Full wwPDB EM Validation Report

Feb 19, 2025 – 06:27 PM JST

PDB ID	:	9JGA
EMDB ID	:	EMD-61460
Title	:	P22 procapsid portal
Authors	:	Liu, H.R.; Xiao, H.
Deposited on	:	2024-09-06
Resolution	:	3.00 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:

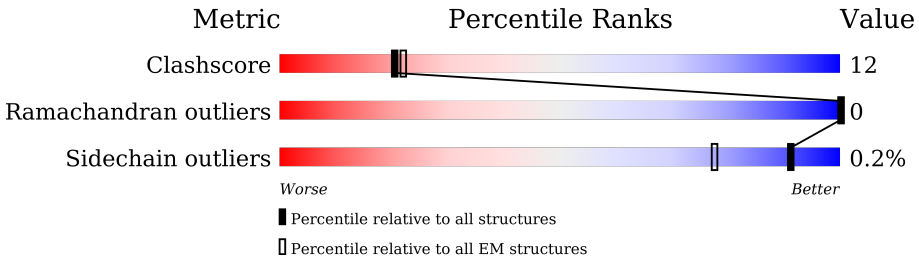
EMDB validation analysis	:	0.0.1.dev117
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41.2

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 3.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	A	725	15% 55% 20% 25%
1	B	725	16% 52% 23% 25%
1	C	725	14% 53% 21% 25%
1	D	725	15% 53% 22% 25%
1	E	725	16% 52% 22% 25%
1	F	725	15% 52% 23% 25%
1	G	725	15% 54% 21% 25%
1	H	725	16% 52% 22% 25%

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Mol	Chain	Length	Quality of chain
1	I	725	15% 53% 22% 25%
1	J	725	15% 55% 20% 25%
1	K	725	15% 53% 21% 25%
1	L	725	15% 53% 22% 25%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 52692 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.

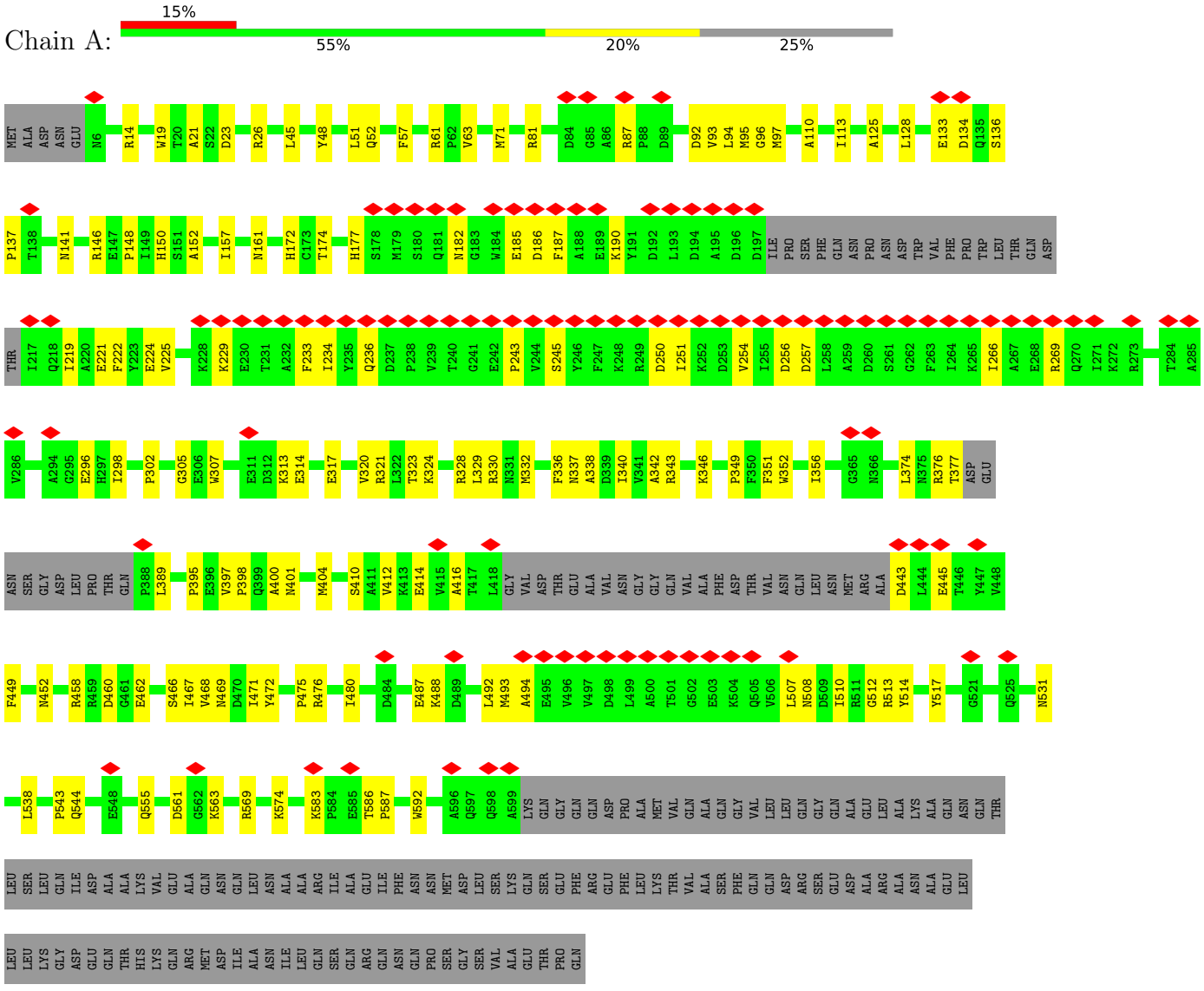
- Molecule 1 is a protein called Portal protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	B	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	C	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	D	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	E	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	F	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	G	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	H	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	I	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	J	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	K	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		
1	L	541	Total	C	N	O	S	0	0
			4391	2769	752	850	20		

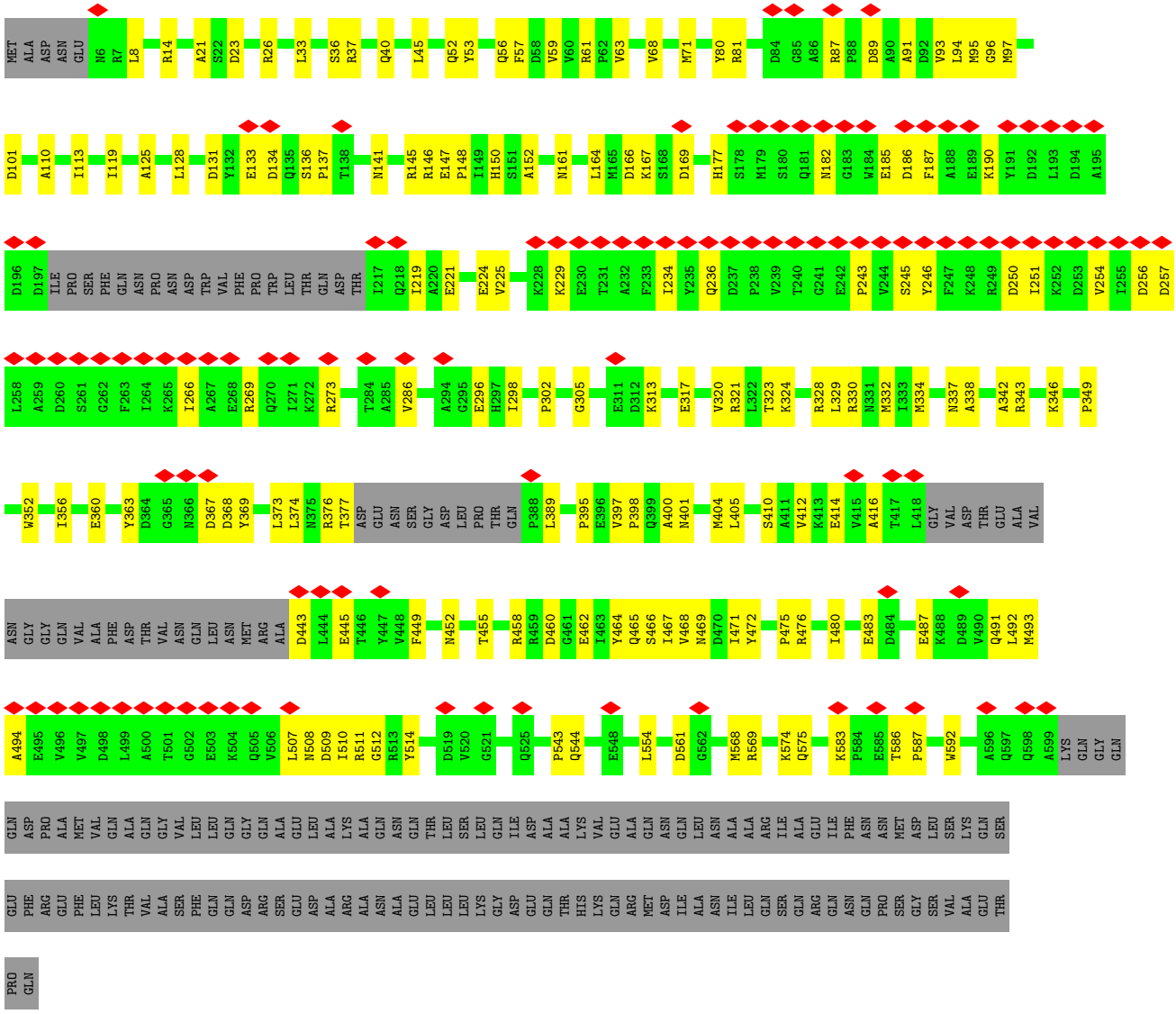
3 Residue-property plots (i)

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: Portal protein

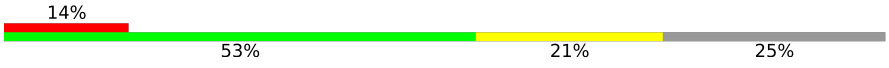


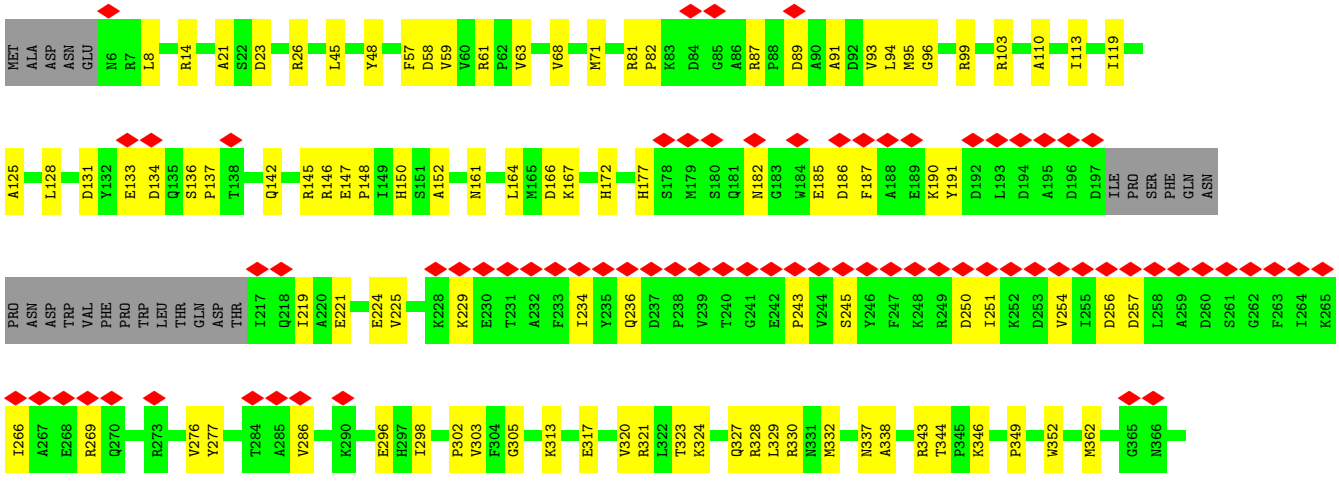
• Molecule 1: Portal protein

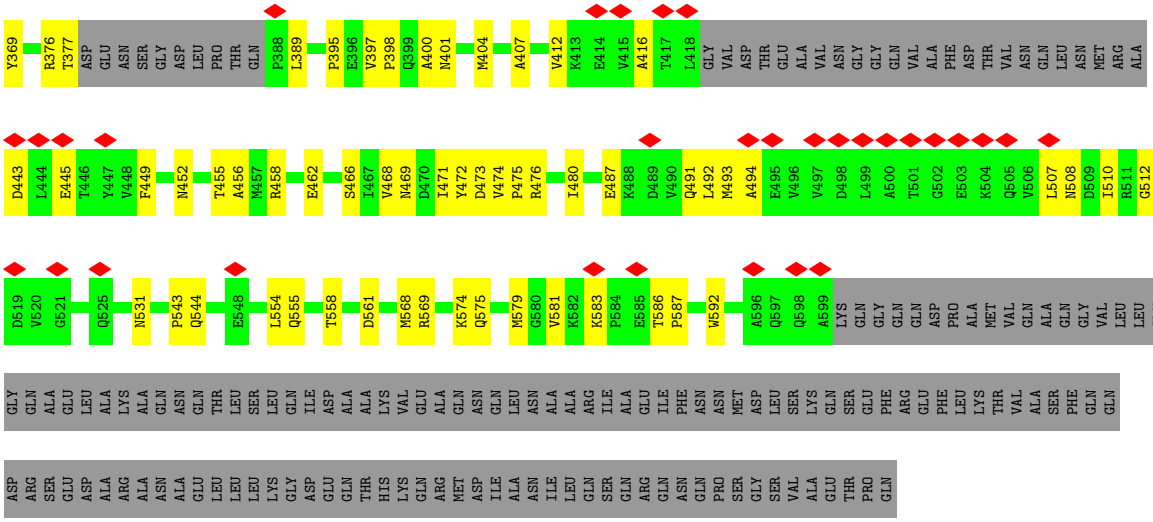


• Molecule 1: Portal protein

Chain C:

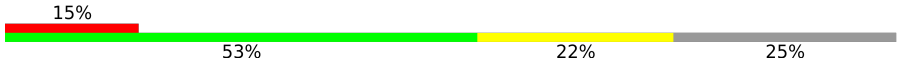


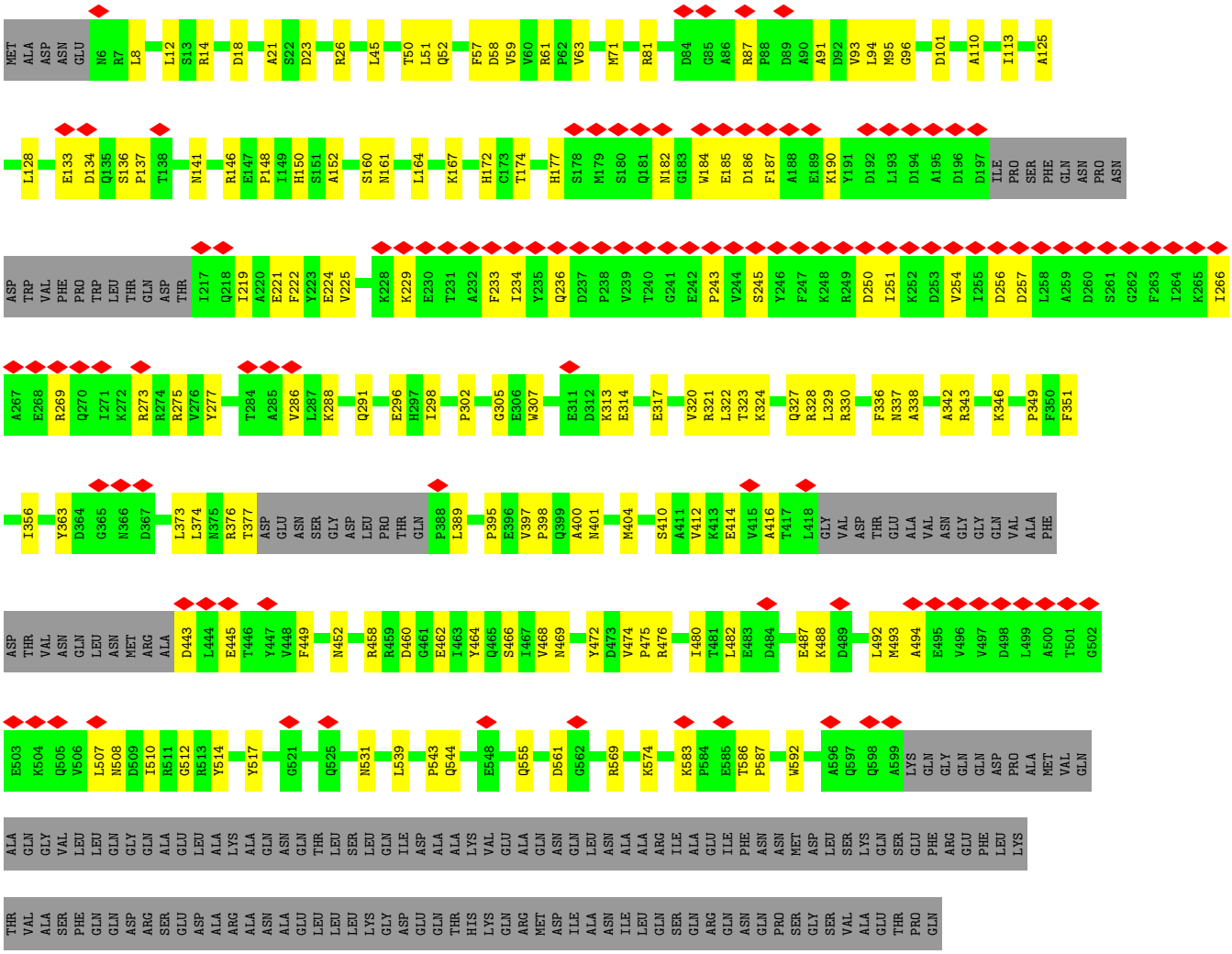




• Molecule 1: Portal protein

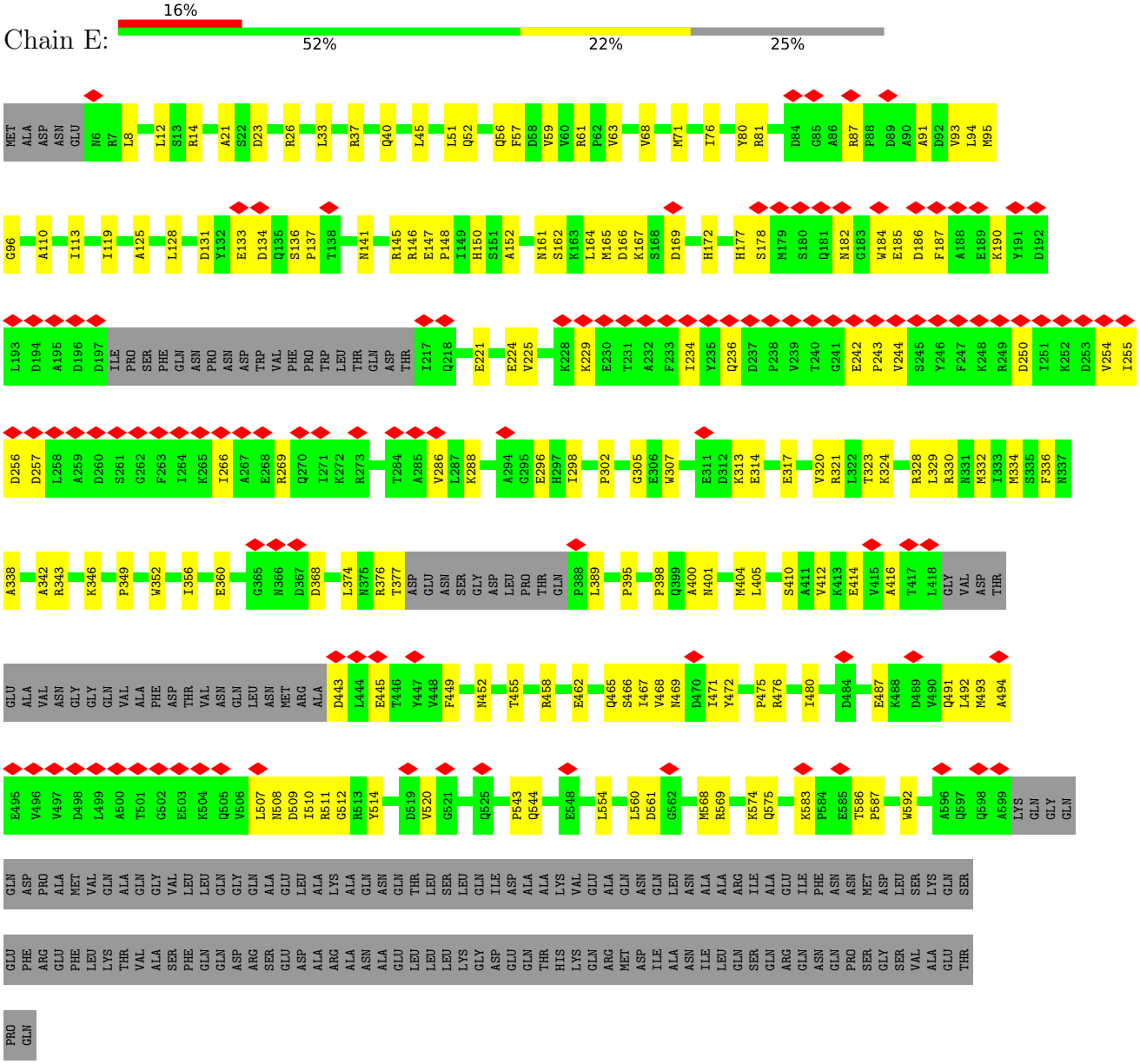
Chain D:





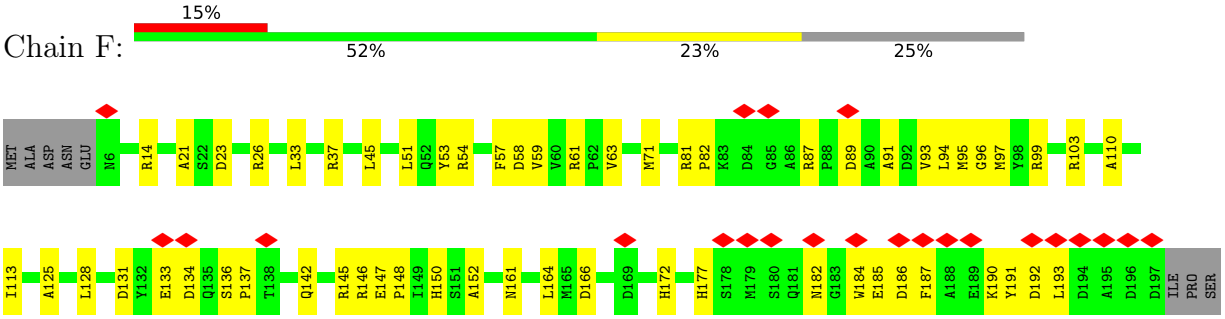
• Molecule 1: Portal protein

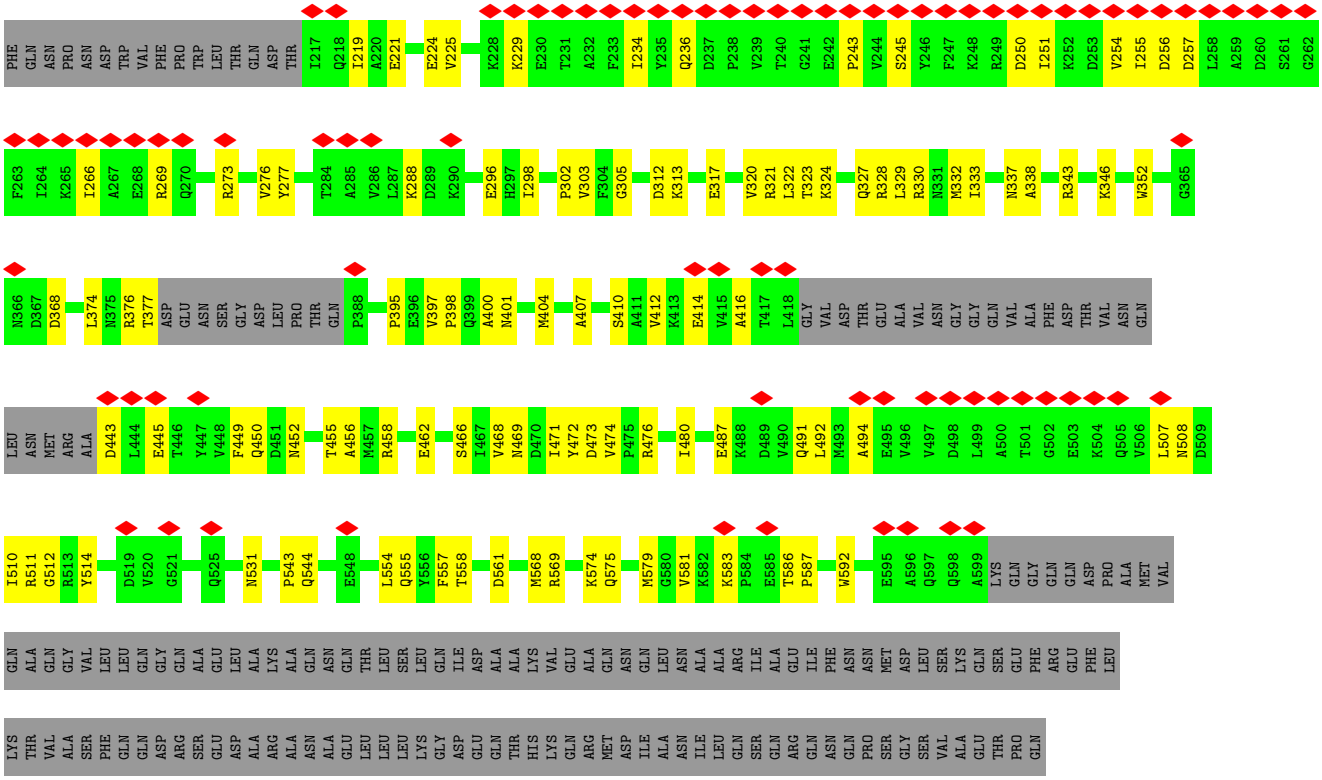
Chain E:



