GLY:HA2	2:Q:152:LEU:HG	1.55	0.86
1:M:95:LEU:HD23	1:M:123:LEU:HA	1.56	0.86
1:G:91:GLU:OE1	1:G:91:GLU:N	2.07	0.85
1:G:102:GLN:CG	1:G:104:SER:O	2.24	0.85
1:O:54:SER:HA	1:O:108:LYS:HE2	1.58	0.85
1:K:120:GLN:OE1	1:K:120:GLN:N	2.09	0.85
1:O:45:LYS:NZ	1:O:46:GLU:O	2.09	0.85
1:G:107:ASP:HB3	2:H:80:SER:OG	1.76	0.85
1:R:60:LYS:CA	1:R:108:LYS:HE3	2.06	0.85
1:A:35:TYR:HE2	1:A:102:GLN:CB	1.84	0.84
1:K:101:SER:HB3	1:K:116:ALA:H	1.42	0.84
1:M:78:GLU:O	1:M:79:ASN:OD1	1.95	0.84
2:D:50:SER:O	2:D:152:LEU:HD23	1.77	0.84
1:R:22:LEU:HD13	1:R:85:MET:HE1	1.58	0.84
1:E:62:TYR:HB2	1:E:67:LYS:HG2	1.60	0.84
2:T:136:GLY:HA2	2:T:152:LEU:HG	1.57	0.84
1:P:63:VAL:HA	1:P:110:ARG:HH12	1.41	0.84
1:G:45:LYS:NZ	1:G:46:GLU:O	2.11	0.83
1:O:64:ASP:HA	1:O:67:LYS:NZ	1.92	0.83
2:L:50:SER:O	2:L:152:LEU:HD23	1.78	0.83
1:P:93:THR:HG23	1:P:125:THR:HA	1.61	0.83
1:A:45:LYS:NZ	1:A:46:GLU:O	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:35:TYR:CD2	1:G:102:GLN:HB2	2.12	0.83
1:M:120:GLN:OE1	1:M:120:GLN:N	2.10	0.83
1:G:4:VAL:HG11	1:G:26:ALA:HB1	1.60	0.83
1:C:13:LEU:HD21	1:K:95:LEU:HD13	1.58	0.83
1:K:109:PRO:HG2	1:K:114:GLU:HG3	1.60	0.83
2:N:50:SER:O	2:N:152:LEU:HD23	1.76	0.83
1:M:88:LEU:HB3	1:M:126:VAL:HG21	1.60	0.82
1:I:24:CYS:O	1:I:80:THR:CG2	2.24	0.82
1:M:93:THR:HG23	1:M:125:THR:HA	1.59	0.82
1:C:105:TYR:CZ	2:D:119:LYS:HD2	2.15	0.82
1:G:64:ASP:HA	1:G:67:LYS:HZ3	1.43	0.82
1:K:8:GLU:OE2	1:K:121:GLY:HA2	1.78	0.82
1:G:62:TYR:HB2	1:G:67:LYS:HG2	1.60	0.82
1:K:36:MET:HA	1:K:36:MET:HE3	1.62	0.82
1:O:36:MET:HA	1:O:36:MET:HE3	1.61	0.82
1:G:36:MET:HE3	1:G:36:MET:HA	1.62	0.82
2:T:100:TRP:CH2	2:T:102:SER:HB3	2.15	0.82
1:E:101:SER:HB2	1:E:116:ALA:H	1.44	0.81
1:M:63:VAL:HA	1:M:110:ARG:HH12	1.45	0.81
1:R:36:MET:HE3	1:R:36:MET:HA	1.61	0.81
1:A:102:GLN:HE21	1:A:104:SER:HB2	1.45	0.81
1:E:45:LYS:NZ	1:E:46:GLU:O	2.13	0.81
1:R:63:VAL:HA	1:R:110:ARG:HH12	1.44	0.81
1:C:120:GLN:OE1	1:C:120:GLN:N	2.13	0.81
1:M:34:HIS:HA	1:M:102:GLN:HB3	1.61	0.81
1:C:54:SER:HB2	1:C:59:ASN:O	1.81	0.80
1:M:41:GLN:HB3	1:M:97:TYR:HE2	1.46	0.80
2:N:4:MET:HG3	2:N:190:LEU:HD21	1.62	0.80
1:R:105:TYR:O	1:R:106:TYR:CG	2.35	0.80
1:C:8:GLU:CG	1:C:98:CYS:SG	2.70	0.80
1:I:17:GLY:HA2	1:I:87:ASN:HA	1.62	0.80
1:I:42:VAL:HB	1:I:45:LYS:HD2	1.64	0.80
1:O:35:TYR:HB2	1:O:108:LYS:HE3	1.62	0.80
1:C:45:LYS:NZ	1:C:46:GLU:O	2.14	0.80
1:K:24:CYS:SG	1:K:98:CYS:CB	2.70	0.80
1:K:71:THR:HG22	1:K:84:GLN:HB3	1.62	0.80
1:C:64:ASP:HA	1:C:67:LYS:HZ3	1.44	0.80
1:M:89:LYS:HB3	1:M:90:PRO:HD2	1.62	0.80
2:N:187:TRP:HA	2:N:190:LEU:HD23	1.64	0.80
1:A:22:LEU:HG	1:A:85:MET:HE1	1.63	0.79
1:K:4:VAL:HA	1:K:27:SER:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:36:MET:HG3	1:P:81:VAL:HG21	1.65	0.79
1:A:78:GLU:OE1	1:A:78:GLU:N	2.15	0.79
1:G:93:THR:HG1	1:G:125:THR:HA	1.46	0.79
1:R:42:VAL:HB	1:R:45:LYS:HD2	1.65	0.79
2:S:183:ASN:OD1	2:S:184:VAL:HG23	1.83	0.78
1:E:54:SER:HB3	1:E:108:LYS:HE2	1.65	0.78
1:M:35:TYR:HB2	1:M:108:LYS:CE	2.12	0.78
2:B:26:LEU:HD21	2:B:30:LEU:HD21	1.64	0.78
1:G:13:LEU:CD2	1:R:95:LEU:CD1	2.61	0.78
2:F:183:ASN:OD1	2:F:184:VAL:HG23	1.84	0.78
1:A:55:GLN:HA	1:A:74:ARG:NH1	1.98	0.78
1:C:54:SER:HB3	1:C:57:GLY:CA	2.13	0.78
1:E:36:MET:HA	1:E:36:MET:HE3	1.65	0.78
1:A:54:SER:HA	1:A:108:LYS:NZ	1.99	0.78
1:G:54:SER:HA	1:G:108:LYS:NZ	1.99	0.78
1:C:46:GLU:N	1:C:46:GLU:OE2	2.17	0.78
1:G:35:TYR:CE2	1:G:102:GLN:HB2	2.19	0.78
1:E:24:CYS:HB3	1:E:81:VAL:CG2	2.14	0.78
1:C:53:ILE:HB	1:C:72:ILE:CD1	2.14	0.78
1:K:88:LEU:HB3	1:K:126:VAL:HG21	1.65	0.78
1:A:36:MET:HA	1:A:36:MET:HE3	1.66	0.77
2:F:54:TYR:HB3	2:F:63:ILE:HB	1.66	0.77
1:R:36:MET:HG3	1:R:81:VAL:HG21	1.67	0.77
2:B:184:VAL:O	2:B:185:LEU:HD23	1.85	0.77
1:R:60:LYS:HA	1:R:108:LYS:HE3	1.64	0.77
1:I:63:VAL:HA	1:I:110:ARG:HH12	1.50	0.77
2:H:183:ASN:OD1	2:H:184:VAL:HG23	1.84	0.77
1:I:109:PRO:HG2	1:I:114:GLU:HG3	1.66	0.77
1:K:63:VAL:HA	1:K:110:ARG:HH12	1.49	0.77
1:M:100:GLY:HA2	1:M:115:TYR:HD2	1.48	0.77
1:C:3:GLU:OE1	1:C:3:GLU:N	2.18	0.77
1:I:93:THR:HG23	1:I:125:THR:HA	1.65	0.77
1:A:24:CYS:HB3	1:A:81:VAL:CG2	2.15	0.77
1:C:36:MET:HG3	1:C:81:VAL:HG11	1.67	0.77
2:B:64:LEU:HD11	2:B:138:GLU:HG2	1.68	0.76
1:E:93:THR:CG2	1:E:125:THR:HA	2.14	0.76
1:R:25:ALA:HA	1:R:80:THR:CG2	2.15	0.76
1:O:36:MET:HE1	1:O:100:GLY:HA3	1.68	0.76
1:K:107:ASP:HA	1:K:108:LYS:HZ2	1.50	0.76
1:A:3:GLU:OE1	1:A:3:GLU:N	2.19	0.76
2:B:64:LEU:CD2	2:B:66:PHE:HB2	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:37:LEU:CD2	2:B:96:ILE:HD11	2.14	0.76
2:B:49:TYR:CD2	2:B:152:LEU:HD13	2.20	0.76
1:M:109:PRO:HG2	1:M:114:GLU:HG3	1.65	0.76
1:P:88:LEU:HB3	1:P:126:VAL:HG21	1.66	0.76
1:R:4:VAL:HA	1:R:27:SER:O	1.85	0.76
2:S:82:ILE:HD12	2:S:121:LEU:HD22	1.67	0.75
1:E:41:GLN:O	1:E:94:ALA:HB1	1.87	0.75
1:K:93:THR:HG23	1:K:125:THR:HA	1.68	0.75
1:O:3:GLU:OE1	1:O:3:GLU:N	2.19	0.75
1:C:123:LEU:HD13	1:K:13:LEU:CD2	2.10	0.75
2:F:22:LEU:HD22	2:F:190:LEU:HD11	1.68	0.75
1:P:41:GLN:HB3	1:P:97:TYR:HE1	1.50	0.75
1:E:3:GLU:OE1	1:E:3:GLU:N	2.19	0.75
1:R:83:LEU:HD22	1:R:85:MET:HE2	1.68	0.75
1:E:30:THR:O	1:E:30:THR:HG22	1.87	0.75
1:A:30:THR:HG22	1:A:30:THR:O	1.84	0.75
1:E:34:HIS:HA	1:E:102:GLN:O	1.87	0.75
1:E:36:MET:HE1	1:E:100:GLY:HA3	1.68	0.75
1:C:78:GLU:O	1:C:80:THR:HG23	1.87	0.75
1:A:13:LEU:HD11	1:M:43:PRO:HD3	1.69	0.75
1:K:36:MET:HG3	1:K:81:VAL:HG21	1.69	0.75
2:T:31:LYS:HG3	2:T:102:SER:OG	1.86	0.74
1:G:13:LEU:HD23	1:R:123:LEU:HD13	1.69	0.74
1:O:30:THR:O	1:O:30:THR:HG22	1.87	0.74
1:G:46:GLU:OE1	1:G:46:GLU:N	2.16	0.74
2:J:14:GLU:HG3	2:J:47:ARG:NH2	2.03	0.74
2:S:22:LEU:HD22	2:S:190:LEU:HD11	1.67	0.74
1:C:36:MET:HE2	1:C:36:MET:HA	1.67	0.74
1:E:55:GLN:NE2	2:F:83:LEU:HD23	2.02	0.74
1:C:105:TYR:HB3	2:D:83:LEU:HG	1.69	0.74
1:G:78:GLU:O	1:G:80:THR:HG23	1.87	0.74
1:K:20:LEU:HD13	1:K:22:LEU:HD11	1.68	0.74
1:A:93:THR:HG23	1:A:125:THR:HA	1.70	0.74
1:E:84:GLN:NE2	1:E:86:ASN:OD1	2.21	0.74
1:A:35:TYR:CD2	1:A:102:GLN:HB3	2.23	0.74
1:O:24:CYS:HB3	1:O:81:VAL:CG2	2.18	0.73
1:C:53:ILE:O	1:C:108:LYS:HE3	1.88	0.73
1:C:54:SER:HB3	1:C:57:GLY:N	2.03	0.73
1:M:35:TYR:HA	1:M:74:ARG:HH22	1.53	0.73
1:C:30:THR:HG22	1:C:30:THR:O	1.86	0.73
1:C:93:THR:HG23	1:C:125:THR:HA	1.69	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:MET:HA	1:I:36:MET:HE3	1.68	0.73
1:P:42:VAL:HG13	1:P:43:PRO:HD2	1.70	0.73
1:G:24:CYS:HB3	1:G:81:VAL:CG2	2.18	0.73
1:A:107:ASP:HB3	2:B:80:SER:OG	1.88	0.73
2:Q:187:TRP:HA	2:Q:190:LEU:HD23	1.69	0.73
1:C:42:VAL:HB	1:C:45:LYS:HE3	1.71	0.73
1:G:3:GLU:N	1:G:3:GLU:OE1	2.22	0.73
1:M:35:TYR:CB	1:M:108:LYS:HE3	2.18	0.73
2:S:87:PRO:HG2	2:S:88:GLU:OE1	1.88	0.73
1:A:41:GLN:O	1:A:94:ALA:HB1	1.88	0.73
1:M:107:ASP:HB3	2:N:80:SER:OG	1.89	0.73
1:G:41:GLN:O	1:G:94:ALA:HB1	1.89	0.73
2:H:158:ASN:O	2:H:160:ASN:ND2	2.22	0.72
1:K:13:LEU:HD12	1:K:13:LEU:O	1.89	0.72
1:P:13:LEU:HD12	1:P:13:LEU:O	1.89	0.72
1:R:38:TRP:CG	1:R:83:LEU:HD12	2.24	0.72
2:B:120:SER:OG	2:D:13:LYS:NZ	2.22	0.72
1:E:78:GLU:O	1:E:80:THR:HG23	1.87	0.72
2:H:22:LEU:HD22	2:H:190:LEU:HD11	1.70	0.72
1:O:4:VAL:CG1	1:O:26:ALA:HB1	2.17	0.72
1:M:36:MET:HG3	1:M:81:VAL:HG21	1.70	0.72
1:P:91:GLU:OE1	1:P:91:GLU:N	2.18	0.72
1:R:41:GLN:HB3	1:R:97:TYR:HE1	1.55	0.72
1:O:89:LYS:HA	1:O:89:LYS:HE3	1.70	0.72
1:O:123:LEU:HD13	1:P:13:LEU:CD2	2.10	0.72
1:G:42:VAL:HG13	1:G:43:PRO:HD2	1.72	0.72
1:E:64:ASP:CA	1:E:67:LYS:HZ3	2.02	0.72
2:H:136:GLY:HA2	2:H:152:LEU:HG	1.71	0.72
1:I:42:VAL:HG13	1:I:43:PRO:HD2	1.71	0.72
1:K:41:GLN:O	1:K:94:ALA:HB1	1.90	0.72
1:K:42:VAL:HG13	1:K:43:PRO:HD2	1.69	0.72
2:H:87:PRO:HG2	2:H:88:GLU:OE1	1.90	0.71
1:I:41:GLN:HB3	1:I:97:TYR:HE1	1.53	0.71
2:S:158:ASN:O	2:S:160:ASN:ND2	2.23	0.71
1:E:35:TYR:CE2	1:E:102:GLN:HB3	2.25	0.71
1:G:30:THR:O	1:G:30:THR:HG22	1.88	0.71
1:G:55:GLN:HA	1:G:74:ARG:NH1	2.06	0.71
1:O:84:GLN:NE2	1:O:86:ASN:OD1	2.23	0.71
2:F:145:ASN:O	2:F:145:ASN:CG	2.33	0.71
1:R:42:VAL:HG13	1:R:43:PRO:HD2	1.71	0.71
1:P:109:PRO:HG2	1:P:114:GLU:HG3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:HG13	1:A:43:PRO:HD2	1.72	0.71
1:E:35:TYR:CE2	1:E:102:GLN:CB	2.74	0.71
2:H:82:ILE:HD11	2:H:121:LEU:HD13	1.72	0.71
1:O:40:ARG:NH2	1:O:96:TYR:OH	2.24	0.71
2:T:14:GLU:HG3	2:T:47:ARG:NH2	2.05	0.71
2:F:87:PRO:HG2	2:F:88:GLU:OE1	1.89	0.70
1:A:54:SER:HA	1:A:108:LYS:CE	2.20	0.70
1:E:42:VAL:HG13	1:E:43:PRO:HD2	1.72	0.70
1:A:35:TYR:CD2	1:A:102:GLN:CB	2.75	0.70
1:C:38:TRP:CZ3	1:C:98:CYS:HB3	2.25	0.70
1:A:89:LYS:HA	1:A:89:LYS:CE	2.19	0.70
1:E:55:GLN:HA	1:E:74:ARG:NH1	2.06	0.70
1:C:42:VAL:HG13	1:C:43:PRO:HD2	1.74	0.70
1:P:59:ASN:ND2	2:Q:79:GLY:O	2.24	0.70
1:O:36:MET:HG3	1:O:81:VAL:CG1	2.21	0.70
1:R:54:SER:N	1:R:108:LYS:HD3	2.07	0.70
1:E:64:ASP:CA	1:E:67:LYS:NZ	2.55	0.70
1:C:62:TYR:HB2	1:C:67:LYS:CG	2.22	0.70
1:O:41:GLN:O	1:O:94:ALA:HB1	1.91	0.70
1:O:105:TYR:C	1:O:106:TYR:CD2	2.70	0.70
1:K:100:GLY:HA2	1:K:115:TYR:HD2	1.57	0.70
1:M:3:GLU:OE2	1:M:34:HIS:CE1	2.44	0.70
1:R:35:TYR:HE1	1:R:102:GLN:HB3	1.57	0.70
1:C:13:LEU:HD23	1:K:123:LEU:HD13	1.74	0.69
1:C:41:GLN:O	1:C:94:ALA:HB1	1.91	0.69
1:G:93:THR:O	1:G:93:THR:HG23	1.91	0.69
1:O:105:TYR:O	1:O:106:TYR:CE2	2.44	0.69
2:Q:172:ASN:O	2:Q:176:LEU:HD23	1.93	0.69
1:C:54:SER:HA	1:C:108:LYS:HZ3	1.54	0.69
1:G:42:VAL:CB	1:G:45:LYS:HE3	2.22	0.69
2:B:46:THR:HG22	2:B:47:ARG:H	1.57	0.69
1:E:35:TYR:HE2	1:E:102:GLN:HB2	1.55	0.69
1:O:42:VAL:HG13	1:O:43:PRO:HD2	1.73	0.69
1:O:64:ASP:HA	1:O:67:LYS:HZ1	1.56	0.69
1:K:24:CYS:HG	1:K:98:CYS:HG	0.76	0.69
1:M:4:VAL:HG11	1:M:26:ALA:HB1	1.73	0.69
1:M:41:GLN:HB3	1:M:97:TYR:CE2	2.27	0.69
1:O:101:SER:HB3	1:O:116:ALA:H	1.57	0.69
1:K:41:GLN:HB3	1:K:97:TYR:HE1	1.57	0.69
1:O:93:THR:HG21	1:O:126:VAL:H	1.56	0.69
1:C:64:ASP:CA	1:C:67:LYS:NZ	2.55	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:36:MET:CG	1:I:81:VAL:HG21	2.19	0.69
1:K:40:ARG:HG3	1:K:96:TYR:HE1	1.57	0.69
2:N:64:LEU:HD21	2:N:66:PHE:HB2	1.75	0.69
1:O:30:THR:CG2	1:O:33:ARG:HB2	2.23	0.69
1:R:88:LEU:CB	1:R:126:VAL:HG21	2.22	0.69
1:O:31:PHE:CE2	1:O:79:ASN:HA	2.28	0.68
1:A:40:ARG:NH2	1:A:96:TYR:OH	2.26	0.68
1:K:54:SER:CB	1:K:108:LYS:HE2	2.23	0.68
2:F:158:ASN:O	2:F:160:ASN:ND2	2.27	0.68
1:M:36:MET:HB2	1:M:53:ILE:HG22	1.76	0.68
2:N:172:ASN:O	2:N:176:LEU:HD23	1.94	0.68
1:M:39:PHE:CD1	1:M:49:PHE:HA	2.27	0.68
2:J:35:VAL:HG22	2:J:161:MET:HG3	1.74	0.68
1:P:39:PHE:CD1	1:P:49:PHE:HA	2.28	0.68
1:C:13:LEU:HD23	1:K:95:LEU:HD12	1.75	0.68
1:K:24:CYS:SG	1:K:98:CYS:HB2	2.34	0.68
1:K:30:THR:OG1	1:K:34:HIS:NE2	2.24	0.68
1:K:24:CYS:HG	1:K:98:CYS:CB	2.05	0.68
2:T:53:SER:HB3	2:T:139:GLN:HE21	1.59	0.68
1:O:54:SER:N	1:O:108:LYS:HE2	2.08	0.68
1:C:111:LEU:HB2	1:C:114:GLU:OE2	1.94	0.68
1:K:24:CYS:HB2	1:K:38:TRP:CH2	2.29	0.68
1:M:93:THR:CG2	1:M:125:THR:HA	2.24	0.68
1:O:42:VAL:HB	1:O:45:LYS:HE3	1.75	0.68
1:O:120:GLN:OE1	1:O:120:GLN:N	2.19	0.68
2:S:136:GLY:HA2	2:S:152:LEU:HG	1.76	0.68
1:A:22:LEU:HG	1:A:85:MET:CE	2.24	0.68
1:C:24:CYS:HB3	1:C:81:VAL:CG2	2.22	0.68
1:E:93:THR:HG23	1:E:125:THR:CA	2.19	0.68
2:L:172:ASN:O	2:L:176:LEU:HD23	1.94	0.68
1:M:22:LEU:HD13	1:M:85:MET:HE1	1.75	0.68
1:P:35:TYR:CE1	1:P:101:SER:HB2	2.28	0.68
1:A:111:LEU:HB2	1:A:114:GLU:OE2	1.93	0.68
1:E:40:ARG:HG3	1:E:96:TYR:HE1	1.59	0.68
2:J:1:GLN:OE1	2:J:1:GLN:N	2.22	0.68
1:K:24:CYS:C	1:K:80:THR:HG23	2.17	0.68
1:K:44:GLY:O	1:K:45:LYS:CG	2.40	0.68
1:R:93:THR:CG2	1:R:125:THR:HA	2.22	0.68
1:R:101:SER:OG	1:R:115:TYR:HA	1.93	0.68
1:A:59:ASN:ND2	2:B:79:GLY:O	2.27	0.68
1:M:54:SER:HA	1:M:108:LYS:CE	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:64:LEU:HD21	2:L:66:PHE:HB2	1.75	0.67
2:T:172:ASN:O	2:T:176:LEU:HD23	1.93	0.67
1:C:64:ASP:CA	1:C:67:LYS:HZ3	2.06	0.67
1:E:111:LEU:HB2	1:E:114:GLU:OE2	1.93	0.67
1:O:95:LEU:HD13	1:P:13:LEU:HD21	1.71	0.67
1:C:105:TYR:CD1	2:D:82:ILE:HG23	2.28	0.67
1:C:107:ASP:HB3	2:D:80:SER:OG	1.94	0.67
1:K:107:ASP:HB3	2:L:80:SER:OG	1.94	0.67
2:N:53:SER:HB3	2:N:139:GLN:HE21	1.58	0.67
1:A:64:ASP:HA	1:A:67:LYS:HZ1	1.58	0.67
1:G:40:ARG:HG3	1:G:96:TYR:HE1	1.60	0.67
2:L:91:VAL:O	2:L:91:VAL:HG13	1.94	0.67
1:G:13:LEU:CD2	1:R:95:LEU:HD12	2.22	0.67
1:K:21:ARG:HE	1:K:84:GLN:HB2	1.58	0.67
1:O:53:ILE:C	1:O:108:LYS:HE2	2.18	0.67
2:S:38:HIS:CE1	2:S:205:TRP:CE3	2.83	0.67
1:A:62:TYR:HB2	1:A:67:LYS:HG2	1.75	0.67
1:E:15:GLN:NE2	1:E:127:SER:OG	2.28	0.67
2:J:172:ASN:O	2:J:176:LEU:HD23	1.94	0.67
1:M:100:GLY:HA2	1:M:115:TYR:CD2	2.30	0.67
1:R:62:TYR:CZ	1:R:72:ILE:HG22	2.29	0.67
1:R:62:TYR:HE2	1:R:71:THR:HA	1.59	0.67
1:O:40:ARG:HG3	1:O:96:TYR:HE1	1.60	0.67
1:O:78:GLU:O	1:O:80:THR:HG23	1.95	0.67
1:I:75:ASP:HB3	1:I:78:GLU:OE2	1.94	0.67
1:M:88:LEU:CB	1:M:126:VAL:HG21	2.24	0.67
1:A:40:ARG:HG3	1:A:96:TYR:HE1	1.60	0.67
1:E:4:VAL:CG1	1:E:26:ALA:HB1	2.25	0.67
1:I:65:SER:O	1:I:69:ARG:NH1	2.26	0.67
1:K:114:GLU:OE1	1:K:114:GLU:N	2.25	0.67
2:S:140:ASP:HB2	2:S:145:ASN:OD1	1.95	0.67
1:A:32:ASN:HB3	1:A:76:ASN:HD21	1.59	0.67
1:A:4:VAL:CG1	1:A:26:ALA:HB1	2.22	0.67
1:C:15:GLN:NE2	1:C:127:SER:OG	2.28	0.67
1:G:15:GLN:NE2	1:G:127:SER:OG	2.28	0.67
1:A:30:THR:CG2	1:A:33:ARG:HB2	2.25	0.66
1:M:62:TYR:CZ	1:M:72:ILE:HG22	2.30	0.66
1:M:95:LEU:HD23	1:M:123:LEU:CA	2.25	0.66
1:K:20:LEU:H	1:K:84:GLN:HE22	1.43	0.66
1:A:15:GLN:NE2	1:A:127:SER:OG	2.28	0.66
1:C:4:VAL:CG1	1:C:26:ALA:HB1	2.24	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:64:LEU:HD21	2:Q:66:PHE:HB2	1.78	0.66
1:R:36:MET:HG3	1:R:81:VAL:CG2	2.25	0.66
1:O:53:ILE:HB	1:O:72:ILE:HD13	1.77	0.66
1:O:54:SER:CA	1:O:108:LYS:HE2	2.24	0.66
2:B:64:LEU:HD23	2:B:66:PHE:HB2	1.77	0.66
1:C:101:SER:CB	1:C:116:ALA:H	2.09	0.66
1:E:36:MET:HG3	1:E:81:VAL:CG1	2.24	0.66
1:E:42:VAL:CB	1:E:45:LYS:HE3	2.23	0.66
1:G:38:TRP:CD1	1:G:83:LEU:HD12	2.30	0.66
2:J:121:LEU:HD12	2:J:122:LYS:N	2.11	0.66
2:T:121:LEU:HD12	2:T:122:LYS:N	2.11	0.66
1:E:13:LEU:HD21	1:I:95:LEU:HD22	1.76	0.66
1:M:91:GLU:OE2	1:M:91:GLU:N	2.21	0.66
1:R:41:GLN:HB2	1:R:47:ARG:HG2	1.77	0.66
2:J:35:VAL:HG22	2:J:161:MET:CG	2.26	0.66
1:O:54:SER:HB2	1:O:59:ASN:HB2	1.76	0.66
1:A:42:VAL:CB	1:A:45:LYS:HE3	2.22	0.66
1:I:101:SER:OG	1:I:115:TYR:HA	1.96	0.66
2:S:38:HIS:ND1	2:S:205:TRP:CD2	2.63	0.66
1:C:63:VAL:C	1:C:67:LYS:HZ3	2.03	0.66
1:E:105:TYR:C	1:E:106:TYR:CD2	2.73	0.66
2:F:82:ILE:HD12	2:F:121:LEU:CD1	2.19	0.66
1:I:8:GLU:H	1:I:120:GLN:HE22	1.43	0.66
2:T:54:TYR:HB3	2:T:63:ILE:HB	1.77	0.66
1:O:64:ASP:HA	1:O:67:LYS:HZ3	1.61	0.65
1:P:31:PHE:CG	1:P:79:ASN:HB2	2.31	0.65
1:G:4:VAL:CG1	1:G:26:ALA:HB1	2.26	0.65
2:H:108:GLU:OE2	2:H:118:ARG:NH1	2.29	0.65
1:K:65:SER:O	1:K:69:ARG:NH1	2.23	0.65
2:Q:121:LEU:HD12	2:Q:122:LYS:N	2.12	0.65
1:O:93:THR:CG2	1:O:126:VAL:H	2.10	0.65
1:G:33:ARG:O	1:G:55:GLN:NE2	2.29	0.65
1:O:15:GLN:NE2	1:O:127:SER:OG	2.29	0.65
1:C:105:TYR:C	1:C:106:TYR:CD2	2.75	0.65
1:K:107:ASP:HA	1:K:108:LYS:NZ	2.12	0.65
1:P:44:GLY:O	1:P:45:LYS:HG3	1.96	0.65
2:B:23:LYS:HE3	2:B:193:GLU:OE1	1.97	0.65
1:C:49:PHE:CE2	1:C:110:ARG:HA	2.32	0.65
1:C:54:SER:HB3	1:C:57:GLY:H	1.61	0.65
1:I:39:PHE:CD1	1:I:49:PHE:HA	2.31	0.65
1:C:64:ASP:HA	1:C:67:LYS:HZ1	1.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:104:SER:OG	1:M:105:TYR:N	2.29	0.65
2:L:183:ASN:OD1	2:L:184:VAL:HG23	1.97	0.65
1:R:109:PRO:HG2	1:R:114:GLU:HG3	1.78	0.65
1:G:40:ARG:NH1	1:G:92:ASP:OD1	2.30	0.65
1:G:120:GLN:OE1	1:G:120:GLN:N	2.19	0.65
1:P:4:VAL:HA	1:P:27:SER:O	1.97	0.65
1:C:40:ARG:NH2	1:C:96:TYR:OH	2.29	0.65
1:C:88:LEU:C	1:C:89:LYS:HZ3	2.04	0.65
1:G:3:GLU:O	1:G:5:GLN:NE2	2.30	0.65
1:K:62:TYR:CZ	1:K:72:ILE:HG22	2.32	0.65
1:M:101:SER:HB3	1:M:117:TYR:H	1.62	0.65
1:A:40:ARG:O	1:A:48:GLU:N	2.29	0.64
2:B:82:ILE:HG21	2:B:119:LYS:HE2	1.79	0.64
2:Q:4:MET:HG3	2:Q:190:LEU:HD21	1.79	0.64
2:T:183:ASN:OD1	2:T:184:VAL:HG23	1.98	0.64
1:O:55:GLN:HE22	1:O:105:TYR:HA	1.61	0.64
1:M:61:ASP:OD1	1:M:110:ARG:NH2	2.30	0.64
1:E:40:ARG:NH2	1:E:96:TYR:OH	2.29	0.64
2:J:64:LEU:HD21	2:J:66:PHE:HB2	1.79	0.64
1:M:55:GLN:NE2	1:M:102:GLN:HG2	2.13	0.64
1:A:93:THR:OG1	1:A:126:VAL:N	2.31	0.64
1:E:35:TYR:HE2	1:E:102:GLN:CB	2.09	0.64
1:E:70:PHE:CE1	1:E:85:MET:HG2	2.32	0.64
1:M:48:GLU:N	1:M:48:GLU:OE1	2.30	0.64
1:E:42:VAL:HG22	1:E:94:ALA:HB2	1.80	0.64
1:G:70:PHE:CE1	1:G:85:MET:HG2	2.33	0.64
1:C:36:MET:CE	1:C:100:GLY:HA3	2.27	0.64
1:A:78:GLU:O	1:A:80:THR:HG23	1.98	0.64
1:C:40:ARG:O	1:C:48:GLU:N	2.30	0.64
2:D:22:LEU:CD2	2:D:190:LEU:HD11	2.28	0.64
2:D:82:ILE:HD12	2:D:121:LEU:HD22	1.80	0.64
1:G:30:THR:HG22	1:G:34:HIS:CD2	2.33	0.64
1:M:53:ILE:O	1:M:108:LYS:HE3	1.98	0.64
1:P:65:SER:O	1:P:69:ARG:NH1	2.20	0.64
1:O:39:PHE:HA	1:O:50:VAL:HG23	1.79	0.63
1:E:64:ASP:HA	1:E:67:LYS:HZ1	1.60	0.63
1:M:54:SER:HA	1:M:108:LYS:HZ1	1.62	0.63
1:R:39:PHE:CD1	1:R:49:PHE:HA	2.34	0.63
2:B:4:MET:HA	2:B:4:MET:HE3	1.79	0.63
1:C:93:THR:OG1	1:C:126:VAL:N	2.30	0.63
2:D:43:LEU:HD11	2:D:153:VAL:HG22	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:4:VAL:HA	1:E:27:SER:O	1.98	0.63
1:O:5:GLN:HB2	1:O:27:SER:OG	1.97	0.63
1:O:24:CYS:HG	1:O:98:CYS:CB	2.11	0.63
1:C:42:VAL:HB	1:C:45:LYS:HG2	1.80	0.63
2:T:125:TYR:CZ	2:T:126:THR:O	2.52	0.63
1:E:35:TYR:CD2	1:E:102:GLN:HB3	2.34	0.63
1:M:54:SER:HA	1:M:108:LYS:NZ	2.13	0.63
1:O:38:TRP:CZ3	1:O:98:CYS:HB3	2.34	0.63
1:G:70:PHE:CZ	1:G:85:MET:HG2	2.34	0.63
1:M:65:SER:O	1:M:69:ARG:NH1	2.26	0.63
1:C:35:TYR:CE1	1:C:102:GLN:HB2	2.33	0.63
1:E:54:SER:CB	1:E:108:LYS:HE2	2.27	0.63
1:K:100:GLY:HA2	1:K:115:TYR:CD2	2.34	0.63
1:M:34:HIS:CA	1:M:102:GLN:HB3	2.28	0.63
1:A:105:TYR:O	1:A:106:TYR:CG	2.51	0.63
2:D:183:ASN:OD1	2:D:184:VAL:HG23	1.99	0.63
1:E:5:GLN:HB2	1:E:27:SER:OG	1.99	0.63
1:E:70:PHE:CZ	1:E:85:MET:HG2	2.33	0.63
1:G:40:ARG:NH2	1:G:96:TYR:OH	2.31	0.63
2:S:82:ILE:CD1	2:S:121:LEU:HD22	2.29	0.63
1:A:46:GLU:OE1	1:A:46:GLU:N	2.29	0.63
1:C:13:LEU:HD11	1:K:43:PRO:HD3	1.81	0.63
1:C:39:PHE:HA	1:C:50:VAL:HG23	1.81	0.63
1:I:102:GLN:HG3	1:I:102:GLN:O	1.99	0.63
2:L:31:LYS:HG3	2:L:102:SER:HB3	1.80	0.63
1:C:53:ILE:C	1:C:108:LYS:HE3	2.24	0.63
1:A:41:GLN:HA	1:A:45:LYS:HZ1	1.64	0.62
2:B:76:THR:HG22	2:B:81:GLU:CB	2.28	0.62
2:Q:125:TYR:CE2	2:Q:126:THR:O	2.52	0.62
2:T:125:TYR:CE2	2:T:126:THR:O	2.52	0.62
1:I:22:LEU:H	1:I:22:LEU:HD12	1.64	0.62
1:K:71:THR:CG2	1:K:84:GLN:HB3	2.29	0.62
1:K:104:SER:CB	1:K:106:TYR:CE2	2.67	0.62
1:M:3:GLU:OE2	1:M:34:HIS:NE2	2.32	0.62
1:P:21:ARG:NE	1:P:84:GLN:HB2	2.13	0.62
1:C:55:GLN:HA	1:C:74:ARG:HH12	1.61	0.62
1:I:4:VAL:HA	1:I:27:SER:O	1.98	0.62
2:J:183:ASN:OD1	2:J:184:VAL:HG23	1.99	0.62
1:K:46:GLU:OE1	1:K:46:GLU:N	2.25	0.62
1:K:53:ILE:HG13	1:K:60:LYS:HG2	1.81	0.62
1:M:35:TYR:CE1	1:M:102:GLN:HB2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:SER:HB2	1:C:116:ALA:H	1.63	0.62
2:D:39:PHE:HE1	2:D:96:ILE:HD12	1.64	0.62
1:A:42:VAL:HG22	1:A:94:ALA:HB2	1.82	0.62
1:K:3:GLU:OE2	1:K:34:HIS:CE1	2.52	0.62
1:A:39:PHE:HA	1:A:50:VAL:HG23	1.82	0.62
1:C:53:ILE:C	1:C:108:LYS:CE	2.72	0.62
1:G:42:VAL:HG22	1:G:94:ALA:HB2	1.82	0.62
1:C:54:SER:CB	1:C:57:GLY:H	2.13	0.62
2:J:83:LEU:HD12	2:J:83:LEU:O	2.00	0.62
1:O:40:ARG:HG3	1:O:96:TYR:CE1	2.35	0.62
1:E:40:ARG:HG3	1:E:96:TYR:CE1	2.35	0.62
1:G:13:LEU:HD21	1:R:95:LEU:HD13	1.80	0.62
1:M:34:HIS:HA	1:M:102:GLN:CB	2.30	0.62
1:P:54:SER:HB3	1:P:108:LYS:HE2	1.81	0.62
1:A:100:GLY:HA2	1:A:115:TYR:CE2	2.35	0.62
2:Q:125:TYR:CZ	2:Q:126:THR:O	2.52	0.62
1:A:49:PHE:CE2	1:A:110:ARG:HA	2.35	0.61
2:B:43:LEU:HD11	2:B:153:VAL:HG22	1.82	0.61
1:C:105:TYR:OH	2:D:119:LYS:HD2	1.99	0.61
1:I:41:GLN:HB2	1:I:47:ARG:HG2	1.82	0.61
1:C:40:ARG:HG3	1:C:96:TYR:HE1	1.64	0.61
1:E:39:PHE:HA	1:E:50:VAL:HG23	1.80	0.61
1:G:40:ARG:HG3	1:G:96:TYR:CE1	2.35	0.61
1:I:41:GLN:HB3	1:I:97:TYR:CE1	2.34	0.61
1:K:21:ARG:HG2	1:K:21:ARG:HH11	1.64	0.61
1:K:101:SER:HB3	1:K:116:ALA:N	2.13	0.61
1:R:65:SER:O	1:R:69:ARG:NH1	2.24	0.61
1:O:41:GLN:HA	1:O:45:LYS:NZ	2.16	0.61
1:C:36:MET:HE1	1:C:100:GLY:HA3	1.83	0.61
2:S:62:GLU:CD	2:S:127:VAL:HG13	2.24	0.61
1:C:38:TRP:CH2	1:C:98:CYS:HB3	2.35	0.61
1:C:112:LEU:O	1:C:112:LEU:HD23	2.00	0.61
1:I:111:LEU:HG	1:I:113:THR:H	1.66	0.61
1:E:112:LEU:O	1:E:112:LEU:HD23	2.00	0.61
2:F:136:GLY:HA2	2:F:152:LEU:HG	1.83	0.61
1:G:83:LEU:HD22	1:G:85:MET:CE	2.27	0.61
2:H:47:ARG:NH1	2:H:149:SER:O	2.34	0.61
2:J:125:TYR:CE2	2:J:126:THR:O	2.53	0.61
1:K:24:CYS:O	1:K:80:THR:CG2	2.39	0.61
2:Q:14:GLU:HG3	2:Q:47:ARG:NH2	2.15	0.61
1:C:36:MET:HG3	1:C:81:VAL:CG1	2.30	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:24:CYS:CB	1:G:98:CYS:SG	2.88	0.61
2:J:105:GLY:O	2:J:121:LEU:N	2.32	0.61
1:K:63:VAL:HG12	1:K:66:ALA:HB3	1.83	0.61
1:M:6:LEU:HD12	1:M:24:CYS:SG	2.40	0.61
1:R:31:PHE:CE1	1:R:79:ASN:HA	2.36	0.61
1:G:13:LEU:HD21	1:R:95:LEU:HD12	1.81	0.61
1:M:35:TYR:HA	1:M:74:ARG:NH2	2.15	0.61
1:E:40:ARG:O	1:E:48:GLU:N	2.34	0.61
2:F:62:GLU:CD	2:F:127:VAL:HG13	2.26	0.61
2:F:108:GLU:OE2	2:F:118:ARG:NH1	2.34	0.61
2:N:2:THR:HG22	2:N:4:MET:HE2	1.81	0.61
2:Q:183:ASN:OD1	2:Q:184:VAL:HG23	2.01	0.61
2:D:184:VAL:HG12	2:D:185:LEU:HD22	1.83	0.61
1:G:112:LEU:HD23	1:G:112:LEU:O	2.01	0.61
1:R:62:TYR:CE2	1:R:71:THR:HA	2.35	0.61
1:A:40:ARG:HG3	1:A:96:TYR:CE1	2.35	0.60
1:R:22:LEU:HD13	1:R:85:MET:CE	2.29	0.60
1:A:38:TRP:CZ3	1:A:98:CYS:HB2	2.36	0.60
1:C:41:GLN:HA	1:C:45:LYS:NZ	2.16	0.60
1:G:49:PHE:CE2	1:G:110:ARG:HA	2.36	0.60
2:J:125:TYR:CZ	2:J:126:THR:O	2.54	0.60
1:M:30:THR:OG1	1:M:34:HIS:NE2	2.33	0.60
1:M:71:THR:HG22	1:M:84:GLN:HB3	1.82	0.60
1:A:112:LEU:HD23	1:A:112:LEU:O	2.01	0.60
1:E:38:TRP:CZ3	1:E:98:CYS:HB2	2.36	0.60
1:G:38:TRP:CG	1:G:83:LEU:HD12	2.37	0.60
1:G:38:TRP:CZ3	1:G:98:CYS:HB2	2.35	0.60
