Full wwPDB EM Validation Report (i)

Jun 1, 2025 – 12:57 AM JST

PDB ID	:	9LR9 / pdb_00009lr9
EMDB ID	:	EMD-63322
Title	:	Local reconstruction of bovine adenovirus type 3 capsid
Authors	:	Xiao, H.; Liu, H.R.
Deposited on	:	2025-01-30
Resolution	:	3.30 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 (i) 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 (i)) were used in the production of this report:

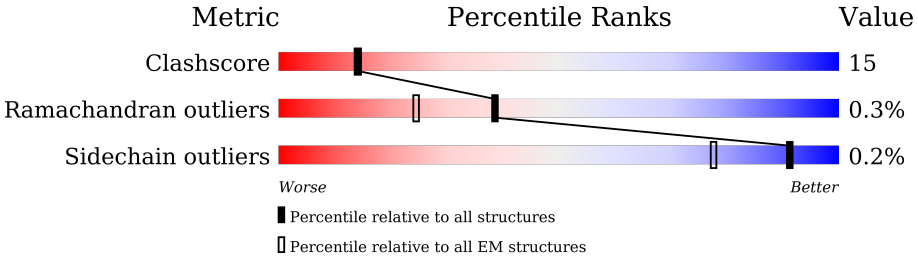
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	911	62% 36%
1	D	911	68% 31%
1	F	911	65% 34%
1	G	911	64% 35%
1	H	911	63% 35%
1	I	911	64% 34%
1	J	911	65% 34%
1	X	911	66% 33%

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Mol	Chain	Length	Quality of chain
1	Y	911	60% 39%
1	g	911	65% 34%
1	h	911	66% 33%
1	i	911	64% 35%
2	B	263	7% 92%
2	L	263	17% 81%
2	S	263	10% 87%
2	T	263	7% 89%
2	Z	263	5% 6% 91%
2	a	263	9% 90%
2	b	263	10% 89%
2	c	263	8% 90%
2	d	263	5% 94%
3	C	171	95%
3	U	171	95%
3	e	171	95%
3	f	171	95%
4	E	80	5% 34% 14% 52%
5	K	568	38% 8% 54%
6	M	410	19% 8% 73%
7	N	216	69% 14% 18%
7	R	216	63% 19% 18%
8	O	125	76% 13% 11%
8	P	125	68% 21% 11%
8	Q	125	66% 22% 11%

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Mol	Chain	Length	Quality of chain
8	V	125	80% 9% 11%
9	j	482	67% 25% 9%

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 101800 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 Hexon protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	900	7183	4544	1257	1351	31	0	0
1	D	903	7223	4574	1264	1354	31	0	0
1	F	905	7238	4583	1267	1357	31	0	0
1	G	907	7248	4589	1269	1359	31	0	0
1	H	901	7209	4566	1262	1351	30	0	0
1	I	899	7174	4539	1254	1351	30	0	0
1	J	909	7260	4596	1271	1362	31	0	0
1	X	904	7230	4579	1265	1355	31	0	0
1	Y	904	7230	4579	1265	1355	31	0	0
1	g	905	7238	4583	1267	1357	31	0	0
1	h	905	7238	4583	1267	1357	31	0	0
1	i	904	7230	4579	1265	1355	31	0	0

- Molecule 2 is a protein called PVI.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	20	152	94	29	28	1	0	0
2	L	50	374	239	65	68	2	0	0
2	S	33	254	156	47	48	3	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	T	28	211	129	40	40	2	0	0
2	Z	24	174	107	35	30	2	0	0
2	a	27	200	123	39	36	2	0	0
2	b	30	229	142	44	41	2	0	0
2	c	26	196	121	38	35	2	0	0
2	d	16	122	74	25	22	1	0	0

- Molecule 3 is a protein called Pre-histone-like nucleoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	8	59	37	10	10	2	0	0
3	U	8	59	37	10	10	2	0	0
3	e	8	59	37	10	10	2	0	0
3	f	8	59	37	10	10	2	0	0

- Molecule 4 is a protein called PX.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
4	E	38	276	184	49	43	0	0

- Molecule 5 is a protein called Pre-hexon-linking protein IIIa.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	K	262	2042	1284	361	395	2	0	0

- Molecule 6 is a protein called PV.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	M	110	837	518	146	169	4	0	0

- Molecule 7 is a protein called Pre-hexon-linking protein VIII.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	N	178	1407	887	254	261	5	0	0
7	R	178	1407	887	254	261	5	0	0

- Molecule 8 is a protein called PIX.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	O	111	863	531	160	169	3	0	0
8	P	111	863	531	160	169	3	0	0
8	Q	111	863	531	160	169	3	0	0
8	V	111	863	531	160	169	3	0	0

- Molecule 9 is a protein called Penton protein.

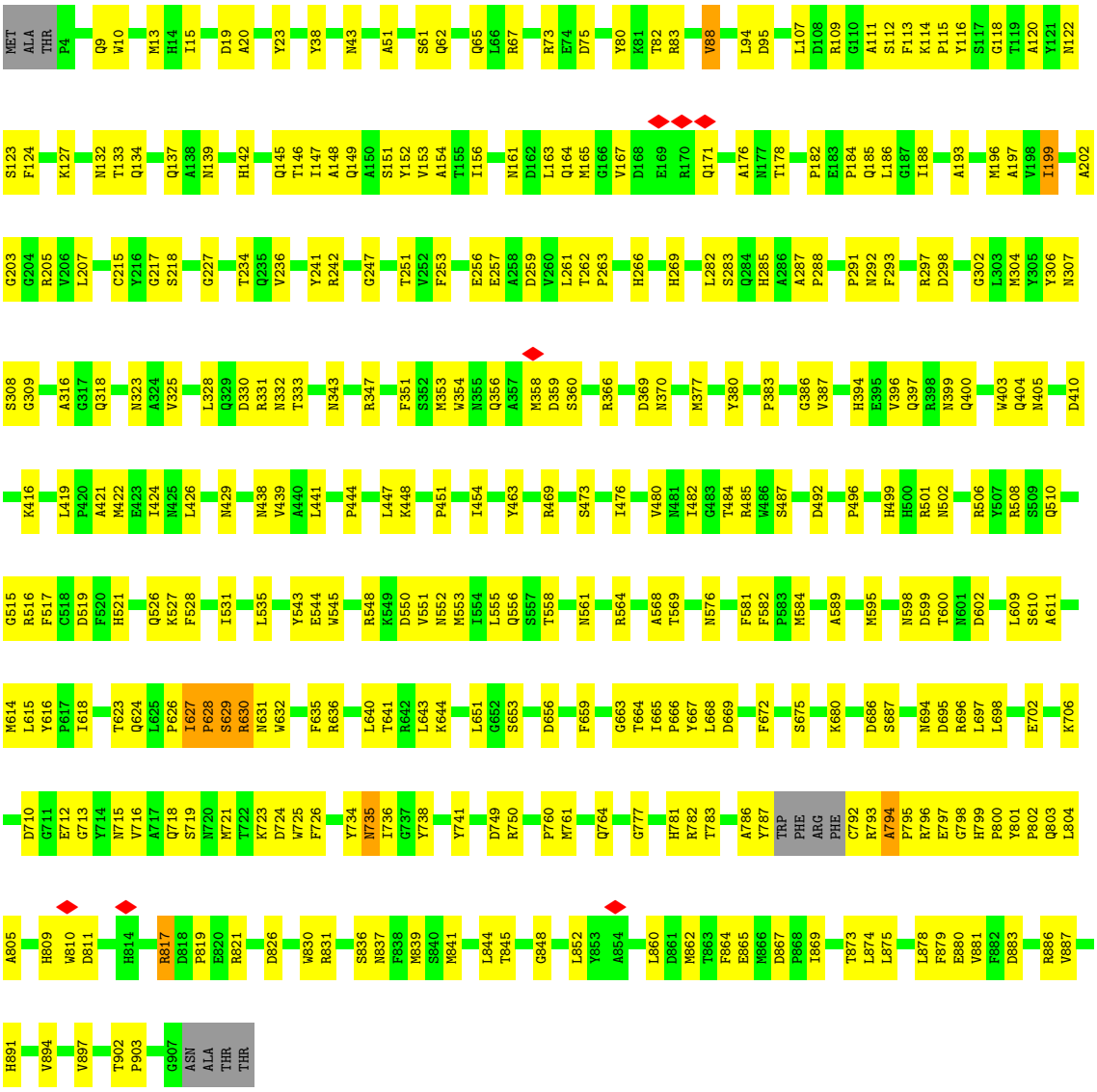
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	j	441	3530	2235	609	675	11	0	0

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: Hexon protein

Chain A:



- Molecule 1: Hexon protein

Chain D: 68% 31%

MET ALA THR PRO S5 M6 L7 P8 Q9 W10 S11 Y12 A16 L24 L28 Q33 E36 S37 Y38 F39 R46 N47 P48 A51 T57 T58 E59 R60 L66 L94 S98 T99 A111 S112 F113 S117 A120 Y121 N122 S123 F124 N131 N132 T133 Q134

Q137 A138 N139 H142 Q145 T146 I147 V153 A154 T155 I156 D162 L163 Q164 M165 Q171 A176 P182 E183 P184 Q185 I188 T192 R205 R208 Q212 T213 P214 C215 Y216 G217 S218 P222 G227 G228 I229 T234 Q235 K238 R242 D245

N246 G247 N248 P249 E250 T251 V252 E256 E257 L261 T262 P263 H269 R276 A277 K278 V279 E280 S283 P288 N289 R290 P291 I294 R297 F300 V301 Y306 V314 L315 N323 L328 Q329 D330 L335 S336 M339 L340 L341 A342 N343 T344 R347 S348

R349 Y350 F351 S352 M353 W354 N355 Q356 A357 M358 I368 D369 N370 V373 E376 Y380 C381 F382 V396 Q397 R398 N399 Q400 Q401 Q402 W403 Q404 N405 S409 I414 L419 M422 N425 L426 A427 A428 R432 V439 A440 L441 P444 D445 N446 L447 K448 T462

Y463 E464 Y465 M466 N467 G468 R469 S473 D477 T478 Y479 V480 N481 I482 G483 T484 S487 M491 D492 L505 R508 L512 G513 I522 K527 I531 L536 E544 R548 K549 D550 V551 I554 L555 Q556 L559 R564 A568 F581 M584 S585

H586 T591 L592 E593 A594 M595 L596 R597 L609 S610 A611 N621 P626 R630 N631 A634 F635 R636 L640 T641 R642 L643 E647 A650 D656 Y661 S662 G663 T664 I665 P666 Y667 L668 S675 H676 T677 F678 R679 Q684 F685 D686 W691 N694 D695

P700 I705 K706 D710 N715 V716 A717 Q718 S719 N720 M721 T722 K723 D724 W725 F726 L731 Y734 N735 I736 D746 Y747 R750 F754 P760 Q764 N767 G777 H781 T784 P785 A786 Y787 W788 F789 C792 R793 R796 E797 P800 Y801 P802 Q803

L804 W810 D811 P812 R813 H814 A815 L816 R817 D818 P819 K822 C825 T828 L829 W830 S836 N837 F838 M839 S840 M841 L844 L847 G848 Q849 H858 D861 F864 D867 P868 I869 T873 F879 E880 V881 F882 V887 H888 Q889 P890 V894 I895 E896 V897

R901 T902 P903 F904 S905 A906 G907 ASN ALA THR THR

- Molecule 1: Hexon protein

Chain F: 65% 34%

MET ALA THR P4 S5 M6 Q9 W10 Q18 D19 A20 S21 E22 Y23 P52 V56 T57 T58 S61 Q62 R63 L66 D72 T76 Q77 Y78 R83 F84 V88 G89 D90 V93 T99 I103 R104 G105 T106 L107 D108 R109 K114 N122 S123 F124

T133 N139 H142 P143 A144 Q145 T146 I147 A148 Q149 V153 L163 A176 T179 Y180 Q181 P182 G187 I188 T192 D200 Q201 A202 G203 G204 R205 V206 L207 R208 N209 P210 T211 C215 Y216 G217 S218 Y219 P222 T223 N224 G228 T234 Y240 Y241 R242

D245 N246 G247 N248 P249 E250 T251 V252 T255 E256 E257 V260 L261 T262 P263 R276 L282 P288 N289 R290 P291 N292 F293 I294 R297 D298 C299 F300 V301 G302 L303 V314 L315 A316 S320 Q321 L322 N323 L328 Q329 D330 E334 L335 S336 M339 L340 T344

R347 S352 M353 W354 N355 Q356 A357 M358 D359 S360 V367 I368 V371 G372 V373 E374 D375 E376 M377 Y380 C381 L384 Q388 V396 N399 Q400 Q401 Q402 W403 Q404 N405 N411 N412 Y413 L419 P420 A421 M422 E423 A427 W431 R432 S433 F434 L435 V439 A440

L441 N446 L447 P451 I454 N459 T462 Y463 E464 N467 S473 Y479 T484 S487 D492 N495 P496 F497 N502 R508 L511 L512 G513 N514 G515 R516 F517 V524 P525 Q526 I531 L534 L535 L536 L537 P538 Y543 E544 R548

V551 N552 M553 I554 L555 Q556 S557 T558 L559 D562 L563 R564 V565 D566 G567 A568 T569 V570 T573 S574 V575 Y578 M584 S585 E593 A594 M595 N601 D602 Q603 S604 F605 Y608 L609 S610 A611 A612 N613 M614 L615 I618 P619 P620 N621 A622 T623 Q624 L625 P626 I627 P628 S629

R630 N631 R636 L640 T641 R642 L643 E647 T648 P649 A650 L651 G652 Y661 S662 G663 T664 I665 P666 D669 F672 S675 R679 K680 V681 A682 D686 S687 N694 D695 R696 L697 E702 I705 D710 N715 V716 K723 D724 W725 F726 Q739 G740 Y741

H742 L743 P744 F758 I759 P760 M761 N767 P768 A769 L776 H781 R782 T783 T784 P785 A786 Y787 W788 F789 R790 F791 C792 R793 R796 E797 G798 Y801 P802 Q803 L804 A805 L806 H809 W810 D811 P812 R813 H814 A815 L816 R817 D818 P819 E820 R821 K822 R827 W830 R831

S836 M839 H858 A859 L860 D861 M862 T863 F864 D867 P868 I869 T873 L874 L875 Y876 E880 V881 V887 V897 R901 T902 P903 N908 ALA THR THR

- Molecule 1: Hexon protein

Chain G: 64% 35%

MET ALA THR P4 A16 G17 Q18 D19 A20 S21 E22 Y23 L24 S25 P26 G27 L28 V29 Q30 P48 P52 V56 S61 Q62 R63 D72 Q77 Y78 K81 T82 R83 F84 Q85 G89 R92 V93 L94 D108 R109 G110 A111 S112 F113 K114 P115 Y121 N122 S123

F124 N131 N132 T133 Q134 Q137 Q145 T146 I147 A148 Q149 V153 I156 L163 Q164 M165 P173 N177 Q181 P182 E183 P184 Q185 L186 G187 I188 E189 G190 W191 M196 G203 G204 R205 V206 L207 P210 T211 Q212 T213 P214 C215 Y219 P222 I229 T230

K231 R242 D245 W246 G247 T251 V252 F253 E256 D259 V260 L261 T262 P263 R276 L282 S283 A286 N289 N292 F293 I294 C295 F296 R297 D298 C299 L303 M304 Y305 Y306 N307 G310 V314 L315 Q318 Q321 L322 N323 A324 Y325 V326 D327 L328

R331 N332 R347 F351 S352 M353 Q356 A357 M358 V365 D369 N370 V371 E376 M377 P378 N379 Y380 C381 F382 P383 L384 R392 V396 Q397 R398 Q401 S409 D410 N411 G415 K416 L419 M422 E423 T424 N425 L426 A427 A428 N429 R432 L435 Y436 S437

N438 Y442 P451 I454 Q455 L456 Y465 M466 N467 G468 R469 S473 I476 D477 T478 Y479 Y480 W481 I482 G483 T484 M491 D492 H499 H500 R501 R508 L511 I512 G513 N514 G515 R516 F517 C518 V524 K527 F528 I531 L534 L535 L536 L537 E544 W545

S546 F547 R548 K549 D550 V551 N552 M553 I554 L555 Q556 S557 N561 R564 A568 F582 P583 M584 E593 A594 M595 L596 R597 N601 N606 N613 M614 L615 Y616 P617 I618 P619 P620 N621 A622 T623 Q624 L625 P626 I627 P628 S629 A633 A634 F635 L640 L643 K644

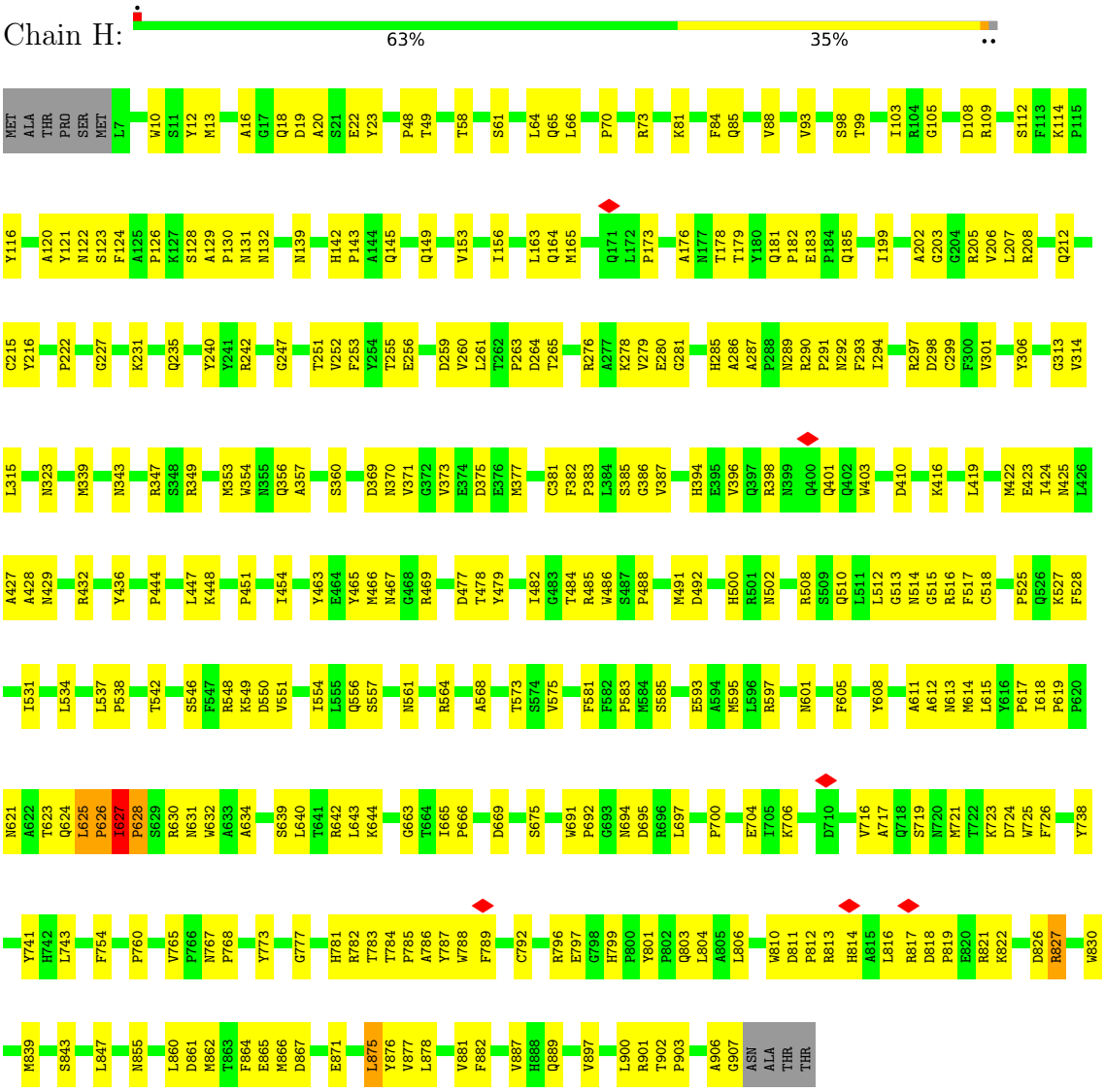
L651 P654 Y658 P666 R679 K680 I683 Q684 S688 V689 T690 W691 P692 G693 N694 D695 R696 L697 E702 F703 E704 I705 K706 V709 D710 G711 E712 N715 V716 N720 M721 T722 K723 D724 W725 F726 L727 V728 Y734 Q739 L743 S753 F754 Q764

P768 Y773 G777 H781 R782 T783 T784 P785 A786 Y787 W788 F789 R790 F791 C792 R793 A794 P795 R796 E797 G798 Y801 P802 Q803 L804 A805 L806 P807 P808 H809 W810 D811 P812 R813 H814 R817 D818 P819 E820 R821 K822 S836 N837 L844 N850 L851 A859 L860 D861 M862

E865 M866 D867 P868 I869 T873 L874 L875 Y876 V881 F882 D883 V884 V887 H888 R892 I895 E896 V897 L900 R901 T902 P903 F904 A909 T910 THR

