Full wwPDB EM Validation Report ⓘ

Nov 4, 2025 – 11:43 AM EST

PDB ID	:	9NGY / pdb_00009ngy
EMDB ID	:	EMD-49396
Title	:	In situ cryo-EM structure of protochannel (DotA-IcmX) of the Legionella Dot/Icm T4SS machine
Authors	:	Yue, J.; Liu, J.
Deposited on	:	2025-02-22
Resolution	:	3.63 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:

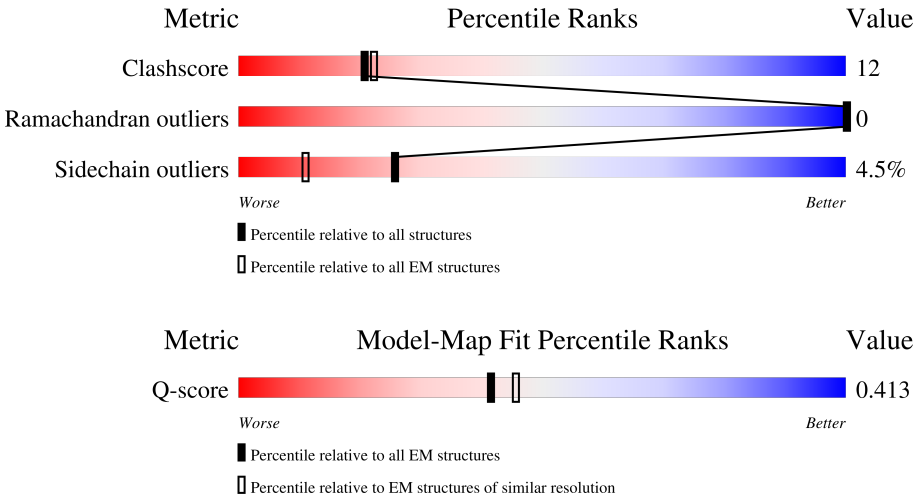
EMDB validation analysis	:	0.0.1.dev129
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.46

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 3.63 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	210492	15764	-
Ramachandran outliers	207382	16835	-
Sidechain outliers	206894	16415	-
Q-score	-	25397	11696 (3.13 - 4.13)

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 <=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	AP1	466	11% 69% 19% • 11%
1	BP1	466	10% 67% 22% • 11%
1	CP1	466	10% 70% 19% • 11%
1	DP1	466	11% 69% 20% • 11%

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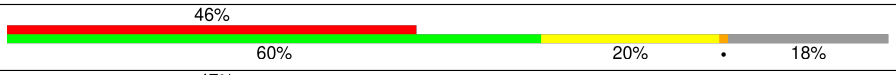
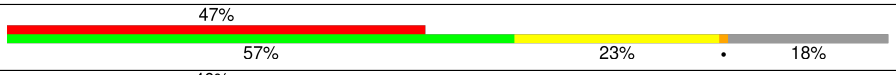
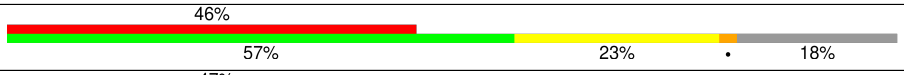
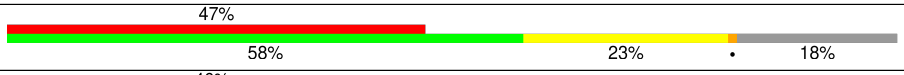
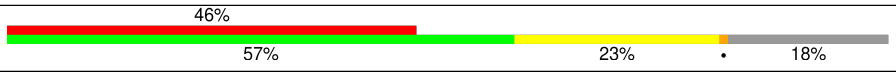
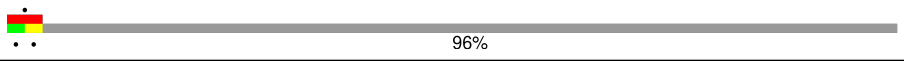
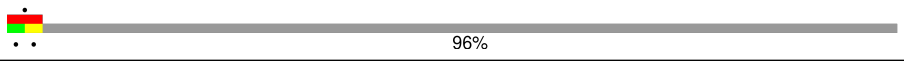
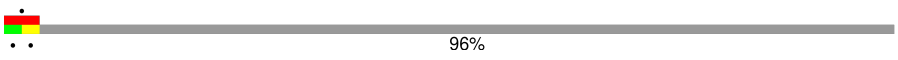
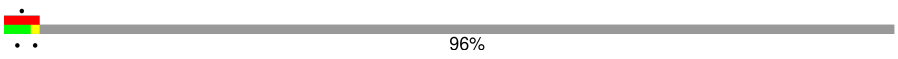
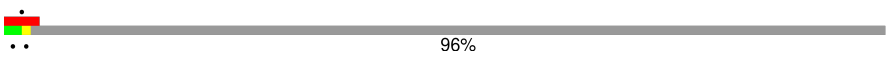
Mol	Chain	Length	Quality of chain
1	EP1	466	
2	FP1	1048	
2	GP1	1048	
2	HP1	1048	
2	IP1	1048	
2	JP1	1048	
3	KP1	1048	
3	LP1	1048	
3	MP1	1048	
3	NP1	1048	
3	OP1	1048	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 50535 atoms, of which 0 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 IcmX (IcmY).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	AP1	417	Total 3213	C 2013	N 542	O 646	S 12	0	0
1	BP1	417	Total 3213	C 2013	N 542	O 646	S 12	0	0
1	CP1	417	Total 3213	C 2013	N 542	O 646	S 12	0	0
1	DP1	417	Total 3213	C 2013	N 542	O 646	S 12	0	0
1	EP1	417	Total 3213	C 2013	N 542	O 646	S 12	0	0

- Molecule 2 is a protein called DotA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	FP1	857	Total 6560	C 4256	N 1051	O 1202	S 51	0	0
2	GP1	857	Total 6560	C 4256	N 1051	O 1202	S 51	0	0
2	HP1	857	Total 6560	C 4256	N 1051	O 1202	S 51	0	0
2	IP1	857	Total 6560	C 4256	N 1051	O 1202	S 51	0	0
2	JP1	857	Total 6560	C 4256	N 1051	O 1202	S 51	0	0

- Molecule 3 is a protein called IcmE (DotG).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	KP1	43	Total 334	C 221	N 58	O 54	S 1	0	0
3	LP1	43	Total 334	C 221	N 58	O 54	S 1	0	0
3	MP1	43	Total 334	C 221	N 58	O 54	S 1	0	0

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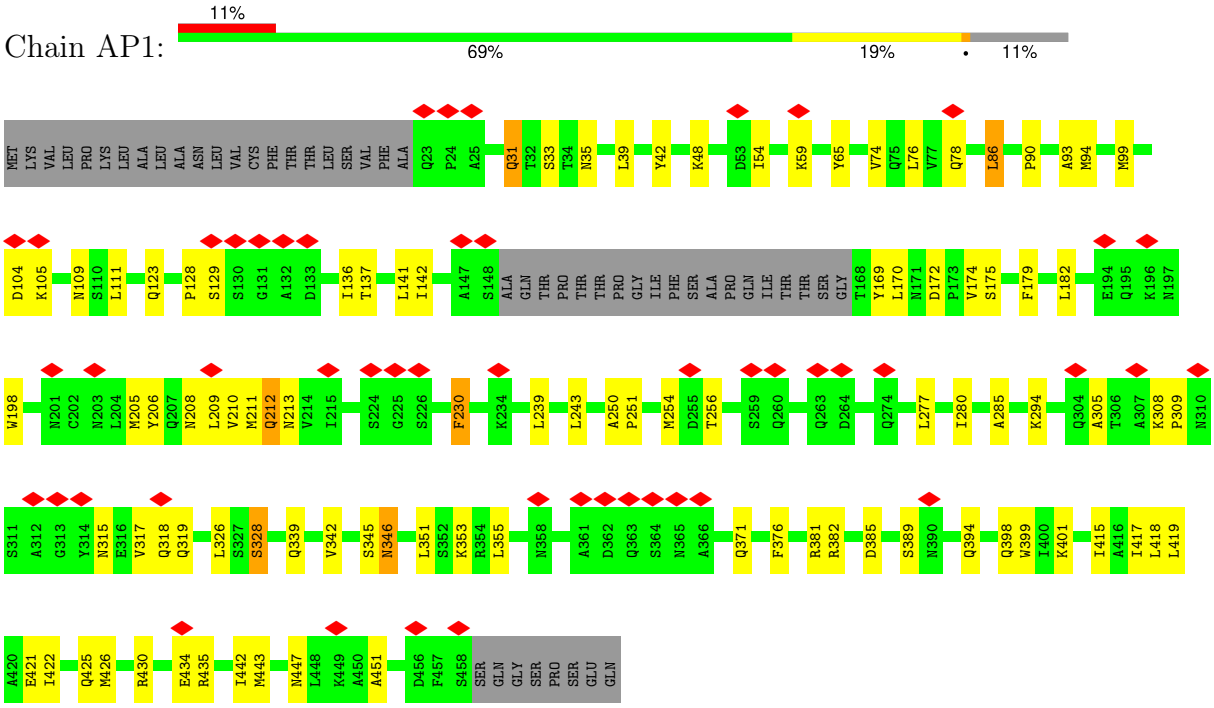
Mol	Chain	Residues	Atoms					AltConf	Trace
3	NP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		
3	OP1	43	Total	C	N	O	S	0	0
			334	221	58	54	1		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and 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.

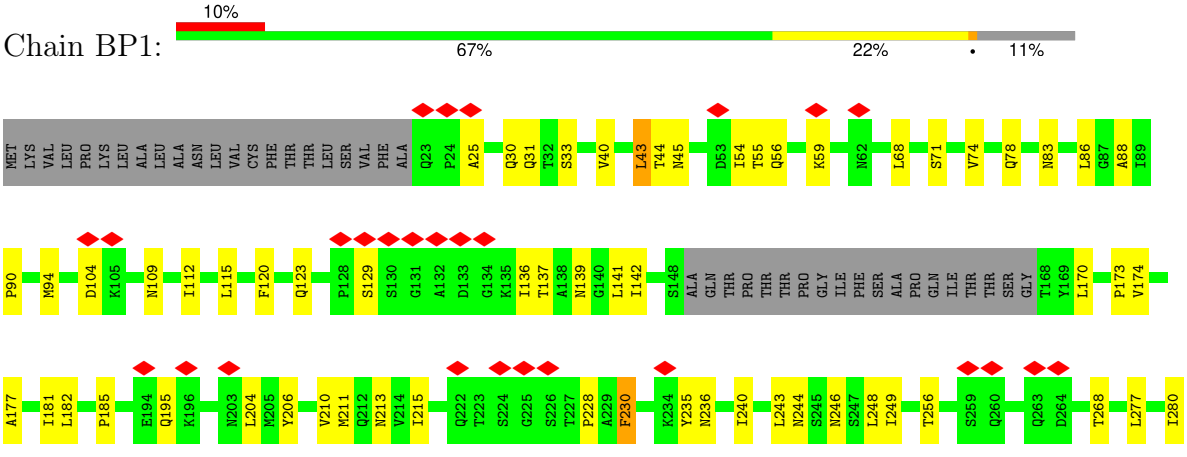
• Molecule 1: IcmX (IcmY)

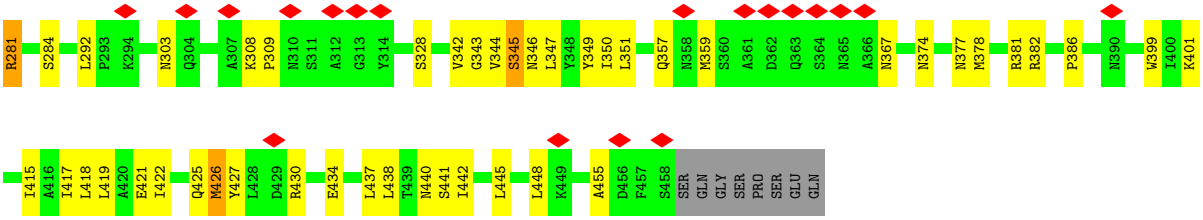
Chain AP1:



• Molecule 1: IcmX (IcmY)

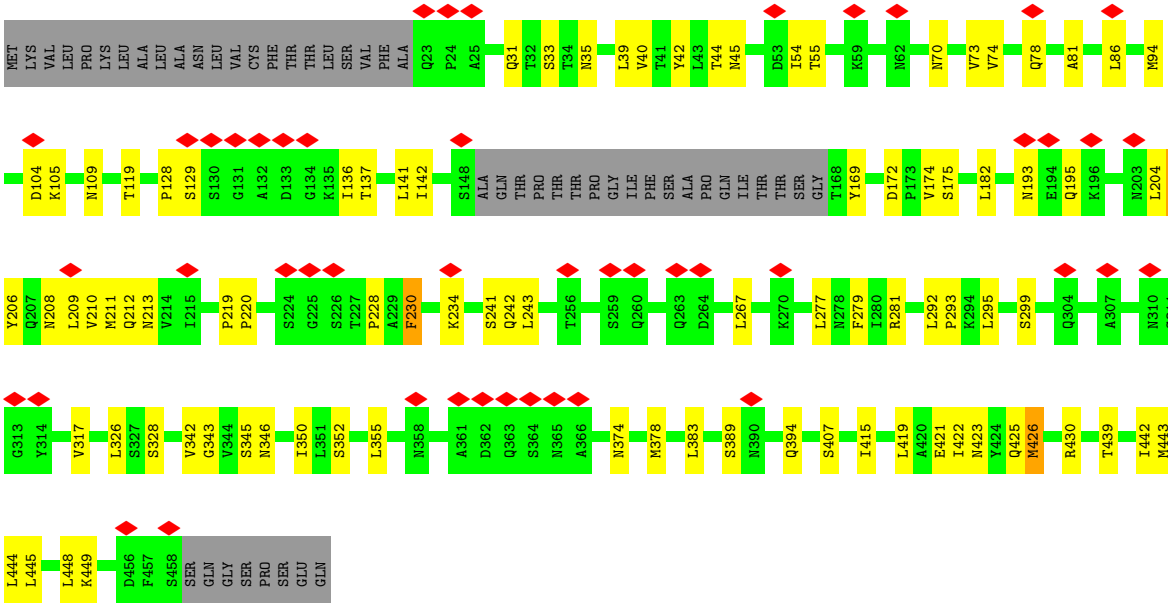
Chain BP1:





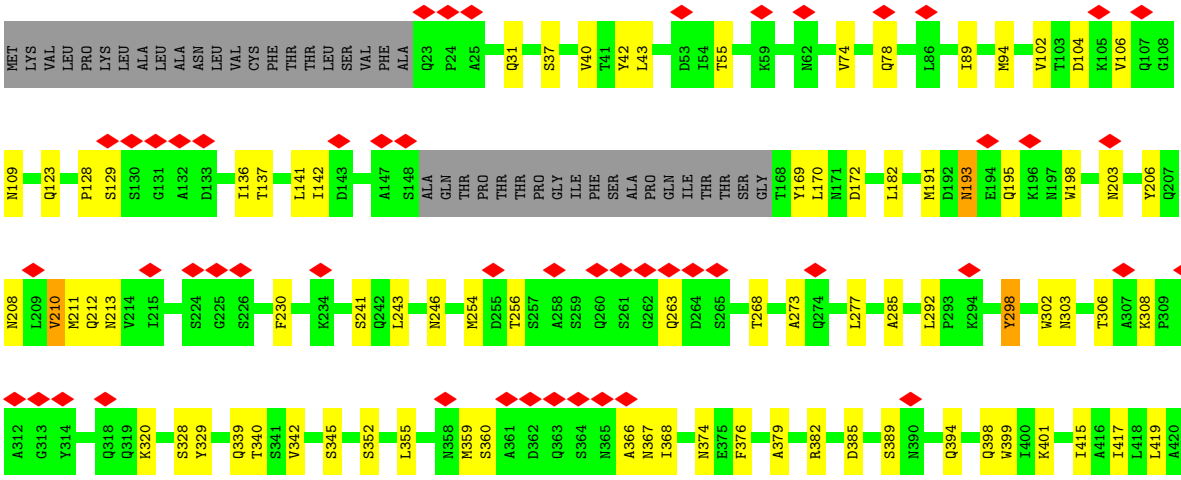
• Molecule 1: IcmX (IcmY)

Chain CP1:



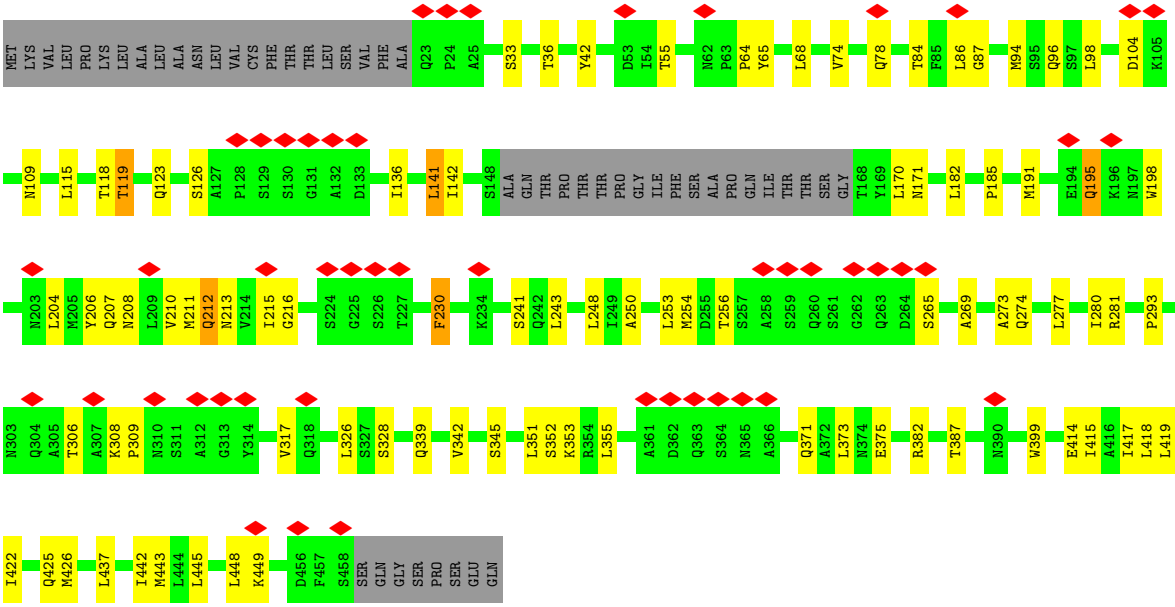
• Molecule 1: IcmX (IcmY)

Chain DP1:



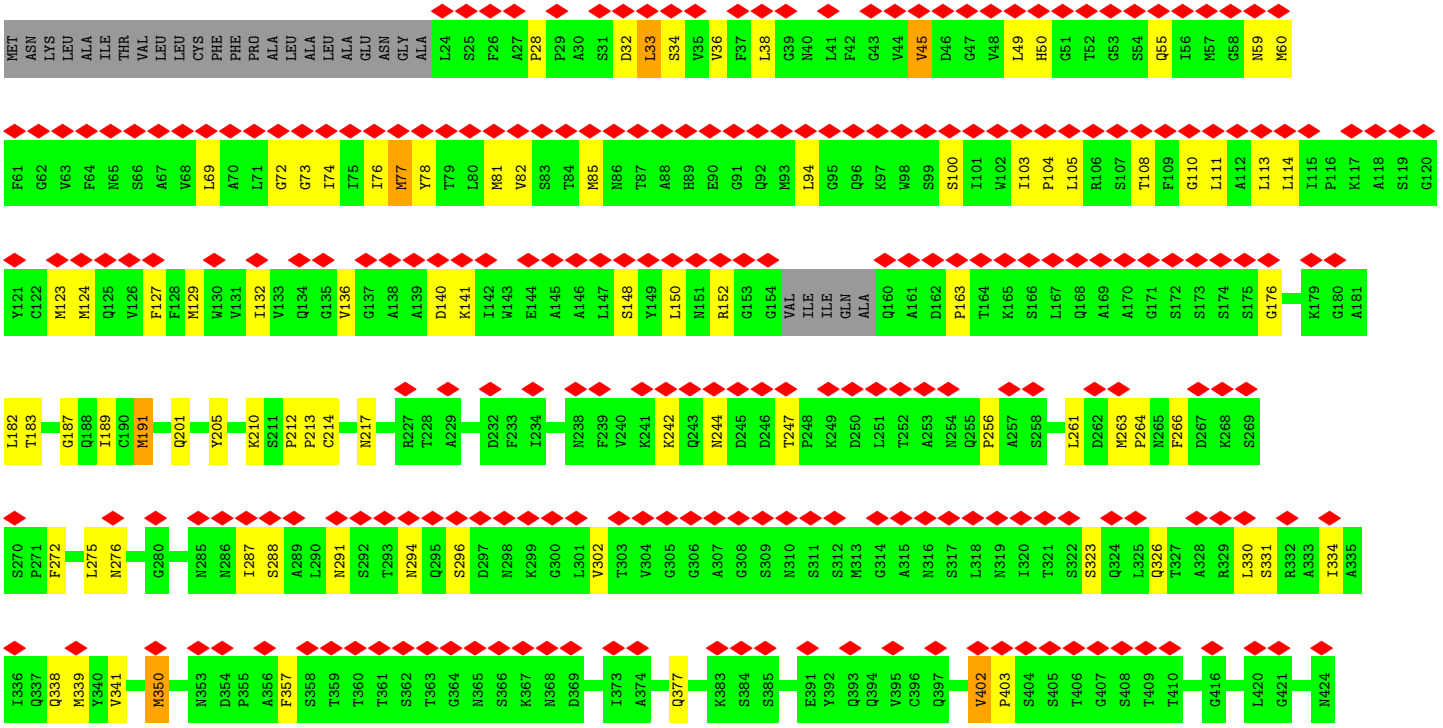
• Molecule 1: IcmX (IcmY)

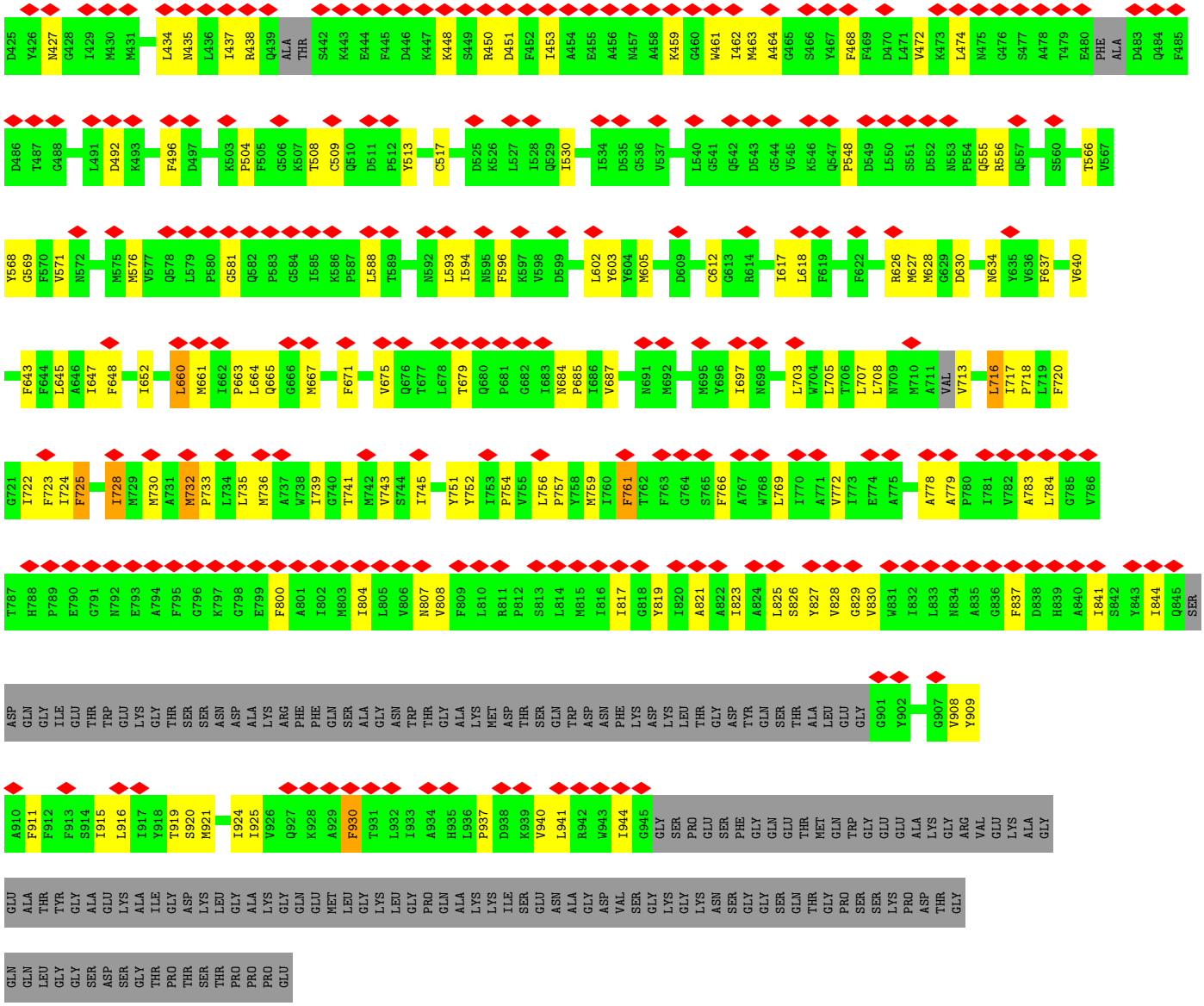
Chain EP1:



• Molecule 2: DotA

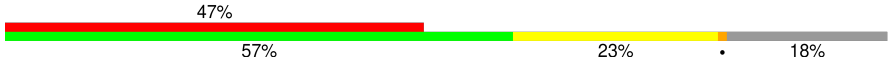
Chain FP1:

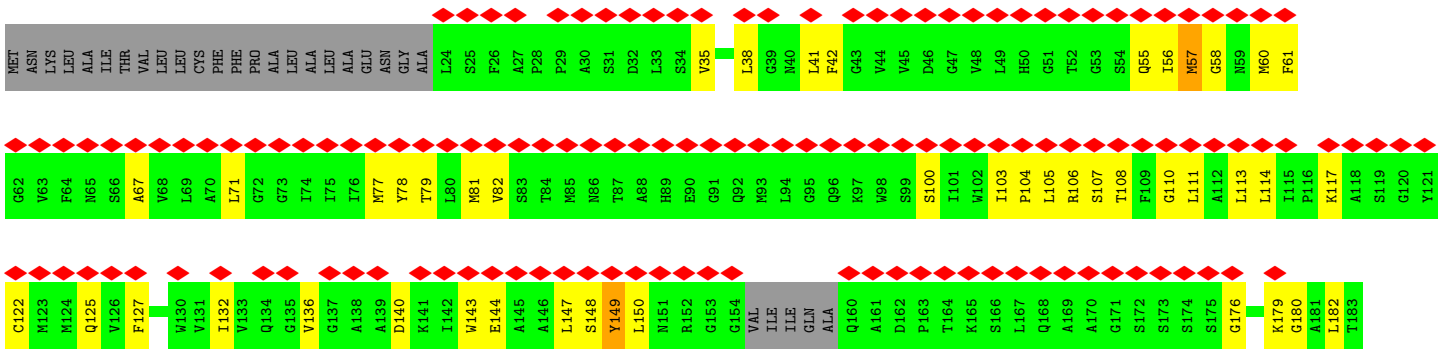


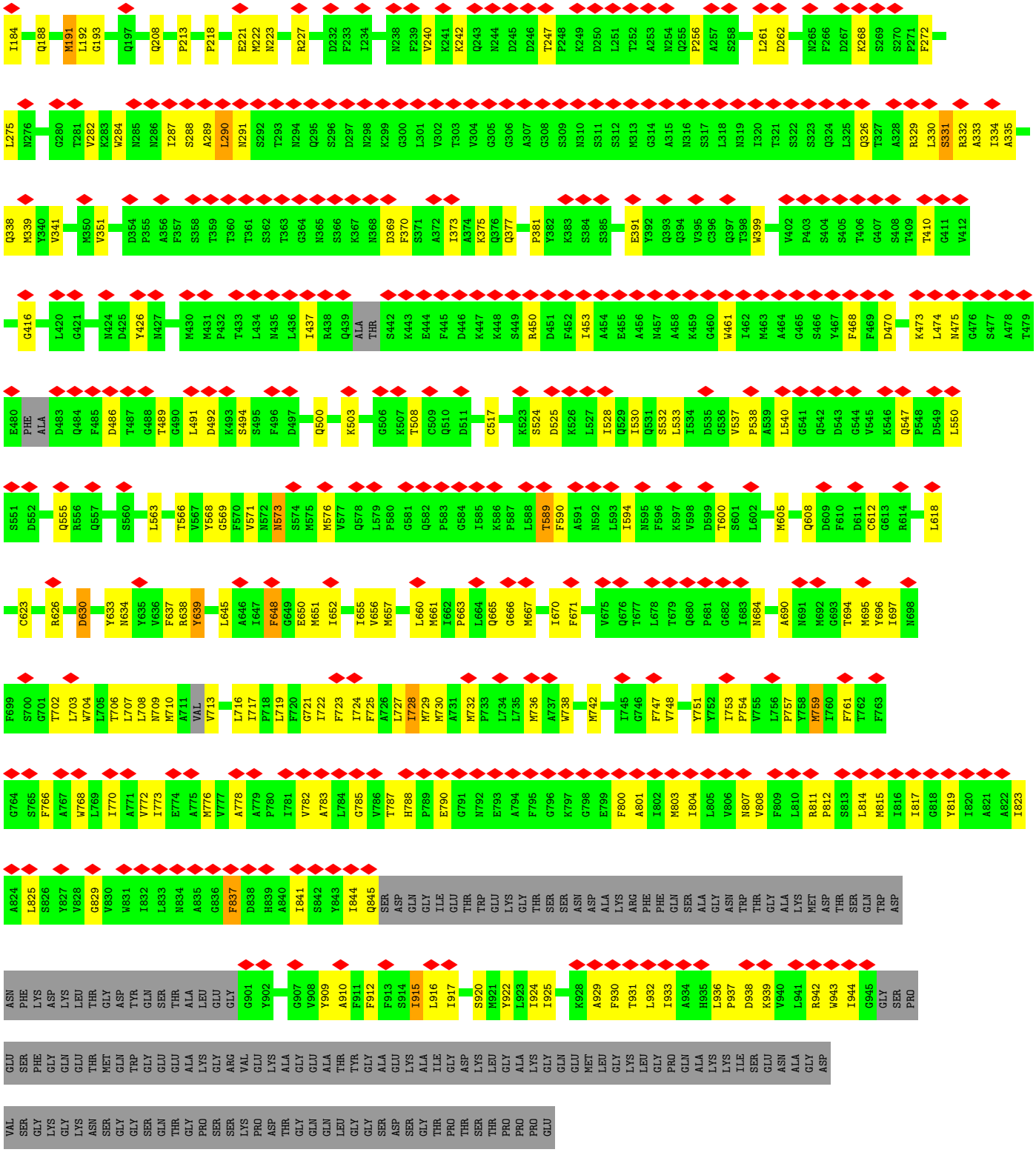


• Molecule 2: DotA

Chain GP1:

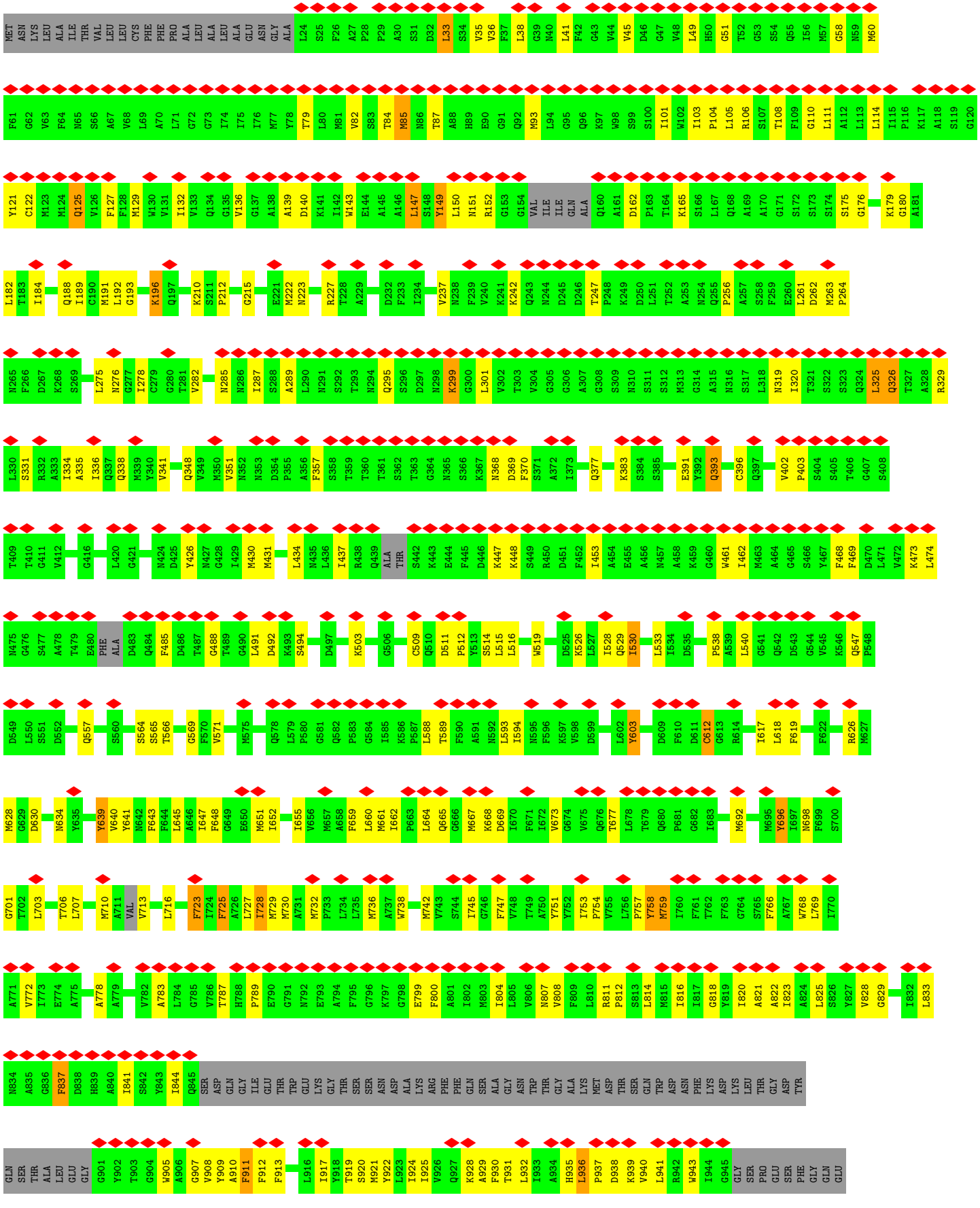


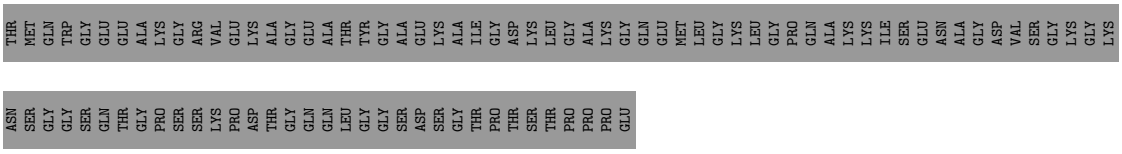




- Molecule 2: DotA

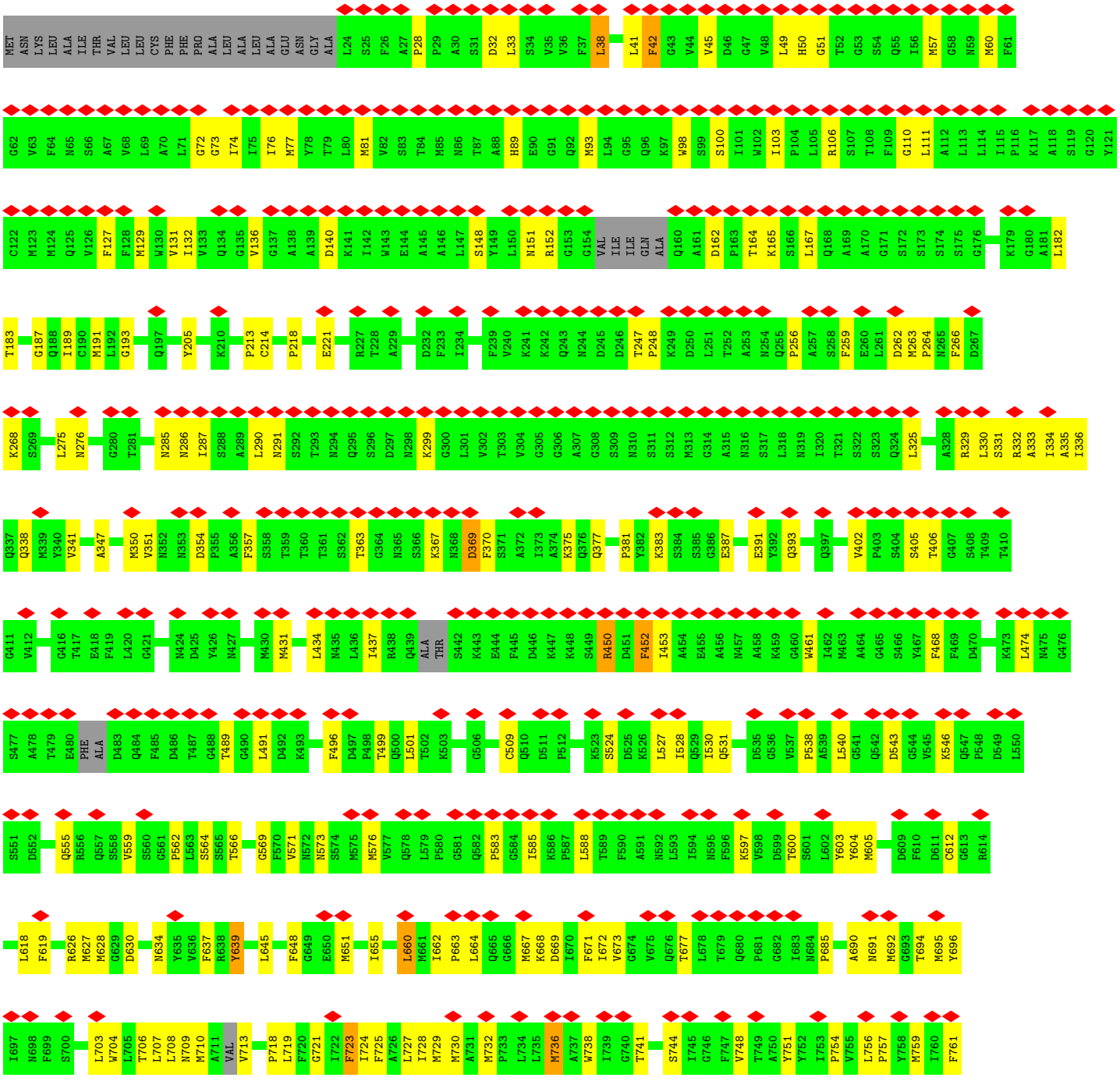
Chain HP1:

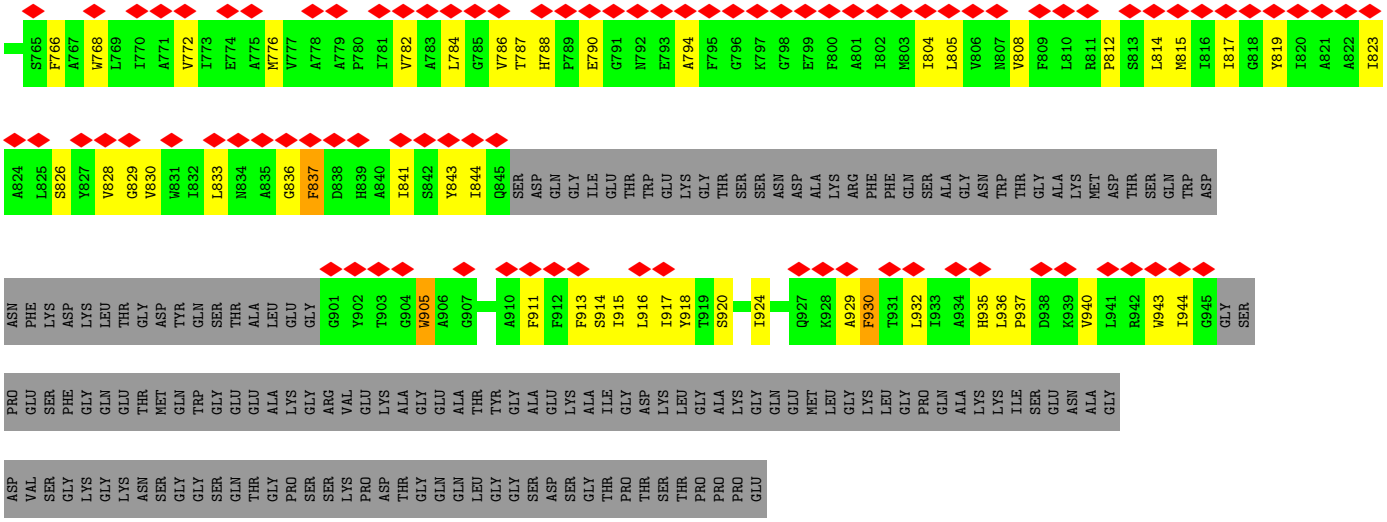

MET ASN LYS LEU ALA ILE THR VAL LEU LEU CYS PHE PHE PRO ALA LEU ALA LEU ALA GLU ASN GLY ALA L24 S25 F26 A27 P28 P29 A30 S31 D32 L33 S34 V35 V36 F37 L38 G39 N40 L41 F42 G43 V44 V45 D46 G47 V48 L49 H50 G51 T52 G53 S54 Q55 I56 M57 G58 N59 M60
F61 G62 V63 F64 N65 S66 A67 V68 L69 A70 L71 G72 G73 I74 I75 I76 M77 Y78 T79 L80 M81 V82 S83 T84 M85 N86 T87 A88 H89 E90 G91 Q92 M93 L94 G95 Q96 K97 W98 S99 S100 I101 W102 I103 P104 L105 R106 S107 T108 F109 G110 L111 A112 L113 L114 I115 P116 K117 A118 S119 G120
Y121 C122 M123 M124 Q125 V126 F127 F128 M129 W130 V131 I132 V133 Q134 G135 V136 G137 A138 A139 D140 K141 I142 W143 E144 A145 A146 L147 S148 Y149 L150 N151 R152 G153 G154 VAL ILE ILE GLN ALA Q160 A161 D162 P163 T164 K165 S166 L167 Q168 A169 A170 G171 S172 S173 S174 S175 G176 K179 G180 A181
L182 T183 I184 Q188 I189 C190 M191 L192 G193 K196 Q197 K210 S211 P212 G215 E221 M222 N223 R227 T228 A229 D232 F233 I234 V237 N238 F239 V240 K241 K242 Q243 N244 D245 D246 T247 P248 K249 D250 L251 T252 A253 N254 Q255 P256 A257 S258 F259 E260 L261 D262 M263 P264
N265 F266 D267 K268 S269 L275 N276 G277 I278 C279 G280 T281 V282 N285 N286 I287 S288 A289 L290 N291 S292 T293 N294 Q295 S296 D297 N298 K299 G300 L301 V302 T303 V304 G305 G306 A307 G308 S309 N310 S311 S312 M313 G314 A315 N316 S317 L318 N319 I320 T321 S322 S323 Q324 L325 Q326 T327 A328 R329
L330 S331 R332 A333 I334 A335 I336 Q337 Q338 M339 Y340 V341 Q348 V349 M350 V351 N352 N353 D354 P355 A356 F357 S358 T359 T360 T361 S362 T363 G364 N365 S366 K367 N368 D369 F370 S371 A372 I373 Q377 K383 S384 S385 E391 Y392 Q393 C396 Q397 V402 P403 S404 S405 T406 G407 S408
T409 T410 G411 V412 G416 L420 G421 N424 D425 Y426 N427 G428 I429 M430 M431 L434 N435 L436 I437 R438 Q439 ALA THR S442 K443 E444 F445 D446 K447 K448 S449 R450 D451 F452 I453 A454 E455 A456 N457 A458 K459 G460 W461 I462 M463 A464 G465 S466 Y467 F468 F469 D470 L471 V472 K473 L474
N475 G476 S477 A478 T479 E480 PHE ALA D483 Q484 F485 D486 T487 G488 T489 G490 L491 D492 K493 S494 D497 K503 G506 C509 Q510 D511 P512 Y513 S514 L515 L516 W519 D525 K526 L527 I528 Q529 I530 L533 I534 D535 P538 A539 L540 G541 Q542 D543 G544 V545 K546 Q547 P548
D549 L550 S551 D552 Q557 S560 S564 S565 T566 G569 F570 V571 M575 Q578 L579 P580 G581 Q582 P583 G584 I585 K586 P587 L588 T589 F590 A591 N592 L593 I594 N595 F596 K597 V598 D599 L602 Y603 D609 F610 D611 G612 G613 R614 I617 L618 F619 F622 R626 M627
M628 G629 D630 M634 Y635 Y639 V640 Y641 N642 F643 F644 L645 A646 I647 F648 G649 E650 M651 I652 I655 V656 M657 A658 F659 L660 M661 I662 P663 L664 Q665 G666 M667 K668 D669 I670 F671 I672 V673 G674 V675 Q676 T677 L678 T679 Q680 P681 G682 I683 M692 M695 Y696 I697 N698 F699 S700
G701 T702 L703 T706 L707 M710 A711 VAL V713 L716 F723 I724 F725 A726 L727 I728 M729 M730 A731 M732 P733 L734 L735 M736 A737 W738 M742 V743 S744 I745 G746 F747 V748 T749 A750 V751 Y752 I753 P754 V755 L756 P757 Y758 M759 I760 F761 T762 F763 G764 S765 F766 A767 W768 L769 I770
A771 V772 I773 E774 A775 A778 A779 V782 A783 L784 G785 V786 T787 H788 P789 E790 G791 N792 E793 A794 F795 G796 K797 G798 E799 F800 A801 I802 M803 I804 L805 V806 N807 V808 F809 L810 R811 P812 S813 L814 M815 I816 I817 G818 Y819 I820 A821 A822 I823 A824 L825 S826 Y827 V828 G829 I832 L833
N834 A835 G836 F837 D838 H839 A840 I841 S842 Y843 I844 Q845 SER ASP GLN GLY ILE GLU THR TRP GLU LYS GLY THR SER SER ASN ASP ALA LYS ARG PHE PHE GLN SER ALA GLY ASN TRP THR THR GLY ALA LYS MET ASP THR SER GLN TRP ASP ASN PHE LYS ASP LYS LEU THR GLY ASP TYR
GLN SER THR ALA LEU GLU GLY G901 Y902 T903 G904 W905 A906 G907 V908 Y909 A910 F911 F912 F913 L916 I917 Y918 T919 S920 M921 Y922 L923 I924 I925 V926 Q927 K928 A929 F930 T931 L932 I933 A934 H935 L936 P937 D938 K939 V940 L941 R942 W943 I944 G945 GLY SER PRO GLU SER PHE GLY GLN GLU



• Molecule 2: DotA

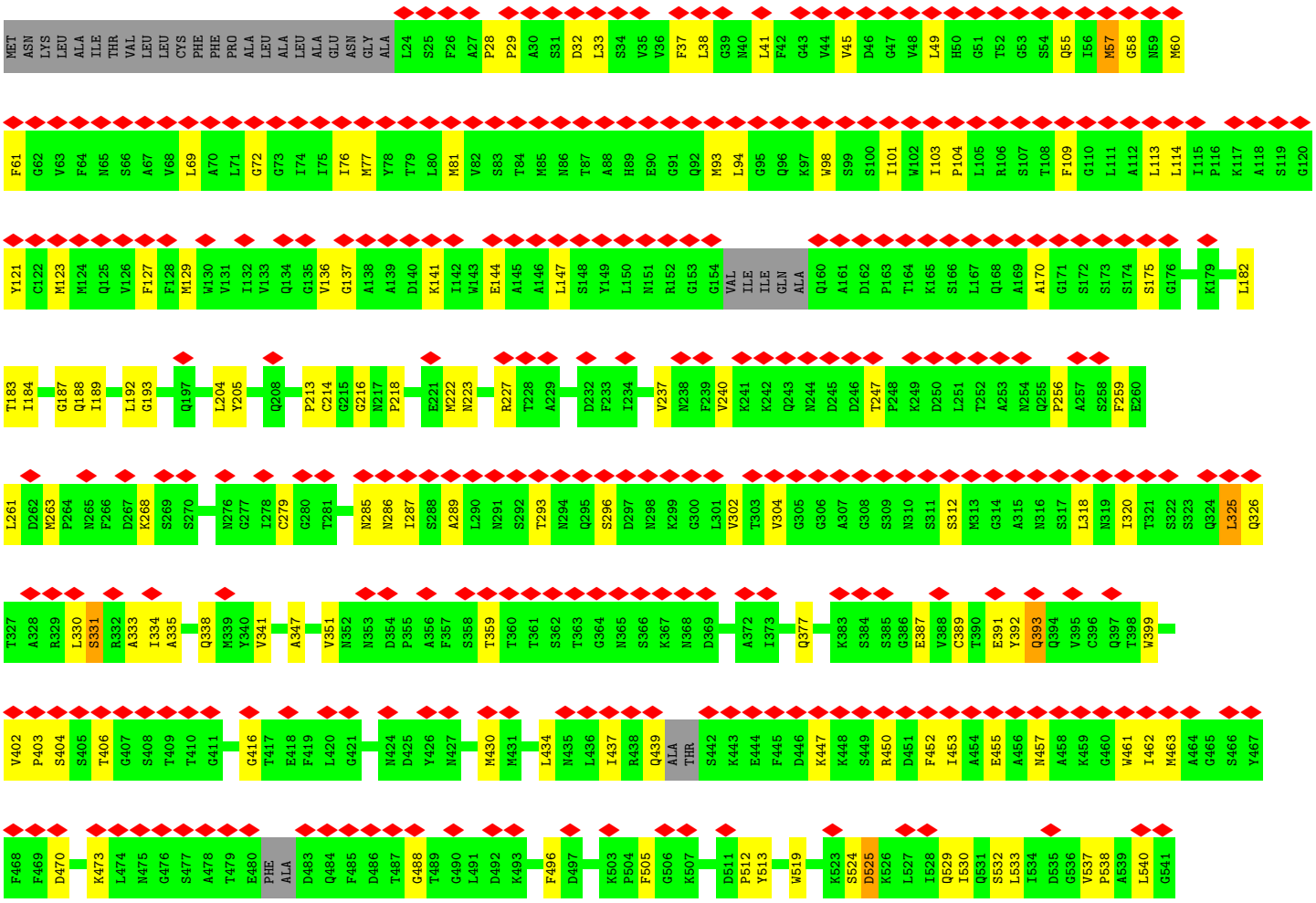
Chain IP1:

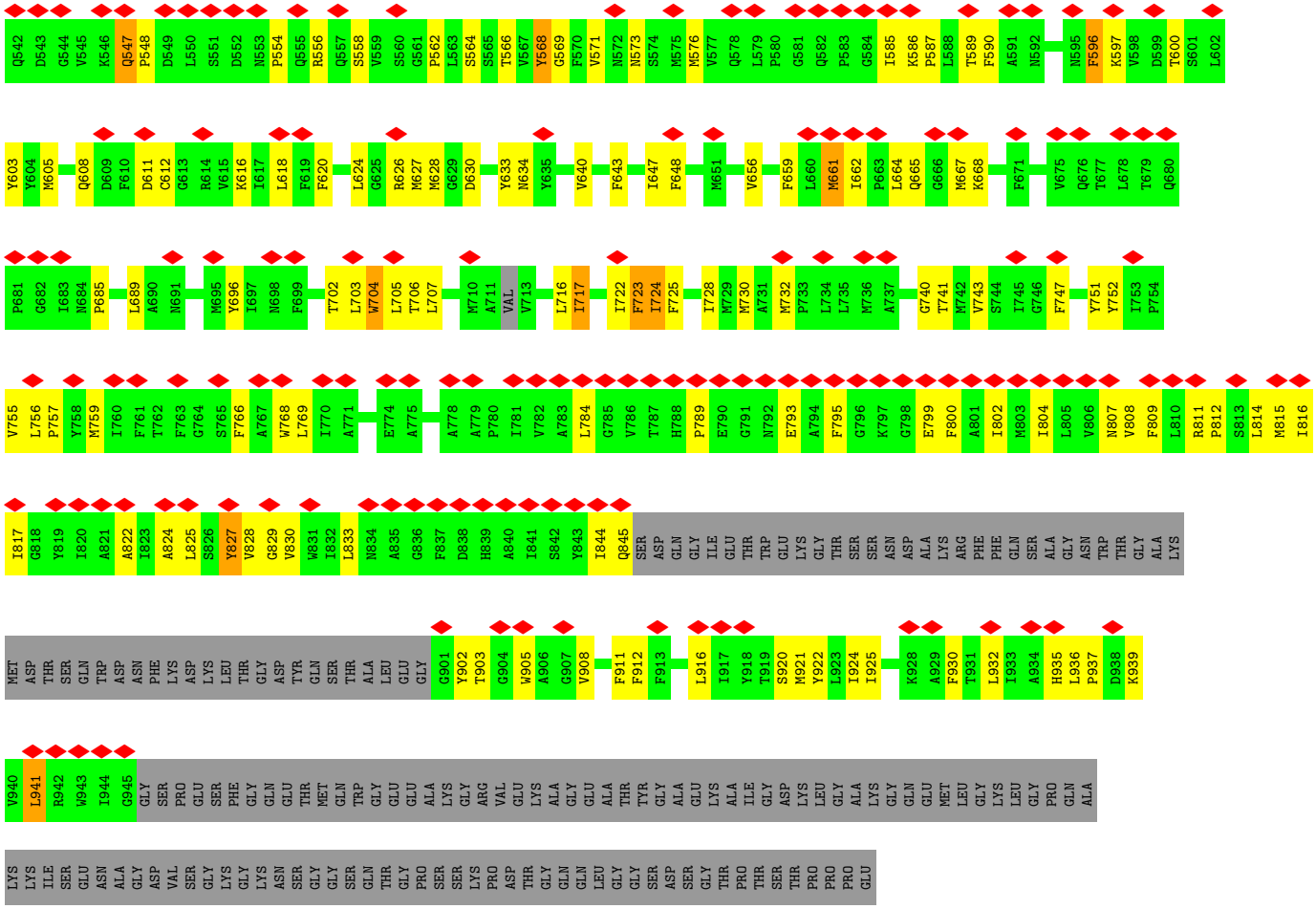


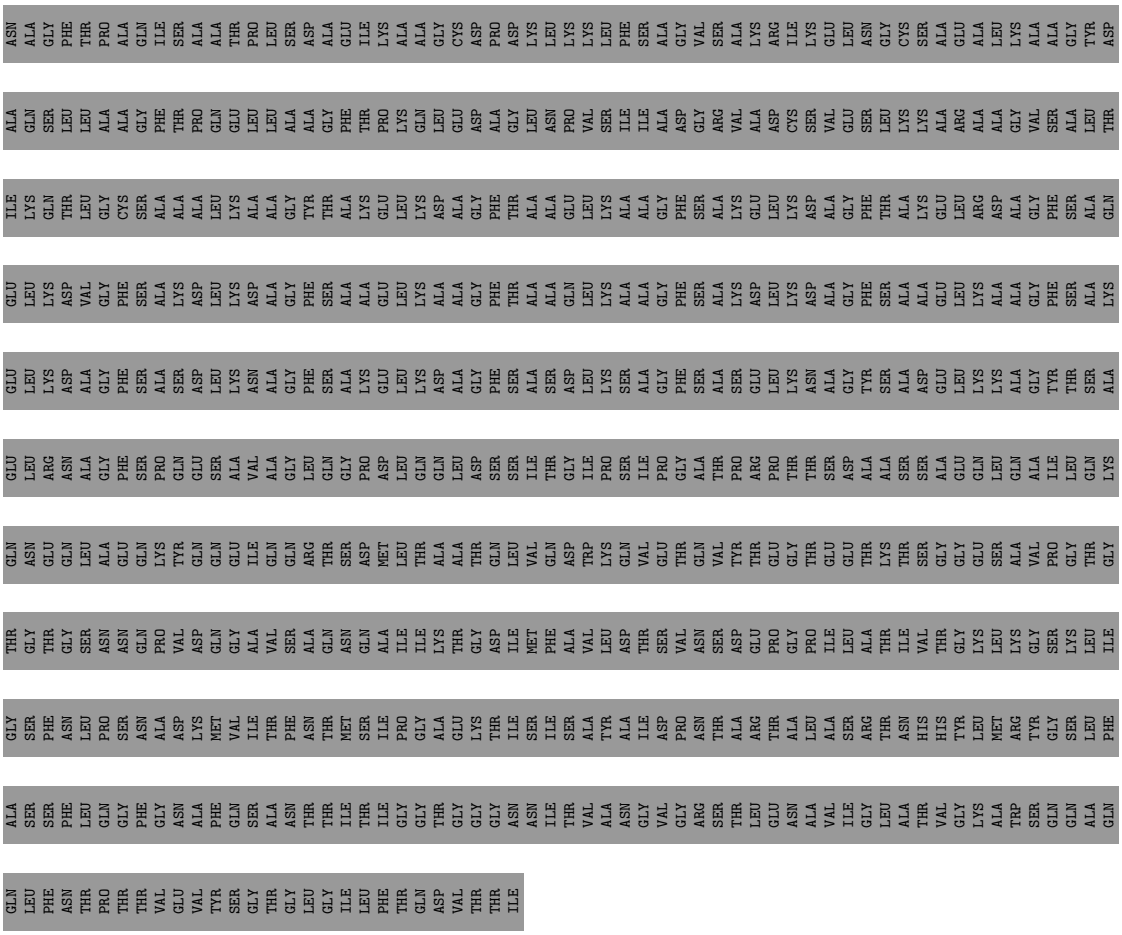


- Molecule 2: DotA

Chain JP1:

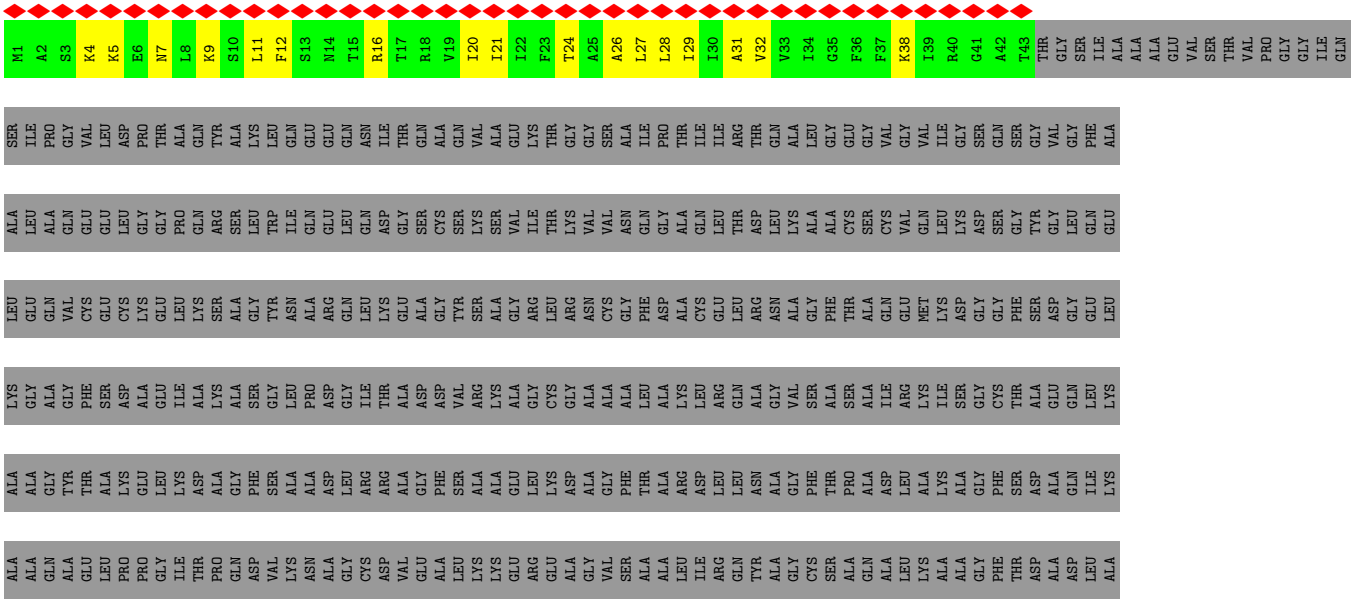


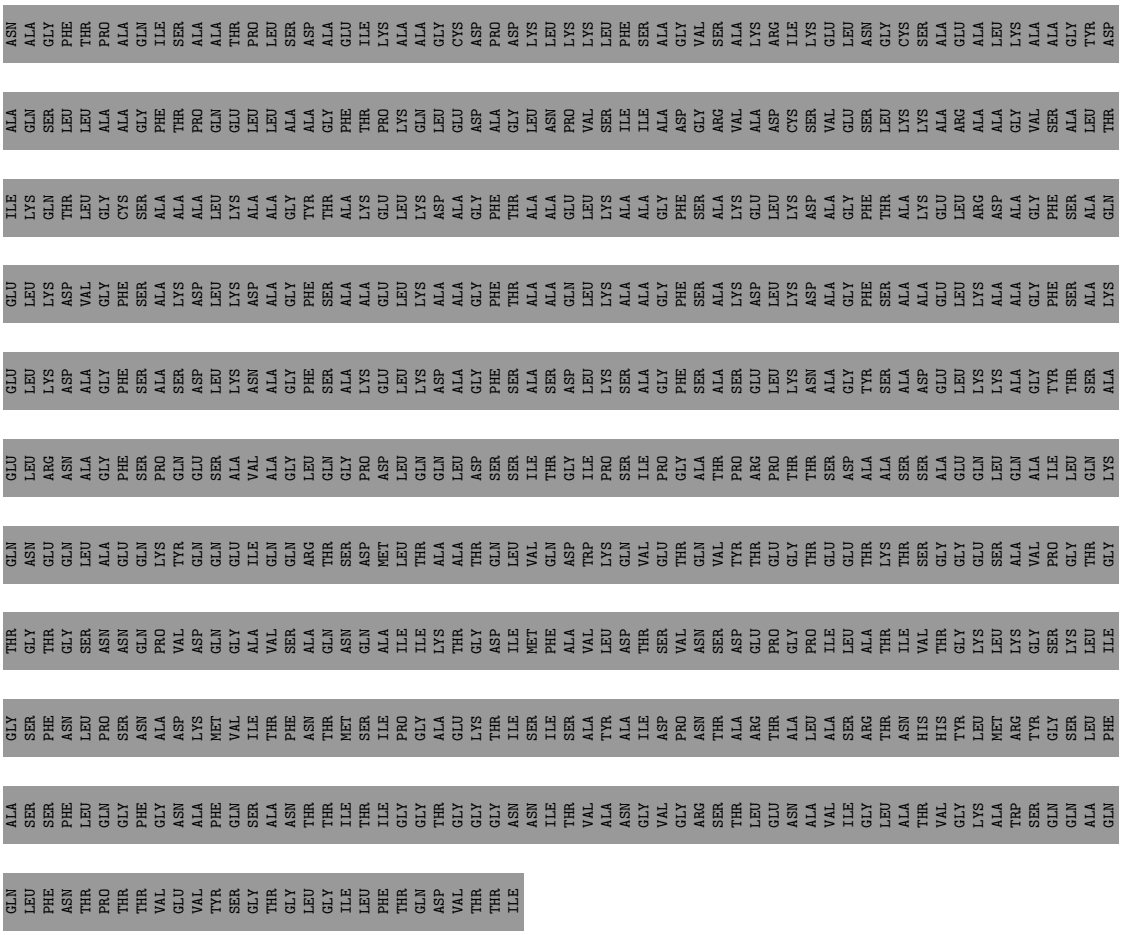




• Molecule 3: IcmE (DotG)

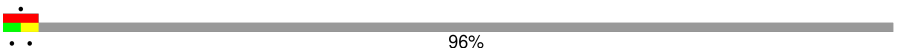
Chain LP1: 96%

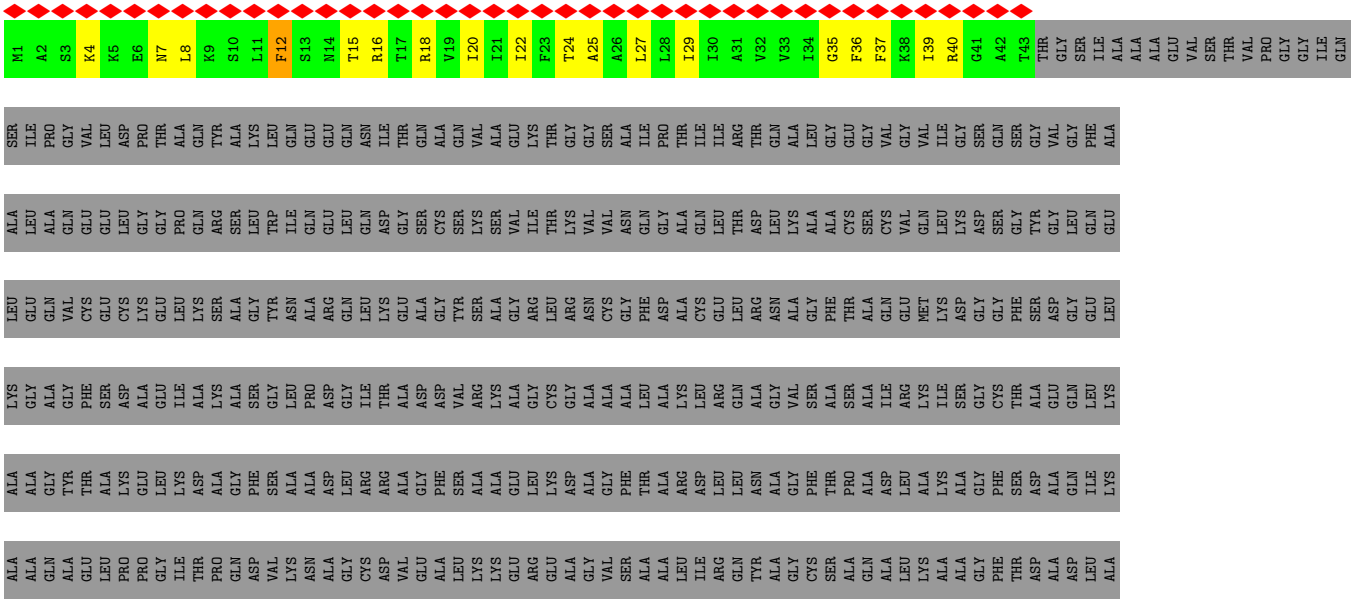


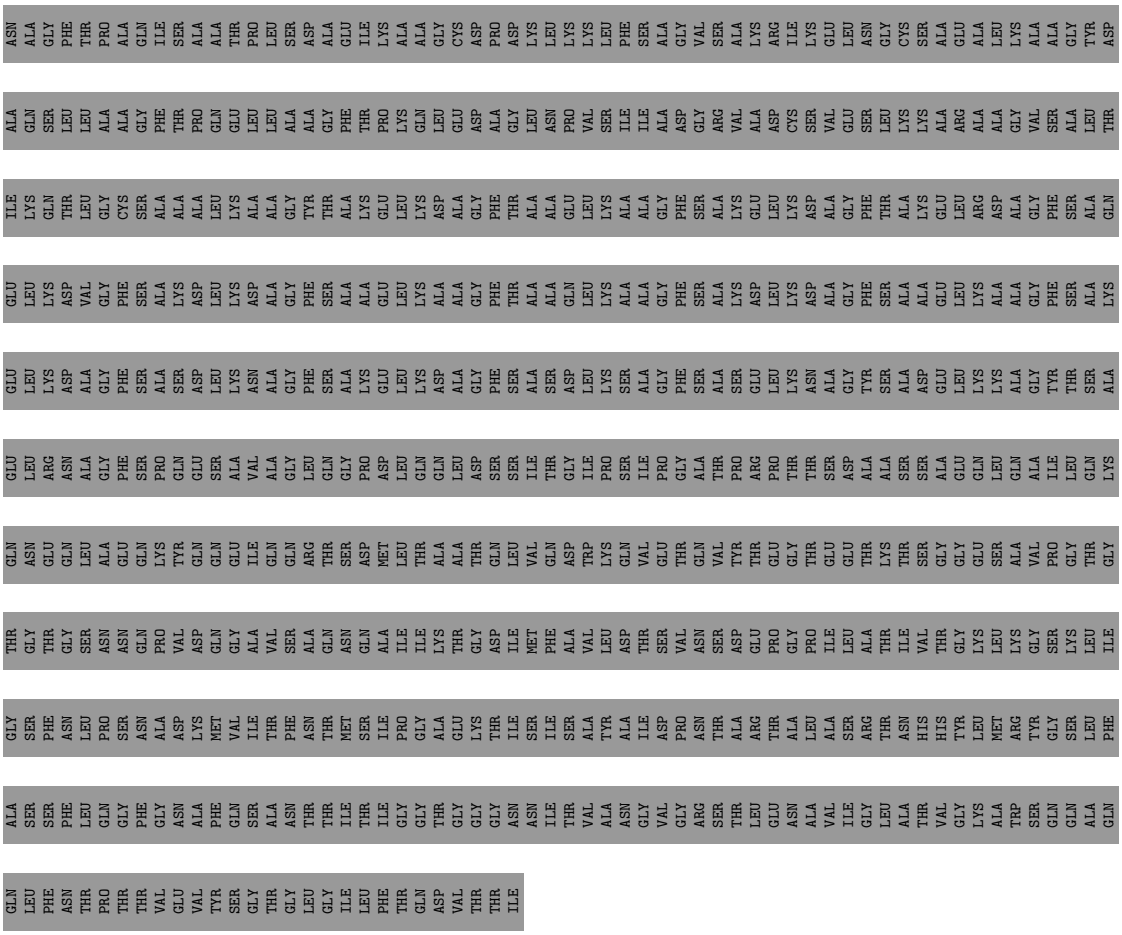


• Molecule 3: IcmE (DotG)

Chain MP1:

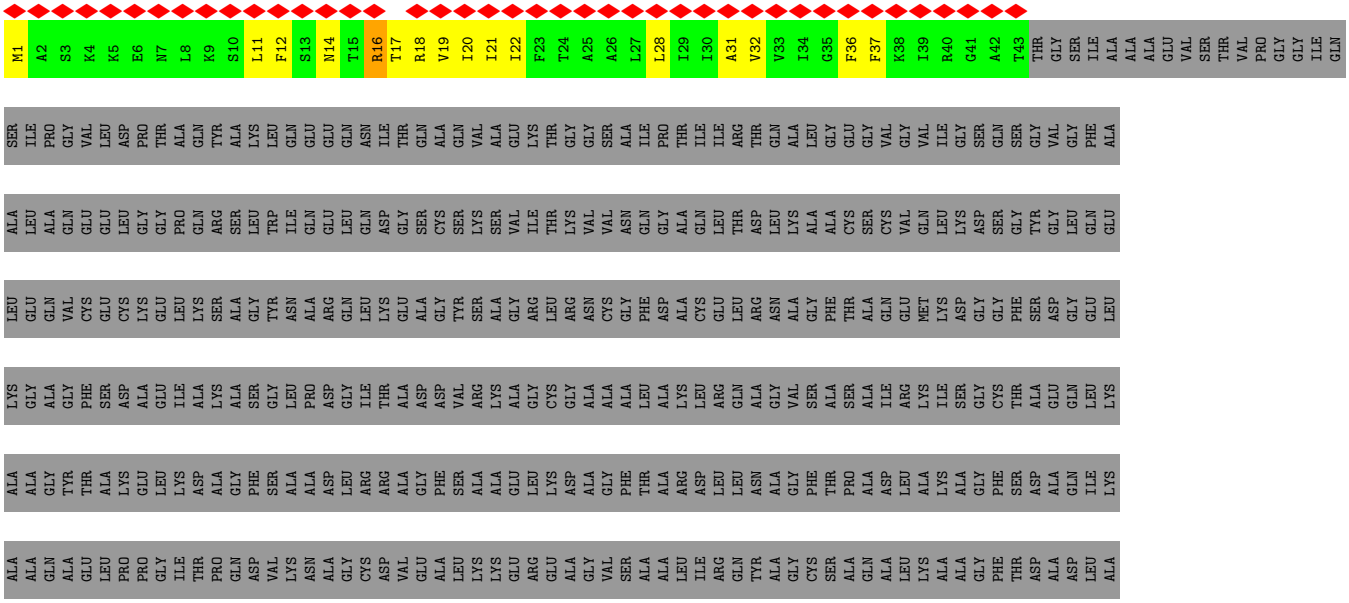


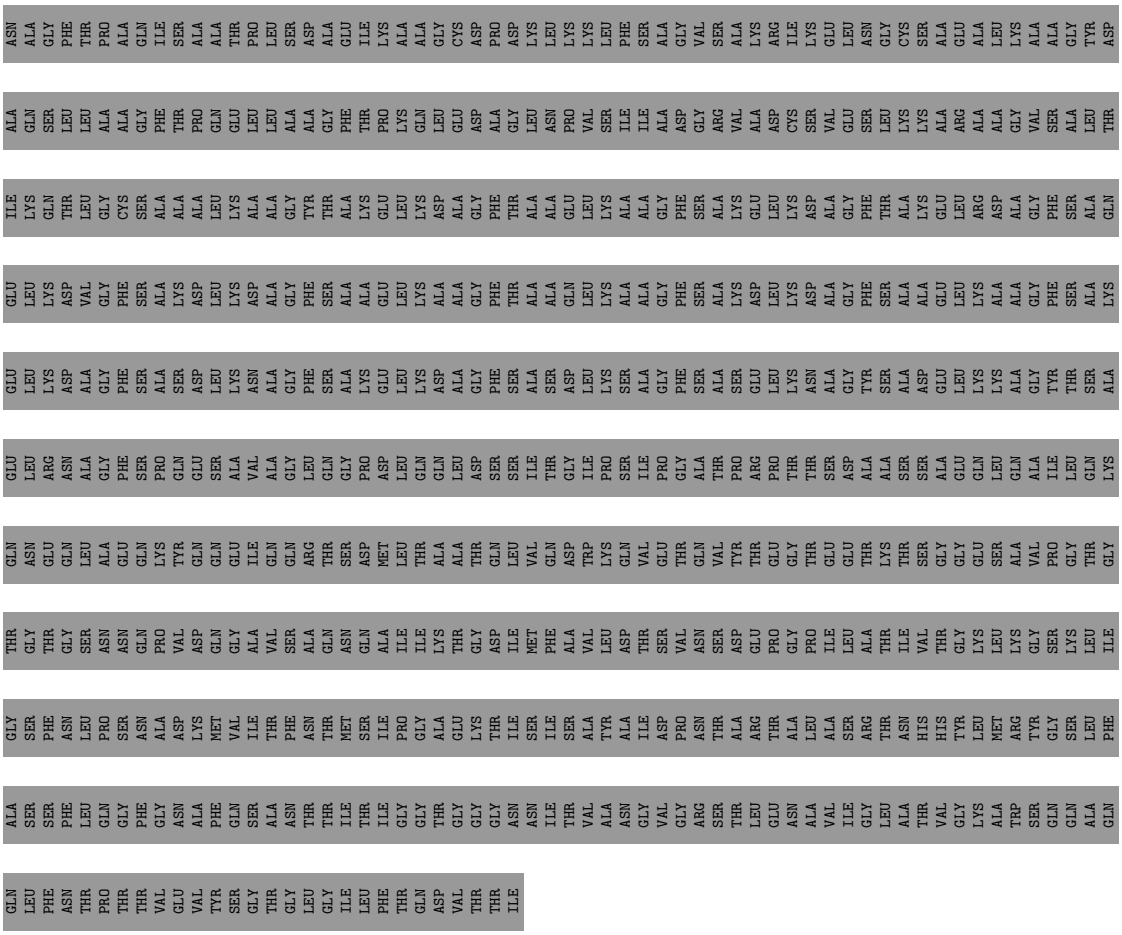




• Molecule 3: IcmE (DotG)

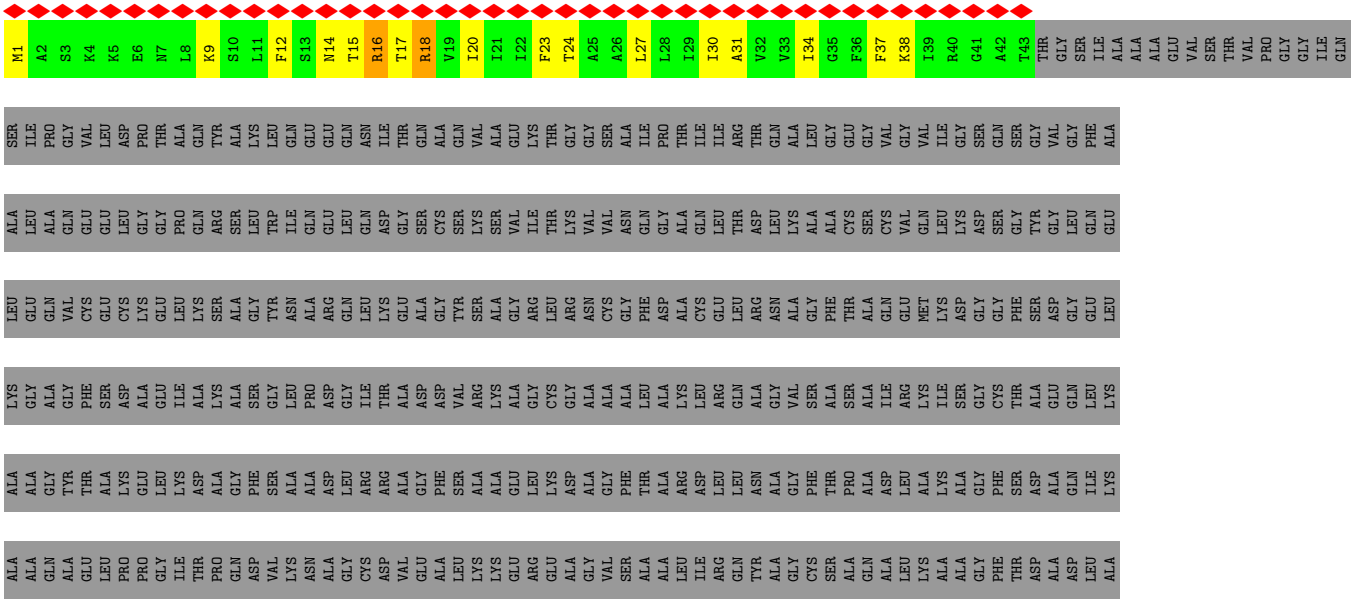
Chain NP1:

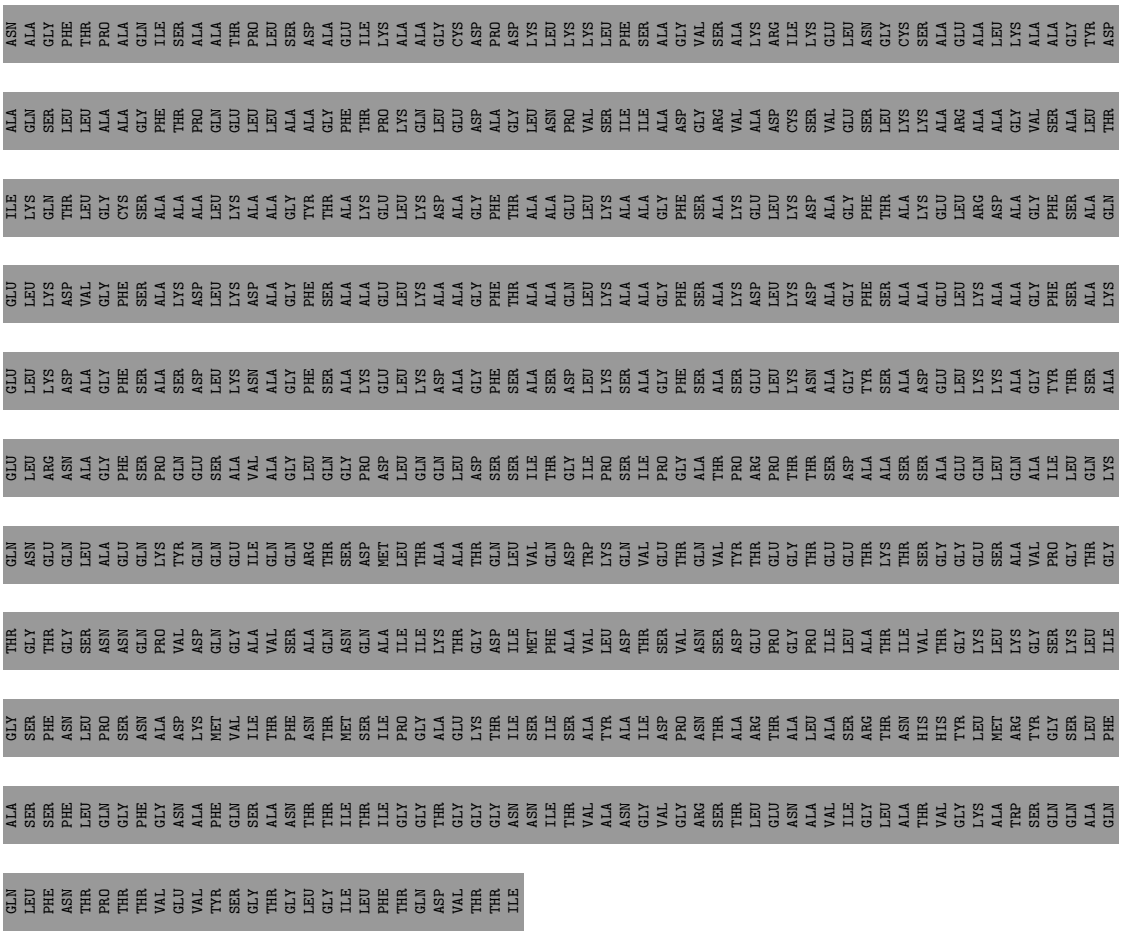




• Molecule 3: IcmE (DotG)

Chain OP1:




ASN ALA GLY PHE THR PRO ALA GLN ILE SER ALA ALA THR PRO LEU SER ASP ALA GLU ILE LYS ALA ALA GLY CYS ASP PRO ASP LYS LEU LYS LYS LEU PHE SER ALA GLY VAL SER ALA LYS ARG ILE LYS GLU LEU ASN GLY CYS SER ALA GLU ALA LEU LYS ALA ALA GLY TYR ASP
ALA GLN SER LEU LEU ALA ALA GLY PHE THR PRO GLN GLU LEU LEU ALA ALA GLY PHE THR PRO LYS GLN LEU GLU GLU ASP ALA GLY LEU ASN PRO VAL SER ILE ILE ALA ASP GLY ARG VAL ALA ASP CYS SER VAL GLU SER LEU LYS LYS ALA ARG ALA ALA ALA GLY VAL SER ALA LEU THR
ILE LYS GLN THR LEU GLY CYS SER ALA ALA ALA LEU LYS ALA ALA ALA GLY TYR THR ALA LYS LYS GLU LEU LYS ASP ALA GLY THR ALA ALA ALA GLU LEU LYS ALA ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA ALA ALA GLN LEU LYS ASP ALA GLY PHE THR ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA ALA GLN
GLU LEU LYS ASP VAL GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE THR ALA ALA ALA GLN LEU LYS ASP ALA GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA ALA LYS
GLU LEU LYS ASP ALA GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA LYS GLU LEU LYS ASP ALA GLY PHE SER ALA LYS ASP LEU LYS ASP ALA GLY PHE SER ALA LYS GLU LEU LYS ASN ALA GLY PHE SER ALA LYS GLU LEU LYS ASN ALA GLY PHE SER ALA LYS GLU LEU LYS ASN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	37503	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TECNAI 12	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	73	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.818	Depositor
Minimum map value	-0.526	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.2	Depositor
Map size (Å)	640.8192, 640.8192, 640.8192	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.2516, 1.2516, 1.2516	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	AP1	0.17	0/3277	0.35	0/4473
1	BP1	0.17	0/3277	0.35	0/4473
1	CP1	0.16	0/3277	0.32	0/4473
1	DP1	0.16	0/3277	0.32	0/4473
1	EP1	0.17	0/3277	0.32	0/4473
2	FP1	0.16	0/6715	0.36	0/9115
2	GP1	0.16	0/6715	0.39	0/9115
2	HP1	0.16	0/6715	0.39	0/9115
2	IP1	0.16	0/6715	0.39	0/9115
2	JP1	0.16	0/6715	0.36	0/9115
3	KP1	0.16	0/337	0.52	0/451
3	LP1	0.09	0/337	0.27	0/451
3	MP1	0.12	0/337	0.38	0/451
3	NP1	0.14	0/337	0.41	0/451
3	OP1	0.18	0/337	0.54	0/451
All	All	0.16	0/51645	0.37	0/70195

There are no bond length outliers.

There are no bond angle outliers.

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	AP1	3213	0	3131	77	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	BP1	3213	0	3131	91	0
1	CP1	3213	0	3131	74	0
1	DP1	3213	0	3131	75	0
1	EP1	3213	0	3131	78	0
2	FP1	6560	0	6545	165	0
2	GP1	6560	0	6545	208	0
2	HP1	6560	0	6545	198	0
2	IP1	6560	0	6545	185	0
2	JP1	6560	0	6545	174	0
3	KP1	334	0	378	15	0
3	LP1	334	0	378	14	0
3	MP1	334	0	378	12	0
3	NP1	334	0	378	11	0
3	OP1	334	0	378	13	0
All	All	50535	0	50270	1188	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 12.