• Molecule 1: Portal protein

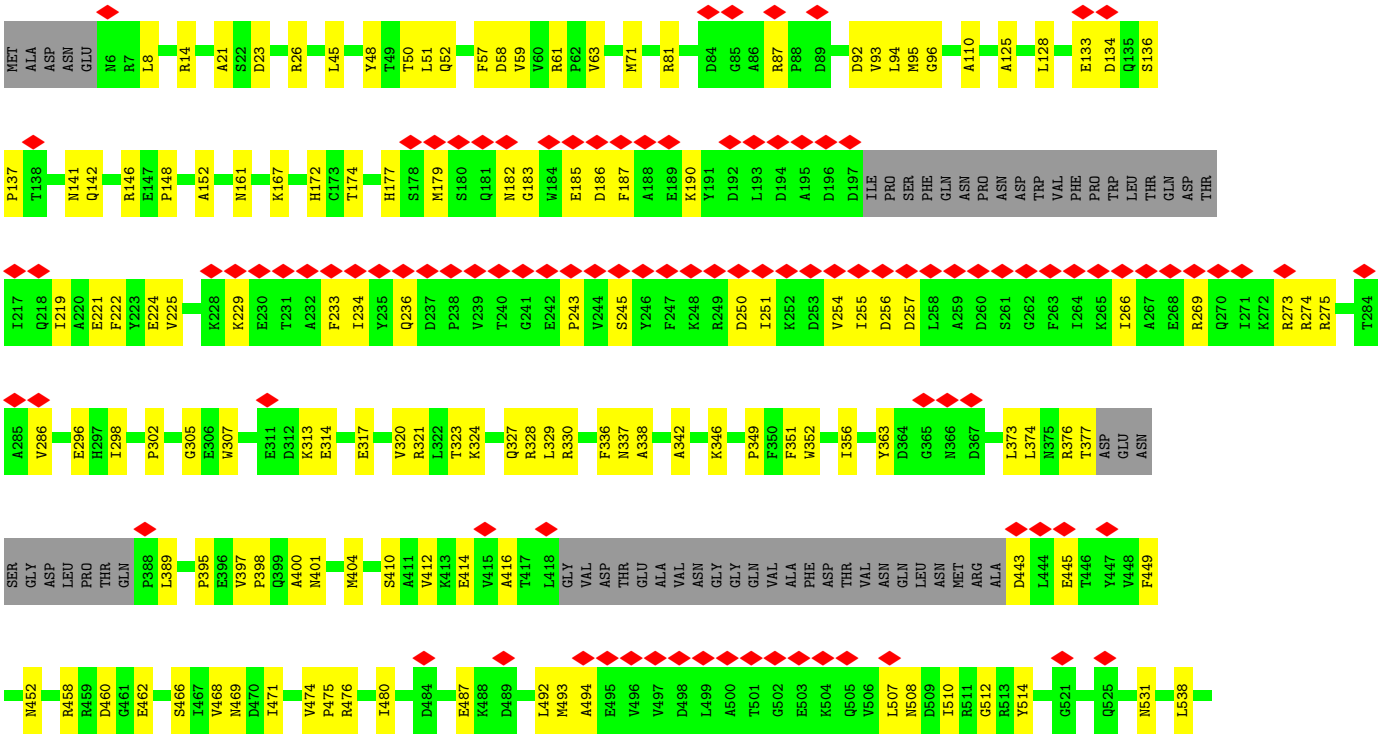
Chain F:

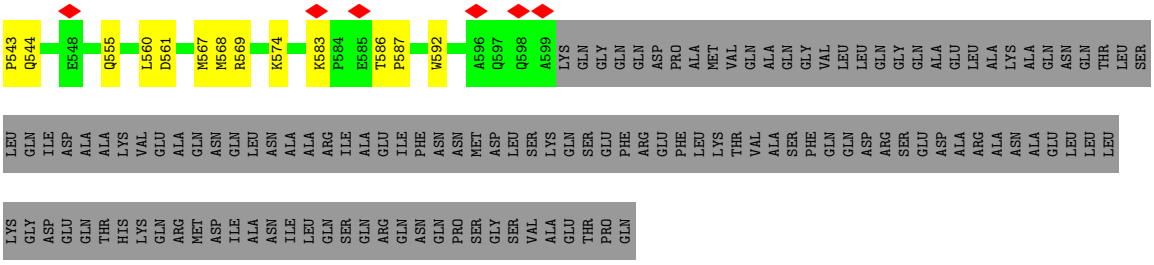




• Molecule 1: Portal protein

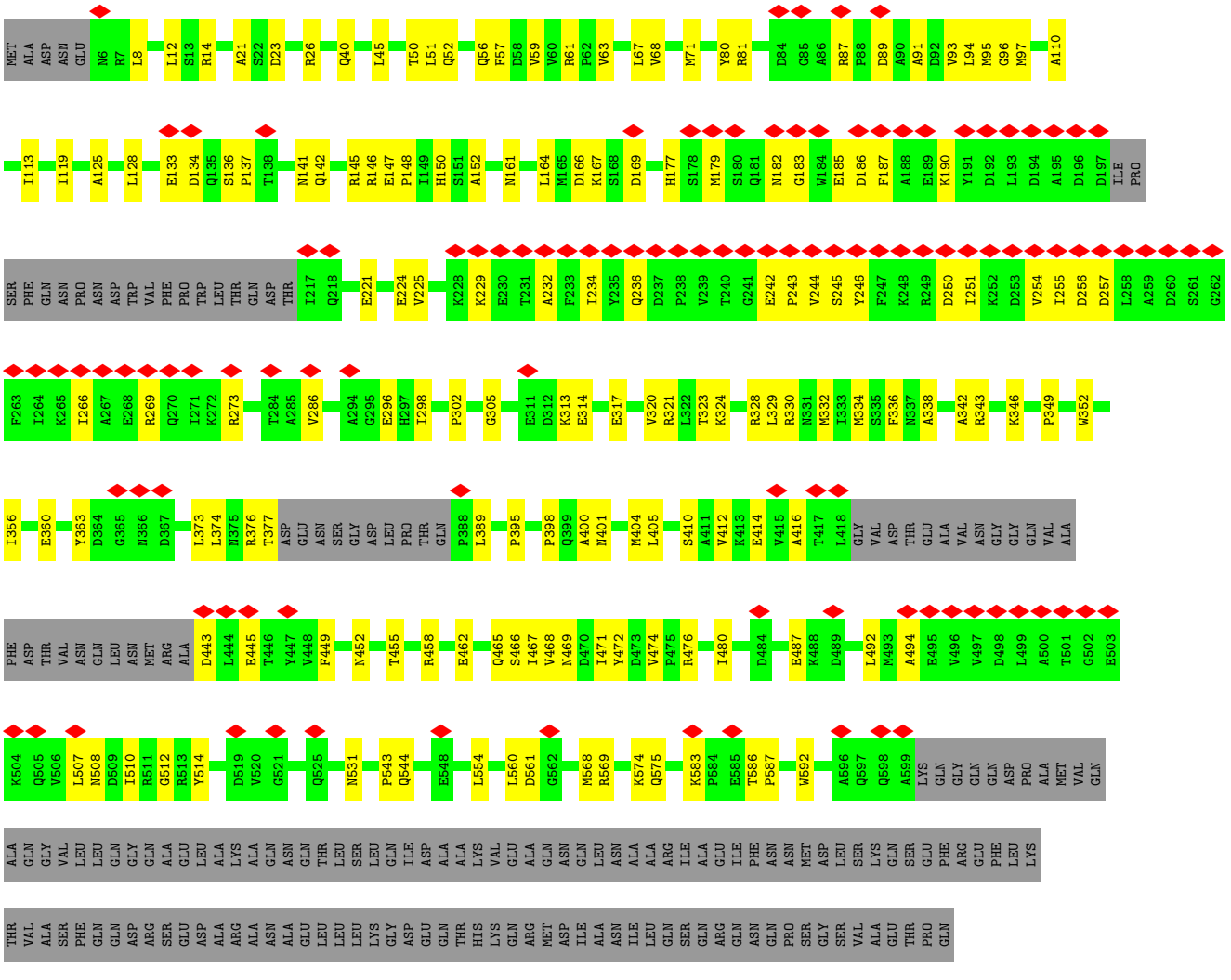
Chain G:





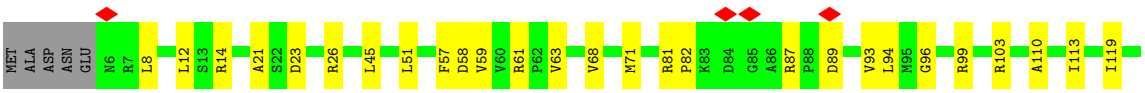
• Molecule 1: Portal protein

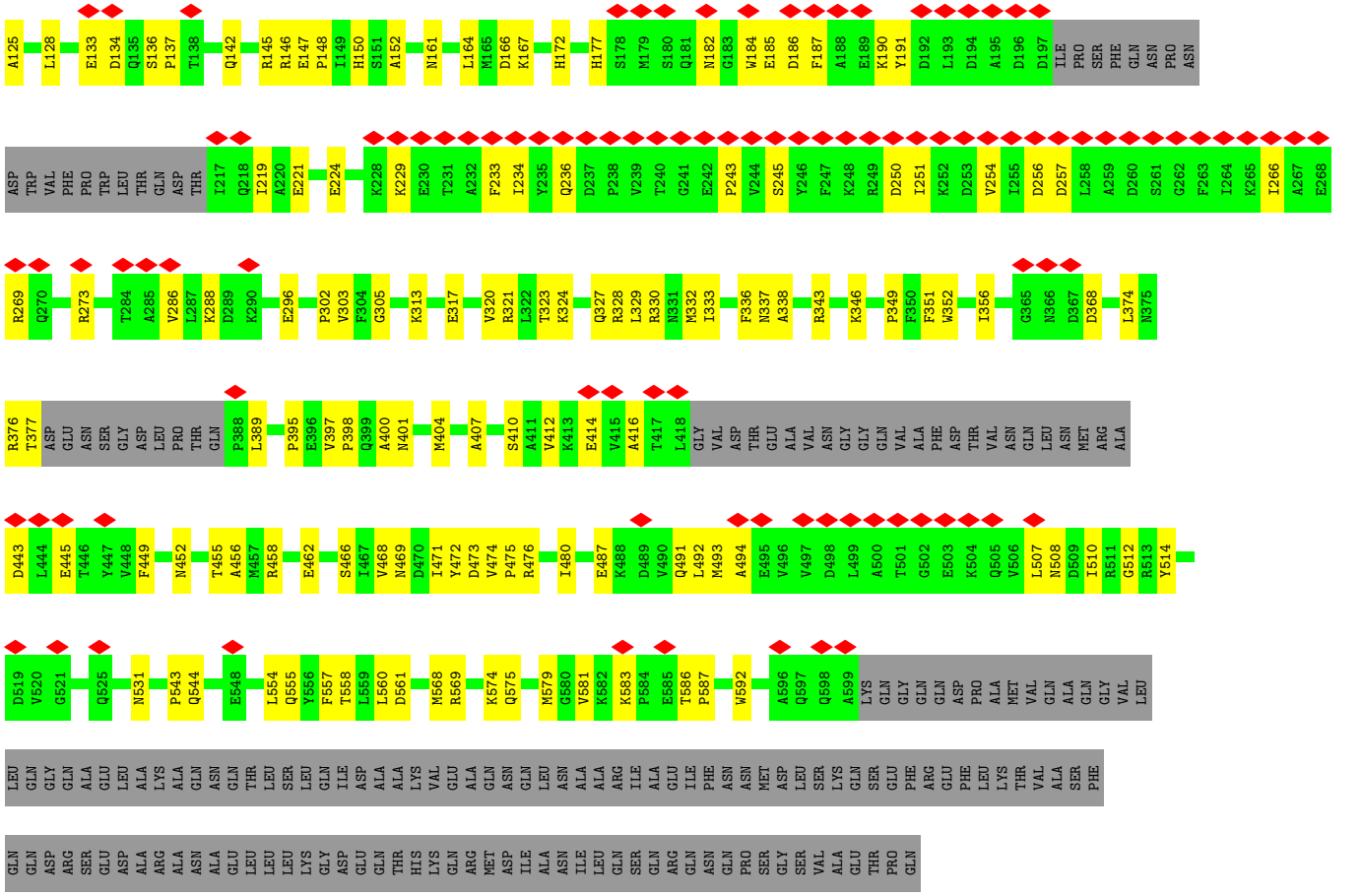
Chain H:



• Molecule 1: Portal protein

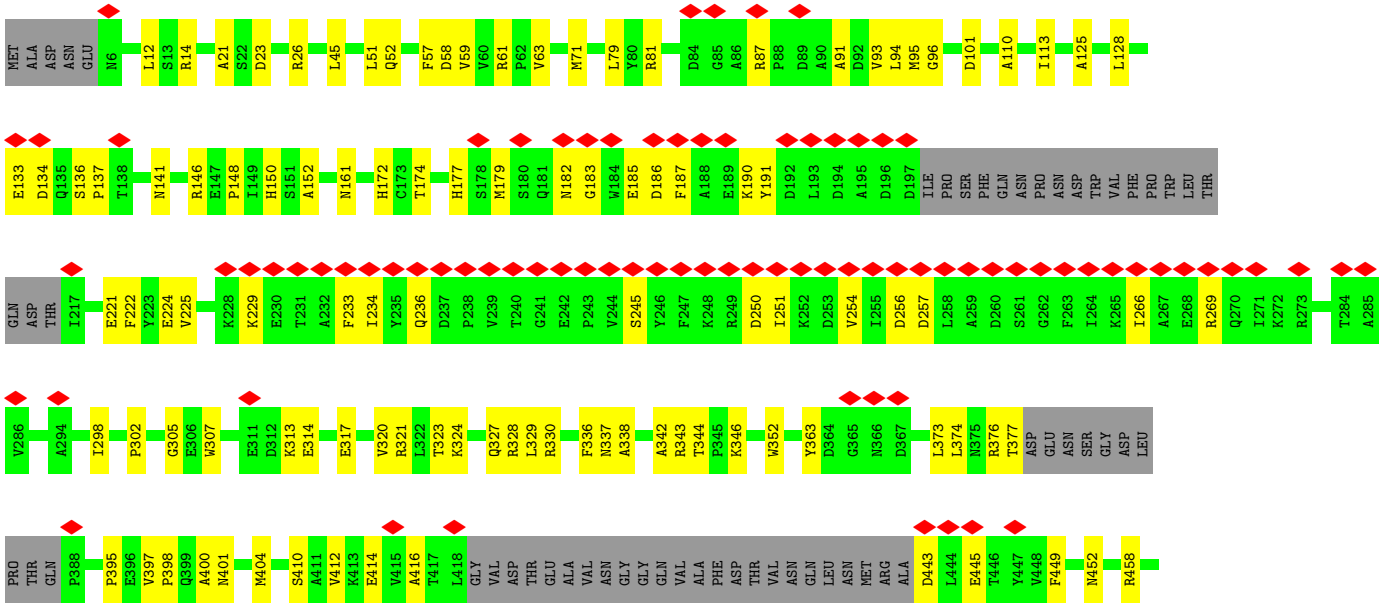
Chain I:

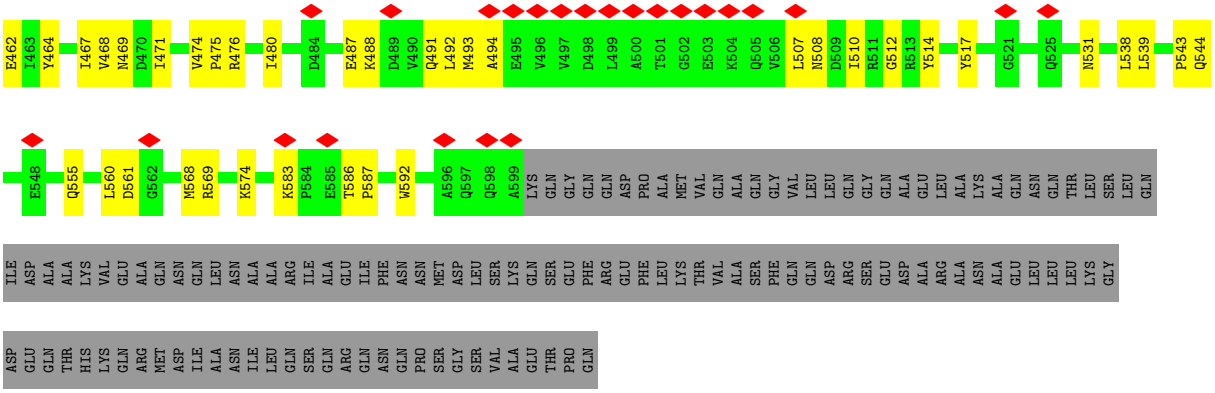




• Molecule 1: Portal protein

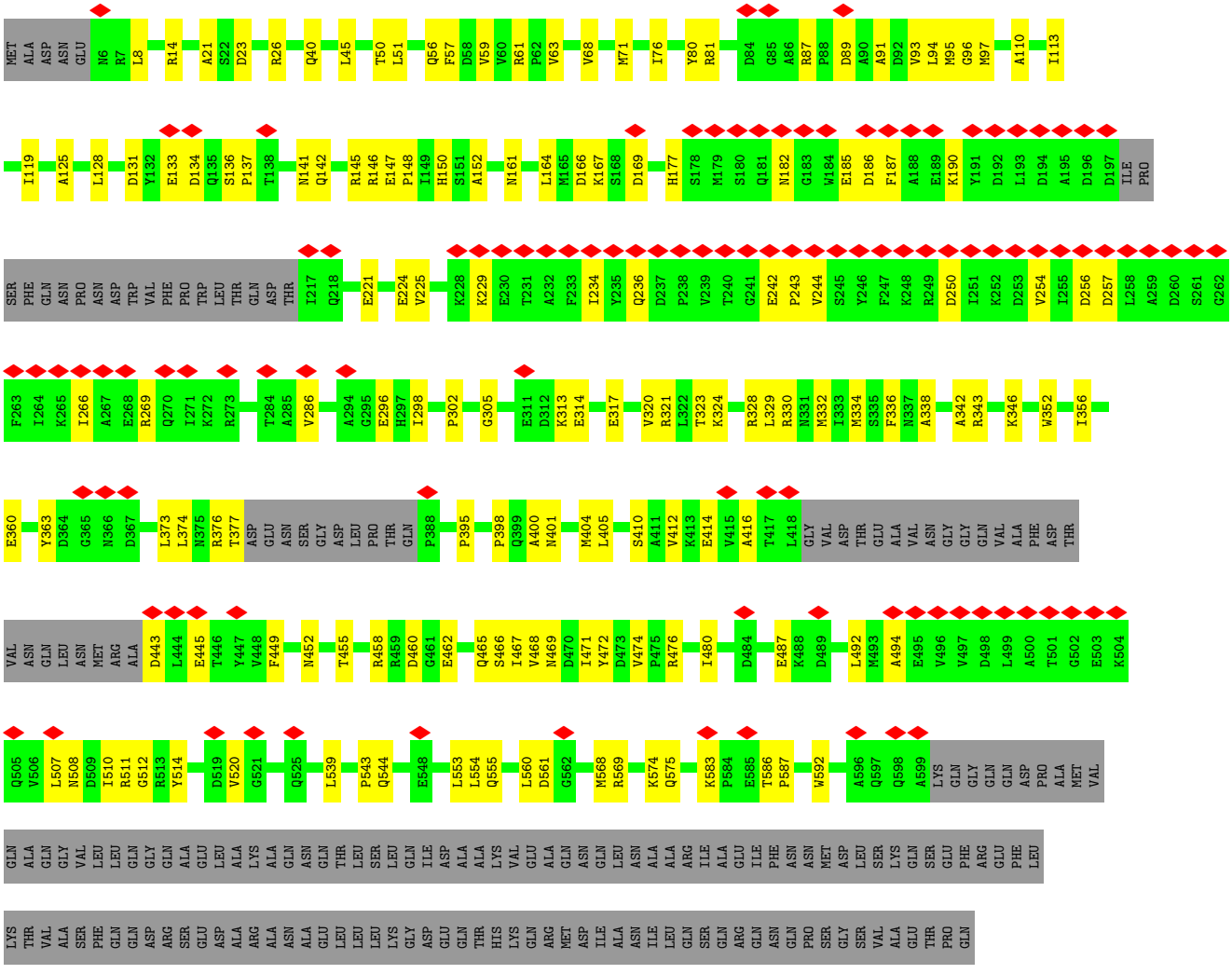
Chain J:





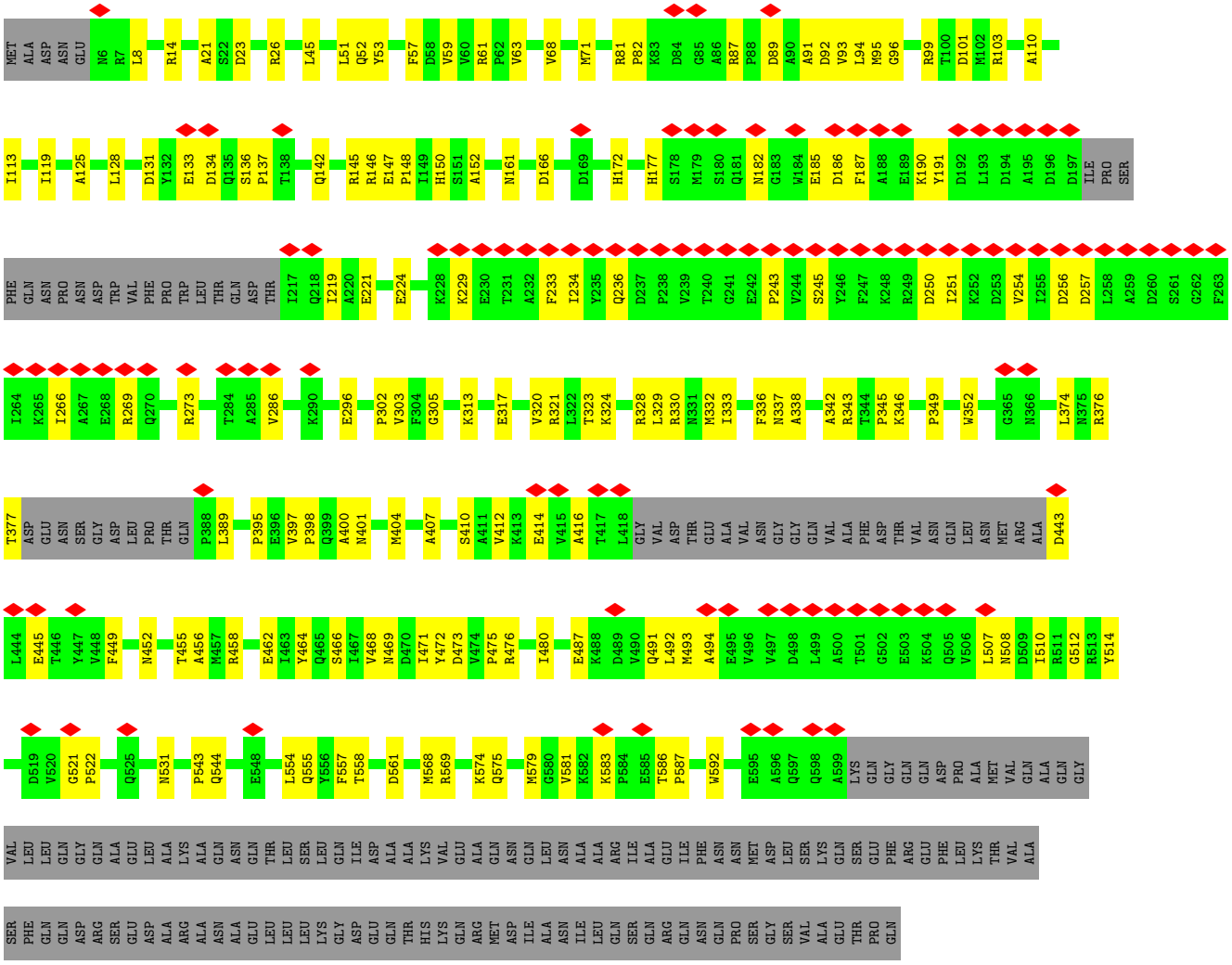
• Molecule 1: Portal protein

Chain K:



• Molecule 1: Portal protein

Chain L:


MET ALA ASP ASN GLU N6 R7 L8 R14 A21 S22 D23 R26 L45 L51 Q52 Y53 F57 D58 V59 V60 R61 P62 V63 V68 M71 R81 P82 K83 D84 G85 A86 R87 P88 D89 A90 A91 D92 V93 L94 M95 G96 R99 T100 D101 M102 R103 A110
I113 I119 A125 L128 D131 Y132 E133 D134 Q135 S136 P137 T138 Q142 R145 R146 E147 P148 I149 H150 S151 A152 N161 D166 D169 H172 H177 S178 M179 S180 Q181 N182 G183 W184 E185 D186 F187 A188 E189 K190 Y191 D192 L193 D194 A195 D196 D197 ILE PRO SER
PHE GLN ASN PRO ASN ASP TRP VAL PHE PRO TRP LEU THR GLN ASP THR I217 Q218 I219 A220 E221 E224 K228 K229 E230 T231 A232 F233 I234 Y235 Q236 D237 P238 V239 T240 G241 E242 P243 V244 S245 Y246 F247 K248 R249 D250 I251 K252 D253 V254 I255 D256 D257 L258 A259 D260 S261 G262 F263
I264 K265 I266 A267 E268 R269 Q270 R273 T284 A285 V286 K290 E296 P302 V303 F304 G305 K313 E317 V320 R321 L322 T323 K324 R328 L329 R330 N331 M332 I333 F336 N337 A338 A342 R343 T344 P345 K346 P349 W352 G365 N366 L374 N375 R376
T377 ASP GLU ASN SER GLY ASP LEU PRO THR GLN P388 L389 P395 E396 V397 P398 Q399 A400 N401 M404 A407 S410 A411 V412 K413 E414 V415 A416 T417 L418 GLY VAL ASP THR GLU ALA VAL ASN GLY GLY GLN VAL ALA PHE ASP THR VAL ASN GLN LEU ASN MET ARG ALA D443
L444 E445 T446 Y447 V448 F449 N452 T455 A456 M457 R458 E462 I463 Y464 Q465 S466 T467 V468 N469 D470 I471 Y472 D473 V474 P475 R476 I480 E487 K488 D489 V490 Q491 L492 M493 A494 E495 V496 V497 D498 L499 A500 T501 G502 E503 K504 Q505 V506 L507 N508 D509 I510 R511 G512 R513 Y514
D519 V520 G521 P522 Q525 N531 P543 Q544 E548 L554 Q555 Y556 F557 T558 D561 M568 R569 K574 Q575 M579 G580 V581 K582 K583 P584 E585 T586 P587 W592 E595 A596 Q597 Q598 A599 LYS GLN GLY GLN GLN ASP PRO ALA MET VAL GLN ALA GLN GLY
VAL LEU LEU GLN GLY GLN ALA GLU LEU ALA ALA LYS ALA ALA GLN ASN ASN GLN GLN THR LEU LEU SER LEU GLN ILE ASP ALA ALA ALA LYS VAL GLU ALA GLN ASN GLN LEU ASN ALA ALA ARG ILE ALA GLU ILE PHE ASN ASN MET ASP LEU SER LYS GLN SER GLU PHE ARG GLU PHE LEU LYS THR VAL ALA
SER PHE GLN GLN ASP ARG SER GLU ASP ALA ARG ALA ASN ALA GLU LEU LEU LEU LYS GLY ASP GLU GLN GLN THR HIS LYS GLN ARG MET ASP ILE ALA ASN ILE LEU GLN SER GLN ARG GLN ASN GLN PRO SER GLY SER VAL ALA GLU THR PRO GLN

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	22169	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	32	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	16.850	Depositor
Minimum map value	-10.584	Depositor
Average map value	0.010	Depositor
Map value standard deviation	0.883	Depositor
Recommended contour level	3.6	Depositor
Map size (Å)	381.59998, 381.59998, 381.59998	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.34	0/4479	0.54	0/6064
1	B	0.35	0/4479	0.54	0/6064
1	C	0.35	0/4479	0.54	0/6064
1	D	0.34	0/4479	0.53	0/6064
1	E	0.34	0/4479	0.54	0/6064
1	F	0.35	0/4479	0.54	0/6064
1	G	0.34	0/4479	0.54	0/6064
1	H	0.34	0/4479	0.54	0/6064
1	I	0.35	0/4479	0.54	0/6064
1	J	0.34	0/4479	0.54	0/6064
1	K	0.34	0/4479	0.54	0/6064
1	L	0.35	0/4479	0.54	0/6064
All	All	0.35	0/53748	0.54	0/72768