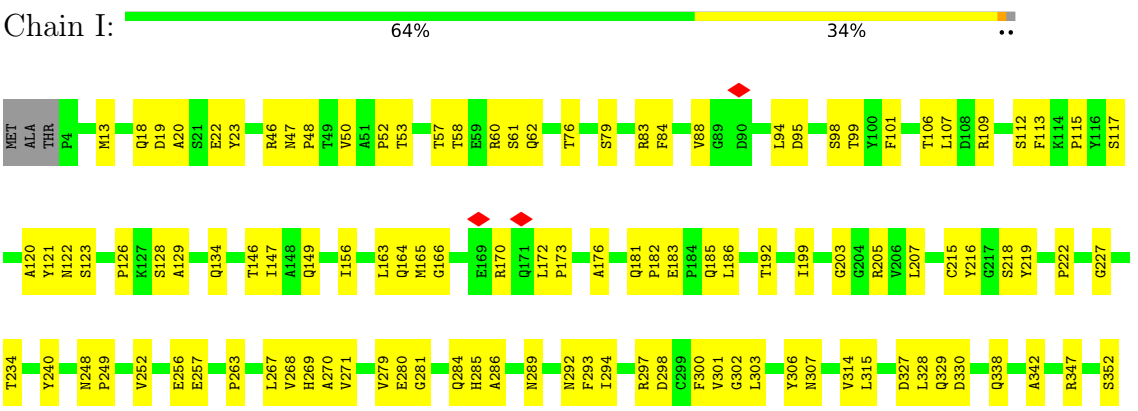
• Molecule 1: Hexon protein

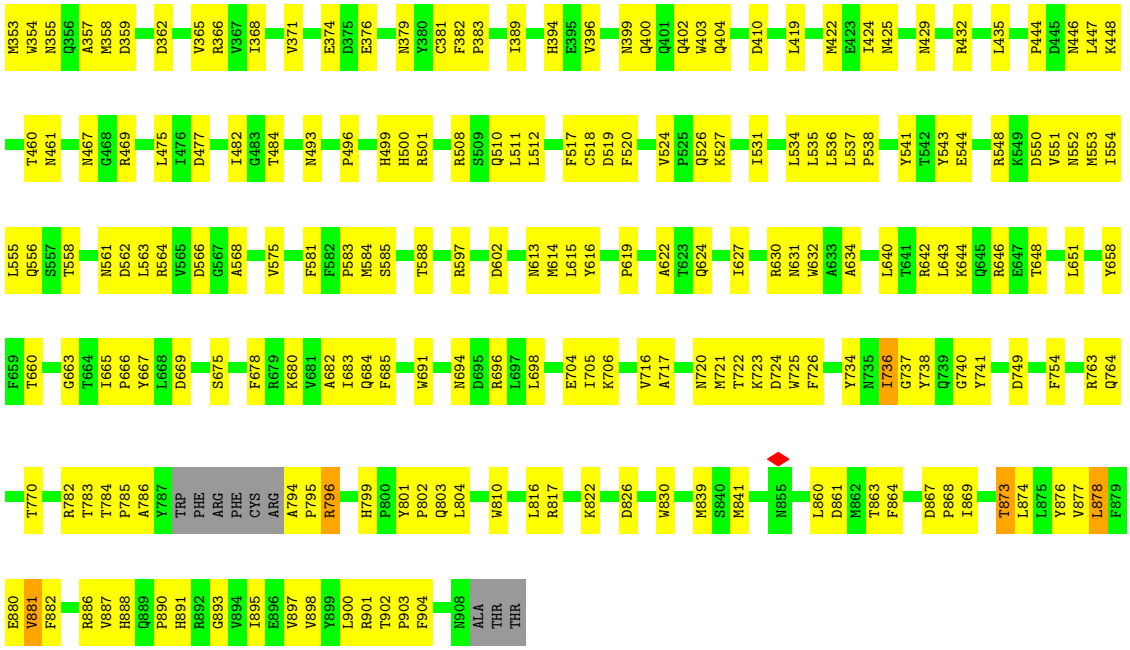
Chain H:



• Molecule 1: Hexon protein

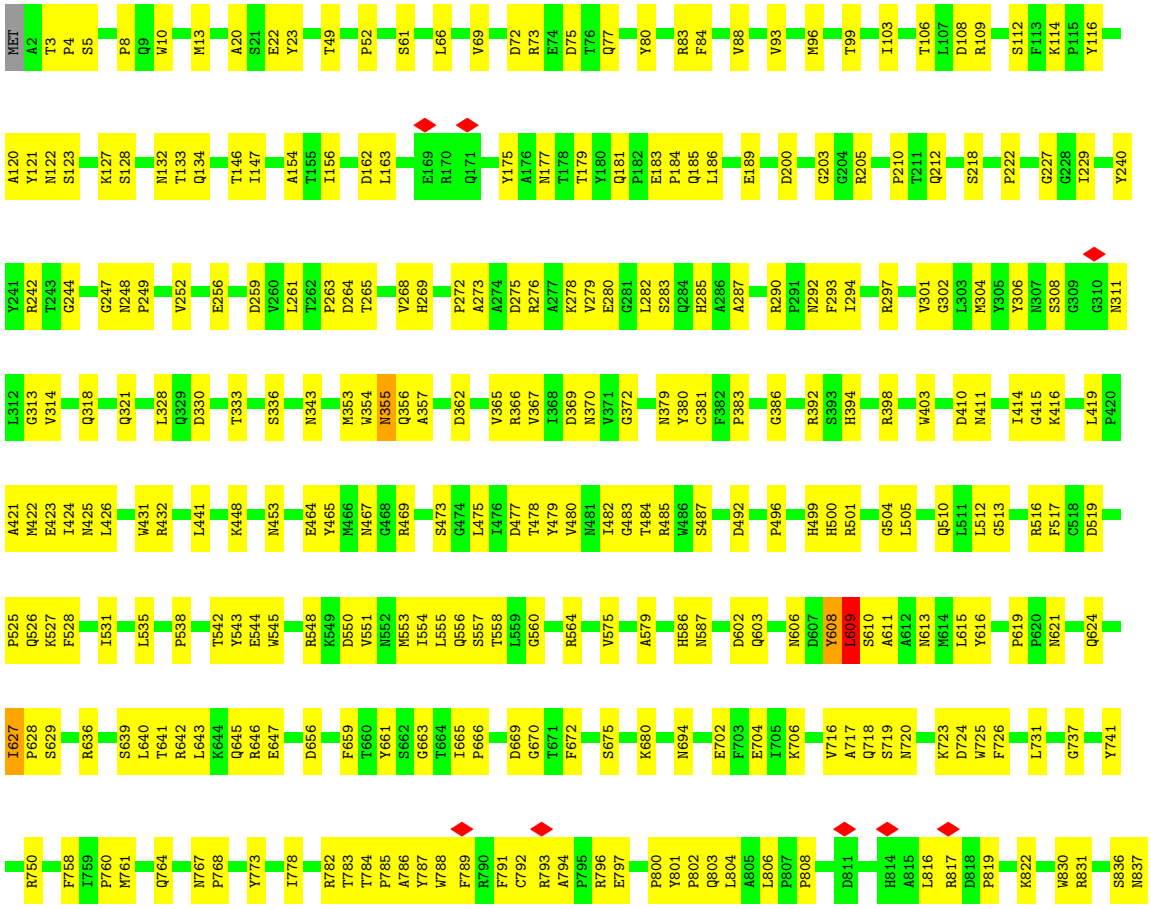
Chain I:





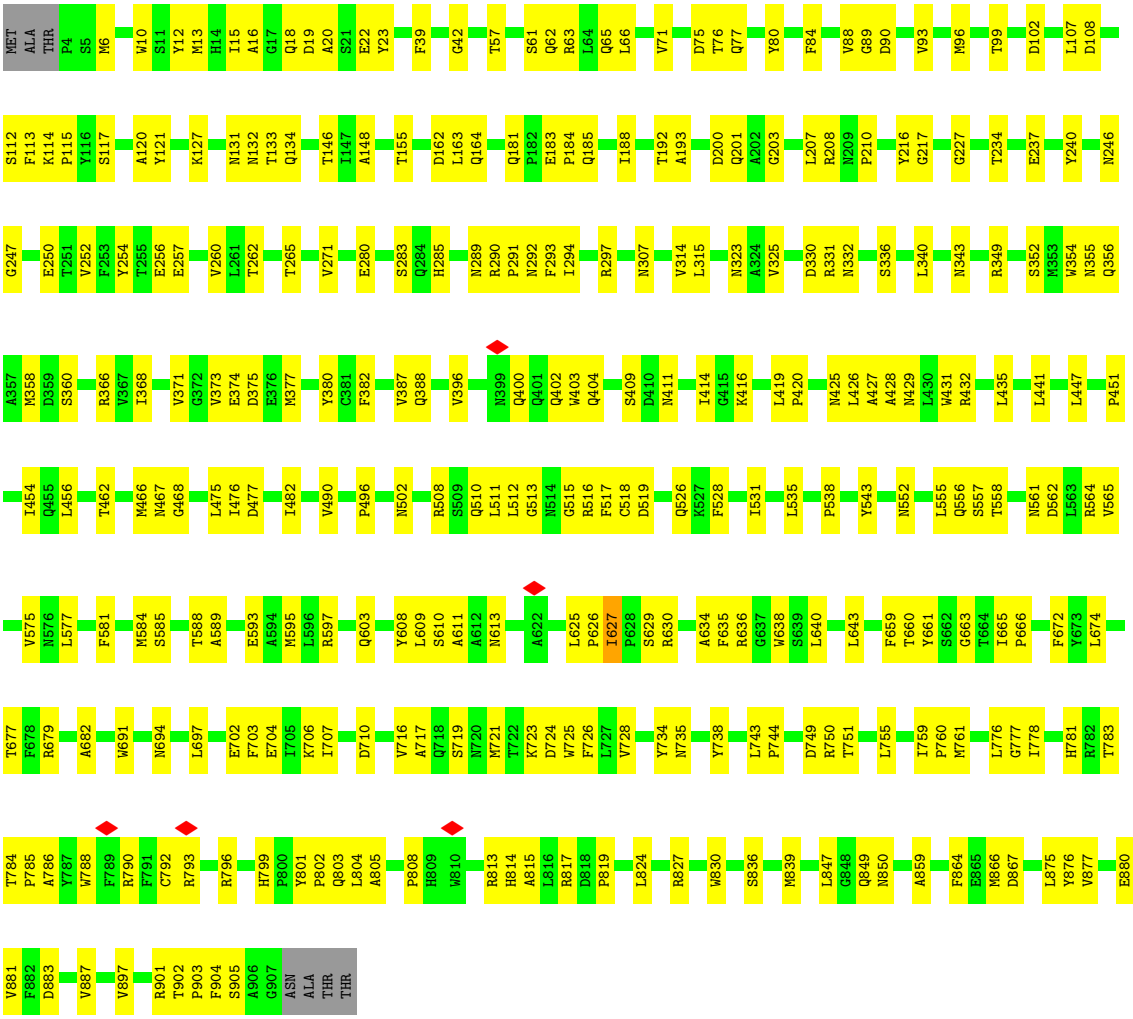
- Molecule 1: Hexon protein

Chain J:



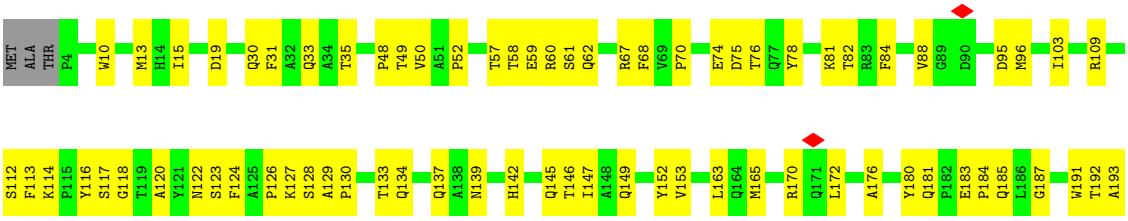
• Molecule 1: Hexon protein

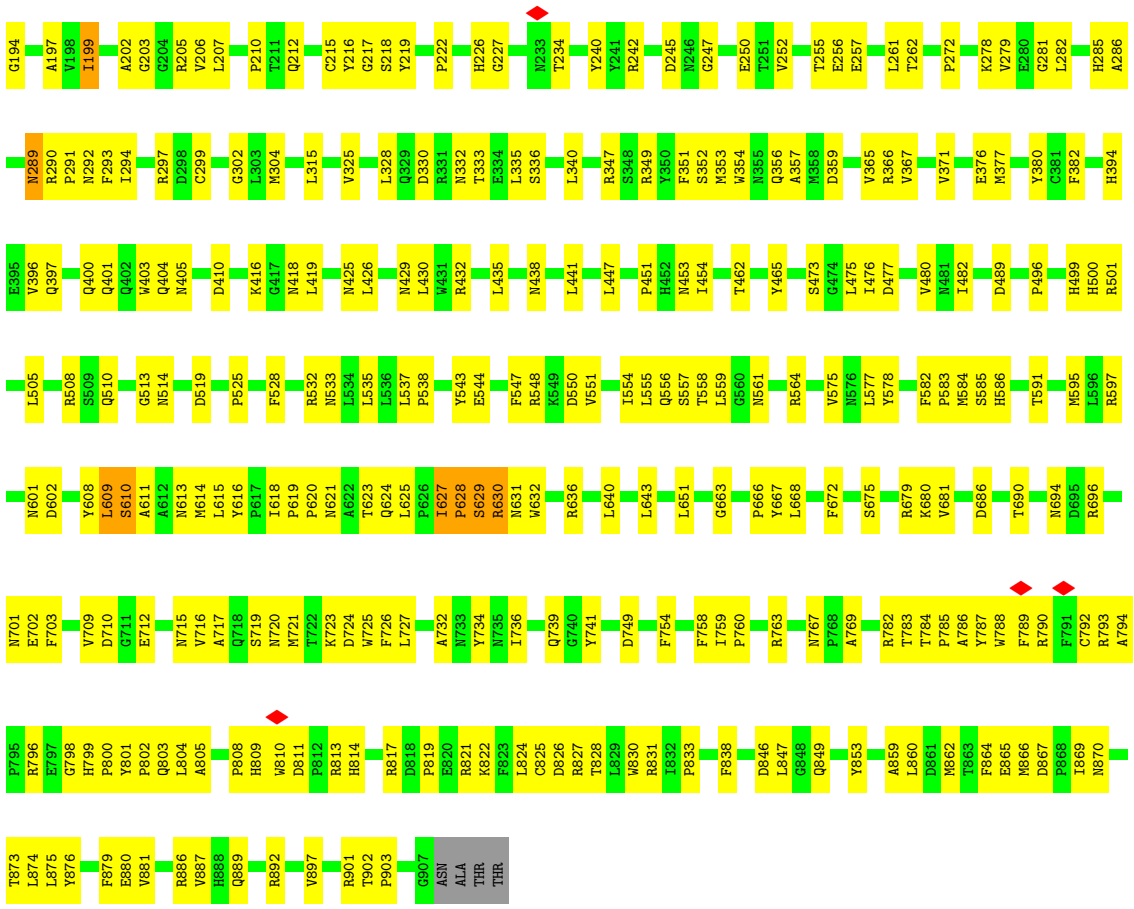
Chain X:



• Molecule 1: Hexon protein

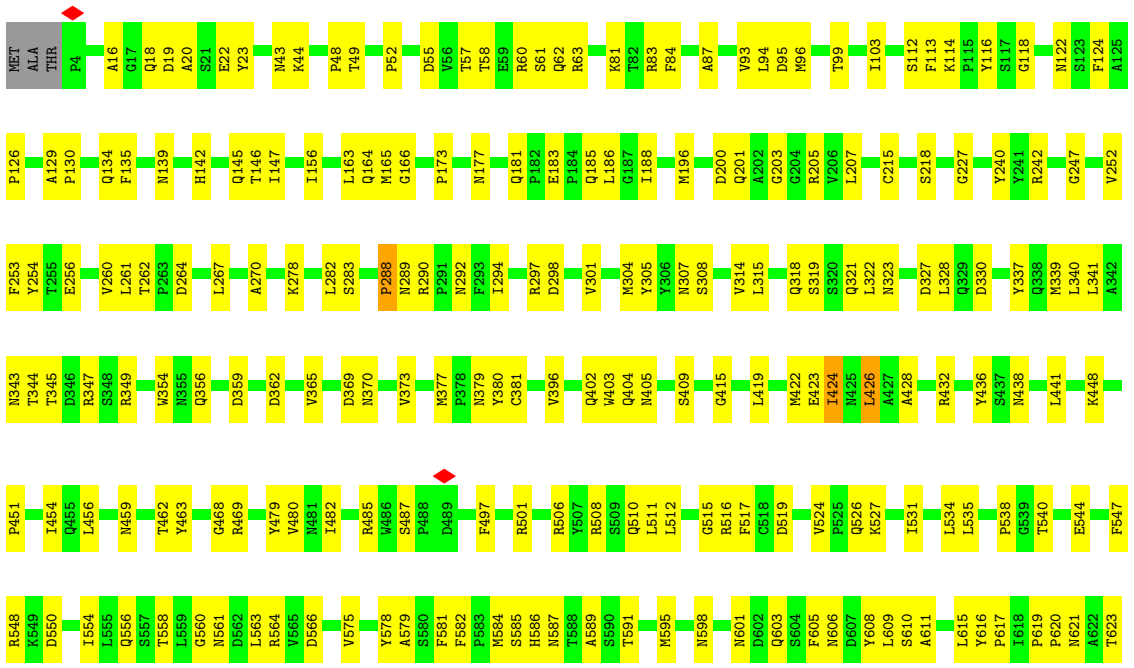
Chain Y:

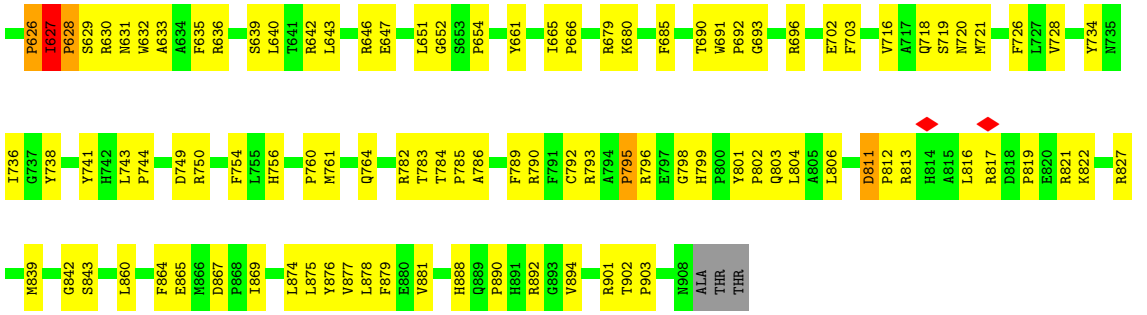




- Molecule 1: Hexon protein

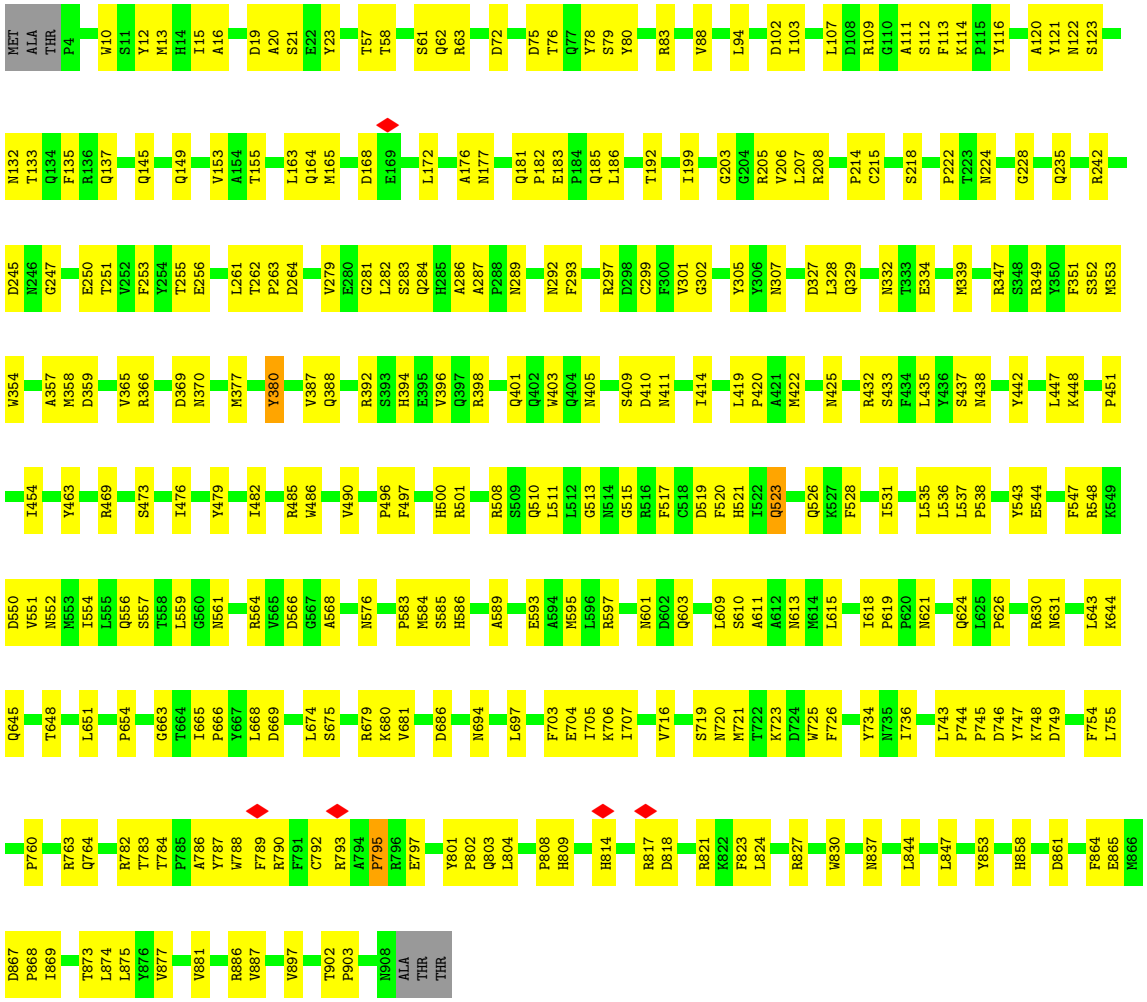
Chain g:





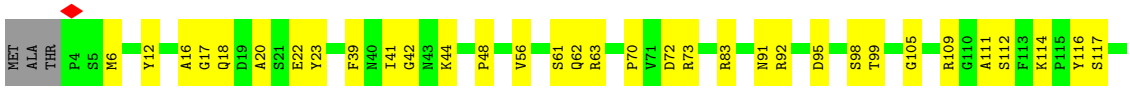
- Molecule 1: Hexon protein

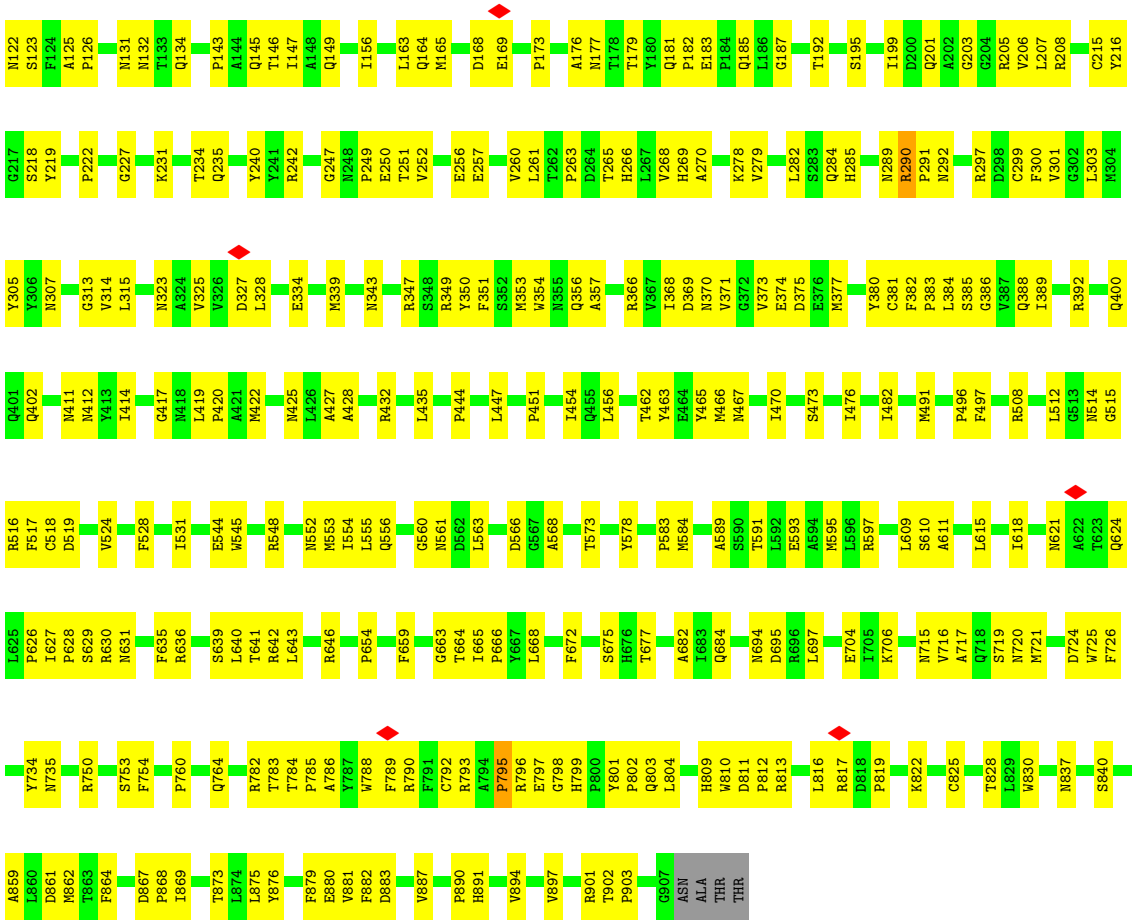
Chain h:



- Molecule 1: Hexon protein

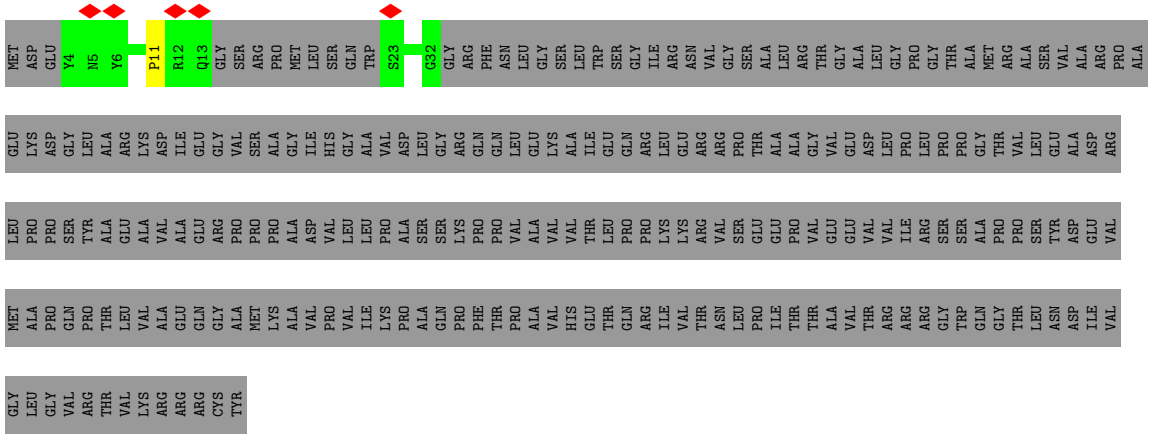
Chain i:





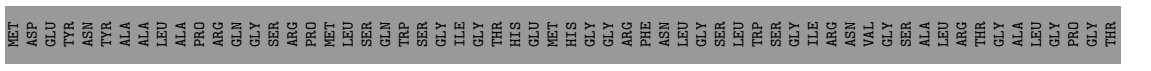
• Molecule 2: PVI

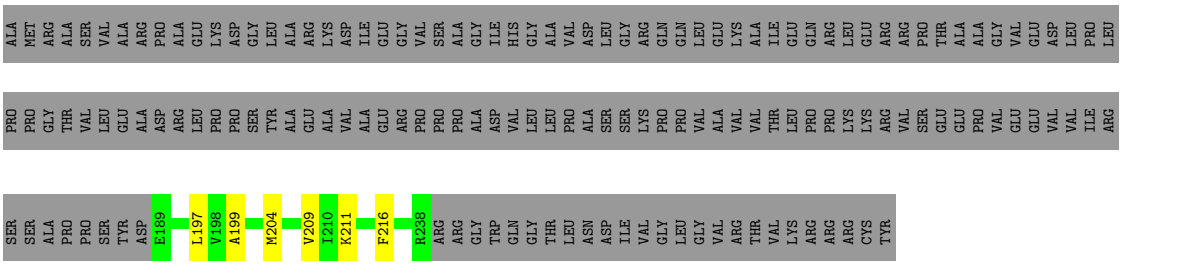
Chain B: 7% 92%



• Molecule 2: PVI

Chain L: 17% 81%



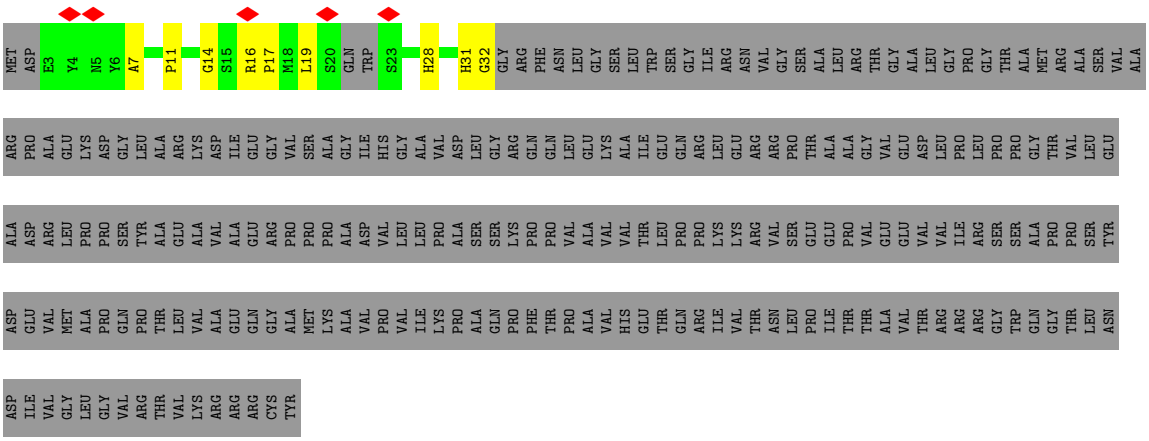


• Molecule 2: PVI

Chain S:

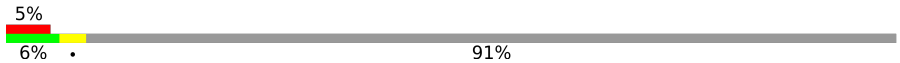
• Molecule 2: PVI

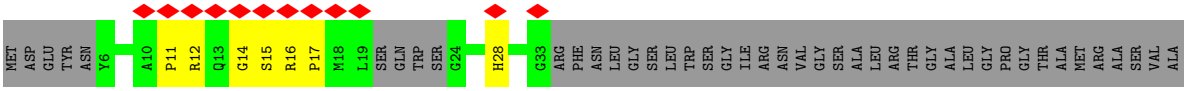
Chain T:

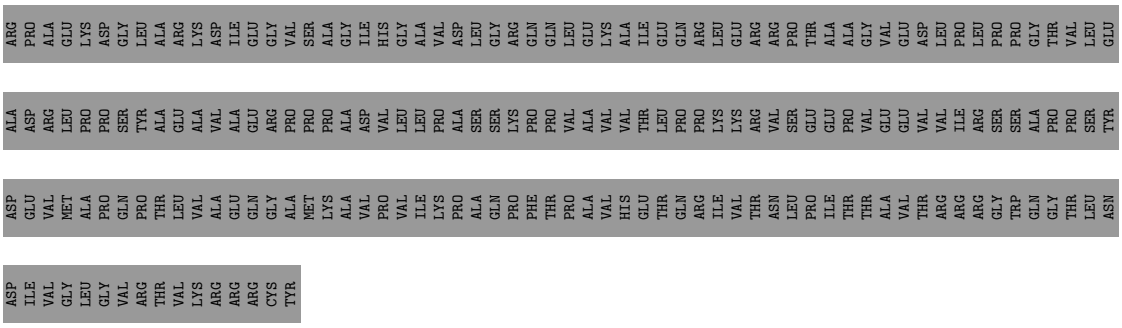


• Molecule 2: PVI

Chain Z:

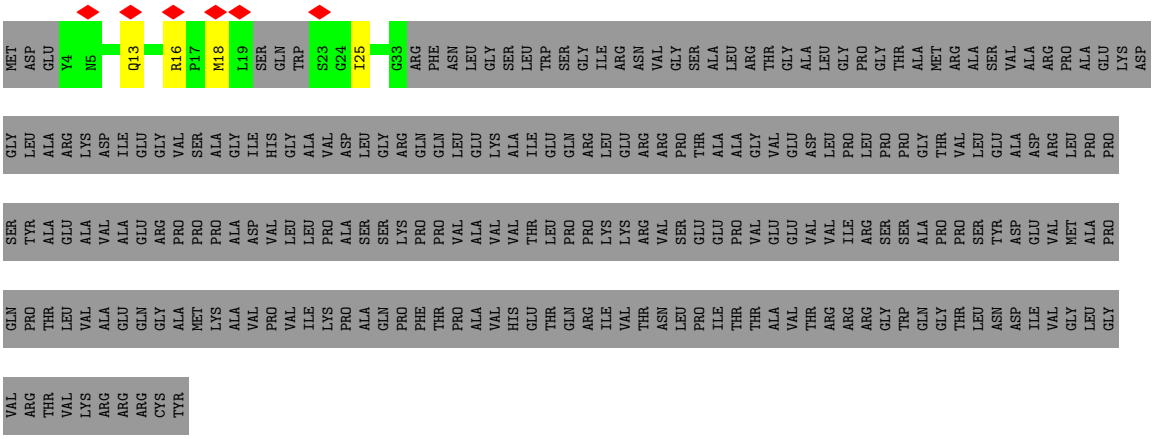






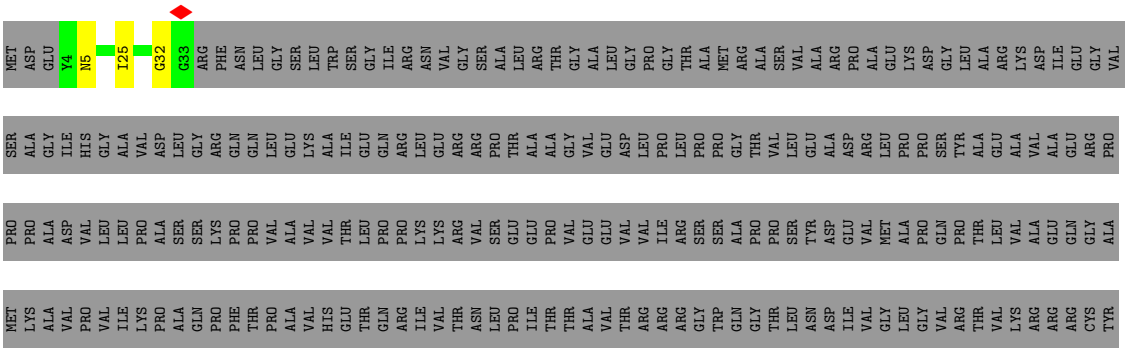
- Molecule 2: PVI

Chain a:



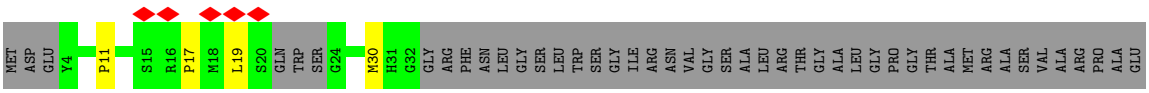
- Molecule 2: PVI

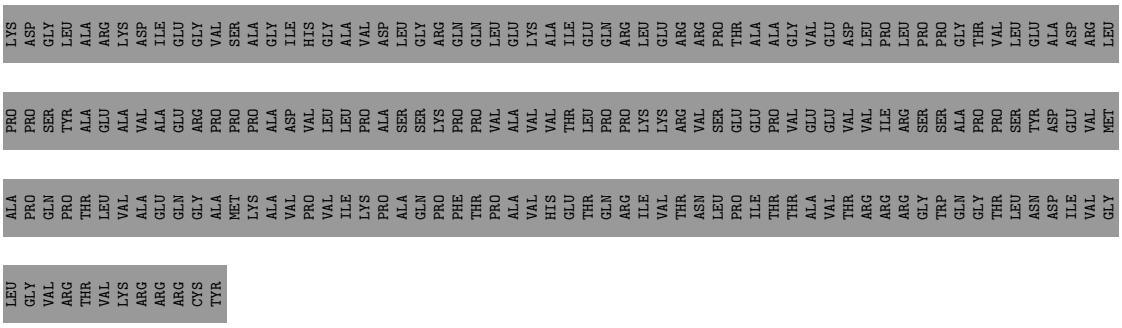
Chain b:



- Molecule 2: PVI

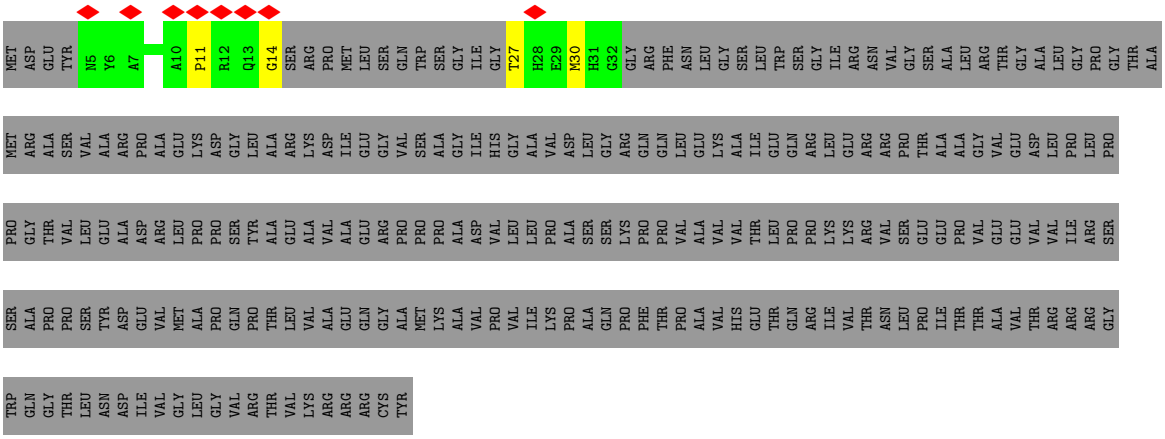
Chain c:





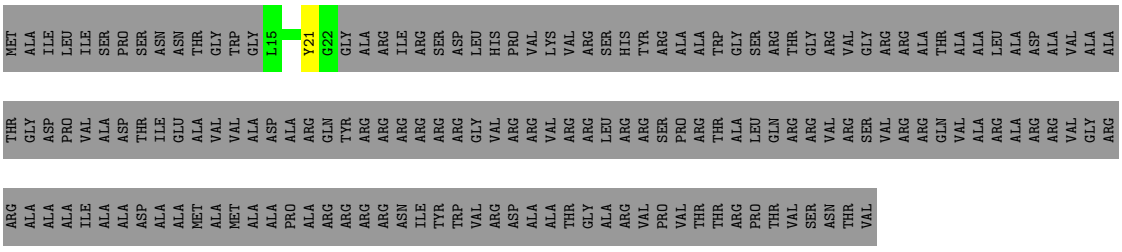
- Molecule 2: PVI

Chain d: 5% 94%



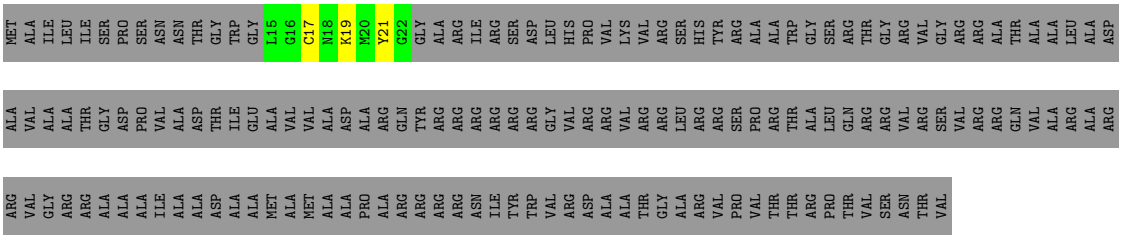
- Molecule 3: Pre-histone-like nucleoprotein

Chain C: 95%



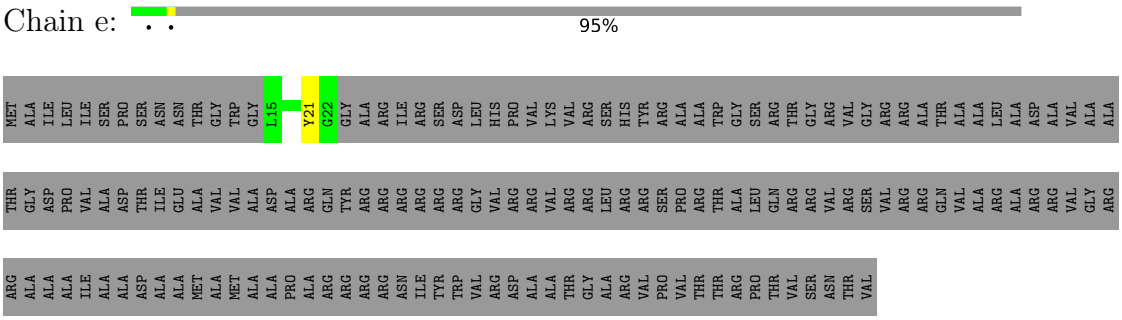
- Molecule 3: Pre-histone-like nucleoprotein

Chain U: 95%



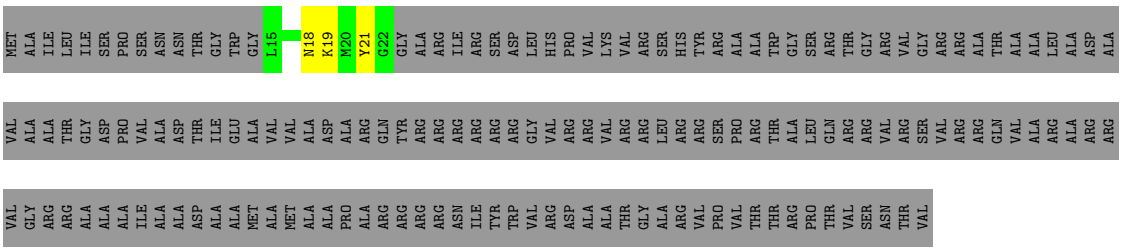
- Molecule 3: Pre-histone-like nucleoprotein

Chain e:



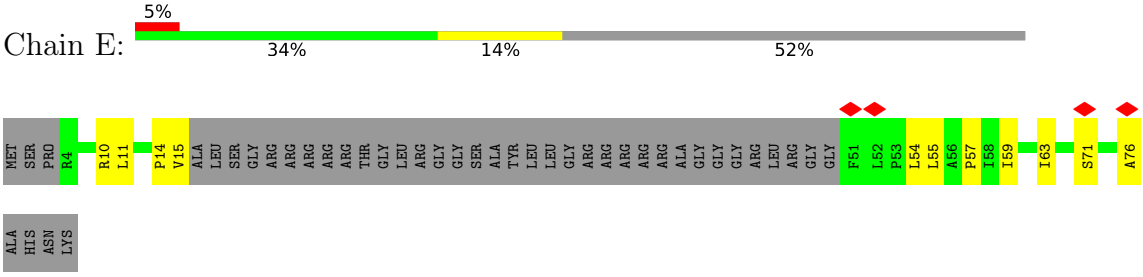
- Molecule 3: Pre-histone-like nucleoprotein

Chain f:



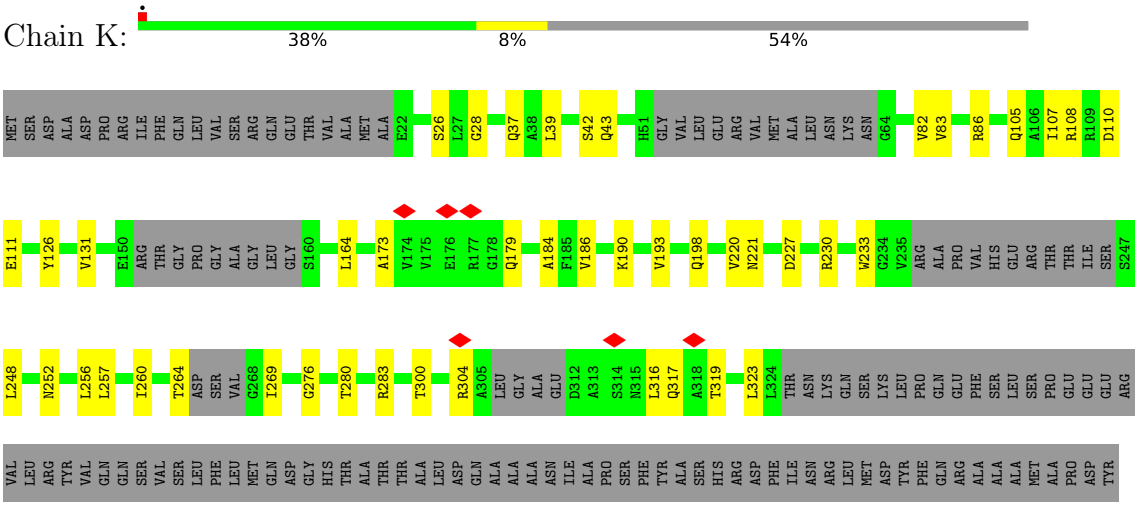
- Molecule 4: PX

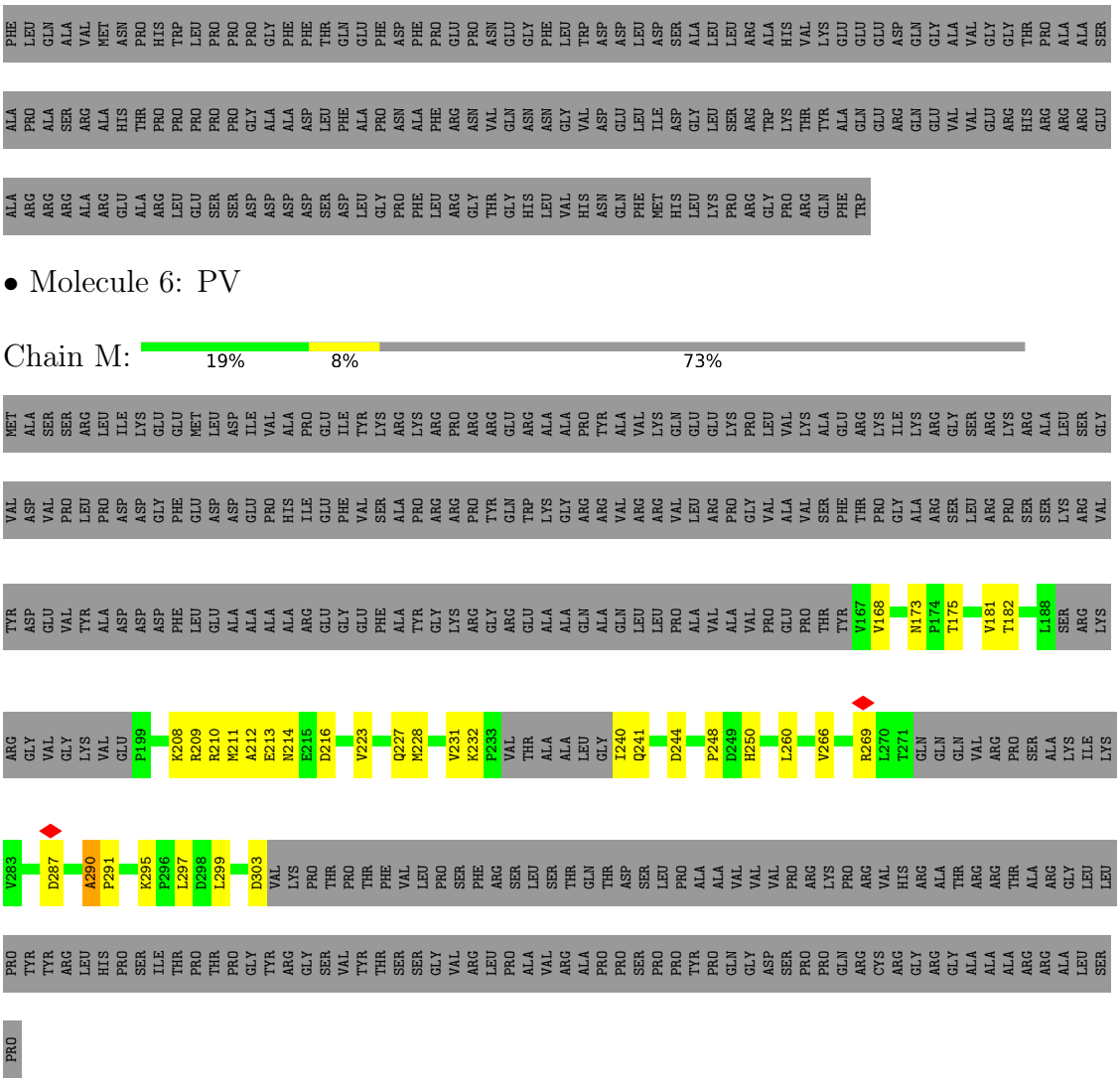
Chain E:



- Molecule 5: Pre-hexon-linking protein IIIa

Chain K:



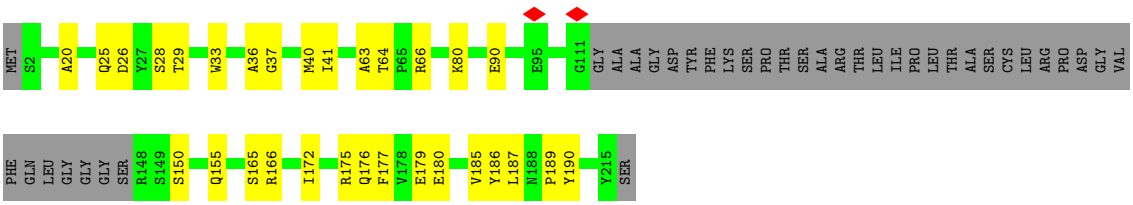


• Molecule 6: PV

Chain M: 19% 8% 73%

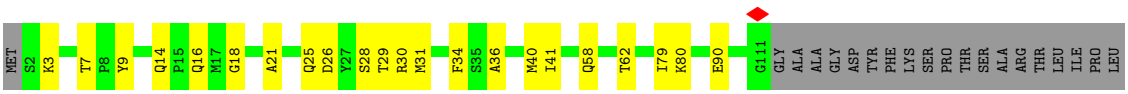
• Molecule 7: Pre-hexon-linking protein VIII

Chain N: 69% 14% 18%



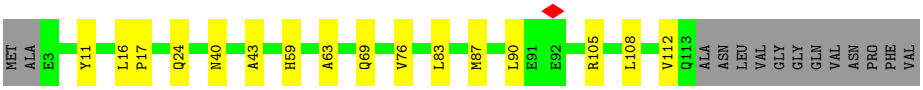
• Molecule 7: Pre-hexon-linking protein VIII

Chain R: 63% 19% 18%



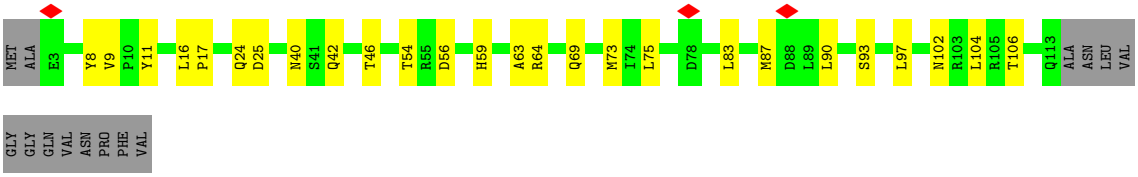
• Molecule 8: PIX

Chain O:



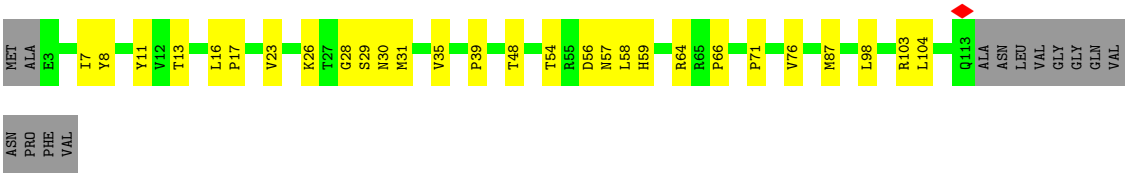
• Molecule 8: PIX

Chain P:



• Molecule 8: PIX

Chain Q:

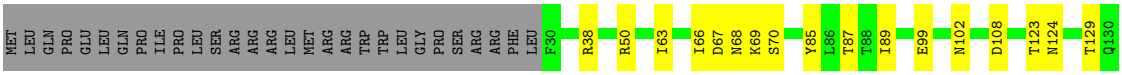


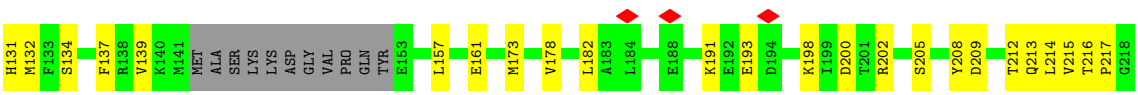
• Molecule 8: PIX

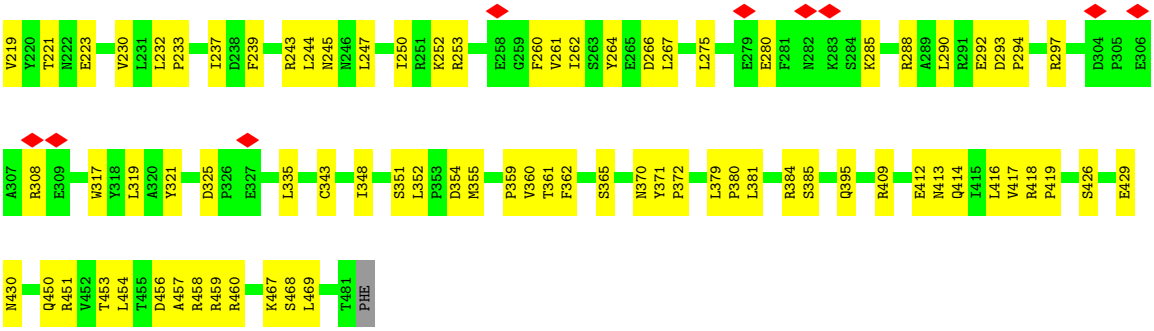
Chain V:

• Molecule 9: Penton protein

Chain j:






V219
Y220
T221
N222
E223
V230
L231
L232
P233
I237
D238
F239
R243
L244
N245
N246
L247
I250
R251
K252
R253
E258
G259
F260
V261
I262
S263
Y264
E265
D266
L267
L275
E279
E280
F281
N282
K283
S284
K285
R288
A289
L290
R291
E292
D293
P294
R297
D304
P305
E306
A307
R308
E309
W317
Y318
L319
A320
Y321
D325
P326
E327
L335
G343
I348
S351
L352
P353
D354
M355
P359
V360
T361
F362
S365
N370
Y371
P372
L379
P380
L381
R384
S385
Q395
R409
E412
N413
Q414
I415
L416
V417
R418
P419
S426
E429
N430
Q450
R451
V452
T453
L454
T455
D456
A457
R458
R459
R460
K467
S468
L469
T481
PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	45262	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	1600	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	51.946	Depositor
Minimum map value	-26.989	Depositor
Average map value	0.019	Depositor
Map value standard deviation	2.759	Depositor
Recommended contour level	5	Depositor
Map size (Å)	467.36, 467.36, 467.36	wwPDB
Map dimensions	368, 368, 368	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.27, 1.27, 1.27	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.22	0/7388	0.40	3/10078 (0.0%)
1	D	0.21	0/7432	0.37	0/10139
1	F	0.25	0/7448	0.40	2/10161 (0.0%)
1	G	0.24	0/7458	0.38	1/10175 (0.0%)
1	H	0.26	0/7418	0.40	3/10121 (0.0%)
1	I	0.22	0/7379	0.40	2/10067 (0.0%)
1	J	0.21	1/7470 (0.0%)	0.38	0/10193
1	X	0.14	0/7440	0.36	0/10150
1	Y	0.27	1/7440 (0.0%)	0.42	2/10150 (0.0%)
1	g	0.33	3/7448 (0.0%)	0.44	4/10161 (0.0%)
1	h	0.14	0/7448	0.33	0/10161
1	i	0.18	1/7440 (0.0%)	0.38	0/10150
2	B	0.11	0/155	0.35	0/207
2	L	0.11	0/382	0.32	0/526
2	S	0.13	0/261	0.38	0/351
2	T	0.11	0/215	0.36	0/287
2	Z	0.10	0/177	0.37	0/235
2	a	0.09	0/204	0.28	0/272
2	b	0.14	0/236	0.35	0/318
2	c	0.11	0/200	0.28	0/267
2	d	0.08	0/124	0.30	0/165
3	C	0.12	0/59	0.42	0/76
3	U	0.13	0/59	0.33	0/76
3	e	0.09	0/59	0.23	0/76
3	f	0.07	0/59	0.17	0/76
4	E	0.11	0/280	0.29	0/382
5	K	0.11	0/2077	0.28	0/2825
6	M	0.19	0/845	0.38	0/1145
7	N	0.14	0/1451	0.32	0/1980
7	R	0.14	0/1451	0.31	0/1980
8	O	0.10	0/876	0.27	0/1187
8	P	0.12	0/876	0.31	0/1187
8	Q	0.14	0/876	0.36	0/1187
8	V	0.11	0/876	0.28	0/1187

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
9	j	0.12	0/3614	0.33	0/4921
All	All	0.22	6/104621 (0.0%)	0.38	17/142619 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	610	SER	CA-C	-7.49	1.43	1.52
1	g	627	ILE	N-CA	6.86	1.55	1.46
1	J	609	LEU	CA-C	-6.27	1.44	1.52
1	g	626	PRO	CA-C	5.57	1.60	1.52
1	i	463	TYR	CA-C	-5.33	1.46	1.52
1	Y	610	SER	CA-C	-5.17	1.45	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	817	ARG	N-CA-C	9.30	121.98	108.86
1	A	629	SER	N-CA-C	8.26	121.75	110.35
1	F	629	SER	N-CA-C	8.14	123.11	109.76
1	g	629	SER	N-CA-C	7.17	121.52	109.76
1	g	627	ILE	N-CA-C	6.94	123.86	108.88
1	Y	629	SER	N-CA-C	6.83	118.66	110.19
1	g	424	ILE	N-CA-C	-6.22	99.25	108.45
1	A	88	VAL	N-CA-C	-6.14	106.52	112.29
1	F	628	PRO	CB-CA-C	-6.07	101.54	111.56
1	I	737	GLY	N-CA-C	5.99	119.89	112.64
1	g	626	PRO	N-CA-C	5.86	124.55	112.47
1	H	625	LEU	CA-C-N	5.48	126.69	119.84
1	H	625	LEU	C-N-CA	5.48	126.69	119.84
1	G	424	ILE	N-CA-C	-5.44	108.55	113.71
1	Y	289	ASN	N-CA-C	-5.43	100.83	109.96
1	H	627	ILE	N-CA-C	5.27	120.27	108.88
1	I	873	THR	N-CA-C	5.26	117.26	109.69

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	7183	0	6847	309	0
1	D	7223	0	6881	235	0
1	F	7238	0	6895	286	0
1	G	7248	0	6902	303	0
1	H	7209	0	6867	291	0
1	I	7174	0	6835	281	0
1	J	7260	0	6913	285	0
1	X	7230	0	6889	257	0
1	Y	7230	0	6889	312	0
1	g	7238	0	6895	300	0
1	h	7238	0	6895	257	0
1	i	7230	0	6889	264	0
2	B	152	0	137	1	0
2	L	374	0	395	4	0
2	S	254	0	234	10	0
2	T	211	0	196	8	0
2	Z	174	0	168	7	0
2	a	200	0	188	5	0
2	b	229	0	212	3	0
2	c	196	0	185	3	0
2	d	122	0	109	6	0
3	C	59	0	58	1	0
3	U	59	0	58	2	0
3	e	59	0	58	1	0
3	f	59	0	58	3	0
4	E	276	0	308	10	0
5	K	2042	0	2015	28	0
6	M	837	0	857	31	0
7	N	1407	0	1331	21	0
7	R	1407	0	1331	37	0
8	O	863	0	860	10	0
8	P	863	0	860	21	0
8	Q	863	0	860	21	0
8	V	863	0	860	7	0
9	j	3530	0	3467	84	0
All	All	101800	0	97402	3057	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 15.