All (1188) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:671:PHE:HE1	2:FP1:915:ILE:HD13	1.29	0.97
2:HP1:193:GLY:HA3	2:HP1:530:ILE:HD11	1.51	0.92
1:DP1:443:MET:HE2	1:EP1:443:MET:HE1	1.53	0.91
2:GP1:929:ALA:O	2:GP1:932:LEU:HB3	1.73	0.88
2:GP1:193:GLY:HA3	2:GP1:530:ILE:HD11	1.55	0.87
3:MP1:16:ARG:HE	3:MP1:20:ILE:HD11	1.37	0.87
2:HP1:326:GLN:HA	2:HP1:329:ARG:HE	1.39	0.86
2:JP1:193:GLY:HA3	2:JP1:530:ILE:HD11	1.57	0.85
2:FP1:594:ILE:HG23	2:JP1:705:LEU:HD11	1.59	0.84
2:FP1:671:PHE:CE1	2:FP1:915:ILE:HD13	2.13	0.84
2:FP1:78:TYR:HA	2:FP1:81:MET:HE2	1.59	0.84
1:BP1:94:MET:HE1	1:BP1:170:LEU:HD23	1.56	0.83
2:GP1:768:TRP:HB2	2:GP1:815:MET:HE1	1.59	0.83
2:IP1:662:ILE:HG23	2:IP1:663:PRO:HD3	1.59	0.83
2:FP1:828:VAL:HG21	2:JP1:41:LEU:HB2	1.62	0.82
1:CP1:426:MET:HE1	1:DP1:422:ILE:HG23	1.64	0.80
2:FP1:766:PHE:HZ	2:GP1:829:GLY:HA2	1.46	0.79
2:FP1:60:MET:HE1	2:GP1:817:ILE:HG12	1.65	0.78
2:IP1:193:GLY:HA3	2:IP1:530:ILE:HD11	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:660:LEU:HD21	2:FP1:661:MET:HE2	1.64	0.78
2:FP1:73:GLY:HA2	2:FP1:76:ILE:HD12	1.64	0.78
2:HP1:909:TYR:O	2:HP1:912:PHE:HB2	1.85	0.76
2:HP1:41:LEU:HB2	2:IP1:828:VAL:HG11	1.66	0.76
2:HP1:917:ILE:HA	2:HP1:920:SER:HB3	1.67	0.75
2:HP1:60:MET:HE3	2:IP1:817:ILE:HD13	1.69	0.75
1:DP1:444:LEU:HD23	1:EP1:443:MET:HB2	1.69	0.74
1:AP1:422:ILE:HG23	1:EP1:426:MET:HE1	1.68	0.74
2:IP1:540:LEU:HD23	2:IP1:562:PRO:HB2	1.69	0.74
1:DP1:94:MET:HE1	1:DP1:170:LEU:HD23	1.67	0.74
2:JP1:302:VAL:HG11	2:JP1:325:LEU:HD13	1.70	0.73
2:IP1:612:CYS:HB2	2:IP1:626:ARG:HE	1.52	0.73
2:HP1:101:ILE:HD13	3:OP1:16:ARG:HH21	1.54	0.73
2:GP1:697:ILE:HD12	2:GP1:751:TYR:HE2	1.53	0.72
2:JP1:612:CYS:HB2	2:JP1:626:ARG:HE	1.53	0.72
2:FP1:72:GLY:HA3	2:FP1:784:LEU:HD21	1.71	0.72
2:IP1:41:LEU:HB2	2:JP1:828:VAL:HG11	1.72	0.72
1:DP1:123:GLN:HE22	1:DP1:256:THR:HG21	1.54	0.72
2:IP1:756:LEU:HA	2:IP1:759:MET:HG3	1.73	0.71
1:DP1:426:MET:HE1	1:EP1:422:ILE:HG23	1.72	0.71
2:IP1:266:PHE:H	2:IP1:276:ASN:HD21	1.36	0.71
2:GP1:759:MET:HE3	2:HP1:917:ILE:HG12	1.71	0.71
2:HP1:103:ILE:HG13	2:HP1:104:PRO:HD3	1.73	0.71
1:BP1:139:ASN:HB2	1:BP1:281:ARG:HH12	1.56	0.70
2:IP1:377:GLN:HE22	2:IP1:402:VAL:HG12	1.56	0.70
2:JP1:627:MET:HG2	2:JP1:628:MET:HE2	1.73	0.70
1:EP1:371:GLN:O	1:EP1:375:GLU:HB2	1.91	0.70
2:GP1:180:GLY:O	2:GP1:184:ILE:HD12	1.90	0.70
1:DP1:328:SER:HA	1:EP1:211:MET:HE2	1.74	0.70
2:FP1:732:MET:HA	2:FP1:732:MET:HE2	1.74	0.69
2:JP1:662:ILE:HG12	2:JP1:703:LEU:HD12	1.74	0.69
2:JP1:920:SER:O	2:JP1:924:ILE:HD12	1.92	0.69
2:GP1:648:PHE:O	2:GP1:652:ILE:HG13	1.93	0.69
1:BP1:94:MET:HG3	1:CP1:241:SER:HB2	1.73	0.69
1:DP1:426:MET:HE3	1:EP1:425:GLN:HB2	1.75	0.69
2:FP1:566:THR:HG23	2:FP1:569:GLY:H	1.56	0.69
2:HP1:377:GLN:HE22	2:HP1:402:VAL:H	1.40	0.69
2:GP1:788:HIS:HB3	2:GP1:790:GLU:HG3	1.75	0.68
2:HP1:320:ILE:HD11	2:HP1:325:LEU:HD12	1.75	0.68
2:IP1:932:LEU:HA	2:IP1:935:HIS:HB3	1.75	0.68
2:FP1:74:ILE:HA	2:FP1:77:MET:HE2	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP1:104:ASP:HA	1:BP1:109:ASN:HD22	1.58	0.68
2:IP1:920:SER:O	2:IP1:924:ILE:HD12	1.94	0.68
2:GP1:716:LEU:HA	2:HP1:723:PHE:CD1	2.29	0.68
1:CP1:342:VAL:HG21	1:CP1:442:ILE:HG13	1.75	0.68
2:IP1:391:GLU:HG3	2:IP1:393:GLN:H	1.59	0.68
2:IP1:741:THR:HG23	2:IP1:916:LEU:HD21	1.75	0.68
1:BP1:342:VAL:HG21	1:BP1:442:ILE:HG13	1.75	0.68
2:IP1:566:THR:HG23	2:IP1:569:GLY:H	1.58	0.68
2:HP1:929:ALA:O	2:HP1:932:LEU:HD12	1.94	0.68
2:FP1:266:PHE:H	2:FP1:276:ASN:HD21	1.42	0.68
1:AP1:104:ASP:HA	1:AP1:109:ASN:HD22	1.59	0.67
2:HP1:757:PRO:HG3	2:HP1:930:PHE:HE1	1.60	0.67
1:EP1:185:PRO:HG3	1:EP1:204:LEU:HD12	1.76	0.67
1:BP1:123:GLN:HE22	1:BP1:256:THR:HG21	1.59	0.67
1:EP1:74:VAL:O	1:EP1:78:GLN:HG2	1.95	0.67
2:GP1:920:SER:O	2:GP1:924:ILE:HD12	1.95	0.67
2:GP1:656:VAL:HG12	2:GP1:660:LEU:HD23	1.76	0.67
2:JP1:723:PHE:CD2	2:JP1:724:ILE:HD13	2.29	0.67
1:AP1:342:VAL:HG21	1:AP1:442:ILE:HG13	1.75	0.67
1:BP1:248:LEU:HD22	1:BP1:249:ILE:HG22	1.75	0.67
2:HP1:192:LEU:HB2	2:HP1:351:VAL:HG21	1.75	0.67
2:HP1:594:ILE:HB	2:HP1:660:LEU:HD12	1.75	0.67
2:FP1:242:LYS:HG2	2:FP1:261:LEU:HD23	1.76	0.67
2:HP1:651:MET:O	2:HP1:655:ILE:HG13	1.95	0.67
3:MP1:25:ALA:O	3:MP1:29:ILE:HG12	1.95	0.67
2:FP1:78:TYR:O	2:FP1:82:VAL:HG23	1.95	0.66
1:BP1:54:ILE:HG22	1:CP1:42:TYR:HD2	1.60	0.66
2:FP1:745:ILE:HG23	2:FP1:919:THR:HG21	1.78	0.66
2:IP1:709:ASN:HD21	2:JP1:597:LYS:H	1.44	0.66
1:CP1:136:ILE:HG23	1:CP1:277:LEU:HD22	1.77	0.66
1:CP1:328:SER:HA	1:DP1:211:MET:HE2	1.78	0.66
2:IP1:72:GLY:O	2:IP1:76:ILE:HG13	1.95	0.66
1:BP1:40:VAL:O	1:BP1:44:THR:HG23	1.96	0.66
2:IP1:759:MET:HA	2:JP1:921:MET:HE1	1.76	0.66
2:GP1:450:ARG:O	2:GP1:453:ILE:HG13	1.96	0.65
2:GP1:651:MET:O	2:GP1:655:ILE:HG12	1.96	0.65
2:HP1:242:LYS:HG2	2:HP1:261:LEU:HD23	1.76	0.65
2:IP1:72:GLY:HA3	2:IP1:784:LEU:HD11	1.76	0.65
2:JP1:566:THR:HG23	2:JP1:569:GLY:H	1.60	0.65
1:BP1:430:ARG:HH21	1:CP1:425:GLN:HB3	1.59	0.65
1:DP1:74:VAL:O	1:DP1:78:GLN:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:627:MET:HG2	2:IP1:628:MET:HE2	1.78	0.65
3:LP1:24:THR:HA	3:LP1:27:LEU:HD12	1.77	0.65
1:AP1:33:SER:HB2	1:BP1:31:GLN:OE1	1.96	0.65
2:GP1:732:MET:HE2	2:GP1:732:MET:HA	1.79	0.65
2:IP1:757:PRO:HG3	2:IP1:930:PHE:CE1	2.32	0.64
2:IP1:841:ILE:HD12	2:IP1:844:ILE:HB	1.79	0.64
2:GP1:702:THR:HG23	2:HP1:905:TRP:HE1	1.61	0.64
2:HP1:180:GLY:O	2:HP1:184:ILE:HD12	1.96	0.64
1:CP1:74:VAL:O	1:CP1:78:GLN:HG2	1.96	0.64
2:GP1:706:THR:HG22	2:GP1:710:MET:HE2	1.80	0.64
2:HP1:662:ILE:HG12	2:HP1:703:LEU:HD11	1.80	0.64
2:JP1:72:GLY:HA3	2:JP1:784:LEU:HD11	1.79	0.64
3:MP1:16:ARG:O	3:MP1:20:ILE:HG13	1.97	0.64
1:AP1:74:VAL:O	1:AP1:78:GLN:HG2	1.98	0.64
2:HP1:738:TRP:CD1	2:HP1:912:PHE:HZ	2.15	0.64
2:HP1:648:PHE:O	2:HP1:652:ILE:HG22	1.98	0.64
2:IP1:639:TYR:HE2	2:JP1:605:MET:HE1	1.61	0.64
2:HP1:932:LEU:HA	2:HP1:935:HIS:CD2	2.33	0.64
2:GP1:132:ILE:HG13	2:GP1:772:VAL:HG13	1.80	0.63
2:GP1:759:MET:HG3	2:HP1:921:MET:HE2	1.78	0.63
2:FP1:667:MET:HE1	2:FP1:915:ILE:HG21	1.80	0.63
2:HP1:182:LEU:HD23	2:HP1:571:VAL:HG21	1.80	0.63
2:IP1:332:ARG:HH21	2:IP1:489:THR:HA	1.63	0.63
2:FP1:741:THR:O	2:FP1:745:ILE:HG13	1.99	0.63
2:GP1:766:PHE:HZ	2:HP1:829:GLY:HA3	1.63	0.63
2:JP1:807:ASN:HD22	2:JP1:941:LEU:HG	1.64	0.63
1:AP1:254:MET:HG3	1:AP1:355:LEU:HD12	1.81	0.63
1:EP1:136:ILE:HG23	1:EP1:277:LEU:HD22	1.81	0.63
2:HP1:728:ILE:HD11	2:IP1:729:MET:HE3	1.80	0.63
1:EP1:141:LEU:HB3	1:EP1:213:ASN:HB3	1.81	0.63
1:AP1:111:LEU:HD23	1:BP1:386:PRO:HB3	1.81	0.62
2:HP1:804:ILE:HD12	2:HP1:807:ASN:HD22	1.64	0.62
2:IP1:45:VAL:HG11	2:IP1:129:MET:HG2	1.81	0.62
1:DP1:129:SER:HB2	1:DP1:137:THR:HG21	1.81	0.62
2:HP1:932:LEU:HB3	2:HP1:936:LEU:HD12	1.82	0.62
2:IP1:100:SER:HA	2:IP1:103:ILE:HD12	1.81	0.62
1:BP1:83:ASN:HB2	1:BP1:359:MET:HE1	1.82	0.62
2:GP1:110:GLY:HA3	2:GP1:787:THR:HG23	1.82	0.62
2:JP1:905:TRP:HA	2:JP1:908:VAL:HB	1.80	0.62
3:MP1:16:ARG:NE	3:MP1:20:ILE:HD11	2.13	0.62
1:AP1:211:MET:HE2	1:EP1:328:SER:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:804:ILE:O	2:HP1:808:VAL:HG22	2.00	0.62
2:IP1:744:SER:O	2:IP1:748:VAL:HG23	2.00	0.62
1:DP1:427:TYR:HA	1:DP1:430:ARG:NH1	2.15	0.62
2:IP1:704:TRP:HA	2:IP1:707:LEU:HD12	1.81	0.62
1:CP1:104:ASP:HA	1:CP1:109:ASN:HD22	1.65	0.61
3:KP1:16:ARG:O	3:KP1:20:ILE:HG12	2.00	0.61
1:AP1:31:GLN:HE21	1:EP1:33:SER:HB2	1.63	0.61
2:JP1:402:VAL:HG12	2:JP1:404:SER:H	1.65	0.61
2:HP1:732:MET:HA	2:HP1:732:MET:HE2	1.80	0.61
2:JP1:616:LYS:HA	2:JP1:620:PHE:O	2.00	0.61
3:MP1:24:THR:HA	3:MP1:27:LEU:HD12	1.82	0.61
1:BP1:142:ILE:HA	1:BP1:210:VAL:HG23	1.83	0.61
2:IP1:131:VAL:HG21	2:IP1:805:LEU:HD11	1.82	0.61
2:JP1:101:ILE:HG12	3:MP1:16:ARG:HH22	1.65	0.61
1:DP1:427:TYR:HA	1:DP1:430:ARG:HH11	1.65	0.61
2:GP1:708:LEU:HD13	2:HP1:730:MET:HB3	1.81	0.61
2:GP1:768:TRP:O	2:GP1:772:VAL:HG23	2.00	0.61
2:IP1:528:ILE:HD11	2:IP1:538:PRO:HD3	1.81	0.61
2:JP1:590:PHE:CE2	2:JP1:664:LEU:HD13	2.35	0.61
2:JP1:630:ASP:HA	2:JP1:634:ASN:HB2	1.82	0.61
1:DP1:427:TYR:HD1	1:DP1:430:ARG:HH12	1.49	0.61
1:EP1:104:ASP:HA	1:EP1:109:ASN:HD22	1.65	0.61
2:FP1:330:LEU:O	2:FP1:334:ILE:HG13	2.00	0.61
2:GP1:721:GLY:HA3	2:HP1:723:PHE:HE1	1.66	0.61
2:IP1:183:THR:HG23	2:IP1:496:PHE:HB2	1.83	0.61
1:DP1:136:ILE:HG23	1:DP1:277:LEU:HD22	1.82	0.61
2:GP1:103:ILE:HG13	2:GP1:104:PRO:HD3	1.82	0.61
3:NP1:16:ARG:HE	3:NP1:17:THR:HG22	1.65	0.61
2:JP1:932:LEU:HA	2:JP1:935:HIS:HB3	1.82	0.61
2:FP1:804:ILE:O	2:FP1:808:VAL:HG22	2.00	0.60
2:GP1:747:PHE:HA	2:GP1:751:TYR:HD2	1.65	0.60
2:IP1:106:ARG:HE	2:IP1:794:ALA:HA	1.67	0.60
1:BP1:129:SER:HB2	1:BP1:137:THR:HG21	1.83	0.60
2:FP1:113:LEU:HD13	2:FP1:123:MET:HG3	1.82	0.60
2:FP1:593:LEU:H	2:FP1:593:LEU:HD23	1.67	0.60
2:GP1:804:ILE:O	2:GP1:808:VAL:HG22	2.00	0.60
2:HP1:816:ILE:O	2:HP1:820:ILE:HG13	2.02	0.60
1:BP1:55:THR:HA	1:CP1:42:TYR:HE2	1.67	0.60
2:HP1:928:LYS:O	2:HP1:931:THR:HG22	2.01	0.60
1:AP1:339:GLN:HB3	1:EP1:448:LEU:HD11	1.84	0.60
1:CP1:81:ALA:HB2	1:CP1:378:MET:HE1	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:470:ASP:HA	2:GP1:473:LYS:HD2	1.84	0.59
1:CP1:40:VAL:O	1:CP1:44:THR:HG23	2.02	0.59
2:GP1:757:PRO:HG3	2:GP1:930:PHE:CE2	2.38	0.59
2:IP1:732:MET:HE2	2:IP1:732:MET:HA	1.84	0.59
1:AP1:174:VAL:HG13	1:BP1:244:ASN:HD21	1.67	0.59
1:CP1:141:LEU:HD22	1:CP1:213:ASN:HB3	1.83	0.59
2:HP1:907:GLY:O	2:HP1:910:ALA:HB3	2.02	0.59
1:DP1:182:LEU:HD11	1:EP1:243:LEU:HD12	1.84	0.59
2:GP1:612:CYS:HB3	2:GP1:626:ARG:HB2	1.85	0.59
2:HP1:391:GLU:HG3	2:HP1:393:GLN:H	1.67	0.59
1:DP1:352:SER:HA	1:DP1:355:LEU:HD23	1.84	0.59
2:FP1:504:PRO:HG3	2:FP1:513:TYR:HB2	1.85	0.59
2:GP1:785:GLY:HA2	2:GP1:788:HIS:CD2	2.37	0.59
1:CP1:352:SER:HA	1:CP1:355:LEU:HD12	1.85	0.59
2:JP1:188:GLN:O	2:JP1:192:LEU:HD13	2.03	0.59
2:FP1:287:ILE:HD12	2:FP1:287:ILE:H	1.68	0.59
2:JP1:287:ILE:HD12	2:JP1:287:ILE:H	1.67	0.59
2:FP1:675:VAL:O	2:FP1:679:THR:HG23	2.03	0.59
2:HP1:566:THR:HG23	2:HP1:569:GLY:H	1.67	0.59
2:JP1:289:ALA:HA	2:JP1:312:SER:HB2	1.84	0.59
2:HP1:150:LEU:HD12	2:HP1:474:LEU:HG	1.85	0.59
2:JP1:136:VAL:HG22	2:JP1:461:TRP:HE1	1.68	0.59
1:BP1:430:ARG:NH2	1:CP1:425:GLN:HB3	2.18	0.58
2:GP1:182:LEU:HD23	2:GP1:571:VAL:HG21	1.85	0.58
2:IP1:38:LEU:HD21	2:IP1:129:MET:HE1	1.85	0.58
2:IP1:77:MET:O	2:IP1:81:MET:HG3	2.02	0.58
2:FP1:722:ILE:O	2:FP1:725:PHE:HB3	2.04	0.58
2:JP1:556:ARG:HD2	2:JP1:576:MET:HG2	1.85	0.58
2:HP1:938:ASP:O	2:HP1:941:LEU:HB2	2.04	0.58
1:DP1:191:MET:HG2	1:DP1:198:TRP:HA	1.86	0.58
2:FP1:403:PRO:HB3	2:JP1:268:LYS:HB3	1.84	0.58
2:FP1:588:LEU:HD13	2:FP1:661:MET:HG3	1.86	0.58
2:FP1:627:MET:HG2	2:FP1:628:MET:HE2	1.84	0.58
2:GP1:147:LEU:HB2	2:GP1:453:ILE:HG23	1.84	0.58
2:JP1:296:SER:HA	2:JP1:302:VAL:HG13	1.86	0.58
3:KP1:38:LYS:HE2	3:KP1:38:LYS:HA	1.86	0.58
2:IP1:367:LYS:HD3	2:IP1:367:LYS:N	2.19	0.58
1:EP1:142:ILE:HA	1:EP1:210:VAL:HG23	1.86	0.58
2:JP1:824:ALA:O	2:JP1:827:TYR:HB2	2.03	0.58
2:GP1:814:LEU:HD23	2:GP1:937:PRO:HA	1.87	0.57
3:OP1:30:ILE:O	3:OP1:34:ILE:HG22	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:242:LYS:HG2	2:GP1:261:LEU:HD23	1.86	0.57
1:CP1:105:LYS:HZ3	1:DP1:367:ASN:HA	1.67	0.57
1:AP1:141:LEU:HD23	1:AP1:213:ASN:HB3	1.86	0.57
1:AP1:94:MET:HE3	1:BP1:240:ILE:HB	1.85	0.57
1:BP1:427:TYR:HD1	1:BP1:430:ARG:HH12	1.51	0.57
2:GP1:528:ILE:HD11	2:GP1:538:PRO:HD3	1.86	0.57
2:IP1:77:MET:HE1	3:NP1:32:VAL:HG11	1.86	0.57
1:BP1:136:ILE:HG23	1:BP1:277:LEU:HD22	1.87	0.57
2:GP1:489:THR:HG23	2:GP1:491:LEU:H	1.70	0.57
2:JP1:512:PRO:HG2	2:JP1:513:TYR:CE1	2.39	0.57
2:JP1:702:THR:O	2:JP1:706:THR:HG23	2.05	0.57
2:GP1:785:GLY:HA2	2:GP1:788:HIS:NE2	2.19	0.57
2:HP1:757:PRO:HG3	2:HP1:930:PHE:CE1	2.40	0.57
2:IP1:402:VAL:HG13	2:IP1:405:SER:HB3	1.86	0.57
1:AP1:353:LYS:HG2	1:AP1:371:GLN:HE21	1.69	0.57
2:FP1:247:THR:HG22	2:FP1:256:PRO:HD2	1.87	0.57
2:HP1:151:ASN:HB3	2:HP1:152:ARG:HH11	1.69	0.56
2:JP1:668:LYS:HA	2:JP1:911:PHE:HE2	1.70	0.56
2:JP1:793:GLU:HG3	2:JP1:795:PHE:H	1.68	0.56
2:GP1:122:CYS:H	2:GP1:125:GLN:HG3	1.71	0.56
2:IP1:766:PHE:CZ	2:JP1:829:GLY:HA2	2.40	0.56
1:DP1:385:ASP:H	1:DP1:398:GLN:HE22	1.52	0.56
2:GP1:770:ILE:HA	2:GP1:773:ILE:HD12	1.87	0.56
2:IP1:766:PHE:CD1	2:JP1:925:ILE:HD11	2.40	0.56
2:IP1:940:VAL:O	2:IP1:944:ILE:HD12	2.05	0.56
2:FP1:807:ASN:HB2	2:FP1:941:LEU:HD11	1.87	0.56
2:HP1:287:ILE:HG22	2:HP1:289:ALA:H	1.71	0.56
2:HP1:766:PHE:HZ	2:IP1:829:GLY:HA2	1.71	0.56
1:BP1:236:ASN:O	1:BP1:240:ILE:HG13	2.05	0.56
2:FP1:33:LEU:HA	2:FP1:36:VAL:HB	1.86	0.56
2:FP1:148:SER:O	2:FP1:152:ARG:HD3	2.05	0.56
2:FP1:660:LEU:HD23	2:FP1:661:MET:H	1.70	0.56
2:HP1:528:ILE:HD11	2:HP1:538:PRO:HD3	1.87	0.56
2:GP1:690:ALA:O	2:GP1:694:THR:HG23	2.06	0.56
2:IP1:837:PHE:O	2:IP1:841:ILE:HG22	2.06	0.56
1:EP1:94:MET:HB2	1:EP1:98:LEU:HD23	1.88	0.56
2:HP1:383:LYS:HA	2:HP1:396:CYS:HA	1.88	0.56
2:JP1:222:MET:HE1	2:JP1:519:TRP:HA	1.87	0.56
2:FP1:685:PRO:HB2	2:FP1:830:VAL:HG11	1.88	0.56
2:IP1:136:VAL:HG13	2:IP1:461:TRP:HE1	1.71	0.56
2:FP1:555:GLN:HE22	2:FP1:588:LEU:HD12	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:684:ASN:HD22	2:FP1:687:VAL:HG23	1.71	0.56
2:GP1:600:THR:HB	2:GP1:645:LEU:HD22	1.87	0.56
1:AP1:426:MET:HE1	1:BP1:422:ILE:HG23	1.88	0.56
2:FP1:640:VAL:HG22	2:GP1:605:MET:HE1	1.88	0.56
2:IP1:434:LEU:HD13	2:IP1:437:ILE:HD12	1.88	0.56
1:AP1:123:GLN:HE22	1:AP1:256:THR:HG21	1.70	0.55
1:DP1:263:GLN:H	1:DP1:268:THR:HG21	1.71	0.55
1:EP1:208:ASN:O	1:EP1:212:GLN:HG2	2.06	0.55
2:HP1:593:LEU:HD21	2:HP1:905:TRP:HB3	1.87	0.55
2:IP1:690:ALA:O	2:IP1:694:THR:HG23	2.05	0.55
2:JP1:590:PHE:HE2	2:JP1:664:LEU:HD13	1.70	0.55
1:CP1:208:ASN:O	1:CP1:212:GLN:HG2	2.06	0.55
2:HP1:630:ASP:HA	2:HP1:634:ASN:HB2	1.87	0.55
3:NP1:14:ASN:HB3	3:NP1:17:THR:HG23	1.88	0.55
1:AP1:285:ALA:HB1	1:EP1:449:LYS:HE3	1.89	0.55
2:GP1:724:ILE:O	2:GP1:728:ILE:HG22	2.06	0.55
2:HP1:35:VAL:HA	2:HP1:38:LEU:HB2	1.87	0.55
2:HP1:331:SER:HA	2:HP1:334:ILE:HD12	1.87	0.55
2:FP1:548:PRO:HD3	2:FP1:568:TYR:CD1	2.41	0.55
2:JP1:844:ILE:HA	2:JP1:902:TYR:HE2	1.72	0.55
1:CP1:142:ILE:HD11	1:CP1:267:LEU:HD22	1.88	0.55
1:BP1:426:MET:HE1	1:CP1:422:ILE:HG23	1.88	0.55
1:EP1:342:VAL:HG21	1:EP1:442:ILE:HG13	1.89	0.55
2:JP1:667:MET:HE2	2:JP1:912:PHE:CD1	2.41	0.55
1:DP1:193:ASN:HD21	2:JP1:216:GLY:HA3	1.71	0.55
2:FP1:821:ALA:HA	2:JP1:57:MET:HE1	1.88	0.55
2:GP1:773:ILE:HD11	2:HP1:825:LEU:HD21	1.88	0.55
2:IP1:618:LEU:HD23	2:JP1:618:LEU:HB2	1.89	0.55
2:GP1:179:LYS:HA	2:GP1:550:LEU:HD23	1.89	0.55
2:JP1:807:ASN:ND2	2:JP1:941:LEU:HG	2.22	0.55
2:GP1:671:PHE:CG	2:GP1:915:ILE:HD11	2.42	0.55
2:IP1:788:HIS:HB3	2:IP1:790:GLU:HG3	1.89	0.54
2:IP1:911:PHE:O	2:IP1:915:ILE:HG22	2.07	0.54
2:JP1:392:TYR:HE2	2:JP1:585:ILE:HG21	1.71	0.54
1:BP1:139:ASN:HB2	1:BP1:281:ARG:NH1	2.22	0.54
2:HP1:180:GLY:HA3	2:HP1:491:LEU:HD23	1.88	0.54
2:HP1:931:THR:HG23	2:HP1:935:HIS:NE2	2.22	0.54
1:EP1:123:GLN:HE22	1:EP1:256:THR:HG21	1.71	0.54
2:IP1:768:TRP:HB2	2:IP1:815:MET:HE1	1.89	0.54
2:FP1:648:PHE:CZ	2:FP1:652:ILE:HD11	2.42	0.54
2:HP1:814:LEU:HD13	2:HP1:937:PRO:HA	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:822:ALA:HB1	2:HP1:930:PHE:HD2	1.72	0.54
1:AP1:93:ALA:HB3	1:AP1:172:ASP:HB2	1.90	0.54
1:CP1:129:SER:H	1:CP1:137:THR:HG21	1.72	0.54
2:HP1:738:TRP:CD1	2:HP1:912:PHE:CZ	2.96	0.54
2:IP1:162:ASP:HB3	2:IP1:165:LYS:HB2	1.90	0.54
2:IP1:932:LEU:HB3	2:IP1:936:LEU:HD23	1.90	0.54
2:GP1:532:SER:HA	2:GP1:537:VAL:H	1.71	0.54
2:HP1:212:PRO:HA	2:HP1:215:GLY:H	1.73	0.54
3:KP1:23:PHE:O	3:KP1:27:LEU:HG	2.07	0.54
2:HP1:745:ILE:HG12	2:HP1:919:THR:HG21	1.89	0.54
2:IP1:287:ILE:HG13	2:IP1:332:ARG:HH12	1.73	0.54
1:AP1:206:TYR:O	1:AP1:210:VAL:HG12	2.08	0.54
1:BP1:185:PRO:HG3	1:BP1:204:LEU:HD22	1.88	0.54
2:IP1:837:PHE:HZ	2:IP1:917:ILE:HG23	1.72	0.54
2:JP1:147:LEU:HD22	2:JP1:453:ILE:HG23	1.90	0.54
2:FP1:60:MET:CE	2:GP1:817:ILE:HG12	2.36	0.54
2:FP1:182:LEU:HD23	2:FP1:571:VAL:HG21	1.89	0.54
2:FP1:556:ARG:HD2	2:FP1:576:MET:HG2	1.90	0.54
2:JP1:554:PRO:HB3	2:JP1:587:PRO:HA	1.89	0.54
1:BP1:280:ILE:HG23	1:BP1:347:LEU:HD23	1.90	0.53
2:GP1:594:ILE:HG21	2:GP1:660:LEU:HD22	1.89	0.53
2:IP1:73:GLY:C	2:IP1:77:MET:HE2	2.32	0.53
2:JP1:187:GLY:HA2	2:JP1:279:CYS:HB3	1.90	0.53
3:OP1:16:ARG:O	3:OP1:20:ILE:HG22	2.08	0.53
3:OP1:38:LYS:HE2	3:OP1:38:LYS:HA	1.89	0.53
2:HP1:822:ALA:HB1	2:HP1:930:PHE:CD2	2.43	0.53
2:JP1:450:ARG:HG2	2:JP1:453:ILE:HD11	1.90	0.53
1:BP1:177:ALA:O	1:BP1:181:ILE:HG12	2.08	0.53
1:DP1:298:TYR:HD1	1:DP1:298:TYR:O	1.91	0.53
2:GP1:648:PHE:HA	2:GP1:651:MET:HB2	1.90	0.53
2:IP1:669:ASP:HA	2:IP1:672:ILE:HG12	1.90	0.53
2:JP1:532:SER:HA	2:JP1:537:VAL:H	1.74	0.53
1:BP1:182:LEU:HD11	1:CP1:243:LEU:HD12	1.89	0.53
2:FP1:45:VAL:HG21	2:FP1:129:MET:HG2	1.90	0.53
2:FP1:548:PRO:HD3	2:FP1:568:TYR:HD1	1.74	0.53
2:GP1:667:MET:HE2	2:GP1:912:PHE:CD2	2.44	0.53
2:HP1:725:PHE:CD1	2:IP1:729:MET:HE1	2.43	0.53
2:HP1:725:PHE:CE1	2:IP1:729:MET:HE1	2.43	0.53
3:OP1:9:LYS:HD3	3:OP1:9:LYS:N	2.23	0.53
2:GP1:261:LEU:HB2	2:GP1:284:TRP:HZ3	1.71	0.53
2:GP1:841:ILE:HD12	2:GP1:844:ILE:HB	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:721:GLY:O	2:IP1:724:ILE:HG22	2.09	0.53
2:FP1:617:ILE:HG22	2:FP1:618:LEU:H	1.73	0.53
2:HP1:725:PHE:CD1	2:HP1:725:PHE:C	2.87	0.53
3:KP1:16:ARG:NH1	3:KP1:20:ILE:HD13	2.24	0.53
1:BP1:141:LEU:HB3	1:BP1:213:ASN:HB3	1.91	0.53
2:HP1:732:MET:O	2:HP1:736:MET:HB2	2.09	0.53
2:IP1:151:ASN:HB2	2:IP1:453:ILE:HD13	1.89	0.53
2:IP1:668:LYS:O	2:IP1:672:ILE:HG23	2.09	0.53
2:FP1:618:LEU:HD23	2:GP1:618:LEU:HB2	1.91	0.53
2:FP1:756:LEU:HA	2:FP1:759:MET:HG3	1.91	0.53
2:IP1:929:ALA:O	2:IP1:932:LEU:HD12	2.09	0.53
1:AP1:90:PRO:HG2	1:BP1:246:ASN:HD21	1.73	0.53
1:CP1:421:GLU:O	1:CP1:425:GLN:HG3	2.09	0.53
2:FP1:630:ASP:HA	2:FP1:634:ASN:HB2	1.89	0.53
2:IP1:164:THR:HG21	2:IP1:583:PRO:HA	1.90	0.53
2:IP1:588:LEU:HD13	2:IP1:660:LEU:HD11	1.90	0.53
2:JP1:94:LEU:HD13	2:JP1:98:TRP:HD1	1.74	0.53
2:JP1:347:ALA:O	2:JP1:351:VAL:HG12	2.08	0.53
2:GP1:221:GLU:CD	2:GP1:221:GLU:H	2.17	0.52
2:GP1:652:ILE:O	2:GP1:656:VAL:HG23	2.09	0.52
2:HP1:920:SER:O	2:HP1:924:ILE:HD12	2.09	0.52
2:HP1:640:VAL:HG22	2:IP1:605:MET:HE1	1.91	0.52
2:IP1:148:SER:O	2:IP1:152:ARG:HD3	2.09	0.52
2:IP1:685:PRO:HB2	2:IP1:830:VAL:HG11	1.92	0.52
2:JP1:33:LEU:HD12	2:JP1:37:PHE:CZ	2.43	0.52
3:OP1:23:PHE:O	3:OP1:27:LEU:HD22	2.09	0.52
2:FP1:722:ILE:HG23	2:FP1:723:PHE:HD1	1.74	0.52
2:GP1:176:GLY:HA3	2:GP1:492:ASP:HB2	1.90	0.52
2:HP1:673:VAL:O	2:HP1:677:THR:HG22	2.10	0.52
2:IP1:213:PRO:O	2:IP1:218:PRO:HB3	2.09	0.52
2:IP1:804:ILE:O	2:IP1:808:VAL:HG22	2.09	0.52
2:JP1:757:PRO:HB3	2:JP1:930:PHE:HE2	1.74	0.52
3:NP1:18:ARG:O	3:NP1:22:ILE:HD13	2.10	0.52
2:FP1:663:PRO:HG3	2:FP1:703:LEU:HD11	1.91	0.52
2:IP1:706:THR:O	2:IP1:710:MET:HG2	2.09	0.52
2:IP1:713:VAL:HG13	2:JP1:723:PHE:CD1	2.44	0.52
1:AP1:305:ALA:HA	1:AP1:319:GLN:HG2	1.91	0.52
1:BP1:328:SER:HA	1:CP1:211:MET:HE2	1.92	0.52
1:CP1:42:TYR:HA	1:CP1:45:ASN:ND2	2.23	0.52
2:FP1:723:PHE:CZ	2:JP1:724:ILE:HG13	2.44	0.52
1:AP1:48:LYS:HG2	1:EP1:64:PRO:HG3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:819:TYR:O	2:FP1:823:ILE:HG22	2.10	0.52
1:AP1:280:ILE:HD11	1:AP1:351:LEU:HB2	1.90	0.52
2:FP1:124:MET:HG3	2:FP1:779:ALA:HB1	1.91	0.52
2:FP1:732:MET:O	2:FP1:736:MET:HB2	2.10	0.52
2:GP1:757:PRO:HG3	2:GP1:930:PHE:CZ	2.45	0.52
2:FP1:725:PHE:CD2	2:GP1:729:MET:HE1	2.44	0.52
2:HP1:122:CYS:H	2:HP1:125:GLN:HG3	1.74	0.52
2:HP1:766:PHE:CZ	2:IP1:829:GLY:HA2	2.45	0.52
2:JP1:304:VAL:HB	2:JP1:318:LEU:H	1.74	0.52
2:JP1:237:VAL:HG13	2:JP1:261:LEU:HD21	1.90	0.52
3:KP1:15:THR:HG22	3:KP1:18:ARG:HH22	1.75	0.52
2:HP1:747:PHE:HA	2:HP1:751:TYR:HD2	1.74	0.52
1:DP1:254:MET:HB3	1:DP1:273:ALA:HB2	1.93	0.51
2:HP1:275:LEU:O	2:HP1:278:ILE:HG22	2.10	0.51
2:HP1:905:TRP:HA	2:HP1:908:VAL:HG13	1.92	0.51
2:JP1:175:SER:HB2	2:JP1:488:GLY:H	1.74	0.51
1:CP1:55:THR:HA	1:DP1:42:TYR:CE1	2.46	0.51
2:GP1:468:PHE:CD1	2:GP1:757:PRO:HG2	2.44	0.51
2:GP1:605:MET:HE2	2:GP1:637:PHE:HE2	1.74	0.51
2:HP1:841:ILE:HD12	2:HP1:844:ILE:HB	1.92	0.51
2:IP1:73:GLY:O	2:IP1:77:MET:HE2	2.11	0.51
2:JP1:183:THR:HG23	2:JP1:496:PHE:HB2	1.92	0.51
2:FP1:77:MET:HG2	3:LP1:28:LEU:HD11	1.91	0.51
2:HP1:33:LEU:HD23	2:HP1:462:ILE:HD11	1.91	0.51
1:AP1:346:ASN:OD1	1:EP1:437:LEU:HD11	2.09	0.51
2:GP1:41:LEU:HD22	2:GP1:42:PHE:CD2	2.45	0.51
2:IP1:182:LEU:HD23	2:IP1:571:VAL:HG21	1.91	0.51
2:IP1:468:PHE:CE1	2:IP1:930:PHE:HZ	2.28	0.51
2:IP1:74:ILE:HA	2:IP1:77:MET:HG2	1.91	0.51
2:JP1:318:LEU:HD11	2:JP1:439:GLN:HB2	1.91	0.51
1:CP1:430:ARG:HH21	1:DP1:425:GLN:HB3	1.76	0.51
2:FP1:718:PRO:HB3	2:GP1:719:LEU:HD11	1.92	0.51
2:GP1:107:SER:HA	2:GP1:787:THR:HG22	1.91	0.51
2:GP1:290:LEU:HB2	2:GP1:329:ARG:NH1	2.26	0.51
2:IP1:673:VAL:O	2:IP1:677:THR:HG22	2.11	0.51
1:AP1:182:LEU:HD11	1:BP1:243:LEU:HD12	1.92	0.51
2:FP1:745:ILE:HD13	2:FP1:915:ILE:HG13	1.93	0.51
2:GP1:656:VAL:HG12	2:GP1:660:LEU:CD2	2.41	0.51
2:GP1:909:TYR:O	2:GP1:912:PHE:HB2	2.11	0.51
2:IP1:944:ILE:HD12	2:IP1:944:ILE:H	1.76	0.51
1:AP1:451:ALA:HB1	2:HP1:619:PHE:HE2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:78:TYR:HA	2:GP1:81:MET:SD	2.51	0.51
2:GP1:179:LYS:HE2	2:GP1:547:GLN:HE22	1.75	0.51
2:GP1:192:LEU:HB2	2:GP1:351:VAL:HG21	1.93	0.51
2:GP1:373:ILE:HG13	2:GP1:533:LEU:HD23	1.92	0.51
2:HP1:713:VAL:O	2:HP1:716:LEU:HD23	2.11	0.51
2:IP1:728:ILE:HD11	2:JP1:730:MET:SD	2.51	0.51
3:OP1:15:THR:HG22	3:OP1:18:ARG:HH22	1.76	0.51
1:AP1:136:ILE:HG23	1:AP1:277:LEU:HD22	1.93	0.51
2:GP1:566:THR:HG23	2:GP1:569:GLY:H	1.76	0.51
2:GP1:670:ILE:HD13	2:GP1:695:MET:HB3	1.93	0.51
2:HP1:222:MET:HE1	2:HP1:519:TRP:HA	1.91	0.51
2:HP1:669:ASP:O	2:HP1:673:VAL:HG13	2.10	0.51
2:IP1:501:LEU:HB3	2:IP1:527:LEU:HD23	1.93	0.51
1:BP1:230:PHE:CD1	1:BP1:230:PHE:C	2.89	0.50
1:DP1:142:ILE:HG22	1:DP1:210:VAL:HG23	1.94	0.50
2:FP1:69:LEU:HD21	3:LP1:31:ALA:HB1	1.94	0.50
2:FP1:150:LEU:HD12	2:FP1:474:LEU:HD23	1.93	0.50
2:FP1:648:PHE:HB2	2:FP1:717:ILE:HD12	1.92	0.50
2:IP1:60:MET:SD	2:JP1:817:ILE:HD13	2.51	0.50
2:IP1:338:GLN:HA	2:IP1:341:VAL:HG22	1.91	0.50
2:JP1:182:LEU:HD23	2:JP1:571:VAL:HG21	1.92	0.50
3:OP1:15:THR:HA	3:OP1:18:ARG:CZ	2.41	0.50
2:FP1:132:ILE:HG12	2:FP1:772:VAL:HG23	1.93	0.50
2:FP1:450:ARG:O	2:FP1:453:ILE:HD12	2.11	0.50
2:JP1:470:ASP:O	2:JP1:473:LYS:HG2	2.11	0.50
1:BP1:206:TYR:O	1:BP1:210:VAL:HG12	2.11	0.50
2:GP1:634:ASN:O	2:GP1:638:ARG:HB3	2.12	0.50
2:HP1:706:THR:O	2:HP1:710:MET:HG2	2.11	0.50
2:HP1:922:TYR:O	2:HP1:925:ILE:HB	2.12	0.50
1:AP1:208:ASN:O	1:AP1:212:GLN:HG2	2.11	0.50
1:CP1:182:LEU:HD11	1:DP1:243:LEU:HD12	1.92	0.50
2:FP1:643:PHE:O	2:FP1:647:ILE:HG22	2.12	0.50
2:IP1:330:LEU:HB3	2:IP1:333:ALA:HB3	1.93	0.50
2:IP1:814:LEU:HD13	2:IP1:937:PRO:HA	1.93	0.50
1:AP1:54:ILE:HG23	1:BP1:45:ASN:OD1	2.12	0.50
1:BP1:174:VAL:HG11	1:BP1:345:SER:HB2	1.94	0.50
2:GP1:630:ASP:HA	2:GP1:634:ASN:HB2	1.93	0.50
2:IP1:468:PHE:HE1	2:IP1:930:PHE:HZ	1.59	0.50
2:GP1:722:ILE:O	2:GP1:725:PHE:HB3	2.11	0.50
2:IP1:370:PHE:CD1	2:IP1:377:GLN:HB3	2.46	0.50
2:IP1:662:ILE:HD13	2:IP1:703:LEU:HD12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JP1:113:LEU:HA	2:JP1:123:MET:HB2	1.93	0.50
2:JP1:392:TYR:CE2	2:JP1:585:ILE:HG21	2.46	0.50
2:JP1:661:MET:O	2:JP1:665:GLN:HB2	2.12	0.50
1:AP1:42:TYR:CE1	1:EP1:55:THR:HA	2.47	0.50
2:FP1:841:ILE:HD12	2:FP1:844:ILE:HB	1.93	0.50
2:GP1:77:MET:HG3	2:GP1:81:MET:HE3	1.93	0.50
2:IP1:167:LEU:HD12	2:IP1:585:ILE:HD11	1.94	0.50
2:IP1:347:ALA:O	2:IP1:351:VAL:HG22	2.11	0.50
2:IP1:655:ILE:HD11	2:IP1:710:MET:HB2	1.92	0.50
3:LP1:7:ASN:O	3:LP1:11:LEU:HG	2.12	0.50
1:AP1:142:ILE:HA	1:AP1:210:VAL:HG23	1.93	0.50
1:BP1:55:THR:HA	1:CP1:42:TYR:CE2	2.47	0.50
1:BP1:347:LEU:HA	1:BP1:350:ILE:HG22	1.91	0.50
2:GP1:370:PHE:HB2	2:GP1:410:THR:HG21	1.93	0.50
1:AP1:179:PHE:HB2	1:BP1:240:ILE:HD13	1.93	0.49
1:DP1:104:ASP:HA	1:DP1:109:ASN:HD22	1.75	0.49
2:HP1:49:LEU:HG	2:HP1:51:GLY:H	1.77	0.49
2:HP1:468:PHE:CD1	2:HP1:757:PRO:HG2	2.47	0.49
2:HP1:939:LYS:HE3	2:HP1:939:LYS:HA	1.94	0.49
1:EP1:280:ILE:HD11	1:EP1:351:LEU:HB2	1.94	0.49
2:GP1:103:ILE:HG22	2:GP1:106:ARG:HH21	1.76	0.49
2:HP1:147:LEU:HB2	2:HP1:453:ILE:HG23	1.94	0.49
1:AP1:35:ASN:O	1:AP1:39:LEU:HD23	2.12	0.49
2:FP1:594:ILE:HB	2:FP1:660:LEU:HD12	1.95	0.49
2:HP1:738:TRP:HD1	2:HP1:912:PHE:CZ	2.29	0.49
2:IP1:268:LYS:HB3	2:JP1:403:PRO:HB3	1.95	0.49
2:JP1:338:GLN:HA	2:JP1:341:VAL:HG12	1.94	0.49
1:AP1:434:GLU:OE2	1:BP1:350:ILE:HD11	2.12	0.49
1:CP1:94:MET:HG3	1:DP1:241:SER:HB3	1.94	0.49
1:DP1:206:TYR:O	1:DP1:210:VAL:HG12	2.12	0.49
2:FP1:183:THR:HG23	2:FP1:496:PHE:HB2	1.94	0.49
2:GP1:381:PRO:HD2	2:GP1:573:ASN:ND2	2.27	0.49
2:HP1:593:LEU:HD11	2:HP1:905:TRP:HB3	1.93	0.49
2:IP1:692:MET:HA	2:IP1:695:MET:HE3	1.94	0.49
2:IP1:718:PRO:O	2:IP1:719:LEU:HB2	2.11	0.49
3:KP1:18:ARG:O	3:KP1:22:ILE:HD13	2.12	0.49
1:CP1:172:ASP:HB3	1:CP1:175:SER:OG	2.12	0.49
1:DP1:342:VAL:HG21	1:DP1:442:ILE:HG13	1.94	0.49
1:EP1:269:ALA:HB1	1:EP1:274:GLN:HB3	1.93	0.49
2:FP1:124:MET:HG2	2:FP1:783:ALA:HB2	1.94	0.49
2:GP1:666:GLY:O	2:GP1:670:ILE:HG13	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:110:GLY:HA3	2:IP1:787:THR:HG22	1.94	0.49
3:MP1:36:PHE:HA	3:MP1:39:ILE:HD11	1.95	0.49
2:GP1:713:VAL:HG22	2:HP1:727:LEU:HB2	1.94	0.49
2:JP1:103:ILE:HG22	2:JP1:104:PRO:HD3	1.93	0.49
3:KP1:28:LEU:O	3:KP1:32:VAL:HG13	2.11	0.49
2:GP1:223:ASN:O	2:GP1:227:ARG:HG2	2.13	0.49
2:GP1:766:PHE:CZ	2:HP1:925:ILE:HG23	2.48	0.49
2:HP1:84:THR:HA	2:HP1:87:THR:HG22	1.94	0.49
2:IP1:663:PRO:HG3	2:IP1:738:TRP:CH2	2.48	0.49
1:BP1:280:ILE:HD11	1:BP1:351:LEU:HB2	1.93	0.49
1:CP1:444:LEU:HD13	1:DP1:443:MET:HB2	1.95	0.49
2:GP1:136:VAL:HG22	2:GP1:461:TRP:HE1	1.78	0.49
2:JP1:259:PHE:HE2	2:JP1:286:ASN:HB2	1.77	0.49
1:AP1:230:PHE:C	1:AP1:230:PHE:CD1	2.91	0.49
2:FP1:605:MET:HE1	2:JP1:640:VAL:HG22	1.95	0.49
2:HP1:664:LEU:O	2:HP1:668:LYS:HB2	2.13	0.49
1:CP1:86:LEU:HD21	1:DP1:376:PHE:CZ	2.48	0.48
1:DP1:455:ALA:HB1	1:EP1:293:PRO:HA	1.95	0.48
1:EP1:382:ARG:HB3	1:EP1:399:TRP:CD2	2.48	0.48
2:GP1:61:PHE:CE1	2:GP1:776:MET:HG3	2.48	0.48
2:JP1:247:THR:HG22	2:JP1:256:PRO:HD2	1.94	0.48
2:JP1:540:LEU:HD23	2:JP1:562:PRO:HB2	1.94	0.48
1:AP1:415:ILE:HG23	1:EP1:419:LEU:HD12	1.96	0.48
2:FP1:78:TYR:HA	2:FP1:81:MET:CE	2.36	0.48
2:FP1:111:LEU:HD13	3:LP1:31:ALA:HB2	1.96	0.48
2:GP1:57:MET:HE1	2:HP1:821:ALA:HA	1.93	0.48
2:IP1:662:ILE:HB	2:IP1:703:LEU:HD11	1.93	0.48
2:FP1:920:SER:O	2:FP1:924:ILE:HD12	2.13	0.48
2:HP1:111:LEU:HD13	3:OP1:31:ALA:HB2	1.95	0.48
2:HP1:176:GLY:HA3	2:HP1:492:ASP:HB2	1.95	0.48
1:CP1:119:THR:HG21	1:CP1:352:SER:HB2	1.96	0.48
2:JP1:184:ILE:HG13	2:JP1:263:MET:HE1	1.96	0.48
1:DP1:141:LEU:HD23	1:DP1:213:ASN:HB3	1.94	0.48
1:EP1:68:LEU:HD11	1:EP1:417:ILE:HD11	1.96	0.48
2:FP1:113:LEU:HD12	2:FP1:124:MET:HE2	1.96	0.48
2:FP1:769:LEU:HA	2:FP1:772:VAL:HG12	1.95	0.48
2:GP1:837:PHE:O	2:GP1:841:ILE:HG22	2.13	0.48
2:JP1:391:GLU:HG3	2:JP1:393:GLN:H	1.79	0.48
1:AP1:308:LYS:HG2	1:AP1:309:PRO:HD2	1.95	0.48
1:AP1:419:LEU:HD12	1:BP1:415:ILE:HG23	1.96	0.48
1:BP1:86:LEU:HD21	1:BP1:112:ILE:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:BP1:292:LEU:HD13	1:CP1:230:PHE:HE2	1.78	0.48
1:BP1:382:ARG:HB3	1:BP1:399:TRP:CE3	2.49	0.48
2:GP1:147:LEU:HB2	2:GP1:453:ILE:CG2	2.43	0.48
2:HP1:132:ILE:HG13	2:HP1:772:VAL:HG23	1.95	0.48
1:AP1:205:MET:HG3	1:AP1:209:LEU:HG	1.94	0.48
2:HP1:589:THR:HG22	2:HP1:664:LEU:HD21	1.96	0.48
2:JP1:461:TRP:CZ2	2:JP1:812:PRO:HB3	2.48	0.48
2:JP1:647:ILE:HG22	2:JP1:717:ILE:HG12	1.95	0.48
1:BP1:419:LEU:HD12	1:CP1:415:ILE:HG23	1.96	0.48
1:CP1:142:ILE:HD12	1:CP1:281:ARG:HD2	1.96	0.48
2:FP1:766:PHE:CE2	2:GP1:925:ILE:HD12	2.49	0.48
2:GP1:468:PHE:CG	2:GP1:757:PRO:HG2	2.49	0.48
2:GP1:612:CYS:HB2	2:GP1:623:CYS:HB2	1.61	0.48
2:HP1:936:LEU:O	2:HP1:940:VAL:HG23	2.14	0.48
2:IP1:450:ARG:HD3	2:IP1:474:LEU:HD11	1.95	0.48
2:FP1:723:PHE:HZ	2:JP1:724:ILE:HG13	1.79	0.48
2:GP1:663:PRO:HG3	2:GP1:703:LEU:HD11	1.96	0.48
2:HP1:338:GLN:HA	2:HP1:341:VAL:HG12	1.95	0.48
2:IP1:129:MET:O	2:IP1:132:ILE:HG13	2.13	0.48
2:JP1:799:GLU:HA	2:JP1:802:ILE:HD12	1.96	0.48
1:AP1:376:PHE:CZ	1:EP1:86:LEU:HD21	2.49	0.48
1:EP1:207:GLN:O	1:EP1:211:MET:HB2	2.13	0.48
2:FP1:434:LEU:HA	2:FP1:437:ILE:HG22	1.95	0.48
2:FP1:707:LEU:HD13	2:FP1:735:LEU:HD21	1.95	0.48
2:GP1:738:TRP:O	2:GP1:742:MET:HG3	2.14	0.48
2:HP1:165:LYS:HB3	2:HP1:485:PHE:HE2	1.78	0.48
2:IP1:136:VAL:HG13	2:IP1:461:TRP:NE1	2.28	0.48
2:IP1:354:ASP:HB3	2:IP1:357:PHE:HD1	1.78	0.48
2:IP1:732:MET:O	2:IP1:736:MET:HB2	2.13	0.48
1:BP1:90:PRO:HG3	1:BP1:349:TYR:HB2	1.95	0.47
1:BP1:421:GLU:O	1:BP1:425:GLN:HG3	2.14	0.47
1:EP1:206:TYR:O	1:EP1:210:VAL:HG12	2.14	0.47
2:GP1:114:LEU:HD21	2:GP1:783:ALA:HB3	1.96	0.47
2:GP1:179:LYS:HG2	2:GP1:492:ASP:HA	1.95	0.47
2:GP1:288:SER:HA	2:GP1:291:ASN:HB3	1.95	0.47
2:HP1:223:ASN:O	2:HP1:227:ARG:HG2	2.14	0.47
1:AP1:418:LEU:HD12	1:AP1:418:LEU:HA	1.77	0.47
1:EP1:126:SER:HB2	1:EP1:171:ASN:HA	1.96	0.47
2:HP1:526:LYS:HA	2:HP1:529:GLN:HE21	1.79	0.47
1:BP1:25:ALA:HB1	1:BP1:30:GLN:HE22	1.80	0.47
2:HP1:60:MET:HE3	2:IP1:817:ILE:CD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:732:MET:O	2:HP1:736:MET:CB	2.62	0.47
2:JP1:768:TRP:HB2	2:JP1:815:MET:HE1	1.96	0.47
2:FP1:829:GLY:HA2	2:JP1:766:PHE:CZ	2.50	0.47
2:FP1:940:VAL:O	2:FP1:944:ILE:HG13	2.14	0.47
2:HP1:188:GLN:O	2:HP1:191:MET:HB2	2.14	0.47
2:IP1:406:THR:O	2:IP1:406:THR:HG22	2.14	0.47
1:EP1:191:MET:HE3	1:EP1:195:GLN:HA	1.96	0.47
2:IP1:41:LEU:HD12	2:JP1:825:LEU:HA	1.96	0.47
3:LP1:5:LYS:O	3:LP1:9:LYS:HG3	2.15	0.47
1:CP1:443:MET:SD	1:DP1:443:MET:HE1	2.55	0.47
1:DP1:389:SER:HB3	1:DP1:394:GLN:OE1	2.15	0.47
2:IP1:189:ILE:HD11	2:IP1:350:MET:HB3	1.95	0.47
2:IP1:524:SER:O	2:IP1:528:ILE:HG22	2.14	0.47
2:JP1:58:GLY:HA2	2:JP1:121:TYR:CE1	2.50	0.47
2:JP1:77:MET:HE3	2:JP1:77:MET:HB2	1.77	0.47
2:JP1:103:ILE:HD11	2:JP1:789:PRO:HA	1.97	0.47