1:M:89:LYS:CE	1:M:91:GLU:OE1	2.49	0.60
1:C:93:THR:CG2	1:C:125:THR:HA	2.30	0.60
2:T:105:GLY:O	2:T:121:LEU:N	2.33	0.60
1:O:40:ARG:HE	1:O:96:TYR:HE1	1.47	0.60
1:C:105:TYR:O	1:C:106:TYR:CE2	2.54	0.60
1:E:35:TYR:CE2	1:E:102:GLN:HB2	2.34	0.60
1:M:7:VAL:HG23	1:M:120:GLN:NE2	2.16	0.60
2:B:26:LEU:CD2	2:B:30:LEU:HD21	2.30	0.60
1:G:40:ARG:O	1:G:48:GLU:N	2.33	0.60
2:H:111:VAL:C	2:H:112:ASP:OD1	2.45	0.60
2:S:152:LEU:HD12	2:S:152:LEU:O	2.02	0.60
1:A:93:THR:CG2	1:A:125:THR:HA	2.32	0.60
1:G:36:MET:HG3	1:G:81:VAL:CG1	2.29	0.60
1:K:21:ARG:HH21	1:K:84:GLN:HB2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:53:ILE:HG12	1:M:74:ARG:HB2	1.84	0.60
2:N:2:THR:CG2	2:N:4:MET:CE	2.80	0.60
1:P:41:GLN:HB3	1:P:97:TYR:CE1	2.35	0.60
1:E:30:THR:CG2	1:E:33:ARG:HB2	2.31	0.60
1:G:39:PHE:HA	1:G:50:VAL:HG23	1.82	0.60
1:O:112:LEU:HD23	1:O:112:LEU:O	2.01	0.60
2:S:111:VAL:C	2:S:112:ASP:OD1	2.45	0.60
1:C:41:GLN:HA	1:C:45:LYS:HZ2	1.67	0.60
1:R:35:TYR:CE1	1:R:102:GLN:HB3	2.37	0.60
2:B:183:ASN:OD1	2:B:184:VAL:HG23	2.02	0.60
1:E:62:TYR:HB2	1:E:67:LYS:CG	2.30	0.60
1:R:75:ASP:O	1:R:79:ASN:HA	2.02	0.60
1:O:22:LEU:HG	1:O:85:MET:HE1	1.84	0.59
1:A:30:THR:HG22	1:A:33:ARG:HB2	1.84	0.59
2:B:49:TYR:HD2	2:B:152:LEU:HD13	1.67	0.59
1:C:95:LEU:HD13	1:K:13:LEU:HD21	1.73	0.59
1:O:88:LEU:C	1:O:89:LYS:HD2	2.27	0.59
2:S:111:VAL:HG23	2:S:112:ASP:OD1	2.03	0.59
1:E:101:SER:HB2	1:E:116:ALA:N	2.15	0.59
1:I:114:GLU:OE1	1:I:114:GLU:N	2.30	0.59
2:L:2:THR:HG22	2:L:4:MET:HE2	1.83	0.59
1:P:44:GLY:O	1:P:45:LYS:CG	2.50	0.59
2:T:64:LEU:HD23	2:T:66:PHE:HB2	1.84	0.59
1:E:96:TYR:CE2	1:E:124:VAL:HG11	2.38	0.59
1:A:40:ARG:CG	1:A:96:TYR:HE1	2.15	0.59
1:C:54:SER:N	1:C:108:LYS:HE2	2.17	0.59
1:E:49:PHE:CE2	1:E:110:ARG:HA	2.37	0.59
1:I:38:TRP:CD1	1:I:83:LEU:HD12	2.38	0.59
1:R:61:ASP:OD1	1:R:110:ARG:NH2	2.34	0.59
1:E:40:ARG:CG	1:E:96:TYR:HE1	2.16	0.59
1:E:40:ARG:HE	1:E:96:TYR:HE1	1.51	0.59
2:F:111:VAL:C	2:F:112:ASP:OD1	2.45	0.59
1:M:62:TYR:HE2	1:M:71:THR:HA	1.67	0.59
2:D:4:MET:HA	2:D:4:MET:HE3	1.84	0.59
1:E:8:GLU:OE1	1:E:121:GLY:N	2.33	0.59
2:N:183:ASN:OD1	2:N:184:VAL:HG23	2.01	0.59
1:R:59:ASN:HB3	1:R:108:LYS:HZ1	1.67	0.59
1:C:40:ARG:HE	1:C:96:TYR:HE1	1.50	0.59
1:G:62:TYR:HB2	1:G:67:LYS:CG	2.30	0.59
1:M:71:THR:CG2	1:M:84:GLN:HB3	2.32	0.59
2:B:130:GLU:OE2	2:B:130:GLU:N	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:LEU:HD11	1:R:43:PRO:HD3	1.85	0.59
1:K:35:TYR:HB2	1:K:53:ILE:O	2.03	0.59
1:E:46:GLU:OE1	1:E:46:GLU:N	2.28	0.59
2:F:1:GLN:OE1	2:F:1:GLN:N	2.25	0.59
1:M:53:ILE:CB	1:M:72:ILE:HD11	2.29	0.59
1:R:38:TRP:CD1	1:R:83:LEU:HD12	2.38	0.59
1:O:36:MET:HA	1:O:36:MET:CE	2.31	0.59
1:O:40:ARG:CG	1:O:96:TYR:HE1	2.15	0.59
1:O:49:PHE:CE2	1:O:110:ARG:HA	2.37	0.59
1:G:4:VAL:HA	1:G:27:SER:O	2.02	0.59
1:I:102:GLN:NE2	1:I:104:SER:HB3	2.18	0.59
2:J:56:THR:HG23	2:J:130:GLU:O	2.02	0.59
1:K:35:TYR:HA	1:K:74:ARG:NH2	2.17	0.59
1:K:112:LEU:HG	1:K:118:TRP:HH2	1.67	0.59
2:Q:105:GLY:O	2:Q:121:LEU:N	2.33	0.59
1:E:123:LEU:HD13	1:I:13:LEU:HD23	1.85	0.58
1:G:41:GLN:HA	1:G:45:LYS:HZ2	1.67	0.58
1:M:20:LEU:HD13	1:M:22:LEU:HD11	1.84	0.58
1:O:42:VAL:HG22	1:O:94:ALA:HB2	1.85	0.58
2:S:38:HIS:CE1	2:S:205:TRP:CB	2.86	0.58
1:G:40:ARG:CG	1:G:96:TYR:HE1	2.15	0.58
1:G:40:ARG:HE	1:G:96:TYR:HE1	1.51	0.58
1:C:13:LEU:CD2	1:K:95:LEU:HD11	2.27	0.58
1:K:3:GLU:N	1:K:117:TYR:HH	2.00	0.58
2:L:43:LEU:HD22	2:L:47:ARG:NH1	2.18	0.58
2:Q:82:ILE:HD12	2:Q:121:LEU:CD2	2.22	0.58
1:R:6:LEU:HD12	1:R:24:CYS:SG	2.42	0.58
1:O:13:LEU:HD11	1:P:43:PRO:HD3	1.85	0.58
1:C:40:ARG:HG3	1:C:96:TYR:CE1	2.38	0.58
1:I:63:VAL:HG12	1:I:66:ALA:HB3	1.85	0.58
1:P:75:ASP:O	1:P:79:ASN:HA	2.02	0.58
1:R:60:LYS:C	1:R:108:LYS:HE3	2.27	0.58
2:H:35:VAL:HG22	2:H:161:MET:HG3	1.84	0.58
1:I:31:PHE:CG	1:I:79:ASN:HB2	2.37	0.58
1:R:36:MET:HE3	1:R:36:MET:CA	2.34	0.58
1:E:30:THR:HG22	1:E:34:HIS:CD2	2.38	0.58
1:E:105:TYR:CD1	2:F:82:ILE:HG23	2.38	0.58
1:I:61:ASP:OD1	1:I:110:ARG:NH2	2.36	0.58
1:O:40:ARG:O	1:O:48:GLU:N	2.37	0.58
1:O:36:MET:HB2	1:O:53:ILE:CG2	2.34	0.58
2:B:76:THR:HG22	2:B:81:GLU:CA	2.34	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:105:TYR:O	1:E:106:TYR:CE2	2.56	0.58
1:O:32:ASN:HB3	1:O:76:ASN:HD21	1.67	0.58
1:O:62:TYR:HB2	1:O:67:LYS:HG2	1.85	0.58
1:C:54:SER:CA	1:C:108:LYS:CE	2.78	0.58
1:C:69:ARG:HE	1:C:87:ASN:HB3	1.69	0.58
2:D:43:LEU:CD1	2:D:153:VAL:HG22	2.34	0.58
1:I:83:LEU:CD2	1:I:85:MET:HG2	2.33	0.58
1:M:34:HIS:O	1:M:55:GLN:HG3	2.03	0.58
1:P:6:LEU:HD12	1:P:24:CYS:SG	2.44	0.58
2:S:35:VAL:HG22	2:S:161:MET:HG3	1.86	0.58
2:D:82:ILE:CD1	2:D:121:LEU:HD22	2.33	0.58
1:K:8:GLU:HB3	1:K:98:CYS:SG	2.44	0.58
1:K:93:THR:CG2	1:K:125:THR:HA	2.34	0.58
1:M:60:LYS:HD3	1:M:62:TYR:HE1	1.69	0.58
2:B:14:GLU:CG	2:B:47:ARG:NH2	2.61	0.57
1:G:101:SER:CB	1:G:116:ALA:H	2.17	0.57
2:H:111:VAL:HG23	2:H:112:ASP:OD1	2.03	0.57
1:I:112:LEU:O	1:I:112:LEU:HD23	2.04	0.57
1:R:40:ARG:HG3	1:R:96:TYR:HE1	1.68	0.57
1:A:123:LEU:HD12	1:A:124:VAL:N	2.19	0.57
1:K:40:ARG:HG2	1:K:41:GLN:N	2.18	0.57
2:T:36:CYS:HG	2:T:97:CYS:CB	2.10	0.57
1:O:13:LEU:HD21	1:P:95:LEU:HD22	1.87	0.57
2:L:105:GLY:O	2:L:121:LEU:N	2.34	0.57
1:E:55:GLN:HG2	1:E:56:THR:N	2.19	0.57
1:G:64:ASP:HA	1:G:67:LYS:HZ1	1.68	0.57
1:I:78:GLU:OE1	1:I:78:GLU:N	2.33	0.57
1:R:63:VAL:HG12	1:R:66:ALA:HB3	1.85	0.57
2:T:31:LYS:CG	2:T:102:SER:OG	2.51	0.57
1:I:16:THR:HG23	1:I:127:SER:O	2.03	0.57
1:K:20:LEU:HB3	1:K:22:LEU:CD1	2.34	0.57
1:M:42:VAL:HG22	1:M:94:ALA:HB2	1.86	0.57
1:P:21:ARG:HH11	1:P:82:TYR:HD2	1.53	0.57
1:A:40:ARG:HE	1:A:96:TYR:HE1	1.48	0.57
2:D:58:ARG:NH1	2:D:58:ARG:HB2	2.19	0.57
1:G:8:GLU:OE1	1:G:121:GLY:N	2.35	0.57
1:I:42:VAL:CB	1:I:45:LYS:HD2	2.33	0.57
1:I:100:GLY:O	1:I:117:TYR:HB2	2.04	0.57
1:M:42:VAL:HB	1:M:45:LYS:HE2	1.86	0.57
1:G:90:PRO:O	1:G:93:THR:HG22	2.04	0.57
2:L:111:VAL:C	2:L:112:ASP:OD1	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:41:GLN:O	1:P:94:ALA:HB1	2.05	0.57
1:R:71:THR:HG22	1:R:84:GLN:HB3	1.85	0.57
2:F:35:VAL:HG22	2:F:161:MET:HG3	1.86	0.57
2:F:82:ILE:CG1	2:F:121:LEU:HD12	2.34	0.57
2:F:133:ILE:O	2:F:134:ILE:HD13	2.05	0.57
1:G:35:TYR:HE2	1:G:102:GLN:OE1	1.88	0.57
1:K:38:TRP:CZ3	1:K:98:CYS:HB3	2.40	0.57
1:M:42:VAL:HG13	1:M:43:PRO:HD2	1.87	0.57
1:M:101:SER:CB	1:M:116:ALA:HB3	2.35	0.57
1:R:107:ASP:HB2	2:T:80:SER:OG	2.05	0.57
1:R:111:LEU:HD12	1:R:112:LEU:H	1.70	0.57
2:S:118:ARG:CZ	2:B:204:LEU:HD21	2.35	0.57
2:F:43:LEU:HD11	2:F:153:VAL:HG22	1.86	0.57
1:G:123:LEU:HD12	1:G:124:VAL:N	2.20	0.57
2:H:82:ILE:HD12	2:H:121:LEU:HD22	1.87	0.57
2:L:22:LEU:HD22	2:L:190:LEU:HD11	1.86	0.57
1:P:48:GLU:N	1:P:48:GLU:OE2	2.37	0.57
1:E:95:LEU:HD23	1:E:97:TYR:OH	2.05	0.56
1:P:21:ARG:HE	1:P:84:GLN:HB2	1.69	0.56
1:R:40:ARG:HG2	1:R:41:GLN:N	2.20	0.56
1:O:70:PHE:CE1	1:O:85:MET:HG2	2.40	0.56
1:E:6:LEU:HD12	1:E:98:CYS:O	2.06	0.56
2:F:132:SER:OG	2:F:134:ILE:HD11	2.05	0.56
1:G:41:GLN:HA	1:G:45:LYS:NZ	2.20	0.56
1:K:40:ARG:HG3	1:K:96:TYR:CE1	2.38	0.56
1:K:40:ARG:N	1:K:48:GLU:O	2.30	0.56
2:T:111:VAL:C	2:T:112:ASP:OD1	2.47	0.56
1:O:30:THR:HG22	1:O:33:ARG:HB2	1.86	0.56
1:O:70:PHE:CZ	1:O:85:MET:HG2	2.40	0.56
1:E:13:LEU:HD11	1:I:43:PRO:HD3	1.87	0.56
2:F:152:LEU:O	2:F:152:LEU:HD12	2.04	0.56
1:G:95:LEU:HD23	1:G:97:TYR:OH	2.05	0.56
2:H:172:ASN:O	2:H:176:LEU:HD23	2.05	0.56
1:I:38:TRP:CZ3	1:I:98:CYS:HB2	2.40	0.56
2:J:91:VAL:HG13	2:J:91:VAL:O	2.05	0.56
1:M:14:VAL:HG22	1:M:15:GLN:N	2.21	0.56
1:M:46:GLU:OE1	1:M:46:GLU:N	2.28	0.56
1:M:111:LEU:HD12	1:M:112:LEU:H	1.69	0.56
1:C:54:SER:HA	1:C:108:LYS:HE2	1.87	0.56
2:H:64:LEU:HD23	2:H:66:PHE:HB2	1.87	0.56
1:I:34:HIS:CE1	1:I:103:SER:OG	2.58	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:SER:O	1:K:81:VAL:HG13	2.06	0.56
2:L:2:THR:CG2	2:L:4:MET:CE	2.82	0.56
1:R:58:LEU:HD12	1:R:59:ASN:ND2	2.20	0.56
1:O:46:GLU:OE1	1:O:46:GLU:N	2.27	0.56
1:O:96:TYR:CE2	1:O:124:VAL:HG11	2.40	0.56
1:C:40:ARG:CG	1:C:96:TYR:HE1	2.19	0.56
1:E:123:LEU:HD12	1:E:124:VAL:N	2.20	0.56
1:K:39:PHE:CD2	1:K:49:PHE:HA	2.41	0.56
2:T:56:THR:HG21	2:T:58:ARG:NH2	2.21	0.56
2:T:91:VAL:O	2:T:91:VAL:HG13	2.05	0.56
1:I:16:THR:HG22	1:I:126:VAL:CG1	2.35	0.56
2:N:45:SER:O	2:N:69:LYS:NZ	2.34	0.56
1:P:32:ASN:HB3	1:P:76:ASN:ND2	2.21	0.56
1:P:111:LEU:HG	1:P:113:THR:H	1.70	0.56
1:O:123:LEU:HD12	1:O:124:VAL:N	2.21	0.56
1:R:42:VAL:CB	1:R:45:LYS:HD2	2.34	0.56
1:R:112:LEU:HD23	1:R:112:LEU:O	2.05	0.56
1:O:38:TRP:CH2	1:O:98:CYS:HB3	2.40	0.56
2:B:118:ARG:CZ	2:D:204:LEU:HD21	2.36	0.56
1:G:64:ASP:CA	1:G:67:LYS:HZ3	2.14	0.56
1:M:54:SER:HB3	1:M:59:ASN:O	2.04	0.56
1:M:63:VAL:HG12	1:M:66:ALA:HB3	1.88	0.56
2:N:91:VAL:O	2:N:91:VAL:HG13	2.06	0.56
1:R:14:VAL:HG22	1:R:15:GLN:N	2.20	0.56
1:R:34:HIS:CE1	1:R:103:SER:OG	2.58	0.56
1:O:6:LEU:HD12	1:O:98:CYS:O	2.06	0.56
1:A:95:LEU:HD23	1:A:97:TYR:OH	2.06	0.56
1:P:112:LEU:O	1:P:112:LEU:HD23	2.06	0.56
1:R:41:GLN:O	1:R:94:ALA:HB1	2.05	0.56
1:O:89:LYS:HA	1:O:89:LYS:CE	2.36	0.56
1:A:41:GLN:HA	1:A:45:LYS:NZ	2.20	0.56
1:A:64:ASP:CA	1:A:67:LYS:HZ3	2.15	0.56
1:E:3:GLU:OE2	1:E:34:HIS:NE2	2.39	0.56
1:K:35:TYR:HA	1:K:74:ARG:HH22	1.70	0.56
2:S:76:THR:HG23	2:S:80:SER:O	2.05	0.55
1:E:41:GLN:HA	1:E:45:LYS:NZ	2.22	0.55
2:F:43:LEU:CD1	2:F:153:VAL:HG22	2.36	0.55
1:M:91:GLU:H	1:M:91:GLU:CD	2.12	0.55
1:R:100:GLY:O	1:R:117:TYR:HB2	2.05	0.55
2:S:50:SER:O	2:S:152:LEU:CD2	2.43	0.55
1:A:123:LEU:HD12	1:A:124:VAL:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:VAL:C	1:C:67:LYS:NZ	2.64	0.55
1:C:84:GLN:HG3	1:C:86:ASN:HD21	1.71	0.55
1:G:7:VAL:HA	1:G:120:GLN:HE22	1.70	0.55
1:M:62:TYR:CE2	1:M:71:THR:HA	2.41	0.55
1:R:105:TYR:C	1:R:106:TYR:CD2	2.83	0.55
1:O:55:GLN:HE22	1:O:106:TYR:H	1.55	0.55
1:O:78:GLU:N	1:O:78:GLU:OE1	2.38	0.55
1:C:96:TYR:CE2	1:C:124:VAL:HG11	2.42	0.55
2:F:172:ASN:O	2:F:176:LEU:HD23	2.05	0.55
1:K:3:GLU:HG2	1:K:4:VAL:HG13	1.87	0.55
1:M:16:THR:HG23	1:M:127:SER:O	2.06	0.55
1:R:96:TYR:O	1:R:121:GLY:HA2	2.06	0.55
2:T:62:GLU:OE1	2:T:63:ILE:HG13	2.06	0.55
2:B:82:ILE:HG21	2:B:119:LYS:CE	2.36	0.55
1:I:35:TYR:CE1	1:I:102:GLN:HB3	2.41	0.55
1:M:33:ARG:CZ	1:M:103:SER:HA	2.36	0.55
2:S:26:LEU:HD21	2:S:30:LEU:HD21	1.89	0.55
1:C:8:GLU:OE1	1:C:121:GLY:N	2.34	0.55
1:I:84:GLN:OE1	1:I:86:ASN:ND2	2.39	0.55
1:I:111:LEU:HD12	1:I:112:LEU:H	1.70	0.55
1:M:38:TRP:O	1:M:50:VAL:HB	2.07	0.55
1:O:8:GLU:OE1	1:O:121:GLY:N	2.35	0.55
1:C:7:VAL:HA	1:C:120:GLN:HE22	1.72	0.55
2:S:132:SER:OG	2:S:134:ILE:HD11	2.07	0.55
2:S:133:ILE:O	2:S:134:ILE:HD13	2.06	0.55
1:A:13:LEU:CD2	1:M:123:LEU:HD13	2.31	0.55
2:D:190:LEU:HD12	2:D:191:LYS:N	2.22	0.55
1:I:24:CYS:CB	1:I:98:CYS:SG	2.95	0.55
1:I:35:TYR:HE1	1:I:102:GLN:HB3	1.71	0.55
1:M:35:TYR:CD1	1:M:102:GLN:HB2	2.42	0.55
2:N:105:GLY:O	2:N:121:LEU:N	2.35	0.55
1:P:24:CYS:HB2	1:P:38:TRP:CZ2	2.41	0.55
1:P:93:THR:CG2	1:P:125:THR:HA	2.32	0.55
1:I:24:CYS:C	1:I:80:THR:HG23	2.24	0.55
1:M:41:GLN:HB2	1:M:47:ARG:HG2	1.87	0.55
2:N:81:GLU:O	2:N:82:ILE:HG13	2.07	0.55
2:N:125:TYR:CE2	2:N:126:THR:O	2.60	0.55
1:P:63:VAL:HG12	1:P:66:ALA:HB3	1.89	0.55
1:A:36:MET:HE1	1:A:100:GLY:HA3	1.88	0.55
1:A:96:TYR:CE2	1:A:124:VAL:HG11	2.42	0.55
1:G:22:LEU:HG	1:G:85:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:78:GLU:N	1:G:78:GLU:OE1	2.40	0.55
1:P:111:LEU:HD12	1:P:112:LEU:H	1.70	0.55
1:P:123:LEU:HD12	1:P:124:VAL:N	2.22	0.55
2:Q:91:VAL:O	2:Q:91:VAL:HG13	2.07	0.55
1:O:35:TYR:CB	1:O:108:LYS:HE3	2.37	0.55
2:S:125:TYR:CE2	2:S:126:THR:O	2.60	0.55
1:C:78:GLU:OE1	1:C:78:GLU:N	2.39	0.55
1:I:34:HIS:CD2	1:I:103:SER:HA	2.42	0.55
2:N:125:TYR:CZ	2:N:126:THR:O	2.60	0.55
1:P:36:MET:CG	1:P:81:VAL:HG21	2.36	0.55
1:A:105:TYR:CD1	2:B:82:ILE:HG23	2.42	0.54
2:F:62:GLU:CD	2:F:63:ILE:HG13	2.33	0.54
2:J:2:THR:CG2	2:J:4:MET:CE	2.85	0.54
1:M:35:TYR:CB	1:M:108:LYS:CE	2.82	0.54
1:P:35:TYR:HA	1:P:74:ARG:HH22	1.72	0.54
1:O:35:TYR:HE1	1:O:115:TYR:CZ	2.25	0.54
1:C:123:LEU:HD12	1:C:124:VAL:N	2.22	0.54
1:G:13:LEU:HD23	1:R:95:LEU:HD12	1.89	0.54
2:H:82:ILE:CD1	2:H:121:LEU:HD13	2.35	0.54
1:I:36:MET:HA	1:I:36:MET:CE	2.37	0.54
1:K:101:SER:HB2	1:K:117:TYR:CD1	2.41	0.54
1:R:16:THR:HG23	1:R:127:SER:O	2.07	0.54
2:T:140:ASP:HB2	2:T:145:ASN:HB3	1.88	0.54
1:O:42:VAL:CB	1:O:45:LYS:HE3	2.38	0.54
1:O:89:LYS:HB2	1:O:91:GLU:OE2	2.08	0.54
1:C:42:VAL:CB	1:C:45:LYS:HE3	2.35	0.54
1:K:53:ILE:HG22	1:K:72:ILE:HD11	1.90	0.54
1:M:30:THR:O	1:M:34:HIS:HD2	1.90	0.54
1:M:89:LYS:HB3	1:M:90:PRO:CD	2.37	0.54
1:O:55:GLN:NE2	1:O:105:TYR:HA	2.23	0.54
1:A:36:MET:HA	1:A:36:MET:CE	2.35	0.54
1:C:14:VAL:HG12	1:C:15:GLN:O	2.08	0.54
1:C:42:VAL:HG22	1:C:94:ALA:HB2	1.88	0.54
1:E:83:LEU:HG	1:E:85:MET:HE2	1.89	0.54
2:F:147:GLU:OE1	2:F:150:GLN:HG3	2.07	0.54
1:G:105:TYR:O	1:G:106:TYR:HD1	1.91	0.54
2:Q:35:VAL:HG22	2:Q:161:MET:SD	2.48	0.54
1:O:30:THR:HG22	1:O:34:HIS:CD2	2.43	0.54
1:O:95:LEU:HD11	1:P:13:LEU:HG	1.89	0.54
1:G:30:THR:CG2	1:G:33:ARG:HB2	2.37	0.54
1:G:105:TYR:HE1	2:H:119:LYS:HE3	1.73	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4:VAL:CG1	1:M:26:ALA:HB1	2.36	0.54
1:M:34:HIS:HA	1:M:102:GLN:CG	2.38	0.54
2:Q:81:GLU:O	2:Q:82:ILE:HG13	2.07	0.54
1:O:123:LEU:HD21	1:P:13:LEU:HB3	1.90	0.54
2:S:12:PRO:HB2	2:H:120:SER:HB2	1.88	0.54
1:G:96:TYR:CE2	1:G:124:VAL:HG11	2.42	0.54
2:H:76:THR:OG1	2:H:80:SER:O	2.24	0.54
1:K:63:VAL:HG13	1:K:66:ALA:H	1.71	0.54
2:T:81:GLU:O	2:T:82:ILE:HG13	2.07	0.54
1:C:15:GLN:OE1	1:C:16:THR:HG23	2.08	0.54
2:D:111:VAL:O	2:D:112:ASP:OD1	2.24	0.54
1:E:78:GLU:OE1	1:E:78:GLU:N	2.40	0.54
2:J:83:LEU:HD12	2:J:83:LEU:C	2.32	0.54
1:M:17:GLY:HA2	1:M:87:ASN:HA	1.90	0.54
2:Q:4:MET:SD	2:Q:190:LEU:HD11	2.48	0.54
1:O:7:VAL:HA	1:O:120:GLN:HE22	1.73	0.54
1:O:107:ASP:HB3	2:S:80:SER:HG	1.69	0.54
1:E:123:LEU:HD12	1:E:124:VAL:H	1.73	0.54
1:C:7:VAL:HG23	1:C:120:GLN:HE22	1.73	0.54
1:E:93:THR:HG21	1:E:125:THR:HG23	1.89	0.54
2:J:170:GLU:O	2:J:174:ILE:HG12	2.07	0.54
2:L:43:LEU:HD11	2:L:153:VAL:HG22	1.89	0.54
1:M:33:ARG:O	1:M:33:ARG:HD2	2.08	0.54
1:M:38:TRP:CZ3	1:M:98:CYS:HB2	2.43	0.54
1:R:34:HIS:CE1	1:R:103:SER:HG	2.26	0.54
1:O:42:VAL:H	1:O:45:LYS:HZ2	1.56	0.54
1:A:102:GLN:C	1:A:104:SER:N	2.63	0.54
1:M:123:LEU:HD12	1:M:124:VAL:N	2.23	0.54
2:B:76:THR:HG22	2:B:81:GLU:HA	1.90	0.53
1:G:123:LEU:HD12	1:G:124:VAL:H	1.73	0.53
1:K:112:LEU:O	1:K:112:LEU:HD23	2.09	0.53
2:Q:50:SER:O	2:Q:152:LEU:CD2	2.49	0.53
2:Q:100:TRP:CH2	2:Q:102:SER:HB2	2.43	0.53
1:O:13:LEU:CD2	1:P:123:LEU:HD13	2.30	0.53
1:O:123:LEU:HD12	1:O:124:VAL:H	1.73	0.53
2:S:140:ASP:HB2	2:S:145:ASN:ND2	2.23	0.53
1:A:36:MET:CE	1:A:100:GLY:HA3	2.37	0.53
1:C:53:ILE:C	1:C:108:LYS:HE2	2.33	0.53
1:I:36:MET:HG3	1:I:81:VAL:CG2	2.27	0.53
2:L:125:TYR:CZ	2:L:126:THR:O	2.61	0.53
1:O:30:THR:HG22	1:O:34:HIS:HD2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ALA:HB3	1:A:78:GLU:OE1	2.08	0.53
1:E:30:THR:O	1:E:30:THR:CG2	2.55	0.53
1:G:32:ASN:HB3	1:G:76:ASN:HD21	1.73	0.53
1:G:38:TRP:CH2	1:G:98:CYS:HB2	2.43	0.53
2:L:125:TYR:CE2	2:L:126:THR:O	2.61	0.53
1:C:7:VAL:HG13	1:C:25:ALA:HB3	1.91	0.53
1:I:34:HIS:NE2	1:I:103:SER:OG	2.41	0.53
1:P:61:ASP:OD1	1:P:110:ARG:NH2	2.39	0.53
2:S:43:LEU:HD21	2:S:153:VAL:HG22	1.90	0.53
1:G:22:LEU:HG	1:G:85:MET:CE	2.37	0.53
1:G:36:MET:HA	1:G:36:MET:CE	2.32	0.53
2:H:132:SER:OG	2:H:134:ILE:HD11	2.08	0.53
1:I:42:VAL:CG1	1:I:45:LYS:HD2	2.37	0.53
2:N:46:THR:HG22	2:N:47:ARG:N	2.24	0.53
1:C:54:SER:HB2	1:C:59:ASN:H	1.72	0.53
1:C:123:LEU:HD21	1:K:13:LEU:HB3	1.90	0.53
2:F:102:SER:OG	2:F:125:TYR:O	2.20	0.53
2:N:2:THR:CG2	2:N:4:MET:HE2	2.39	0.53
1:O:14:VAL:HG12	1:O:15:GLN:O	2.09	0.53
1:C:34:HIS:C	1:C:55:GLN:HG2	2.34	0.53
1:I:36:MET:HE3	1:I:36:MET:CA	2.39	0.53
1:K:33:ARG:O	1:K:55:GLN:HG2	2.08	0.53
1:R:16:THR:N	1:R:127:SER:O	2.41	0.53
1:R:93:THR:HG23	1:R:125:THR:CA	2.34	0.53
1:O:30:THR:O	1:O:30:THR:CG2	2.57	0.53
2:S:172:ASN:O	2:S:176:LEU:HD23	2.08	0.53
1:C:86:ASN:O	1:C:87:ASN:C	2.52	0.53
1:G:14:VAL:HG12	1:G:15:GLN:O	2.09	0.53
2:H:1:GLN:OE1	2:H:1:GLN:N	2.30	0.53
1:P:35:TYR:HA	1:P:74:ARG:NH2	2.24	0.53
2:T:43:LEU:HD11	2:T:153:VAL:HG22	1.91	0.53
2:T:45:SER:O	2:T:69:LYS:NZ	2.38	0.53
1:O:22:LEU:HG	1:O:85:MET:CE	2.39	0.53
1:A:120:GLN:OE1	1:A:120:GLN:N	2.29	0.53
1:G:105:TYR:CD2	2:H:83:LEU:HD11	2.43	0.53
1:I:85:MET:HB2	1:I:88:LEU:HD11	1.90	0.53
1:A:8:GLU:OE1	1:A:121:GLY:N	2.34	0.53
1:C:123:LEU:HD12	1:C:124:VAL:H	1.74	0.53
1:E:101:SER:HB2	1:E:115:TYR:HA	1.91	0.53
2:H:37:LEU:C	2:H:37:LEU:HD12	2.34	0.53
2:J:81:GLU:O	2:J:82:ILE:HG13	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:96:TYR:O	1:P:121:GLY:HA2	2.08	0.53
1:C:75:ASP:O	1:C:79:ASN:N	2.43	0.52
1:C:95:LEU:HD11	1:K:13:LEU:HG	1.91	0.52
1:I:41:GLN:O	1:I:94:ALA:HB1	2.09	0.52
2:L:121:LEU:HD12	2:L:122:LYS:N	2.24	0.52
1:M:4:VAL:HA	1:M:27:SER:O	2.10	0.52
1:M:123:LEU:HD11	1:M:125:THR:HG22	1.91	0.52
1:P:102:GLN:HG3	1:P:102:GLN:O	2.08	0.52
2:B:26:LEU:HD21	2:B:30:LEU:CD2	2.35	0.52
1:C:13:LEU:HD23	1:K:95:LEU:CD1	2.29	0.52
1:I:91:GLU:HG2	1:I:92:ASP:H	1.74	0.52
1:K:62:TYR:CE2	1:K:72:ILE:HG22	2.44	0.52
2:L:141:SER:HB2	2:L:145:ASN:CG	2.35	0.52
1:M:4:VAL:HG13	1:M:27:SER:O	2.09	0.52
1:M:78:GLU:C	1:M:79:ASN:OD1	2.50	0.52
2:N:121:LEU:HD12	2:N:122:LYS:N	2.24	0.52
2:S:1:GLN:OE1	2:S:1:GLN:N	2.30	0.52
1:A:30:THR:O	1:A:30:THR:CG2	2.54	0.52
1:M:22:LEU:HD13	1:M:85:MET:CE	2.37	0.52
2:N:2:THR:HG21	2:N:4:MET:CE	2.40	0.52
2:N:35:VAL:HG22	2:N:161:MET:HG3	1.92	0.52
1:P:24:CYS:SG	1:P:98:CYS:CB	2.97	0.52
1:A:54:SER:HB2	1:A:59:ASN:O	2.08	0.52
2:D:34:THR:HG23	2:D:99:SER:HB3	1.92	0.52
1:E:8:GLU:H	1:E:120:GLN:HE22	1.58	0.52
1:I:24:CYS:HB2	1:I:38:TRP:CH2	2.44	0.52
1:A:14:VAL:HG12	1:A:15:GLN:O	2.09	0.52
2:D:136:GLY:HA2	2:D:152:LEU:HG	1.92	0.52
2:F:133:ILE:C	2:F:134:ILE:HD13	2.34	0.52
1:G:101:SER:HB3	1:G:116:ALA:H	1.73	0.52
1:R:31:PHE:CE1	1:R:76:ASN:HA	2.45	0.52
1:O:3:GLU:OE2	1:O:30:THR:HB	2.09	0.52
1:K:62:TYR:CE2	1:K:71:THR:HA	2.44	0.52
2:L:168:PRO:HA	2:L:171:ILE:HD12	1.91	0.52
2:Q:80:SER:HB3	2:Q:122:LYS:HD3	1.90	0.52
1:R:42:VAL:CG1	1:R:45:LYS:HD2	2.39	0.52
2:B:43:LEU:CD1	2:B:153:VAL:HG22	2.40	0.52
1:C:30:THR:O	1:C:30:THR:CG2	2.54	0.52
1:G:105:TYR:CG	2:H:83:LEU:HG	2.45	0.52
2:H:183:ASN:OD1	2:H:184:VAL:N	2.43	0.52
2:J:80:SER:HB3	2:J:122:LYS:HD3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:168:PRO:HA	2:J:171:ILE:HD12	1.91	0.52
2:L:2:THR:CG2	2:L:4:MET:HE2	2.40	0.52
1:C:7:VAL:HG23	1:C:120:GLN:NE2	2.24	0.52
1:E:15:GLN:OE1	1:E:16:THR:HG23	2.10	0.52
1:G:15:GLN:OE1	1:G:16:THR:HG23	2.09	0.52
1:G:30:THR:O	1:G:30:THR:CG2	2.56	0.52
1:I:63:VAL:HG13	1:I:66:ALA:H	1.73	0.52
1:I:93:THR:CG2	1:I:125:THR:HA	2.38	0.52
1:K:4:VAL:HG22	1:K:117:TYR:HD2	1.75	0.52
1:K:111:LEU:HD12	1:K:112:LEU:H	1.74	0.52
1:A:62:TYR:HB2	1:A:67:LYS:CG	2.39	0.52
1:E:7:VAL:HA	1:E:120:GLN:HE22	1.75	0.52
1:E:65:SER:O	1:E:69:ARG:NH1	2.43	0.52
2:N:4:MET:CG	2:N:190:LEU:HD21	2.34	0.52
2:Q:43:LEU:HD22	2:Q:47:ARG:NH1	2.24	0.52
1:R:21:ARG:HG3	1:R:21:ARG:O	2.09	0.52
1:R:91:GLU:HG2	1:R:92:ASP:H	1.75	0.52
1:A:36:MET:HG3	1:A:81:VAL:CG1	2.33	0.51
1:E:42:VAL:H	1:E:45:LYS:HZ2	1.57	0.51
2:F:169:ASP:O	2:F:173:THR:HG23	2.10	0.51
2:H:169:ASP:O	2:H:173:THR:HG23	2.10	0.51
2:J:56:THR:HG22	2:J:57:LYS:H	1.75	0.51
2:L:37:LEU:C	2:L:37:LEU:HD12	2.35	0.51
1:M:14:VAL:HG13	1:M:126:VAL:HG22	1.93	0.51
1:P:88:LEU:CB	1:P:126:VAL:HG21	2.39	0.51
2:Q:125:TYR:CE2	2:Q:126:THR:C	2.88	0.51
1:R:34:HIS:NE2	1:R:103:SER:HA	2.25	0.51
1:O:15:GLN:OE1	1:O:16:THR:HG23	2.11	0.51
1:O:56:THR:HB	1:O:58:LEU:HD13	1.93	0.51
2:S:108:GLU:OE2	2:S:118:ARG:NH1	2.41	0.51
2:S:168:PRO:HA	2:S:171:ILE:HD12	1.93	0.51
1:E:101:SER:CB	1:E:115:TYR:HA	2.41	0.51
2:F:26:LEU:HD21	2:F:30:LEU:HD21	1.92	0.51
2:F:168:PRO:HA	2:F:171:ILE:HD12	1.92	0.51
1:G:5:GLN:HB2	1:G:27:SER:HB3	1.92	0.51
1:G:13:LEU:HD23	1:R:95:LEU:CD1	2.40	0.51
1:M:43:PRO:O	1:M:45:LYS:NZ	2.43	0.51
2:Q:168:PRO:HA	2:Q:171:ILE:HD12	1.92	0.51
2:T:80:SER:HB3	2:T:122:LYS:HD3	1.92	0.51
2:T:125:TYR:CE2	2:T:126:THR:C	2.88	0.51
1:O:75:ASP:O	1:O:79:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:152:LEU:HD13	2:D:156:ILE:HD11	1.92	0.51
1:K:33:ARG:NE	1:K:103:SER:HA	2.26	0.51
1:P:36:MET:HE1	1:P:100:GLY:HA2	1.91	0.51
1:O:90:PRO:O	1:O:93:THR:HG23	2.10	0.51
1:O:105:TYR:HB3	2:S:83:LEU:HG	1.91	0.51
2:S:183:ASN:OD1	2:S:184:VAL:N	2.43	0.51
1:C:3:GLU:OE2	1:C:30:THR:HB	2.11	0.51
1:E:78:GLU:C	1:E:79:ASN:OD1	2.54	0.51
1:K:74:ARG:HG2	1:K:75:ASP:N	2.25	0.51
1:M:112:LEU:O	1:M:112:LEU:HD23	2.10	0.51
1:O:42:VAL:HB	1:O:45:LYS:HG2	1.92	0.51
1:O:123:LEU:HD11	1:P:13:LEU:HD23	1.88	0.51
2:S:169:ASP:O	2:S:173:THR:HG23	2.10	0.51
1:A:22:LEU:CG	1:A:85:MET:HE1	2.39	0.51
1:A:35:TYR:HD2	1:A:102:GLN:HB3	1.72	0.51
1:C:41:GLN:OE1	1:C:42:VAL:N	2.41	0.51
1:C:75:ASP:CG	1:C:78:GLU:HB2	2.35	0.51
2:F:62:GLU:O	2:F:77:VAL:HA	2.10	0.51
2:H:133:ILE:O	2:H:134:ILE:HD13	2.09	0.51
2:H:153:VAL:HG23	2:H:153:VAL:O	2.11	0.51
1:O:7:VAL:HG23	1:O:120:GLN:NE2	2.25	0.51
2:S:125:TYR:CZ	2:S:126:THR:O	2.63	0.51
2:F:183:ASN:OD1	2:F:184:VAL:N	2.43	0.51
1:G:93:THR:O	1:G:93:THR:CG2	2.58	0.51
2:H:168:PRO:HA	2:H:171:ILE:HD12	1.92	0.51
1:P:35:TYR:HB2	1:P:53:ILE:O	2.10	0.51
1:P:38:TRP:CZ3	1:P:98:CYS:HB2	2.45	0.51
1:O:95:LEU:CD1	1:P:13:LEU:CG	2.88	0.51
1:O:101:SER:OG	1:O:115:TYR:HA	2.10	0.51
1:O:102:GLN:NE2	1:O:106:TYR:CD2	2.78	0.51
2:S:54:TYR:HB3	2:S:63:ILE:HB	1.93	0.51
2:D:22:LEU:HD22	2:D:190:LEU:HD11	1.93	0.51
1:E:14:VAL:HG12	1:E:15:GLN:O	2.10	0.51
1:E:36:MET:HA	1:E:36:MET:CE	2.34	0.51
1:G:65:SER:O	1:G:69:ARG:NH1	2.44	0.51
1:I:34:HIS:C	1:I:55:GLN:HG3	2.36	0.51