All (3057) 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:F:627:ILE:HD12	1:F:628:PRO:HD2	1.28	1.10
1:A:627:ILE:HG23	1:A:860:LEU:O	1.49	1.09
1:A:623:THR:CG2	1:A:865:GLU:HG3	1.83	1.07
1:F:627:ILE:HG23	1:F:860:LEU:O	1.54	1.05
1:H:626:PRO:HB3	1:H:862:MET:H	1.19	1.04
1:X:425:ASN:O	1:X:429:ASN:HB2	1.60	1.01
1:F:817:ARG:HH21	1:g:517:PHE:H	1.11	0.97
1:A:782:ARG:HB3	1:X:185:GLN:HE21	1.30	0.96
1:A:623:THR:HG22	1:A:865:GLU:HG3	1.47	0.95
1:F:625:LEU:HG	1:F:863:THR:HG22	1.49	0.94
1:I:616:TYR:HB3	1:I:624:GLN:HE22	1.35	0.90
1:A:627:ILE:CG2	1:A:860:LEU:O	2.22	0.87
1:F:627:ILE:CD1	1:F:628:PRO:HD2	2.05	0.87
1:F:618:ILE:HD11	1:F:875:LEU:HB2	1.57	0.86
1:A:623:THR:HG21	1:A:865:GLU:HG3	1.54	0.86
1:D:426:LEU:HB2	1:g:426:LEU:HD21	1.57	0.86
1:H:782:ARG:HB2	1:J:185:GLN:HE21	1.40	0.86
1:D:122:ASN:HD21	1:g:803:GLN:HE22	1.20	0.86
1:I:630:ARG:HH22	1:I:904:PHE:HA	1.41	0.85
1:G:716:VAL:HG11	1:G:726:PHE:HB2	1.59	0.85
1:g:627:ILE:HD12	1:g:628:PRO:HD2	1.58	0.85
1:G:89:GLY:HA3	1:G:92:ARG:HE	1.43	0.83
1:Y:627:ILE:HG23	1:Y:860:LEU:O	1.76	0.83
1:G:784:THR:HG22	1:h:122:ASN:HA	1.60	0.83
1:F:743:LEU:HD12	1:F:744:PRO:HD2	1.61	0.82
1:J:785:PRO:HD2	1:J:803:GLN:HE21	1.42	0.82
1:G:299:CYS:SG	1:G:347:ARG:NH2	2.52	0.82
1:H:697:LEU:HD12	1:H:724:ASP:HB2	1.62	0.82
1:A:185:GLN:HE21	1:Y:782:ARG:HB2	1.43	0.82
1:Y:290:ARG:NH1	1:Y:441:LEU:HB3	1.95	0.82
1:A:623:THR:CG2	1:A:865:GLU:CG	2.57	0.81
1:g:627:ILE:HG12	1:g:860:LEU:HB2	1.62	0.81
1:H:299:CYS:SG	1:H:347:ARG:NH2	2.54	0.81
1:I:185:GLN:HE21	1:J:782:ARG:HB3	1.43	0.81
1:Y:212:GLN:HE22	1:Y:282:LEU:HD23	1.44	0.80
1:A:627:ILE:HG21	1:A:860:LEU:CD2	2.11	0.80
1:D:817:ARG:HB3	1:F:517:PHE:HB2	1.64	0.80
3:U:17:CYS:SG	3:U:19:LYS:NZ	2.55	0.80
1:A:347:ARG:NH1	1:A:358:MET:SD	2.56	0.79
1:G:347:ARG:NH1	1:G:358:MET:SD	2.55	0.79
1:g:611:ALA:HA	1:g:881:VAL:HG22	1.64	0.79
1:h:804:LEU:HD12	1:i:222:PRO:HB3	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:132:ASN:HD22	1:G:148:ALA:HA	1.46	0.79
1:H:623:THR:HG21	1:H:865:GLU:CD	2.08	0.79
1:A:515:GLY:HA2	1:Y:809:HIS:HB3	1.64	0.78
1:F:817:ARG:HH21	1:g:517:PHE:N	1.81	0.78
1:J:716:VAL:HG11	1:J:726:PHE:HB2	1.64	0.78
1:F:299:CYS:SG	1:F:347:ARG:NH2	2.57	0.78
1:i:289:ASN:HB3	1:i:467:ASN:HD21	1.48	0.78
1:F:58:THR:HG21	1:F:62:GLN:HG2	1.66	0.78
1:G:694:ASN:HB3	1:h:61:SER:HA	1.66	0.77
1:F:627:ILE:CG2	1:F:860:LEU:O	2.33	0.77
1:G:134:GLN:HG2	1:G:146:THR:HG22	1.67	0.77
1:h:535:LEU:HB3	1:h:603:GLN:HE22	1.50	0.77
1:A:623:THR:HG22	1:A:865:GLU:CG	2.14	0.77
1:D:422:MET:SD	1:g:422:MET:HE2	2.24	0.77
1:F:784:THR:HG22	1:g:122:ASN:HA	1.67	0.77
1:h:366:ARG:HD3	1:h:496:PRO:HB3	1.65	0.77
1:G:690:THR:HG22	1:G:692:PRO:HD2	1.66	0.76
2:S:28:HIS:HE2	1:g:843:SER:HG	1.25	0.76
1:G:817:ARG:HD3	1:h:517:PHE:HB3	1.67	0.76
1:I:783:THR:HA	1:I:803:GLN:HG2	1.68	0.76
1:Y:618:ILE:HD13	1:Y:866:MET:HE1	1.68	0.76
1:Y:292:ASN:HD21	1:Y:561:ASN:HD21	1.33	0.75
1:A:122:ASN:ND2	1:A:218:SER:OG	2.20	0.75
1:D:122:ASN:HA	1:g:784:THR:HG22	1.67	0.75
1:D:122:ASN:ND2	1:g:803:GLN:HE22	1.84	0.75
1:G:784:THR:OG1	1:G:788:TRP:NE1	2.20	0.75
1:D:716:VAL:HG11	1:D:726:PHE:HB2	1.66	0.75
6:M:214:ASN:HB3	1:g:60:ARG:HH21	1.51	0.75
1:Y:432:ARG:NH2	1:Y:792:CYS:SG	2.59	0.75
1:X:373:VAL:HG21	1:X:428:ALA:HB2	1.68	0.75
1:A:444:PRO:HG2	1:A:447:LEU:HD13	1.68	0.75
9:j:139:VAL:HG22	9:j:237:ILE:HG22	1.68	0.75
1:F:625:LEU:CG	1:F:863:THR:HG22	2.16	0.74
1:g:381:CYS:SG	1:g:424:ILE:HD11	2.27	0.74
1:F:402:GLN:HE22	1:F:404:GLN:HB3	1.51	0.74
1:h:784:THR:OG1	1:h:788:TRP:NE1	2.20	0.74
1:X:716:VAL:HG11	1:X:726:PHE:HB2	1.67	0.74
1:i:122:ASN:ND2	1:i:215:CYS:O	2.21	0.74
1:i:784:THR:OG1	1:i:788:TRP:NE1	2.20	0.74
1:G:321:GLN:HE22	1:g:633:ALA:HB3	1.53	0.74
1:J:784:THR:HG1	1:J:788:TRP:CD1	2.05	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:165:MET:HE3	1:i:176:ALA:HB2	1.68	0.74
1:G:383:PRO:HA	1:h:422:MET:HG2	1.69	0.74
1:G:618:ILE:HD11	1:G:875:LEU:HB2	1.70	0.74
1:A:716:VAL:HG11	1:A:726:PHE:HB2	1.70	0.74
1:X:39:PHE:O	1:Y:739:GLN:NE2	2.20	0.74
1:A:298:ASP:OD2	1:A:347:ARG:NH2	2.21	0.73
1:H:721:MET:HE1	1:H:754:PHE:HZ	1.53	0.73
1:D:222:PRO:HB3	1:g:804:LEU:HD12	1.68	0.73
1:F:694:ASN:HB3	1:g:61:SER:HA	1.68	0.73
1:H:123:SER:O	1:I:425:ASN:ND2	2.21	0.73
1:A:627:ILE:HG21	1:A:860:LEU:HD23	1.71	0.73
1:i:132:ASN:ND2	1:i:205:ARG:O	2.22	0.73
1:F:200:ASP:OD1	1:F:201:GLN:N	2.21	0.73
1:G:626:PRO:HD2	1:G:862:MET:O	1.88	0.73
1:X:813:ARG:HD2	1:Y:261:LEU:HD22	1.70	0.73
1:H:716:VAL:HG11	1:H:726:PHE:HB2	1.69	0.73
1:A:122:ASN:ND2	1:A:215:CYS:O	2.21	0.73
1:I:122:ASN:ND2	1:I:215:CYS:SG	2.62	0.73
1:G:122:ASN:ND2	1:G:215:CYS:O	2.20	0.73
1:I:52:PRO:HD3	2:Z:11:PRO:HA	1.70	0.73
1:F:630:ARG:HG2	1:F:631:ASN:H	1.52	0.72
1:i:618:ILE:HD11	1:i:875:LEU:HB2	1.70	0.72
1:I:493:ASN:O	1:I:644:LYS:NZ	2.23	0.72
1:X:784:THR:H	1:X:803:GLN:HG2	1.54	0.72
1:G:205:ARG:O	1:i:799:HIS:NE2	2.22	0.72
1:H:18:GLN:HG2	1:H:22:GLU:HG3	1.71	0.72
1:H:444:PRO:HG2	1:H:447:LEU:HD13	1.72	0.72
1:A:697:LEU:HD23	1:A:724:ASP:HB2	1.72	0.72
1:D:694:ASN:HB3	1:F:61:SER:HA	1.72	0.72
1:I:716:VAL:HG11	1:I:726:PHE:HB2	1.71	0.72
7:R:80:LYS:HG2	7:R:176:GLN:HG3	1.72	0.72
1:Y:70:PRO:HA	1:Y:84:PHE:HB3	1.71	0.72
1:g:783:THR:HA	1:g:803:GLN:HG2	1.71	0.72
1:F:6:MET:SD	1:F:9:GLN:NE2	2.63	0.72
1:J:5:SER:HA	7:R:174:SER:HB3	1.71	0.71
1:g:817:ARG:HD2	1:g:819:PRO:HD3	1.72	0.71
1:H:784:THR:OG1	1:H:788:TRP:NE1	2.22	0.71
1:i:641:THR:HG21	1:i:672:PHE:HB3	1.72	0.71
1:H:626:PRO:CB	1:H:861:ASP:HA	2.20	0.71
1:A:424:ILE:O	1:A:429:ASN:ND2	2.23	0.71
1:Y:716:VAL:HG11	1:Y:726:PHE:HB2	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:297:ARG:NH1	1:A:663:GLY:O	2.24	0.71
1:D:6:MET:SD	1:D:10:TRP:NE1	2.63	0.71
1:Y:299:CYS:SG	1:Y:347:ARG:NH2	2.64	0.71
1:g:308:SER:HA	1:g:652:GLY:HA2	1.71	0.71
1:g:640:LEU:HD22	1:g:864:PHE:HE2	1.53	0.71
2:b:5:ASN:O	2:b:5:ASN:ND2	2.23	0.71
1:h:618:ILE:HD11	1:h:875:LEU:HB2	1.73	0.71
1:A:499:HIS:HD2	1:A:501:ARG:H	1.37	0.71
1:F:339:MET:HE1	2:T:32:GLY:HA3	1.73	0.71
1:A:764:GLN:NE2	1:X:512:LEU:O	2.23	0.71
1:D:630:ARG:HG3	1:D:631:ASN:H	1.56	0.71
9:j:173:MET:HE2	9:j:244:LEU:HD12	1.73	0.71
1:A:185:GLN:HB3	1:Y:790:ARG:HH11	1.56	0.70
1:F:784:THR:H	1:F:803:GLN:HE21	1.38	0.70
1:I:785:PRO:HD3	1:I:803:GLN:HE21	1.55	0.70
1:D:591:THR:HG22	1:D:595:MET:HE2	1.74	0.70
1:g:359:ASP:OD1	1:g:508:ARG:NH2	2.25	0.70
1:A:734:TYR:HB2	1:A:736:ILE:HG12	1.73	0.70
1:F:492:ASP:OD2	1:F:822:LYS:NZ	2.22	0.70
1:F:803:GLN:NE2	1:g:122:ASN:H	1.90	0.70
1:G:145:GLN:HE21	1:h:409:SER:HA	1.55	0.70
1:I:616:TYR:HB3	1:I:624:GLN:NE2	2.05	0.70
1:X:425:ASN:ND2	1:Y:123:SER:O	2.24	0.70
1:X:719:SER:HB3	1:X:760:PRO:HB3	1.74	0.70
8:P:73:MET:HE2	8:P:75:LEU:HD21	1.72	0.70
2:S:30:MET:SD	1:g:636:ARG:NH1	2.64	0.70
1:X:234:THR:HG21	1:X:257:GLU:HB2	1.73	0.70
1:X:564:ARG:HH22	1:X:659:PHE:HB3	1.57	0.70
1:J:784:THR:HG1	1:J:788:TRP:NE1	1.90	0.70
1:F:626:PRO:HD2	1:F:862:MET:O	1.91	0.69
7:N:90:GLU:OE2	7:N:155:GLN:NE2	2.25	0.69
1:Y:52:PRO:HD3	2:d:11:PRO:HA	1.74	0.69
1:A:127:LYS:HD2	1:A:793:ARG:HH21	1.57	0.69
1:D:122:ASN:ND2	1:D:215:CYS:SG	2.65	0.69
1:J:680:LYS:HD3	1:J:702:GLU:HG3	1.74	0.69
1:I:123:SER:O	1:J:425:ASN:ND2	2.26	0.69
1:J:109:ARG:NH2	1:J:513:GLY:O	2.25	0.69
1:A:123:SER:O	1:Y:425:ASN:ND2	2.24	0.69
1:g:183:GLU:HG2	1:g:186:LEU:HD23	1.74	0.69
1:g:716:VAL:HG11	1:g:726:PHE:HB2	1.74	0.69
9:j:232:LEU:HD12	9:j:233:PRO:HD2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:347:ARG:HD3	1:F:358:MET:HE3	1.73	0.69
1:G:61:SER:HA	1:i:694:ASN:HB2	1.73	0.69
1:J:784:THR:OG1	1:J:788:TRP:NE1	2.25	0.69
1:i:297:ARG:NH1	1:i:663:GLY:O	2.22	0.69
1:A:377:MET:HE1	1:X:432:ARG:HD3	1.75	0.69
1:F:432:ARG:NH2	1:F:792:CYS:SG	2.66	0.69
1:G:122:ASN:HA	1:i:784:THR:HG22	1.73	0.69
1:i:83:ARG:HG3	1:i:544:GLU:HB3	1.75	0.69
1:H:289:ASN:OD1	1:H:467:ASN:ND2	2.26	0.69
1:H:626:PRO:HB2	1:H:861:ASP:HA	1.73	0.69
1:D:39:PHE:O	1:F:739:GLN:NE2	2.25	0.68
1:H:61:SER:HA	1:I:694:ASN:HB3	1.73	0.68
1:Y:613:ASN:HB3	1:Y:876:TYR:HE1	1.58	0.68
1:i:435:LEU:HD21	1:i:476:ILE:HG13	1.75	0.68
1:H:623:THR:HB	1:H:864:PHE:O	1.93	0.68
1:g:479:TYR:HB2	1:g:806:LEU:HD22	1.75	0.68
1:A:113:PHE:HE2	1:A:515:GLY:H	1.41	0.68
1:H:626:PRO:HB3	1:H:862:MET:N	2.02	0.68
1:i:716:VAL:HG11	1:i:726:PHE:HB2	1.75	0.68
1:A:623:THR:HG21	1:A:865:GLU:CG	2.21	0.68
1:G:323:ASN:ND2	1:G:325:VAL:O	2.27	0.68
1:J:112:SER:OG	1:J:292:ASN:ND2	2.27	0.68
1:i:339:MET:HE1	1:i:609:LEU:HD13	1.73	0.68
9:j:215:VAL:HG22	9:j:217:PRO:HD2	1.74	0.68
1:F:623:THR:HB	1:F:864:PHE:O	1.93	0.68
1:G:688:SER:HB2	7:R:16:GLN:HE22	1.58	0.68
1:Y:432:ARG:NH1	1:Y:477:ASP:OD1	2.26	0.68
1:i:112:SER:OG	1:i:292:ASN:ND2	2.26	0.68
1:F:551:VAL:HG11	1:F:568:ALA:HB3	1.76	0.68
1:H:817:ARG:HB3	1:J:517:PHE:HB2	1.76	0.68
1:J:448:LYS:O	1:J:469:ARG:NH2	2.26	0.68
1:g:362:ASP:HB3	1:g:365:VAL:HG12	1.76	0.68
1:A:738:TYR:HD2	1:A:839:MET:HE3	1.59	0.68
1:F:72:ASP:HB3	1:X:71:VAL:HA	1.74	0.68
1:G:739:GLN:NE2	1:i:39:PHE:O	2.26	0.68
1:i:299:CYS:SG	1:i:347:ARG:NH2	2.67	0.68
1:A:134:GLN:HG2	1:A:146:THR:HG22	1.76	0.67
1:H:122:ASN:ND2	1:H:215:CYS:O	2.25	0.67
1:X:706:LYS:NZ	1:X:867:ASP:OD2	2.26	0.67
1:Y:336:SER:HA	1:Y:609:LEU:HD23	1.75	0.67
9:j:360:VAL:HG22	9:j:361:THR:HG23	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:297:ARG:HH12	1:H:665:ILE:HD12	1.59	0.67
1:G:392:ARG:HD2	1:G:411:ASN:HA	1.76	0.67
1:J:354:TRP:O	1:J:356:GLN:N	2.27	0.67
1:Y:114:LYS:NZ	1:Y:116:TYR:O	2.27	0.67
1:g:721:MET:HE1	1:g:754:PHE:HZ	1.58	0.67
1:A:629:SER:O	1:A:630:ARG:HB2	1.95	0.67
1:Y:591:THR:O	1:Y:595:MET:HG3	1.95	0.67
1:A:193:ALA:HA	1:A:197:ALA:HB3	1.77	0.67
1:A:792:CYS:SG	1:A:793:ARG:N	2.66	0.67
1:X:814:HIS:ND1	1:X:815:ALA:O	2.24	0.67
1:g:163:LEU:HD21	1:g:203:GLY:HA3	1.76	0.67
1:g:122:ASN:ND2	1:g:218:SER:OG	2.24	0.67
1:A:61:SER:HA	1:Y:694:ASN:HB2	1.77	0.67
1:A:463:TYR:HB2	1:A:561:ASN:HD22	1.59	0.67
1:A:800:PRO:O	1:X:132:ASN:ND2	2.27	0.67
1:G:432:ARG:NH2	1:G:792:CYS:SG	2.65	0.67
1:H:626:PRO:CB	1:H:862:MET:H	2.03	0.67
8:Q:23:VAL:HG21	8:Q:26:LYS:HD3	1.77	0.67
1:X:400:GLN:H	1:X:404:GLN:HE22	1.42	0.67
1:i:591:THR:HG22	1:i:595:MET:HE2	1.77	0.67
9:j:137:PHE:HB3	9:j:157:LEU:HB2	1.77	0.67
1:G:896:GLU:HB2	7:R:36:ALA:HA	1.75	0.67
1:H:432:ARG:NH2	1:H:792:CYS:SG	2.68	0.67
1:J:535:LEU:HB3	1:J:603:GLN:HE22	1.60	0.67
1:G:328:LEU:HD11	1:G:901:ARG:HH11	1.59	0.67
1:H:164:GLN:HE22	1:H:173:PRO:HB3	1.60	0.67
1:g:130:PRO:HG3	1:g:282:LEU:HB3	1.75	0.67
1:i:643:LEU:HD22	1:i:666:PRO:HB2	1.75	0.67
9:j:123:THR:HG22	9:j:380:PRO:HG2	1.77	0.67
1:A:227:GLY:HA2	1:Y:804:LEU:HD11	1.76	0.67
1:F:205:ARG:NH1	1:F:256:GLU:OE1	2.27	0.67
1:G:422:MET:HG3	1:i:381:CYS:SG	2.36	0.67
1:J:792:CYS:SG	1:J:793:ARG:N	2.65	0.67
1:A:332:ASN:ND2	1:A:667:TYR:O	2.24	0.66
1:D:784:THR:OG1	1:D:788:TRP:NE1	2.27	0.66
1:J:212:GLN:HE22	1:J:282:LEU:HD23	1.59	0.66
1:J:432:ARG:NH2	1:J:792:CYS:SG	2.68	0.66
1:Y:640:LEU:HD22	1:Y:864:PHE:HE2	1.59	0.66
1:g:359:ASP:O	1:g:827:ARG:NH2	2.28	0.66
1:A:869:ILE:HD11	1:A:873:THR:HG21	1.77	0.66
1:D:785:PRO:HD2	1:D:803:GLN:HE21	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:881:VAL:HB	1:g:903:PRO:HD2	1.75	0.66
1:A:902:THR:O	1:J:321:GLN:NE2	2.28	0.66
1:F:58:THR:HA	1:F:585:SER:HA	1.77	0.66
1:G:307:ASN:ND2	1:G:331:ARG:O	2.29	0.66
1:H:804:LEU:HD12	1:J:222:PRO:HB3	1.77	0.66
1:I:279:VAL:O	1:I:280:GLU:HG3	1.96	0.66
1:h:803:GLN:HE22	1:i:122:ASN:HD21	1.44	0.66
1:H:623:THR:HG22	1:H:865:GLU:HA	1.77	0.66
1:J:83:ARG:NH1	1:J:544:GLU:OE2	2.28	0.66
1:X:112:SER:OG	1:X:292:ASN:ND2	2.28	0.66
9:j:200:ASP:HA	9:j:419:PRO:HB3	1.77	0.66
1:D:205:ARG:NH1	1:D:256:GLU:OE1	2.28	0.66
1:H:623:THR:HG21	1:H:865:GLU:OE2	1.95	0.66
1:I:362:ASP:HB3	1:I:365:VAL:HG12	1.78	0.66
1:h:149:GLN:NE2	1:i:417:GLY:O	2.27	0.66
1:D:513:GLY:HA3	1:g:764:GLN:HE22	1.61	0.66
1:F:508:ARG:NH2	1:F:556:GLN:OE1	2.28	0.66
1:G:616:TYR:HB3	1:G:624:GLN:HE22	1.61	0.66
1:G:796:ARG:NH2	1:i:419:LEU:O	2.29	0.66
1:I:122:ASN:HA	1:J:784:THR:HG22	1.78	0.66
1:h:783:THR:HA	1:h:803:GLN:HG2	1.77	0.66
1:G:289:ASN:OD1	1:G:467:ASN:ND2	2.29	0.66
1:Y:112:SER:OG	1:Y:292:ASN:ND2	2.28	0.66
1:A:307:ASN:ND2	1:A:331:ARG:O	2.29	0.65
1:A:112:SER:O	1:A:292:ASN:ND2	2.29	0.65
1:D:154:ALA:HB1	1:D:164:GLN:HB3	1.78	0.65
1:I:399:ASN:ND2	1:I:404:GLN:OE1	2.29	0.65
1:I:564:ARG:HH21	1:I:660:THR:H	1.43	0.65
1:D:347:ARG:NH1	1:D:358:MET:SD	2.69	0.65
1:D:508:ARG:NH1	1:D:556:GLN:OE1	2.22	0.65
1:I:112:SER:OG	1:I:292:ASN:ND2	2.29	0.65
1:g:738:TYR:HD2	1:g:839:MET:HE3	1.62	0.65
1:H:65:GLN:HB2	1:I:698:LEU:HD13	1.79	0.65
1:I:164:GLN:NE2	1:I:166:GLY:O	2.29	0.65
1:G:432:ARG:HD3	1:i:377:MET:HE1	1.78	0.65
1:i:432:ARG:NH2	1:i:792:CYS:SG	2.70	0.65
1:G:321:GLN:HE21	1:g:631:ASN:ND2	1.94	0.65