2:JP1:558:SER:HB3	2:JP1:576:MET:HE1	1.97	0.47
2:JP1:732:MET:HE2	2:JP1:732:MET:HA	1.95	0.47
1:BP1:437:LEU:HD11	1:CP1:346:ASN:HB3	1.96	0.47
2:FP1:94:LEU:HD21	3:LP1:21:ILE:HD11	1.96	0.47
2:GP1:608:GLN:HG2	2:GP1:633:TYR:CE2	2.50	0.47
2:HP1:79:THR:HA	2:HP1:82:VAL:HG22	1.97	0.47
2:HP1:713:VAL:HG22	2:IP1:727:LEU:HB2	1.96	0.47
2:JP1:462:ILE:HG13	2:JP1:463:MET:SD	2.55	0.47
2:JP1:833:LEU:HD21	2:JP1:921:MET:HB3	1.97	0.47
3:KP1:35:GLY:O	3:KP1:39:ILE:HG12	2.15	0.47
3:OP1:24:THR:HA	3:OP1:27:LEU:HD23	1.95	0.47
1:BP1:88:ALA:HB2	1:BP1:357:GLN:HE22	1.80	0.47
2:GP1:338:GLN:HA	2:GP1:341:VAL:HG12	1.97	0.47
2:HP1:82:VAL:HA	2:HP1:85:MET:HG3	1.96	0.47
2:HP1:106:ARG:HH11	2:HP1:789:PRO:HA	1.80	0.47
1:BP1:68:LEU:HD11	1:BP1:417:ILE:HD11	1.96	0.47
2:FP1:716:LEU:HD13	2:GP1:648:PHE:HE2	1.80	0.47
2:FP1:826:SER:O	2:FP1:830:VAL:HG23	2.15	0.47
2:GP1:213:PRO:HB2	2:GP1:222:MET:HE2	1.96	0.47
2:HP1:759:MET:HE3	2:IP1:917:ILE:HD11	1.96	0.47
1:AP1:243:LEU:HD12	1:EP1:182:LEU:HD11	1.97	0.46
2:GP1:117:LYS:HA	2:GP1:117:LYS:HD3	1.66	0.46
2:IP1:111:LEU:HD13	3:NP1:31:ALA:HB2	1.96	0.46
2:IP1:287:ILE:HG13	2:IP1:332:ARG:NH1	2.29	0.46
2:IP1:559:VAL:HG22	2:IP1:573:ASN:OD1	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JP1:72:GLY:O	2:JP1:76:ILE:HG12	2.14	0.46
2:JP1:189:ILE:HD11	2:JP1:533:LEU:HD21	1.96	0.46
2:JP1:747:PHE:HA	2:JP1:751:TYR:HD2	1.81	0.46
1:AP1:35:ASN:HB3	1:EP1:36:THR:HB	1.96	0.46
2:HP1:189:ILE:HD11	2:HP1:533:LEU:HD21	1.96	0.46
1:BP1:228:PRO:HB2	1:BP1:235:TYR:HB2	1.97	0.46
2:FP1:829:GLY:HA2	2:JP1:766:PHE:HZ	1.79	0.46
2:GP1:55:GLN:HB3	2:HP1:149:TYR:OH	2.15	0.46
2:HP1:778:ALA:HB2	2:IP1:943:TRP:CH2	2.50	0.46
2:IP1:336:ILE:HD11	2:IP1:491:LEU:HD21	1.97	0.46
2:IP1:826:SER:O	2:IP1:830:VAL:HG23	2.14	0.46
3:LP1:28:LEU:O	3:LP1:32:VAL:HG13	2.15	0.46
1:CP1:445:LEU:HD11	1:DP1:340:THR:HG23	1.97	0.46
2:JP1:69:LEU:HD21	2:JP1:114:LEU:HB3	1.97	0.46
1:AP1:430:ARG:NH2	1:BP1:425:GLN:HE21	2.14	0.46
2:FP1:338:GLN:HA	2:FP1:341:VAL:HG12	1.97	0.46
2:GP1:150:LEU:HD12	2:GP1:474:LEU:HG	1.97	0.46
2:HP1:196:LYS:NZ	2:HP1:357:PHE:HB3	2.31	0.46
3:LP1:4:LYS:H	3:LP1:4:LYS:HD3	1.79	0.46
1:BP1:30:GLN:CD	1:BP1:30:GLN:H	2.24	0.46
1:EP1:254:MET:HG3	1:EP1:355:LEU:HD23	1.97	0.46
2:FP1:55:GLN:HB3	2:GP1:149:TYR:OH	2.16	0.46
2:FP1:925:ILE:HG12	2:JP1:766:PHE:CE2	2.51	0.46
2:GP1:41:LEU:HB2	2:HP1:828:VAL:HG21	1.97	0.46
2:GP1:111:LEU:HD13	3:KP1:31:ALA:HB2	1.98	0.46
2:GP1:475:ASN:HB3	2:GP1:684:ASN:HD21	1.80	0.46
2:HP1:698:ASN:HA	2:IP1:905:TRP:CZ3	2.50	0.46
2:HP1:751:TYR:HB3	2:IP1:913:PHE:CD2	2.50	0.46
2:JP1:757:PRO:HB3	2:JP1:930:PHE:CE2	2.51	0.46
2:JP1:811:ARG:O	2:JP1:815:MET:HE3	2.14	0.46
1:BP1:94:MET:HE2	1:BP1:94:MET:HA	1.97	0.46
1:BP1:438:LEU:HD12	1:CP1:350:ILE:HD13	1.98	0.46
2:FP1:464:ALA:HB3	2:FP1:761:PHE:HE2	1.80	0.46
2:IP1:663:PRO:HB3	2:IP1:738:TRP:CD2	2.50	0.46
2:JP1:434:LEU:HA	2:JP1:437:ILE:HG22	1.97	0.46
2:JP1:608:GLN:HG3	2:JP1:633:TYR:HE2	1.80	0.46
2:JP1:659:PHE:CZ	2:JP1:707:LEU:HD11	2.51	0.46
3:KP1:23:PHE:CZ	3:KP1:27:LEU:HD21	2.51	0.46
1:CP1:419:LEU:HD12	1:DP1:415:ILE:HG23	1.98	0.46
1:DP1:419:LEU:HD12	1:EP1:415:ILE:HG23	1.98	0.46
2:FP1:189:ILE:HD11	2:FP1:350:MET:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:659:PHE:HA	2:HP1:662:ILE:HD11	1.97	0.46
2:IP1:667:MET:HE2	2:IP1:915:ILE:HD13	1.98	0.46
1:DP1:89:ILE:HD11	1:EP1:250:ALA:HA	1.98	0.46
2:FP1:357:PHE:HZ	2:FP1:530:ILE:HD13	1.80	0.46
2:IP1:77:MET:SD	3:NP1:28:LEU:HD21	2.56	0.46
1:DP1:421:GLU:O	1:DP1:425:GLN:HG3	2.16	0.46
2:FP1:741:THR:HG23	2:FP1:916:LEU:HD21	1.97	0.46
2:FP1:757:PRO:HG3	2:FP1:930:PHE:CE2	2.51	0.46
2:GP1:589:THR:H	2:GP1:665:GLN:HE22	1.64	0.46
2:GP1:944:ILE:HD12	2:GP1:944:ILE:H	1.81	0.46
2:HP1:212:PRO:HB3	2:HP1:215:GLY:O	2.16	0.46
2:IP1:708:LEU:HA	2:JP1:730:MET:HG2	1.97	0.46
2:IP1:713:VAL:HG13	2:JP1:723:PHE:HD1	1.81	0.46
2:IP1:819:TYR:CZ	2:IP1:823:ILE:HD11	2.51	0.46
2:JP1:28:PRO:HB2	2:JP1:32:ASP:OD2	2.16	0.46
2:JP1:184:ILE:O	2:JP1:188:GLN:HG3	2.16	0.46
1:CP1:242:GLN:O	1:CP1:279:PHE:HB2	2.16	0.45
1:DP1:382:ARG:HD3	1:DP1:399:TRP:CE2	2.51	0.45
1:DP1:401:LYS:HA	1:DP1:401:LYS:HD2	1.79	0.45
2:GP1:330:LEU:O	2:GP1:334:ILE:HG13	2.16	0.45
2:GP1:399:TRP:CE3	2:GP1:416:GLY:HA3	2.51	0.45
2:IP1:132:ILE:HG22	2:IP1:808:VAL:HB	1.98	0.45
2:JP1:49:LEU:HD23	2:JP1:129:MET:HE3	1.98	0.45
2:JP1:822:ALA:HB1	2:JP1:930:PHE:CD1	2.51	0.45
1:BP1:78:GLN:HB3	1:CP1:383:LEU:HD13	1.98	0.45
1:BP1:377:ASN:O	1:BP1:381:ARG:HB2	2.15	0.45
2:FP1:94:LEU:HD23	2:FP1:94:LEU:HA	1.81	0.45
2:IP1:132:ILE:HG21	2:IP1:772:VAL:HG23	1.97	0.45
2:JP1:377:GLN:OE1	2:JP1:402:VAL:HB	2.16	0.45
2:JP1:643:PHE:O	2:JP1:647:ILE:HG13	2.16	0.45
1:CP1:326:LEU:HD23	1:CP1:326:LEU:HA	1.82	0.45
2:FP1:201:GLN:O	2:FP1:205:TYR:HD1	1.99	0.45
2:FP1:697:ILE:HG13	2:FP1:751:TYR:HE2	1.81	0.45
2:FP1:708:LEU:HA	2:GP1:730:MET:HG2	1.97	0.45
2:GP1:55:GLN:NE2	2:GP1:58:GLY:HA3	2.32	0.45
2:GP1:247:THR:HG22	2:GP1:256:PRO:HD2	1.98	0.45
2:HP1:143:TRP:O	2:HP1:147:LEU:HG	2.16	0.45
2:IP1:247:THR:HG22	2:IP1:256:PRO:HD2	1.97	0.45
2:IP1:618:LEU:HD11	2:IP1:619:PHE:CE2	2.51	0.45
2:JP1:740:GLY:HA2	2:JP1:743:VAL:HG12	1.98	0.45
3:OP1:16:ARG:NH1	3:OP1:20:ILE:HG21	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:CP1:277:LEU:HD21	1:CP1:281:ARG:HH21	1.81	0.45
1:CP1:292:LEU:HD13	1:DP1:230:PHE:HE1	1.81	0.45
1:DP1:170:LEU:HD12	1:DP1:170:LEU:H	1.81	0.45
2:FP1:28:PRO:HB2	2:FP1:32:ASP:OD2	2.16	0.45
2:FP1:602:LEU:HD23	2:JP1:647:ILE:HD13	1.99	0.45
2:HP1:468:PHE:CE2	2:HP1:930:PHE:HZ	2.34	0.45
2:JP1:103:ILE:HD12	2:JP1:103:ILE:HA	1.88	0.45
1:EP1:353:LYS:HE3	1:EP1:353:LYS:HB3	1.68	0.45
2:HP1:473:LYS:HE3	2:IP1:843:TYR:CZ	2.52	0.45
2:HP1:659:PHE:CE1	2:HP1:707:LEU:HD22	2.51	0.45
1:AP1:105:LYS:HZ3	1:BP1:367:ASN:HA	1.82	0.45
1:BP1:74:VAL:O	1:BP1:78:GLN:HG2	2.16	0.45
1:CP1:81:ALA:CB	1:CP1:378:MET:HE1	2.45	0.45
1:DP1:55:THR:HA	1:EP1:42:TYR:CE1	2.52	0.45
1:DP1:208:ASN:O	1:DP1:212:GLN:HG2	2.17	0.45
2:FP1:103:ILE:N	2:FP1:104:PRO:HD2	2.32	0.45
2:FP1:435:ASN:HA	2:FP1:438:ARG:HD2	1.98	0.45
2:FP1:908:VAL:HG23	2:FP1:909:TYR:HD1	1.82	0.45
2:GP1:290:LEU:HB2	2:GP1:329:ARG:HH12	1.82	0.45
2:JP1:223:ASN:O	2:JP1:227:ARG:HG2	2.16	0.45
1:AP1:328:SER:HA	1:BP1:211:MET:CE	2.46	0.45
1:AP1:417:ILE:O	1:AP1:421:GLU:HG2	2.16	0.45
1:CP1:378:MET:HE3	1:CP1:378:MET:HB2	1.69	0.45
1:DP1:94:MET:HG3	1:EP1:241:SER:HB3	1.98	0.45
1:EP1:248:LEU:HD13	1:EP1:280:ILE:HD11	1.98	0.45
2:FP1:612:CYS:HB2	2:FP1:626:ARG:HE	1.82	0.45
2:GP1:819:TYR:CZ	2:GP1:823:ILE:HD11	2.52	0.45
2:IP1:461:TRP:CZ2	2:IP1:812:PRO:HB3	2.52	0.45
2:JP1:334:ILE:HD12	2:JP1:335:ALA:N	2.32	0.45
1:BP1:343:GLY:HA2	1:BP1:346:ASN:HD22	1.82	0.45
2:GP1:105:LEU:HD12	2:GP1:106:ARG:N	2.32	0.45
2:GP1:326:GLN:O	2:GP1:329:ARG:HB2	2.17	0.45
2:GP1:667:MET:CE	2:GP1:915:ILE:HD12	2.47	0.45
2:HP1:511:ASP:HB3	2:HP1:512:PRO:HA	1.98	0.45
2:HP1:905:TRP:O	2:HP1:908:VAL:HG22	2.16	0.45
2:JP1:330:LEU:O	2:JP1:334:ILE:HG13	2.17	0.45
2:JP1:741:THR:HG23	2:JP1:916:LEU:HG	1.99	0.45
1:AP1:389:SER:HB3	1:AP1:394:GLN:OE1	2.17	0.45
1:DP1:142:ILE:C	1:DP1:142:ILE:HD12	2.42	0.45
1:EP1:104:ASP:HA	1:EP1:109:ASN:ND2	2.32	0.45
2:FP1:288:SER:HA	2:FP1:291:ASN:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:820:ILE:HA	2:HP1:823:ILE:HG22	1.98	0.45
2:IP1:290:LEU:HB3	2:IP1:329:ARG:NH1	2.31	0.45
2:IP1:648:PHE:HE1	2:IP1:723:PHE:CD2	2.35	0.45
2:JP1:809:PHE:CD1	2:JP1:809:PHE:C	2.95	0.45
1:AP1:385:ASP:H	1:AP1:398:GLN:HE22	1.65	0.45
2:GP1:284:TRP:CD1	2:GP1:332:ARG:HG2	2.52	0.45
2:HP1:628:MET:HA	2:HP1:628:MET:HE2	1.99	0.45
1:BP1:378:MET:HE3	1:BP1:378:MET:HB2	1.65	0.44
1:CP1:389:SER:HB3	1:CP1:394:GLN:OE1	2.17	0.44
1:EP1:141:LEU:H	1:EP1:141:LEU:HD12	1.82	0.44
1:EP1:399:TRP:HE1	1:EP1:414:GLU:CD	2.25	0.44
2:FP1:100:SER:C	3:LP1:16:ARG:HH12	2.25	0.44
2:FP1:713:VAL:HG21	2:GP1:727:LEU:HD12	1.99	0.44
2:GP1:287:ILE:HG13	2:GP1:332:ARG:NH2	2.33	0.44
2:GP1:778:ALA:HB2	2:HP1:943:TRP:CH2	2.52	0.44
2:HP1:191:MET:CE	2:HP1:263:MET:HB3	2.47	0.44
2:HP1:932:LEU:HA	2:HP1:935:HIS:HD2	1.81	0.44
2:IP1:725:PHE:CZ	2:JP1:722:ILE:HG23	2.53	0.44
3:KP1:16:ARG:HA	3:KP1:19:VAL:HG22	1.98	0.44
1:EP1:302:TRP:NE1	1:EP1:306:THR:HG21	2.32	0.44
2:GP1:667:MET:HE2	2:GP1:912:PHE:HD2	1.82	0.44
2:GP1:930:PHE:O	2:GP1:933:ILE:HB	2.17	0.44
1:AP1:421:GLU:O	1:AP1:425:GLN:HG3	2.18	0.44
2:FP1:176:GLY:HA3	2:FP1:492:ASP:HB2	1.99	0.44
2:FP1:472:VAL:HG13	2:FP1:827:TYR:HE1	1.83	0.44
2:JP1:452:PHE:O	2:JP1:455:GLU:HG3	2.17	0.44
2:JP1:689:LEU:HD23	2:JP1:922:TYR:CE2	2.52	0.44
2:FP1:605:MET:HE3	2:FP1:605:MET:HB3	1.81	0.44
2:GP1:563:LEU:HD23	2:GP1:563:LEU:HA	1.82	0.44
2:GP1:639:TYR:CD1	2:GP1:639:TYR:C	2.94	0.44
2:HP1:247:THR:HG22	2:HP1:256:PRO:HD2	2.00	0.44
2:HP1:282:VAL:HA	2:HP1:494:SER:HB3	2.00	0.44
2:IP1:450:ARG:HD2	2:IP1:453:ILE:HD11	1.99	0.44
1:AP1:315:ASN:OD1	1:AP1:318:GLN:HB3	2.17	0.44
1:BP1:43:LEU:HD12	1:CP1:39:LEU:HD13	2.00	0.44
1:EP1:418:LEU:HD12	1:EP1:418:LEU:HA	1.80	0.44
2:FP1:34:SER:HA	2:FP1:462:ILE:HD13	1.99	0.44
2:GP1:213:PRO:O	2:GP1:218:PRO:HB3	2.17	0.44
2:GP1:369:ASP:OD1	2:GP1:369:ASP:N	2.51	0.44
2:GP1:525:ASP:HA	2:GP1:528:ILE:HG22	2.00	0.44
2:HP1:639:TYR:CD1	2:HP1:639:TYR:C	2.94	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:833:LEU:O	2:IP1:837:PHE:HB2	2.17	0.44
2:FP1:49:LEU:HD22	2:FP1:50:HIS:H	1.83	0.44
2:FP1:77:MET:O	2:FP1:81:MET:HG3	2.17	0.44
2:FP1:331:SER:HA	2:FP1:334:ILE:HD12	1.99	0.44
2:GP1:370:PHE:CD1	2:GP1:377:GLN:HB3	2.52	0.44
2:GP1:651:MET:HE1	2:GP1:655:ILE:HD11	2.00	0.44
2:HP1:753:ILE:HG13	2:HP1:922:TYR:CE2	2.52	0.44
2:IP1:555:GLN:NE2	2:IP1:588:LEU:HD12	2.32	0.44
2:IP1:664:LEU:O	2:IP1:668:LYS:HB2	2.18	0.44
2:JP1:537:VAL:HA	2:JP1:538:PRO:HA	1.86	0.44
3:KP1:40:ARG:HD2	3:KP1:40:ARG:HA	1.78	0.44
1:BP1:359:MET:HB2	1:BP1:367:ASN:OD1	2.18	0.44
1:DP1:104:ASP:HA	1:DP1:109:ASN:ND2	2.33	0.44
1:DP1:424:TYR:CZ	1:DP1:428:LEU:HD11	2.52	0.44
1:DP1:448:LEU:HD11	1:EP1:339:GLN:HB3	1.99	0.44
2:FP1:323:SER:O	2:FP1:326:GLN:HG3	2.18	0.44
2:GP1:766:PHE:CZ	2:HP1:829:GLY:HA3	2.49	0.44
2:IP1:461:TRP:CH2	2:IP1:812:PRO:HB3	2.52	0.44
2:JP1:600:THR:HG22	2:JP1:648:PHE:HE2	1.82	0.44
2:JP1:608:GLN:HG3	2:JP1:633:TYR:CE2	2.52	0.44
1:CP1:174:VAL:HG21	1:DP1:246:ASN:HD21	1.82	0.44
1:DP1:417:ILE:O	1:DP1:421:GLU:HG2	2.17	0.44
2:FP1:272:PHE:HD2	2:FP1:275:LEU:HD12	1.83	0.44
2:GP1:272:PHE:HD2	2:GP1:275:LEU:HD12	1.82	0.44
2:GP1:290:LEU:HD11	2:GP1:437:ILE:HD11	2.00	0.44
2:GP1:939:LYS:HA	2:GP1:939:LYS:HD2	1.86	0.44
2:JP1:240:VAL:HA	2:JP1:333:ALA:HB1	1.99	0.44
1:AP1:128:PRO:HB3	1:AP1:169:TYR:CE2	2.53	0.44
1:AP1:443:MET:HE1	1:EP1:443:MET:CE	2.48	0.44
2:FP1:377:GLN:HE22	2:FP1:402:VAL:HB	1.83	0.44
2:FP1:751:TYR:C	2:FP1:754:PRO:HD2	2.43	0.44
2:HP1:110:GLY:HA3	2:HP1:787:THR:HG22	2.00	0.44
2:HP1:516:LEU:HD23	2:HP1:516:LEU:HA	1.78	0.44
2:HP1:617:ILE:O	2:HP1:618:LEU:C	2.61	0.44
2:IP1:49:LEU:HD13	2:IP1:51:GLY:N	2.33	0.44
1:AP1:435:ARG:NH1	1:BP1:249:ILE:HD11	2.32	0.43
1:DP1:102:VAL:HG21	1:DP1:106:VAL:HG12	2.00	0.43
1:EP1:87:GLY:HA3	1:EP1:118:THR:HG22	2.00	0.43
2:FP1:33:LEU:HD12	2:FP1:459:LYS:O	2.19	0.43
2:FP1:921:MET:HA	2:FP1:924:ILE:HD12	2.00	0.43
2:GP1:188:GLN:O	2:GP1:191:MET:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:335:ALA:HB1	2:GP1:426:TYR:CD1	2.53	0.43
2:GP1:612:CYS:HB3	2:GP1:626:ARG:H	1.83	0.43
2:GP1:704:TRP:CZ2	2:HP1:730:MET:HE3	2.52	0.43
2:GP1:753:ILE:HG13	2:GP1:922:TYR:CE2	2.53	0.43
2:GP1:811:ARG:HE	2:GP1:815:MET:HE2	1.82	0.43
2:IP1:89:HIS:HA	3:NP1:1:MET:HG2	1.99	0.43
2:IP1:452:PHE:CE1	2:IP1:453:ILE:HG13	2.53	0.43
1:CP1:448:LEU:HD11	1:DP1:339:GLN:HB3	2.00	0.43
2:FP1:38:LEU:HD12	2:FP1:38:LEU:HA	1.79	0.43
2:GP1:113:LEU:O	2:GP1:122:CYS:HB3	2.19	0.43
2:HP1:175:SER:HB2	2:HP1:488:GLY:H	1.82	0.43
2:HP1:643:PHE:CZ	2:HP1:647:ILE:HD11	2.53	0.43
1:AP1:419:LEU:HA	1:AP1:419:LEU:HD23	1.80	0.43
1:BP1:401:LYS:HD2	1:BP1:401:LYS:HA	1.75	0.43
1:CP1:33:SER:HB2	1:DP1:31:GLN:OE1	2.17	0.43
1:CP1:206:TYR:CZ	1:CP1:209:LEU:HB2	2.53	0.43
1:DP1:37:SER:O	1:DP1:40:VAL:HG12	2.18	0.43
2:HP1:818:GLY:HA2	2:HP1:936:LEU:HD13	2.01	0.43
2:IP1:667:MET:HE3	2:IP1:696:TYR:OH	2.18	0.43
2:IP1:917:ILE:HD12	2:IP1:917:ILE:HA	1.82	0.43
1:BP1:455:ALA:HB1	1:CP1:293:PRO:HA	2.01	0.43
1:EP1:119:THR:HG21	1:EP1:352:SER:OG	2.19	0.43
2:FP1:73:GLY:O	2:FP1:77:MET:HG3	2.18	0.43
2:FP1:205:TYR:HE2	2:FP1:213:PRO:HG2	1.83	0.43
2:FP1:720:PHE:HD1	2:JP1:716:LEU:HD12	1.83	0.43
2:FP1:766:PHE:CZ	2:GP1:829:GLY:HA2	2.36	0.43
2:GP1:261:LEU:HB2	2:GP1:284:TRP:CZ3	2.52	0.43
2:GP1:725:PHE:O	2:GP1:728:ILE:HG23	2.18	0.43
2:HP1:188:GLN:O	2:HP1:192:LEU:HG	2.18	0.43
2:IP1:334:ILE:HD12	2:IP1:335:ALA:N	2.33	0.43
2:IP1:381:PRO:HD3	2:IP1:573:ASN:HB3	1.99	0.43
2:IP1:756:LEU:O	2:IP1:759:MET:HB2	2.17	0.43
3:OP1:14:ASN:HB3	3:OP1:17:THR:HB	1.99	0.43
1:EP1:115:LEU:HD23	1:EP1:115:LEU:HA	1.79	0.43
1:EP1:123:GLN:NE2	1:EP1:256:THR:HG21	2.33	0.43
2:FP1:645:LEU:HD12	2:FP1:645:LEU:HA	1.84	0.43
2:FP1:716:LEU:HA	2:GP1:723:PHE:CG	2.54	0.43
2:FP1:778:ALA:HB2	2:GP1:943:TRP:CH2	2.53	0.43
2:GP1:79:THR:HA	2:GP1:82:VAL:HG12	2.01	0.43
2:GP1:125:GLN:H	2:GP1:125:GLN:HG2	1.66	0.43
2:HP1:139:ALA:HB2	2:HP1:812:PRO:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:152:ARG:N	2:HP1:152:ARG:HD3	2.33	0.43
2:HP1:264:PRO:O	2:HP1:276:ASN:ND2	2.51	0.43
2:HP1:434:LEU:O	2:HP1:437:ILE:HG22	2.18	0.43
2:HP1:769:LEU:HD23	2:HP1:769:LEU:HA	1.82	0.43
2:HP1:807:ASN:O	2:HP1:811:ARG:HG2	2.18	0.43
2:JP1:259:PHE:CE2	2:JP1:286:ASN:HB2	2.54	0.43
2:JP1:548:PRO:HD3	2:JP1:568:TYR:HD2	1.82	0.43
2:JP1:586:LYS:HB3	2:JP1:586:LYS:HE3	1.90	0.43
1:BP1:308:LYS:HG2	1:BP1:309:PRO:HD2	2.01	0.43
1:CP1:328:SER:HA	1:DP1:211:MET:CE	2.48	0.43
1:EP1:170:LEU:H	1:EP1:170:LEU:HD12	1.83	0.43
1:EP1:445:LEU:HD13	1:EP1:445:LEU:HA	1.84	0.43
2:GP1:105:LEU:HA	2:GP1:108:THR:HG22	2.00	0.43
2:JP1:45:VAL:HG12	2:JP1:49:LEU:HB2	2.01	0.43
1:CP1:423:ASN:HD21	1:DP1:379:ALA:HA	1.83	0.43
1:EP1:419:LEU:HD23	1:EP1:419:LEU:HA	1.81	0.43
2:GP1:717:ILE:HD12	2:GP1:717:ILE:O	2.19	0.43
2:HP1:377:GLN:HE22	2:HP1:402:VAL:HB	1.83	0.43
2:IP1:383:LYS:HG3	2:IP1:387:GLU:O	2.18	0.43
2:JP1:38:LEU:HD23	2:JP1:38:LEU:HA	1.80	0.43
1:AP1:86:LEU:HA	1:AP1:86:LEU:HD12	1.81	0.43
1:AP1:123:GLN:NE2	1:AP1:256:THR:HG21	2.33	0.43
1:CP1:206:TYR:O	1:CP1:210:VAL:HG12	2.18	0.43
1:EP1:355:LEU:HD23	1:EP1:355:LEU:HA	1.85	0.43
2:FP1:163:PRO:HG2	2:FP1:581:GLY:HA3	1.99	0.43
2:HP1:136:VAL:HG13	2:HP1:461:TRP:HE1	1.84	0.43
2:JP1:399:TRP:CE3	2:JP1:416:GLY:HA3	2.54	0.43
2:JP1:447:LYS:HE2	2:JP1:447:LYS:HB2	1.87	0.43
3:LP1:26:ALA:HA	3:LP1:29:ILE:HG12	2.01	0.43
3:NP1:16:ARG:HA	3:NP1:19:VAL:HG22	2.01	0.43
1:AP1:211:MET:CE	1:EP1:328:SER:HA	2.48	0.43
1:CP1:205:MET:HA	1:CP1:209:LEU:HD23	2.00	0.43
1:CP1:449:LYS:HE2	1:DP1:285:ALA:HB1	1.99	0.43
1:EP1:84:THR:HB	1:EP1:371:GLN:HA	2.01	0.43
2:HP1:103:ILE:HA	2:HP1:106:ARG:HG2	2.01	0.43
2:HP1:922:TYR:HA	2:HP1:925:ILE:HD12	2.00	0.43
2:IP1:766:PHE:HZ	2:JP1:829:GLY:HA2	1.81	0.43
1:AP1:31:GLN:HE22	1:AP1:35:ASN:ND2	2.16	0.43
1:AP1:99:MET:HE2	1:AP1:99:MET:HB2	1.86	0.43
1:EP1:142:ILE:HD13	1:EP1:281:ARG:HD3	2.01	0.43
2:FP1:716:LEU:HA	2:GP1:723:PHE:CD1	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:FP1:739:ILE:O	2:FP1:743:VAL:HG22	2.19	0.43
2:GP1:725:PHE:HE1	2:HP1:729:MET:SD	2.42	0.43
2:HP1:503:LYS:HE2	2:HP1:503:LYS:HB2	1.73	0.43
2:IP1:330:LEU:O	2:IP1:334:ILE:HG13	2.19	0.43
2:IP1:612:CYS:HB2	2:IP1:626:ARG:NE	2.27	0.43
2:JP1:573:ASN:HA	2:JP1:576:MET:HE2	2.01	0.43
1:AP1:175:SER:HB3	1:BP1:244:ASN:HD22	1.84	0.42
1:BP1:351:LEU:C	1:BP1:351:LEU:HD23	2.44	0.42
1:DP1:359:MET:HB2	1:DP1:367:ASN:OD1	2.19	0.42
2:FP1:205:TYR:HB3	2:FP1:214:CYS:SG	2.59	0.42
2:GP1:67:ALA:O	2:GP1:71:LEU:HD12	2.18	0.42
2:GP1:125:GLN:HB3	2:GP1:776:MET:SD	2.59	0.42
2:GP1:547:GLN:HA	2:GP1:568:TYR:CD2	2.54	0.42
2:HP1:45:VAL:HG11	2:HP1:129:MET:HG2	2.00	0.42
2:HP1:692:MET:HE3	2:HP1:696:TYR:HE2	1.83	0.42
2:IP1:766:PHE:CG	2:JP1:925:ILE:HD11	2.54	0.42
2:JP1:331:SER:HA	2:JP1:334:ILE:HD11	2.01	0.42
2:JP1:725:PHE:HA	2:JP1:728:ILE:HG22	2.01	0.42
2:HP1:143:TRP:HB2	2:HP1:816:ILE:HG12	2.00	0.42
2:IP1:370:PHE:CE2	2:IP1:562:PRO:HA	2.53	0.42
2:JP1:213:PRO:O	2:JP1:218:PRO:HB3	2.19	0.42
2:JP1:612:CYS:HB2	2:JP1:626:ARG:NE	2.27	0.42
2:JP1:922:TYR:O	2:JP1:925:ILE:HG22	2.19	0.42
1:AP1:172:ASP:HB3	1:AP1:175:SER:OG	2.18	0.42
2:FP1:664:LEU:HD23	2:FP1:664:LEU:HA	1.89	0.42
2:FP1:769:LEU:HA	2:FP1:769:LEU:HD23	1.87	0.42
2:IP1:41:LEU:HD23	2:IP1:42:PHE:CD1	2.54	0.42
2:IP1:708:LEU:HD13	2:JP1:730:MET:HB3	2.01	0.42
2:JP1:525:ASP:OD2	2:JP1:525:ASP:N	2.52	0.42
1:BP1:56:GLN:HB3	1:BP1:59:LYS:HG3	2.01	0.42
1:BP1:445:LEU:HD21	1:CP1:343:GLY:HA3	2.01	0.42
1:CP1:317:VAL:HA	1:DP1:198:TRP:HE1	1.84	0.42
1:DP1:320:LYS:HD2	1:EP1:198:TRP:CE2	2.55	0.42
2:FP1:588:LEU:HD22	2:FP1:665:GLN:HE22	1.83	0.42
2:FP1:817:ILE:HD13	2:JP1:60:MET:HE3	2.00	0.42
2:HP1:33:LEU:HA	2:HP1:36:VAL:HB	2.01	0.42
1:BP1:328:SER:HA	1:CP1:211:MET:CE	2.50	0.42
2:FP1:724:ILE:O	2:FP1:728:ILE:HG22	2.19	0.42
2:GP1:268:LYS:HB3	2:HP1:403:PRO:HB3	2.01	0.42
2:GP1:375:LYS:HE3	2:GP1:375:LYS:HB2	1.91	0.42
2:GP1:391:GLU:OE1	2:GP1:391:GLU:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:GP1:461:TRP:CH2	2:GP1:812:PRO:HB3	2.55	0.42
2:GP1:751:TYR:HB3	2:HP1:913:PHE:CD2	2.55	0.42
2:HP1:162:ASP:HB3	2:HP1:165:LYS:HB3	2.02	0.42
2:HP1:299:LYS:H	2:HP1:299:LYS:HG2	1.67	0.42
2:HP1:768:TRP:O	2:HP1:772:VAL:HG12	2.20	0.42
2:HP1:837:PHE:O	2:HP1:841:ILE:HG22	2.18	0.42
1:BP1:33:SER:HB2	1:CP1:31:GLN:OE1	2.20	0.42
1:CP1:54:ILE:HD13	1:CP1:54:ILE:HA	1.87	0.42
1:EP1:216:GLY:HA3	1:EP1:265:SER:O	2.20	0.42
2:FP1:103:ILE:HD11	3:LP1:20:ILE:HD12	2.00	0.42
2:HP1:162:ASP:H	2:HP1:485:PHE:HZ	1.67	0.42
2:HP1:617:ILE:HG22	2:HP1:618:LEU:H	1.85	0.42
2:JP1:101:ILE:O	2:JP1:104:PRO:HD2	2.19	0.42
2:JP1:204:LEU:HD23	2:JP1:204:LEU:HA	1.75	0.42
2:JP1:589:THR:HG23	2:JP1:590:PHE:CD1	2.55	0.42
2:JP1:755:VAL:O	2:JP1:759:MET:HG3	2.19	0.42
2:JP1:936:LEU:N	2:JP1:937:PRO:HD2	2.34	0.42
1:AP1:382:ARG:HB3	1:AP1:399:TRP:CE3	2.55	0.42
1:BP1:204:LEU:HD23	1:BP1:204:LEU:HA	1.82	0.42
1:DP1:308:LYS:HA	1:DP1:308:LYS:HD2	1.75	0.42
2:GP1:35:VAL:HA	2:GP1:38:LEU:HB2	2.02	0.42
2:GP1:524:SER:O	2:GP1:528:ILE:HG22	2.19	0.42
2:GP1:657:MET:O	2:GP1:661:MET:HG2	2.19	0.42
2:GP1:667:MET:HE3	2:GP1:915:ILE:HD12	2.01	0.42
2:HP1:237:VAL:HG13	2:HP1:261:LEU:HD11	2.01	0.42
2:IP1:725:PHE:CE2	2:JP1:722:ILE:HG23	2.55	0.42
3:KP1:24:THR:HA	3:KP1:27:LEU:HD12	2.02	0.42
1:BP1:292:LEU:HD13	1:CP1:230:PHE:CE2	2.55	0.42
2:FP1:187:GLY:HA3	2:FP1:263:MET:HE3	2.02	0.42
2:GP1:334:ILE:HD12	2:GP1:335:ALA:N	2.34	0.42
2:HP1:728:ILE:HD12	2:IP1:730:MET:SD	2.60	0.42
2:IP1:751:TYR:C	2:IP1:754:PRO:HD2	2.45	0.42
2:JP1:804:ILE:O	2:JP1:808:VAL:HG22	2.20	0.42
3:LP1:38:LYS:HA	3:LP1:38:LYS:HD2	1.77	0.42
3:MP1:35:GLY:O	3:MP1:39:ILE:HG13	2.20	0.42
1:AP1:430:ARG:NH2	1:BP1:425:GLN:NE2	2.68	0.42
2:FP1:617:ILE:O	2:FP1:618:LEU:C	2.63	0.42
2:FP1:730:MET:O	2:FP1:733:PRO:HD2	2.20	0.42
2:FP1:759:MET:HE1	2:GP1:917:ILE:HD12	2.01	0.42
2:GP1:240:VAL:HA	2:GP1:333:ALA:HB1	2.01	0.42
2:GP1:573:ASN:O	2:GP1:576:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:EP1:96:GLN:OE1	1:EP1:96:GLN:N	2.52	0.42
1:EP1:230:PHE:C	1:EP1:230:PHE:CD2	2.97	0.42
2:FP1:191:MET:HE1	2:FP1:264:PRO:HA	2.02	0.42
2:GP1:41:LEU:HD22	2:GP1:42:PHE:CE2	2.55	0.42
2:GP1:143:TRP:CE2	2:GP1:147:LEU:HD23	2.55	0.42
2:GP1:782:VAL:HG11	2:GP1:801:ALA:HB2	2.02	0.42
2:HP1:667:MET:HE3	2:HP1:911:PHE:HD2	1.84	0.42
2:HP1:799:GLU:HG2	2:HP1:800:PHE:H	1.85	0.42
3:LP1:4:LYS:HB2	3:LP1:4:LYS:HE2	1.83	0.42
1:BP1:303:ASN:HD22	2:GP1:208:GLN:CD	2.28	0.41
1:CP1:219:PRO:HA	1:CP1:220:PRO:HD3	1.91	0.41
1:DP1:298:TYR:HE2	1:EP1:230:PHE:CD1	2.38	0.41
2:FP1:105:LEU:HA	2:FP1:108:THR:HG22	2.02	0.41
2:GP1:703:LEU:O	2:GP1:707:LEU:HG	2.20	0.41
2:HP1:179:LYS:HE3	2:HP1:547:GLN:HE22	1.84	0.41
2:HP1:336:ILE:HD11	2:HP1:491:LEU:HD11	2.01	0.41
2:FP1:59:ASN:HD22	2:GP1:149:TYR:HB2	1.84	0.41
2:GP1:330:LEU:HB3	2:GP1:333:ALA:HB3	2.01	0.41
2:HP1:335:ALA:HB1	2:HP1:426:TYR:CD1	2.55	0.41
2:HP1:448:LYS:HE2	2:HP1:448:LYS:HB2	1.66	0.41
2:HP1:588:LEU:HD22	2:HP1:665:GLN:CD	2.45	0.41
2:IP1:259:PHE:HE1	2:IP1:286:ASN:HB2	1.85	0.41
2:IP1:331:SER:O	2:IP1:334:ILE:HD12	2.19	0.41
2:IP1:837:PHE:CE2	2:IP1:918:TYR:HB2	2.55	0.41
2:JP1:57:MET:SD	2:JP1:61:PHE:HE1	2.43	0.41
2:JP1:137:GLY:O	2:JP1:141:LYS:HG3	2.21	0.41
2:JP1:141:LYS:HA	2:JP1:144:GLU:HG2	2.02	0.41
1:DP1:128:PRO:HB3	1:DP1:169:TYR:CE2	2.55	0.41
1:EP1:215:ILE:HD13	1:EP1:215:ILE:HA	1.75	0.41
1:EP1:253:LEU:HD22	1:EP1:373:LEU:HD22	2.02	0.41
2:HP1:753:ILE:HD13	2:HP1:753:ILE:HA	1.94	0.41
2:HP1:758:TYR:OH	2:IP1:836:GLY:HA3	2.21	0.41
2:JP1:547:GLN:HA	2:JP1:568:TYR:CE2	2.55	0.41
1:AP1:250:ALA:HB3	1:AP1:251:PRO:HD3	2.02	0.41
1:AP1:419:LEU:HD23	1:AP1:422:ILE:HD12	2.02	0.41
2:FP1:136:VAL:HG13	2:FP1:461:TRP:HE1	1.85	0.41
2:GP1:144:GLU:HA	2:GP1:147:LEU:HG	2.01	0.41
2:GP1:329:ARG:HA	2:GP1:329:ARG:HD3	1.81	0.41
2:HP1:105:LEU:HA	2:HP1:108:THR:HG22	2.02	0.41
2:HP1:603:TYR:O	2:HP1:641:TYR:HE2	2.04	0.41
2:HP1:645:LEU:HD23	2:HP1:645:LEU:HA	1.90	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:701:GLY:HA3	2:IP1:905:TRP:CH2	2.55	0.41
2:IP1:131:VAL:HG11	2:IP1:805:LEU:HG	2.01	0.41
2:IP1:600:THR:HB	2:IP1:645:LEU:HD22	2.01	0.41
2:JP1:939:LYS:HE3	2:JP1:939:LYS:HB3	1.86	0.41
3:NP1:21:ILE:HD13	3:NP1:21:ILE:HA	1.84	0.41
1:AP1:104:ASP:OD1	1:AP1:104:ASP:C	2.64	0.41
1:BP1:115:LEU:HD23	1:BP1:115:LEU:HA	1.88	0.41
1:DP1:102:VAL:HG23	1:EP1:253:LEU:HD23	2.01	0.41
1:DP1:302:TRP:O	1:DP1:306:THR:HG22	2.21	0.41
1:DP1:368:ILE:HD13	1:DP1:368:ILE:HA	1.88	0.41
2:FP1:468:PHE:CE1	2:FP1:757:PRO:HG2	2.56	0.41
2:FP1:705:LEU:HD12	2:GP1:594:ILE:HG23	2.03	0.41
2:GP1:147:LEU:HD12	2:GP1:148:SER:N	2.34	0.41
2:GP1:290:LEU:HD12	2:GP1:290:LEU:H	1.85	0.41
2:GP1:671:PHE:CD1	2:GP1:915:ILE:HD11	2.55	0.41
2:GP1:841:ILE:HG13	2:GP1:845:GLN:HG2	2.01	0.41
2:HP1:612:CYS:HB2	2:HP1:626:ARG:HE	1.85	0.41
2:HP1:833:LEU:O	2:HP1:837:PHE:HB2	2.20	0.41
2:IP1:187:GLY:O	2:IP1:191:MET:HG2	2.20	0.41
2:IP1:499:THR:HA	2:IP1:531:GLN:NE2	2.35	0.41
2:IP1:630:ASP:HA	2:IP1:634:ASN:HB2	2.01	0.41
2:JP1:505:PHE:CG	2:JP1:524:SER:HB3	2.56	0.41
3:MP1:36:PHE:O	3:MP1:39:ILE:HD12	2.19	0.41
1:CP1:228:PRO:HG3	1:CP1:234:LYS:HD2	2.01	0.41
2:GP1:184:ILE:HD12	2:GP1:184:ILE:H	1.85	0.41
2:GP1:282:VAL:HA	2:GP1:494:SER:HB3	2.03	0.41
2:GP1:589:THR:HG23	2:GP1:590:PHE:CD1	2.55	0.41
2:GP1:751:TYR:C	2:GP1:754:PRO:HD2	2.46	0.41
2:HP1:210:LYS:HE2	2:HP1:210:LYS:HB2	1.81	0.41
2:IP1:205:TYR:HB3	2:IP1:214:CYS:SG	2.60	0.41
2:IP1:369:ASP:HB3	2:IP1:375:LYS:HA	2.02	0.41
2:IP1:782:VAL:O	2:IP1:786:VAL:HG23	2.20	0.41
2:JP1:685:PRO:HB2	2:JP1:830:VAL:HG11	2.02	0.41
2:JP1:816:ILE:HD13	2:JP1:816:ILE:HA	1.83	0.41
3:MP1:15:THR:HG22	3:MP1:18:ARG:HH22	1.85	0.41
1:AP1:206:TYR:CZ	1:AP1:209:LEU:HB2	2.56	0.41
1:AP1:294:LYS:H	1:AP1:294:LYS:HG2	1.61	0.41
2:GP1:100:SER:HB3	3:KP1:16:ARG:HH12	1.85	0.41
2:GP1:748:VAL:O	2:GP1:753:ILE:HG12	2.20	0.41
2:GP1:803:MET:HE3	2:GP1:804:ILE:N	2.36	0.41
2:HP1:469:PHE:O	2:HP1:473:LYS:HG2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:IP1:691:ASN:HA	2:IP1:694:THR:HG23	2.02	0.41
2:IP1:841:ILE:HG12	2:IP1:914:SER:HB3	2.03	0.41
2:JP1:302:VAL:HB	2:JP1:320:ILE:HG13	2.02	0.41
3:MP1:4:LYS:O	3:MP1:8:LEU:HG	2.20	0.41
3:NP1:16:ARG:O	3:NP1:20:ILE:HG23	2.21	0.41
1:AP1:239:LEU:O	1:AP1:243:LEU:HG	2.21	0.41
1:AP1:339:GLN:HG2	1:AP1:442:ILE:HG23	2.02	0.41
1:AP1:443:MET:HE1	1:EP1:443:MET:HE2	2.01	0.41
1:CP1:70:ASN:HB3	1:CP1:73:VAL:HG22	2.02	0.41
2:FP1:334:ILE:HG13	2:FP1:334:ILE:H	1.69	0.41
2:IP1:98:TRP:CD1	2:IP1:103:ILE:HD11	2.56	0.41
2:JP1:170:ALA:HA	2:JP1:175:SER:H	1.84	0.41
2:JP1:205:TYR:HB3	2:JP1:214:CYS:SG	2.61	0.41
1:AP1:170:LEU:HD12	1:AP1:170:LEU:H	1.86	0.41
1:AP1:326:LEU:HD23	1:AP1:326:LEU:HA	1.81	0.41
1:BP1:104:ASP:OD2	1:BP1:104:ASP:C	2.64	0.41
1:BP1:418:LEU:HD12	1:BP1:418:LEU:HA	1.84	0.41
1:BP1:440:ASN:HB3	1:CP1:439:THR:HG21	2.03	0.41
1:BP1:441:SER:O	1:BP1:445:LEU:HD23	2.19	0.41
1:CP1:448:LEU:HD23	1:CP1:448:LEU:HA	1.77	0.41
1:DP1:292:LEU:HD13	1:DP1:329:TYR:OH	2.21	0.41
1:DP1:360:SER:HB2	1:DP1:366:ALA:HA	2.02	0.41
1:EP1:254:MET:HB3	1:EP1:273:ALA:HB2	2.03	0.41
1:EP1:426:MET:HB2	1:EP1:426:MET:HE3	1.71	0.41
2:FP1:725:PHE:CD2	2:FP1:725:PHE:C	2.98	0.41
2:FP1:725:PHE:CE2	2:GP1:729:MET:HE1	2.55	0.41
2:FP1:937:PRO:HA	2:FP1:940:VAL:HG22	2.03	0.41
2:GP1:56:ILE:O	2:GP1:60:MET:HB2	2.21	0.41
2:GP1:184:ILE:O	2:GP1:188:GLN:HG3	2.20	0.41
2:GP1:287:ILE:HD12	2:GP1:287:ILE:H	1.86	0.41
2:GP1:331:SER:HA	2:GP1:334:ILE:HD11	2.03	0.41
2:GP1:766:PHE:CE2	2:HP1:925:ILE:HG23	2.55	0.41
2:HP1:103:ILE:HG13	2:HP1:104:PRO:CD	2.47	0.41
2:HP1:114:LEU:HD21	2:HP1:783:ALA:HB3	2.03	0.41
2:HP1:301:LEU:HD21	2:HP1:319:ASN:HD21	1.86	0.41
2:HP1:696:TYR:CD1	2:HP1:742:MET:HG2	2.55	0.41
2:HP1:751:TYR:C	2:HP1:754:PRO:HD2	2.46	0.41
2:IP1:28:PRO:HB2	2:IP1:32:ASP:OD2	2.21	0.41
2:IP1:191:MET:HE1	2:IP1:264:PRO:N	2.36	0.41
2:IP1:651:MET:HB2	2:IP1:651:MET:HE2	1.79	0.41
2:IP1:713:VAL:HG11	2:JP1:596:PHE:HE2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:JP1:752:TYR:HE1	2:JP1:756:LEU:HD22	1.86	0.41
1:BP1:284:SER:HB2	1:BP1:344:VAL:HG22	2.03	0.41
1:BP1:419:LEU:HD23	1:BP1:419:LEU:HA	1.84	0.41
1:DP1:43:LEU:HD12	1:DP1:43:LEU:HA	1.92	0.41
2:FP1:210:LYS:HB2	2:FP1:210:LYS:HE2	1.76	0.41
2:IP1:660:LEU:O	2:IP1:663:PRO:HD2	2.21	0.41
2:JP1:704:TRP:CD1	2:JP1:704:TRP:C	3.00	0.41
3:MP1:12:PHE:CZ	3:MP1:22:ILE:HD11	2.56	0.41
1:BP1:120:PHE:CZ	1:BP1:173:PRO:HG3	2.56	0.40
1:BP1:215:ILE:HD12	1:BP1:215:ILE:HA	1.80	0.40
1:EP1:142:ILE:HG22	1:EP1:210:VAL:HG23	2.03	0.40
2:FP1:751:TYR:CE1	2:GP1:910:ALA:HA	2.56	0.40
2:HP1:447:LYS:HD2	2:HP1:447:LYS:H	1.86	0.40
2:IP1:191:MET:CE	2:IP1:263:MET:HB3	2.51	0.40
2:JP1:525:ASP:O	2:JP1:529:GLN:HG3	2.21	0.40
2:JP1:814:LEU:O	2:JP1:817:ILE:HB	2.21	0.40
1:AP1:129:SER:HB3	1:AP1:137:THR:HG21	2.04	0.40
2:FP1:110:GLY:O	2:FP1:114:LEU:HD23	2.21	0.40
2:FP1:296:SER:HA	2:FP1:302:VAL:HG13	2.03	0.40
2:FP1:588:LEU:HD22	2:FP1:665:GLN:NE2	2.35	0.40
2:FP1:708:LEU:O	2:FP1:713:VAL:HG23	2.21	0.40
2:GP1:149:TYR:C	2:GP1:149:TYR:CD2	2.99	0.40
2:GP1:650:GLU:CD	2:GP1:650:GLU:H	2.30	0.40
2:HP1:816:ILE:HD12	2:HP1:816:ILE:HA	1.94	0.40
2:IP1:248:PRO:HD2	2:IP1:256:PRO:HD3	2.03	0.40
2:IP1:597:LYS:HA	2:IP1:597:LYS:HD2	1.79	0.40
2:IP1:725:PHE:O	2:IP1:728:ILE:HG22	2.21	0.40
2:IP1:844:ILE:N	2:IP1:844:ILE:HD13	2.36	0.40
2:JP1:331:SER:O	2:JP1:334:ILE:HD12	2.21	0.40
2:JP1:547:GLN:HA	2:JP1:568:TYR:HE2	1.86	0.40
1:BP1:448:LEU:HD23	1:BP1:448:LEU:HA	1.95	0.40
2:FP1:462:ILE:HG13	2:FP1:463:MET:SD	2.61	0.40
2:FP1:752:TYR:CE1	2:FP1:756:LEU:HB2	2.56	0.40
2:GP1:732:MET:O	2:GP1:736:MET:HB2	2.21	0.40
2:HP1:377:GLN:NE2	2:HP1:402:VAL:H	2.13	0.40
2:IP1:528:ILE:CD1	2:IP1:538:PRO:HD3	2.50	0.40
2:JP1:664:LEU:HD23	2:JP1:664:LEU:HA	1.67	0.40
2:JP1:769:LEU:HD23	2:JP1:769:LEU:HA	1.84	0.40
3:OP1:30:ILE:HD13	3:OP1:30:ILE:HA	1.94	0.40
2:FP1:844:ILE:HD13	2:FP1:844:ILE:N	2.37	0.40
2:HP1:58:GLY:HA2	2:HP1:121:TYR:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:HP1:370:PHE:HE2	2:HP1:565:SER:HB3	1.87	0.40
2:IP1:290:LEU:HD11	2:IP1:437:ILE:HG12	2.02	0.40
2:JP1:935:HIS:HE1	2:JP1:939:LYS:HD2	1.86	0.40
1:AP1:198:TRP:CD1	1:EP1:317:VAL:HG22	2.56	0.40
1:AP1:401:LYS:HD2	1:AP1:401:LYS:HA	1.70	0.40
1:CP1:35:ASN:O	1:CP1:39:LEU:HD23	2.22	0.40
1:CP1:128:PRO:HG3	1:CP1:169:TYR:CE2	2.56	0.40
1:CP1:295:LEU:HD11	2:FP1:212:PRO:HG3	2.03	0.40
1:EP1:308:LYS:HG2	1:EP1:309:PRO:HD2	2.03	0.40
1:EP1:326:LEU:HD23	1:EP1:326:LEU:HA	1.81	0.40
2:FP1:448:LYS:HA	2:FP1:451:ASP:OD2	2.21	0.40
2:FP1:915:ILE:HD12	2:FP1:915:ILE:HA	1.93	0.40
2:GP1:289:ALA:HB3	2:GP1:437:ILE:HD13	2.04	0.40
2:GP1:500:GLN:HA	2:GP1:503:LYS:HB2	2.02	0.40
2:GP1:800:PHE:HZ	2:HP1:943:TRP:CE2	2.39	0.40
2:GP1:939:LYS:HA	2:GP1:942:ARG:HG3	2.02	0.40
2:HP1:617:ILE:HG22	2:HP1:618:LEU:N	2.37	0.40
2:HP1:619:PHE:HD1	2:HP1:619:PHE:HA	1.76	0.40
2:IP1:93:MET:HE1	3:NP1:17:THR:HG22	2.03	0.40
2:JP1:596:PHE:CD2	2:JP1:656:VAL:HG21	2.56	0.40
3:KP1:5:LYS:HG3	3:KP1:6:GLU:N	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	AP1	413/466 (89%)	401 (97%)	12 (3%)	0	100	100
1	BP1	413/466 (89%)	405 (98%)	8 (2%)	0	100	100
1	CP1	413/466 (89%)	406 (98%)	7 (2%)	0	100	100
1	DP1	413/466 (89%)	402 (97%)	11 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	EP1	413/466 (89%)	406 (98%)	7 (2%)	0	100	100
2	FP1	847/1048 (81%)	816 (96%)	31 (4%)	0	100	100
2	GP1	847/1048 (81%)	813 (96%)	34 (4%)	0	100	100
2	HP1	847/1048 (81%)	807 (95%)	40 (5%)	0	100	100
2	IP1	847/1048 (81%)	813 (96%)	34 (4%)	0	100	100
2	JP1	847/1048 (81%)	811 (96%)	36 (4%)	0	100	100
3	KP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	LP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	MP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	NP1	41/1048 (4%)	41 (100%)	0	0	100	100
3	OP1	41/1048 (4%)	41 (100%)	0	0	100	100
All	All	6505/12810 (51%)	6285 (97%)	220 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	AP1	360/401 (90%)	347 (96%)	13 (4%)	30	55
1	BP1	360/401 (90%)	350 (97%)	10 (3%)	38	60
1	CP1	360/401 (90%)	350 (97%)	10 (3%)	38	60
1	DP1	360/401 (90%)	350 (97%)	10 (3%)	38	60
1	EP1	360/401 (90%)	352 (98%)	8 (2%)	47	66
2	FP1	715/858 (83%)	683 (96%)	32 (4%)	23	49
2	GP1	715/858 (83%)	683 (96%)	32 (4%)	23	49
2	HP1	715/858 (83%)	674 (94%)	41 (6%)	17	43
2	IP1	715/858 (83%)	678 (95%)	37 (5%)	19	45
2	JP1	715/858 (83%)	677 (95%)	38 (5%)	19	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	KP1	36/765 (5%)	32 (89%)	4 (11%)	5 22
3	LP1	36/765 (5%)	35 (97%)	1 (3%)	38 60
3	MP1	36/765 (5%)	32 (89%)	4 (11%)	5 22
3	NP1	36/765 (5%)	31 (86%)	5 (14%)	3 15
3	OP1	36/765 (5%)	31 (86%)	5 (14%)	3 15
All	All	5555/10120 (55%)	5305 (96%)	250 (4%)	26 49