1:M:42:VAL:HB	1:M:45:LYS:CE	2.40	0.51
2:S:153:VAL:HG23	2:S:153:VAL:O	2.11	0.51
1:A:65:SER:O	1:A:69:ARG:NH1	2.44	0.51
1:E:24:CYS:HB2	1:E:38:TRP:CH2	2.46	0.51
2:F:82:ILE:HG21	2:F:119:LYS:CE	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:44:GLY:O	1:M:45:LYS:HG3	2.10	0.51
1:A:15:GLN:OE1	1:A:16:THR:HG23	2.10	0.51
1:C:95:LEU:CD1	1:K:13:LEU:CG	2.89	0.51
2:H:50:SER:O	2:H:152:LEU:CD2	2.51	0.51
2:H:54:TYR:HB3	2:H:63:ILE:HB	1.93	0.51
1:I:54:SER:CB	1:I:108:LYS:HE2	2.33	0.51
2:J:2:THR:HG22	2:J:4:MET:HE2	1.92	0.51
1:K:4:VAL:HG22	1:K:117:TYR:CD2	2.46	0.51
1:K:15:GLN:HA	1:K:127:SER:OG	2.11	0.51
1:K:78:GLU:C	1:K:79:ASN:OD1	2.54	0.51
2:L:81:GLU:O	2:L:82:ILE:HG13	2.10	0.51
2:S:36:CYS:HG	2:S:97:CYS:CB	2.17	0.51
2:J:43:LEU:HD11	2:J:153:VAL:HG22	1.93	0.51
1:M:24:CYS:SG	1:M:98:CYS:HB3	2.50	0.51
1:M:41:GLN:O	1:M:94:ALA:HB1	2.11	0.51
1:M:101:SER:CB	1:M:116:ALA:H	2.24	0.51
1:K:8:GLU:HA	1:K:24:CYS:HA	1.91	0.50
1:K:41:GLN:HB3	1:K:97:TYR:CE1	2.42	0.50
2:N:187:TRP:CE3	2:N:190:LEU:CD2	2.94	0.50
1:R:53:ILE:HB	1:R:72:ILE:HD13	1.93	0.50
1:O:41:GLN:HA	1:O:45:LYS:HZ1	1.76	0.50
1:A:123:LEU:HD11	1:M:13:LEU:HD12	1.94	0.50
2:D:76:THR:HG23	2:D:80:SER:O	2.12	0.50
1:E:35:TYR:HE1	1:E:115:TYR:CZ	2.28	0.50
1:R:59:ASN:HB3	1:R:108:LYS:NZ	2.26	0.50
1:I:40:ARG:HH22	1:I:92:ASP:HB2	1.75	0.50
1:I:58:LEU:HD12	1:I:59:ASN:ND2	2.26	0.50
1:I:63:VAL:HG22	1:I:64:ASP:OD1	2.11	0.50
1:K:123:LEU:HD12	1:K:124:VAL:N	2.27	0.50
2:S:38:HIS:CE1	2:S:205:TRP:HB3	2.47	0.50
2:D:197:GLU:OE1	2:D:197:GLU:HA	2.10	0.50
2:N:168:PRO:HA	2:N:171:ILE:HD12	1.92	0.50
1:P:89:LYS:HB2	1:P:91:GLU:CD	2.36	0.50
2:T:186:ASN:O	2:T:190:LEU:HD13	2.12	0.50
1:O:64:ASP:OD1	1:O:65:SER:N	2.44	0.50
1:O:93:THR:HB	1:O:125:THR:HA	1.92	0.50
1:C:30:THR:HG22	1:C:34:HIS:CD2	2.47	0.50
2:D:46:THR:HG22	2:D:47:ARG:HG2	1.92	0.50
2:D:96:ILE:HG12	2:D:111:VAL:HG13	1.94	0.50
2:D:152:LEU:HD12	2:D:152:LEU:O	2.12	0.50
1:G:24:CYS:HB2	1:G:38:TRP:CH2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:50:SER:O	2:N:152:LEU:CD2	2.56	0.50
2:Q:4:MET:HA	2:Q:4:MET:HE3	1.93	0.50
1:O:34:HIS:CD2	1:O:103:SER:HA	2.47	0.50
1:C:38:TRP:O	1:C:50:VAL:HB	2.12	0.50
1:G:62:TYR:OH	1:G:72:ILE:N	2.44	0.50
1:P:31:PHE:CD1	1:P:79:ASN:HB2	2.46	0.50
1:R:40:ARG:HG3	1:R:96:TYR:CE1	2.47	0.50
2:T:168:PRO:HA	2:T:171:ILE:HD12	1.92	0.50
1:O:59:ASN:HD21	2:S:76:THR:HG21	1.75	0.50
1:O:65:SER:O	1:O:69:ARG:NH1	2.45	0.50
1:E:13:LEU:HB3	1:I:123:LEU:CD1	2.42	0.50
1:E:38:TRP:O	1:E:50:VAL:HB	2.11	0.50
2:F:125:TYR:CE2	2:F:126:THR:O	2.65	0.50
1:K:8:GLU:OE2	1:K:121:GLY:C	2.54	0.50
1:K:33:ARG:CD	1:K:103:SER:HA	2.42	0.50
1:K:101:SER:HB2	1:K:117:TYR:CG	2.46	0.50
2:N:170:GLU:O	2:N:174:ILE:HG12	2.12	0.50
1:P:38:TRP:O	1:P:50:VAL:HB	2.11	0.50
1:O:107:ASP:CB	2:S:80:SER:OG	2.53	0.50
2:B:64:LEU:HD11	2:B:138:GLU:CG	2.40	0.50
1:K:36:MET:CG	1:K:81:VAL:HG21	2.39	0.50
2:T:170:GLU:O	2:T:174:ILE:HG12	2.12	0.50
1:A:42:VAL:HG22	1:A:94:ALA:CB	2.42	0.50
1:E:41:GLN:HA	1:E:45:LYS:HZ2	1.76	0.50
2:F:120:SER:HB2	2:H:12:PRO:HB2	1.93	0.50
2:L:170:GLU:O	2:L:174:ILE:HG12	2.12	0.50
1:R:14:VAL:HG13	1:R:126:VAL:HG22	1.93	0.50
1:R:17:GLY:N	1:R:88:LEU:O	2.26	0.50
1:E:58:LEU:HD21	2:F:66:PHE:CG	2.47	0.49
2:H:102:SER:OG	2:H:125:TYR:O	2.22	0.49
1:P:39:PHE:HD1	1:P:49:PHE:HA	1.75	0.49
2:Q:170:GLU:O	2:Q:174:ILE:HG12	2.12	0.49
1:O:42:VAL:HG22	1:O:94:ALA:CB	2.42	0.49
1:A:64:ASP:OD1	1:A:65:SER:N	2.45	0.49
1:G:78:GLU:C	1:G:79:ASN:OD1	2.55	0.49
2:H:75:PHE:N	2:H:82:ILE:O	2.42	0.49
1:K:7:VAL:HG23	1:K:7:VAL:O	2.12	0.49
1:P:7:VAL:HG13	1:P:7:VAL:O	2.10	0.49
1:R:16:THR:HA	1:R:126:VAL:CG1	2.43	0.49
1:R:123:LEU:HD12	1:R:124:VAL:N	2.27	0.49
1:O:102:GLN:NE2	1:O:106:TYR:CE2	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:120:SER:HB2	2:B:12:PRO:HB2	1.93	0.49
1:A:8:GLU:H	1:A:120:GLN:HE22	1.59	0.49
1:C:36:MET:CG	1:C:81:VAL:HG11	2.38	0.49
1:C:64:ASP:OD1	1:C:65:SER:N	2.46	0.49
1:G:90:PRO:HA	1:G:126:VAL:HB	1.94	0.49
1:I:20:LEU:HB3	1:I:22:LEU:HD11	1.95	0.49
2:J:125:TYR:CE2	2:J:126:THR:C	2.90	0.49
1:P:16:THR:OG1	1:P:127:SER:O	2.26	0.49
1:R:16:THR:HA	1:R:126:VAL:HG13	1.95	0.49
2:S:133:ILE:C	2:S:134:ILE:HD13	2.37	0.49
1:A:38:TRP:O	1:A:50:VAL:HB	2.12	0.49
2:D:169:ASP:O	2:D:173:THR:HG23	2.13	0.49
1:E:89:LYS:C	1:E:126:VAL:HG11	2.38	0.49
2:F:153:VAL:O	2:F:153:VAL:HG23	2.12	0.49
1:K:53:ILE:HB	1:K:72:ILE:HD13	1.93	0.49
1:M:95:LEU:HD21	1:M:123:LEU:HB2	1.94	0.49
1:O:53:ILE:C	1:O:108:LYS:CE	2.86	0.49
1:O:59:ASN:C	1:O:60:LYS:HG3	2.38	0.49
1:A:38:TRP:CH2	1:A:98:CYS:HB2	2.48	0.49
2:F:147:GLU:OE1	2:F:150:GLN:CD	2.56	0.49
2:L:136:GLY:HA2	2:L:152:LEU:CG	2.36	0.49
1:M:63:VAL:HG13	1:M:66:ALA:H	1.76	0.49
2:Q:26:LEU:CD2	2:Q:30:LEU:HD21	2.43	0.49
2:B:153:VAL:HG23	2:B:153:VAL:O	2.13	0.49
1:E:13:LEU:HD21	1:I:95:LEU:CD2	2.40	0.49
1:E:105:TYR:C	1:E:106:TYR:CG	2.88	0.49
2:F:50:SER:O	2:F:152:LEU:CD2	2.44	0.49
1:G:22:LEU:CD1	1:G:85:MET:HE1	2.42	0.49
2:H:197:GLU:OE2	2:H:197:GLU:HA	2.11	0.49
1:P:85:MET:SD	1:P:96:TYR:HE2	2.36	0.49
1:R:71:THR:CG2	1:R:84:GLN:HB3	2.43	0.49
1:C:32:ASN:HB3	1:C:76:ASN:HD21	1.76	0.49
1:C:36:MET:HE2	1:C:100:GLY:HA3	1.94	0.49
2:D:14:GLU:O	2:D:14:GLU:OE2	2.30	0.49
1:E:3:GLU:OE2	1:E:4:VAL:HG23	2.13	0.49
1:E:30:THR:HG23	1:E:33:ARG:HB2	1.95	0.49
1:G:13:LEU:CD2	1:R:123:LEU:HD13	2.42	0.49
2:N:35:VAL:HG22	2:N:161:MET:CG	2.42	0.49
2:N:136:GLY:HA2	2:N:152:LEU:CG	2.36	0.49
2:B:37:LEU:C	2:B:37:LEU:HD12	2.37	0.49
1:C:63:VAL:O	1:C:67:LYS:HG3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:17:THR:O	2:D:17:THR:HG22	2.12	0.49
2:F:125:TYR:CZ	2:F:126:THR:O	2.66	0.49
2:L:2:THR:HG21	2:L:4:MET:CE	2.42	0.49
1:M:40:ARG:HG2	1:M:41:GLN:N	2.26	0.49
2:N:82:ILE:HD12	2:N:121:LEU:CD2	2.23	0.49
1:P:13:LEU:HD12	1:P:13:LEU:C	2.38	0.49
1:O:38:TRP:O	1:O:50:VAL:HB	2.12	0.49
2:S:111:VAL:O	2:S:112:ASP:OD1	2.31	0.49
1:A:54:SER:HA	1:A:108:LYS:HZ1	1.72	0.49
1:I:40:ARG:HG2	1:I:41:GLN:N	2.27	0.49
1:M:40:ARG:HH12	1:M:92:ASP:HA	1.78	0.49
1:M:40:ARG:HG3	1:M:96:TYR:CE1	2.47	0.49
1:O:89:LYS:HD2	1:O:89:LYS:N	2.28	0.49
1:O:89:LYS:C	1:O:126:VAL:HG11	2.38	0.49
2:J:50:SER:O	2:J:152:LEU:CD2	2.55	0.49
1:K:21:ARG:HH21	1:K:84:GLN:CB	2.25	0.49
1:O:54:SER:CA	1:O:108:LYS:HZ3	2.13	0.48
1:O:95:LEU:HD11	1:P:13:LEU:CG	2.43	0.48
1:A:30:THR:HG23	1:A:33:ARG:CG	2.43	0.48
1:C:110:ARG:C	1:C:111:LEU:HD22	2.38	0.48
2:D:54:TYR:HB3	2:D:63:ILE:HB	1.94	0.48
1:G:54:SER:HA	1:G:108:LYS:HE2	1.88	0.48
1:G:101:SER:OG	1:G:116:ALA:HB3	2.13	0.48
1:I:31:PHE:CE1	1:I:79:ASN:HA	2.48	0.48
1:R:40:ARG:HH22	1:R:92:ASP:HB2	1.78	0.48
1:E:41:GLN:OE1	1:E:42:VAL:N	2.46	0.48
1:I:38:TRP:O	1:I:50:VAL:HB	2.14	0.48
1:I:105:TYR:HE2	2:J:119:LYS:HE3	1.79	0.48
1:P:74:ARG:HG2	1:P:75:ASP:N	2.28	0.48
1:G:89:LYS:C	1:G:126:VAL:HG11	2.38	0.48
1:I:66:ALA:HA	1:I:69:ARG:NH2	2.28	0.48
2:J:82:ILE:HD12	2:J:121:LEU:CD2	2.25	0.48
1:K:34:HIS:C	1:K:55:GLN:HG3	2.38	0.48
2:L:43:LEU:CD2	2:L:47:ARG:NH1	2.76	0.48
1:R:63:VAL:HG13	1:R:66:ALA:H	1.76	0.48
1:C:89:LYS:C	1:C:126:VAL:HG11	2.39	0.48
1:E:63:VAL:C	1:E:67:LYS:HZ3	2.21	0.48
2:F:111:VAL:O	2:F:112:ASP:OD1	2.31	0.48
1:G:38:TRP:O	1:G:50:VAL:HB	2.12	0.48
2:J:45:SER:O	2:J:69:LYS:NZ	2.41	0.48
1:K:104:SER:O	1:K:106:TYR:HD2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HG21	1:A:98:CYS:SG	2.53	0.48
1:A:105:TYR:HB3	2:B:83:LEU:HG	1.95	0.48
1:I:75:ASP:HB3	1:I:78:GLU:CD	2.37	0.48
1:M:42:VAL:HG22	1:M:94:ALA:CB	2.43	0.48
1:P:89:LYS:O	1:P:126:VAL:HB	2.14	0.48
2:S:140:ASP:CB	2:S:145:ASN:ND2	2.77	0.48
1:A:8:GLU:H	1:A:120:GLN:NE2	2.12	0.48
1:C:105:TYR:HB2	2:D:82:ILE:HG23	1.95	0.48
1:E:8:GLU:H	1:E:120:GLN:NE2	2.12	0.48
1:G:42:VAL:HG22	1:G:94:ALA:CB	2.42	0.48
1:M:40:ARG:HG3	1:M:96:TYR:HE1	1.78	0.48
1:A:42:VAL:H	1:A:45:LYS:HZ1	1.62	0.48
2:B:64:LEU:HD21	2:B:66:PHE:HB2	1.94	0.48
1:C:62:TYR:CB	1:C:67:LYS:HG2	2.35	0.48
1:E:4:VAL:HG13	1:E:27:SER:O	2.14	0.48
1:G:7:VAL:HG23	1:G:120:GLN:NE2	2.28	0.48
1:K:53:ILE:HB	1:K:72:ILE:CD1	2.43	0.48
1:O:53:ILE:O	1:O:108:LYS:HE3	2.14	0.48
1:C:35:TYR:HE1	1:C:102:GLN:HE21	1.62	0.48
1:E:34:HIS:ND1	1:E:101:SER:O	2.47	0.48
1:E:64:ASP:OD1	1:E:65:SER:N	2.47	0.48
2:H:111:VAL:O	2:H:112:ASP:OD1	2.31	0.48
1:I:34:HIS:NE2	1:I:103:SER:HA	2.28	0.48
1:I:89:LYS:O	1:I:126:VAL:HB	2.14	0.48
2:L:26:LEU:CD2	2:L:30:LEU:HD21	2.44	0.48
1:P:40:ARG:HG2	1:P:41:GLN:N	2.28	0.48
1:P:93:THR:HG21	1:P:125:THR:HG23	1.96	0.48
2:Q:56:THR:HG22	2:Q:130:GLU:O	2.14	0.48
1:R:91:GLU:HG2	1:R:92:ASP:N	2.29	0.48
1:R:114:GLU:OE1	1:R:114:GLU:N	2.33	0.48
1:O:13:LEU:HD21	1:P:95:LEU:CD2	2.44	0.48
2:S:58:ARG:NH1	2:S:58:ARG:HB2	2.29	0.48
1:A:64:ASP:CA	1:A:67:LYS:NZ	2.66	0.48
1:C:20:LEU:H	1:C:84:GLN:HE22	1.62	0.48
1:G:6:LEU:HD12	1:G:98:CYS:O	2.13	0.48
1:K:105:TYR:O	1:K:106:TYR:CG	2.67	0.48
1:M:36:MET:CG	1:M:81:VAL:HG21	2.41	0.48
1:R:59:ASN:C	1:R:108:LYS:NZ	2.72	0.48
1:R:66:ALA:HA	1:R:69:ARG:NH2	2.29	0.48
1:O:110:ARG:C	1:O:111:LEU:HD22	2.39	0.48
1:C:24:CYS:HB2	1:C:38:TRP:CH2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:104:SER:HB3	1:C:106:TYR:HE2	1.79	0.48
1:G:32:ASN:OD1	1:G:33:ARG:HD3	2.14	0.48
1:P:89:LYS:HB2	1:P:91:GLU:OE2	2.13	0.48
2:Q:125:TYR:CG	2:Q:126:THR:N	2.81	0.48
1:O:7:VAL:HG23	1:O:120:GLN:HE22	1.78	0.47
2:S:82:ILE:HD11	2:S:121:LEU:HB2	1.95	0.47
1:E:22:LEU:CD1	1:E:85:MET:HE1	2.44	0.47
1:G:52:SER:C	1:G:72:ILE:HD13	2.39	0.47
2:H:26:LEU:HD21	2:H:30:LEU:HD21	1.96	0.47
1:K:70:PHE:CD1	1:K:85:MET:HA	2.49	0.47
2:L:140:ASP:HB2	2:L:145:ASN:HB3	1.95	0.47
1:M:16:THR:N	1:M:127:SER:O	2.46	0.47
2:Q:83:LEU:HD12	2:Q:83:LEU:O	2.14	0.47
1:R:31:PHE:CG	1:R:79:ASN:HB2	2.49	0.47
1:P:85:MET:HB3	1:P:88:LEU:HD11	1.94	0.47
2:T:26:LEU:CD2	2:T:30:LEU:HD21	2.44	0.47
2:B:83:LEU:HD12	2:B:83:LEU:O	2.14	0.47
1:C:54:SER:HB3	1:C:57:GLY:HA2	1.96	0.47
1:E:13:LEU:HB3	1:I:123:LEU:HD11	1.95	0.47
1:E:13:LEU:HD23	1:I:123:LEU:HD12	1.95	0.47
1:E:42:VAL:HG22	1:E:94:ALA:CB	2.43	0.47
2:H:57:LYS:NZ	2:H:142:PHE:CE2	2.82	0.47
1:I:70:PHE:CE1	1:I:85:MET:HB3	2.49	0.47
1:K:85:MET:HB3	1:K:88:LEU:HD11	1.97	0.47
1:R:4:VAL:HG23	1:R:6:LEU:CD2	2.45	0.47
1:R:24:CYS:HB2	1:R:38:TRP:CH2	2.50	0.47
2:T:125:TYR:CG	2:T:126:THR:N	2.82	0.47
1:A:5:GLN:HB2	1:A:27:SER:HB2	1.97	0.47
1:I:85:MET:CB	1:I:88:LEU:HD11	2.44	0.47
1:I:88:LEU:HB3	1:I:126:VAL:HG21	1.96	0.47
1:K:8:GLU:OE2	1:K:121:GLY:N	2.47	0.47
1:K:40:ARG:HH22	1:K:92:ASP:HB2	1.79	0.47
1:K:93:THR:HG23	1:K:124:VAL:O	2.15	0.47
1:P:16:THR:HA	1:P:126:VAL:HG13	1.96	0.47
1:P:55:GLN:HE22	1:P:106:TYR:H	1.61	0.47
1:O:36:MET:HE3	1:O:99:ALA:O	2.15	0.47
1:A:7:VAL:HA	1:A:120:GLN:HE22	1.78	0.47
1:A:95:LEU:HD12	1:A:122:THR:O	2.14	0.47
1:C:64:ASP:N	1:C:67:LYS:NZ	2.63	0.47
2:D:82:ILE:HG22	2:D:83:LEU:N	2.29	0.47
1:E:120:GLN:OE1	1:E:120:GLN:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:6:LEU:HD12	1:I:24:CYS:SG	2.55	0.47
1:K:36:MET:HG3	1:K:81:VAL:CG2	2.41	0.47
1:R:38:TRP:O	1:R:50:VAL:HB	2.14	0.47
1:R:59:ASN:C	1:R:108:LYS:HZ2	2.22	0.47
2:S:76:THR:HG23	2:S:80:SER:C	2.39	0.47
2:S:82:ILE:HG21	2:S:119:LYS:CE	2.44	0.47
1:A:93:THR:OG1	1:A:125:THR:HA	2.14	0.47
2:B:76:THR:HG22	2:B:81:GLU:CG	2.44	0.47
1:I:14:VAL:O	1:I:126:VAL:HA	2.14	0.47
2:J:169:ASP:O	2:J:173:THR:HG23	2.14	0.47
1:K:31:PHE:HZ	1:K:81:VAL:HG23	1.79	0.47
1:K:105:TYR:HE2	2:L:119:LYS:HE3	1.79	0.47
1:P:20:LEU:HB3	1:P:22:LEU:CD1	2.45	0.47
1:P:55:GLN:OE1	1:P:105:TYR:HA	2.14	0.47
1:P:63:VAL:HG13	1:P:66:ALA:H	1.77	0.47
1:O:30:THR:HG23	1:O:33:ARG:HB2	1.94	0.47
1:O:40:ARG:NE	1:O:96:TYR:HE1	2.13	0.47
1:O:41:GLN:OE1	1:O:42:VAL:N	2.47	0.47
1:A:52:SER:C	1:A:72:ILE:HD13	2.39	0.47
1:A:58:LEU:HD21	2:B:66:PHE:CE2	2.50	0.47
1:A:102:GLN:C	1:A:104:SER:H	2.21	0.47
2:D:160:ASN:OD1	2:D:182:PRO:HG2	2.14	0.47
1:E:36:MET:HE3	1:E:99:ALA:O	2.15	0.47
1:E:108:LYS:HA	1:E:108:LYS:HD3	1.68	0.47
2:F:170:GLU:O	2:F:173:THR:OG1	2.25	0.47
1:G:7:VAL:CG1	1:G:25:ALA:HB3	2.45	0.47
2:H:81:GLU:O	2:H:82:ILE:HG13	2.15	0.47
1:I:88:LEU:C	1:I:89:LYS:HD3	2.40	0.47
1:K:16:THR:HA	1:K:126:VAL:HG13	1.97	0.47
1:K:36:MET:HE3	1:K:36:MET:CA	2.37	0.47
1:K:101:SER:OG	1:K:116:ALA:HB3	2.14	0.47
2:L:26:LEU:HD21	2:L:30:LEU:HD21	1.97	0.47
1:M:39:PHE:CE1	1:M:49:PHE:HA	2.50	0.47
1:M:63:VAL:HG22	1:M:64:ASP:OD1	2.15	0.47
2:Q:36:CYS:SG	2:Q:97:CYS:CB	3.03	0.47
2:T:4:MET:HA	2:T:4:MET:HE3	1.96	0.47
2:D:59:GLN:OE1	2:D:59:GLN:HA	2.15	0.47
1:I:63:VAL:HG23	1:I:110:ARG:NH1	2.30	0.47
2:J:136:GLY:HA2	2:J:152:LEU:CG	2.38	0.47
1:K:63:VAL:HG22	1:K:64:ASP:OD1	2.15	0.47
2:N:53:SER:CB	2:N:139:GLN:HE21	2.26	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:67:LYS:HB2	1:P:67:LYS:HE2	1.62	0.47
2:Q:187:TRP:CE3	2:Q:190:LEU:CD2	2.98	0.47
2:T:50:SER:O	2:T:152:LEU:CD2	2.55	0.47
1:G:30:THR:O	1:G:34:HIS:HD2	1.98	0.47
2:J:131:ALA:HA	2:J:142:PHE:HE1	1.80	0.47
1:K:91:GLU:HG2	1:K:92:ASP:N	2.30	0.47
1:P:54:SER:CB	1:P:108:LYS:HE2	2.43	0.47
1:O:22:LEU:CD1	1:O:85:MET:HE1	2.45	0.47
1:O:93:THR:CG2	1:O:126:VAL:N	2.77	0.47
1:E:22:LEU:HG	1:E:85:MET:CE	2.45	0.47
2:F:26:LEU:HG	2:F:129:ALA:HB1	1.96	0.47
1:I:31:PHE:CE1	1:I:76:ASN:HA	2.50	0.47
2:J:186:ASN:HD22	2:J:189:ALA:HB3	1.80	0.47
1:M:75:ASP:OD1	1:M:80:THR:N	2.43	0.47
1:O:16:THR:HB	1:O:89:LYS:NZ	2.30	0.46
2:S:62:GLU:OE1	2:S:63:ILE:HG13	2.15	0.46
1:A:20:LEU:HD12	1:A:20:LEU:HA	1.82	0.46
2:B:90:THR:HG23	2:B:91:VAL:N	2.29	0.46
1:C:32:ASN:OD1	1:C:33:ARG:HD3	2.15	0.46
1:C:78:GLU:C	1:C:79:ASN:OD1	2.58	0.46
1:C:101:SER:OG	1:C:116:ALA:HB3	2.15	0.46
2:H:26:LEU:HG	2:H:129:ALA:HB1	1.96	0.46
2:H:133:ILE:C	2:H:134:ILE:HD13	2.40	0.46
1:I:105:TYR:CE2	2:J:119:LYS:HE3	2.50	0.46
1:K:13:LEU:HD12	1:K:13:LEU:C	2.39	0.46
2:L:46:THR:OG1	2:L:47:ARG:N	2.47	0.46
1:M:60:LYS:HD3	1:M:62:TYR:CE1	2.49	0.46
1:R:76:ASN:O	1:R:79:ASN:HB3	2.15	0.46
1:R:101:SER:HB3	1:R:116:ALA:N	2.19	0.46
1:O:16:THR:HG22	1:O:126:VAL:CG1	2.44	0.46
1:A:101:SER:HB2	1:A:117:TYR:HD1	1.80	0.46
1:C:93:THR:OG1	1:C:125:THR:HA	2.14	0.46
1:C:123:LEU:HD11	1:K:13:LEU:HD23	1.88	0.46
2:D:82:ILE:HD11	2:D:121:LEU:HD13	1.96	0.46
2:J:125:TYR:CG	2:J:126:THR:N	2.82	0.46
1:K:26:ALA:CB	1:K:31:PHE:CD1	2.98	0.46
1:M:114:GLU:OE1	1:M:114:GLU:N	2.34	0.46
1:R:36:MET:CG	1:R:81:VAL:HG21	2.42	0.46
2:S:57:LYS:NZ	2:S:142:PHE:CE2	2.83	0.46
1:A:35:TYR:HB3	1:A:55:GLN:OE1	2.15	0.46
2:D:190:LEU:HG	2:D:192:TYR:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:122:THR:HG22	1:E:123:LEU:N	2.30	0.46
1:K:85:MET:HE1	1:K:96:TYR:HE2	1.81	0.46
2:L:43:LEU:HD21	2:L:153:VAL:HG22	1.97	0.46
1:M:7:VAL:HG23	1:M:120:GLN:HE22	1.77	0.46
1:M:42:VAL:CG1	1:M:43:PRO:HD2	2.45	0.46
2:T:83:LEU:HD12	2:T:83:LEU:O	2.16	0.46
1:A:101:SER:HB3	1:A:116:ALA:H	1.81	0.46
1:A:122:THR:HG22	1:A:123:LEU:N	2.30	0.46
1:C:42:VAL:HG22	1:C:94:ALA:CB	2.46	0.46
2:D:109:PHE:HB3	2:D:116:ARG:HB2	1.97	0.46
1:K:24:CYS:HB2	1:K:38:TRP:CZ2	2.51	0.46
1:K:40:ARG:HG2	1:K:41:GLN:H	1.80	0.46
1:M:78:GLU:O	1:M:80:THR:HG23	2.15	0.46
1:P:24:CYS:HB2	1:P:38:TRP:CH2	2.50	0.46
1:P:105:TYR:CB	2:Q:83:LEU:HG	2.45	0.46
2:Q:136:GLY:HA2	2:Q:152:LEU:CG	2.37	0.46
1:R:53:ILE:HG22	1:R:72:ILE:HD11	1.97	0.46
1:R:83:LEU:HD22	1:R:85:MET:CE	2.42	0.46
2:S:121:LEU:HD12	2:S:122:LYS:N	2.30	0.46
1:A:90:PRO:HA	1:A:126:VAL:CG1	2.46	0.46
1:E:95:LEU:HD12	1:E:122:THR:O	2.16	0.46
1:I:38:TRP:CG	1:I:83:LEU:HD12	2.50	0.46
2:J:2:THR:HG22	2:J:4:MET:CE	2.45	0.46
2:L:31:LYS:CG	2:L:102:SER:HB3	2.42	0.46
1:O:122:THR:HG22	1:O:123:LEU:N	2.31	0.46
2:S:26:LEU:CD2	2:S:30:LEU:HD21	2.45	0.46
2:S:26:LEU:HG	2:S:129:ALA:HB1	1.97	0.46
2:S:38:HIS:HE1	2:S:205:TRP:CE3	2.33	0.46
2:S:47:ARG:HG2	2:S:48:GLY:N	2.31	0.46
1:A:32:ASN:HB3	1:A:76:ASN:ND2	2.27	0.46
1:C:65:SER:O	1:C:69:ARG:NH1	2.49	0.46
1:I:24:CYS:SG	1:I:98:CYS:CB	3.03	0.46
1:K:17:GLY:HA2	1:K:87:ASN:HA	1.98	0.46
1:K:58:LEU:HD12	1:K:59:ASN:ND2	2.31	0.46
2:L:135:LEU:HD13	2:L:156:ILE:HD11	1.98	0.46
1:R:53:ILE:C	1:R:108:LYS:HD3	2.40	0.46
2:T:111:VAL:O	2:T:112:ASP:OD1	2.33	0.46
1:O:4:VAL:HG13	1:O:27:SER:O	2.16	0.46
1:O:33:ARG:HB3	1:O:103:SER:O	2.15	0.46
2:S:14:GLU:OE1	2:S:14:GLU:C	2.59	0.46
1:A:88:LEU:C	1:A:89:LYS:HD2	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:LEU:HD22	2:J:190:LEU:HD11	1.97	0.46
2:L:52:PHE:CZ	2:L:54:TYR:HB2	2.51	0.46
1:M:16:THR:HA	1:M:126:VAL:HG13	1.98	0.46
1:M:52:SER:OG	1:M:61:ASP:HB3	2.16	0.46
1:P:15:GLN:HA	1:P:127:SER:OG	2.16	0.46
2:S:36:CYS:SG	2:S:97:CYS:CB	3.04	0.46
2:F:82:ILE:HD11	2:F:121:LEU:HD12	1.87	0.46
1:I:78:GLU:O	1:I:79:ASN:OD1	2.34	0.46
1:K:61:ASP:OD1	1:K:110:ARG:NH2	2.49	0.46
2:N:36:CYS:SG	2:N:97:CYS:CB	3.04	0.46
2:D:175:TYR:HD2	2:D:176:LEU:HD22	1.80	0.46
1:E:38:TRP:CH2	1:E:98:CYS:HB2	2.51	0.46
2:H:163:ASP:OD1	2:H:183:ASN:ND2	2.49	0.46
1:I:20:LEU:HD23	1:I:20:LEU:HA	1.80	0.46
1:M:66:ALA:HA	1:M:69:ARG:NH2	2.31	0.46
1:M:95:LEU:CD2	1:M:123:LEU:HB2	2.46	0.46
1:R:105:TYR:C	1:R:106:TYR:CG	2.94	0.46
2:T:82:ILE:HD12	2:T:121:LEU:CD2	2.24	0.46
1:O:20:LEU:HD12	1:O:20:LEU:HA	1.86	0.46
1:A:4:VAL:HG13	1:A:27:SER:O	2.16	0.46
1:E:16:THR:HG22	1:E:126:VAL:CG1	2.45	0.46
1:K:63:VAL:HG23	1:K:110:ARG:NH1	2.31	0.46
2:L:125:TYR:CG	2:L:126:THR:N	2.84	0.46
1:M:39:PHE:HD1	1:M:49:PHE:HA	1.76	0.46
1:M:101:SER:OG	1:M:116:ALA:N	2.43	0.46
1:O:8:GLU:H	1:O:120:GLN:NE2	2.14	0.45
2:D:43:LEU:CG	2:D:153:VAL:HG22	2.45	0.45
2:D:105:GLY:O	2:D:120:SER:HA	2.16	0.45
1:E:85:MET:HB3	1:E:88:LEU:HD21	1.99	0.45
2:F:62:GLU:OE1	2:F:63:ILE:HG13	2.16	0.45
1:G:42:VAL:H	1:G:45:LYS:HZ2	1.63	0.45
1:G:101:SER:CB	1:G:116:ALA:HB3	2.46	0.45
1:I:89:LYS:CB	1:I:90:PRO:HD2	2.46	0.45
2:J:26:LEU:CD2	2:J:30:LEU:HD21	2.47	0.45
1:K:17:GLY:N	1:K:88:LEU:O	2.35	0.45
2:N:125:TYR:CG	2:N:126:THR:N	2.84	0.45
2:B:170:GLU:O	2:B:174:ILE:HG12	2.16	0.45
1:C:54:SER:C	1:C:57:GLY:H	2.25	0.45
1:C:95:LEU:HD11	1:K:13:LEU:CG	2.46	0.45
2:F:170:GLU:O	2:F:174:ILE:HG12	2.16	0.45
2:H:137:GLN:HB3	2:H:146:PHE:CD2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:153:VAL:HG23	2:J:153:VAL:O	2.16	0.45
2:L:111:VAL:O	2:L:112:ASP:OD1	2.33	0.45
1:P:34:HIS:CD2	1:P:103:SER:HA	2.50	0.45
1:P:88:LEU:C	1:P:89:LYS:HD3	2.41	0.45
1:P:89:LYS:HB2	1:P:91:GLU:OE1	2.16	0.45
1:A:24:CYS:SG	1:A:98:CYS:HB3	2.56	0.45
1:C:54:SER:CA	1:C:108:LYS:HE2	2.44	0.45
1:C:122:THR:HG22	1:C:123:LEU:N	2.31	0.45
1:E:104:SER:OG	1:E:106:TYR:HE2	1.99	0.45
1:E:110:ARG:C	1:E:111:LEU:HD22	2.41	0.45
2:F:57:LYS:NZ	2:F:142:PHE:CE2	2.84	0.45
2:H:36:CYS:SG	2:H:97:CYS:CB	3.05	0.45
1:K:20:LEU:H	1:K:84:GLN:NE2	2.12	0.45
1:M:89:LYS:O	1:M:126:VAL:HB	2.16	0.45
1:P:4:VAL:HG23	1:P:6:LEU:CD2	2.46	0.45
1:P:15:GLN:HA	1:P:127:SER:HG	1.81	0.45
1:R:63:VAL:HG22	1:R:64:ASP:OD1	2.15	0.45
2:S:125:TYR:CG	2:S:126:THR:N	2.84	0.45
1:A:58:LEU:HD21	2:B:66:PHE:CZ	2.52	0.45
2:B:36:CYS:SG	2:B:97:CYS:CB	3.03	0.45
1:G:95:LEU:HD12	1:G:122:THR:O	2.16	0.45
1:G:123:LEU:HD11	1:R:13:LEU:HD12	1.98	0.45
1:K:101:SER:CB	1:K:116:ALA:HB3	2.46	0.45
2:N:26:LEU:CD2	2:N:30:LEU:HD21	2.46	0.45
1:R:102:GLN:OE1	1:R:104:SER:HB3	2.16	0.45
1:O:31:PHE:CD2	1:O:79:ASN:CB	3.00	0.45
1:O:85:MET:HE3	1:O:85:MET:HB2	1.85	0.45
1:M:16:THR:HA	1:M:126:VAL:CG1	2.47	0.45
1:R:75:ASP:O	1:R:79:ASN:CA	2.64	0.45
1:O:24:CYS:HB2	1:O:38:TRP:CH2	2.52	0.45
1:A:52:SER:O	1:A:72:ILE:HD13	2.16	0.45
1:A:110:ARG:C	1:A:111:LEU:HD22	2.41	0.45
2:F:46:THR:HG23	2:F:47:ARG:N	2.31	0.45
1:G:7:VAL:HG23	1:G:120:GLN:HE22	1.81	0.45
1:G:63:VAL:C	1:G:67:LYS:HZ3	2.25	0.45
1:G:64:ASP:CA	1:G:67:LYS:NZ	2.69	0.45
2:H:98:THR:HG22	2:H:109:PHE:CD1	2.52	0.45
1:I:102:GLN:HE22	1:I:104:SER:HB3	1.81	0.45
2:Q:135:LEU:HD13	2:Q:156:ILE:HD11	1.99	0.45
1:R:59:ASN:O	1:R:108:LYS:NZ	2.48	0.45
1:E:42:VAL:HB	1:E:45:LYS:CE	2.36	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:105:TYR:HD1	2:H:82:ILE:HG23	1.81	0.45
2:H:26:LEU:CD2	2:H:30:LEU:HD21	2.47	0.45
2:L:36:CYS:SG	2:L:97:CYS:CB	3.03	0.45
1:M:54:SER:CA	1:M:108:LYS:CE	2.93	0.45
1:M:54:SER:CA	1:M:108:LYS:NZ	2.80	0.45
2:N:106:ILE:HA	2:N:119:LYS:O	2.17	0.45
1:P:39:PHE:CE1	1:P:49:PHE:HA	2.52	0.45
1:P:78:GLU:O	1:P:80:THR:HG23	2.15	0.45
2:T:11:PHE:CE2	2:T:198:VAL:HG13	2.52	0.45
2:T:102:SER:O	2:T:103:ALA:C	2.55	0.45
1:O:24:CYS:SG	1:O:98:CYS:CB	3.03	0.45
1:E:30:THR:O	1:E:34:HIS:HD2	2.00	0.45
2:F:26:LEU:CD2	2:F:30:LEU:HD21	2.46	0.45
1:G:24:CYS:SG	1:G:98:CYS:CB	3.03	0.45
1:G:122:THR:HG22	1:G:123:LEU:N	2.32	0.45
1:M:34:HIS:CB	1:M:102:GLN:HB3	2.47	0.45
2:N:55:ALA:HB3	2:N:139:GLN:OE1	2.17	0.45
1:R:20:LEU:HG	1:R:22:LEU:CD1	2.47	0.45
1:R:107:ASP:CG	1:R:108:LYS:H	2.25	0.45
2:B:59:GLN:HA	2:B:59:GLN:OE1	2.17	0.45
2:B:135:LEU:HD22	2:B:156:ILE:HD12	1.99	0.45
1:C:88:LEU:HB3	1:C:126:VAL:CG2	2.47	0.45
1:G:101:SER:HB3	1:G:116:ALA:N	2.32	0.45
1:K:38:TRP:O	1:K:50:VAL:HB	2.17	0.45
2:L:140:ASP:HB2	2:L:145:ASN:CB	2.47	0.45
1:M:38:TRP:CH2	1:M:98:CYS:HB2	2.51	0.45
2:N:83:LEU:HD12	2:N:83:LEU:O	2.17	0.45
1:P:17:GLY:HA2	1:P:87:ASN:HA	1.99	0.45
1:P:78:GLU:O	1:P:79:ASN:OD1	2.34	0.45
2:S:170:GLU:O	2:S:174:ILE:HG12	2.16	0.45
1:A:30:THR:O	1:A:34:HIS:HD2	1.99	0.45
2:F:14:GLU:C	2:F:14:GLU:OE1	2.59	0.45
2:F:137:GLN:HB3	2:F:146:PHE:CD2	2.52	0.45
2:H:170:GLU:O	2:H:174:ILE:HG12	2.16	0.45
2:H:186:ASN:OD1	2:H:188:ARG:N	2.49	0.45
1:I:34:HIS:CE1	1:I:103:SER:HG	2.34	0.45
1:I:80:THR:HG22	1:I:81:VAL:N	2.32	0.45
2:J:52:PHE:CZ	2:J:54:TYR:HB2	2.52	0.45
2:L:64:LEU:CD2	2:L:66:PHE:HB2	2.46	0.45
1:M:53:ILE:C	1:M:108:LYS:HE2	2.42	0.45
1:P:36:MET:CE	1:P:100:GLY:HA2	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:108:LYS:N	1:P:108:LYS:HD3	2.31	0.45
1:A:101:SER:OG	1:A:116:ALA:HB3	2.18	0.44
2:D:36:CYS:SG	2:D:97:CYS:CB	3.04	0.44