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	A	4391	0	4279	118	0
1	B	4391	0	4279	131	0
1	C	4391	0	4279	119	0
1	D	4391	0	4279	123	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	E	4391	0	4279	129	0
1	F	4391	0	4279	128	0
1	G	4391	0	4279	118	0
1	H	4391	0	4279	124	0
1	I	4391	0	4279	125	0
1	J	4391	0	4279	115	0
1	K	4391	0	4279	122	0
1	L	4391	0	4279	124	0
All	All	52692	0	51348	1233	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 (1233) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:186:ASP:OD2	1:J:161:ASN:ND2	2.10	0.84
1:H:186:ASP:OD2	1:I:161:ASN:ND2	2.11	0.83
1:C:401:ASN:ND2	1:C:404:MET:SD	2.58	0.77
1:B:401:ASN:ND2	1:B:404:MET:SD	2.58	0.77
1:A:186:ASP:OD2	1:B:161:ASN:ND2	2.17	0.77
1:K:401:ASN:ND2	1:K:404:MET:SD	2.58	0.76
1:A:343:ARG:HH21	1:L:346:LYS:HZ1	1.33	0.76
1:H:401:ASN:ND2	1:H:404:MET:SD	2.58	0.76
1:I:333:ILE:HD11	1:I:404:MET:HG2	1.68	0.76
1:L:333:ILE:HD11	1:L:404:MET:HG2	1.68	0.76
1:A:401:ASN:ND2	1:A:404:MET:SD	2.59	0.76
1:A:96:GLY:HA3	1:A:480:ILE:HG23	1.67	0.75
1:F:333:ILE:HD11	1:F:404:MET:HG2	1.68	0.75
1:D:141:ASN:HB3	1:D:476:ARG:HE	1.52	0.75
1:E:401:ASN:ND2	1:E:404:MET:SD	2.59	0.75
1:J:401:ASN:ND2	1:J:404:MET:SD	2.60	0.75
1:G:401:ASN:ND2	1:G:404:MET:SD	2.60	0.74
1:C:346:LYS:HZ1	1:D:343:ARG:HH21	1.33	0.74
1:D:401:ASN:ND2	1:D:404:MET:SD	2.60	0.74
1:F:96:GLY:HA3	1:F:480:ILE:HG23	1.69	0.74
1:K:186:ASP:OD2	1:L:161:ASN:ND2	2.17	0.74
1:A:342:ALA:O	1:A:343:ARG:NH1	2.22	0.73
1:E:186:ASP:OD2	1:F:161:ASN:ND2	2.19	0.73
1:K:186:ASP:OD1	1:K:187:PHE:N	2.22	0.73
1:J:342:ALA:O	1:J:343:ARG:NH1	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:VAL:HG13	1:D:472:TYR:HD2	1.54	0.72
1:B:186:ASP:OD1	1:B:187:PHE:N	2.22	0.72
1:D:61:ARG:NH1	1:E:317:GLU:OE1	2.23	0.72
1:A:61:ARG:NH1	1:B:317:GLU:OE1	2.23	0.71
1:C:61:ARG:NH1	1:D:317:GLU:OE1	2.23	0.71
1:A:317:GLU:OE1	1:L:61:ARG:NH1	2.23	0.71
1:L:186:ASP:OD1	1:L:187:PHE:N	2.23	0.71
1:I:346:LYS:HZ1	1:J:343:ARG:HH21	1.39	0.71
1:G:61:ARG:NH1	1:H:317:GLU:OE1	2.23	0.71
1:J:186:ASP:OD2	1:K:161:ASN:ND2	2.24	0.70
1:J:186:ASP:OD1	1:J:187:PHE:N	2.23	0.70
1:J:61:ARG:NH1	1:K:317:GLU:OE1	2.23	0.70
1:G:141:ASN:HB3	1:G:476:ARG:HE	1.56	0.70
1:I:61:ARG:NH1	1:J:317:GLU:OE2	2.23	0.70
1:C:186:ASP:OD2	1:D:161:ASN:ND2	2.25	0.70
1:F:61:ARG:NH1	1:G:317:GLU:OE1	2.24	0.70
1:H:246:TYR:OH	1:H:273:ARG:NH1	2.25	0.70
1:E:186:ASP:OD1	1:E:187:PHE:N	2.24	0.70
1:L:93:VAL:HG13	1:L:480:ILE:HD11	1.74	0.69
1:G:92:ASP:HA	1:G:95:MET:HG3	1.72	0.69
1:G:186:ASP:OD1	1:G:187:PHE:N	2.24	0.69
1:A:92:ASP:HA	1:A:95:MET:HG3	1.74	0.69
1:B:468:VAL:HG13	1:B:472:TYR:HD2	1.56	0.69
1:I:186:ASP:OD1	1:I:187:PHE:N	2.25	0.69
1:I:93:VAL:HG13	1:I:480:ILE:HD11	1.75	0.69
1:B:246:TYR:OH	1:B:273:ARG:NH1	2.25	0.68
1:C:186:ASP:OD1	1:C:187:PHE:N	2.27	0.68
1:F:186:ASP:OD1	1:F:187:PHE:N	2.26	0.68
1:J:305:GLY:O	1:J:452:ASN:ND2	2.26	0.68
1:F:133:GLU:O	1:G:269:ARG:NH2	2.27	0.68
1:J:141:ASN:HB3	1:J:476:ARG:HE	1.59	0.68
1:A:133:GLU:O	1:B:269:ARG:NH2	2.27	0.68
1:A:269:ARG:NH2	1:L:133:GLU:O	2.27	0.68
1:G:186:ASP:OD2	1:H:161:ASN:ND2	2.27	0.68
1:B:305:GLY:O	1:B:452:ASN:ND2	2.27	0.67
1:G:125:ALA:HA	1:G:302:PRO:HA	1.76	0.67
1:B:133:GLU:O	1:C:269:ARG:NH2	2.27	0.67
1:B:186:ASP:OD2	1:C:161:ASN:ND2	2.19	0.67
1:C:14:ARG:NH2	1:C:224:GLU:OE2	2.28	0.67
1:K:133:GLU:O	1:L:269:ARG:NH2	2.27	0.67
1:L:14:ARG:NH2	1:L:224:GLU:OE2	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:125:ALA:HA	1:D:302:PRO:HA	1.77	0.67
1:J:125:ALA:HA	1:J:302:PRO:HA	1.77	0.67
1:A:305:GLY:O	1:A:452:ASN:ND2	2.27	0.67
1:D:133:GLU:O	1:E:269:ARG:NH2	2.26	0.67
1:F:14:ARG:NH2	1:F:224:GLU:OE2	2.28	0.67
1:C:93:VAL:HG13	1:C:480:ILE:HD11	1.76	0.67
1:F:93:VAL:HG13	1:F:480:ILE:HD11	1.75	0.67
1:H:133:GLU:O	1:I:269:ARG:NH2	2.28	0.67
1:A:125:ALA:HA	1:A:302:PRO:HA	1.76	0.67
1:C:133:GLU:O	1:D:269:ARG:NH2	2.27	0.67
1:E:133:GLU:O	1:F:269:ARG:NH2	2.27	0.67
1:E:305:GLY:O	1:E:452:ASN:ND2	2.27	0.67
1:D:186:ASP:OD2	1:E:161:ASN:ND2	2.28	0.67
1:J:133:GLU:O	1:K:269:ARG:NH2	2.28	0.67
1:I:14:ARG:NH2	1:I:224:GLU:OE2	2.28	0.66
1:D:14:ARG:NH2	1:D:224:GLU:OE2	2.28	0.66
1:K:305:GLY:O	1:K:452:ASN:ND2	2.27	0.66
1:A:351:PHE:HE2	1:A:356:ILE:HD13	1.60	0.66
1:D:186:ASP:OD1	1:D:187:PHE:N	2.28	0.66
1:E:14:ARG:NH2	1:E:224:GLU:OE2	2.28	0.66
1:J:14:ARG:NH2	1:J:224:GLU:OE2	2.28	0.66
1:J:93:VAL:HG13	1:J:480:ILE:HD11	1.77	0.66
1:A:14:ARG:NH2	1:A:224:GLU:OE2	2.28	0.66
1:A:186:ASP:OD1	1:A:187:PHE:N	2.28	0.66
1:I:487:GLU:OE2	1:J:81:ARG:NH1	2.28	0.66
1:F:186:ASP:OD2	1:G:161:ASN:ND2	2.29	0.66
1:F:445:GLU:HG2	1:F:450:GLN:HE21	1.60	0.66
1:H:14:ARG:NH2	1:H:224:GLU:OE2	2.29	0.66
1:I:133:GLU:O	1:J:269:ARG:NH2	2.28	0.66
1:H:93:VAL:HG13	1:H:480:ILE:HD11	1.78	0.66
1:H:305:GLY:O	1:H:452:ASN:ND2	2.27	0.66
1:A:161:ASN:ND2	1:L:186:ASP:OD2	2.29	0.65
1:D:351:PHE:HE2	1:D:356:ILE:HD13	1.61	0.65
1:B:14:ARG:NH2	1:B:224:GLU:OE2	2.29	0.65
1:G:14:ARG:NH2	1:G:224:GLU:OE2	2.29	0.65
1:G:351:PHE:HE2	1:G:356:ILE:HD13	1.61	0.65
1:H:125:ALA:HA	1:H:302:PRO:HA	1.79	0.65
1:D:133:GLU:OE2	1:D:476:ARG:NH2	2.30	0.65
1:D:305:GLY:O	1:D:452:ASN:ND2	2.30	0.65
1:E:487:GLU:OE2	1:F:81:ARG:NE	2.21	0.65
1:E:125:ALA:HA	1:E:302:PRO:HA	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:351:PHE:HE2	1:I:356:ILE:HD13	1.62	0.65
1:F:305:GLY:O	1:F:452:ASN:ND2	2.30	0.65
1:K:14:ARG:NH2	1:K:224:GLU:OE2	2.29	0.65
1:K:93:VAL:HG13	1:K:480:ILE:HD11	1.79	0.65
1:H:186:ASP:OD1	1:H:187:PHE:N	2.30	0.65
1:E:468:VAL:HG13	1:E:472:TYR:HD2	1.61	0.65
1:B:125:ALA:HA	1:B:302:PRO:HA	1.79	0.65
1:C:125:ALA:HA	1:C:302:PRO:HA	1.79	0.64
1:C:305:GLY:O	1:C:452:ASN:ND2	2.30	0.64
1:D:93:VAL:HG13	1:D:480:ILE:HD11	1.77	0.64
1:F:125:ALA:HA	1:F:302:PRO:HA	1.79	0.64
1:H:468:VAL:HG13	1:H:472:TYR:HD2	1.61	0.64
1:A:93:VAL:HG13	1:A:480:ILE:HD11	1.78	0.64
1:I:96:GLY:HA3	1:I:480:ILE:HG23	1.78	0.64
1:J:182:ASN:OD1	1:J:183:GLY:N	2.30	0.64
1:G:93:VAL:HG13	1:G:480:ILE:HD11	1.79	0.64
1:J:487:GLU:OE1	1:K:81:ARG:NH1	2.19	0.64
1:K:125:ALA:HA	1:K:302:PRO:HA	1.79	0.64
1:G:305:GLY:O	1:G:452:ASN:ND2	2.29	0.64
1:F:469:ASN:ND2	1:F:512:GLY:O	2.28	0.64
1:L:125:ALA:HA	1:L:302:PRO:HA	1.79	0.64
1:B:93:VAL:HG13	1:B:480:ILE:HD11	1.80	0.64
1:G:96:GLY:HA3	1:G:480:ILE:HG23	1.80	0.63
1:D:277:TYR:HD2	1:D:291:GLN:HB3	1.63	0.63
1:I:125:ALA:HA	1:I:302:PRO:HA	1.81	0.63
1:I:305:GLY:O	1:I:452:ASN:ND2	2.31	0.63
1:G:133:GLU:O	1:H:269:ARG:NH2	2.32	0.63
1:L:305:GLY:O	1:L:452:ASN:ND2	2.32	0.62
1:K:468:VAL:HG13	1:K:472:TYR:HD2	1.63	0.62
1:L:57:PHE:O	1:L:330:ARG:NH1	2.32	0.62
1:D:346:LYS:NZ	1:E:52:GLN:OE1	2.23	0.62
1:H:96:GLY:HA3	1:H:480:ILE:HG23	1.82	0.62
1:E:96:GLY:HA3	1:E:480:ILE:HG23	1.82	0.61
1:G:323:THR:HB	1:G:412:VAL:HG13	1.82	0.61
1:C:57:PHE:O	1:C:330:ARG:NH1	2.31	0.61
1:E:93:VAL:HG13	1:E:480:ILE:HD11	1.82	0.61
1:I:323:THR:HB	1:I:412:VAL:HG13	1.83	0.61
1:A:81:ARG:NH1	1:L:487:GLU:OE2	2.34	0.61
1:K:8:LEU:HD13	1:K:286:VAL:HA	1.83	0.61
1:H:8:LEU:HD13	1:H:286:VAL:HA	1.83	0.61
1:H:61:ARG:NH1	1:I:317:GLU:OE2	2.34	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:487:GLU:OE2	1:H:81:ARG:NH1	2.34	0.60
1:L:323:THR:HB	1:L:412:VAL:HG13	1.83	0.60
1:G:475:PRO:HA	1:G:493:MET:HG2	1.83	0.60
1:A:57:PHE:O	1:A:330:ARG:NH1	2.31	0.60
1:F:323:THR:HB	1:F:412:VAL:HG13	1.83	0.60
1:K:61:ARG:NH1	1:L:317:GLU:OE2	2.34	0.60
1:B:8:LEU:HD13	1:B:286:VAL:HA	1.83	0.60
1:C:323:THR:HB	1:C:412:VAL:HG13	1.82	0.60
1:J:323:THR:HB	1:J:412:VAL:HG13	1.84	0.60
1:D:561:ASP:O	1:D:569:ARG:NH1	2.34	0.60
1:I:57:PHE:O	1:I:330:ARG:NH1	2.32	0.60
1:B:61:ARG:NH1	1:C:317:GLU:OE2	2.34	0.60
1:K:76:ILE:HG12	1:K:520:VAL:HG22	1.84	0.60
1:K:323:THR:HB	1:K:412:VAL:HG13	1.84	0.60
1:A:323:THR:HB	1:A:412:VAL:HG13	1.83	0.60
1:E:61:ARG:NH1	1:F:317:GLU:OE1	2.35	0.59
1:L:410:SER:O	1:L:414:GLU:HG3	2.02	0.59
1:D:94:LEU:HD21	1:D:468:VAL:HG11	1.83	0.59
1:F:57:PHE:O	1:F:330:ARG:NH1	2.34	0.59
1:F:579:MET:HG2	1:F:581:VAL:HG23	1.85	0.59
1:C:579:MET:HG2	1:C:581:VAL:HG23	1.84	0.59
1:H:136:SER:O	1:I:269:ARG:NH1	2.35	0.59
1:A:410:SER:O	1:A:414:GLU:HG3	2.03	0.59
1:D:475:PRO:HA	1:D:493:MET:HG2	1.85	0.59
1:H:323:THR:HB	1:H:412:VAL:HG13	1.84	0.59
1:K:136:SER:O	1:L:269:ARG:NH1	2.35	0.59
1:D:410:SER:O	1:D:414:GLU:HG3	2.03	0.59
1:E:323:THR:HB	1:E:412:VAL:HG13	1.83	0.59
1:J:410:SER:O	1:J:414:GLU:HG3	2.03	0.59
1:L:96:GLY:HA3	1:L:480:ILE:HG23	1.85	0.59
1:L:177:HIS:NE2	1:L:221:GLU:OE2	2.36	0.59
1:A:561:ASP:O	1:A:569:ARG:NH1	2.33	0.58
1:J:177:HIS:NE2	1:J:221:GLU:OE2	2.35	0.58
1:E:8:LEU:HD12	1:E:286:VAL:HA	1.85	0.58
1:F:51:LEU:O	1:F:54:ARG:NH1	2.36	0.58
1:I:177:HIS:NE2	1:I:221:GLU:OE2	2.36	0.58
1:I:579:MET:HG2	1:I:581:VAL:HG23	1.84	0.58
1:D:323:THR:HB	1:D:412:VAL:HG13	1.84	0.58
1:E:76:ILE:HG12	1:E:520:VAL:HG22	1.84	0.58
1:E:134:ASP:O	1:F:269:ARG:NH2	2.37	0.58
1:J:561:ASP:O	1:J:569:ARG:NH1	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:579:MET:HG2	1:L:581:VAL:HG23	1.84	0.58
1:E:136:SER:O	1:F:269:ARG:NH1	2.36	0.58
1:J:307:TRP:NE1	1:J:314:GLU:OE1	2.31	0.58
1:J:94:LEU:HD21	1:J:468:VAL:HG11	1.86	0.58
1:D:134:ASP:O	1:E:269:ARG:NH2	2.37	0.58
1:E:190:LYS:O	1:F:229:LYS:NZ	2.36	0.58
1:J:125:ALA:HB3	1:J:152:ALA:HB1	1.86	0.57
1:D:177:HIS:NE2	1:D:221:GLU:OE2	2.37	0.57
1:D:307:TRP:NE1	1:D:314:GLU:OE1	2.31	0.57
1:J:94:LEU:HG	1:J:510:ILE:HD12	1.86	0.57
1:E:468:VAL:HG13	1:E:472:TYR:CD2	2.40	0.57
1:G:190:LYS:O	1:H:229:LYS:NZ	2.37	0.57
1:B:134:ASP:O	1:C:269:ARG:NH2	2.37	0.57
1:G:177:HIS:NE2	1:G:221:GLU:OE2	2.37	0.57
1:A:177:HIS:NE2	1:A:221:GLU:OE2	2.37	0.57
1:B:468:VAL:HG13	1:B:472:TYR:CD2	2.38	0.57
1:G:125:ALA:HB3	1:G:152:ALA:HB1	1.86	0.57
1:G:410:SER:O	1:G:414:GLU:HG3	2.03	0.57
1:L:125:ALA:HB3	1:L:152:ALA:HB1	1.87	0.57
1:I:337:ASN:HB3	1:J:404:MET:HE3	1.86	0.57
1:F:346:LYS:NZ	1:G:52:GLN:OE1	2.24	0.57
1:G:136:SER:O	1:H:269:ARG:NH1	2.38	0.57
1:C:125:ALA:HB3	1:C:152:ALA:HB1	1.87	0.57
1:A:125:ALA:HB3	1:A:152:ALA:HB1	1.86	0.57
1:B:136:SER:O	1:C:269:ARG:NH1	2.37	0.57
1:C:177:HIS:NE2	1:C:221:GLU:OE2	2.35	0.57
1:G:134:ASP:O	1:H:269:ARG:NH2	2.37	0.57
1:I:190:LYS:O	1:J:229:LYS:NZ	2.37	0.57
1:A:190:LYS:O	1:B:229:LYS:NZ	2.37	0.57
1:A:404:MET:HE3	1:L:337:ASN:HB3	1.87	0.57
1:D:190:LYS:O	1:E:229:LYS:NZ	2.37	0.57
1:F:177:HIS:NE2	1:F:221:GLU:OE2	2.36	0.57
1:K:134:ASP:O	1:L:269:ARG:NH2	2.38	0.57
1:B:323:THR:HB	1:B:412:VAL:HG13	1.85	0.56
1:C:487:GLU:OE2	1:D:81:ARG:NH1	2.37	0.56
1:D:96:GLY:HA3	1:D:480:ILE:HG23	1.86	0.56
1:C:337:ASN:HB3	1:D:404:MET:HE3	1.87	0.56
1:F:487:GLU:OE1	1:G:81:ARG:NH1	2.38	0.56
1:J:96:GLY:HA3	1:J:480:ILE:HG23	1.88	0.56
1:F:93:VAL:HB	1:F:510:ILE:HD11	1.87	0.56
1:H:134:ASP:O	1:I:269:ARG:NH2	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:96:GLY:HA3	1:K:480:ILE:HG23	1.88	0.56
1:K:254:VAL:HB	1:K:257:ASP:HB3	1.87	0.56
1:B:491:GLN:O	1:B:508:ASN:ND2	2.39	0.56
1:F:337:ASN:HB3	1:G:404:MET:HE3	1.86	0.56
1:B:254:VAL:HB	1:B:257:ASP:HB3	1.87	0.56
1:D:125:ALA:HB3	1:D:152:ALA:HB1	1.86	0.56
1:I:368:ASP:OD1	1:K:50:THR:HG21	2.06	0.56
1:E:57:PHE:O	1:E:330:ARG:NH1	2.36	0.56
1:H:94:LEU:HG	1:H:510:ILE:HD12	1.88	0.56
1:J:134:ASP:O	1:K:269:ARG:NH2	2.39	0.56
1:A:134:ASP:O	1:B:269:ARG:NH2	2.39	0.56
1:A:254:VAL:HB	1:A:257:ASP:HB3	1.88	0.56
1:G:469:ASN:ND2	1:G:512:GLY:O	2.39	0.56
1:K:346:LYS:NZ	1:L:52:GLN:OE1	2.22	0.56
1:D:254:VAL:HB	1:D:257:ASP:HB3	1.88	0.55
1:F:125:ALA:HB3	1:F:152:ALA:HB1	1.87	0.55
1:H:125:ALA:HB3	1:H:152:ALA:HB1	1.87	0.55
1:J:254:VAL:HB	1:J:257:ASP:HB3	1.88	0.55
1:F:91:ALA:O	1:F:95:MET:HG3	2.05	0.55
1:A:71:MET:HE1	1:A:449:PHE:HB3	1.88	0.55
1:E:491:GLN:O	1:E:508:ASN:ND2	2.40	0.55
1:F:97:MET:HE1	1:F:510:ILE:HG13	1.87	0.55
1:L:21:ALA:O	1:L:313:LYS:NZ	2.39	0.55
1:A:229:LYS:NZ	1:L:190:LYS:O	2.39	0.55
1:F:134:ASP:O	1:G:269:ARG:NH2	2.40	0.55
1:I:125:ALA:HB3	1:I:152:ALA:HB1	1.87	0.55
1:I:458:ARG:NH1	1:I:462:GLU:OE2	2.40	0.55
1:K:469:ASN:ND2	1:K:512:GLY:O	2.38	0.55
1:L:561:ASP:O	1:L:569:ARG:NH1	2.37	0.55
1:B:96:GLY:HA3	1:B:480:ILE:HG23	1.87	0.55
1:B:125:ALA:HB3	1:B:152:ALA:HB1	1.87	0.55
1:B:177:HIS:NE2	1:B:221:GLU:OE2	2.40	0.55
1:K:125:ALA:HB3	1:K:152:ALA:HB1	1.88	0.55
1:C:190:LYS:O	1:D:229:LYS:NZ	2.39	0.55
1:C:475:PRO:HA	1:C:493:MET:HG2	1.86	0.55
1:G:254:VAL:HB	1:G:257:ASP:HB3	1.88	0.55
1:A:269:ARG:NH2	1:L:134:ASP:O	2.40	0.55
1:C:128:LEU:HD13	1:C:146:ARG:HG2	1.89	0.55
1:C:134:ASP:O	1:D:269:ARG:NH2	2.40	0.55
1:G:458:ARG:NH1	1:G:462:GLU:OE2	2.40	0.55
1:A:458:ARG:NH1	1:A:462:GLU:OE2	2.40	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:21:ALA:O	1:C:313:LYS:NZ	2.40	0.55
1:D:458:ARG:NH1	1:D:462:GLU:OE2	2.40	0.55
1:F:190:LYS:O	1:G:229:LYS:NZ	2.40	0.55
1:J:458:ARG:NH1	1:J:462:GLU:OE2	2.40	0.54
1:H:57:PHE:O	1:H:330:ARG:NH1	2.37	0.54
1:A:475:PRO:HA	1:A:493:MET:HG2	1.90	0.54
1:E:254:VAL:HB	1:E:257:ASP:HB3	1.88	0.54
1:K:342:ALA:HB2	1:L:332:MET:SD	2.48	0.54
1:H:338:ALA:HB2	1:I:329:LEU:HD13	1.89	0.54
1:I:82:PRO:HA	1:I:514:TYR:CE1	2.41	0.54
1:K:94:LEU:HG	1:K:510:ILE:HD12	1.89	0.54
1:B:458:ARG:NH1	1:B:462:GLU:OE2	2.40	0.54
1:E:91:ALA:O	1:E:95:MET:HG3	2.08	0.54
1:E:125:ALA:HB3	1:E:152:ALA:HB1	1.87	0.54
1:H:190:LYS:O	1:I:229:LYS:NZ	2.40	0.54
1:H:458:ARG:NH1	1:H:462:GLU:OE2	2.41	0.54
1:I:134:ASP:O	1:J:269:ARG:NH2	2.40	0.54
1:D:94:LEU:HG	1:D:510:ILE:HD12	1.90	0.54
1:B:190:LYS:O	1:C:229:LYS:NZ	2.40	0.54
1:H:561:ASP:O	1:H:569:ARG:NH1	2.40	0.54
1:I:469:ASN:ND2	1:I:512:GLY:O	2.39	0.54
1:A:234:ILE:HD13	1:L:137:PRO:O	2.08	0.54
1:B:145:ARG:NH1	1:B:147:GLU:OE2	2.41	0.54
1:E:338:ALA:HB2	1:F:329:LEU:HD13	1.89	0.54
1:H:254:VAL:HB	1:H:257:ASP:HB3	1.88	0.54
1:H:91:ALA:O	1:H:95:MET:HG3	2.08	0.54
1:H:342:ALA:HB2	1:I:332:MET:SD	2.48	0.54
1:I:21:ALA:O	1:I:313:LYS:NZ	2.38	0.54
1:I:137:PRO:O	1:J:234:ILE:HD13	2.08	0.54
1:K:338:ALA:HB2	1:L:329:LEU:HD13	1.88	0.54
1:K:458:ARG:NH1	1:K:462:GLU:OE2	2.41	0.54
1:L:45:LEU:HD22	1:L:328:ARG:HD3	1.90	0.54
1:D:21:ALA:O	1:D:313:LYS:NZ	2.40	0.54
1:E:177:HIS:NE2	1:E:221:GLU:OE2	2.41	0.54
1:E:342:ALA:HB2	1:F:332:MET:SD	2.48	0.54
1:E:458:ARG:NH1	1:E:462:GLU:OE2	2.40	0.54
1:I:142:GLN:H	1:I:476:ARG:HH12	1.56	0.54
1:J:91:ALA:O	1:J:95:MET:HG3	2.07	0.54
1:F:45:LEU:HD22	1:F:328:ARG:HD3	1.90	0.53
1:B:87:ARG:NH2	1:B:507:LEU:O	2.41	0.53
1:E:87:ARG:NH2	1:E:507:LEU:O	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:128:LEU:HD13	1:F:146:ARG:HG2	1.90	0.53
1:B:338:ALA:HB2	1:C:329:LEU:HD13	1.89	0.53
1:C:458:ARG:NH1	1:C:462:GLU:OE2	2.41	0.53
1:F:317:GLU:HG2	1:F:321:ARG:HD2	1.90	0.53
1:G:71:MET:HE1	1:G:449:PHE:HB3	1.88	0.53
1:L:458:ARG:NH1	1:L:462:GLU:OE2	2.41	0.53
1:D:57:PHE:O	1:D:330:ARG:NH1	2.37	0.53
1:F:82:PRO:HA	1:F:514:TYR:CE1	2.43	0.53
1:L:91:ALA:O	1:L:95:MET:HG3	2.09	0.53
1:B:94:LEU:HD12	1:B:514:TYR:CE2	2.44	0.53
1:F:458:ARG:NH1	1:F:462:GLU:OE2	2.42	0.53
1:I:184:TRP:HH2	1:I:288:LYS:HE3	1.74	0.53
1:A:307:TRP:NE1	1:A:314:GLU:OE1	2.31	0.53
1:C:137:PRO:O	1:D:234:ILE:HD13	2.08	0.53
1:K:145:ARG:NH1	1:K:147:GLU:OE2	2.42	0.53
1:L:401:ASN:ND2	1:L:404:MET:SD	2.82	0.53
1:A:21:ALA:O	1:A:313:LYS:NZ	2.41	0.53
1:I:561:ASP:O	1:I:569:ARG:NH1	2.37	0.53
1:D:128:LEU:HD13	1:D:146:ARG:HG2	1.91	0.53
1:E:145:ARG:NH1	1:E:147:GLU:OE2	2.42	0.53
1:F:401:ASN:ND2	1:F:404:MET:SD	2.81	0.53
1:I:45:LEU:HD22	1:I:328:ARG:HD3	1.90	0.53
1:C:82:PRO:HA	1:C:514:TYR:CE1	2.44	0.53
1:E:94:LEU:HD12	1:E:514:TYR:CE2	2.44	0.53
1:J:21:ALA:O	1:J:313:LYS:NZ	2.40	0.53
1:L:128:LEU:HD13	1:L:146:ARG:HG2	1.90	0.53
1:K:190:LYS:O	1:L:229:LYS:NZ	2.42	0.53
1:E:561:ASP:OD1	1:F:531:ASN:ND2	2.41	0.52
1:F:23:ASP:OD1	1:F:26:ARG:NH2	2.42	0.52
1:F:561:ASP:O	1:F:569:ARG:NH1	2.37	0.52
1:L:92:ASP:HA	1:L:95:MET:HG3	1.91	0.52
1:G:128:LEU:HD13	1:G:146:ARG:HG2	1.91	0.52
1:J:101:ASP:OD2	1:J:464:TYR:OH	2.22	0.52
1:A:332:MET:SD	1:L:342:ALA:HB2	2.48	0.52
1:C:23:ASP:OD1	1:C:26:ARG:NH2	2.43	0.52
1:F:136:SER:O	1:G:269:ARG:NH1	2.43	0.52
1:G:57:PHE:O	1:G:330:ARG:NH1	2.37	0.52
1:L:71:MET:CE	1:L:449:PHE:HB3	2.40	0.52
1:B:57:PHE:O	1:B:330:ARG:NH1	2.40	0.52
1:E:94:LEU:HD21	1:E:468:VAL:HG11	1.92	0.52
1:K:94:LEU:HD12	1:K:514:TYR:CE2	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:410:SER:O	1:F:414:GLU:HG3	2.10	0.52
1:I:71:MET:CE	1:I:449:PHE:HB3	2.40	0.52
1:I:128:LEU:HD13	1:I:146:ARG:HG2	1.90	0.52
1:A:269:ARG:NH1	1:L:136:SER:O	2.42	0.52
1:C:110:ALA:HA	1:C:148:PRO:HB3	1.92	0.52
1:H:469:ASN:ND2	1:H:512:GLY:O	2.42	0.52
1:I:401:ASN:ND2	1:I:404:MET:SD	2.82	0.52
1:L:23:ASP:OD1	1:L:26:ARG:NH2	2.42	0.52
1:F:110:ALA:HA	1:F:148:PRO:HB3	1.92	0.52
1:F:137:PRO:O	1:G:234:ILE:HD13	2.09	0.52
1:H:467:ILE:O	1:H:471:ILE:HG12	2.10	0.52
1:K:561:ASP:O	1:K:569:ARG:NH1	2.41	0.52
1:A:513:ARG:HG2	1:A:513:ARG:HH11	1.75	0.52
1:I:23:ASP:OD1	1:I:26:ARG:NH2	2.43	0.52
1:L:110:ALA:HA	1:L:148:PRO:HB3	1.92	0.52
1:A:338:ALA:HB2	1:B:329:LEU:HD13	1.91	0.52
1:B:492:LEU:O	1:B:508:ASN:HB2	2.10	0.52
1:F:71:MET:CE	1:F:449:PHE:HB3	2.39	0.52
1:J:344:THR:HG23	1:K:50:THR:OG1	2.08	0.52
1:L:142:GLN:H	1:L:476:ARG:HH12	1.57	0.52
1:L:254:VAL:HB	1:L:257:ASP:HB3	1.92	0.52
1:B:94:LEU:HD21	1:B:468:VAL:HG11	1.92	0.52
1:C:469:ASN:ND2	1:C:512:GLY:O	2.43	0.52
1:H:376:ARG:HG3	1:H:377:THR:H	1.75	0.52
1:I:136:SER:O	1:J:269:ARG:NH1	2.42	0.52
1:I:410:SER:O	1:I:414:GLU:HG3	2.10	0.52
1:J:190:LYS:O	1:K:229:LYS:NZ	2.43	0.52
1:B:376:ARG:HG3	1:B:377:THR:H	1.75	0.51
1:E:376:ARG:HG3	1:E:377:THR:H	1.75	0.51
1:F:561:ASP:OD1	1:G:531:ASN:ND2	2.40	0.51
1:G:94:LEU:HG	1:G:510:ILE:HD12	1.92	0.51
1:G:142:GLN:HB2	1:G:471:ILE:HD11	1.93	0.51
1:C:136:SER:O	1:D:269:ARG:NH1	2.42	0.51
1:J:475:PRO:HA	1:J:493:MET:HG2	1.91	0.51
1:K:177:HIS:NE2	1:K:221:GLU:OE2	2.42	0.51
1:K:376:ARG:HG3	1:K:377:THR:H	1.75	0.51
1:A:94:LEU:HD12	1:A:514:TYR:CD2	2.45	0.51
1:F:21:ALA:O	1:F:313:LYS:NZ	2.40	0.51
1:F:184:TRP:HH2	1:F:288:LYS:HE3	1.75	0.51
1:L:317:GLU:HG2	1:L:321:ARG:HD2	1.93	0.51
1:E:492:LEU:O	1:E:508:ASN:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:177:HIS:NE2	1:H:221:GLU:OE2	2.41	0.51
1:I:110:ALA:HA	1:I:148:PRO:HB3	1.92	0.51
1:J:137:PRO:O	1:K:234:ILE:HD13	2.11	0.51
1:A:492:LEU:O	1:A:508:ASN:HB2	2.11	0.51
1:I:317:GLU:HG2	1:I:321:ARG:HD2	1.93	0.51
1:I:492:LEU:O	1:I:508:ASN:HB2	2.10	0.51
1:L:82:PRO:HA	1:L:514:TYR:CE1	2.46	0.51
1:E:410:SER:O	1:E:414:GLU:HG3	2.11	0.51
1:G:137:PRO:O	1:H:234:ILE:HD13	2.11	0.51
1:I:254:VAL:HB	1:I:257:ASP:HB3	1.92	0.51
1:I:338:ALA:HB2	1:J:329:LEU:HD13	1.92	0.51
1:J:128:LEU:HD13	1:J:146:ARG:HG2	1.91	0.51
1:A:376:ARG:HG3	1:A:377:THR:H	1.76	0.51
1:A:467:ILE:O	1:A:471:ILE:HG12	2.10	0.51
1:B:137:PRO:O	1:C:234:ILE:HD13	2.11	0.51
1:C:376:ARG:HG3	1:C:377:THR:H	1.76	0.51
1:D:376:ARG:HG3	1:D:377:THR:H	1.76	0.51
1:D:492:LEU:O	1:D:508:ASN:HB2	2.11	0.51
1:E:509:ASP:OD1	1:E:511:ARG:NH2	2.44	0.51
1:F:376:ARG:HG3	1:F:377:THR:H	1.76	0.51
1:G:376:ARG:HG3	1:G:377:THR:H	1.76	0.51
1:H:87:ARG:NH2	1:H:507:LEU:O	2.43	0.51