All (250) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AP1	31	GLN
1	AP1	59	LYS
1	AP1	65	TYR
1	AP1	76	LEU
1	AP1	86	LEU
1	AP1	212	GLN
1	AP1	230	PHE
1	AP1	317	VAL
1	AP1	328	SER
1	AP1	345	SER
1	AP1	346	ASN
1	AP1	381	ARG
1	AP1	447	ASN
1	BP1	43	LEU
1	BP1	71	SER
1	BP1	195	GLN
1	BP1	230	PHE
1	BP1	268	THR
1	BP1	281	ARG
1	BP1	345	SER
1	BP1	374	ASN
1	BP1	426	MET
1	BP1	434	GLU
1	CP1	193	ASN
1	CP1	195	GLN
1	CP1	204	LEU
1	CP1	205	MET
1	CP1	230	PHE
1	CP1	299	SER
1	CP1	345	SER

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Mol	Chain	Res	Type
1	CP1	374	ASN
1	CP1	407	SER
1	CP1	426	MET
1	DP1	172	ASP
1	DP1	193	ASN
1	DP1	195	GLN
1	DP1	203	ASN
1	DP1	210	VAL
1	DP1	298	TYR
1	DP1	303	ASN
1	DP1	345	SER
1	DP1	374	ASN
1	DP1	456	ASP
1	EP1	65	TYR
1	EP1	119	THR
1	EP1	141	LEU
1	EP1	195	GLN
1	EP1	212	GLN
1	EP1	230	PHE
1	EP1	345	SER
1	EP1	387	THR
2	FP1	33	LEU
2	FP1	45	VAL
2	FP1	77	MET
2	FP1	85	MET
2	FP1	127	PHE
2	FP1	140	ASP
2	FP1	141	LYS
2	FP1	191	MET
2	FP1	217	ASN
2	FP1	244	ASN
2	FP1	294	ASN
2	FP1	339	MET
2	FP1	350	MET
2	FP1	402	VAL
2	FP1	427	ASN
2	FP1	508	THR
2	FP1	509	CYS
2	FP1	517	CYS
2	FP1	596	PHE
2	FP1	603	TYR
2	FP1	637	PHE