2:D:184:VAL:HG12	2:D:185:LEU:CD2	2.48	0.44
1:G:31:PHE:CE2	1:G:79:ASN:HA	2.52	0.44
1:I:8:GLU:OE1	1:I:121:GLY:N	2.44	0.44
1:I:91:GLU:HG2	1:I:92:ASP:N	2.30	0.44
2:J:36:CYS:SG	2:J:97:CYS:CB	3.05	0.44
1:K:38:TRP:CH2	1:K:98:CYS:HB3	2.52	0.44
1:K:88:LEU:CB	1:K:126:VAL:HG21	2.41	0.44
2:L:91:VAL:O	2:L:91:VAL:CG1	2.65	0.44
1:M:63:VAL:HG23	1:M:110:ARG:NH1	2.33	0.44
1:M:78:GLU:OE1	1:M:78:GLU:N	2.38	0.44
2:N:64:LEU:CD2	2:N:66:PHE:HB2	2.46	0.44
2:Q:64:LEU:HB3	2:Q:76:THR:CG2	2.47	0.44
1:O:8:GLU:H	1:O:120:GLN:HE22	1.66	0.44
1:O:88:LEU:HB3	1:O:126:VAL:CG2	2.46	0.44
1:C:64:ASP:N	1:C:67:LYS:HZ3	2.16	0.44
1:E:32:ASN:HB3	1:E:76:ASN:HD21	1.81	0.44
1:I:70:PHE:CD1	1:I:85:MET:HA	2.53	0.44
1:I:83:LEU:HD22	1:I:85:MET:HG2	1.99	0.44
1:P:63:VAL:HG23	1:P:110:ARG:NH1	2.32	0.44
2:T:59:GLN:HG3	2:T:62:GLU:N	2.32	0.44
2:S:26:LEU:HD23	2:S:129:ALA:HA	1.99	0.44
1:A:42:VAL:HB	1:A:45:LYS:CE	2.36	0.44
1:C:55:GLN:CA	1:C:74:ARG:NH1	2.68	0.44
1:E:22:LEU:HG	1:E:85:MET:HE1	1.98	0.44
2:F:83:LEU:HD12	2:F:83:LEU:O	2.17	0.44
2:H:33:PHE:CZ	2:H:63:ILE:HD11	2.52	0.44
2:H:141:SER:HB3	2:H:145:ASN:HD22	1.83	0.44
2:J:2:THR:HG21	2:J:4:MET:CE	2.48	0.44
1:K:67:LYS:HE2	1:K:67:LYS:HB2	1.61	0.44
1:K:96:TYR:CE2	1:K:124:VAL:HG21	2.52	0.44
2:L:43:LEU:HD21	2:L:153:VAL:CG2	2.47	0.44
1:M:53:ILE:HB	1:M:72:ILE:CG1	2.48	0.44
2:N:83:LEU:HD12	2:N:83:LEU:C	2.42	0.44
2:Q:147:GLU:N	2:Q:147:GLU:OE2	2.49	0.44
2:T:131:ALA:HA	2:T:142:PHE:HE1	1.82	0.44
1:O:35:TYR:CE2	1:O:102:GLN:HB3	2.52	0.44
1:A:4:VAL:HA	1:A:27:SER:O	2.18	0.44
1:A:32:ASN:OD1	1:A:33:ARG:HD3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:133:ILE:HD12	2:B:133:ILE:N	2.33	0.44
1:G:75:ASP:O	1:G:79:ASN:N	2.50	0.44
2:H:26:LEU:HD23	2:H:129:ALA:HA	1.99	0.44
2:N:4:MET:CG	2:N:190:LEU:HD11	2.47	0.44
1:P:35:TYR:CD1	1:P:101:SER:HB2	2.53	0.44
1:P:114:GLU:OE1	1:P:114:GLU:N	2.31	0.44
1:R:3:GLU:OE2	1:R:4:VAL:HG13	2.17	0.44
1:R:8:GLU:OE1	1:R:121:GLY:N	2.48	0.44
1:R:78:GLU:C	1:R:79:ASN:OD1	2.61	0.44
1:A:11:GLY:HA3	1:A:122:THR:CG2	2.48	0.44
1:A:39:PHE:CD2	1:A:49:PHE:HA	2.53	0.44
1:A:53:ILE:O	1:A:108:LYS:HE3	2.17	0.44
2:D:43:LEU:HG	2:D:153:VAL:HG22	1.99	0.44
1:G:39:PHE:CD2	1:G:49:PHE:HA	2.53	0.44
1:G:110:ARG:C	1:G:111:LEU:HD22	2.42	0.44
2:L:11:PHE:CE2	2:L:198:VAL:HG13	2.52	0.44
1:M:33:ARG:HD2	1:M:102:GLN:O	2.16	0.44
1:O:4:VAL:HA	1:O:27:SER:O	2.18	0.44
2:S:170:GLU:O	2:S:173:THR:OG1	2.24	0.44
2:D:64:LEU:HD12	2:D:65:ILE:N	2.32	0.44
2:F:37:LEU:C	2:F:37:LEU:HD12	2.43	0.44
2:F:186:ASN:OD1	2:F:188:ARG:N	2.48	0.44
2:H:82:ILE:HD11	2:H:121:LEU:HB2	1.99	0.44
1:M:93:THR:HG23	1:M:125:THR:CA	2.38	0.44
2:N:1:GLN:OE1	2:N:189:ALA:O	2.36	0.44
1:P:63:VAL:HG22	1:P:64:ASP:OD1	2.18	0.44
1:P:93:THR:HG23	1:P:125:THR:CA	2.39	0.44
1:R:34:HIS:C	1:R:55:GLN:HG3	2.42	0.44
1:O:62:TYR:HB2	1:O:67:LYS:CG	2.47	0.44
1:C:31:PHE:CE2	1:C:79:ASN:HA	2.53	0.44
1:C:49:PHE:HZ	1:C:52:SER:OG	1.99	0.44
1:C:101:SER:HB3	1:C:115:TYR:HA	2.00	0.44
2:D:34:THR:HG23	2:D:99:SER:CB	2.46	0.44
1:E:52:SER:OG	1:E:61:ASP:HB3	2.18	0.44
1:I:93:THR:HG23	1:I:124:VAL:O	2.17	0.44
1:K:26:ALA:HB3	1:K:31:PHE:CD1	2.52	0.44
1:M:13:LEU:HG	1:M:125:THR:OG1	2.17	0.44
1:M:20:LEU:HB3	1:M:22:LEU:CD1	2.48	0.44
1:R:107:ASP:CG	1:R:108:LYS:N	2.75	0.44
2:T:26:LEU:HD21	2:T:30:LEU:HD21	2.00	0.44
1:A:15:GLN:HA	1:A:127:SER:OG	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:PHE:CE2	1:A:79:ASN:HA	2.52	0.44
1:A:40:ARG:NE	1:A:96:TYR:HE1	2.14	0.44
2:F:163:ASP:OD1	2:F:183:ASN:ND2	2.50	0.44
1:G:88:LEU:HB3	1:G:126:VAL:HG21	2.00	0.44
2:J:121:LEU:HD12	2:J:122:LYS:H	1.83	0.44
1:K:33:ARG:HE	1:K:34:HIS:CE1	2.35	0.44
1:K:42:VAL:HG13	1:K:43:PRO:CD	2.46	0.44
1:M:28:GLY:O	1:M:29:ARG:HD3	2.18	0.44
1:P:109:PRO:HB2	1:P:114:GLU:OE2	2.17	0.44
1:R:89:LYS:O	1:R:126:VAL:HB	2.18	0.44
2:D:38:HIS:HD1	2:D:95:HIS:HB2	1.81	0.44
2:D:55:ALA:O	2:D:131:ALA:HB1	2.18	0.44
1:G:63:VAL:HG22	1:G:64:ASP:H	1.83	0.44
2:H:95:HIS:HE1	2:H:97:CYS:SG	2.41	0.44
1:I:78:GLU:C	1:I:79:ASN:OD1	2.61	0.44
1:K:89:LYS:O	1:K:126:VAL:HB	2.18	0.44
1:M:20:LEU:HD23	1:M:20:LEU:HA	1.78	0.44
2:N:131:ALA:HA	2:N:142:PHE:HE1	1.83	0.44
1:O:32:ASN:OD1	1:O:33:ARG:HD3	2.18	0.43
2:S:163:ASP:OD1	2:S:183:ASN:ND2	2.51	0.43
1:A:41:GLN:OE1	1:A:42:VAL:N	2.47	0.43
1:C:24:CYS:SG	1:C:98:CYS:CB	3.06	0.43
1:E:15:GLN:HA	1:E:127:SER:OG	2.18	0.43
2:F:36:CYS:SG	2:F:97:CYS:CB	3.06	0.43
2:F:58:ARG:HB2	2:F:58:ARG:HH11	1.81	0.43
1:K:93:THR:HG21	1:K:125:THR:HG23	2.00	0.43
2:L:64:LEU:HB3	2:L:76:THR:CG2	2.47	0.43
1:P:92:ASP:OD1	1:P:92:ASP:N	2.51	0.43
1:O:39:PHE:CA	1:O:50:VAL:HG23	2.48	0.43
1:A:89:LYS:HE3	1:A:90:PRO:HD3	1.99	0.43
2:D:82:ILE:HG21	2:D:119:LYS:HE2	1.99	0.43
2:D:170:GLU:O	2:D:174:ILE:HG12	2.17	0.43
1:E:54:SER:O	1:E:74:ARG:NH1	2.47	0.43
2:H:58:ARG:HB2	2:H:58:ARG:HH11	1.82	0.43
2:L:35:VAL:HG22	2:L:161:MET:HG3	2.00	0.43
2:L:186:ASN:HD22	2:L:189:ALA:HB3	1.83	0.43
2:N:100:TRP:CZ2	2:N:102:SER:HB2	2.52	0.43
1:R:93:THR:HG23	1:R:124:VAL:O	2.19	0.43
1:O:24:CYS:SG	1:O:98:CYS:HB2	2.57	0.43
1:C:54:SER:CB	1:C:59:ASN:H	2.31	0.43
2:J:35:VAL:HG22	2:J:161:MET:HG2	1.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:55:ALA:HB3	2:J:139:GLN:OE1	2.18	0.43
1:K:21:ARG:NE	1:K:84:GLN:HB2	2.31	0.43
1:M:96:TYR:CE2	1:M:124:VAL:HG21	2.53	0.43
1:M:112:LEU:HG	1:M:118:TRP:HH2	1.83	0.43
1:P:3:GLU:OE2	1:P:4:VAL:HG13	2.19	0.43
1:P:105:TYR:O	1:P:106:TYR:CG	2.71	0.43
2:Q:26:LEU:HD21	2:Q:30:LEU:HD21	2.00	0.43
2:Q:44:SER:O	2:Q:45:SER:HB3	2.18	0.43
1:O:53:ILE:HB	1:O:72:ILE:CD1	2.46	0.43
1:I:31:PHE:O	1:I:74:ARG:NH2	2.51	0.43
1:K:8:GLU:OE1	1:K:98:CYS:SG	2.76	0.43
1:K:44:GLY:C	1:K:45:LYS:HG3	2.40	0.43
2:L:1:GLN:OE1	2:L:189:ALA:O	2.35	0.43
2:L:147:GLU:OE2	2:L:147:GLU:N	2.52	0.43
1:M:5:GLN:OE1	1:M:5:GLN:HA	2.18	0.43
2:N:135:LEU:HD13	2:N:156:ILE:HD11	2.00	0.43
1:P:93:THR:HG23	1:P:124:VAL:O	2.18	0.43
1:R:41:GLN:HE22	1:R:46:GLU:HA	1.84	0.43
2:T:53:SER:CB	2:T:139:GLN:HE21	2.28	0.43
1:A:102:GLN:NE2	1:A:104:SER:HB2	2.24	0.43
1:E:40:ARG:NE	1:E:96:TYR:HE1	2.16	0.43
1:G:15:GLN:HA	1:G:127:SER:OG	2.18	0.43
1:I:20:LEU:HB3	1:I:22:LEU:CD1	2.48	0.43
1:K:53:ILE:CG2	1:K:72:ILE:HD11	2.47	0.43
2:L:43:LEU:HD22	2:L:47:ARG:CZ	2.48	0.43
2:N:2:THR:HG22	2:N:4:MET:CE	2.46	0.43
1:A:101:SER:CB	1:A:116:ALA:H	2.32	0.43
1:C:8:GLU:OE2	1:C:119:GLY:HA3	2.19	0.43
1:C:54:SER:N	1:C:108:LYS:CE	2.81	0.43
1:E:62:TYR:OH	1:E:72:ILE:N	2.51	0.43
2:F:125:TYR:CG	2:F:126:THR:N	2.87	0.43
1:G:40:ARG:NE	1:G:96:TYR:HE1	2.17	0.43
1:I:101:SER:HB3	1:I:116:ALA:N	2.18	0.43
2:J:135:LEU:HD13	2:J:156:ILE:HD11	2.00	0.43
1:K:8:GLU:OE1	1:K:8:GLU:N	2.50	0.43
1:P:38:TRP:CG	1:P:83:LEU:HD22	2.54	0.43
1:O:52:SER:OG	1:O:61:ASP:HB3	2.19	0.43
1:C:58:LEU:HD21	2:D:66:PHE:CE2	2.54	0.43
1:E:84:GLN:NE2	1:E:85:MET:O	2.51	0.43
1:G:62:TYR:CZ	1:G:72:ILE:HG22	2.54	0.43
1:K:35:TYR:HE2	1:K:109:PRO:HD2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:64:LEU:HB3	2:N:76:THR:CG2	2.48	0.43
1:R:16:THR:HG23	1:R:127:SER:C	2.43	0.43
1:O:41:GLN:HA	1:O:45:LYS:HZ2	1.84	0.43
1:E:30:THR:HG22	1:E:33:ARG:HB2	1.99	0.43
1:E:75:ASP:O	1:E:79:ASN:N	2.51	0.43
2:H:81:GLU:C	2:H:82:ILE:HG13	2.44	0.43
2:J:36:CYS:HG	2:J:97:CYS:CB	2.19	0.43
2:J:100:TRP:CZ2	2:J:102:SER:HB2	2.51	0.43
1:K:88:LEU:C	1:K:89:LYS:HD3	2.44	0.43
1:M:56:THR:OG1	1:M:58:LEU:HG	2.19	0.43
1:M:109:PRO:HB2	1:M:114:GLU:OE2	2.19	0.43
2:N:125:TYR:CE2	2:N:126:THR:C	2.97	0.43
1:P:114:GLU:HG2	1:P:115:TYR:N	2.33	0.43
1:R:63:VAL:HG23	1:R:110:ARG:NH1	2.34	0.43
1:O:8:GLU:OE2	1:O:119:GLY:HA3	2.19	0.43
1:A:70:PHE:CE1	1:A:85:MET:HB3	2.54	0.43
1:E:39:PHE:CD2	1:E:49:PHE:HA	2.54	0.43
2:F:81:GLU:C	2:F:82:ILE:HG13	2.44	0.43
2:F:121:LEU:HD23	2:F:122:LYS:CB	2.49	0.43
1:G:30:THR:HG22	1:G:33:ARG:HB2	2.00	0.43
1:I:15:GLN:OE1	1:I:15:GLN:HA	2.18	0.43
1:K:3:GLU:OE1	1:K:117:TYR:OH	2.31	0.43
1:K:20:LEU:N	1:K:84:GLN:HE22	2.14	0.43
1:P:62:TYR:OH	1:P:72:ILE:HG22	2.19	0.43
1:R:20:LEU:HG	1:R:22:LEU:HD12	2.01	0.43
1:R:42:VAL:HG22	1:R:94:ALA:HB2	2.00	0.43
1:R:111:LEU:HG	1:R:113:THR:H	1.84	0.43
1:A:30:THR:HG22	1:A:34:HIS:CD2	2.54	0.43
1:A:84:GLN:NE2	1:A:85:MET:O	2.51	0.43
1:E:31:PHE:CE1	1:E:79:ASN:HA	2.53	0.43
1:E:32:ASN:OD1	1:E:33:ARG:HD3	2.19	0.43
1:G:4:VAL:HG13	1:G:27:SER:O	2.19	0.43
1:G:42:VAL:HB	1:G:45:LYS:CE	2.36	0.43
1:G:90:PRO:O	1:G:93:THR:CG2	2.67	0.43
2:H:141:SER:CB	2:H:145:ASN:HD22	2.32	0.43
1:I:22:LEU:HD12	1:I:22:LEU:N	2.31	0.43
1:I:73:SER:O	1:I:81:VAL:HG13	2.19	0.43
1:M:105:TYR:HD2	2:N:82:ILE:HG23	1.84	0.43
2:N:54:TYR:HB3	2:N:63:ILE:HB	2.01	0.43
1:O:39:PHE:CD2	1:O:49:PHE:HA	2.54	0.42
1:O:40:ARG:CZ	1:O:96:TYR:OH	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:S:62:GLU:O	2:S:77:VAL:HA	2.18	0.42
1:A:3:GLU:OE2	1:A:30:THR:HB	2.19	0.42
1:A:47:ARG:HD3	1:A:118:TRP:CZ3	2.54	0.42
2:B:95:HIS:HE1	2:B:97:CYS:SG	2.41	0.42
1:E:63:VAL:O	1:E:67:LYS:HG3	2.19	0.42
1:G:105:TYR:CD1	2:H:82:ILE:HG23	2.54	0.42
1:I:89:LYS:HB3	1:I:90:PRO:HD2	2.01	0.42
2:L:52:PHE:CE2	2:L:54:TYR:HB2	2.54	0.42
1:P:24:CYS:HB3	1:P:81:VAL:HB	2.00	0.42
2:T:135:LEU:HD13	2:T:156:ILE:HD11	2.00	0.42
1:A:24:CYS:HB2	1:A:38:TRP:CH2	2.54	0.42
1:C:34:HIS:CG	1:C:102:GLN:O	2.71	0.42
1:E:39:PHE:CA	1:E:50:VAL:HG23	2.49	0.42
1:I:7:VAL:HG13	1:I:25:ALA:HB3	2.00	0.42
1:I:67:LYS:HB2	1:I:67:LYS:HE2	1.55	0.42
2:J:54:TYR:HB3	2:J:63:ILE:HB	2.01	0.42
1:A:8:GLU:OE2	1:A:119:GLY:HA3	2.18	0.42
2:H:104:SER:HA	2:H:123:LYS:NZ	2.34	0.42
1:I:54:SER:HB3	1:I:108:LYS:CE	2.37	0.42
1:K:111:LEU:HG	1:K:113:THR:H	1.84	0.42
1:M:111:LEU:HG	1:M:113:THR:H	1.85	0.42
1:P:24:CYS:SG	1:P:98:CYS:HB3	2.59	0.42
1:P:36:MET:HG3	1:P:81:VAL:CG2	2.40	0.42
1:P:89:LYS:CB	1:P:90:PRO:HD2	2.50	0.42
2:Q:84:PHE:CE2	2:Q:119:LYS:NZ	2.88	0.42
1:R:70:PHE:CD1	1:R:85:MET:HA	2.54	0.42
1:O:42:VAL:HB	1:O:45:LYS:CE	2.47	0.42
2:B:163:ASP:OD1	2:B:183:ASN:ND2	2.45	0.42
1:C:7:VAL:CG1	1:C:25:ALA:HB3	2.49	0.42
2:F:46:THR:HG23	2:F:47:ARG:HG2	2.02	0.42
1:G:105:TYR:O	1:G:106:TYR:CD1	2.72	0.42
2:L:183:ASN:OD1	2:L:184:VAL:N	2.51	0.42
1:M:55:GLN:HE22	1:M:102:GLN:HG2	1.84	0.42
2:N:84:PHE:CE2	2:N:119:LYS:NZ	2.88	0.42
1:P:17:GLY:N	1:P:88:LEU:O	2.39	0.42
1:R:89:LYS:CB	1:R:90:PRO:HD2	2.49	0.42
1:O:15:GLN:HA	1:O:127:SER:OG	2.18	0.42
2:S:152:LEU:HD12	2:S:152:LEU:C	2.44	0.42
1:A:20:LEU:HG	1:A:22:LEU:CD2	2.50	0.42
2:H:67:TRP:CZ2	2:H:89:VAL:HG11	2.55	0.42
1:I:42:VAL:HG13	1:I:43:PRO:CD	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:81:VAL:HG12	1:I:82:TYR:N	2.35	0.42
1:I:92:ASP:N	1:I:92:ASP:OD1	2.50	0.42
1:I:109:PRO:HB2	1:I:114:GLU:OE2	2.19	0.42
2:J:64:LEU:HB3	2:J:76:THR:CG2	2.49	0.42
1:K:35:TYR:CE1	1:K:102:GLN:HG3	2.54	0.42
2:N:117:VAL:HG12	2:Q:42:GLU:OE2	2.20	0.42
2:T:55:ALA:HB3	2:T:139:GLN:OE1	2.19	0.42
2:T:64:LEU:HB3	2:T:76:THR:CG2	2.49	0.42
2:T:183:ASN:OD1	2:T:184:VAL:N	2.53	0.42
1:O:11:GLY:HA3	1:O:122:THR:CG2	2.50	0.42
1:O:42:VAL:CG1	1:O:43:PRO:HD2	2.47	0.42
1:O:54:SER:HB3	1:O:59:ASN:H	1.85	0.42
1:O:111:LEU:HB2	1:O:114:GLU:OE1	2.18	0.42
1:A:58:LEU:N	1:A:58:LEU:HD12	2.35	0.42
1:C:58:LEU:HD21	2:D:66:PHE:CD2	2.54	0.42
2:D:152:LEU:CD1	2:D:156:ILE:HD11	2.50	0.42
1:E:58:LEU:HD12	1:E:58:LEU:N	2.35	0.42
1:G:3:GLU:OE2	1:G:34:HIS:NE2	2.53	0.42
2:J:11:PHE:CE2	2:J:198:VAL:HG13	2.54	0.42
1:K:89:LYS:CB	1:K:90:PRO:HD2	2.50	0.42
1:M:36:MET:CB	1:M:53:ILE:HG22	2.46	0.42
1:M:123:LEU:HD12	1:M:124:VAL:H	1.85	0.42
2:Q:54:TYR:CD1	2:Q:54:TYR:C	2.98	0.42
1:R:42:VAL:O	1:R:45:LYS:HG2	2.19	0.42
1:R:93:THR:HG23	1:R:125:THR:HG22	2.01	0.42
1:A:93:THR:HA	1:A:124:VAL:O	2.20	0.42
2:B:120:SER:HB2	2:D:12:PRO:HB2	2.02	0.42
1:C:11:GLY:HA3	1:C:122:THR:CG2	2.50	0.42
1:C:20:LEU:HG	1:C:22:LEU:CD2	2.50	0.42
2:D:71:ILE:O	2:D:85:GLU:HA	2.19	0.42
1:K:36:MET:HA	1:K:36:MET:CE	2.38	0.42
1:R:42:VAL:HG13	1:R:43:PRO:CD	2.46	0.42
1:R:43:PRO:O	1:R:45:LYS:NZ	2.52	0.42
1:R:114:GLU:HG2	1:R:115:TYR:N	2.35	0.42
2:T:62:GLU:O	2:T:77:VAL:HA	2.19	0.42
1:O:58:LEU:HD21	2:S:66:PHE:CG	2.55	0.42
1:A:16:THR:HG23	1:A:127:SER:O	2.20	0.42
1:C:62:TYR:OH	1:C:72:ILE:N	2.51	0.42
1:C:93:THR:HA	1:C:124:VAL:O	2.19	0.42
1:G:35:TYR:HE1	1:G:115:TYR:CZ	2.37	0.42
2:H:43:LEU:HG	2:H:153:VAL:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:101:SER:HB2	1:K:117:TYR:N	2.35	0.42
1:R:70:PHE:CZ	1:R:85:MET:HG2	2.55	0.42
1:R:88:LEU:C	1:R:89:LYS:HD3	2.45	0.42
2:S:82:ILE:CD1	2:S:121:LEU:HB2	2.50	0.42
1:A:30:THR:HG23	1:A:33:ARG:HB2	2.01	0.42
1:A:62:TYR:OH	1:A:72:ILE:N	2.51	0.42
1:C:5:GLN:HB2	1:C:27:SER:HB3	2.00	0.42
1:E:7:VAL:CG1	1:E:25:ALA:HB3	2.49	0.42
1:G:41:GLN:OE1	1:G:42:VAL:N	2.50	0.42
1:K:39:PHE:HA	1:K:50:VAL:HG23	2.01	0.42
1:K:123:LEU:HD12	1:K:124:VAL:H	1.85	0.42
2:L:2:THR:HG22	2:L:4:MET:CE	2.49	0.42
2:L:54:TYR:CD1	2:L:54:TYR:C	2.98	0.42
2:L:125:TYR:CE2	2:L:126:THR:C	2.98	0.42
2:Q:82:ILE:CD1	2:Q:121:LEU:HB2	2.50	0.42
2:Q:120:SER:HB2	2:T:12:PRO:HB2	2.01	0.42
1:R:4:VAL:HG22	1:R:117:TYR:HD2	1.85	0.42
2:T:153:VAL:HG23	2:T:153:VAL:O	2.20	0.42
1:A:78:GLU:N	1:A:78:GLU:CD	2.78	0.42
2:J:120:SER:HB2	2:L:12:PRO:HB2	2.02	0.42
2:L:82:ILE:CD1	2:L:121:LEU:HB2	2.50	0.42
1:M:45:LYS:HE2	1:M:45:LYS:HB2	1.82	0.42
1:R:3:GLU:HG2	1:R:4:VAL:HG13	2.02	0.42
1:O:110:ARG:HG2	1:O:110:ARG:O	2.20	0.41
2:S:186:ASN:OD1	2:S:188:ARG:N	2.52	0.41
1:A:5:GLN:C	1:A:6:LEU:HD23	2.45	0.41
2:B:54:TYR:HD2	2:B:62:GLU:HB3	1.85	0.41
2:B:58:ARG:O	2:B:58:ARG:CG	2.67	0.41
1:C:39:PHE:CD2	1:C:49:PHE:HA	2.55	0.41
1:E:100:GLY:O	1:E:117:TYR:HD2	2.03	0.41
2:F:26:LEU:HD23	2:F:129:ALA:HA	2.01	0.41
2:F:43:LEU:CG	2:F:153:VAL:HG22	2.50	0.41
2:F:95:HIS:HE1	2:F:97:CYS:SG	2.43	0.41
1:G:83:LEU:HD23	1:G:83:LEU:C	2.44	0.41
1:I:64:ASP:OD1	1:I:64:ASP:N	2.53	0.41
2:J:12:PRO:HB2	2:T:120:SER:HB2	2.02	0.41
2:N:54:TYR:CD1	2:N:54:TYR:C	2.98	0.41
1:R:4:VAL:HG22	1:R:117:TYR:CD2	2.55	0.41
1:O:31:PHE:CD2	1:O:79:ASN:HA	2.54	0.41
1:A:58:LEU:HD21	2:B:66:PHE:CD2	2.55	0.41
1:A:93:THR:HG21	1:A:125:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:O	1:C:47:ARG:HA	2.20	0.41
2:D:152:LEU:HD12	2:D:152:LEU:C	2.45	0.41
1:G:63:VAL:O	1:G:67:LYS:HG3	2.20	0.41
2:J:26:LEU:HD21	2:J:30:LEU:HD21	2.02	0.41
2:J:147:GLU:N	2:J:147:GLU:OE2	2.53	0.41
1:K:105:TYR:O	1:K:106:TYR:CD2	2.73	0.41
2:L:55:ALA:HB3	2:L:139:GLN:OE1	2.20	0.41
2:L:132:SER:HB2	2:L:142:PHE:CE2	2.55	0.41
1:M:17:GLY:N	1:M:88:LEU:O	2.27	0.41
1:M:21:ARG:HB2	1:M:84:GLN:OE1	2.21	0.41
2:S:18:SER:HA	2:S:195:GLN:O	2.20	0.41
1:E:35:TYR:HB2	1:E:53:ILE:O	2.19	0.41
2:N:26:LEU:HD21	2:N:30:LEU:HD21	2.02	0.41
2:N:98:THR:HG22	2:N:109:PHE:CD2	2.55	0.41
1:R:34:HIS:CD2	1:R:103:SER:HA	2.55	0.41
1:C:39:PHE:CA	1:C:50:VAL:HG23	2.50	0.41
1:C:85:MET:HE2	1:C:85:MET:HB2	1.71	0.41
1:E:11:GLY:HA3	1:E:122:THR:CG2	2.50	0.41
1:K:105:TYR:CD1	1:K:105:TYR:N	2.88	0.41
1:R:8:GLU:H	1:R:8:GLU:CD	2.28	0.41
1:R:38:TRP:CZ3	1:R:98:CYS:HB2	2.56	0.41
1:R:84:GLN:OE1	1:R:86:ASN:ND2	2.53	0.41
2:T:33:PHE:CZ	2:T:63:ILE:HD11	2.55	0.41
1:O:42:VAL:CG2	1:O:45:LYS:HE3	2.51	0.41
2:S:38:HIS:HE1	2:S:205:TRP:HB3	1.85	0.41
2:S:43:LEU:HB2	2:S:49:TYR:CD2	2.55	0.41
1:A:20:LEU:HG	1:A:22:LEU:HD21	2.03	0.41
1:A:40:ARG:CZ	1:A:96:TYR:OH	2.68	0.41
2:B:170:GLU:O	2:B:173:THR:OG1	2.27	0.41
2:D:133:ILE:HD12	2:D:133:ILE:N	2.35	0.41
1:G:53:ILE:O	1:G:108:LYS:HE3	2.21	0.41
2:J:36:CYS:HG	2:J:97:CYS:HG	0.43	0.41
1:M:3:GLU:N	1:M:3:GLU:OE1	2.54	0.41
1:P:31:PHE:CE1	1:P:79:ASN:HA	2.55	0.41
1:P:54:SER:HA	1:P:108:LYS:CE	2.50	0.41
2:Q:64:LEU:CD2	2:Q:66:PHE:HB2	2.49	0.41
2:T:54:TYR:CD1	2:T:54:TYR:C	2.98	0.41
1:A:4:VAL:HG13	1:A:27:SER:C	2.45	0.41
2:B:104:SER:HA	2:B:123:LYS:NZ	2.35	0.41
1:C:15:GLN:HA	1:C:127:SER:OG	2.20	0.41
1:C:30:THR:HG23	1:C:33:ARG:CG	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:40:ARG:NH1	1:C:92:ASP:OD1	2.54	0.41
2:D:153:VAL:O	2:D:153:VAL:HG23	2.20	0.41
1:E:4:VAL:HG13	1:E:27:SER:C	2.45	0.41
1:E:20:LEU:HD12	1:E:20:LEU:HA	1.85	0.41
2:F:43:LEU:HG	2:F:153:VAL:HG22	2.02	0.41
2:F:85:GLU:OE1	2:F:87:PRO:HD3	2.20	0.41
2:H:85:GLU:OE1	2:H:87:PRO:HD3	2.21	0.41
1:I:46:GLU:OE1	1:I:46:GLU:N	2.50	0.41
1:I:102:GLN:O	1:I:102:GLN:CG	2.68	0.41
1:I:105:TYR:CD2	2:J:82:ILE:HG23	2.55	0.41
1:M:36:MET:HE3	1:M:99:ALA:O	2.21	0.41
1:P:36:MET:HE3	1:P:99:ALA:O	2.21	0.41
2:Q:137:GLN:OE1	2:Q:151:SER:HB3	2.20	0.41
1:R:17:GLY:HA2	1:R:87:ASN:HA	2.02	0.41
1:O:5:GLN:C	1:O:6:LEU:HD23	2.46	0.41
1:O:38:TRP:CG	1:O:83:LEU:HD22	2.56	0.41
1:C:30:THR:O	1:C:34:HIS:HD2	2.03	0.41
1:G:58:LEU:HD21	2:H:66:PHE:CD1	2.56	0.41
2:J:37:LEU:C	2:J:37:LEU:HD12	2.45	0.41
1:K:4:VAL:HG23	1:K:6:LEU:CD2	2.51	0.41
1:M:54:SER:CB	1:M:108:LYS:NZ	2.84	0.41
1:M:93:THR:HG23	1:M:124:VAL:O	2.20	0.41
1:P:95:LEU:C	1:P:96:TYR:HD1	2.29	0.41
1:O:34:HIS:NE2	1:O:103:SER:OG	2.53	0.41
2:B:58:ARG:O	2:B:58:ARG:HG3	2.20	0.41
1:C:64:ASP:CA	1:C:67:LYS:HZ1	2.26	0.41
1:C:110:ARG:O	1:C:110:ARG:HG2	2.19	0.41
1:E:110:ARG:O	1:E:110:ARG:HG2	2.21	0.41
2:F:67:TRP:CZ2	2:F:89:VAL:HG11	2.56	0.41
1:G:5:GLN:C	1:G:6:LEU:HD23	2.46	0.41
1:G:110:ARG:HG2	1:G:110:ARG:O	2.21	0.41
1:G:123:LEU:CD2	1:R:13:LEU:HB2	2.51	0.41
2:H:14:GLU:OE2	2:H:14:GLU:C	2.64	0.41
1:I:63:VAL:HG12	1:I:66:ALA:CB	2.47	0.41
2:J:54:TYR:CD1	2:J:54:TYR:C	2.98	0.41
1:K:3:GLU:OE2	1:K:34:HIS:HE1	2.03	0.41
1:K:3:GLU:N	1:K:3:GLU:OE1	2.53	0.41
1:M:13:LEU:HD23	1:M:14:VAL:N	2.35	0.41
1:M:24:CYS:SG	1:M:98:CYS:SG	3.19	0.41
1:M:35:TYR:HB3	1:M:108:LYS:NZ	2.36	0.41
1:P:53:ILE:HG12	1:P:54:SER:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Q:121:LEU:HD12	2:Q:122:LYS:H	1.84	0.41
1:R:93:THR:HA	1:R:124:VAL:O	2.21	0.41
1:O:20:LEU:HG	1:O:22:LEU:CD2	2.51	0.41
1:O:31:PHE:CG	1:O:79:ASN:HB2	2.55	0.41
2:S:36:CYS:HG	2:S:97:CYS:HG	0.43	0.41
2:S:52:PHE:CE1	2:S:54:TYR:HB2	2.56	0.41
1:A:16:THR:HG22	1:A:126:VAL:CG1	2.50	0.41
1:A:16:THR:HB	1:A:89:LYS:NZ	2.36	0.41
2:B:69:LYS:O	2:B:70:ASP:HB2	2.21	0.41
2:D:26:LEU:HD21	2:D:30:LEU:HG	2.02	0.41
2:D:146:PHE:N	2:D:146:PHE:CD1	2.89	0.41
2:F:117:VAL:HB	2:H:42:GLU:HG3	2.02	0.41
2:F:145:ASN:O	2:F:145:ASN:OD1	2.39	0.41
1:G:34:HIS:C	1:G:55:GLN:HG2	2.46	0.41
2:H:170:GLU:O	2:H:173:THR:OG1	2.24	0.41
1:I:55:GLN:HA	1:I:74:ARG:CZ	2.51	0.41
1:I:62:TYR:CE1	1:I:71:THR:HA	2.55	0.41
2:J:64:LEU:HD21	2:J:66:PHE:CB	2.50	0.41
1:K:35:TYR:CE2	1:K:109:PRO:HD2	2.56	0.41
1:K:74:ARG:HG3	1:K:81:VAL:HG22	2.03	0.41
2:N:82:ILE:CD1	2:N:121:LEU:HB2	2.50	0.41
2:N:153:VAL:O	2:N:153:VAL:HG23	2.21	0.41
1:P:38:TRP:CD1	1:P:83:LEU:HD22	2.56	0.41
1:C:35:TYR:N	1:C:55:GLN:HG2	2.36	0.41
1:G:84:GLN:NE2	1:G:85:MET:O	2.54	0.41
1:I:35:TYR:HE1	1:I:102:GLN:CG	2.34	0.41
1:K:63:VAL:HG12	1:K:66:ALA:CB	2.50	0.41
1:P:22:LEU:N	1:P:22:LEU:HD12	2.36	0.41
1:R:63:VAL:HG12	1:R:66:ALA:CB	2.51	0.41
2:T:31:LYS:HG3	2:T:102:SER:HG	1.85	0.41
1:O:62:TYR:OH	1:O:72:ILE:N	2.51	0.40
1:C:17:GLY:H	1:C:89:LYS:NZ	2.19	0.40
1:G:8:GLU:H	1:G:120:GLN:NE2	2.19	0.40
1:G:16:THR:HG22	1:G:126:VAL:CG1	2.51	0.40
1:I:62:TYR:OH	1:I:72:ILE:N	2.41	0.40
1:I:114:GLU:HG2	1:I:115:TYR:N	2.36	0.40
2:J:82:ILE:CD1	2:J:121:LEU:HB2	2.50	0.40
1:K:33:ARG:C	1:K:33:ARG:HD2	2.46	0.40
1:K:41:GLN:HB2	1:K:47:ARG:HG2	2.02	0.40
1:A:105:TYR:O	1:A:106:TYR:CE1	2.70	0.40
1:C:40:ARG:NE	1:C:96:TYR:HE1	2.17	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:PHE:CD2	1:C:110:ARG:HA	2.57	0.40
1:E:53:ILE:HG22	1:E:72:ILE:HD11	2.04	0.40
2:F:111:VAL:HG23	2:F:112:ASP:OD1	2.22	0.40
2:F:138:GLU:O	2:F:146:PHE:CD1	2.74	0.40
1:G:32:ASN:CB	1:G:76:ASN:HD21	2.34	0.40
1:G:58:LEU:HD12	1:G:58:LEU:N	2.35	0.40
1:G:90:PRO:N	1:G:126:VAL:HG11	2.36	0.40
1:M:64:ASP:OD1	1:M:64:ASP:N	2.54	0.40
2:T:136:GLY:HA2	2:T:152:LEU:CG	2.40	0.40
1:O:58:LEU:HD21	2:S:66:PHE:CD1	2.56	0.40
2:B:87:PRO:HG2	2:B:88:GLU:OE1	2.22	0.40
1:G:58:LEU:HD21	2:H:66:PHE:CG	2.56	0.40
2:J:108:GLU:OE2	2:J:118:ARG:NH1	2.55	0.40
2:L:57:LYS:HG2	2:L:142:PHE:CD1	2.57	0.40
2:L:82:ILE:HG21	2:L:119:LYS:CE	2.51	0.40
2:L:130:GLU:O	2:L:130:GLU:HG2	2.21	0.40
1:P:42:VAL:HG13	1:P:43:PRO:CD	2.44	0.40
1:P:111:LEU:HB3	1:P:114:GLU:OE1	2.21	0.40
1:P:123:LEU:HD12	1:P:124:VAL:H	1.86	0.40
1:O:31:PHE:CD2	1:O:79:ASN:HB2	2.56	0.40
1:O:40:ARG:NE	1:O:96:TYR:OH	2.55	0.40
1:O:58:LEU:N	1:O:58:LEU:HD12	2.36	0.40
1:O:62:TYR:CZ	1:O:72:ILE:HG22	2.57	0.40
2:B:58:ARG:NH1	2:B:58:ARG:HB2	2.37	0.40
2:D:130:GLU:HG2	2:D:130:GLU:O	2.21	0.40
2:D:204:LEU:N	2:D:204:LEU:HD23	2.36	0.40
1:I:105:TYR:CD1	1:I:105:TYR:N	2.88	0.40
1:M:67:LYS:HB2	1:M:67:LYS:HE2	1.54	0.40
2:Q:54:TYR:HB3	2:Q:63:ILE:HB	2.04	0.40
1:R:64:ASP:OD1	1:R:64:ASP:N	2.54	0.40
1:O:4:VAL:HG13	1:O:27:SER:C	2.46	0.40
2:S:43:LEU:HD11	2:S:153:VAL:H	1.86	0.40
2:S:67:TRP:CZ2	2:S:89:VAL:HG11	2.56	0.40
1:A:7:VAL:CG1	1:A:25:ALA:HB3	2.52	0.40
1:A:110:ARG:HG2	1:A:110:ARG:O	2.21	0.40
2:B:14:GLU:CG	2:B:47:ARG:HH21	2.32	0.40
2:B:62:GLU:O	2:B:77:VAL:HA	2.21	0.40
2:D:112:ASP:OD1	2:D:114:LYS:HG2	2.21	0.40
1:E:16:THR:HG22	1:E:126:VAL:HG13	2.04	0.40
1:E:120:GLN:H	1:E:120:GLN:CD	2.21	0.40
2:J:183:ASN:OD1	2:J:184:VAL:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:42:VAL:HG22	1:K:94:ALA:HB2	2.04	0.40
1:K:92:ASP:N	1:K:92:ASP:OD1	2.54	0.40
2:L:137:GLN:OE1	2:L:151:SER:HB3	2.21	0.40
1:M:114:GLU:HG2	1:M:115:TYR:N	2.35	0.40
2:N:18:SER:HA	2:N:195:GLN:O	2.22	0.40
2:N:26:LEU:HG	2:N:129:ALA:HB1	2.04	0.40
1:P:53:ILE:HG12	1:P:54:SER:H	1.87	0.40
1:P:89:LYS:HB3	1:P:90:PRO:HD2	2.04	0.40
2:Q:183:ASN:OD1	2:Q:184:VAL:N	2.54	0.40
1:R:14:VAL:CG2	1:R:15:GLN:N	2.85	0.40
2:T:36:CYS:SG	2:T:97:CYS:CB	3.04	0.40
2:T:137:GLN:HB3	2:T:146:PHE:CG	2.56	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 PDB entries followed by that with respect to all EM entries.