1:C:561:ASP:O	1:C:569:ARG:NH1	2.36	0.51
1:G:561:ASP:O	1:G:569:ARG:NH1	2.41	0.51
1:K:561:ASP:OD1	1:L:531:ASN:ND2	2.41	0.51
1:A:45:LEU:HD22	1:A:328:ARG:HD3	1.91	0.51
1:A:128:LEU:HD13	1:A:146:ARG:HG2	1.92	0.51
1:A:177:HIS:HB2	1:A:219:ILE:HG22	1.92	0.51
1:B:250:ASP:O	1:B:254:VAL:HG22	2.11	0.51
1:D:137:PRO:O	1:E:234:ILE:HD13	2.11	0.51
1:G:23:ASP:OD1	1:G:26:ARG:NH2	2.44	0.51
1:H:94:LEU:HD12	1:H:514:TYR:CE2	2.45	0.51
1:H:410:SER:O	1:H:414:GLU:HG3	2.11	0.51
1:I:296:GLU:HB3	1:I:466:SER:OG	2.11	0.51
1:J:376:ARG:HG3	1:J:377:THR:H	1.76	0.51
1:K:250:ASP:O	1:K:254:VAL:HG22	2.11	0.51
1:K:492:LEU:O	1:K:508:ASN:HB2	2.10	0.51
1:L:376:ARG:HG3	1:L:377:THR:H	1.76	0.51
1:A:110:ALA:HA	1:A:148:PRO:HB3	1.93	0.51
1:C:254:VAL:HB	1:C:257:ASP:HB3	1.93	0.51
1:E:469:ASN:ND2	1:E:512:GLY:O	2.42	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:142:GLN:H	1:F:476:ARG:HH12	1.56	0.51
1:J:338:ALA:HB2	1:K:329:LEU:HD13	1.91	0.51
1:K:410:SER:O	1:K:414:GLU:HG3	2.11	0.51
1:A:23:ASP:OD1	1:A:26:ARG:NH2	2.44	0.50
1:B:509:ASP:OD1	1:B:511:ARG:NH2	2.44	0.50
1:D:23:ASP:OD1	1:D:26:ARG:NH2	2.44	0.50
1:D:110:ALA:HA	1:D:148:PRO:HB3	1.94	0.50
1:G:338:ALA:HB2	1:H:329:LEU:HD13	1.92	0.50
1:A:94:LEU:HD21	1:A:468:VAL:HG11	1.93	0.50
1:A:531:ASN:ND2	1:L:561:ASP:OD1	2.40	0.50
1:C:317:GLU:HG2	1:C:321:ARG:HD2	1.93	0.50
1:E:137:PRO:O	1:F:234:ILE:HD13	2.11	0.50
1:E:554:LEU:HD21	1:E:575:GLN:HB3	1.93	0.50
1:H:145:ARG:NH1	1:H:147:GLU:OE2	2.44	0.50
1:K:57:PHE:O	1:K:330:ARG:NH1	2.38	0.50
1:C:346:LYS:NZ	1:D:52:GLN:OE1	2.24	0.50
1:G:21:ALA:O	1:G:313:LYS:NZ	2.40	0.50
1:I:376:ARG:HG3	1:I:377:THR:H	1.76	0.50
1:A:137:PRO:O	1:B:234:ILE:HD13	2.11	0.50
1:C:142:GLN:H	1:C:476:ARG:HH12	1.59	0.50
1:C:346:LYS:HA	1:D:395:PRO:HG3	1.94	0.50
1:D:338:ALA:HB2	1:E:329:LEU:HD13	1.94	0.50
1:D:494:ALA:HB3	1:D:507:LEU:HB2	1.94	0.50
1:G:346:LYS:HA	1:H:395:PRO:HG3	1.93	0.50
1:G:494:ALA:HB3	1:G:507:LEU:HB2	1.93	0.50
1:J:492:LEU:O	1:J:508:ASN:HB2	2.10	0.50
1:I:468:VAL:HG13	1:I:472:TYR:CD2	2.46	0.50
1:L:492:LEU:O	1:L:508:ASN:HB2	2.11	0.50
1:E:561:ASP:O	1:E:569:ARG:NH1	2.41	0.50
1:G:273:ARG:NH2	1:G:275:ARG:HE	2.10	0.50
1:H:137:PRO:O	1:I:234:ILE:HD13	2.12	0.50
1:H:137:PRO:HB2	1:I:243:PRO:HB3	1.94	0.50
1:K:346:LYS:HA	1:L:395:PRO:HG3	1.93	0.50
1:D:136:SER:O	1:E:269:ARG:NH1	2.44	0.50
1:A:395:PRO:HG3	1:L:346:LYS:HA	1.94	0.50
1:F:338:ALA:HB2	1:G:329:LEU:HD13	1.94	0.50
1:H:128:LEU:HD13	1:H:146:ARG:HG2	1.93	0.50
1:H:250:ASP:O	1:H:254:VAL:HG22	2.11	0.50
1:H:256:ASP:OD1	1:H:257:ASP:N	2.45	0.50
1:J:23:ASP:OD1	1:J:26:ARG:NH2	2.44	0.50
1:J:110:ALA:HA	1:J:148:PRO:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:469:ASN:ND2	1:L:512:GLY:O	2.43	0.50
1:B:256:ASP:OD1	1:B:257:ASP:N	2.45	0.50
1:E:250:ASP:O	1:E:254:VAL:HG22	2.11	0.50
1:J:57:PHE:O	1:J:330:ARG:NH1	2.36	0.50
1:K:137:PRO:O	1:L:234:ILE:HD13	2.12	0.50
1:K:164:LEU:HD13	1:K:169:ASP:OD2	2.12	0.49
1:B:137:PRO:HB2	1:C:243:PRO:HB3	1.94	0.49
1:E:128:LEU:HD13	1:E:146:ARG:HG2	1.94	0.49
1:G:110:ALA:HA	1:G:148:PRO:HB3	1.94	0.49
1:K:467:ILE:O	1:K:471:ILE:HG12	2.12	0.49
1:E:256:ASP:OD1	1:E:257:ASP:N	2.45	0.49
1:J:346:LYS:HA	1:K:395:PRO:HG3	1.94	0.49
1:B:469:ASN:ND2	1:B:512:GLY:O	2.43	0.49
1:C:491:GLN:O	1:C:508:ASN:ND2	2.45	0.49
1:D:91:ALA:O	1:D:95:MET:HG3	2.11	0.49
1:D:101:ASP:OD2	1:D:464:TYR:OH	2.21	0.49
1:F:254:VAL:HB	1:F:257:ASP:HB3	1.93	0.49
1:H:23:ASP:OD1	1:H:26:ARG:NH2	2.45	0.49
1:H:164:LEU:HD13	1:H:169:ASP:OD2	2.12	0.49
1:E:23:ASP:OD1	1:E:26:ARG:NH2	2.46	0.49
1:E:137:PRO:HB2	1:F:243:PRO:HB3	1.94	0.49
1:F:494:ALA:HB3	1:F:507:LEU:HB2	1.94	0.49
1:A:87:ARG:NH2	1:A:507:LEU:O	2.46	0.49
1:A:469:ASN:ND2	1:A:512:GLY:O	2.45	0.49
1:B:164:LEU:HD13	1:B:169:ASP:OD2	2.13	0.49
1:C:338:ALA:HB2	1:D:329:LEU:HD13	1.94	0.49
1:F:99:ARG:HG2	1:F:103:ARG:HH21	1.77	0.49
1:J:136:SER:O	1:K:269:ARG:NH1	2.45	0.49
1:A:329:LEU:HD13	1:L:338:ALA:HB2	1.92	0.49
1:B:23:ASP:OD1	1:B:26:ARG:NH2	2.46	0.49
1:G:182:ASN:O	1:G:185:GLU:HG3	2.13	0.49
1:H:494:ALA:HB3	1:H:507:LEU:HB2	1.94	0.49
1:I:45:LEU:HD11	1:I:332:MET:CE	2.43	0.49
1:I:346:LYS:HA	1:J:395:PRO:HG3	1.94	0.49
1:B:398:PRO:C	1:B:400:ALA:H	2.16	0.49
1:B:410:SER:O	1:B:414:GLU:HG3	2.12	0.49
1:K:87:ARG:NH2	1:K:507:LEU:O	2.45	0.49
1:C:492:LEU:O	1:C:508:ASN:HB2	2.12	0.49
1:G:544:GLN:HB3	1:H:543:PRO:HG3	1.94	0.49
1:H:94:LEU:HD21	1:H:468:VAL:HG11	1.95	0.49
1:B:561:ASP:O	1:B:569:ARG:NH1	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:256:ASP:OD1	1:C:257:ASP:N	2.46	0.49
1:E:467:ILE:O	1:E:471:ILE:HG12	2.13	0.49
1:A:346:LYS:HZ1	1:B:343:ARG:NH2	2.11	0.48
1:B:128:LEU:HD13	1:B:146:ARG:HG2	1.94	0.48
1:C:71:MET:CE	1:C:449:PHE:HB3	2.42	0.48
1:D:544:GLN:HB3	1:E:543:PRO:HG3	1.95	0.48
1:H:182:ASN:HA	1:H:185:GLU:OE1	2.13	0.48
1:J:469:ASN:ND2	1:J:512:GLY:O	2.46	0.48
1:J:494:ALA:HB3	1:J:507:LEU:HB2	1.95	0.48
1:D:346:LYS:HA	1:E:395:PRO:HG3	1.96	0.48
1:E:165:MET:HE2	1:E:307:TRP:CE3	2.48	0.48
1:F:346:LYS:HA	1:G:395:PRO:HG3	1.95	0.48
1:H:492:LEU:O	1:H:508:ASN:HB2	2.13	0.48
1:L:45:LEU:HD11	1:L:332:MET:CE	2.43	0.48
1:B:475:PRO:HG3	1:B:493:MET:HG3	1.95	0.48
1:H:141:ASN:HB3	1:H:476:ARG:CZ	2.43	0.48
1:B:110:ALA:HA	1:B:148:PRO:HB3	1.95	0.48
1:D:273:ARG:NH2	1:D:275:ARG:HE	2.10	0.48
1:F:45:LEU:HD11	1:F:332:MET:CE	2.43	0.48
1:F:256:ASP:OD1	1:F:257:ASP:N	2.46	0.48
1:G:137:PRO:HB2	1:H:243:PRO:HB3	1.95	0.48
1:K:23:ASP:OD1	1:K:26:ARG:NH2	2.46	0.48
1:K:137:PRO:HB2	1:L:243:PRO:HB3	1.95	0.48
1:K:398:PRO:C	1:K:400:ALA:H	2.16	0.48
1:C:443:ASP:C	1:C:445:GLU:H	2.16	0.48
1:K:141:ASN:HB3	1:K:476:ARG:CZ	2.43	0.48
1:K:443:ASP:C	1:K:445:GLU:H	2.17	0.48
1:K:494:ALA:HB3	1:K:507:LEU:HB2	1.96	0.48
1:C:346:LYS:HZ1	1:D:343:ARG:NH2	2.06	0.48
1:G:307:TRP:NE1	1:G:314:GLU:OE1	2.31	0.48
1:H:474:VAL:O	1:H:476:ARG:HG3	2.14	0.48
1:A:468:VAL:HG13	1:A:472:TYR:CD2	2.49	0.48
1:B:494:ALA:HB3	1:B:507:LEU:HB2	1.95	0.48
1:E:443:ASP:C	1:E:445:GLU:H	2.17	0.48
1:E:494:ALA:HB3	1:E:507:LEU:HB2	1.96	0.48
1:G:492:LEU:O	1:G:508:ASN:HB2	2.13	0.48
1:H:110:ALA:HA	1:H:148:PRO:HB3	1.96	0.48
1:K:81:ARG:HG3	1:K:81:ARG:HH11	1.79	0.48
1:B:561:ASP:OD1	1:C:531:ASN:ND2	2.40	0.48
1:D:443:ASP:C	1:D:445:GLU:H	2.17	0.48
1:E:110:ALA:HA	1:E:148:PRO:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:492:LEU:O	1:F:508:ASN:HB2	2.13	0.48
1:K:110:ALA:HA	1:K:148:PRO:HB3	1.96	0.48
1:F:468:VAL:HG13	1:F:472:TYR:CD2	2.48	0.48
1:J:63:VAL:HG11	1:J:416:ALA:HB1	1.96	0.48
1:K:296:GLU:HB3	1:K:466:SER:HB3	1.96	0.48
1:B:94:LEU:HG	1:B:510:ILE:HD12	1.96	0.48
1:D:182:ASN:O	1:D:185:GLU:HG3	2.13	0.48
1:E:574:LYS:HG3	1:E:592:TRP:CE3	2.49	0.48
1:I:82:PRO:HA	1:I:514:TYR:HE1	1.78	0.48
1:I:236:GLN:HB2	1:I:266:ILE:HG13	1.96	0.48
1:I:494:ALA:HB3	1:I:507:LEU:HB2	1.96	0.48
1:A:94:LEU:HG	1:A:510:ILE:HD12	1.96	0.47
1:B:342:ALA:HB2	1:C:332:MET:HE2	1.96	0.47
1:C:99:ARG:HG2	1:C:103:ARG:HH21	1.77	0.47
1:G:346:LYS:NZ	1:H:52:GLN:OE1	2.26	0.47
1:K:128:LEU:HD13	1:K:146:ARG:HG2	1.95	0.47
1:K:256:ASP:OD1	1:K:257:ASP:N	2.46	0.47
1:K:474:VAL:O	1:K:476:ARG:HG3	2.13	0.47
1:L:87:ARG:NH2	1:L:507:LEU:O	2.46	0.47
1:A:494:ALA:HB3	1:A:507:LEU:HB2	1.96	0.47
1:A:544:GLN:HB3	1:B:543:PRO:HG3	1.95	0.47
1:D:469:ASN:ND2	1:D:512:GLY:O	2.46	0.47
1:F:443:ASP:C	1:F:445:GLU:H	2.17	0.47
1:G:177:HIS:HB2	1:G:219:ILE:HG22	1.94	0.47
1:G:321:ARG:O	1:G:324:LYS:HB3	2.14	0.47
1:H:63:VAL:HG11	1:H:416:ALA:CB	2.44	0.47
1:J:467:ILE:O	1:J:471:ILE:HG12	2.13	0.47
1:B:21:ALA:O	1:B:313:LYS:NZ	2.46	0.47
1:C:468:VAL:HG13	1:C:472:TYR:CD2	2.50	0.47
1:E:346:LYS:HA	1:F:395:PRO:HG3	1.96	0.47
1:H:236:GLN:HB2	1:H:266:ILE:HG13	1.97	0.47
1:L:443:ASP:C	1:L:445:GLU:H	2.17	0.47
1:C:166:ASP:OD2	1:C:455:THR:HG22	2.15	0.47
1:F:236:GLN:HB2	1:F:266:ILE:HG13	1.97	0.47
1:G:94:LEU:HD12	1:G:514:TYR:CD2	2.48	0.47
1:G:363:TYR:OH	1:G:373:LEU:O	2.31	0.47
1:H:179:MET:SD	1:H:183:GLY:HA3	2.54	0.47
1:A:136:SER:O	1:B:269:ARG:NH1	2.47	0.47
1:A:137:PRO:HB2	1:B:243:PRO:HB3	1.96	0.47
1:C:561:ASP:OD1	1:D:531:ASN:ND2	2.40	0.47
1:E:94:LEU:HG	1:E:510:ILE:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:178:SER:OG	1:F:312:ASP:OD2	2.32	0.47
1:F:87:ARG:NH2	1:F:507:LEU:O	2.46	0.47
1:H:398:PRO:C	1:H:400:ALA:H	2.16	0.47
1:H:561:ASP:OD1	1:I:531:ASN:ND2	2.41	0.47
1:J:544:GLN:HB3	1:K:543:PRO:HG3	1.95	0.47
1:K:182:ASN:HA	1:K:185:GLU:OE1	2.15	0.47
1:L:256:ASP:OD1	1:L:257:ASP:N	2.47	0.47
1:D:256:ASP:OD1	1:D:257:ASP:N	2.47	0.47
1:E:296:GLU:HB3	1:E:466:SER:HB3	1.95	0.47
1:G:256:ASP:OD1	1:G:257:ASP:N	2.48	0.47
1:K:131:ASP:OD2	1:K:145:ARG:NE	2.33	0.47
1:A:63:VAL:HG11	1:A:416:ALA:CB	2.45	0.47
1:A:93:VAL:HB	1:A:510:ILE:HD11	1.97	0.47
1:A:182:ASN:O	1:A:185:GLU:HG3	2.13	0.47
1:B:182:ASN:HA	1:B:185:GLU:OE1	2.15	0.47
1:C:63:VAL:HG11	1:C:416:ALA:CB	2.45	0.47
1:E:236:GLN:HB2	1:E:266:ILE:HG13	1.97	0.47
1:E:398:PRO:C	1:E:400:ALA:H	2.16	0.47
1:E:544:GLN:HB3	1:F:543:PRO:HG3	1.96	0.47
1:H:544:GLN:HB3	1:I:543:PRO:HG3	1.96	0.47
1:I:256:ASP:OD1	1:I:257:ASP:N	2.47	0.47
1:I:544:GLN:HB3	1:J:543:PRO:HG3	1.97	0.47
1:J:45:LEU:HD22	1:J:328:ARG:HD3	1.95	0.47
1:J:443:ASP:C	1:J:445:GLU:H	2.17	0.47
1:A:256:ASP:OD1	1:A:257:ASP:N	2.48	0.47
1:B:53:TYR:HB2	1:C:48:TYR:CE2	2.50	0.47
1:I:443:ASP:C	1:I:445:GLU:H	2.17	0.47
1:K:236:GLN:HB2	1:K:266:ILE:HG13	1.96	0.47
1:L:236:GLN:HB2	1:L:266:ILE:HG13	1.96	0.47
1:B:467:ILE:O	1:B:471:ILE:HG12	2.15	0.47
1:E:321:ARG:O	1:E:324:LYS:HB3	2.14	0.47
1:G:63:VAL:HG11	1:G:416:ALA:HB1	1.96	0.47
1:G:225:VAL:HG23	1:G:298:ILE:HG23	1.97	0.47
1:K:63:VAL:HG11	1:K:416:ALA:CB	2.44	0.47
1:K:544:GLN:HB3	1:L:543:PRO:HG3	1.96	0.47
1:A:63:VAL:HG11	1:A:416:ALA:HB1	1.97	0.47
1:B:296:GLU:HB3	1:B:466:SER:HB3	1.95	0.47
1:B:346:LYS:HA	1:C:395:PRO:HG3	1.97	0.47
1:B:346:LYS:HE2	1:C:343:ARG:NH1	2.29	0.47
1:D:63:VAL:HG11	1:D:416:ALA:CB	2.45	0.47
1:E:164:LEU:HD13	1:E:169:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:321:ARG:O	1:F:324:LYS:HB3	2.15	0.47
1:H:346:LYS:HA	1:I:395:PRO:HG3	1.97	0.47
1:K:321:ARG:O	1:K:324:LYS:HB3	2.15	0.47
1:B:63:VAL:HG11	1:B:416:ALA:CB	2.45	0.46
1:C:96:GLY:HA3	1:C:480:ILE:HG23	1.97	0.46
1:C:236:GLN:HB2	1:C:266:ILE:HG13	1.96	0.46
1:D:63:VAL:HG11	1:D:416:ALA:HB1	1.96	0.46
1:H:321:ARG:O	1:H:324:LYS:HB3	2.15	0.46
1:H:346:LYS:HE2	1:I:343:ARG:NH1	2.30	0.46
1:A:45:LEU:HA	1:A:45:LEU:HD12	1.66	0.46
1:A:45:LEU:HD11	1:A:332:MET:CE	2.45	0.46
1:A:225:VAL:HG23	1:A:298:ILE:HG23	1.97	0.46
1:A:337:ASN:HB3	1:B:404:MET:HE2	1.97	0.46
1:D:363:TYR:OH	1:D:373:LEU:O	2.32	0.46
1:F:544:GLN:HB3	1:G:543:PRO:HG3	1.97	0.46
1:H:296:GLU:HB3	1:H:466:SER:HB3	1.97	0.46
1:K:568:MET:SD	1:L:555:GLN:HG2	2.55	0.46
1:A:487:GLU:CD	1:B:81:ARG:HH12	2.19	0.46
1:E:63:VAL:HG11	1:E:416:ALA:CB	2.45	0.46
1:E:320:VAL:O	1:E:324:LYS:HB2	2.15	0.46
1:G:87:ARG:NH2	1:G:507:LEU:O	2.48	0.46
1:H:443:ASP:C	1:H:445:GLU:H	2.17	0.46
1:K:554:LEU:HD21	1:K:575:GLN:HB3	1.97	0.46
1:K:574:LYS:HG3	1:K:592:TRP:CE3	2.51	0.46
1:L:321:ARG:O	1:L:324:LYS:HB3	2.14	0.46
1:C:544:GLN:HB3	1:D:543:PRO:HG3	1.97	0.46
1:D:225:VAL:HG23	1:D:298:ILE:HG23	1.98	0.46
1:F:471:ILE:O	1:F:473:ASP:N	2.48	0.46
1:I:321:ARG:O	1:I:324:LYS:HB3	2.15	0.46
1:J:137:PRO:HB2	1:K:243:PRO:HB3	1.96	0.46
1:L:494:ALA:HB3	1:L:507:LEU:HB2	1.97	0.46
1:B:544:GLN:HB3	1:C:543:PRO:HG3	1.96	0.46
1:C:63:VAL:HG11	1:C:416:ALA:HB1	1.97	0.46
1:E:80:TYR:HE2	1:E:465:GLN:HB2	1.81	0.46
1:E:475:PRO:HG3	1:E:493:MET:HG3	1.96	0.46
1:H:334:MET:HE1	1:I:407:ALA:HB1	1.96	0.46
1:H:468:VAL:HG13	1:H:472:TYR:CD2	2.48	0.46
1:I:63:VAL:HG11	1:I:416:ALA:CB	2.45	0.46
1:K:80:TYR:HE2	1:K:465:GLN:HB2	1.80	0.46
1:L:398:PRO:C	1:L:400:ALA:H	2.19	0.46
1:D:51:LEU:HD11	1:D:336:PHE:HA	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:443:ASP:C	1:G:445:GLU:H	2.17	0.46
1:J:256:ASP:OD1	1:J:257:ASP:N	2.48	0.46
1:A:343:ARG:HH21	1:L:346:LYS:NZ	2.09	0.46
1:A:346:LYS:HA	1:B:395:PRO:HG3	1.98	0.46
1:A:443:ASP:C	1:A:445:GLU:H	2.18	0.46
1:F:59:VAL:HG23	1:F:412:VAL:HG11	1.97	0.46
1:H:320:VAL:O	1:H:324:LYS:HB2	2.15	0.46
1:B:321:ARG:O	1:B:324:LYS:HB3	2.16	0.46
1:B:324:LYS:HD2	1:B:328:ARG:HH21	1.81	0.46
1:B:334:MET:HE1	1:C:407:ALA:HB1	1.97	0.46
1:F:94:LEU:HD21	1:F:468:VAL:HG11	1.98	0.46
1:J:363:TYR:OH	1:J:373:LEU:O	2.32	0.46
1:K:560:LEU:HD23	1:K:560:LEU:HA	1.81	0.46
1:B:80:TYR:HE2	1:B:465:GLN:HB2	1.81	0.46
1:B:574:LYS:HG3	1:B:592:TRP:CE3	2.51	0.46
1:E:164:LEU:O	1:E:167:LYS:HD3	2.16	0.46
1:G:94:LEU:HD12	1:G:514:TYR:CE2	2.51	0.46
1:H:97:MET:HE1	1:H:472:TYR:CE2	2.51	0.46
1:H:568:MET:SD	1:I:555:GLN:HG2	2.55	0.46
1:I:561:ASP:OD1	1:J:531:ASN:ND2	2.40	0.46
1:K:346:LYS:HZ1	1:L:343:ARG:NH2	2.13	0.46
1:L:63:VAL:HG11	1:L:416:ALA:CB	2.46	0.46
1:L:166:ASP:OD2	1:L:455:THR:HG22	2.16	0.46
1:B:554:LEU:HD21	1:B:575:GLN:HB3	1.98	0.46
1:B:568:MET:SD	1:C:555:GLN:HG2	2.56	0.46
1:D:184:TRP:CH2	1:D:288:LYS:HE3	2.51	0.46
1:D:487:GLU:CD	1:E:81:ARG:HH12	2.19	0.46
1:E:178:SER:OG	1:E:178:SER:O	2.33	0.46
1:A:543:PRO:HG3	1:L:544:GLN:HB3	1.98	0.45
1:B:337:ASN:HB3	1:C:404:MET:HE2	1.98	0.45
1:E:568:MET:SD	1:F:555:GLN:HG2	2.56	0.45
1:G:236:GLN:HB2	1:G:266:ILE:HG13	1.98	0.45
1:K:21:ALA:O	1:K:313:LYS:NZ	2.46	0.45
1:A:346:LYS:HZ1	1:B:343:ARG:HH21	1.64	0.45
1:B:443:ASP:C	1:B:445:GLU:H	2.17	0.45
1:D:137:PRO:HB2	1:E:243:PRO:HB3	1.97	0.45
1:D:236:GLN:HB2	1:D:266:ILE:HG13	1.98	0.45
1:H:166:ASP:OD1	1:H:455:THR:HG22	2.16	0.45
1:I:87:ARG:NH2	1:I:507:LEU:O	2.49	0.45
1:K:45:LEU:HD22	1:K:328:ARG:HD3	1.98	0.45
1:K:81:ARG:NH1	1:K:81:ARG:HG3	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:63:VAL:HG11	1:L:416:ALA:HB1	1.99	0.45
1:A:574:LYS:HG3	1:A:592:TRP:CE3	2.52	0.45
1:G:63:VAL:HG11	1:G:416:ALA:CB	2.45	0.45
1:I:398:PRO:C	1:I:400:ALA:H	2.19	0.45
1:J:225:VAL:HG23	1:J:298:ILE:HG23	1.97	0.45
1:A:97:MET:HE1	1:A:510:ILE:HG13	1.99	0.45
1:B:236:GLN:HB2	1:B:266:ILE:HG13	1.97	0.45
1:C:94:LEU:HG	1:C:510:ILE:HD12	1.99	0.45
1:D:45:LEU:HD22	1:D:328:ARG:HD3	1.97	0.45
1:D:177:HIS:HB2	1:D:219:ILE:HG22	1.98	0.45
1:F:398:PRO:C	1:F:400:ALA:H	2.19	0.45
1:H:164:LEU:O	1:H:167:LYS:HD3	2.17	0.45
1:J:236:GLN:HB2	1:J:266:ILE:HG13	1.99	0.45
1:K:334:MET:HE1	1:L:407:ALA:HB1	1.97	0.45
1:D:87:ARG:NH2	1:D:507:LEU:O	2.49	0.45
1:D:574:LYS:HG3	1:D:592:TRP:CE3	2.52	0.45
1:F:397:VAL:HG21	1:G:404:MET:SD	2.57	0.45
1:J:63:VAL:HG11	1:J:416:ALA:CB	2.45	0.45
1:L:59:VAL:HG23	1:L:412:VAL:HG11	1.99	0.45
1:A:48:TYR:CE2	1:L:53:TYR:HB2	2.52	0.45
1:B:166:ASP:OD1	1:B:455:THR:HG22	2.16	0.45
1:G:233:PHE:HD2	1:G:251:ILE:HG13	1.81	0.45
1:H:356:ILE:HD12	1:H:360:GLU:HG2	1.99	0.45
1:H:487:GLU:OE2	1:I:81:ARG:NH2	2.48	0.45
1:J:568:MET:HE2	1:K:555:GLN:HG2	1.99	0.45
1:J:574:LYS:HG3	1:J:592:TRP:CE3	2.52	0.45
1:K:94:LEU:HD21	1:K:468:VAL:HG11	1.99	0.45
1:L:89:ASP:O	1:L:93:VAL:HG23	2.17	0.45
1:L:296:GLU:HB3	1:L:466:SER:HB3	1.99	0.45
1:B:487:GLU:OE2	1:C:81:ARG:NE	2.43	0.45
1:D:346:LYS:HZ1	1:E:343:ARG:NH2	2.15	0.45
1:F:63:VAL:HG11	1:F:416:ALA:CB	2.45	0.45
1:F:491:GLN:O	1:F:508:ASN:ND2	2.50	0.45
1:G:51:LEU:HD11	1:G:336:PHE:HA	1.99	0.45
1:G:342:ALA:HB2	1:H:332:MET:CE	2.47	0.45
1:I:63:VAL:HG11	1:I:416:ALA:HB1	1.99	0.45
1:K:320:VAL:O	1:K:324:LYS:HB2	2.15	0.45
1:A:236:GLN:HB2	1:A:266:ILE:HG13	1.98	0.45
1:A:510:ILE:HD13	1:A:510:ILE:HA	1.83	0.45
1:D:342:ALA:HB2	1:E:332:MET:CE	2.47	0.45
1:E:356:ILE:HD12	1:E:360:GLU:HG2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:94:LEU:HD21	1:I:468:VAL:HG11	1.97	0.45
1:J:321:ARG:O	1:J:324:LYS:HB3	2.17	0.45
1:K:164:LEU:O	1:K:167:LYS:HD3	2.17	0.45
1:E:182:ASN:O	1:E:185:GLU:HG3	2.17	0.45
1:G:296:GLU:HB3	1:G:466:SER:HB3	1.98	0.45
1:H:21:ALA:O	1:H:313:LYS:NZ	2.46	0.45
1:I:397:VAL:HG21	1:J:404:MET:SD	2.57	0.45
1:K:166:ASP:OD1	1:K:455:THR:HG22	2.16	0.45
1:A:233:PHE:HD2	1:A:251:ILE:HG13	1.82	0.45
1:B:164:LEU:O	1:B:167:LYS:HD3	2.16	0.45
1:C:45:LEU:HD22	1:C:328:ARG:HD3	1.98	0.45
1:C:321:ARG:O	1:C:324:LYS:HB3	2.16	0.45
1:D:94:LEU:HD12	1:D:514:TYR:CE2	2.52	0.45
1:G:45:LEU:HD22	1:G:328:ARG:HD3	1.98	0.45
1:I:166:ASP:OD2	1:I:455:THR:HG22	2.16	0.45
1:J:179:MET:SD	1:J:183:GLY:HA3	2.57	0.45
1:J:233:PHE:HD2	1:J:251:ILE:HG13	1.82	0.45
1:J:337:ASN:HB3	1:K:404:MET:HE2	1.98	0.45
1:A:141:ASN:HB3	1:A:476:ARG:CZ	2.47	0.44
1:C:87:ARG:NH2	1:C:507:LEU:O	2.49	0.44
1:E:225:VAL:HG23	1:E:298:ILE:HG23	1.99	0.44
1:E:334:MET:HE1	1:F:407:ALA:HB1	1.98	0.44
1:F:473:ASP:OD1	1:F:511:ARG:NE	2.50	0.44
1:J:71:MET:HE1	1:J:449:PHE:HB3	1.98	0.44
1:A:51:LEU:HD11	1:A:336:PHE:HA	1.99	0.44
1:F:166:ASP:OD2	1:F:455:THR:HG22	2.17	0.44
1:H:45:LEU:HD22	1:H:328:ARG:HD3	1.98	0.44
1:I:182:ASN:HA	1:I:185:GLU:OE2	2.17	0.44
1:J:94:LEU:HD12	1:J:514:TYR:CE2	2.52	0.44
1:A:321:ARG:O	1:A:324:LYS:HB3	2.17	0.44
1:B:45:LEU:HD22	1:B:328:ARG:HD3	1.98	0.44
1:B:94:LEU:HD12	1:B:514:TYR:CD2	2.53	0.44
1:B:94:LEU:HD23	1:B:94:LEU:HA	1.80	0.44
1:B:131:ASP:OD2	1:B:145:ARG:NE	2.33	0.44
1:B:356:ILE:HD12	1:B:360:GLU:HG2	1.98	0.44
1:J:87:ARG:NH2	1:J:507:LEU:O	2.49	0.44
1:L:45:LEU:HD12	1:L:45:LEU:HA	1.65	0.44
1:C:245:SER:HB3	1:C:251:ILE:HG12	2.00	0.44
1:D:94:LEU:HD23	1:D:94:LEU:HA	1.83	0.44
1:E:21:ALA:O	1:E:313:LYS:NZ	2.45	0.44
1:J:81:ARG:HG3	1:J:517:TYR:CE1	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:97:MET:HE1	1:K:472:TYR:CE2	2.53	0.44
1:K:167:LYS:NZ	1:K:314:GLU:OE2	2.48	0.44
1:L:101:ASP:OD2	1:L:464:TYR:OH	2.21	0.44
1:B:59:VAL:HG23	1:B:412:VAL:HG11	1.99	0.44
1:E:166:ASP:OD1	1:E:455:THR:HG22	2.18	0.44
1:E:184:TRP:CZ3	1:E:288:LYS:HE3	2.52	0.44
1:F:94:LEU:HG	1:F:510:ILE:HD12	1.98	0.44
1:G:93:VAL:CG1	1:G:510:ILE:HD11	2.47	0.44
1:I:346:LYS:NZ	1:J:52:GLN:OE1	2.27	0.44
1:K:63:VAL:HG11	1:K:416:ALA:HB1	1.99	0.44
1:B:363:TYR:OH	1:B:373:LEU:O	2.35	0.44
1:D:233:PHE:HD2	1:D:251:ILE:HG13	1.81	0.44
1:E:45:LEU:HD22	1:E:328:ARG:HD3	1.99	0.44
1:J:51:LEU:HD11	1:J:336:PHE:HA	1.98	0.44
1:J:59:VAL:HG23	1:J:412:VAL:HG11	1.99	0.44
1:A:398:PRO:C	1:A:400:ALA:H	2.20	0.44
1:F:190:LYS:HE2	1:F:191:TYR:HE2	1.83	0.44
1:G:94:LEU:HD23	1:G:94:LEU:HA	1.85	0.44
1:H:63:VAL:HG11	1:H:416:ALA:HB1	1.99	0.44
1:J:398:PRO:C	1:J:400:ALA:H	2.20	0.44
1:K:94:LEU:HD12	1:K:514:TYR:CD2	2.53	0.44
1:K:356:ILE:HD12	1:K:360:GLU:HG2	1.99	0.44
1:A:404:MET:SD	1:L:397:VAL:HG21	2.57	0.44
1:B:141:ASN:HB3	1:B:476:ARG:NH1	2.32	0.44
1:I:59:VAL:HG23	1:I:412:VAL:HG11	2.00	0.44
1:I:560:LEU:HD23	1:I:560:LEU:HA	1.85	0.44
1:K:225:VAL:HG23	1:K:298:ILE:HG23	1.99	0.44
1:K:476:ARG:HE	1:K:476:ARG:HB3	1.52	0.44
1:K:539:LEU:HD21	1:K:553:LEU:HD13	1.99	0.44
1:B:320:VAL:O	1:B:324:LYS:HB2	2.17	0.44
1:D:398:PRO:C	1:D:400:ALA:H	2.20	0.44
1:G:245:SER:HB3	1:G:251:ILE:HG12	2.00	0.44
1:G:398:PRO:C	1:G:400:ALA:H	2.20	0.44
1:H:225:VAL:HG23	1:H:298:ILE:HG23	1.99	0.44
1:I:250:ASP:O	1:I:254:VAL:HG22	2.18	0.44
1:L:190:LYS:HE2	1:L:191:TYR:HE2	1.83	0.44
1:C:82:PRO:HA	1:C:514:TYR:HE1	1.82	0.43
1:D:321:ARG:O	1:D:324:LYS:HB3	2.17	0.43
1:E:63:VAL:HG11	1:E:416:ALA:HB1	1.99	0.43