1:H:419:LEU:HD13	1:J:786:ALA:HB1	1.78	0.65
1:J:22:GLU:HB2	7:R:166:ARG:HG2	1.78	0.65
1:A:506:ARG:O	1:A:510:GLN:HG2	1.95	0.65
1:A:598:ASN:OD1	7:N:25:GLN:NE2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:205:ARG:NH1	1:h:256:GLU:OE1	2.29	0.65
1:h:643:LEU:HD22	1:h:666:PRO:HB2	1.79	0.65
1:A:419:LEU:O	1:X:796:ARG:NH2	2.29	0.65
1:D:425:ASN:ND2	1:F:123:SER:O	2.30	0.65
1:J:114:LYS:NZ	1:J:116:TYR:O	2.29	0.65
1:A:165:MET:HE3	1:A:176:ALA:HB2	1.78	0.65
1:D:289:ASN:OD1	1:D:467:ASN:ND2	2.29	0.65
1:D:796:ARG:NH2	1:g:419:LEU:O	2.25	0.65
1:F:817:ARG:NH2	1:g:516:ARG:HB3	2.12	0.65
1:H:112:SER:OG	1:H:561:ASN:ND2	2.30	0.65
1:I:94:LEU:HD13	1:I:581:PHE:HE1	1.61	0.65
1:I:400:GLN:NE2	1:I:402:GLN:OE1	2.29	0.65
1:Y:783:THR:HA	1:Y:803:GLN:HG2	1.79	0.65
1:F:625:LEU:CD2	1:F:863:THR:HG22	2.27	0.64
1:G:684:GLN:HE22	1:H:907:GLY:H	1.43	0.64
1:G:517:PHE:HB2	1:i:817:ARG:HG3	1.77	0.64
1:D:227:GLY:HA2	1:g:804:LEU:HD11	1.78	0.64
1:D:448:LYS:O	1:D:469:ARG:NH1	2.30	0.64
1:F:234:THR:HG21	1:F:257:GLU:HB2	1.79	0.64
1:G:253:PHE:HE2	1:h:414:ILE:HD12	1.61	0.64
1:H:112:SER:OG	1:H:292:ASN:ND2	2.30	0.64
1:H:227:GLY:HA2	1:I:804:LEU:HD11	1.79	0.64
1:J:122:ASN:ND2	1:J:218:SER:OG	2.30	0.64
1:H:465:TYR:OH	1:H:469:ARG:NH1	2.30	0.64
1:g:267:LEU:HB3	1:g:270:ALA:HB2	1.80	0.64
1:A:149:GLN:HB2	1:X:387:VAL:HG12	1.80	0.64
1:F:340:LEU:HD12	1:F:608:TYR:HB2	1.78	0.64
1:I:822:LYS:HD3	8:P:46:THR:HG22	1.79	0.64
1:A:623:THR:HB	1:A:864:PHE:O	1.97	0.64
1:D:746:ASP:OD1	1:D:747:TYR:N	2.31	0.64
1:I:163:LEU:HD21	1:I:203:GLY:HA3	1.79	0.64
1:J:586:HIS:HB2	6:M:216:ASP:HB2	1.80	0.64
1:J:629:SER:HA	1:J:859:ALA:HA	1.80	0.64
1:h:113:PHE:HE2	1:h:515:GLY:H	1.45	0.64
1:A:359:ASP:OD1	1:A:508:ARG:NH2	2.31	0.64
1:A:615:LEU:HB3	1:A:874:LEU:HD13	1.80	0.64
1:F:422:MET:SD	1:g:422:MET:HE1	2.38	0.64
1:F:776:LEU:HD22	1:F:804:LEU:HD13	1.78	0.64
1:H:382:PHE:HZ	1:J:796:ARG:HG3	1.62	0.64
1:A:694:ASN:HB3	1:X:61:SER:HA	1.79	0.64
1:F:630:ARG:HG2	1:F:631:ASN:N	2.12	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:640:LEU:HD22	1:X:864:PHE:HE1	1.62	0.64
1:g:18:GLN:HG2	1:g:22:GLU:HG3	1.80	0.64
1:g:96:MET:O	1:g:526:GLN:NE2	2.30	0.64
1:g:643:LEU:HD22	1:g:666:PRO:HB2	1.78	0.64
1:h:679:ARG:NH1	1:h:867:ASP:OD1	2.31	0.64
1:G:163:LEU:HD11	1:G:203:GLY:HA3	1.80	0.64
1:I:640:LEU:HD22	1:I:864:PHE:HE1	1.63	0.64
9:j:280:GLU:OE1	9:j:288:ARG:NE	2.31	0.64
1:F:710:ASP:OD2	1:F:715:ASN:ND2	2.31	0.64
1:G:419:LEU:HA	1:i:149:GLN:HE22	1.63	0.64
1:g:595:MET:O	1:g:601:ASN:ND2	2.27	0.64
1:h:425:ASN:ND2	1:i:123:SER:O	2.31	0.64
1:D:719:SER:HB3	1:D:760:PRO:HB3	1.80	0.63
1:J:261:LEU:HG	1:J:263:PRO:HD3	1.80	0.63
1:A:261:LEU:HD12	1:A:263:PRO:HD3	1.79	0.63
1:G:398:ARG:HH21	1:G:401:GLN:HA	1.61	0.63
1:J:103:ILE:HG12	1:J:575:VAL:HG22	1.81	0.63
1:h:508:ARG:NH1	1:h:556:GLN:OE1	2.30	0.63
1:I:602:ASP:HB2	1:I:886:ARG:HE	1.63	0.63
1:X:785:PRO:HD2	1:X:803:GLN:HE21	1.64	0.63
1:Y:332:ASN:HB2	1:Y:613:ASN:ND2	2.13	0.63
1:i:785:PRO:HD2	1:i:803:GLN:HE21	1.62	0.63
1:A:718:GLN:O	1:A:821:ARG:NH1	2.30	0.63
6:M:232:LYS:O	6:M:240:ILE:N	2.31	0.63
1:g:319:SER:HB3	1:g:894:VAL:HG22	1.80	0.63
1:D:113:PHE:HB2	1:D:294:ILE:HD12	1.81	0.63
1:D:432:ARG:NH2	1:D:792:CYS:SG	2.72	0.63
1:I:881:VAL:HB	1:I:903:PRO:HD2	1.81	0.63
1:i:444:PRO:HG2	1:i:447:LEU:HD23	1.79	0.63
1:A:627:ILE:HG21	1:A:860:LEU:HD22	1.77	0.63
1:X:428:ALA:HA	1:X:431:TRP:HB3	1.80	0.63
1:h:716:VAL:HG21	1:h:726:PHE:CG	2.34	0.63
1:A:712:GLU:HG2	1:A:713:GLY:H	1.63	0.63
1:H:199:ILE:O	1:J:416:LYS:NZ	2.27	0.63
1:H:383:PRO:HA	1:J:422:MET:HG2	1.79	0.63
1:I:444:PRO:HG2	1:I:447:LEU:HD23	1.80	0.63
6:M:213:GLU:O	1:g:60:ARG:NH2	2.32	0.63
1:X:694:ASN:HB3	1:Y:61:SER:HA	1.80	0.63
1:Y:801:TYR:O	1:Y:803:GLN:NE2	2.31	0.63
1:F:320:SER:HA	1:X:90:ASP:HB2	1.80	0.63
1:D:825:CYS:HG	1:D:828:THR:HG1	1.47	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:675:SER:O	1:I:830:TRP:NE1	2.27	0.63
1:h:398:ARG:NH1	1:h:401:GLN:O	2.32	0.63
1:H:516:ARG:HB2	1:I:810:TRP:HA	1.79	0.62
1:h:359:ASP:OD1	1:h:508:ARG:NH2	2.29	0.62
1:G:365:VAL:HG21	1:G:501:ARG:HD2	1.80	0.62
1:H:294:ILE:HG12	1:H:557:SER:HB3	1.82	0.62
1:I:658:TYR:HA	8:Q:28:GLY:HA2	1.81	0.62
5:K:319:THR:O	5:K:323:LEU:HB2	1.99	0.62
1:h:388:GLN:HB2	1:h:420:PRO:HG3	1.81	0.62
1:G:804:LEU:HB2	1:h:222:PRO:HG3	1.81	0.62
1:J:328:LEU:HD11	1:J:901:ARG:HH11	1.64	0.62
6:M:290:ALA:HB3	6:M:291:PRO:HD3	1.82	0.62
8:Q:30:ASN:ND2	8:Q:54:THR:O	2.31	0.62
1:g:264:ASP:HA	1:g:289:ASN:HD21	1.64	0.62
1:i:816:LEU:HG	1:i:817:ARG:H	1.65	0.62
1:J:640:LEU:HD22	1:J:864:PHE:HE2	1.65	0.62
1:g:785:PRO:HD2	1:g:803:GLN:HE21	1.64	0.62
1:D:192:THR:HG23	1:g:283:SER:HB3	1.82	0.62
1:D:640:LEU:HD22	1:D:864:PHE:HE2	1.63	0.62
1:D:810:TRP:HA	1:F:516:ARG:HG3	1.80	0.62
1:F:716:VAL:HG11	1:F:726:PHE:HB2	1.81	0.62
1:X:188:ILE:HG21	1:X:193:ALA:HB3	1.79	0.62
1:G:303:LEU:HD22	1:G:524:VAL:HG11	1.82	0.62
1:F:375:ASP:HB3	1:F:427:ALA:HB3	1.82	0.62
1:H:625:LEU:HD22	1:H:626:PRO:HD3	1.82	0.62
7:R:9:TYR:OH	1:g:598:ASN:ND2	2.33	0.62
1:Y:290:ARG:HH11	1:Y:441:LEU:HB3	1.64	0.62
1:F:626:PRO:CD	1:F:862:MET:O	2.48	0.62
1:H:369:ASP:HB3	1:H:485:ARG:HB3	1.80	0.62
1:I:338:GLN:OE1	1:I:347:ARG:NH1	2.32	0.62
1:I:552:ASN:HD21	1:I:563:LEU:H	1.48	0.62
1:X:426:LEU:HD13	1:Y:430:LEU:HG	1.80	0.62
1:D:643:LEU:HD22	1:D:666:PRO:HB2	1.82	0.62
1:I:720:ASN:HB2	1:I:822:LYS:HA	1.82	0.62
1:A:397:GLN:HE22	1:A:399:ASN:HB2	1.65	0.62
1:D:314:VAL:HG22	1:D:544:GLU:HG3	1.82	0.62
1:A:680:LYS:HD3	1:A:702:GLU:HG3	1.81	0.61
1:H:297:ARG:HE	1:H:556:GLN:HB2	1.63	0.61
1:J:602:ASP:OD2	1:J:886:ARG:NH1	2.33	0.61
1:J:881:VAL:HB	1:J:903:PRO:HD2	1.82	0.61
8:V:16:LEU:HD12	8:V:17:PRO:HD2	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:58:THR:HA	1:Y:585:SER:HA	1.80	0.61
1:h:297:ARG:HD3	1:h:556:GLN:HB2	1.82	0.61
1:h:535:LEU:HB2	1:i:44:LYS:HE2	1.81	0.61
1:X:332:ASN:HB2	1:X:613:ASN:HD21	1.66	0.61
1:h:122:ASN:ND2	1:h:215:CYS:SG	2.73	0.61
1:X:749:ASP:OD2	1:Y:349:ARG:NH1	2.33	0.61
1:g:801:TYR:O	1:g:803:GLN:NE2	2.33	0.61
1:A:817:ARG:HH22	1:X:518:CYS:HA	1.65	0.61
1:F:242:ARG:NH1	1:F:247:GLY:O	2.32	0.61
1:J:465:TYR:OH	1:J:469:ARG:NH1	2.32	0.61
1:X:134:GLN:HG2	1:X:146:THR:HG22	1.82	0.61
1:G:149:GLN:HB2	1:h:387:VAL:HG12	1.83	0.61
1:I:667:TYR:HE1	1:I:876:TYR:CE1	2.17	0.61
1:Y:49:THR:HG21	3:f:18:ASN:HD22	1.66	0.61
1:Y:792:CYS:SG	1:Y:793:ARG:N	2.73	0.61
1:h:13:MET:HB2	1:h:15:ILE:HG12	1.81	0.61
1:D:626:PRO:HB3	1:D:861:ASP:HA	1.83	0.61
1:F:315:LEU:HD23	1:F:531:ILE:HD12	1.82	0.61
1:F:381:CYS:HB3	1:g:424:ILE:HG12	1.82	0.61
1:H:644:LYS:NZ	1:H:871:GLU:OE2	2.21	0.61
1:I:460:THR:HG22	8:Q:71:PRO:HG3	1.81	0.61
1:h:864:PHE:CD2	1:h:875:LEU:HD11	2.35	0.61
1:A:297:ARG:NH2	1:A:552:ASN:O	2.33	0.61
1:F:122:ASN:ND2	1:F:215:CYS:O	2.27	0.61
1:H:261:LEU:HG	1:H:263:PRO:HD3	1.81	0.61
1:I:801:TYR:O	1:I:803:GLN:NE2	2.34	0.61
1:J:602:ASP:OD1	1:J:888:HIS:ND1	2.33	0.61
1:h:448:LYS:O	1:h:469:ARG:NH1	2.34	0.61
1:A:551:VAL:HG11	1:A:568:ALA:HB3	1.83	0.61
1:G:211:THR:OG1	1:G:276:ARG:NH1	2.34	0.61
1:H:508:ARG:NH2	1:H:556:GLN:OE1	2.31	0.61
5:K:173:ALA:O	5:K:179:GLN:NE2	2.33	0.61
1:Y:165:MET:HE2	1:Y:181:GLN:HG3	1.81	0.61
1:Y:613:ASN:HB3	1:Y:876:TYR:CE1	2.36	0.61
1:i:208:ARG:NH2	1:i:235:GLN:O	2.34	0.61
1:G:416:LYS:NZ	1:i:199:ILE:O	2.34	0.61
1:H:349:ARG:NH2	1:I:749:ASP:OD2	2.34	0.61
2:S:28:HIS:NE2	1:g:843:SER:OG	2.26	0.61
1:Y:505:LEU:HD22	1:Y:556:GLN:HE21	1.65	0.61
1:h:208:ARG:NH2	1:h:235:GLN:O	2.34	0.61
1:i:91:ASN:O	1:i:92:ARG:HG2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:a:25:ILE:HG13	1:i:42:GLY:HA2	1.82	0.61
3:e:21:TYR:O	1:i:636:ARG:NH1	2.33	0.61
1:h:261:LEU:HD12	1:h:263:PRO:HD3	1.84	0.60
1:i:240:TYR:HD1	1:i:252:VAL:HG22	1.65	0.60
1:F:290:ARG:NH1	1:F:441:LEU:O	2.33	0.60
1:G:627:ILE:HG21	1:G:860:LEU:HB3	1.84	0.60
1:H:222:PRO:HB3	1:I:804:LEU:HD12	1.81	0.60
1:H:381:CYS:HB3	1:H:424:ILE:HD11	1.83	0.60
1:H:694:ASN:HB3	1:J:61:SER:HA	1.83	0.60
1:J:608:TYR:O	1:J:609:LEU:C	2.43	0.60
1:Y:595:MET:O	1:Y:601:ASN:ND2	2.33	0.60
1:Y:869:ILE:HD11	1:Y:873:THR:HG21	1.82	0.60
9:j:297:ARG:NH1	9:j:412:GLU:OE2	2.33	0.60
5:K:227:ASP:OD1	5:K:230:ARG:NH2	2.33	0.60
1:Y:643:LEU:HD22	1:Y:666:PRO:HB2	1.82	0.60
1:h:297:ARG:NH1	1:h:663:GLY:O	2.34	0.60
1:i:626:PRO:HB3	1:i:862:MET:H	1.66	0.60
1:A:196:MET:HE1	1:Y:282:LEU:HD12	1.82	0.60
1:F:321:GLN:HB2	1:X:89:GLY:HA2	1.83	0.60
1:G:109:ARG:NH2	1:G:518:CYS:SG	2.70	0.60
1:G:644:LYS:HA	1:G:873:THR:HG22	1.84	0.60
1:I:721:MET:HE1	1:I:754:PHE:HZ	1.66	0.60
1:J:205:ARG:NH2	1:J:256:GLU:OE1	2.28	0.60
1:g:615:LEU:HD23	1:g:876:TYR:HA	1.82	0.60
9:j:243:ARG:NH1	9:j:343:CYS:O	2.34	0.60
9:j:132:MET:HB3	9:j:243:ARG:HH21	1.65	0.60
1:G:112:SER:OG	1:G:292:ASN:ND2	2.34	0.60
1:G:205:ARG:NH1	1:G:256:GLU:OE1	2.35	0.60
1:H:297:ARG:HB3	1:H:301:VAL:HG12	1.83	0.60
5:K:230:ARG:HA	5:K:233:TRP:NE1	2.17	0.60
8:O:90:LEU:HD13	8:P:90:LEU:HD22	1.83	0.60
2:S:30:MET:HE3	1:g:606:ASN:HD22	1.67	0.60
1:i:869:ILE:HD11	1:i:873:THR:HG21	1.82	0.60
1:A:482:ILE:HD13	1:X:120:ALA:HB2	1.83	0.60
1:G:836:SER:HB2	1:h:57:THR:HG21	1.82	0.60
1:I:868:PRO:HG3	8:P:40:ASN:HA	1.81	0.60
1:h:165:MET:HE3	1:h:181:GLN:HG3	1.83	0.60
1:I:330:ASP:HB2	1:I:901:ARG:HH12	1.67	0.60
1:i:373:VAL:HG11	1:i:428:ALA:HA	1.83	0.60
1:A:323:ASN:ND2	1:A:325:VAL:O	2.34	0.60
1:F:630:ARG:CG	1:F:631:ASN:H	2.14	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:719:SER:HB3	1:H:760:PRO:HB3	1.84	0.60
1:I:613:ASN:ND2	1:I:876:TYR:OH	2.35	0.60
5:K:26:SER:HB3	5:K:37:GLN:HE22	1.67	0.60
1:X:784:THR:HB	1:X:788:TRP:HE1	1.66	0.60
1:g:344:THR:HG23	1:g:345:THR:HG23	1.83	0.60
1:F:289:ASN:OD1	1:F:467:ASN:ND2	2.35	0.60
1:G:415:GLY:O	1:i:149:GLN:HG3	2.02	0.60
1:G:697:LEU:HD22	1:G:724:ASP:HB2	1.83	0.60
1:H:642:ARG:NH2	1:H:866:MET:SD	2.75	0.60
1:X:354:TRP:O	1:X:356:GLN:N	2.35	0.60
1:h:790:ARG:HD3	1:i:185:GLN:HG2	1.83	0.60
1:A:205:ARG:NH1	1:A:256:GLU:OE1	2.33	0.59
1:J:163:LEU:HD11	1:J:203:GLY:HA3	1.82	0.59
1:h:697:LEU:O	1:i:63:ARG:NH2	2.35	0.59
9:j:85:TYR:HH	9:j:468:SER:HG	1.49	0.59
1:D:792:CYS:SG	1:D:793:ARG:N	2.74	0.59
1:F:163:LEU:HD11	1:F:203:GLY:HA3	1.83	0.59
1:F:381:CYS:SG	1:g:422:MET:HE3	2.42	0.59
1:G:697:LEU:O	1:h:63:ARG:NH1	2.35	0.59
1:H:843:SER:H	1:J:49:THR:HG22	1.67	0.59
1:g:113:PHE:HB2	1:g:294:ILE:HD12	1.85	0.59
1:A:797:GLU:HA	1:Y:418:ASN:ND2	2.18	0.59
1:H:298:ASP:OD2	1:H:347:ARG:NH2	2.36	0.59
1:X:112:SER:OG	1:X:561:ASN:ND2	2.35	0.59
1:X:340:LEU:HD12	1:X:608:TYR:HB2	1.84	0.59
1:G:501:ARG:NH2	1:i:374:GLU:OE2	2.35	0.59
1:G:803:GLN:HE22	1:h:122:ASN:HD21	1.50	0.59
1:X:297:ARG:NH2	1:X:555:LEU:O	2.36	0.59
1:g:55:ASP:OD1	1:g:587:ASN:ND2	2.35	0.59
1:G:792:CYS:SG	1:G:793:ARG:N	2.75	0.59
1:H:419:LEU:O	1:J:796:ARG:NH2	2.36	0.59
1:X:163:LEU:HD11	1:X:203:GLY:HA3	1.84	0.59
1:X:535:LEU:HB3	1:X:603:GLN:HE22	1.68	0.59
1:X:682:ALA:HB2	1:X:702:GLU:HG3	1.84	0.59
1:h:435:LEU:HD21	1:h:476:ILE:HG22	1.85	0.59
1:i:801:TYR:O	1:i:803:GLN:NE2	2.36	0.59
1:D:147:ILE:HG13	1:D:147:ILE:O	2.02	0.59
1:D:439:VAL:HG13	1:D:491:MET:HE2	1.84	0.59
1:F:816:LEU:C	1:F:817:ARG:HD3	2.27	0.59
1:H:357:ALA:O	1:H:508:ARG:NH1	2.36	0.59
1:H:375:ASP:HB3	1:H:427:ALA:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:508:ARG:NH1	1:X:556:GLN:OE1	2.30	0.59
1:X:836:SER:HB2	1:Y:57:THR:HG21	1.84	0.59
1:h:473:SER:HB3	1:h:792:CYS:H	1.67	0.59
1:D:176:ALA:HB1	1:D:182:PRO:HD3	1.84	0.59
1:D:797:GLU:OE1	1:F:187:GLY:N	2.36	0.59
1:D:804:LEU:HD12	1:F:222:PRO:HB3	1.85	0.59
1:F:354:TRP:HB2	1:F:356:GLN:HG3	1.84	0.59
1:G:473:SER:HB3	1:G:792:CYS:H	1.68	0.59
1:H:721:MET:HE3	1:H:726:PHE:HD1	1.67	0.59
1:H:881:VAL:HG21	1:H:901:ARG:HD2	1.84	0.59
1:I:121:TYR:O	1:J:783:THR:OG1	2.20	0.59
1:J:370:ASN:HB3	1:J:482:ILE:HG13	1.85	0.59
1:g:813:ARG:NH1	1:g:813:ARG:HA	2.17	0.59
1:F:697:LEU:O	1:g:63:ARG:NH1	2.35	0.59
1:I:631:ASN:OD1	1:I:632:TRP:N	2.36	0.59
1:I:644:LYS:HA	1:I:873:THR:HG22	1.83	0.59
1:J:479:TYR:HB2	1:J:806:LEU:HD22	1.84	0.59
1:X:375:ASP:HB3	1:X:427:ALA:HB3	1.85	0.59
1:F:103:ILE:HG12	1:F:575:VAL:HG22	1.85	0.59
1:F:743:LEU:HG	1:g:349:ARG:HH21	1.67	0.59
1:F:881:VAL:HB	1:F:903:PRO:HD2	1.85	0.59
1:X:703:PHE:HE1	1:X:728:VAL:HG21	1.68	0.59
1:Y:435:LEU:HD21	1:Y:476:ILE:HG13	1.84	0.59
1:g:561:ASN:ND2	1:g:566:ASP:OD2	2.36	0.59
1:h:801:TYR:O	1:h:803:GLN:NE2	2.35	0.59
1:i:642:ARG:NH2	1:i:873:THR:OG1	2.33	0.59
1:F:497:PHE:HB2	1:F:664:THR:HG21	1.84	0.59
1:G:628:PRO:CG	1:g:319:SER:HA	2.32	0.59
1:G:844:LEU:HD13	1:h:16:ALA:HB2	1.84	0.59
1:J:318:GLN:HA	1:J:542:THR:HG23	1.84	0.59
1:J:610:SER:OG	1:J:636:ARG:NH1	2.36	0.59
2:a:16:ARG:NH2	1:h:19:ASP:OD2	2.36	0.59
1:g:685:PHE:HD2	1:g:691:TRP:HB2	1.67	0.59
9:j:379:LEU:HD12	9:j:380:PRO:HD2	1.84	0.59
1:A:802:PRO:HG3	1:X:131:ASN:HD22	1.68	0.58