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	123/128 (96%)	114 (93%)	9 (7%)	0	100	100
1	C	123/128 (96%)	115 (94%)	8 (6%)	0	100	100
1	E	123/128 (96%)	115 (94%)	8 (6%)	0	100	100
1	G	123/128 (96%)	116 (94%)	7 (6%)	0	100	100
1	I	123/128 (96%)	112 (91%)	11 (9%)	0	100	100
1	K	123/128 (96%)	117 (95%)	6 (5%)	0	100	100
1	M	123/128 (96%)	118 (96%)	5 (4%)	0	100	100
1	O	123/128 (96%)	114 (93%)	9 (7%)	0	100	100
1	P	123/128 (96%)	118 (96%)	5 (4%)	0	100	100
1	R	123/128 (96%)	111 (90%)	12 (10%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	204/206 (99%)	189 (93%)	15 (7%)	0	100	100
2	D	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
2	F	204/206 (99%)	195 (96%)	9 (4%)	0	100	100
2	H	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
2	J	204/206 (99%)	194 (95%)	10 (5%)	0	100	100
2	L	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
2	N	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
2	Q	204/206 (99%)	193 (95%)	11 (5%)	0	100	100
2	S	204/206 (99%)	196 (96%)	8 (4%)	0	100	100
2	T	204/206 (99%)	197 (97%)	7 (3%)	0	100	100
All	All	3270/3340 (98%)	3093 (95%)	177 (5%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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	104/106 (98%)	104 (100%)	0	100	100
1	C	104/106 (98%)	101 (97%)	3 (3%)	37	56
1	E	104/106 (98%)	104 (100%)	0	100	100
1	G	104/106 (98%)	103 (99%)	1 (1%)	68	72
1	I	104/106 (98%)	102 (98%)	2 (2%)	50	64
1	K	104/106 (98%)	104 (100%)	0	100	100
1	M	104/106 (98%)	102 (98%)	2 (2%)	50	64
1	O	104/106 (98%)	103 (99%)	1 (1%)	68	72
1	P	104/106 (98%)	104 (100%)	0	100	100
1	R	104/106 (98%)	103 (99%)	1 (1%)	68	72
2	B	180/180 (100%)	179 (99%)	1 (1%)	78	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	180/180 (100%)	179 (99%)	1 (1%)	78	78
2	F	180/180 (100%)	180 (100%)	0	100	100
2	H	180/180 (100%)	179 (99%)	1 (1%)	78	78
2	J	180/180 (100%)	180 (100%)	0	100	100
2	L	180/180 (100%)	180 (100%)	0	100	100
2	N	180/180 (100%)	180 (100%)	0	100	100
2	Q	180/180 (100%)	180 (100%)	0	100	100
2	S	180/180 (100%)	179 (99%)	1 (1%)	78	78
2	T	180/180 (100%)	180 (100%)	0	100	100
All	All	2840/2860 (99%)	2826 (100%)	14 (0%)	78	79