1:E:324:LYS:HD2	1:E:328:ARG:HH21	1.83	0.43
1:F:245:SER:HB3	1:F:251:ILE:HG12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:554:LEU:HD21	1:F:575:GLN:HB3	2.00	0.43
1:I:346:LYS:NZ	1:J:343:ARG:HH21	2.13	0.43
1:J:174:THR:HG22	1:J:222:PHE:HD1	1.83	0.43
1:J:539:LEU:HD23	1:J:539:LEU:HA	1.85	0.43
1:B:68:VAL:HG22	1:B:119:ILE:HD12	2.00	0.43
1:C:190:LYS:HE2	1:C:191:TYR:HE2	1.83	0.43
1:C:507:LEU:HD23	1:C:507:LEU:HA	1.88	0.43
1:E:475:PRO:HA	1:E:493:MET:HG2	2.00	0.43
1:E:586:THR:OG1	1:E:587:PRO:HD2	2.18	0.43
1:F:320:VAL:O	1:F:324:LYS:HB2	2.18	0.43
1:H:324:LYS:HD2	1:H:328:ARG:HH21	1.83	0.43
1:H:554:LEU:HD21	1:H:575:GLN:HG2	2.00	0.43
1:I:164:LEU:HD23	1:I:164:LEU:HA	1.91	0.43
1:J:93:VAL:CG1	1:J:510:ILE:HD11	2.48	0.43
1:J:182:ASN:HA	1:J:185:GLU:CD	2.38	0.43
1:K:487:GLU:OE2	1:L:81:ARG:NE	2.45	0.43
1:B:225:VAL:HG23	1:B:298:ILE:HG23	1.99	0.43
1:C:397:VAL:HG21	1:D:404:MET:SD	2.58	0.43
1:E:12:LEU:HD23	1:E:12:LEU:HA	1.83	0.43
1:F:53:TYR:HB2	1:G:48:TYR:CE2	2.53	0.43
1:F:63:VAL:HG11	1:F:416:ALA:HB1	1.99	0.43
1:F:586:THR:OG1	1:F:587:PRO:HD2	2.19	0.43
1:G:8:LEU:HD13	1:G:286:VAL:HA	2.01	0.43
1:G:574:LYS:HG3	1:G:592:TRP:CE3	2.53	0.43
1:H:12:LEU:HD23	1:H:12:LEU:HA	1.83	0.43
1:I:554:LEU:HD21	1:I:575:GLN:HB3	2.01	0.43
1:K:59:VAL:HG23	1:K:412:VAL:HG11	2.00	0.43
1:K:363:TYR:OH	1:K:373:LEU:O	2.35	0.43
1:L:245:SER:HB3	1:L:251:ILE:HG12	1.99	0.43
1:L:468:VAL:HG13	1:L:472:TYR:CD2	2.54	0.43
1:C:398:PRO:C	1:C:400:ALA:H	2.21	0.43
1:E:40:GLN:HB2	1:E:56:GLN:HG2	2.01	0.43
1:E:334:MET:HE1	1:E:405:LEU:HD11	1.99	0.43
1:G:320:VAL:O	1:G:324:LYS:HB2	2.18	0.43
1:H:94:LEU:HD12	1:H:514:TYR:CD2	2.52	0.43
1:J:342:ALA:HB2	1:K:332:MET:CE	2.49	0.43
1:L:250:ASP:O	1:L:254:VAL:HG22	2.18	0.43
1:A:94:LEU:HD12	1:A:514:TYR:CE2	2.54	0.43
1:A:174:THR:HG22	1:A:222:PHE:HD1	1.83	0.43
1:C:250:ASP:O	1:C:254:VAL:HG22	2.19	0.43
1:C:296:GLU:HB3	1:C:466:SER:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:277:TYR:CD2	1:D:291:GLN:HB3	2.47	0.43
1:E:94:LEU:HD12	1:E:514:TYR:CD2	2.52	0.43
1:G:128:LEU:HD21	1:G:460:ASP:OD1	2.19	0.43
1:H:93:VAL:CG1	1:H:510:ILE:HD11	2.49	0.43
1:L:273:ARG:HA	1:L:273:ARG:HD2	1.90	0.43
1:L:333:ILE:CD1	1:L:404:MET:HG2	2.45	0.43
1:E:141:ASN:HB3	1:E:476:ARG:NH1	2.33	0.43
1:G:346:LYS:HZ1	1:H:343:ARG:NH2	2.17	0.43
1:H:40:GLN:HB2	1:H:56:GLN:HG2	2.01	0.43
1:I:273:ARG:HA	1:I:273:ARG:HD2	1.90	0.43
1:I:471:ILE:O	1:I:473:ASP:N	2.49	0.43
1:K:40:GLN:HB2	1:K:56:GLN:HG2	2.00	0.43
1:K:68:VAL:HG22	1:K:119:ILE:HD12	2.00	0.43
1:K:334:MET:HE1	1:K:405:LEU:HD11	2.01	0.43
1:L:8:LEU:HD13	1:L:286:VAL:HA	2.01	0.43
1:L:491:GLN:O	1:L:508:ASN:ND2	2.52	0.43
1:A:349:PRO:HB2	1:A:389:LEU:HD12	2.00	0.43
1:B:586:THR:OG1	1:B:587:PRO:HD2	2.19	0.43
1:C:91:ALA:O	1:C:95:MET:HG3	2.19	0.43
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.92	0.43
1:D:8:LEU:HD13	1:D:286:VAL:HA	2.00	0.43
1:D:245:SER:HB3	1:D:251:ILE:HG12	2.01	0.43
1:F:368:ASP:OD2	1:H:50:THR:HG21	2.19	0.43
1:G:474:VAL:O	1:G:476:ARG:HG3	2.18	0.43
1:H:574:LYS:HG3	1:H:592:TRP:CE3	2.54	0.43
1:I:190:LYS:HE2	1:I:191:TYR:HE2	1.83	0.43
1:J:324:LYS:HD2	1:J:328:ARG:HH21	1.84	0.43
1:A:346:LYS:HE2	1:B:343:ARG:HE	1.83	0.43
1:C:324:LYS:HD2	1:C:328:ARG:HH21	1.84	0.43
1:C:586:THR:OG1	1:C:587:PRO:HD2	2.19	0.43
1:E:334:MET:CE	1:E:405:LEU:HD11	2.49	0.43
1:I:586:THR:OG1	1:I:587:PRO:HD2	2.19	0.43
1:J:12:LEU:HD23	1:J:12:LEU:HA	1.83	0.43
1:J:560:LEU:HD23	1:J:560:LEU:HA	1.85	0.43
1:A:342:ALA:HB2	1:B:332:MET:CE	2.48	0.43
1:D:18:ASP:HA	1:D:160:SER:HB3	2.01	0.43
1:D:81:ARG:HG3	1:D:517:TYR:CE1	2.54	0.43
1:E:68:VAL:HG22	1:E:119:ILE:HD12	2.00	0.43
1:G:174:THR:HG22	1:G:222:PHE:HD1	1.83	0.43
1:H:59:VAL:HG23	1:H:412:VAL:HG11	2.00	0.43
1:H:586:THR:OG1	1:H:587:PRO:HD2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:167:LYS:HD2	1:I:167:LYS:HA	1.87	0.43
1:I:245:SER:HB3	1:I:251:ILE:HG12	2.00	0.43
1:L:324:LYS:HD2	1:L:328:ARG:HH21	1.84	0.43
1:B:40:GLN:HB2	1:B:56:GLN:HG2	2.00	0.43
1:B:63:VAL:HG11	1:B:416:ALA:HB1	2.00	0.43
1:C:14:ARG:HD2	1:C:172:HIS:CE1	2.54	0.43
1:C:320:VAL:O	1:C:324:LYS:HB2	2.19	0.43
1:F:33:LEU:HD11	1:F:37:ARG:NH1	2.34	0.43
1:F:276:VAL:C	1:F:277:TYR:HD2	2.22	0.43
1:F:324:LYS:HD2	1:F:328:ARG:HH21	1.83	0.43
1:G:14:ARG:HD2	1:G:172:HIS:CE1	2.54	0.43
1:K:71:MET:CE	1:K:449:PHE:HB3	2.49	0.43
1:K:586:THR:OG1	1:K:587:PRO:HD2	2.19	0.43
1:A:250:ASP:O	1:A:254:VAL:HG22	2.19	0.42
1:B:397:VAL:HG21	1:C:404:MET:SD	2.59	0.42
1:D:586:THR:OG1	1:D:587:PRO:HD2	2.19	0.42
1:F:250:ASP:O	1:F:254:VAL:HG22	2.19	0.42
1:H:167:LYS:NZ	1:H:314:GLU:OE2	2.48	0.42
1:K:93:VAL:CG1	1:K:510:ILE:HD11	2.49	0.42
1:L:94:LEU:HD23	1:L:94:LEU:HA	1.89	0.42
1:C:93:VAL:CG1	1:C:510:ILE:HD11	2.49	0.42
1:D:71:MET:HE1	1:D:449:PHE:HB3	2.01	0.42
1:D:167:LYS:HD2	1:D:167:LYS:HA	1.84	0.42
1:D:324:LYS:HD2	1:D:328:ARG:HH21	1.84	0.42
1:G:71:MET:CE	1:G:449:PHE:HB3	2.49	0.42
1:G:468:VAL:HA	1:G:471:ILE:HG22	2.00	0.42
1:J:586:THR:OG1	1:J:587:PRO:HD2	2.19	0.42
1:K:324:LYS:HD2	1:K:328:ARG:HH21	1.83	0.42
1:L:554:LEU:HD21	1:L:575:GLN:HB3	2.00	0.42
1:D:320:VAL:O	1:D:324:LYS:HB2	2.20	0.42
1:E:14:ARG:HD2	1:E:172:HIS:CE1	2.53	0.42
1:F:131:ASP:OD2	1:F:145:ARG:NE	2.37	0.42
1:G:561:ASP:OD1	1:H:531:ASN:ND2	2.45	0.42
1:B:71:MET:CE	1:B:449:PHE:HB3	2.49	0.42
1:C:276:VAL:C	1:C:277:TYR:HD2	2.22	0.42
1:C:554:LEU:HD21	1:C:575:GLN:HB3	2.00	0.42
1:C:555:GLN:HA	1:C:558:THR:HG22	2.02	0.42
1:D:337:ASN:HB3	1:E:404:MET:HE3	2.01	0.42
1:E:368:ASP:OD1	1:G:50:THR:OG1	2.26	0.42
1:F:14:ARG:HD2	1:F:172:HIS:CE1	2.55	0.42
1:F:555:GLN:HA	1:F:558:THR:HG22	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:324:LYS:HD2	1:I:328:ARG:HH21	1.84	0.42
1:J:14:ARG:HD2	1:J:172:HIS:CE1	2.55	0.42
1:L:320:VAL:O	1:L:324:LYS:HB2	2.18	0.42
1:L:586:THR:OG1	1:L:587:PRO:HD2	2.19	0.42
1:A:81:ARG:HG3	1:A:517:TYR:CE1	2.55	0.42
1:B:368:ASP:OD1	1:D:50:THR:HG21	2.19	0.42
1:C:89:ASP:O	1:C:93:VAL:HG23	2.19	0.42
1:C:167:LYS:HD2	1:C:167:LYS:HA	1.87	0.42
1:D:12:LEU:HD23	1:D:12:LEU:HA	1.83	0.42
1:D:71:MET:CE	1:D:449:PHE:HB3	2.49	0.42
1:D:128:LEU:HD21	1:D:460:ASP:OD1	2.20	0.42
1:E:71:MET:CE	1:E:449:PHE:HB3	2.49	0.42
1:G:337:ASN:HB3	1:H:404:MET:HE2	2.01	0.42
1:H:68:VAL:HG22	1:H:119:ILE:HD12	2.00	0.42
1:I:349:PRO:HB2	1:I:389:LEU:HD12	2.01	0.42
1:I:492:LEU:HD23	1:I:492:LEU:HA	1.85	0.42
1:J:190:LYS:HE2	1:J:191:TYR:HE2	1.85	0.42
1:J:250:ASP:O	1:J:254:VAL:HG22	2.20	0.42
1:L:555:GLN:HA	1:L:558:THR:HG22	2.01	0.42
1:A:14:ARG:HD2	1:A:172:HIS:CE1	2.54	0.42
1:B:334:MET:CE	1:B:405:LEU:HD11	2.50	0.42
1:C:8:LEU:HD13	1:C:286:VAL:HA	2.02	0.42
1:D:14:ARG:HD2	1:D:172:HIS:CE1	2.54	0.42
1:D:59:VAL:HG23	1:D:412:VAL:HG11	2.00	0.42
1:D:322:LEU:HD23	1:D:322:LEU:HA	1.87	0.42
1:D:474:VAL:O	1:D:476:ARG:HG3	2.20	0.42
1:E:349:PRO:HB2	1:E:389:LEU:HD12	2.01	0.42
1:I:8:LEU:HD13	1:I:286:VAL:HA	2.01	0.42
1:K:334:MET:CE	1:K:405:LEU:HD11	2.49	0.42
1:L:14:ARG:HD2	1:L:172:HIS:CE1	2.55	0.42
1:L:145:ARG:NH1	1:L:147:GLU:OE2	2.52	0.42
1:D:93:VAL:CG1	1:D:510:ILE:HD11	2.49	0.42
1:D:250:ASP:O	1:D:254:VAL:HG22	2.20	0.42
1:E:8:LEU:CD1	1:E:286:VAL:HA	2.50	0.42
1:G:492:LEU:HD23	1:G:492:LEU:HA	1.86	0.42
1:H:80:TYR:HE2	1:H:465:GLN:HB2	1.85	0.42
1:K:510:ILE:HD13	1:K:510:ILE:HA	1.86	0.42
1:B:91:ALA:O	1:B:95:MET:HG3	2.20	0.42
1:C:323:THR:CG2	1:C:416:ALA:HB2	2.50	0.42
1:E:59:VAL:HG23	1:E:412:VAL:HG11	2.01	0.42
1:E:94:LEU:HD23	1:E:94:LEU:HA	1.81	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:296:GLU:HB3	1:F:466:SER:HB3	2.01	0.42
1:G:374:LEU:O	1:H:352:TRP:HA	2.20	0.42
1:I:555:GLN:HA	1:I:558:THR:HG22	2.02	0.42
1:B:89:ASP:O	1:B:93:VAL:HG23	2.20	0.42
1:C:131:ASP:OD2	1:C:145:ARG:NE	2.35	0.42
1:C:145:ARG:NH1	1:C:147:GLU:OE2	2.52	0.42
1:F:333:ILE:CD1	1:F:404:MET:HG2	2.45	0.42
1:G:167:LYS:HD2	1:G:167:LYS:HA	1.84	0.42
1:G:323:THR:CG2	1:G:416:ALA:HB2	2.49	0.42
1:G:586:THR:OG1	1:G:587:PRO:HD2	2.19	0.42
1:H:255:ILE:H	1:H:255:ILE:HG13	1.70	0.42
1:H:320:VAL:O	1:H:324:LYS:CB	2.68	0.42
1:I:320:VAL:O	1:I:324:LYS:HB2	2.19	0.42
1:I:491:GLN:O	1:I:508:ASN:ND2	2.53	0.42
1:J:346:LYS:HZ3	1:K:343:ARG:NH2	2.18	0.42
1:J:374:LEU:O	1:K:352:TRP:HA	2.20	0.42
1:K:89:ASP:O	1:K:93:VAL:HG23	2.20	0.42
1:K:320:VAL:O	1:K:324:LYS:CB	2.68	0.42
1:A:320:VAL:O	1:A:324:LYS:HB2	2.19	0.42
1:A:374:LEU:O	1:B:352:TRP:HA	2.20	0.42
1:A:586:THR:OG1	1:A:587:PRO:HD2	2.20	0.42
1:D:174:THR:HG22	1:D:222:PHE:HD1	1.83	0.42
1:E:255:ILE:H	1:E:255:ILE:HG13	1.70	0.42
1:F:182:ASN:HA	1:F:185:GLU:OE2	2.20	0.42
1:F:192:ASP:OD1	1:F:193:LEU:N	2.50	0.42
1:K:51:LEU:HD11	1:K:336:PHE:HA	2.00	0.42
1:L:131:ASP:OD2	1:L:145:ARG:NE	2.37	0.42
1:B:472:TYR:HE1	1:B:476:ARG:CZ	2.33	0.41
1:C:344:THR:HG23	1:D:50:THR:OG1	2.20	0.41
1:C:574:LYS:HG3	1:C:592:TRP:CE3	2.55	0.41
1:E:320:VAL:O	1:E:324:LYS:CB	2.68	0.41
1:H:51:LEU:HD11	1:H:336:PHE:HA	2.01	0.41
1:I:145:ARG:NH1	1:I:147:GLU:OE2	2.53	0.41
1:K:91:ALA:O	1:K:95:MET:HG3	2.20	0.41
1:L:323:THR:CG2	1:L:416:ALA:HB2	2.50	0.41
1:B:475:PRO:HA	1:B:493:MET:HG2	2.01	0.41
1:D:349:PRO:HB2	1:D:389:LEU:HD12	2.02	0.41
1:E:45:LEU:HD12	1:E:45:LEU:HA	1.86	0.41
1:F:164:LEU:HD23	1:F:164:LEU:HA	1.92	0.41
1:F:255:ILE:H	1:F:255:ILE:HG13	1.68	0.41
1:H:113:ILE:HD13	1:H:150:HIS:NE2	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:334:MET:CE	1:H:405:LEU:HD11	2.50	0.41
1:I:58:ASP:HA	1:I:327:GLN:NE2	2.35	0.41
1:I:333:ILE:CD1	1:I:404:MET:HG2	2.45	0.41
1:J:94:LEU:HA	1:J:94:LEU:HD23	1.84	0.41
1:L:182:ASN:HA	1:L:185:GLU:CD	2.40	0.41
1:L:233:PHE:HD2	1:L:251:ILE:HG13	1.85	0.41
1:A:323:THR:CG2	1:A:416:ALA:HB2	2.51	0.41
1:A:352:TRP:HA	1:L:374:LEU:O	2.21	0.41
1:B:97:MET:HE1	1:B:472:TYR:CE2	2.55	0.41
1:C:182:ASN:HA	1:C:185:GLU:OE2	2.20	0.41
1:C:494:ALA:HB3	1:C:507:LEU:HB2	2.01	0.41
1:E:560:LEU:HD23	1:E:560:LEU:HA	1.81	0.41
1:F:45:LEU:HA	1:F:45:LEU:HD12	1.65	0.41
1:G:59:VAL:HG23	1:G:412:VAL:HG11	2.01	0.41
1:G:567:MET:SD	1:G:568:MET:HG3	2.60	0.41
1:I:89:ASP:O	1:I:93:VAL:HG23	2.21	0.41
1:L:303:VAL:HG12	1:L:456:ALA:CB	2.51	0.41
1:L:471:ILE:O	1:L:473:ASP:N	2.50	0.41
1:A:245:SER:HB3	1:A:251:ILE:HG12	2.01	0.41
1:B:245:SER:HB3	1:B:251:ILE:HD13	2.02	0.41
1:B:349:PRO:HB2	1:B:389:LEU:HD12	2.02	0.41
1:D:397:VAL:HG21	1:E:404:MET:SD	2.60	0.41
1:E:93:VAL:CG1	1:E:510:ILE:HD11	2.50	0.41
1:F:89:ASP:O	1:F:93:VAL:HG23	2.20	0.41
1:F:145:ARG:NH1	1:F:147:GLU:OE2	2.53	0.41
1:H:89:ASP:O	1:H:93:VAL:HG23	2.20	0.41
1:H:363:TYR:OH	1:H:373:LEU:O	2.35	0.41
1:J:320:VAL:O	1:J:324:LYS:HB2	2.19	0.41
1:J:491:GLN:O	1:J:508:ASN:ND2	2.54	0.41
1:A:52:GLN:OE1	1:L:346:LYS:NZ	2.28	0.41
1:A:128:LEU:HD21	1:A:460:ASP:OD1	2.21	0.41
1:B:167:LYS:HD2	1:B:167:LYS:HA	1.89	0.41
1:B:320:VAL:O	1:B:324:LYS:CB	2.68	0.41
1:D:164:LEU:HD23	1:D:164:LEU:HA	1.93	0.41
1:D:323:THR:CG2	1:D:416:ALA:HB2	2.51	0.41
1:E:131:ASP:OD2	1:E:145:ARG:NE	2.34	0.41
1:F:82:PRO:HA	1:F:514:TYR:HE1	1.82	0.41
1:F:225:VAL:HG23	1:F:298:ILE:HG23	2.02	0.41
1:F:322:LEU:HD23	1:F:322:LEU:HA	1.89	0.41
1:G:255:ILE:H	1:G:255:ILE:HG13	1.69	0.41
1:J:58:ASP:HA	1:J:327:GLN:NE2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:324:LYS:HD2	1:A:328:ARG:HH21	1.84	0.41
1:A:555:GLN:HG2	1:L:568:MET:SD	2.60	0.41
1:B:33:LEU:HD11	1:B:37:ARG:NH1	2.36	0.41
1:G:560:LEU:HD23	1:G:560:LEU:HA	1.85	0.41
1:H:71:MET:CE	1:H:449:PHE:HB3	2.50	0.41
1:H:245:SER:HB3	1:H:251:ILE:HD13	2.03	0.41
1:H:560:LEU:HD23	1:H:560:LEU:HA	1.81	0.41
1:I:12:LEU:HD23	1:I:12:LEU:HA	1.85	0.41
1:I:14:ARG:HD2	1:I:172:HIS:CE1	2.56	0.41
1:L:349:PRO:HB2	1:L:389:LEU:HD12	2.01	0.41
1:A:563:LYS:HD3	1:B:483:GLU:OE1	2.20	0.41
1:B:113:ILE:HD13	1:B:150:HIS:NE2	2.36	0.41
1:B:323:THR:CG2	1:B:416:ALA:HB2	2.51	0.41
1:D:58:ASP:HA	1:D:327:GLN:NE2	2.36	0.41
1:D:296:GLU:HB3	1:D:466:SER:HB3	2.01	0.41
1:F:137:PRO:HB2	1:G:243:PRO:HB3	2.02	0.41
1:F:557:PHE:HE1	1:G:538:LEU:HD13	1.85	0.41
1:G:324:LYS:HD2	1:G:328:ARG:HH21	1.86	0.41
1:G:397:VAL:HG21	1:H:404:MET:SD	2.60	0.41
1:I:475:PRO:HA	1:I:493:MET:HG2	2.02	0.41
1:J:492:LEU:HD23	1:J:492:LEU:HA	1.86	0.41
1:B:36:SER:O	1:B:36:SER:OG	2.34	0.41
1:B:245:SER:HB3	1:B:251:ILE:CD1	2.51	0.41
1:C:177:HIS:HB2	1:C:219:ILE:HG22	2.03	0.41
1:C:568:MET:SD	1:D:555:GLN:HG2	2.60	0.41
1:E:184:TRP:HZ3	1:E:288:LYS:HE3	1.86	0.41
1:F:374:LEU:O	1:G:352:TRP:HA	2.21	0.41
1:G:250:ASP:O	1:G:254:VAL:HG22	2.20	0.41
1:G:507:LEU:HD23	1:G:507:LEU:HA	1.89	0.41
1:H:376:ARG:HG3	1:H:377:THR:N	2.36	0.41
1:I:51:LEU:HD11	1:I:336:PHE:HA	2.02	0.41
1:I:233:PHE:HD2	1:I:251:ILE:HG13	1.86	0.41
1:I:303:VAL:HG12	1:I:456:ALA:CB	2.51	0.41
1:I:323:THR:CG2	1:I:416:ALA:HB2	2.50	0.41
1:I:374:LEU:O	1:J:352:TRP:HA	2.21	0.41
1:I:568:MET:SD	1:J:555:GLN:HG2	2.60	0.41
1:J:397:VAL:HG21	1:K:404:MET:SD	2.60	0.41
1:K:242:GLU:O	1:K:244:VAL:HG23	2.21	0.41
1:K:469:ASN:OD1	1:K:511:ARG:HG2	2.21	0.41
1:L:93:VAL:CG1	1:L:510:ILE:HD11	2.50	0.41
1:L:99:ARG:HG2	1:L:103:ARG:HH21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:PRO:HB3	1:L:137:PRO:HB2	2.03	0.41
1:A:397:VAL:HG21	1:B:404:MET:SD	2.60	0.41
1:A:507:LEU:HD23	1:A:507:LEU:HA	1.88	0.41
1:A:538:LEU:HD13	1:L:557:PHE:HE1	1.85	0.41
1:C:58:ASP:HA	1:C:327:GLN:NE2	2.36	0.41
1:C:225:VAL:HG23	1:C:298:ILE:HG23	2.03	0.41
1:C:303:VAL:HG12	1:C:456:ALA:CB	2.51	0.41
1:C:471:ILE:O	1:C:473:ASP:N	2.49	0.41
1:D:374:LEU:O	1:E:352:TRP:HA	2.20	0.41
1:E:346:LYS:HE2	1:F:343:ARG:NH1	2.35	0.41
1:F:58:ASP:HA	1:F:327:GLN:NE2	2.36	0.41
1:F:113:ILE:HD13	1:F:150:HIS:NE2	2.36	0.41
1:F:303:VAL:HG12	1:F:456:ALA:CB	2.50	0.41
1:F:568:MET:SD	1:G:555:GLN:HG2	2.61	0.41
1:F:574:LYS:HG3	1:F:592:TRP:CE3	2.56	0.41
1:H:142:GLN:H	1:H:476:ARG:NH1	2.19	0.41
1:H:232:ALA:HB3	1:H:269:ARG:O	2.21	0.41
1:H:374:LEU:O	1:I:352:TRP:HA	2.21	0.41
1:I:68:VAL:HG22	1:I:119:ILE:HD12	2.03	0.41
1:I:474:VAL:O	1:I:476:ARG:HG3	2.20	0.41
1:J:79:LEU:HA	1:J:95:MET:HE2	2.02	0.41
1:J:245:SER:HB3	1:J:251:ILE:HG12	2.01	0.41
1:J:474:VAL:O	1:J:476:ARG:HG3	2.21	0.41
1:J:488:LYS:HB2	1:J:488:LYS:HE3	1.85	0.41
1:L:492:LEU:HA	1:L:492:LEU:HD23	1.85	0.41
1:A:488:LYS:HB2	1:A:488:LYS:HE3	1.86	0.41
1:B:45:LEU:HD12	1:B:45:LEU:HA	1.86	0.41
1:B:367:ASP:HB2	1:B:369:TYR:CE1	2.56	0.41
1:C:349:PRO:HB2	1:C:389:LEU:HD12	2.03	0.41
1:C:474:VAL:O	1:C:476:ARG:HG3	2.21	0.41
1:F:273:ARG:HA	1:F:273:ARG:HD2	1.91	0.41
1:H:67:LEU:HD23	1:H:67:LEU:HA	1.90	0.41
1:H:323:THR:CG2	1:H:416:ALA:HB2	2.51	0.41
1:I:94:LEU:HG	1:I:510:ILE:HD12	2.03	0.41
1:L:68:VAL:HG22	1:L:119:ILE:HD12	2.03	0.41
1:L:521:GLY:HA3	1:L:522:PRO:HD3	1.94	0.41
1:A:296:GLU:HB3	1:A:466:SER:HB3	2.03	0.40
1:B:374:LEU:O	1:C:352:TRP:HA	2.21	0.40
1:E:162:SER:OG	1:E:167:LYS:HD2	2.21	0.40
1:E:167:LYS:NZ	1:E:314:GLU:OE2	2.49	0.40
1:E:323:THR:CG2	1:E:416:ALA:HB2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:474:VAL:O	1:F:476:ARG:HG3	2.21	0.40
1:G:179:MET:SD	1:G:183:GLY:HA3	2.62	0.40
1:H:242:GLU:O	1:H:244:VAL:HG23	2.21	0.40
1:I:113:ILE:HD13	1:I:150:HIS:NE2	2.35	0.40
1:I:507:LEU:HD23	1:I:507:LEU:HA	1.89	0.40
1:I:510:ILE:HD13	1:I:510:ILE:HA	1.86	0.40
1:J:45:LEU:HD12	1:J:45:LEU:HA	1.75	0.40
1:K:374:LEU:O	1:L:352:TRP:HA	2.21	0.40
1:L:94:LEU:HG	1:L:510:ILE:HD12	2.03	0.40
1:L:177:HIS:HB2	1:L:219:ILE:HG22	2.03	0.40
1:A:346:LYS:NZ	1:B:52:GLN:OE1	2.29	0.40
1:B:101:ASP:OD2	1:B:464:TYR:OH	2.26	0.40
1:B:177:HIS:HB2	1:B:219:ILE:HG22	2.03	0.40
1:C:59:VAL:HG23	1:C:412:VAL:HG11	2.03	0.40
1:C:68:VAL:HG22	1:C:119:ILE:HD12	2.03	0.40
1:C:113:ILE:HD13	1:C:150:HIS:NE2	2.36	0.40
1:C:137:PRO:HB2	1:D:243:PRO:HB3	2.02	0.40
1:D:482:LEU:HD11	1:D:488:LYS:HD2	2.04	0.40
1:D:488:LYS:HE3	1:D:488:LYS:HB2	1.86	0.40
1:E:33:LEU:HD11	1:E:37:ARG:NH1	2.36	0.40
1:E:51:LEU:HD11	1:E:336:PHE:HA	2.02	0.40
1:E:113:ILE:HD13	1:E:150:HIS:NE2	2.36	0.40
1:E:554:LEU:CD2	1:E:575:GLN:HB3	2.51	0.40
1:F:323:THR:CG2	1:F:416:ALA:HB2	2.51	0.40
1:G:376:ARG:HG3	1:G:377:THR:N	2.36	0.40
1:A:19:TRP:HE3	1:A:157:ILE:HG12	1.86	0.40
1:A:113:ILE:HD13	1:A:150:HIS:NE2	2.37	0.40
1:D:113:ILE:HD13	1:D:150:HIS:NE2	2.37	0.40
1:E:374:LEU:O	1:F:352:TRP:HA	2.21	0.40
1:F:177:HIS:HB2	1:F:219:ILE:HG22	2.03	0.40
1:H:94:LEU:HA	1:H:94:LEU:HD23	1.82	0.40
1:H:349:PRO:HB2	1:H:389:LEU:HD12	2.02	0.40
1:I:99:ARG:HG2	1:I:103:ARG:HH21	1.85	0.40
1:I:177:HIS:HB2	1:I:219:ILE:HG22	2.03	0.40
1:J:376:ARG:HG3	1:J:377:THR:N	2.36	0.40
1:K:113:ILE:HD13	1:K:150:HIS:NE2	2.36	0.40
1:L:113:ILE:HD13	1:L:150:HIS:NE2	2.35	0.40
1:L:475:PRO:HA	1:L:493:MET:HG2	2.02	0.40
1:L:574:LYS:HG3	1:L:592:TRP:CE3	2.56	0.40
1:C:71:MET:HE2	1:C:449:PHE:HB3	2.03	0.40
1:D:94:LEU:HD12	1:D:514:TYR:CD2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:242:GLU:O	1:E:244:VAL:HG23	2.21	0.40
1:F:184:TRP:CH2	1:F:288:LYS:HE3	2.56	0.40
1:F:510:ILE:HD13	1:F:510:ILE:HA	1.85	0.40
1:G:58:ASP:HA	1:G:327:GLN:NE2	2.36	0.40
1:H:487:GLU:OE2	1:I:81:ARG:NE	2.52	0.40
1:I:557:PHE:HE1	1:J:538:LEU:HD13	1.87	0.40
1:I:574:LYS:HG3	1:I:592:TRP:CE3	2.56	0.40
1:K:128:LEU:HD21	1:K:460:ASP:OD1	2.21	0.40
1:A:340:ILE:HG13	1:L:345:PRO:HG3	2.03	0.40
1:B:128:LEU:HD21	1:B:460:ASP:OD1	2.22	0.40
1:B:376:ARG:HG3	1:B:377:THR:N	2.36	0.40
1:C:362:MET:HA	1:C:369:TYR:CE2	2.56	0.40
1:D:539:LEU:HD23	1:D:539:LEU:HA	1.85	0.40
1:G:273:ARG:HD2	1:G:274:ARG:H	1.85	0.40
1:G:349:PRO:HB2	1:G:389:LEU:HD12	2.02	0.40
1:J:113:ILE:HD13	1:J:150:HIS:NE2	2.37	0.40
1:J:507:LEU:HD23	1:J:507:LEU:HA	1.90	0.40
1:K:142:GLN:O	1:K:476:ARG:NH1	2.36	0.40
1:L:51:LEU:HD11	1:L:336:PHE:HA	2.02	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	A	533/725 (74%)	482 (90%)	51 (10%)	0	100	100
1	B	533/725 (74%)	486 (91%)	47 (9%)	0	100	100
1	C	533/725 (74%)	483 (91%)	50 (9%)	0	100	100
1	D	533/725 (74%)	485 (91%)	48 (9%)	0	100	100
1	E	533/725 (74%)	487 (91%)	46 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	533/725 (74%)	483 (91%)	50 (9%)	0	100	100
1	G	533/725 (74%)	479 (90%)	54 (10%)	0	100	100
1	H	533/725 (74%)	485 (91%)	48 (9%)	0	100	100
1	I	533/725 (74%)	484 (91%)	49 (9%)	0	100	100
1	J	533/725 (74%)	484 (91%)	49 (9%)	0	100	100
1	K	533/725 (74%)	486 (91%)	47 (9%)	0	100	100
1	L	533/725 (74%)	483 (91%)	50 (9%)	0	100	100
All	All	6396/8700 (74%)	5807 (91%)	589 (9%)	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	A	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	B	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	C	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	D	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	E	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	F	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	G	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	H	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	I	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	J	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	K	476/630 (76%)	475 (100%)	1 (0%)	92	97
1	L	476/630 (76%)	475 (100%)	1 (0%)	92	97
All	All	5712/7560 (76%)	5700 (100%)	12 (0%)	91	97