1:H:665:ILE:O	1:H:669:ASP:HB2	2.03	0.58
6:M:211:MET:O	1:g:587:ASN:ND2	2.36	0.58
6:M:227:GLN:HB3	6:M:244:ASP:HB2	1.85	0.58
6:M:231:VAL:HG22	6:M:241:GLN:HG2	1.85	0.58
1:g:340:LEU:HD12	1:g:608:TYR:HB2	1.85	0.58
1:A:118:GLY:HA2	1:A:288:PRO:HB3	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ASN:HA	1:Y:784:THR:HG22	1.84	0.58
1:G:616:TYR:HB3	1:G:624:GLN:NE2	2.17	0.58
1:I:353:MET:HA	1:J:717:ALA:HA	1.85	0.58
1:J:362:ASP:HB3	1:J:365:VAL:HG22	1.84	0.58
7:N:80:LYS:HE2	7:N:175:ARG:HH12	1.67	0.58
1:g:114:LYS:NZ	1:g:118:GLY:O	2.32	0.58
1:i:109:ARG:NH2	1:i:518:CYS:SG	2.71	0.58
1:A:51:ALA:O	1:Y:849:GLN:NE2	2.27	0.58
1:D:122:ASN:OD1	1:g:803:GLN:NE2	2.36	0.58
1:I:706:LYS:NZ	1:I:867:ASP:OD2	2.33	0.58
7:R:200:GLN:HE22	7:R:207:VAL:HG13	1.69	0.58
1:Y:299:CYS:HG	1:Y:347:ARG:HH22	1.51	0.58
1:h:112:SER:OG	1:h:292:ASN:ND2	2.36	0.58
1:i:163:LEU:HD11	1:i:203:GLY:HA3	1.84	0.58
1:G:133:THR:HB	1:G:210:PRO:HG3	1.84	0.58
1:Y:60:ARG:O	1:Y:60:ARG:HG2	2.03	0.58
1:Y:790:ARG:HH11	1:Y:790:ARG:HG2	1.68	0.58
9:j:66:ILE:HD11	9:j:69:LYS:HE2	1.83	0.58
9:j:395:GLN:HE21	9:j:418:ARG:HE	1.52	0.58
1:A:439:VAL:HG12	1:A:476:ILE:HD13	1.85	0.58
1:F:627:ILE:HD12	1:F:628:PRO:CD	2.19	0.58
1:G:19:ASP:OD1	1:G:20:ALA:N	2.36	0.58
1:g:264:ASP:HA	1:g:289:ASN:ND2	2.18	0.58
1:i:811:ASP:OD1	1:i:812:PRO:HD2	2.02	0.58
1:A:261:LEU:HD22	1:Y:813:ARG:HE	1.69	0.58
1:D:145:GLN:HG2	1:F:411:ASN:HB2	1.84	0.58
1:F:618:ILE:HB	1:F:873:THR:O	2.04	0.58
1:F:790:ARG:HG2	1:F:790:ARG:HH11	1.69	0.58
1:X:552:ASN:HD21	1:X:661:TYR:H	1.51	0.58
1:h:523:GLN:HE21	1:h:523:GLN:N	2.00	0.58
1:i:351:PHE:HB3	1:i:356:GLN:HB3	1.85	0.58
1:D:12:TYR:HE2	1:G:909:ALA:HB3	1.69	0.58
1:D:222:PRO:HD3	1:g:804:LEU:HB2	1.86	0.58
1:A:316:ALA:HB2	1:A:323:ASN:HA	1.84	0.58
1:G:479:TYR:CD1	1:G:806:LEU:HD11	2.39	0.58
1:I:58:THR:HG22	1:I:60:ARG:H	1.69	0.58
1:g:205:ARG:NH1	1:g:256:GLU:OE1	2.36	0.58
1:g:782:ARG:HG2	1:g:803:GLN:HG3	1.85	0.58
1:A:73:ARG:NE	1:A:80:TYR:OH	2.32	0.58
1:F:360:SER:N	1:F:502:ASN:OD1	2.27	0.58
8:O:105:ARG:HH22	8:Q:103:ARG:HH22	1.52	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:359:ASP:OD1	1:Y:508:ARG:NH2	2.28	0.58
1:D:621:ASN:OD1	1:D:868:PRO:HB2	2.02	0.58
1:G:465:TYR:CZ	1:G:469:ARG:HD2	2.39	0.58
1:H:425:ASN:ND2	1:J:123:SER:O	2.37	0.58
1:I:357:ALA:HB3	1:I:508:ARG:HG3	1.85	0.58
1:J:93:VAL:HG12	1:J:538:PRO:HD3	1.84	0.58
1:J:609:LEU:HD11	1:J:878:LEU:HD11	1.86	0.58
1:J:831:ARG:NH2	1:J:880:GLU:OE1	2.36	0.58
1:X:93:VAL:HG12	1:X:538:PRO:HD3	1.85	0.58
1:X:849:GLN:HE22	1:Y:50:VAL:HB	1.68	0.58
1:g:58:THR:HA	1:g:585:SER:HA	1.84	0.58
1:h:347:ARG:HE	1:h:358:MET:HG3	1.69	0.58
1:A:640:LEU:HD23	1:A:640:LEU:H	1.68	0.57
1:I:115:PRO:HB2	1:J:483:GLY:HA3	1.85	0.57
1:J:392:ARG:HD2	1:J:411:ASN:HA	1.85	0.57
8:P:102:ASN:O	8:P:106:THR:HG23	2.04	0.57
1:i:289:ASN:CB	1:i:467:ASN:HD21	2.16	0.57
1:i:366:ARG:HD3	1:i:496:PRO:HB3	1.85	0.57
9:j:131:HIS:O	9:j:460:ARG:NH2	2.37	0.57
1:A:147:ILE:HG21	1:A:282:LEU:HD21	1.85	0.57
1:A:484:THR:HA	1:X:510:GLN:HG2	1.85	0.57
1:I:694:ASN:HB2	1:I:696:ARG:HG2	1.86	0.57
1:g:200:ASP:OD1	1:g:201:GLN:N	2.37	0.57
1:g:623:THR:HB	1:g:864:PHE:O	2.04	0.57
1:i:560:GLY:O	1:i:646:ARG:NH2	2.37	0.57
1:A:234:THR:HG21	1:A:257:GLU:HB3	1.86	0.57
1:D:122:ASN:ND2	1:g:803:GLN:NE2	2.52	0.57
4:E:10:ARG:HH22	6:M:175:THR:HG22	1.70	0.57
1:F:813:ARG:HD2	1:g:261:LEU:HD13	1.86	0.57
1:I:134:GLN:HG2	1:I:146:THR:HG22	1.87	0.57
5:K:164:LEU:HD22	5:K:193:VAL:HG11	1.85	0.57
1:h:279:VAL:HG23	1:h:282:LEU:HD13	1.85	0.57
1:A:242:ARG:NH1	1:A:247:GLY:O	2.36	0.57
1:D:7:LEU:HD11	2:L:204:MET:HE2	1.86	0.57
1:I:227:GLY:HA2	1:J:804:LEU:HD11	1.87	0.57
1:X:307:ASN:HD21	1:X:332:ASN:HA	1.68	0.57
1:A:347:ARG:HG2	1:A:358:MET:HG2	1.86	0.57
1:H:289:ASN:O	1:H:463:TYR:OH	2.21	0.57
1:J:706:LYS:NZ	1:J:867:ASP:OD2	2.37	0.57
6:M:299:LEU:HD13	1:X:595:MET:HE3	1.86	0.57
1:X:20:ALA:HA	1:X:23:TYR:CE2	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:620:PRO:HB3	1:g:869:ILE:O	2.04	0.57
1:h:94:LEU:O	1:h:536:LEU:N	2.36	0.57
1:h:168:ASP:OD1	1:h:172:LEU:N	2.34	0.57
1:D:816:LEU:HG	1:D:817:ARG:H	1.69	0.57
1:F:242:ARG:NH2	1:g:405:ASN:OD1	2.37	0.57
1:F:563:LEU:HA	1:F:566:ASP:HB2	1.86	0.57
1:I:170:ARG:HB3	1:I:172:LEU:HD23	1.86	0.57
1:J:179:THR:O	1:J:205:ARG:NH2	2.37	0.57
1:h:58:THR:HA	1:h:585:SER:HA	1.85	0.57
1:h:359:ASP:O	1:h:827:ARG:NH2	2.36	0.57
1:h:681:VAL:HG13	1:h:703:PHE:HB2	1.87	0.57
1:i:497:PHE:HB2	1:i:664:THR:HG21	1.86	0.57
1:A:881:VAL:HB	1:A:903:PRO:HD2	1.86	0.57
1:D:487:SER:OG	1:D:492:ASP:OD1	2.20	0.57
1:D:786:ALA:HB1	1:g:419:LEU:HD13	1.86	0.57
1:F:88:VAL:HB	1:F:538:PRO:HA	1.87	0.57
1:H:640:LEU:HD22	1:H:864:PHE:HE2	1.68	0.57
1:I:164:GLN:HE22	1:I:173:PRO:HA	1.69	0.57
1:I:218:SER:HB3	1:J:802:PRO:HA	1.87	0.57
1:Y:109:ARG:NH2	1:Y:513:GLY:O	2.37	0.57
1:Y:332:ASN:HB2	1:Y:613:ASN:HD22	1.69	0.57
1:Y:602:ASP:HB2	1:Y:886:ARG:HH21	1.69	0.57
1:A:153:VAL:HA	1:A:202:ALA:HA	1.87	0.57
1:G:640:LEU:HD23	1:G:640:LEU:H	1.69	0.57
1:H:139:ASN:HD22	1:H:142:HIS:HE1	1.53	0.57
1:H:178:THR:O	1:H:205:ARG:NH2	2.38	0.57
1:X:297:ARG:NH1	1:X:663:GLY:O	2.27	0.57
1:i:207:LEU:HD21	1:i:260:VAL:HG21	1.87	0.57
1:D:256:GLU:OE2	1:g:801:TYR:OH	2.22	0.57
1:I:447:LEU:HD12	1:I:475:LEU:HD11	1.86	0.57
1:X:562:ASP:HB3	1:X:565:VAL:HG12	1.86	0.57
1:Y:629:SER:OG	1:Y:630:ARG:N	2.37	0.57
1:i:314:VAL:HG12	1:i:544:GLU:HG2	1.86	0.57
9:j:68:ASN:OD1	9:j:467:LYS:NZ	2.37	0.57
1:F:109:ARG:NH2	1:F:294:ILE:O	2.26	0.57
1:F:176:ALA:HB1	1:F:182:PRO:HD3	1.86	0.57
7:R:14:GLN:HB2	7:R:21:ALA:HB2	1.86	0.57
1:X:801:TYR:O	1:X:803:GLN:NE2	2.38	0.57
1:g:95:ASP:HA	1:g:535:LEU:HA	1.87	0.57
9:j:209:ASP:HB3	9:j:212:THR:HG22	1.85	0.57
1:F:620:PRO:HB3	1:F:869:ILE:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:679:ARG:NH1	1:Y:867:ASP:OD1	2.38	0.56
1:D:706:LYS:NZ	1:D:867:ASP:OD2	2.33	0.56
1:D:813:ARG:HH22	1:F:261:LEU:HB2	1.70	0.56
1:F:122:ASN:ND2	1:F:215:CYS:SG	2.78	0.56
1:F:380:TYR:HE1	1:F:423:GLU:HG2	1.70	0.56
1:F:831:ARG:NH2	1:F:880:GLU:OE1	2.38	0.56
1:G:222:PRO:HG3	1:i:804:LEU:HB2	1.85	0.56
1:I:682:ALA:HB3	1:I:863:THR:HB	1.85	0.56
1:X:626:PRO:HB2	1:X:627:ILE:HG12	1.87	0.56
1:i:265:THR:C	1:i:289:ASN:HD21	2.13	0.56
1:A:810:TRP:HE1	1:X:114:LYS:HB2	1.71	0.56
1:D:492:ASP:OD2	1:D:822:LYS:NZ	2.31	0.56
4:E:14:PRO:HA	6:M:240:ILE:HG22	1.85	0.56
1:F:93:VAL:HG12	1:F:538:PRO:HD3	1.87	0.56
1:F:869:ILE:HD11	1:F:873:THR:HB	1.88	0.56
1:G:321:GLN:HE21	1:g:631:ASN:HB3	1.69	0.56
1:H:595:MET:O	1:H:601:ASN:ND2	2.36	0.56
5:K:42:SER:O	5:K:43:GLN:NE2	2.38	0.56
2:S:13:GLN:HG3	2:S:13:GLN:O	2.06	0.56
1:X:42:GLY:HA2	2:b:25:ILE:HG13	1.88	0.56
1:g:139:ASN:HD22	1:g:142:HIS:HE1	1.54	0.56
1:g:902:THR:HB	1:g:903:PRO:HD3	1.86	0.56
1:i:105:GLY:HA2	1:i:573:THR:HG23	1.87	0.56
1:G:133:THR:HG22	1:G:207:LEU:HB2	1.86	0.56
1:G:783:THR:HA	1:G:803:GLN:HG3	1.88	0.56
1:G:810:TRP:NE1	1:h:264:ASP:OD1	2.39	0.56
8:P:97:LEU:HD21	8:Q:98:LEU:HD12	1.88	0.56
1:Y:784:THR:OG1	1:Y:788:TRP:NE1	2.38	0.56
1:A:804:LEU:HD11	1:X:227:GLY:HA2	1.87	0.56
1:G:716:VAL:HB	1:G:723:LYS:HA	1.88	0.56
1:J:556:GLN:HG3	1:J:663:GLY:HA2	1.87	0.56
1:Y:332:ASN:ND2	1:Y:667:TYR:O	2.38	0.56
1:g:631:ASN:O	1:g:632:TRP:HB2	2.05	0.56
1:A:185:GLN:HB3	1:Y:790:ARG:NH1	2.20	0.56
1:D:38:TYR:HB2	1:F:839:MET:HE3	1.87	0.56
1:I:562:ASP:OD2	8:Q:29:SER:OG	2.22	0.56
1:J:615:LEU:HB3	1:J:874:LEU:HD12	1.88	0.56
1:Y:48:PRO:HG2	2:d:14:GLY:HA2	1.87	0.56
1:h:694:ASN:HB3	1:i:61:SER:HA	1.87	0.56
1:i:289:ASN:HB3	1:i:467:ASN:ND2	2.19	0.56
1:D:784:THR:HG22	1:F:122:ASN:HA	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:261:LEU:HD23	1:F:261:LEU:H	1.70	0.56
1:G:94:LEU:O	1:G:536:LEU:N	2.36	0.56
1:J:903:PRO:O	7:N:28:SER:OG	2.22	0.56
1:X:761:MET:HE2	1:X:824:LEU:HB2	1.86	0.56
1:A:132:ASN:ND2	1:Y:800:PRO:O	2.39	0.56
1:A:675:SER:O	1:A:830:TRP:NE1	2.34	0.56
1:A:845:THR:HG23	1:A:848:GLY:H	1.70	0.56
1:D:234:THR:HG21	1:D:257:GLU:HB3	1.88	0.56
1:G:112:SER:O	1:G:292:ASN:ND2	2.38	0.56
1:G:436:TYR:OH	1:G:793:ARG:HD3	2.06	0.56
1:I:667:TYR:CE1	1:I:876:TYR:CE1	2.94	0.56
1:i:114:LYS:NZ	1:i:116:TYR:O	2.35	0.56
1:i:131:ASN:HB3	1:i:215:CYS:HA	1.87	0.56
1:D:462:THR:HG22	1:D:464:GLU:H	1.69	0.56
1:D:724:ASP:OD1	1:D:725:TRP:N	2.39	0.56
1:F:790:ARG:HH11	1:g:185:GLN:HB3	1.70	0.56
1:G:643:LEU:HD22	1:G:666:PRO:HB2	1.88	0.56
1:Y:76:THR:HG23	1:Y:78:TYR:H	1.71	0.56
1:g:370:ASN:ND2	1:g:480:VAL:O	2.38	0.56
1:h:218:SER:H	1:h:262:THR:HG22	1.71	0.56
1:h:746:ASP:OD1	1:h:747:TYR:N	2.39	0.56
9:j:178:VAL:HG11	9:j:409:ARG:HD3	1.87	0.56
1:H:782:ARG:O	1:H:803:GLN:OE1	2.23	0.56
1:H:902:THR:HB	1:H:903:PRO:HD3	1.88	0.56
1:I:50:VAL:HG22	1:J:844:LEU:HD12	1.88	0.56
1:J:608:TYR:O	1:J:610:SER:N	2.38	0.56
8:Q:30:ASN:OD1	8:Q:31:MET:N	2.37	0.56
1:i:706:LYS:NZ	1:i:867:ASP:OD2	2.35	0.56
1:A:67:ARG:NH2	1:A:576:ASN:OD1	2.39	0.55
1:D:735:ASN:HB3	1:D:839:MET:HE3	1.88	0.55
1:H:623:THR:CB	1:H:864:PHE:O	2.54	0.55
1:H:724:ASP:OD1	1:H:725:TRP:N	2.38	0.55
1:J:242:ARG:HG2	1:J:244:GLY:H	1.71	0.55
7:R:79:ILE:HG21	7:R:168:ARG:HH21	1.71	0.55
1:X:691:TRP:HH2	1:X:847:LEU:HD22	1.71	0.55
1:h:743:LEU:HD12	1:h:744:PRO:HD2	1.86	0.55
1:F:462:THR:HG22	1:F:464:GLU:H	1.72	0.55
1:G:83:ARG:HG3	1:G:544:GLU:HB3	1.88	0.55
1:G:396:VAL:HG21	1:i:249:PRO:HG3	1.89	0.55
1:H:70:PRO:HG2	1:H:73:ARG:HH21	1.71	0.55
1:H:803:GLN:HG2	1:J:121:TYR:CD1	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:122:ASN:ND2	1:Y:218:SER:OG	2.39	0.55
1:g:680:LYS:HG2	1:g:865:GLU:HB3	1.87	0.55
1:h:593:GLU:O	1:h:597:ARG:HG2	2.06	0.55
1:i:297:ARG:NH2	1:i:555:LEU:O	2.39	0.55
1:A:288:PRO:HG2	1:Y:376:GLU:HA	1.88	0.55
1:D:382:PHE:O	1:F:423:GLU:N	2.39	0.55
1:H:256:GLU:OE2	1:I:801:TYR:OH	2.24	0.55
1:H:826:ASP:O	1:H:827:ARG:HB2	2.05	0.55
1:J:297:ARG:HH12	1:J:665:ILE:HD12	1.72	0.55
7:R:26:ASP:OD2	7:R:29:THR:OG1	2.25	0.55
1:Y:240:TYR:HD1	1:Y:252:VAL:HG22	1.70	0.55
1:Y:623:THR:HB	1:Y:864:PHE:O	2.07	0.55
1:Y:736:ILE:HG13	1:Y:736:ILE:O	2.07	0.55
1:g:508:ARG:NH1	1:g:556:GLN:OE1	2.35	0.55
1:h:821:ARG:NH2	1:i:519:ASP:O	2.39	0.55
1:i:168:ASP:OD1	1:i:169:GLU:N	2.37	0.55
1:F:479:TYR:HB2	1:F:806:LEU:HD22	1.88	0.55
1:i:250:GLU:HG3	1:i:251:THR:HG23	1.88	0.55
1:A:902:THR:OG1	1:A:903:PRO:HD3	2.06	0.55
1:H:875:LEU:CD2	1:H:876:TYR:H	2.19	0.55
1:J:162:ASP:HB2	1:J:175:TYR:HD2	1.70	0.55
1:X:307:ASN:ND2	1:X:331:ARG:O	2.38	0.55
1:X:366:ARG:HD3	1:X:496:PRO:HB3	1.88	0.55
1:X:643:LEU:HD22	1:X:666:PRO:HB2	1.87	0.55
1:Y:330:ASP:HB2	1:Y:901:ARG:HH12	1.72	0.55
1:Y:609:LEU:HD12	1:Y:611:ALA:HB3	1.88	0.55
1:h:528:PHE:HD2	1:h:531:ILE:HG12	1.71	0.55
1:h:706:LYS:HE3	1:h:720:ASN:HD22	1.71	0.55
1:i:675:SER:OG	1:i:825:CYS:SG	2.63	0.55
1:F:298:ASP:OD1	1:F:347:ARG:NH2	2.40	0.55
1:H:643:LEU:HD22	1:H:666:PRO:HB2	1.87	0.55
1:A:448:LYS:O	1:A:469:ARG:NH2	2.40	0.55
1:A:686:ASP:O	1:F:630:ARG:NH1	2.40	0.55
1:I:795:PRO:O	1:I:796:ARG:HG3	2.07	0.55
1:J:641:THR:HG21	1:J:672:PHE:HB3	1.89	0.55
1:X:672:PHE:O	1:X:827:ARG:N	2.31	0.55
1:Y:831:ARG:NH1	1:Y:880:GLU:OE1	2.40	0.55
1:h:706:LYS:NZ	1:h:867:ASP:OD2	2.35	0.55
1:i:156:ILE:HD13	1:i:252:VAL:HG23	1.89	0.55
1:D:477:ASP:OD1	1:D:478:THR:N	2.33	0.55
1:D:710:ASP:OD2	1:D:715:ASN:ND2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:890:PRO:HD2	1:D:894:VAL:HG23	1.89	0.55
1:F:538:PRO:HD2	1:F:593:GLU:HG3	1.89	0.55
1:I:396:VAL:HG11	1:I:403:TRP:HB3	1.89	0.55
1:X:377:MET:HA	1:Y:793:ARG:HG2	1.89	0.55
1:Y:335:LEU:HG	1:Y:609:LEU:HD22	1.88	0.55
1:g:134:GLN:HG2	1:g:146:THR:HG22	1.88	0.55
1:h:619:PRO:O	1:h:621:ASN:N	2.39	0.55
1:A:176:ALA:HB1	1:A:182:PRO:HD3	1.88	0.55
1:A:641:THR:HG21	1:A:672:PHE:HB3	1.89	0.55
1:A:793:ARG:HD3	1:A:794:ALA:N	2.21	0.55
1:A:795:PRO:HG2	1:A:797:GLU:HG3	1.89	0.55
1:H:182:PRO:HG2	1:H:205:ARG:HE	1.72	0.55
1:J:616:TYR:HB3	1:J:624:GLN:NE2	2.22	0.55
1:J:882:PHE:O	1:J:901:ARG:HA	2.06	0.55
1:X:183:GLU:HB3	1:X:185:GLN:OE1	2.07	0.55
1:X:734:TYR:HE2	1:X:755:LEU:HB2	1.72	0.55
1:Y:315:LEU:HD12	1:Y:543:TYR:CD1	2.42	0.55
1:h:351:PHE:CE2	1:h:353:MET:HB2	2.42	0.55
1:h:451:PRO:HG2	1:h:454:ILE:HG21	1.89	0.55
1:i:98:SER:O	1:i:99:THR:OG1	2.22	0.55
1:i:735:ASN:HD21	1:i:840:SER:HB2	1.71	0.55
1:A:602:ASP:HB2	1:A:886:ARG:HE	1.72	0.55
1:D:836:SER:HB2	1:F:57:THR:HG21	1.89	0.55
1:I:619:PRO:HB2	8:Q:8:TYR:HE2	1.72	0.55
1:X:289:ASN:OD1	1:X:467:ASN:ND2	2.37	0.55
1:Y:709:VAL:HG23	1:Y:710:ASP:H	1.72	0.55
1:A:643:LEU:HD22	1:A:666:PRO:HB2	1.89	0.54
1:A:764:GLN:HB3	1:A:817:ARG:CD	2.37	0.54
1:D:183:GLU:HG2	1:D:185:GLN:OE1	2.07	0.54
1:D:400:GLN:HG2	1:D:401:GLN:H	1.72	0.54
1:F:381:CYS:CB	1:g:424:ILE:HG12	2.36	0.54
1:F:810:TRP:O	1:F:811:ASP:HB2	2.06	0.54
1:Y:152:TYR:HD1	1:Y:187:GLY:HA2	1.71	0.54
1:h:610:SER:OG	1:h:881:VAL:O	2.21	0.54
1:h:630:ARG:HG3	1:h:631:ASN:H	1.71	0.54