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	81	VAL
2	S	198	VAL
2	B	171	ILE
1	C	53	ILE
1	C	81	VAL
1	C	89	LYS
2	D	147	GLU
1	G	81	VAL
2	H	197	GLU
1	I	67	LYS
1	I	85	MET
1	M	67	LYS
1	M	72	ILE
1	R	7	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	O	15	GLN
1	O	55	GLN
1	O	59	ASN
1	O	102	GLN
2	S	38	HIS
2	S	95	HIS

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Mol	Chain	Res	Type
2	S	150	GLN
2	S	160	ASN
2	S	203	GLN
1	A	15	GLN
1	A	34	HIS
1	A	84	GLN
1	A	87	ASN
1	A	102	GLN
2	B	1	GLN
2	B	61	ASN
2	B	95	HIS
2	B	150	GLN
1	C	15	GLN
1	C	34	HIS
1	C	84	GLN
1	C	86	ASN
1	C	87	ASN
1	E	15	GLN
1	E	59	ASN
1	E	87	ASN
2	F	61	ASN
2	F	95	HIS
2	F	150	GLN
2	F	158	ASN
2	F	160	ASN
2	F	203	GLN
1	G	15	GLN
1	G	55	GLN
1	G	87	ASN
2	H	61	ASN
2	H	95	HIS
2	H	145	ASN
2	H	150	GLN
2	H	158	ASN
2	H	160	ASN
2	H	203	GLN
1	I	59	ASN
1	I	86	ASN
1	I	87	ASN
2	J	61	ASN
2	J	186	ASN
2	J	203	GLN