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	583	LYS
1	B	583	LYS
1	C	583	LYS
1	D	583	LYS
1	E	583	LYS
1	F	583	LYS
1	G	583	LYS
1	H	583	LYS
1	I	583	LYS
1	J	583	LYS
1	K	583	LYS
1	L	583	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	161	ASN
1	K	578	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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.

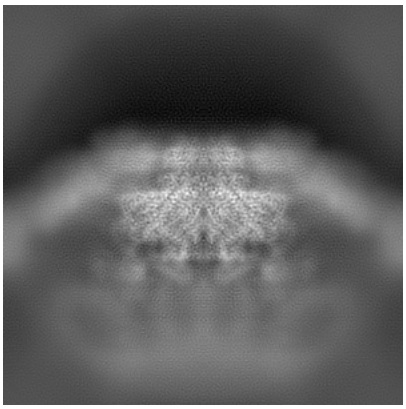
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-61460. These allow visual inspection of the internal detail of the map and identification of artifacts.

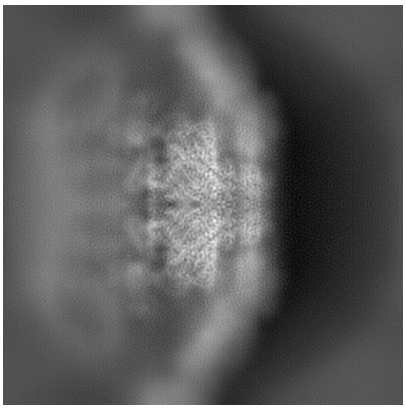
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

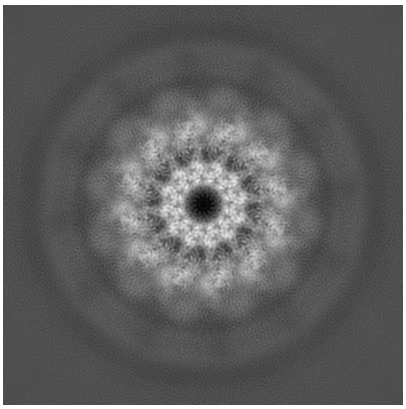
6.1.1 Primary map



X

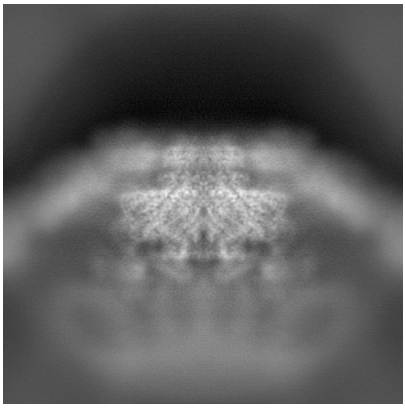


Y

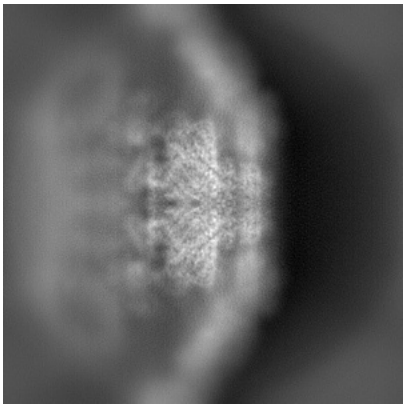


Z

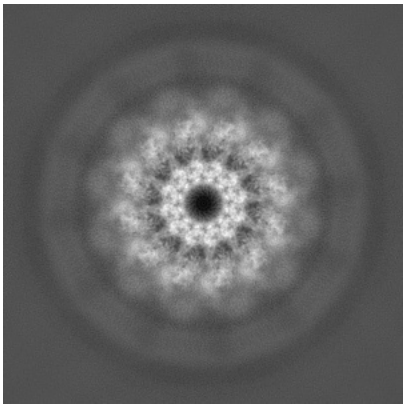
6.1.2 Raw map



X



Y

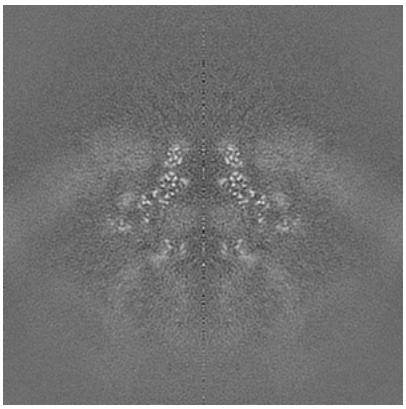


Z

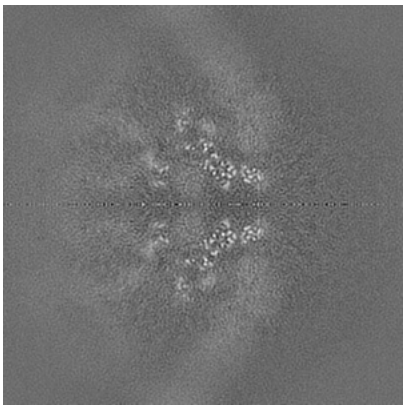
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

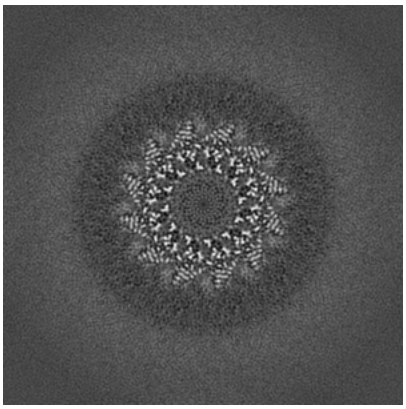
6.2.1 Primary map



X Index: 180

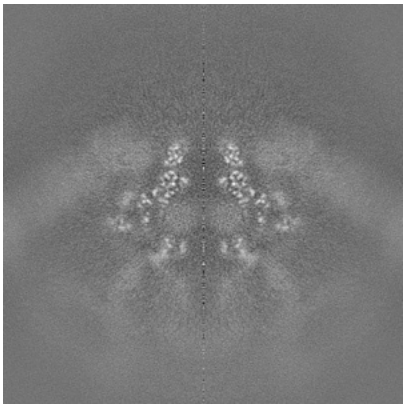


Y Index: 180

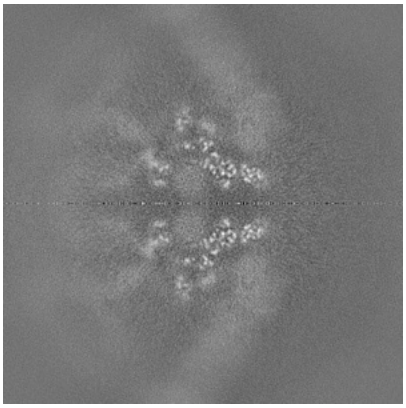


Z Index: 180

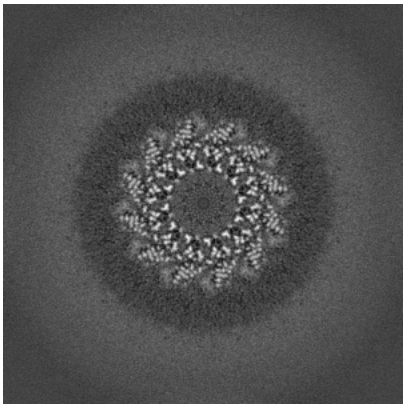
6.2.2 Raw map



X Index: 180



Y Index: 180

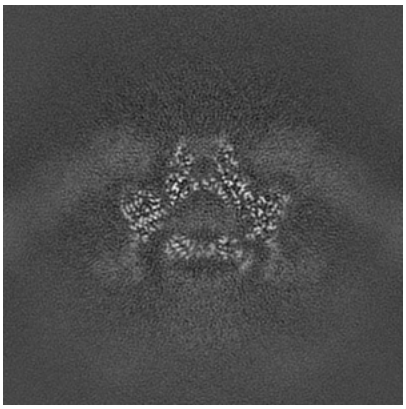


Z Index: 180

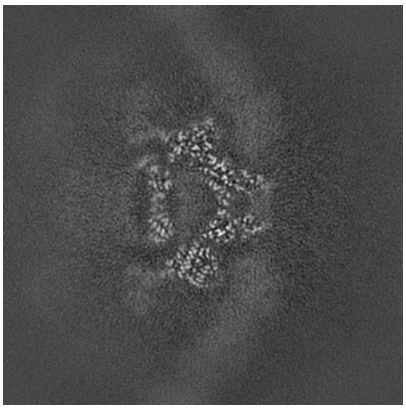
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

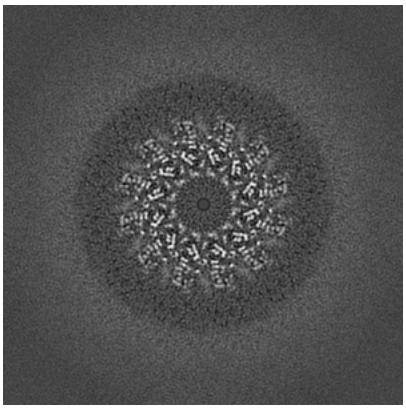
6.3.1 Primary map



X Index: 197

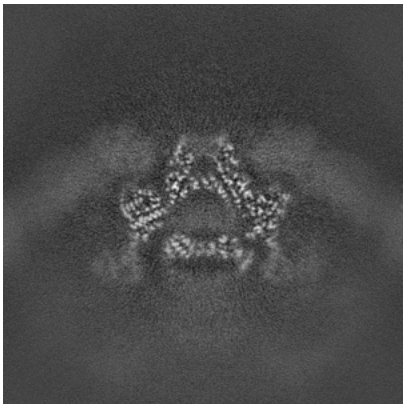


Y Index: 163

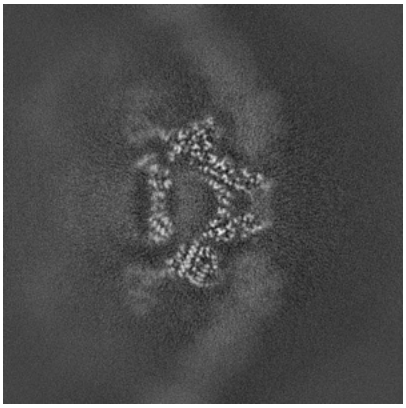


Z Index: 183

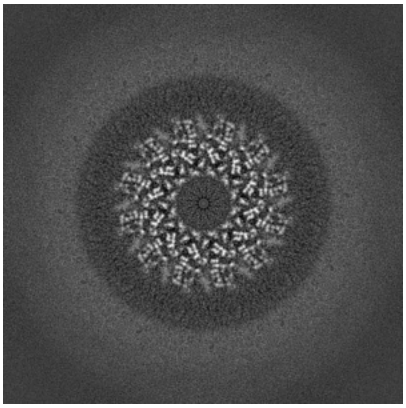
6.3.2 Raw map



X Index: 197



Y Index: 163

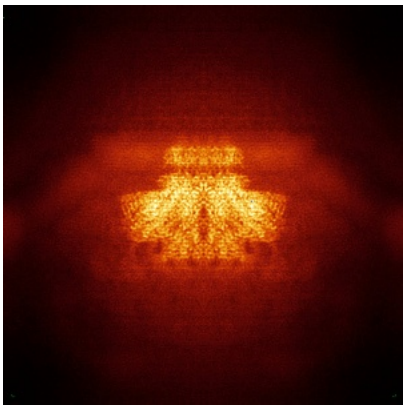


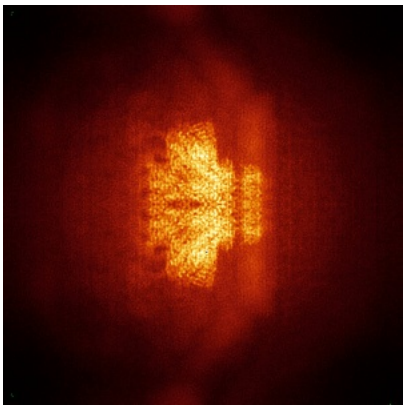
Z Index: 183

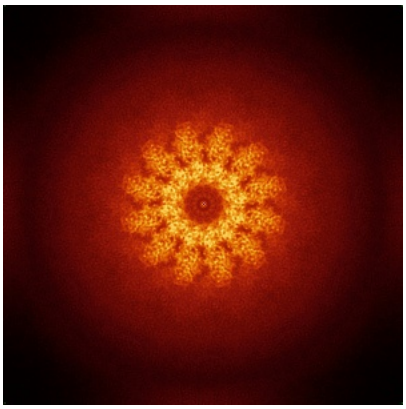
The images above show the largest variance slices of the map in three orthogonal directions.

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

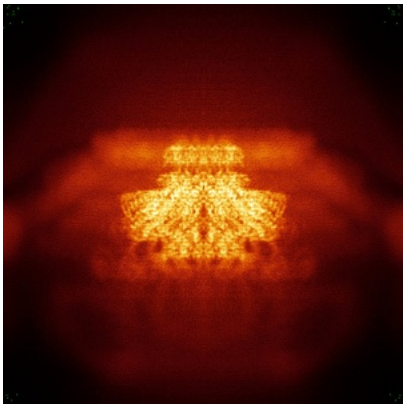
6.4.1 Primary map

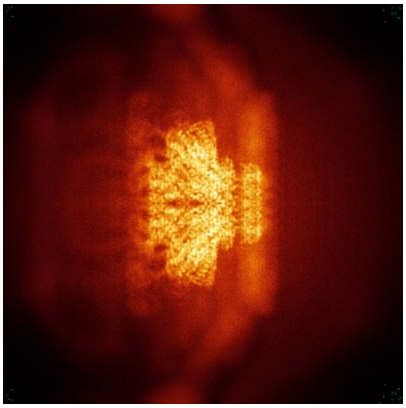

X

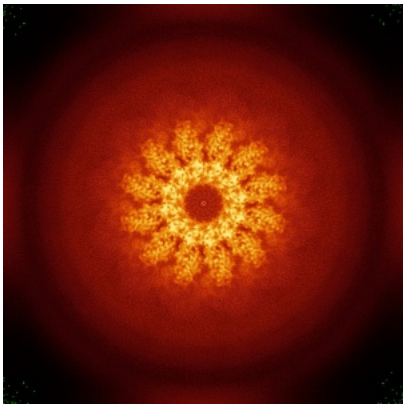

Y


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 3.6. 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.