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Mol	Chain	Res	Type
2	FP1	660	LEU
2	FP1	716	LEU
2	FP1	725	PHE
2	FP1	728	ILE
2	FP1	732	MET
2	FP1	761	PHE
2	FP1	800	PHE
2	FP1	825	LEU
2	FP1	837	PHE
2	FP1	911	PHE
2	FP1	930	PHE
2	GP1	57	MET
2	GP1	127	PHE
2	GP1	140	ASP
2	GP1	149	TYR
2	GP1	191	MET
2	GP1	262	ASP
2	GP1	290	LEU
2	GP1	331	SER
2	GP1	339	MET
2	GP1	486	ASP
2	GP1	508	THR
2	GP1	517	CYS
2	GP1	540	LEU
2	GP1	555	GLN
2	GP1	573	ASN
2	GP1	589	THR
2	GP1	630	ASP
2	GP1	639	TYR
2	GP1	648	PHE
2	GP1	696	TYR
2	GP1	709	ASN
2	GP1	728	ILE
2	GP1	759	MET
2	GP1	761	PHE
2	GP1	807	ASN
2	GP1	825	LEU
2	GP1	837	PHE
2	GP1	915	ILE
2	GP1	916	LEU
2	GP1	931	THR
2	GP1	936	LEU

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Mol	Chain	Res	Type
2	GP1	938	ASP
2	HP1	33	LEU
2	HP1	85	MET
2	HP1	93	MET
2	HP1	125	GLN
2	HP1	127	PHE
2	HP1	140	ASP
2	HP1	147	LEU
2	HP1	149	TYR
2	HP1	196	LYS
2	HP1	262	ASP
2	HP1	285	ASN
2	HP1	295	GLN
2	HP1	299	LYS
2	HP1	325	LEU
2	HP1	326	GLN
2	HP1	348	GLN
2	HP1	368	ASN
2	HP1	369	ASP
2	HP1	393	GLN
2	HP1	430	MET
2	HP1	431	MET
2	HP1	509	CYS
2	HP1	514	SER
2	HP1	515	LEU
2	HP1	530	ILE
2	HP1	540	LEU
2	HP1	557	GLN
2	HP1	564	SER
2	HP1	603	TYR
2	HP1	612	CYS
2	HP1	639	TYR
2	HP1	661	MET
2	HP1	696	TYR
2	HP1	723	PHE
2	HP1	725	PHE
2	HP1	728	ILE
2	HP1	758	TYR
2	HP1	759	MET
2	HP1	837	PHE
2	HP1	911	PHE
2	HP1	936	LEU

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Mol	Chain	Res	Type
2	IP1	33	LEU
2	IP1	38	LEU
2	IP1	42	PHE
2	IP1	50	HIS
2	IP1	57	MET
2	IP1	127	PHE
2	IP1	140	ASP
2	IP1	221	GLU
2	IP1	262	ASP
2	IP1	275	LEU
2	IP1	285	ASN
2	IP1	291	ASN
2	IP1	299	LYS
2	IP1	325	LEU
2	IP1	363	THR
2	IP1	369	ASP
2	IP1	431	MET
2	IP1	450	ARG
2	IP1	452	PHE
2	IP1	509	CYS
2	IP1	543	ASP
2	IP1	546	LYS
2	IP1	564	SER
2	IP1	576	MET
2	IP1	603	TYR
2	IP1	604	TYR
2	IP1	637	PHE
2	IP1	639	TYR
2	IP1	660	LEU
2	IP1	671	PHE
2	IP1	723	PHE
2	IP1	736	MET
2	IP1	761	PHE
2	IP1	776	MET
2	IP1	837	PHE
2	IP1	905	TRP
2	IP1	930	PHE
2	JP1	29	PRO
2	JP1	55	GLN
2	JP1	57	MET
2	JP1	81	MET
2	JP1	93	MET

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Mol	Chain	Res	Type
2	JP1	109	PHE
2	JP1	127	PHE
2	JP1	285	ASN
2	JP1	293	THR
2	JP1	325	LEU
2	JP1	326	GLN
2	JP1	331	SER
2	JP1	359	THR
2	JP1	387	GLU
2	JP1	389	CYS
2	JP1	393	GLN
2	JP1	406	THR
2	JP1	430	MET
2	JP1	457	ASN
2	JP1	525	ASP
2	JP1	547	GLN
2	JP1	564	SER
2	JP1	568	TYR
2	JP1	596	PHE
2	JP1	603	TYR
2	JP1	611	ASP
2	JP1	624	LEU
2	JP1	661	MET
2	JP1	696	TYR
2	JP1	704	TRP
2	JP1	717	ILE
2	JP1	723	PHE
2	JP1	724	ILE
2	JP1	800	PHE
2	JP1	827	TYR
2	JP1	845	GLN
2	JP1	903	THR
2	JP1	941	LEU
3	KP1	12	PHE
3	KP1	16	ARG
3	KP1	36	PHE
3	KP1	38	LYS
3	LP1	12	PHE
3	MP1	7	ASN
3	MP1	12	PHE
3	MP1	37	PHE
3	MP1	40	ARG

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Mol	Chain	Res	Type
3	NP1	11	LEU
3	NP1	12	PHE
3	NP1	16	ARG
3	NP1	36	PHE
3	NP1	37	PHE
3	OP1	1	MET
3	OP1	12	PHE
3	OP1	16	ARG
3	OP1	18	ARG
3	OP1	37	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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.

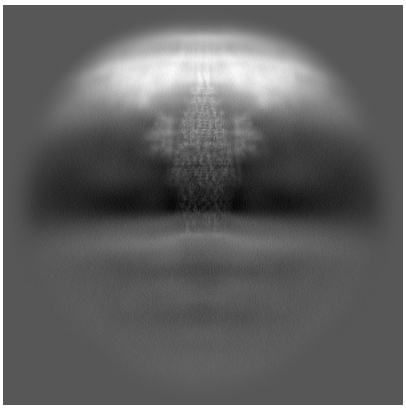
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-49396. These allow visual inspection of the internal detail of the map and identification of artifacts.

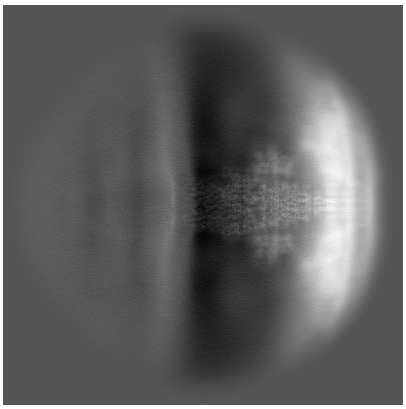
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

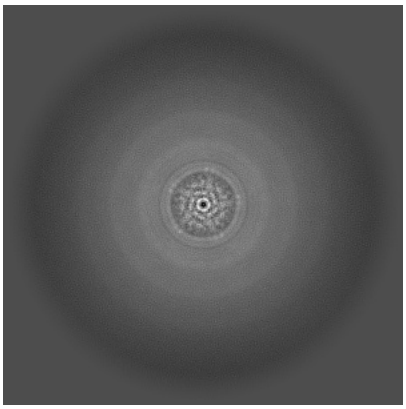
6.1.1 Primary map



X

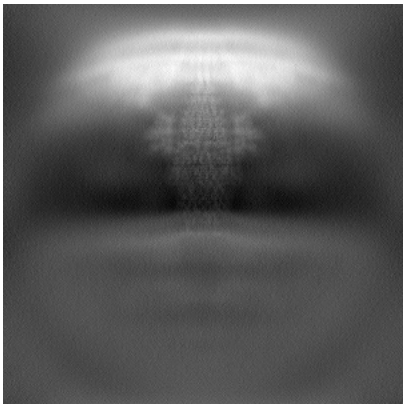


Y

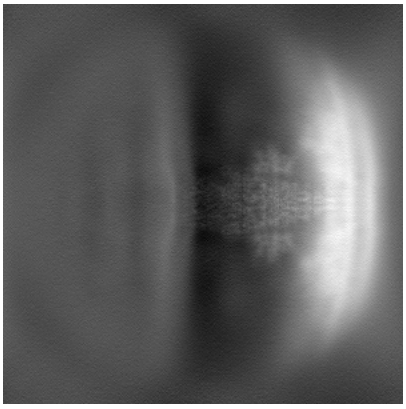


Z

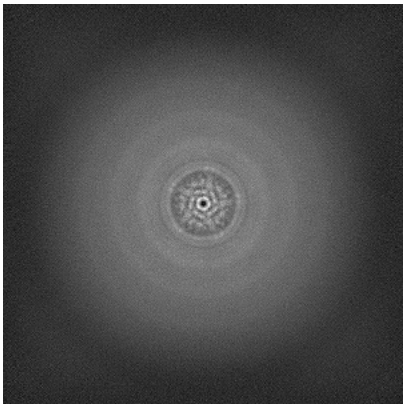
6.1.2 Raw map



X



Y

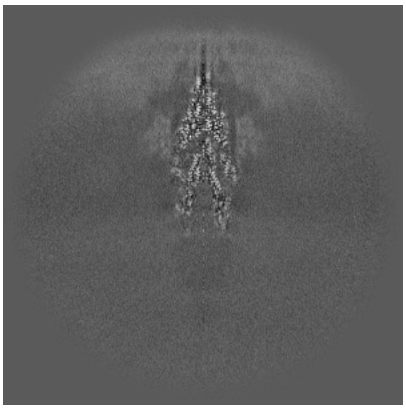


Z

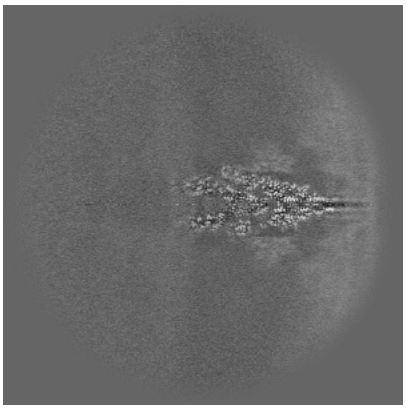
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

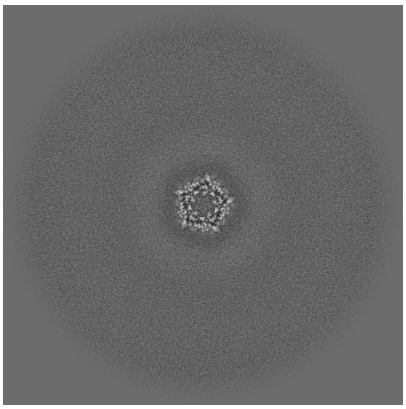
6.2.1 Primary map



X Index: 256

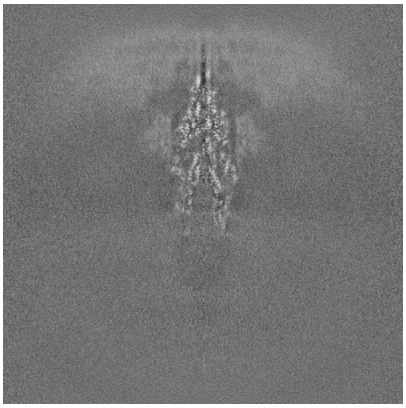


Y Index: 256

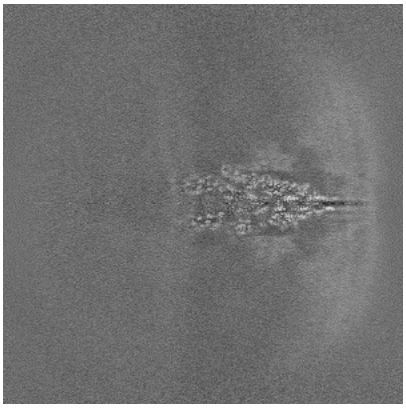


Z Index: 256

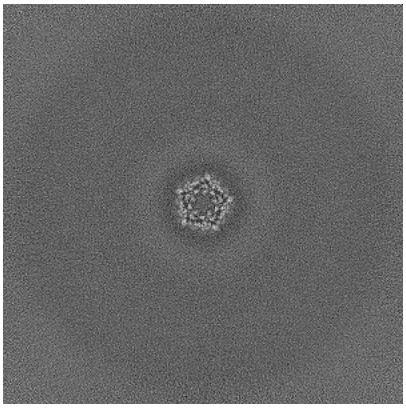
6.2.2 Raw map



X Index: 256



Y Index: 256

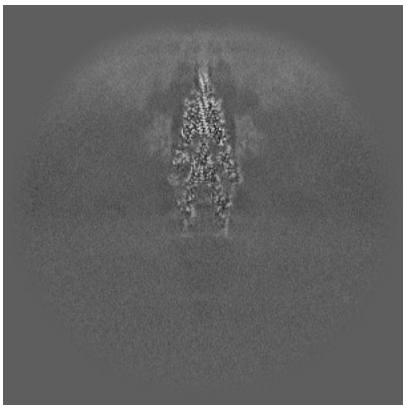


Z Index: 256

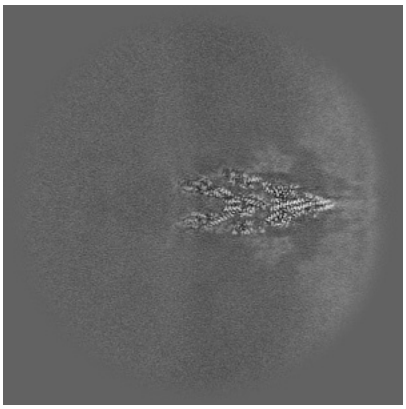
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