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Mol	Chain	Res	Type
1	K	59	ASN
1	K	84	GLN
1	K	86	ASN
1	K	87	ASN
2	L	61	ASN
2	L	139	GLN
2	L	160	ASN
2	L	186	ASN
2	L	203	GLN
1	M	15	GLN
1	M	84	GLN
1	M	87	ASN
2	N	61	ASN
2	N	139	GLN
2	N	145	ASN
2	N	160	ASN
2	N	186	ASN
2	N	203	GLN
1	P	86	ASN
1	P	87	ASN
2	Q	139	GLN
2	Q	160	ASN
2	Q	186	ASN
2	Q	203	GLN
1	R	15	GLN
1	R	59	ASN
1	R	86	ASN
1	R	87	ASN
2	T	61	ASN
2	T	95	HIS
2	T	139	GLN
2	T	158	ASN
2	T	186	ASN
2	T	203	GLN

5.3.3 RNA ⓘ

There are no RNA molecules 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

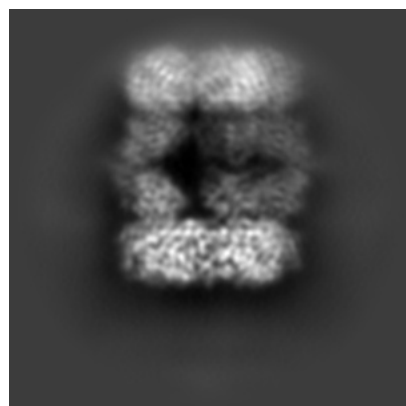
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-61648. These allow visual inspection of the internal detail of the map and identification of artifacts.

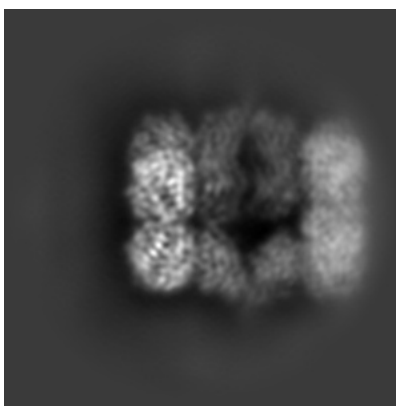
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

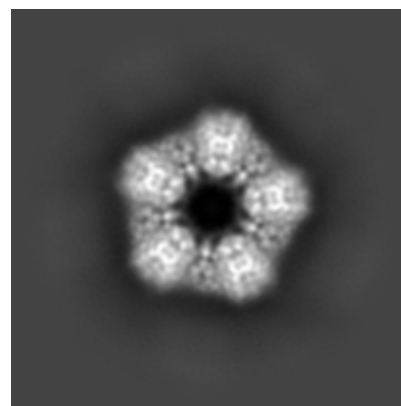
6.1.1 Primary map



X

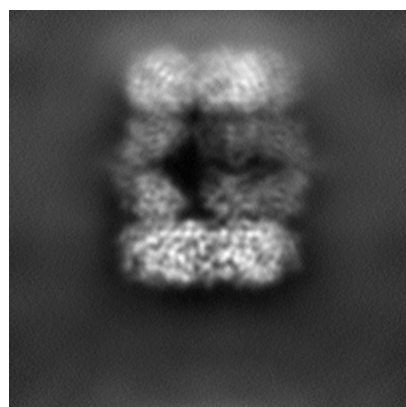


Y

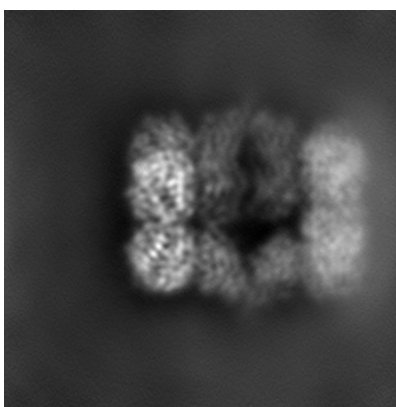


Z

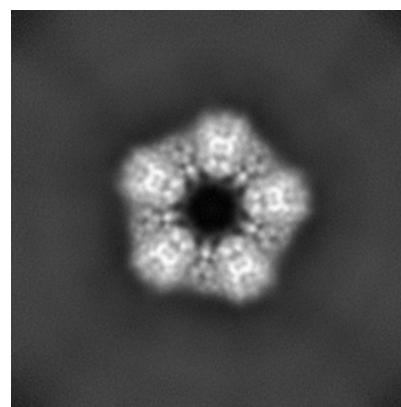
6.1.2 Raw map



X



Y

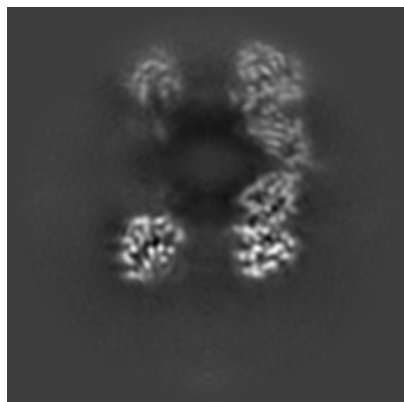


Z

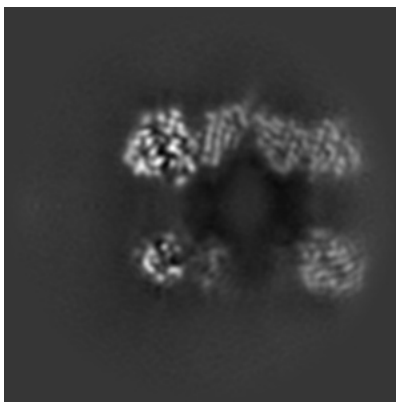
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

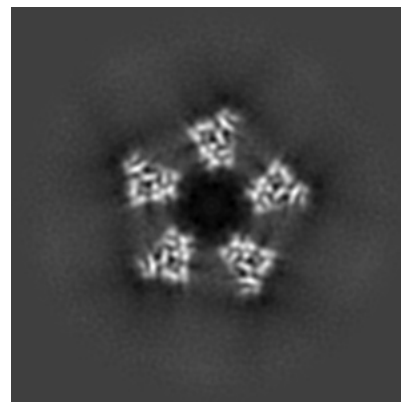
6.2.1 Primary map



X Index: 128

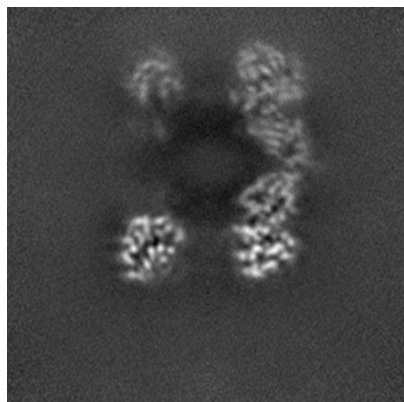


Y Index: 128

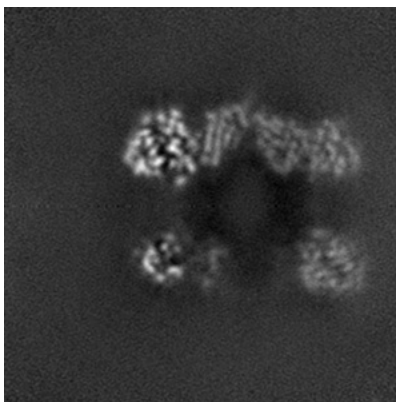


Z Index: 128

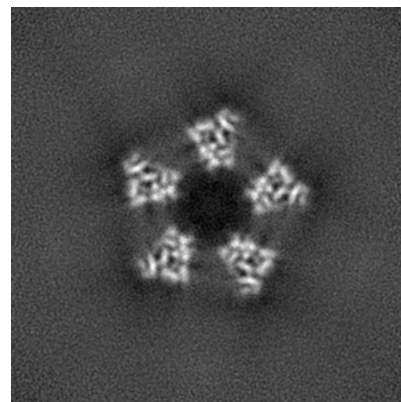
6.2.2 Raw map



X Index: 128



Y Index: 128

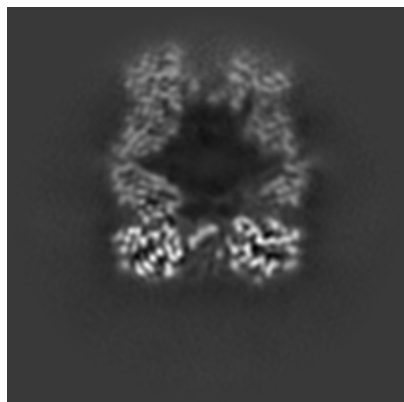


Z Index: 128

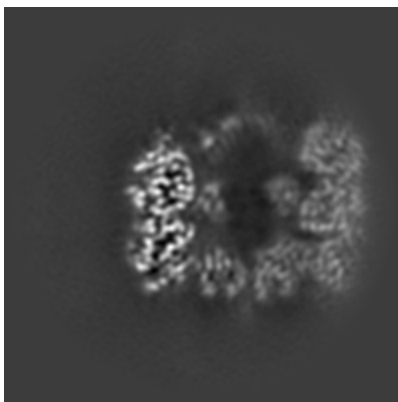
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

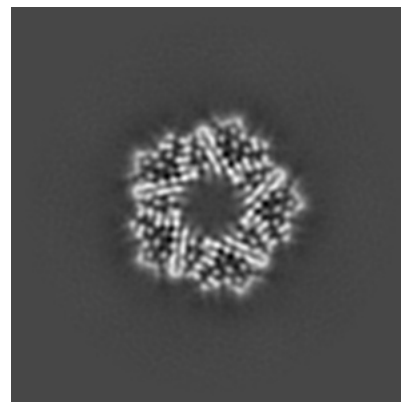
6.3.1 Primary map



X Index: 145

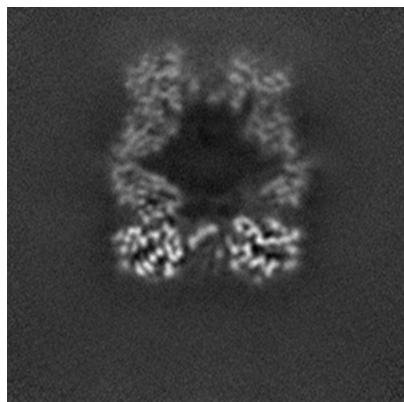


Y Index: 154

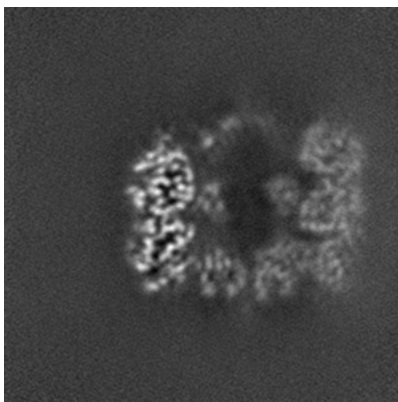


Z Index: 100

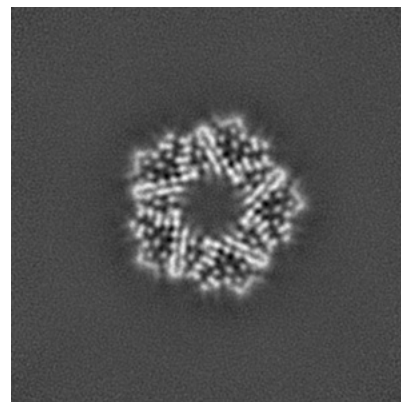
6.3.2 Raw map



X Index: 145



Y Index: 154

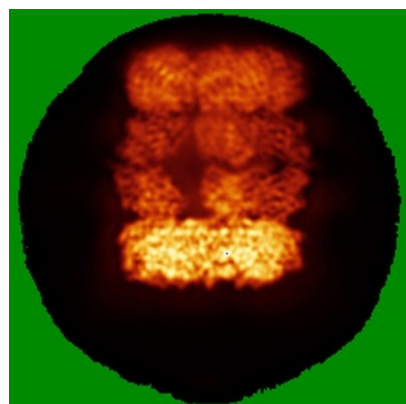


Z Index: 100

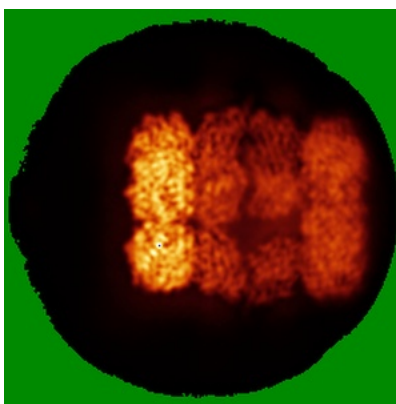
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

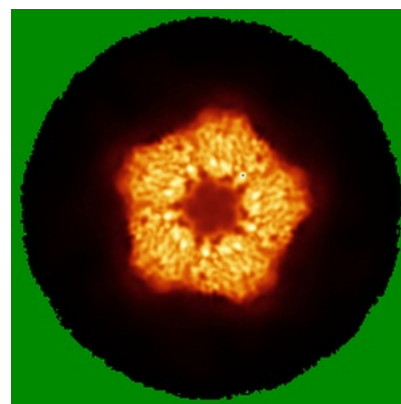
6.4.1 Primary map



X

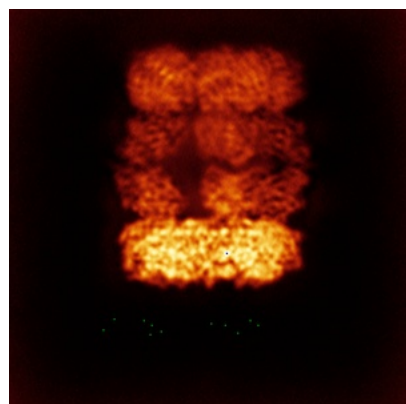


Y

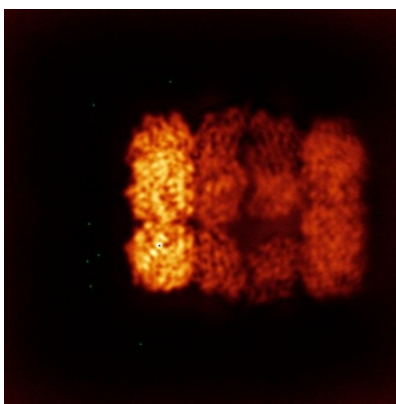


Z

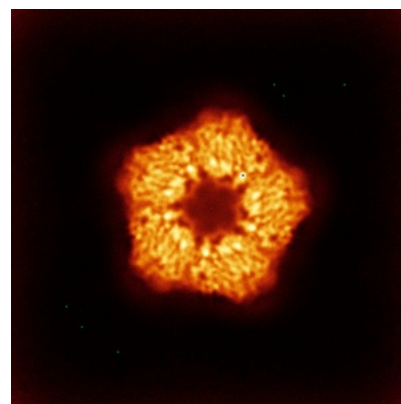
6.4.2 Raw map



X



Y

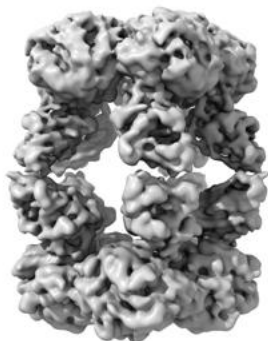


Z

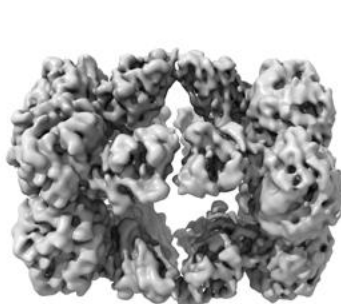
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