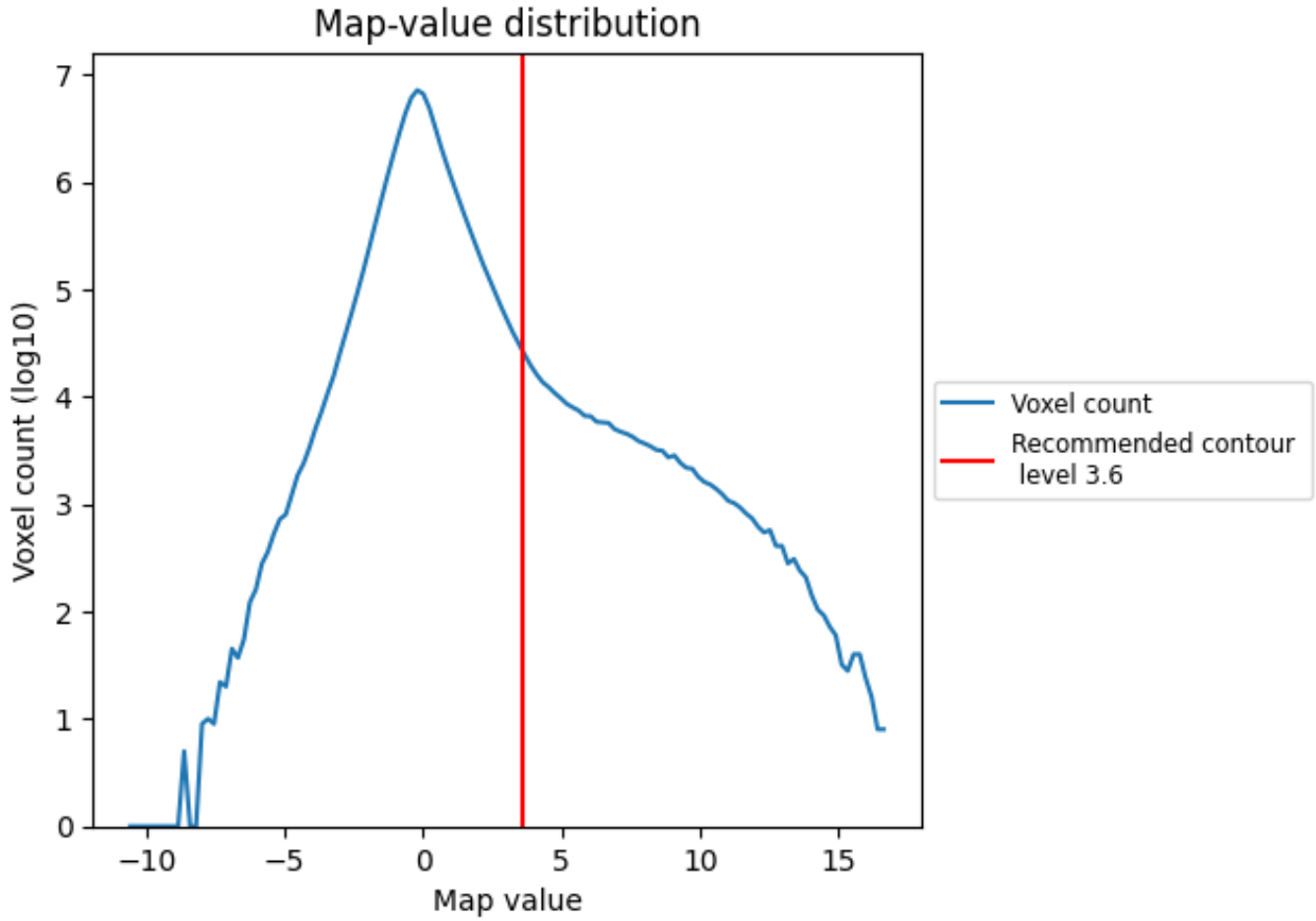
6.6 Mask visualisation (i)

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

7 Map analysis

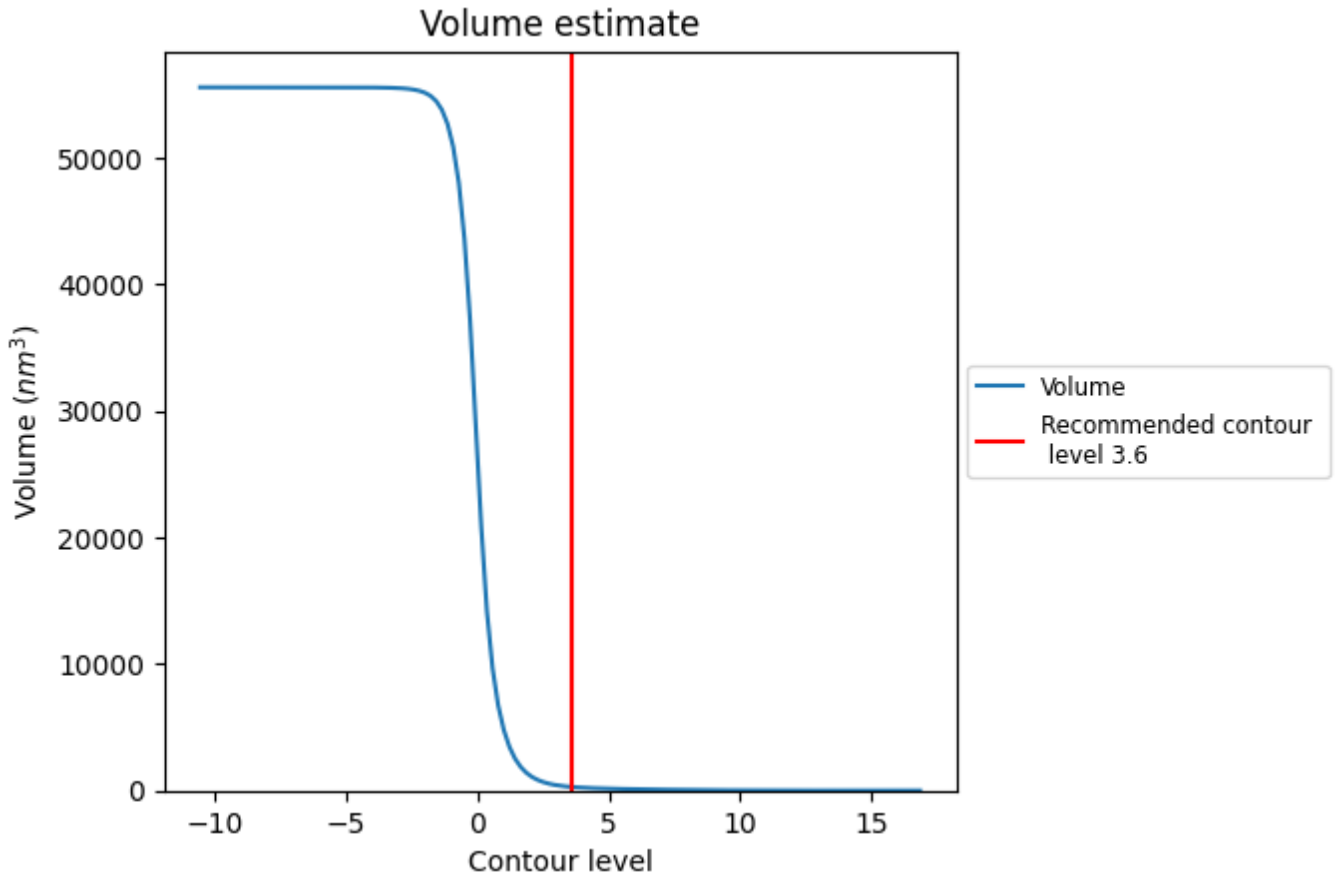
This section contains the results of statistical analysis of the map.

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.

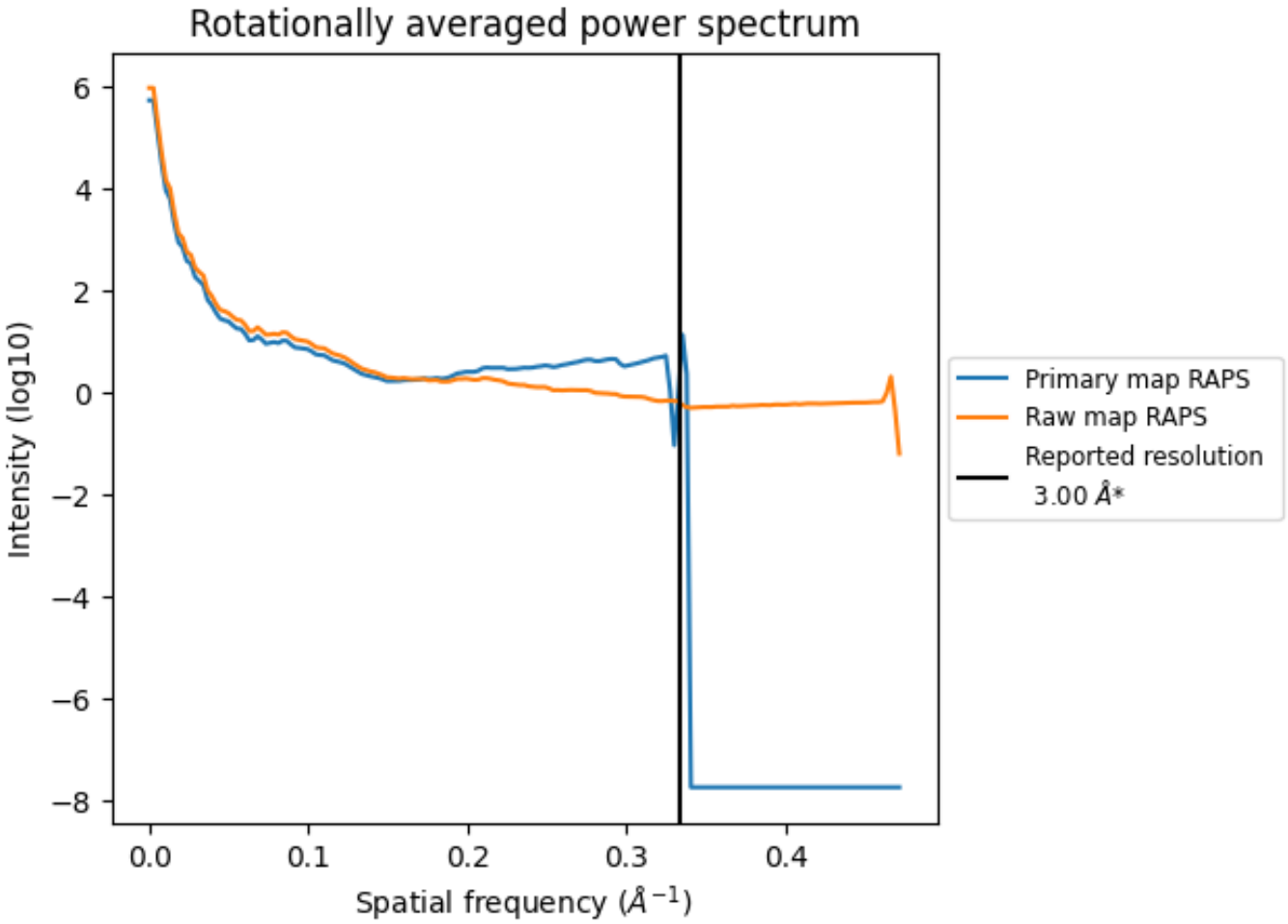
7.2 Volume estimate



The volume at the recommended contour level is 279 nm^3; this corresponds to an approximate mass of 252 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)

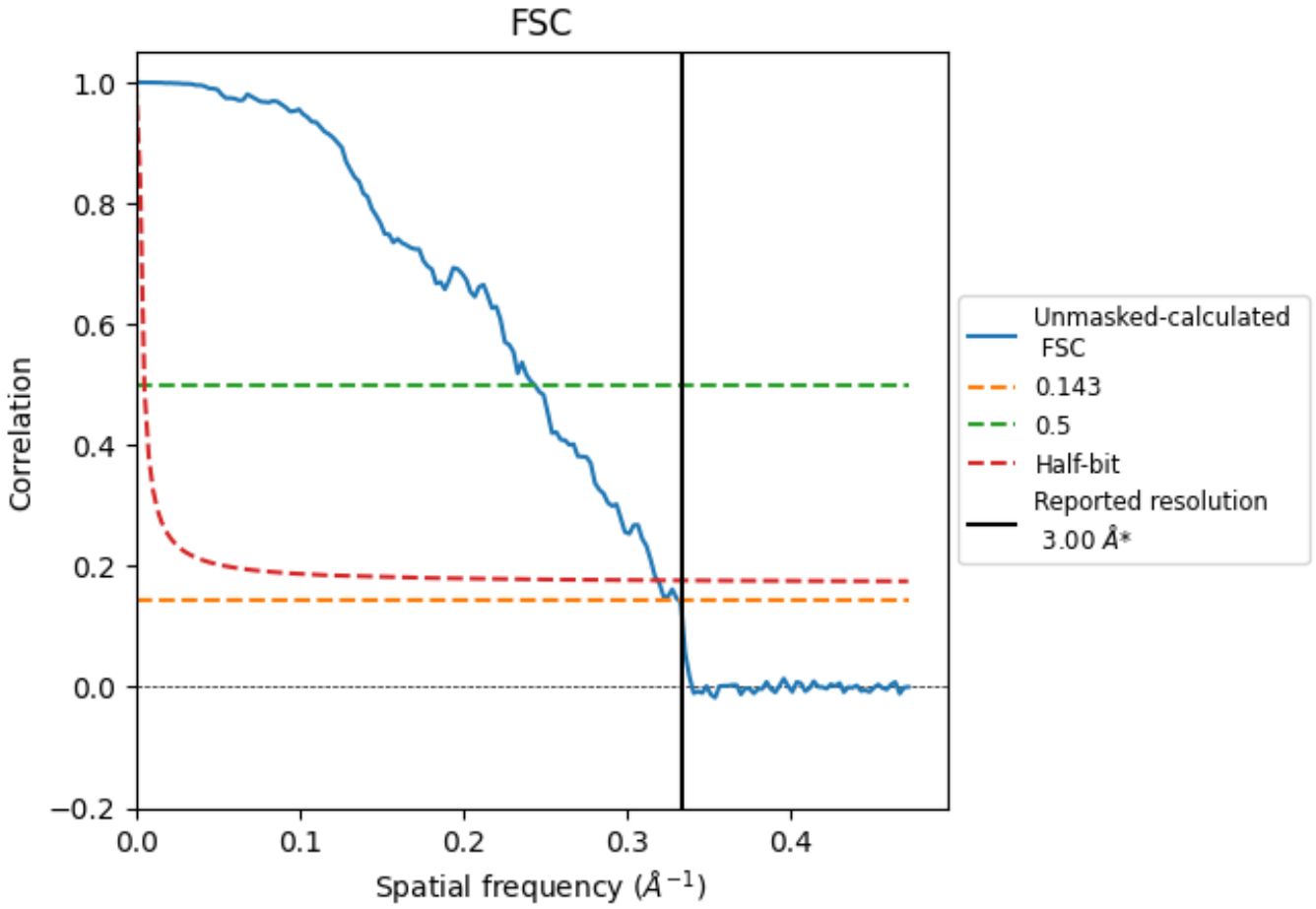


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

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 0.333 Å^{-1}

8.2 Resolution estimates (i)

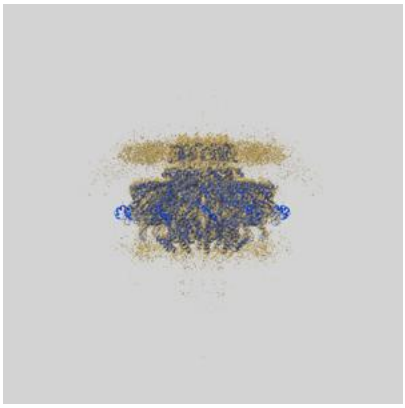
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.01	4.11	3.14

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

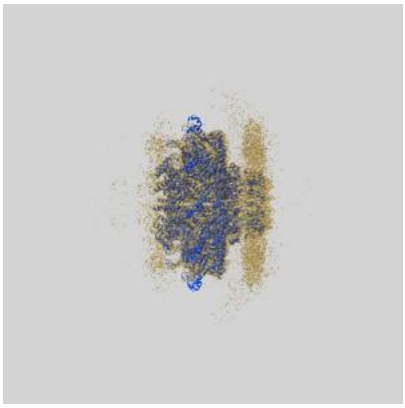
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61460 and PDB model 9JGA. Per-residue inclusion information can be found in section 3 on page 5.

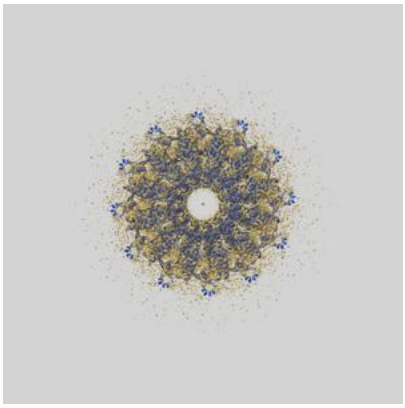
9.1 Map-model overlay



X



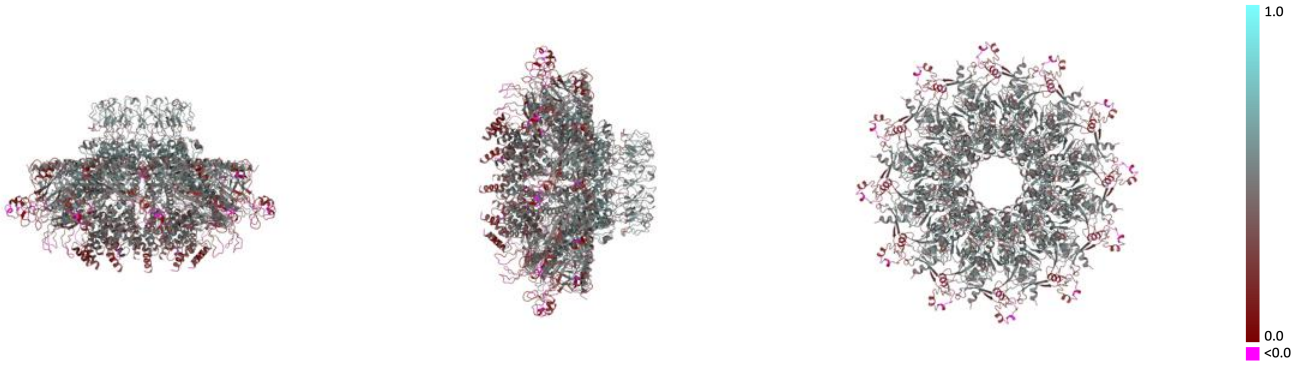
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.6 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.

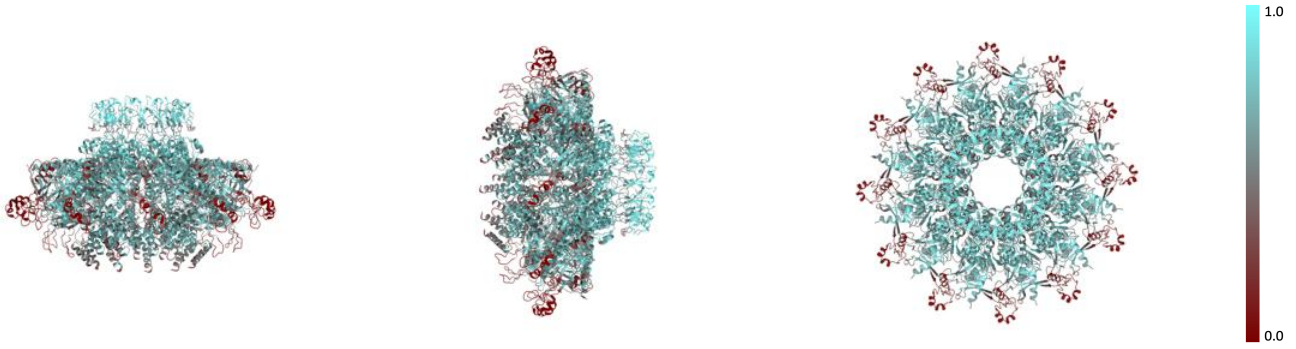
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

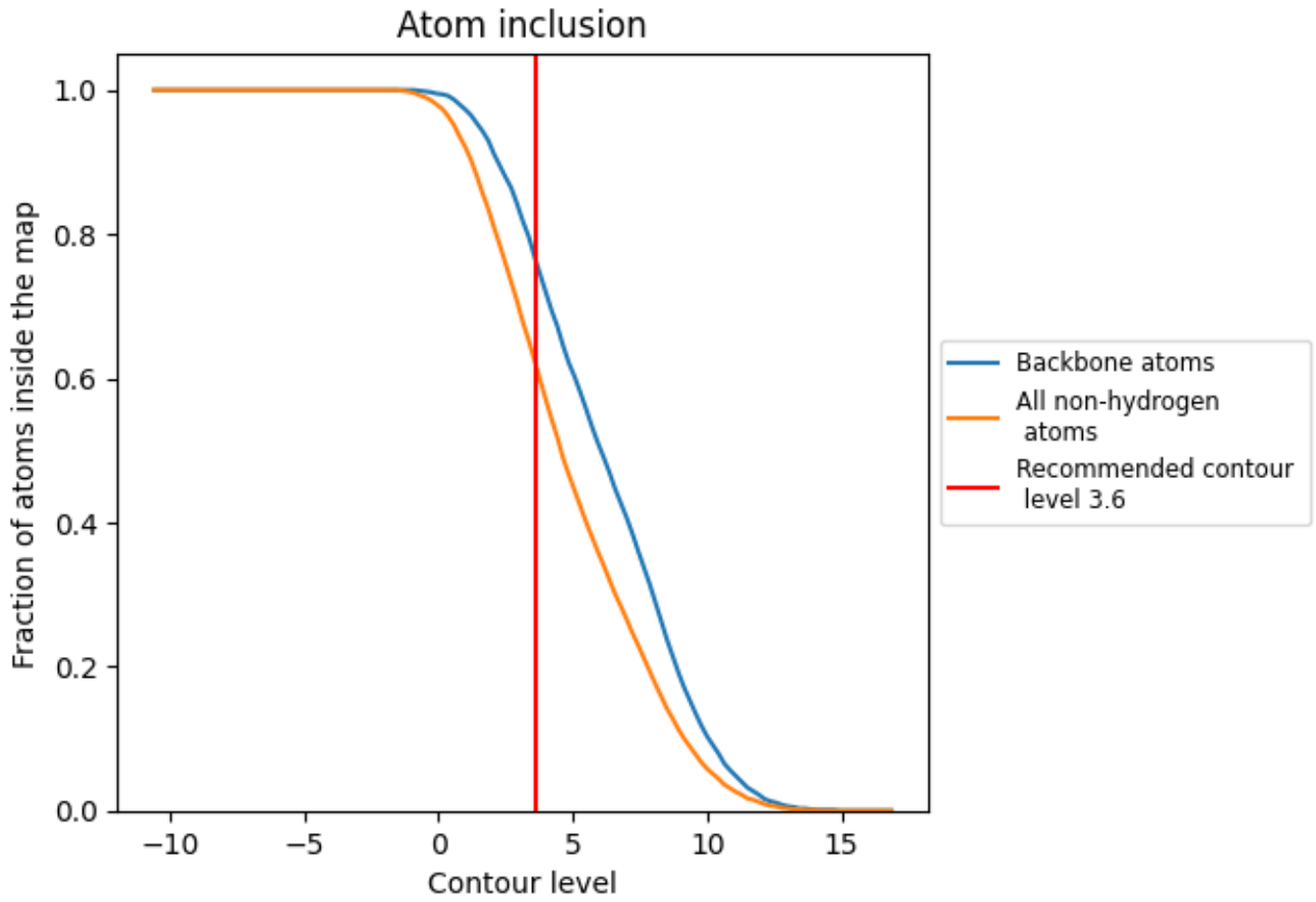
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (3.6).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 62% 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 (3.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6200	0.4110
A	0.6190	0.4110
B	0.6200	0.4110
C	0.6210	0.4120
D	0.6210	0.4110
E	0.6190	0.4100
F	0.6210	0.4110
G	0.6230	0.4100
H	0.6180	0.4110
I	0.6200	0.4130
J	0.6220	0.4110
K	0.6200	0.4120
L	0.6180	0.4120