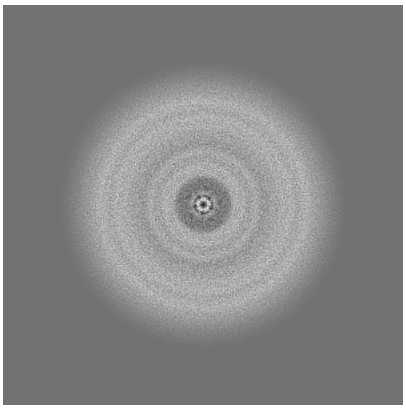
6.3.1 Primary map



X Index: 262

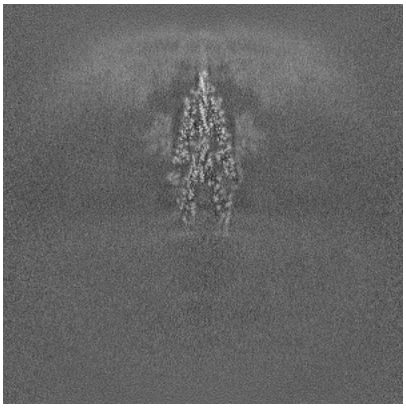


Y Index: 262

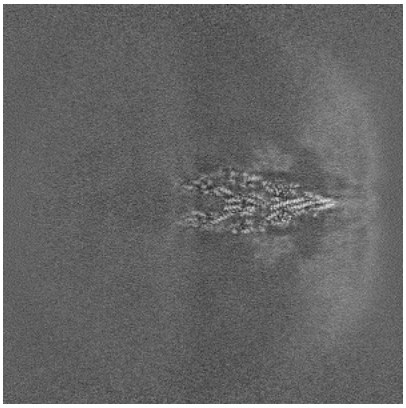


Z Index: 428

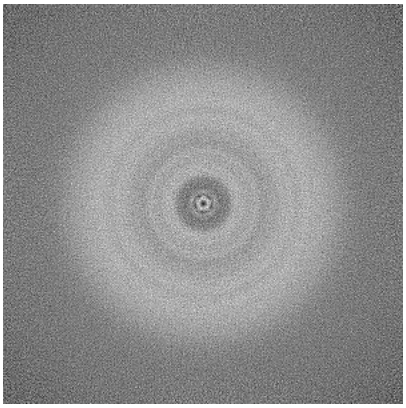
6.3.2 Raw map



X Index: 263



Y Index: 262

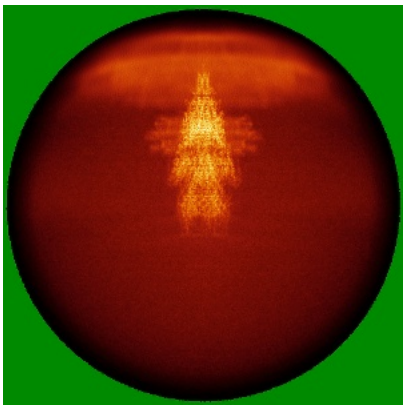


Z Index: 429

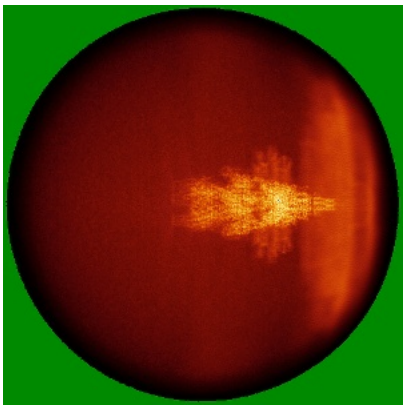
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

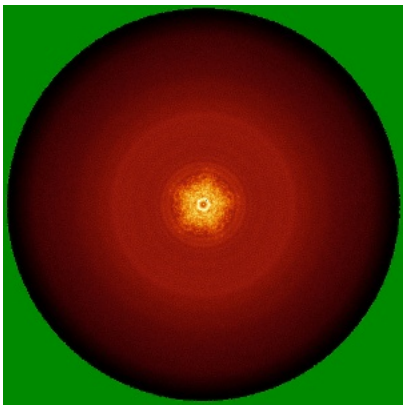
6.4.1 Primary map



X

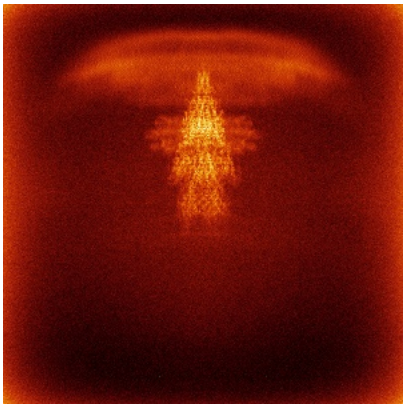


Y

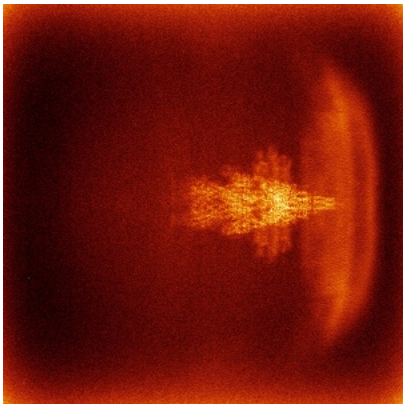


Z

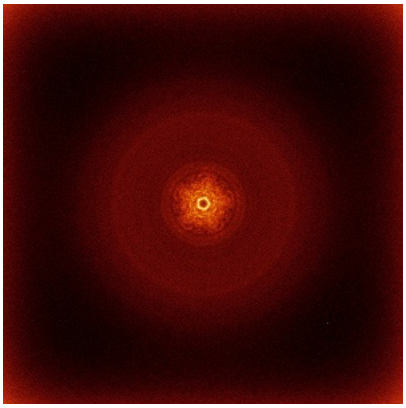
6.4.2 Raw map



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 0.2. 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.

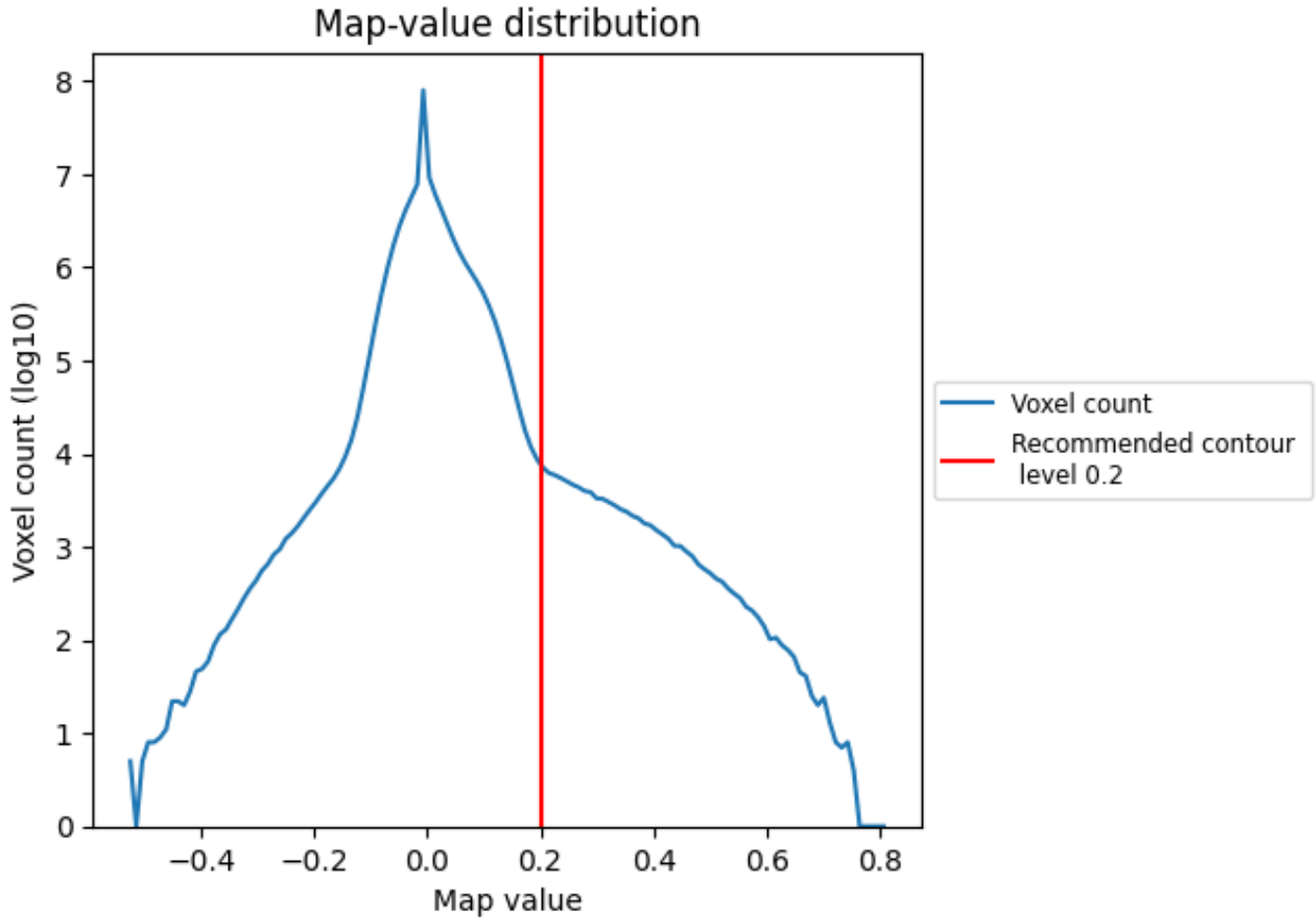
6.6 Mask visualisation (i)

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

7 Map analysis

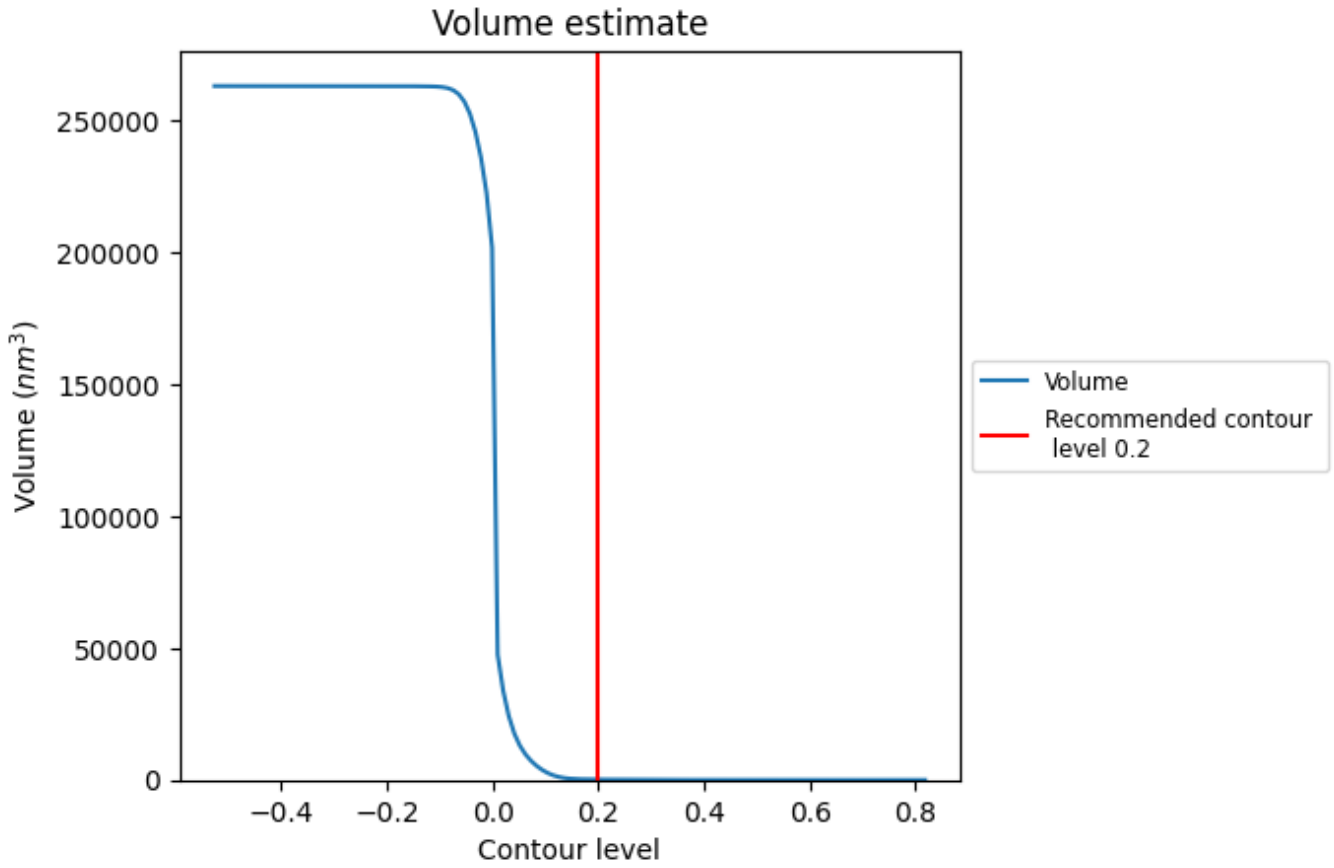
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

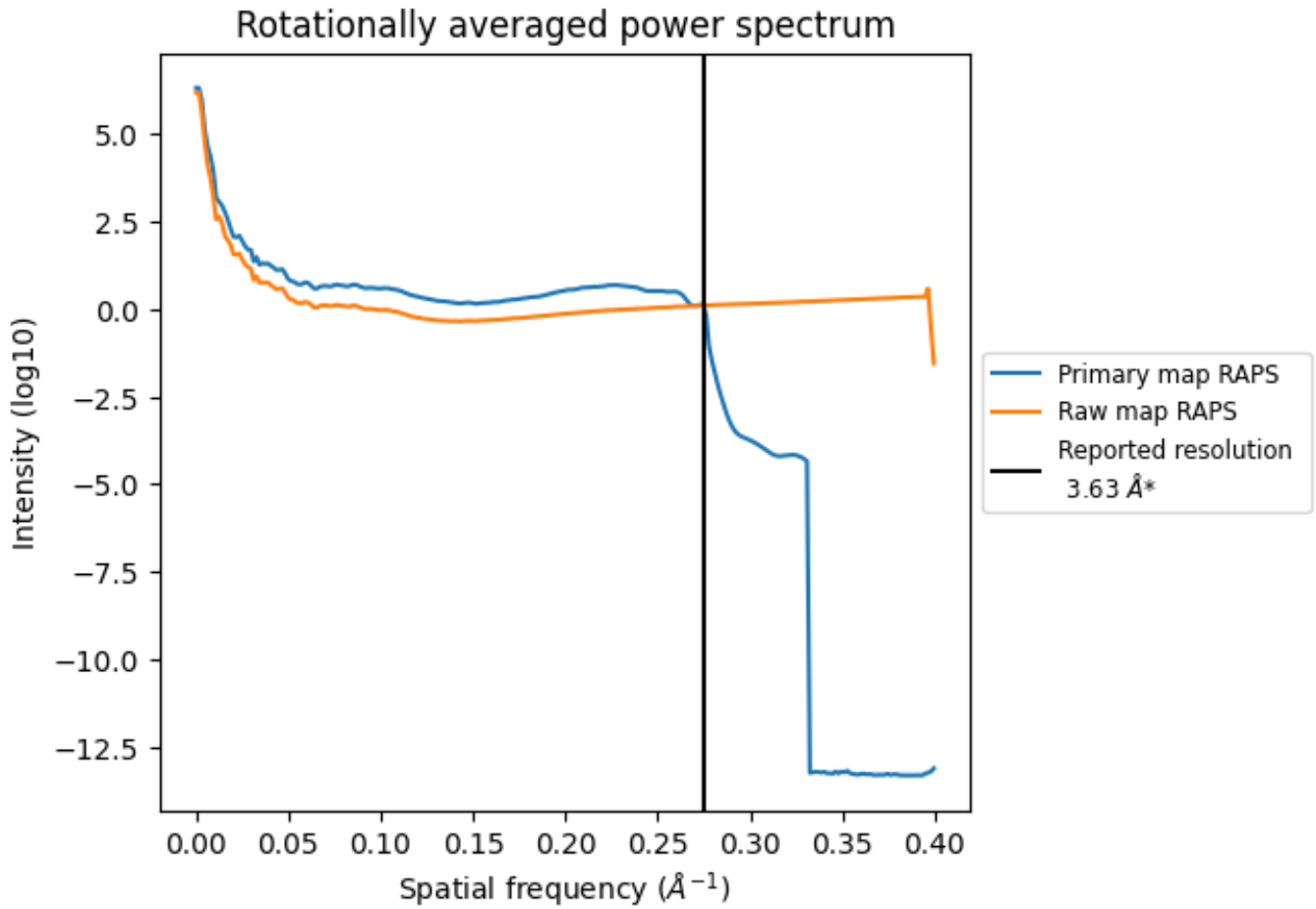
7.2 Volume estimate



The volume at the recommended contour level is 173 nm^3; this corresponds to an approximate mass of 156 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 (i)

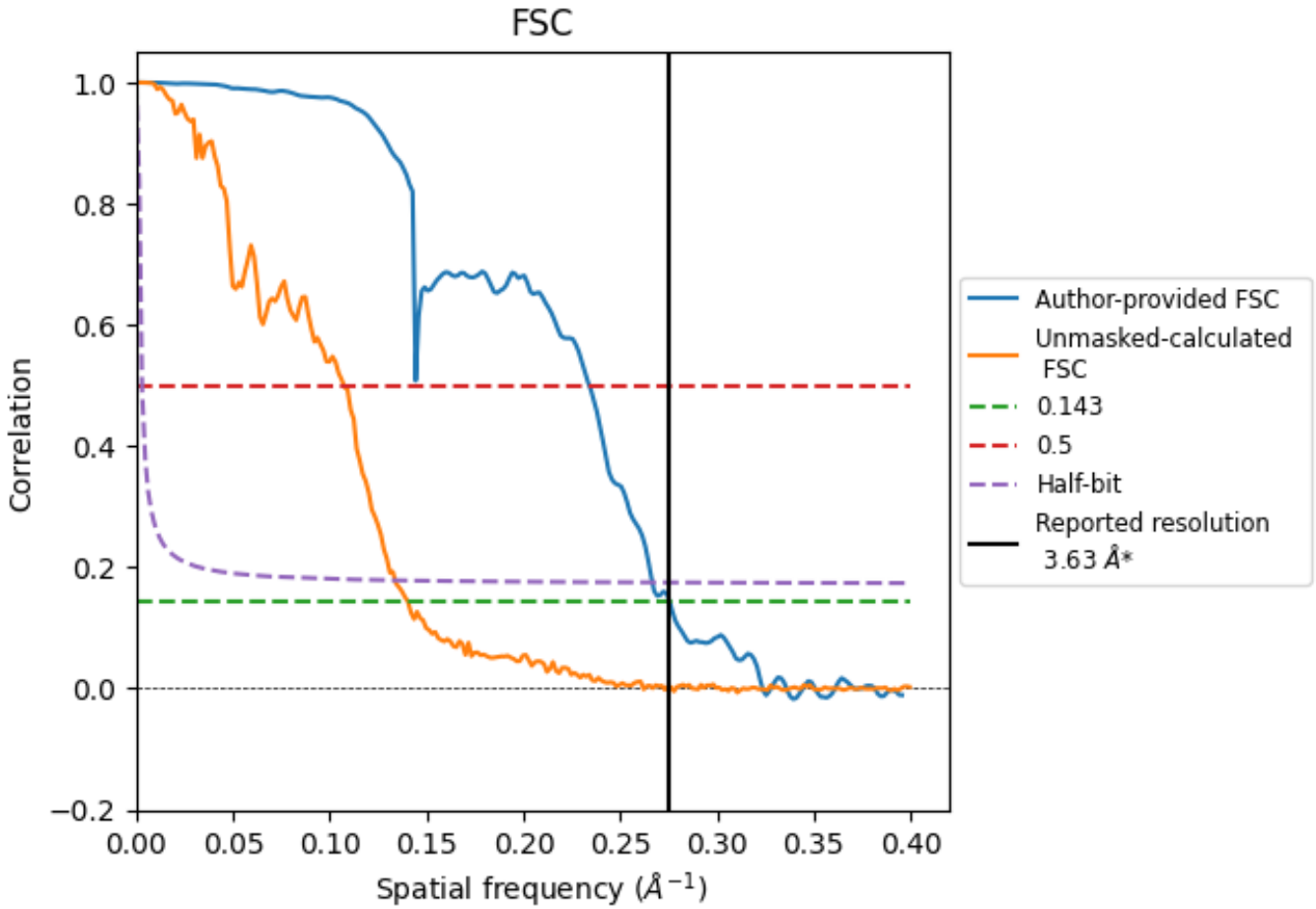


*Reported resolution corresponds to spatial frequency of 0.275 $Å^{-1}$

8 Fourier-Shell correlation

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



*Reported resolution corresponds to spatial frequency of 0.275 Å^{-1}

8.2 Resolution estimates (i)

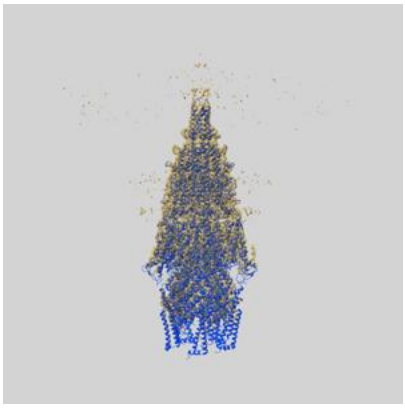
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.63	-	-
Author-provided FSC curve	3.63	4.27	3.75
Unmasked-calculated*	7.12	9.32	7.47

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.12 differs from the reported value 3.63 by more than 10 %

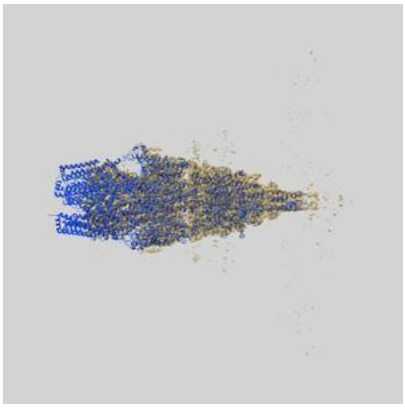
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-49396 and PDB model 9NGY. Per-residue inclusion information can be found in section 3 on page 6.

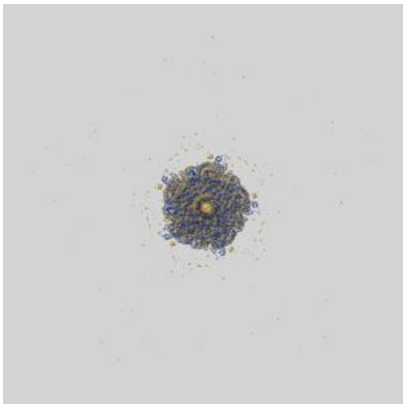
9.1 Map-model overlay



X



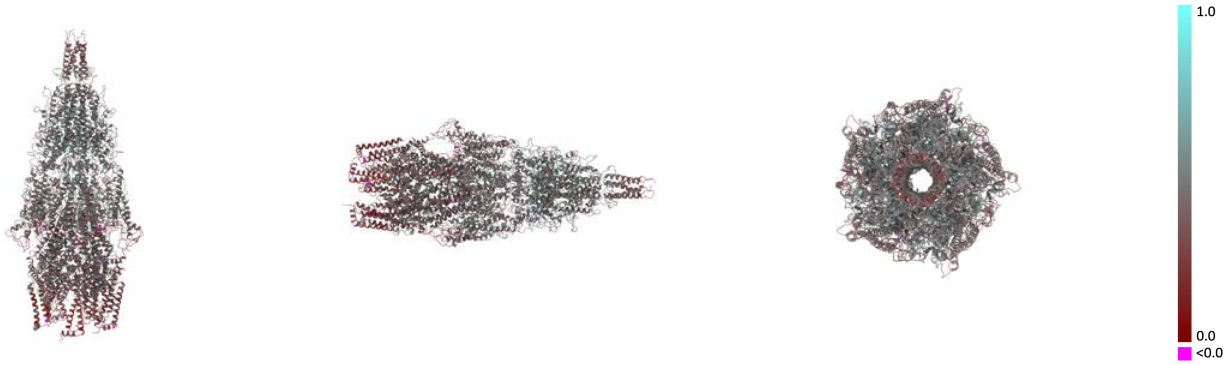
Y



Z

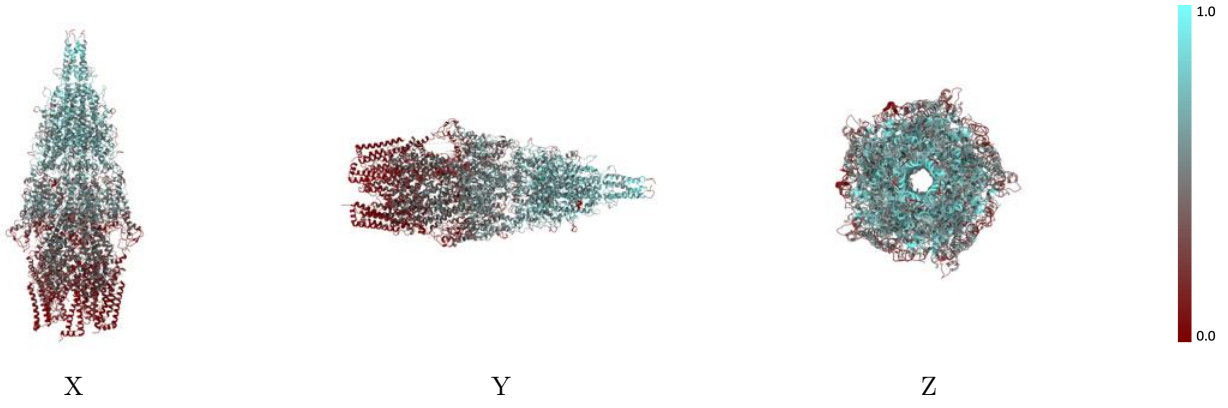
The images above show the 3D surface view of the map at the recommended contour level 0.2 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



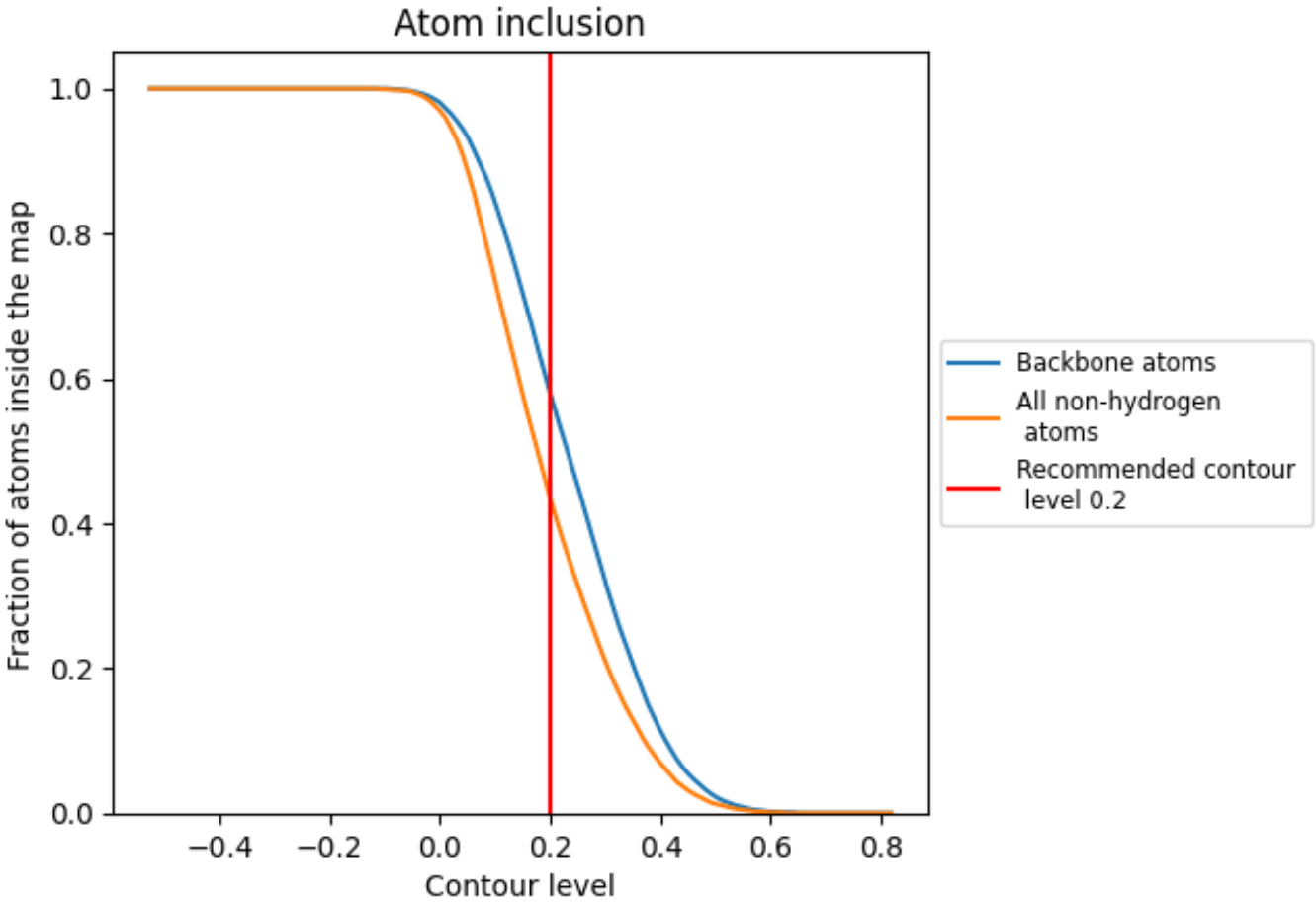
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.2).

9.4 Atom inclusion (i)



At the recommended contour level, 58% of all backbone atoms, 43% 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 (0.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4340	0.4130
AP1	0.6400	0.4630
BP1	0.6390	0.4630
CP1	0.6390	0.4630
DP1	0.6380	0.4640
EP1	0.6410	0.4630
FP1	0.3560	0.3990
GP1	0.3560	0.3970
HP1	0.3540	0.3970
IP1	0.3510	0.3960
JP1	0.3510	0.3960
KP1	0.0400	0.2680
LP1	0.0490	0.2740
MP1	0.0400	0.2680
NP1	0.0520	0.2460
OP1	0.0370	0.2420