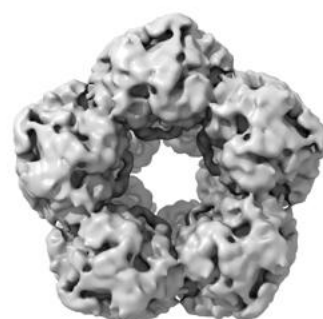
6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0959. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X



Y



Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

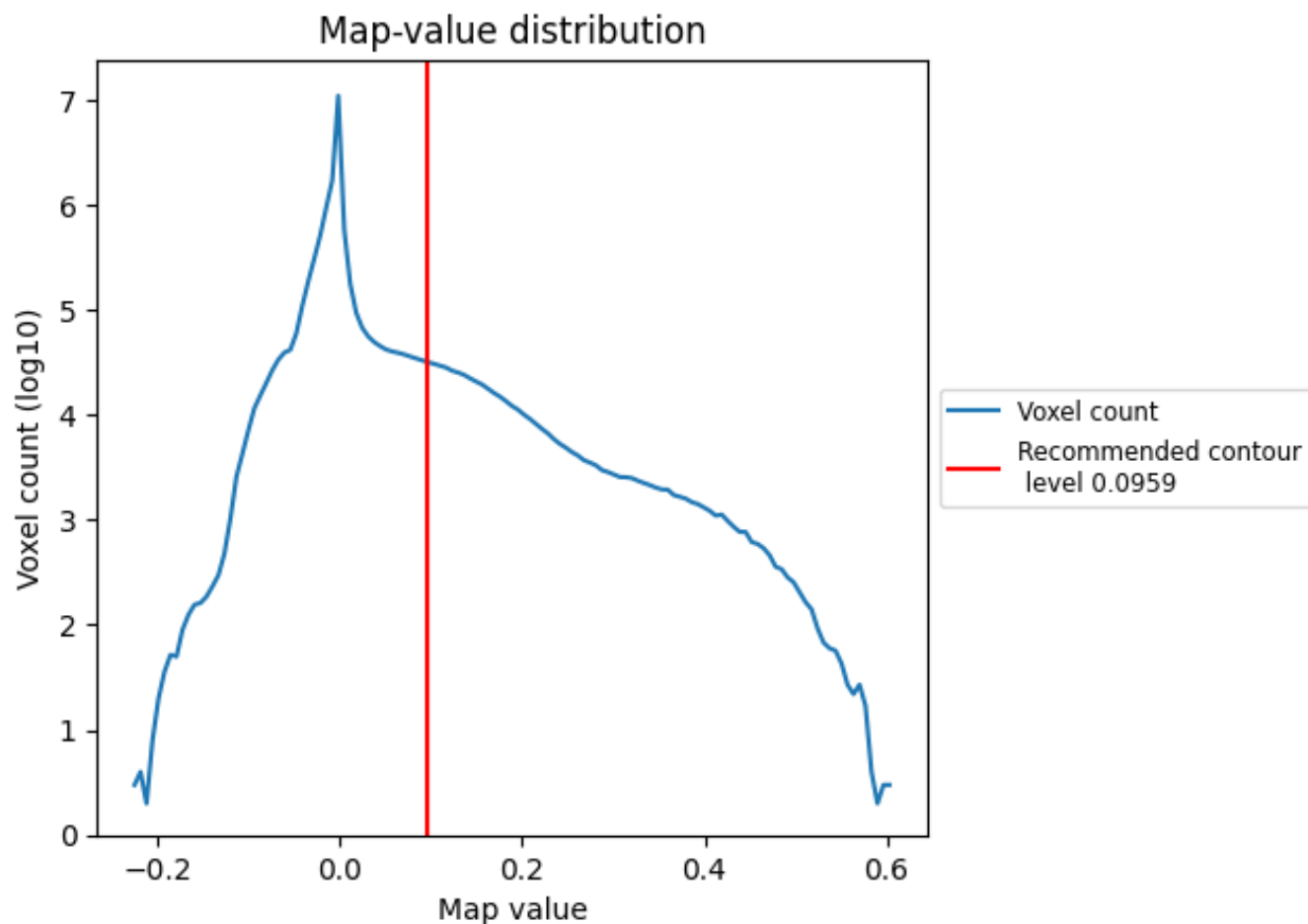
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

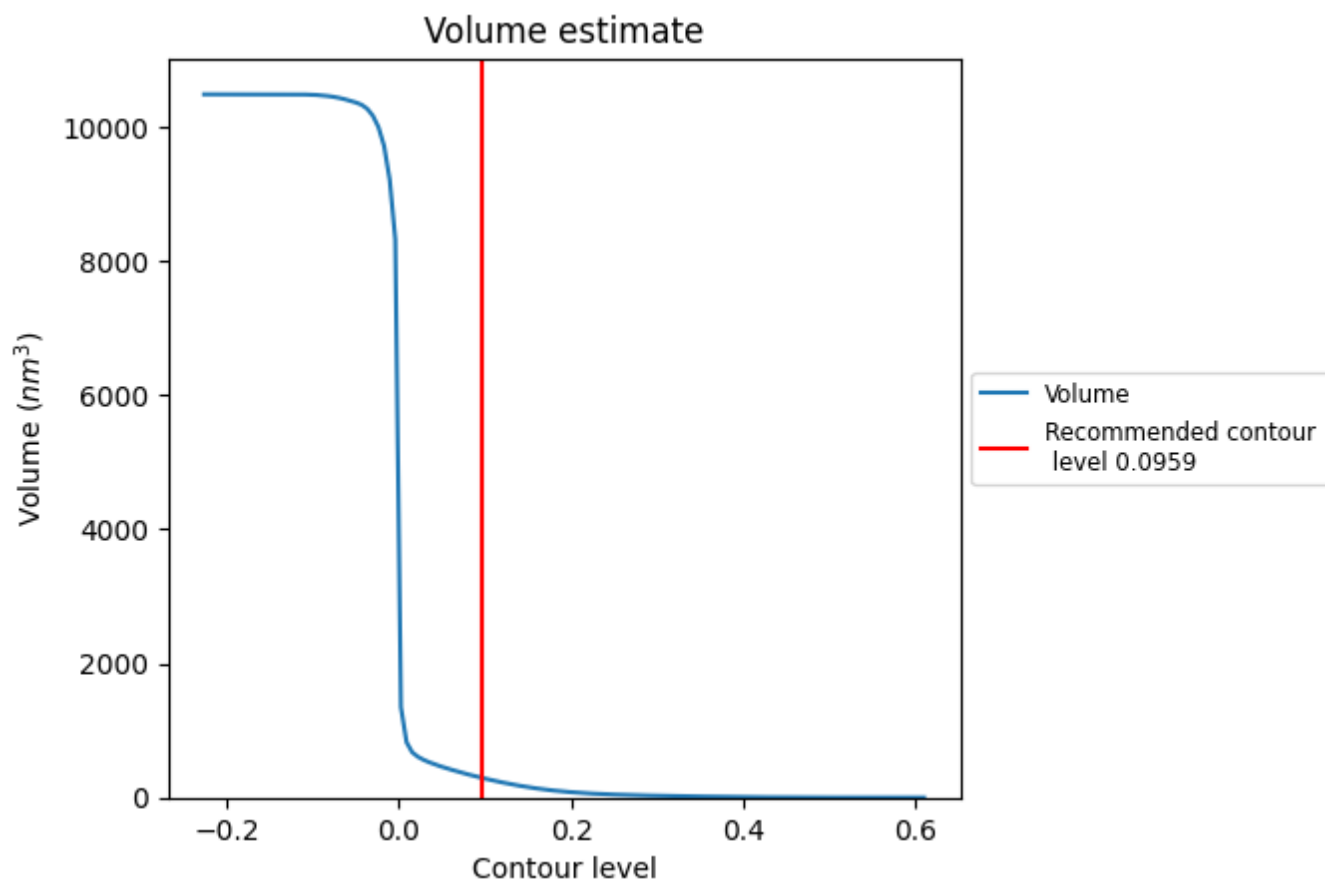
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

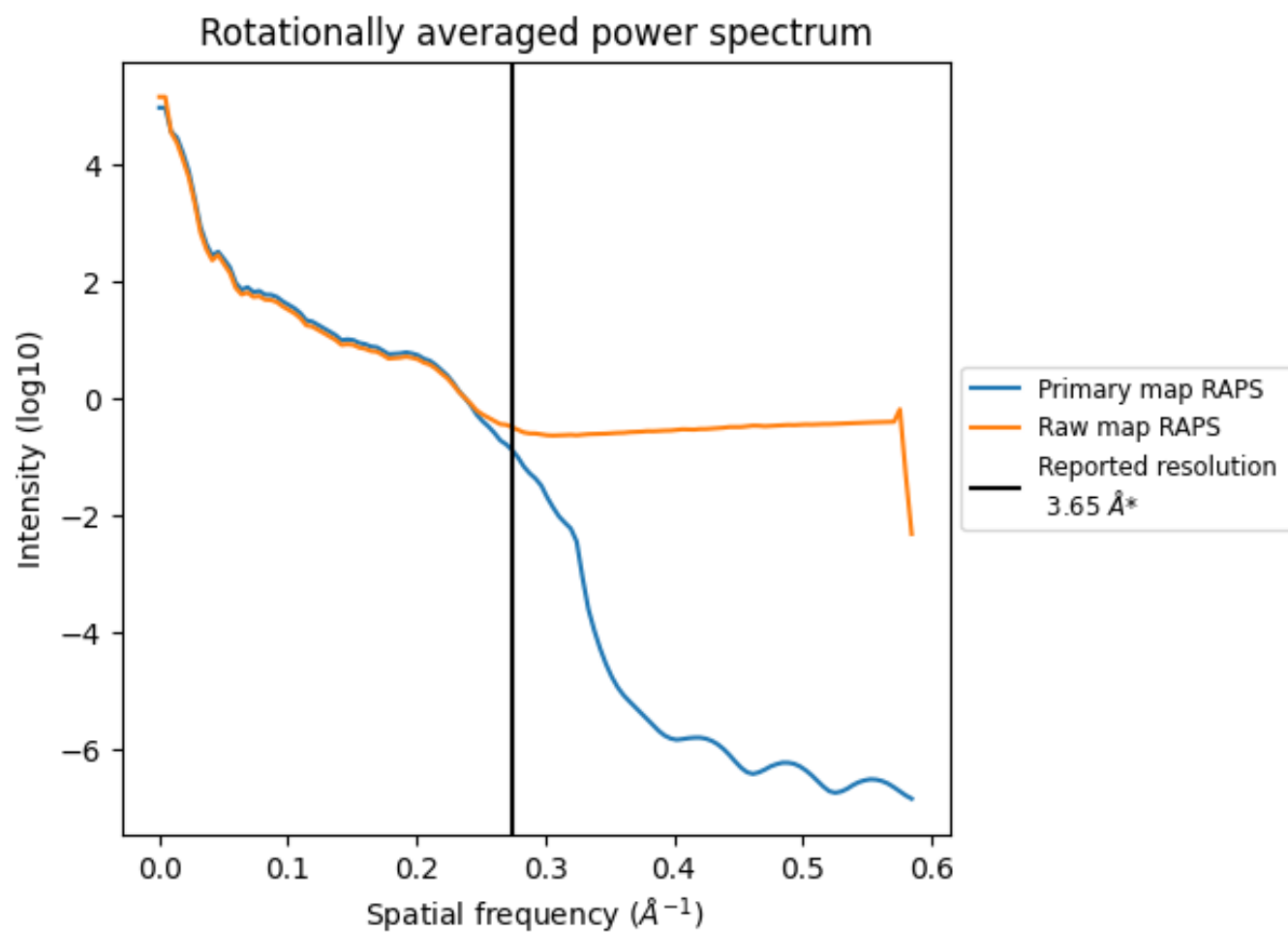
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 296 nm^3 ; this corresponds to an approximate mass of 267 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

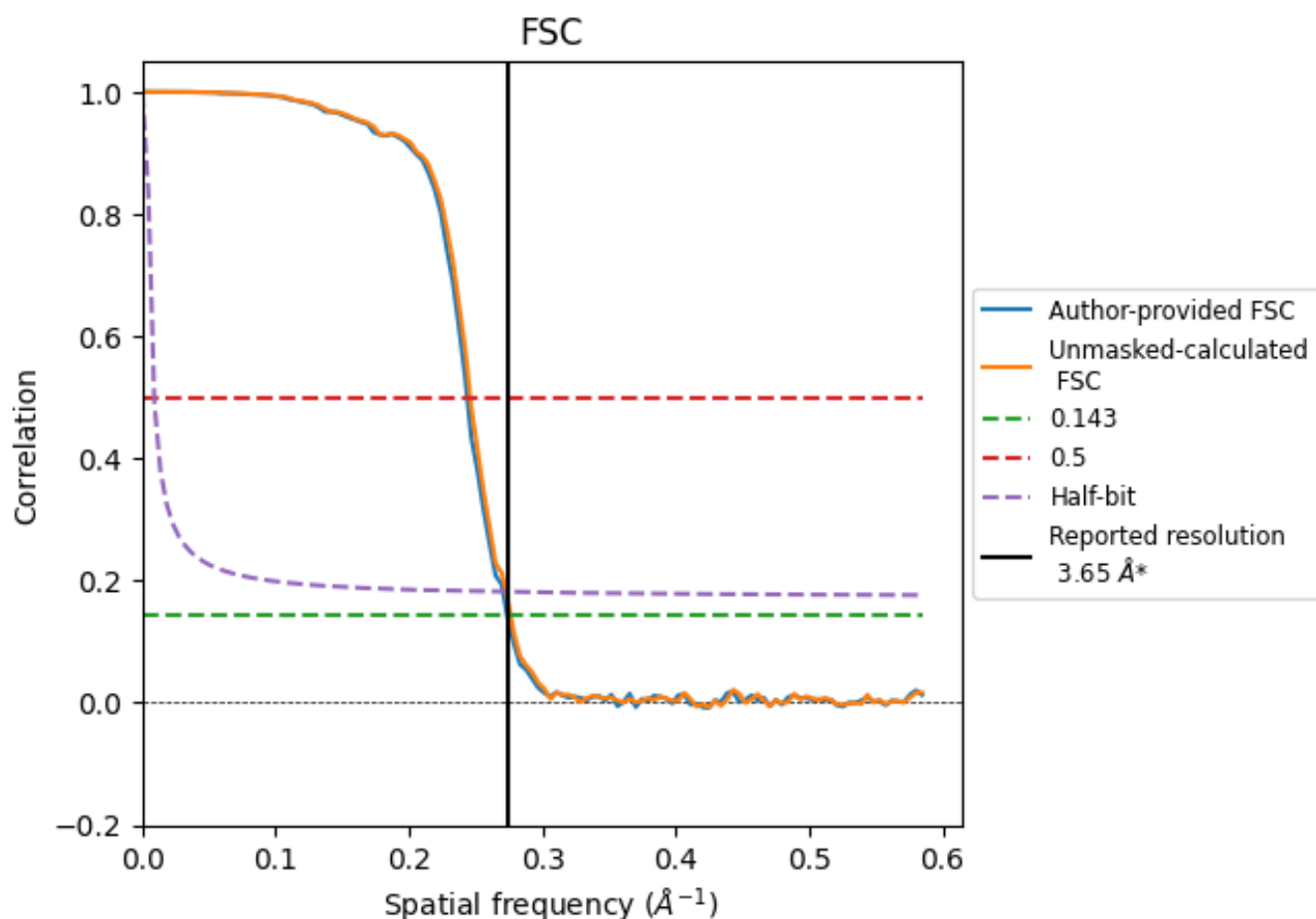


*Reported resolution corresponds to spatial frequency of 0.274 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.274 $\text{\AA}^{-1}$

8.2 Resolution estimates

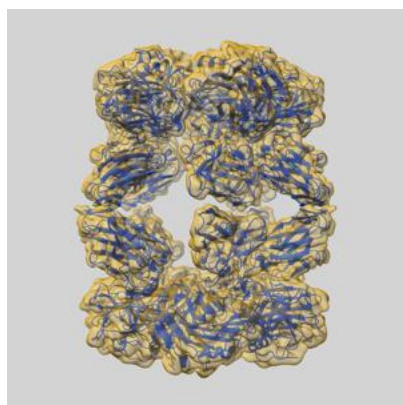
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.65	-	-
Author-provided FSC curve	3.65	4.10	3.70
Unmasked-calculated*	3.62	4.07	3.67

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

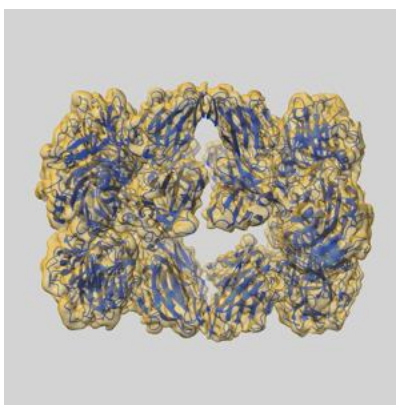
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-61648 and PDB model 9JO9. Per-residue inclusion information can be found in section [3](#) on page [6](#).

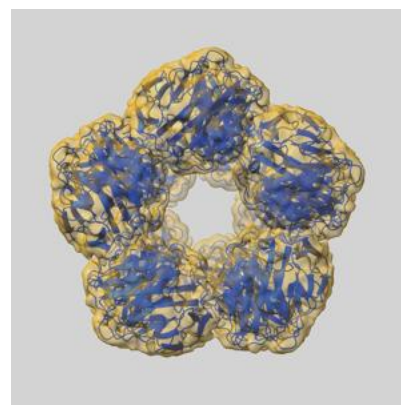
9.1 Map-model overlay [i](#)



X



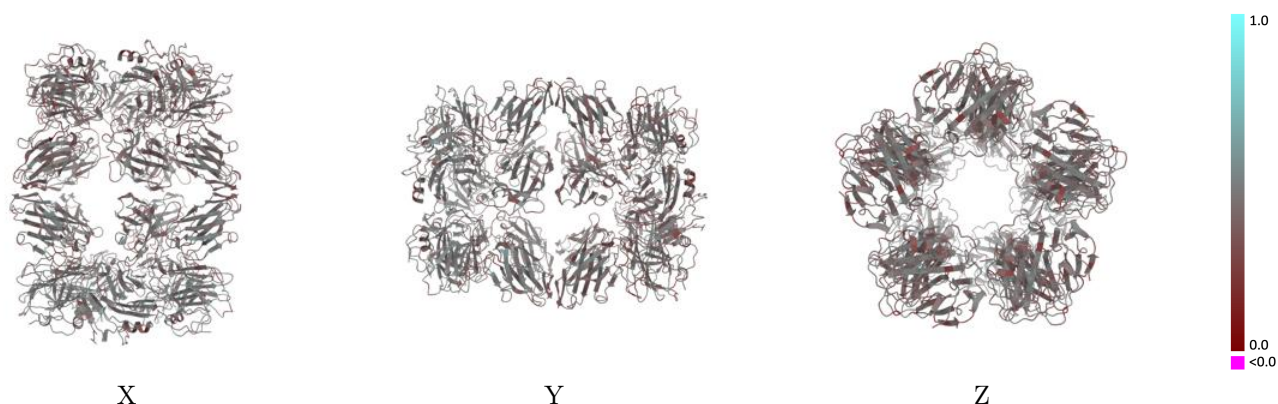
Y



Z

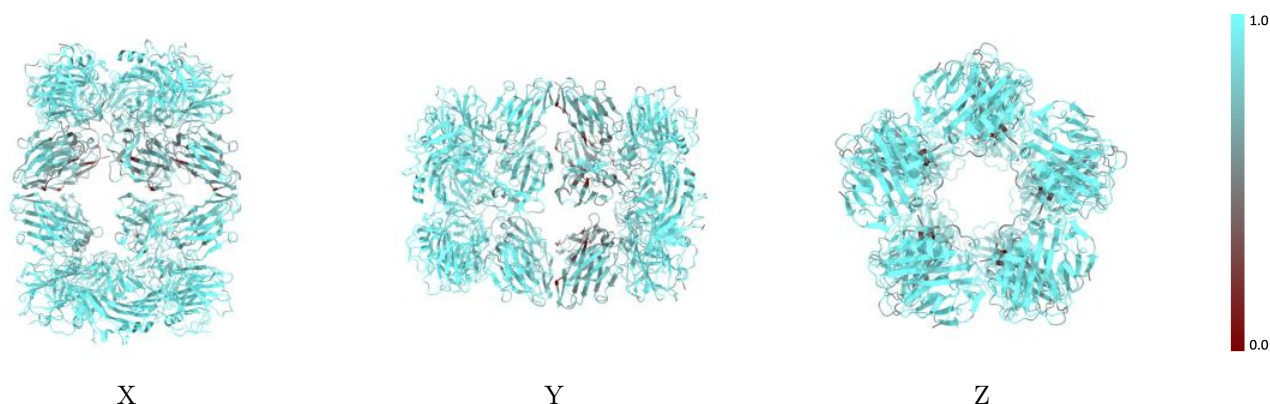
The images above show the 3D surface view of the map at the recommended contour level 0.0959 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



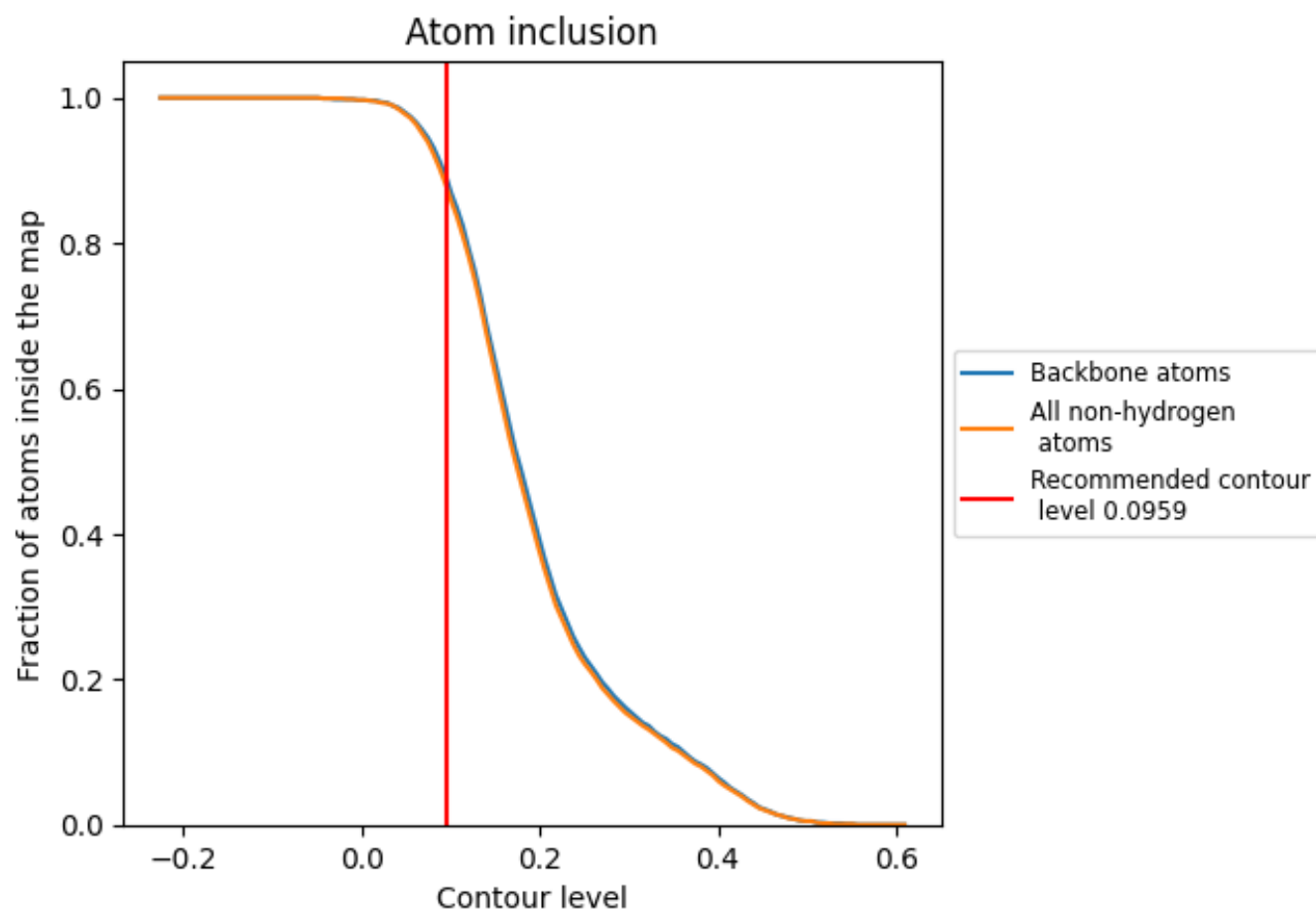
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0959).

9.4 Atom inclusion [i](#)



At the recommended contour level, 89% of all backbone atoms, 88% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0959) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8760	 0.4250
A	 0.8730	 0.4230
B	 0.9580	 0.4560
C	 0.8660	 0.4170
D	 0.9580	 0.4560
E	 0.8710	 0.4270
F	 0.9560	 0.4480
G	 0.8680	 0.4200
H	 0.9580	 0.4500
I	 0.7190	 0.4050
J	 0.9090	 0.4130
K	 0.7100	 0.4050
L	 0.9110	 0.4130
M	 0.7230	 0.4010
N	 0.9090	 0.4130
O	 0.8700	 0.4270
P	 0.7190	 0.4040
Q	 0.9140	 0.4130
R	 0.7180	 0.4000
S	 0.9580	 0.4500
T	 0.9110	 0.4110