1:i:176:ALA:HB1	1:i:181:GLN:HB3	1.89	0.54
1:D:869:ILE:HD11	1:D:873:THR:HG21	1.88	0.54
1:G:26:PRO:O	1:G:30:GLN:HG3	2.08	0.54
1:G:377:MET:HE3	1:h:433:SER:HA	1.87	0.54
1:J:487:SER:OG	1:J:492:ASP:OD1	2.22	0.54
1:h:153:VAL:HG11	1:h:199:ILE:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:782:ARG:HG2	1:A:804:LEU:HD23	1.89	0.54
1:G:476:ILE:HD12	1:G:480:VAL:HG21	1.89	0.54
1:H:12:TYR:O	1:I:886:ARG:NH1	2.37	0.54
5:K:108:ARG:NH2	5:K:110:ASP:OD2	2.40	0.54
8:P:16:LEU:HD12	8:P:17:PRO:HD2	1.89	0.54
1:X:323:ASN:ND2	1:X:325:VAL:O	2.40	0.54
1:Y:811:ASP:O	1:Y:814:HIS:ND1	2.40	0.54
1:i:902:THR:OG1	1:i:903:PRO:HD3	2.07	0.54
1:D:283:SER:HB3	1:F:192:THR:HG23	1.89	0.54
1:D:328:LEU:HD13	1:D:906:ALA:HB2	1.88	0.54
1:I:510:GLN:HG2	1:J:484:THR:HA	1.89	0.54
1:g:242:ARG:NH1	1:g:247:GLY:O	2.36	0.54
1:h:253:PHE:HE2	1:i:414:ILE:HG12	1.72	0.54
1:A:844:LEU:HD22	1:X:16:ALA:HB2	1.88	0.54
1:D:382:PHE:N	1:F:423:GLU:O	2.38	0.54
1:F:696:ARG:NH1	1:g:62:GLN:O	2.38	0.54
1:G:515:GLY:HA2	1:i:809:HIS:HB3	1.89	0.54
1:J:248:ASN:OD1	1:J:249:PRO:HD2	2.08	0.54
6:M:173:ASN:ND2	6:M:175:THR:O	2.40	0.54
1:X:360:SER:N	1:X:502:ASN:OD1	2.33	0.54
1:X:801:TYR:OH	1:Y:256:GLU:OE2	2.23	0.54
1:Y:680:LYS:HD3	1:Y:702:GLU:HG2	1.90	0.54
1:g:627:ILE:CG2	1:g:860:LEU:HB2	2.37	0.54
1:h:183:GLU:OE1	1:h:185:GLN:NE2	2.40	0.54
1:h:817:ARG:HE	1:h:818:ASP:H	1.55	0.54
4:E:15:VAL:HG11	6:M:241:GLN:HG3	1.89	0.54
1:F:640:LEU:HD23	1:F:640:LEU:H	1.73	0.54
1:F:817:ARG:NH2	1:g:517:PHE:CD2	2.75	0.54
1:H:510:GLN:HG2	1:I:484:THR:HA	1.89	0.54
1:H:548:ARG:HG2	1:H:550:ASP:H	1.71	0.54
1:J:279:VAL:HG13	1:J:280:GLU:OE1	2.07	0.54
8:P:54:THR:OG1	8:P:56:ASP:OD1	2.25	0.54
7:R:3:LYS:HG2	7:R:189:PRO:HD2	1.90	0.54
1:g:341:LEU:HB3	1:g:347:ARG:HD2	1.90	0.54
1:g:691:TRP:O	1:g:693:GLY:N	2.41	0.54
1:i:343:ASN:HA	1:i:750:ARG:HD3	1.90	0.54
9:j:359:PRO:HG2	9:j:362:PHE:CD2	2.43	0.54
1:A:145:GLN:HG2	1:X:411:ASN:HB3	1.90	0.54
1:A:618:ILE:HD11	1:A:875:LEU:HB2	1.89	0.54
1:D:315:LEU:HD23	1:D:531:ILE:HD12	1.90	0.54
1:F:629:SER:HB2	1:F:859:ALA:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:809:HIS:CD2	1:F:817:ARG:HD2	2.43	0.54
1:G:321:GLN:HE21	1:g:631:ASN:HD22	1.55	0.54
1:G:425:ASN:ND2	1:h:123:SER:O	2.40	0.54
1:H:448:LYS:O	1:H:469:ARG:NH2	2.34	0.54
1:H:675:SER:O	1:H:830:TRP:NE1	2.33	0.54
1:I:113:PHE:CE2	1:I:115:PRO:HG3	2.42	0.54
1:I:630:ARG:NH1	1:I:903:PRO:O	2.41	0.54
1:h:283:SER:HB3	1:i:192:THR:HG23	1.90	0.54
1:h:802:PRO:HA	1:i:218:SER:HB3	1.89	0.54
1:i:792:CYS:SG	1:i:793:ARG:N	2.81	0.54
9:j:321:TYR:HE2	9:j:335:LEU:HA	1.73	0.54
1:A:628:PRO:HG3	1:J:72:ASP:OD2	2.08	0.54
1:D:153:VAL:HG21	1:D:188:ILE:HD13	1.90	0.54
1:I:83:ARG:HG3	1:I:544:GLU:HB3	1.89	0.54
1:g:734:TYR:HB2	1:g:736:ILE:HG12	1.90	0.54
1:h:242:ARG:NH1	1:h:247:GLY:O	2.37	0.54
1:h:645:GLN:HG2	1:h:874:LEU:HD23	1.90	0.54
1:h:749:ASP:OD2	1:i:349:ARG:NH1	2.36	0.54
9:j:371:TYR:O	9:j:459:ARG:NH2	2.33	0.54
1:D:593:GLU:OE2	1:D:597:ARG:NH1	2.39	0.54
1:F:314:VAL:HB	1:F:544:GLU:HG2	1.90	0.54
1:G:212:GLN:HE22	1:G:282:LEU:HD23	1.72	0.54
8:P:90:LEU:HD13	8:Q:87:MET:HE1	1.90	0.54
7:R:200:GLN:HE22	7:R:207:VAL:HG22	1.73	0.54
1:X:629:SER:HA	1:X:859:ALA:HA	1.90	0.54
1:g:114:LYS:HE2	1:g:289:ASN:HB2	1.90	0.54
1:g:402:GLN:HE22	1:g:404:GLN:HB3	1.72	0.54
1:G:132:ASN:ND2	1:G:148:ALA:HA	2.19	0.54
1:G:419:LEU:HD13	1:h:786:ALA:HB1	1.89	0.54
1:X:734:TYR:CE2	1:X:744:PRO:HG3	2.43	0.54
1:A:706:LYS:NZ	1:A:867:ASP:OD2	2.42	0.53
1:A:809:HIS:HB3	1:X:515:GLY:HA2	1.90	0.53
1:G:315:LEU:HD23	1:G:531:ILE:HD12	1.89	0.53
1:H:528:PHE:HD2	1:H:531:ILE:HG12	1.73	0.53
1:I:366:ARG:HD3	1:I:496:PRO:HB3	1.89	0.53
1:J:297:ARG:O	1:J:355:ASN:ND2	2.39	0.53
1:J:302:GLY:O	1:J:548:ARG:NH1	2.39	0.53
1:g:679:ARG:NH1	1:g:867:ASP:OD1	2.41	0.53
1:i:721:MET:HE3	1:i:726:PHE:HD1	1.73	0.53
1:D:212:GLN:HG3	1:D:276:ARG:O	2.08	0.53
1:F:380:TYR:CE1	1:F:423:GLU:HG2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:619:PRO:O	1:G:621:ASN:N	2.35	0.53
1:G:790:ARG:HD2	1:h:185:GLN:HG3	1.89	0.53
1:J:73:ARG:NH1	1:J:80:TYR:OH	2.41	0.53
1:J:656:ASP:HB3	1:J:659:PHE:HB2	1.90	0.53
1:h:76:THR:HG23	1:h:78:TYR:H	1.72	0.53
1:h:297:ARG:NH2	1:h:552:ASN:O	2.41	0.53
1:i:266:HIS:N	1:i:289:ASN:HD21	2.07	0.53
1:D:51:ALA:HB2	1:g:842:GLY:HA3	1.91	0.53
1:D:137:GLN:NE2	1:D:145:GLN:OE1	2.32	0.53
1:D:314:VAL:HG12	1:D:323:ASN:ND2	2.24	0.53
1:D:484:THR:HG23	1:F:514:ASN:HB3	1.91	0.53
1:F:303:LEU:HD23	1:F:524:VAL:HG21	1.89	0.53
1:F:836:SER:HB2	1:g:57:THR:HG21	1.90	0.53
1:H:821:ARG:NH2	1:J:519:ASP:O	2.40	0.53
1:J:290:ARG:NH1	1:J:441:LEU:O	2.41	0.53
1:Y:82:THR:O	1:Y:544:GLU:HB2	2.08	0.53
1:A:366:ARG:NH1	1:A:826:ASP:OD1	2.42	0.53
1:A:764:GLN:HB3	1:A:817:ARG:NE	2.24	0.53
1:D:340:LEU:O	1:D:344:THR:HG23	2.07	0.53
1:G:149:GLN:O	1:i:799:HIS:ND1	2.41	0.53
1:H:93:VAL:HG22	1:H:538:PRO:HD3	1.90	0.53
1:H:783:THR:HG22	1:H:784:THR:HG23	1.90	0.53
1:I:19:ASP:OD1	2:Z:14:GLY:HA3	2.08	0.53
1:I:422:MET:HG2	1:J:383:PRO:HA	1.90	0.53
1:Y:206:VAL:HB	1:Y:255:THR:HG22	1.89	0.53
1:h:789:PHE:CD1	1:h:797:GLU:HB2	2.42	0.53
1:h:881:VAL:HB	1:h:903:PRO:HD2	1.90	0.53
1:D:134:GLN:HG2	1:D:146:THR:HG22	1.90	0.53
1:F:487:SER:H	1:F:761:MET:HE3	1.73	0.53
1:G:123:SER:O	1:i:425:ASN:ND2	2.42	0.53
1:I:526:GLN:OE1	1:I:543:TYR:OH	2.27	0.53
1:X:435:LEU:HD21	1:X:476:ILE:HG13	1.89	0.53
9:j:198:LYS:NZ	9:j:417:VAL:O	2.41	0.53
1:A:616:TYR:HB3	1:A:624:GLN:NE2	2.23	0.53
1:A:630:ARG:HG2	1:A:631:ASN:N	2.23	0.53
1:A:712:GLU:HG2	1:A:713:GLY:N	2.23	0.53
1:G:18:GLN:HG3	1:G:23:TYR:HB3	1.91	0.53
1:G:196:MET:HE2	1:i:282:LEU:HD12	1.91	0.53
1:H:19:ASP:OD1	1:H:20:ALA:N	2.42	0.53
1:H:105:GLY:HA2	1:H:573:THR:HG23	1.91	0.53
1:H:153:VAL:HA	1:H:202:ALA:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:611:ALA:HA	1:H:881:VAL:HG22	1.91	0.53
1:I:394:HIS:ND1	1:I:410:ASP:OD1	2.38	0.53
1:I:738:TYR:HD2	1:I:839:MET:HE3	1.72	0.53
7:R:7:THR:OG1	7:R:25:GLN:OE1	2.23	0.53
1:X:875:LEU:HD23	1:X:877:VAL:H	1.73	0.53
1:Y:58:THR:HG21	1:Y:62:GLN:HG2	1.91	0.53
1:Y:902:THR:OG1	1:Y:903:PRO:HD3	2.08	0.53
1:g:83:ARG:HA	1:g:544:GLU:HA	1.91	0.53
1:h:584:MET:HG3	1:h:589:ALA:HB2	1.90	0.53
1:h:809:HIS:HB3	1:i:515:GLY:HA2	1.90	0.53
1:i:303:LEU:HD23	1:i:524:VAL:HG11	1.91	0.53
1:F:218:SER:H	1:F:262:THR:HG22	1.73	0.53
1:G:706:LYS:HG3	1:G:720:ASN:HB3	1.89	0.53
1:H:240:TYR:HD1	1:H:252:VAL:HG22	1.74	0.53
1:H:814:HIS:CG	1:J:517:PHE:HE2	2.27	0.53
1:H:875:LEU:HD22	1:H:876:TYR:H	1.74	0.53
1:I:534:LEU:HD13	1:I:887:VAL:HG21	1.91	0.53
1:J:526:GLN:OE1	1:J:543:TYR:OH	2.25	0.53
1:J:665:ILE:O	1:J:669:ASP:HB3	2.09	0.53
1:X:402:GLN:NE2	1:X:404:GLN:OE1	2.42	0.53
1:X:630:ARG:NH2	1:X:904:PHE:HA	2.24	0.53
1:g:720:ASN:HB2	1:g:822:LYS:HA	1.90	0.53
1:A:215:CYS:O	1:A:218:SER:OG	2.27	0.53
1:A:800:PRO:HD2	1:X:132:ASN:HD21	1.72	0.53
1:F:484:THR:HA	1:g:510:GLN:HG2	1.91	0.53
1:G:869:ILE:HD11	1:G:873:THR:HG21	1.91	0.53
1:Y:623:THR:HG22	1:Y:865:GLU:HA	1.91	0.53
1:Y:817:ARG:HG3	1:Y:819:PRO:HD3	1.90	0.53
1:i:675:SER:O	1:i:830:TRP:NE1	2.33	0.53
1:A:297:ARG:NH2	1:A:555:LEU:O	2.41	0.53
1:F:612:ALA:HB1	1:F:614:MET:HE2	1.91	0.53
1:G:211:THR:HG1	1:G:276:ARG:HH12	1.57	0.53
1:G:803:GLN:NE2	1:h:122:ASN:OD1	2.42	0.53
1:H:394:HIS:ND1	1:H:410:ASP:OD1	2.34	0.53
1:H:551:VAL:HG11	1:H:568:ALA:HB3	1.91	0.53
1:H:782:ARG:HB2	1:J:185:GLN:NE2	2.18	0.53
1:I:122:ASN:ND2	1:I:215:CYS:O	2.29	0.53
1:I:643:LEU:HD22	1:I:666:PRO:HB2	1.91	0.53
1:J:229:ILE:HG13	1:J:229:ILE:O	2.09	0.53
1:g:783:THR:HG22	1:g:784:THR:HG23	1.91	0.53
1:i:131:ASN:ND2	1:i:218:SER:OG	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:j:325:ASP:N	9:j:325:ASP:OD1	2.42	0.53
1:F:208:ARG:NH1	1:F:255:THR:O	2.41	0.53
1:H:315:LEU:HA	1:H:542:THR:O	2.09	0.53
1:g:207:LEU:HD21	1:g:260:VAL:HG21	1.89	0.53
1:g:692:PRO:HB3	1:g:703:PHE:CE2	2.44	0.53
9:j:99:GLU:OE2	9:j:102:ASN:ND2	2.42	0.53
9:j:191:LYS:HD2	9:j:193:GLU:HG3	1.90	0.53
1:F:783:THR:HG22	1:F:784:THR:HG23	1.91	0.52
1:G:812:PRO:HD3	1:h:111:ALA:HB1	1.92	0.52
1:H:279:VAL:O	1:H:280:GLU:HG3	2.09	0.52
1:H:293:PHE:HZ	1:I:371:VAL:HG23	1.74	0.52
1:I:342:ALA:HA	1:I:347:ARG:HG3	1.91	0.52
1:J:367:VAL:HG12	1:J:761:MET:HE1	1.90	0.52
1:J:492:ASP:OD2	1:J:822:LYS:NZ	2.31	0.52
8:P:104:LEU:HD21	8:Q:104:LEU:HD22	1.91	0.52
2:Z:12:ARG:NH1	2:Z:14:GLY:O	2.38	0.52
1:h:72:ASP:OD2	1:h:83:ARG:NH2	2.39	0.52
1:h:380:TYR:CE2	1:i:796:ARG:HB3	2.44	0.52
1:h:680:LYS:HB2	1:h:704:GLU:HA	1.91	0.52
9:j:129:THR:H	9:j:134:SER:HB3	1.73	0.52
1:A:137:GLN:HG3	1:A:142:HIS:HB2	1.91	0.52
1:A:837:ASN:HD21	1:A:841:MET:HE1	1.73	0.52
1:G:551:VAL:HG13	1:G:555:LEU:HD12	1.91	0.52
8:V:34:GLY:H	8:V:55:ARG:HG3	1.74	0.52
1:X:332:ASN:HB2	1:X:613:ASN:ND2	2.24	0.52
1:Y:126:PRO:HB2	1:Y:129:ALA:HB2	1.91	0.52
1:h:83:ARG:HG3	1:h:544:GLU:HB2	1.91	0.52
9:j:129:THR:HA	9:j:161:GLU:HG2	1.90	0.52
1:A:178:THR:HB	1:A:236:VAL:HG21	1.91	0.52
1:A:718:GLN:HG3	1:X:511:LEU:HD13	1.92	0.52
1:G:629:SER:HA	1:G:859:ALA:HA	1.91	0.52
6:M:287:ASP:O	6:M:291:PRO:HD2	2.09	0.52
1:X:217:GLY:HA3	1:X:262:THR:HG22	1.92	0.52
1:X:707:ILE:HG21	1:X:710:ASP:HB3	1.91	0.52
1:Y:400:GLN:HG2	1:Y:401:GLN:N	2.23	0.52
1:A:163:LEU:HD11	1:A:203:GLY:HA3	1.90	0.52
1:A:640:LEU:HD13	1:A:864:PHE:HE2	1.73	0.52
1:A:653:SER:HB3	1:J:77:GLN:HE21	1.75	0.52
1:D:133:THR:O	1:D:147:ILE:HG22	2.09	0.52
1:G:242:ARG:NH1	1:G:247:GLY:O	2.40	0.52
1:G:703:PHE:HE1	1:G:728:VAL:HG21	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:801:TYR:O	1:G:803:GLN:NE2	2.42	0.52
1:G:887:VAL:HA	1:G:897:VAL:HG12	1.92	0.52
1:J:88:VAL:HB	1:J:538:PRO:HA	1.90	0.52
1:J:366:ARG:HD3	1:J:496:PRO:HB3	1.91	0.52
1:X:396:VAL:HG12	1:X:403:TRP:HE3	1.74	0.52
1:Y:170:ARG:HB3	1:Y:172:LEU:HD22	1.91	0.52
1:Y:365:VAL:HG21	1:Y:501:ARG:HD2	1.92	0.52
1:g:16:ALA:HA	1:g:48:PRO:HB3	1.90	0.52
1:h:302:GLY:O	1:h:548:ARG:NH1	2.42	0.52
9:j:275:LEU:HG	9:j:290:LEU:HD23	1.91	0.52
1:G:528:PHE:HD2	1:G:531:ILE:HG12	1.73	0.52
1:I:564:ARG:NH2	1:I:660:THR:H	2.08	0.52
1:h:804:LEU:HD11	1:i:227:GLY:HA2	1.90	0.52
1:F:347:ARG:NH2	1:F:356:GLN:HA	2.24	0.52
1:G:384:LEU:HD13	1:h:380:TYR:HE1	1.75	0.52
1:X:75:ASP:HB3	1:X:80:TYR:HD1	1.73	0.52
1:Y:548:ARG:HB3	1:Y:554:ILE:HD11	1.90	0.52
1:h:332:ASN:HB2	1:h:613:ASN:ND2	2.24	0.52
1:h:595:MET:O	1:h:601:ASN:ND2	2.40	0.52
1:A:627:ILE:CG2	1:A:860:LEU:HD23	2.40	0.52
1:F:216:TYR:HE2	1:F:288:PRO:HG3	1.73	0.52
1:F:347:ARG:HH21	1:F:356:GLN:HA	1.74	0.52
1:H:13:MET:HE1	1:I:898:VAL:HG13	1.92	0.52
1:H:139:ASN:HD22	1:H:142:HIS:CE1	2.26	0.52
1:X:66:LEU:HD12	1:X:581:PHE:CE1	2.45	0.52
1:X:112:SER:O	1:X:292:ASN:ND2	2.35	0.52
1:g:330:ASP:HB2	1:g:901:ARG:HH12	1.75	0.52
1:i:72:ASP:OD2	1:i:83:ARG:NH2	2.42	0.52
1:A:473:SER:HB3	1:A:792:CYS:HA	1.91	0.52
1:F:19:ASP:OD1	1:F:20:ALA:N	2.42	0.52
1:F:297:ARG:NH1	1:F:663:GLY:O	2.28	0.52
1:F:368:ILE:HD11	1:F:439:VAL:HG11	1.91	0.52
1:H:500:HIS:NE2	1:I:374:GLU:OE1	2.41	0.52
1:I:665:ILE:O	1:I:669:ASP:HB3	2.10	0.52
8:P:59:HIS:O	8:P:64:ARG:NH2	2.43	0.52
1:X:426:LEU:HD21	1:Y:426:LEU:HD22	1.90	0.52
1:h:837:ASN:HB3	1:i:583:PRO:HG2	1.92	0.52
1:A:819:PRO:HG3	1:X:519:ASP:HB2	1.90	0.52
1:D:801:TYR:O	1:D:803:GLN:NE2	2.43	0.52
1:F:18:GLN:HB3	1:F:22:GLU:HG3	1.92	0.52
1:F:248:ASN:OD1	1:F:249:PRO:HD2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:301:VAL:HG23	1:F:334:GLU:OE1	2.10	0.52
1:F:526:GLN:NE2	1:F:543:TYR:OH	2.33	0.52
1:F:665:ILE:O	1:F:669:ASP:HB2	2.10	0.52
1:I:58:THR:HA	1:I:585:SER:HA	1.92	0.52
1:J:3:THR:HB	1:J:4:PRO:HD3	1.92	0.52
1:Y:127:LYS:HD3	1:Y:793:ARG:NH2	2.25	0.52
1:i:719:SER:HB3	1:i:760:PRO:HB3	1.92	0.52
1:A:83:ARG:HG3	1:A:544:GLU:HB2	1.92	0.52
1:A:800:PRO:HG3	1:Y:419:LEU:HD11	1.92	0.52
1:F:108:ASP:HB3	1:F:568:ALA:O	2.10	0.52
1:F:595:MET:O	1:F:601:ASN:ND2	2.28	0.52
1:F:686:ASP:OD2	1:F:858:HIS:ND1	2.40	0.52
1:G:551:VAL:HG21	1:G:568:ALA:HB3	1.92	0.52
1:H:799:HIS:HB2	1:J:132:ASN:HD21	1.74	0.52
1:I:734:TYR:HB2	1:I:736:ILE:HG13	1.91	0.52
1:J:550:ASP:CG	1:J:564:ARG:HH21	2.18	0.52
1:X:292:ASN:HD21	1:X:561:ASN:HD21	1.57	0.52
1:X:294:ILE:HG12	1:X:557:SER:HB3	1.92	0.52
1:X:630:ARG:HH21	1:X:904:PHE:HA	1.75	0.52
1:g:307:ASN:ND2	1:g:327:ASP:OD2	2.42	0.52
1:i:164:GLN:HE21	1:i:173:PRO:HB3	1.75	0.52
1:i:301:VAL:HG23	1:i:334:GLU:OE2	2.10	0.52
1:D:111:ALA:HB1	1:g:812:PRO:HD3	1.92	0.51
1:D:844:LEU:HD21	1:D:849:GLN:HG3	1.92	0.51
1:g:611:ALA:CA	1:g:881:VAL:HG22	2.38	0.51
9:j:355:MET:HE3	9:j:450:GLN:HE22	1.75	0.51
1:A:405:ASN:ND2	1:Y:245:ASP:OD1	2.40	0.51
1:A:764:GLN:HG2	1:A:817:ARG:CZ	2.40	0.51
1:A:764:GLN:HG2	1:A:817:ARG:NH1	2.26	0.51
1:G:606:ASN:HB3	1:G:884:VAL:HG22	1.91	0.51
1:G:712:GLU:OE1	1:G:712:GLU:N	2.43	0.51
1:i:825:CYS:SG	1:i:828:THR:OG1	2.68	0.51
9:j:66:ILE:HA	9:j:469:LEU:HD13	1.92	0.51
9:j:216:THR:OG1	9:j:217:PRO:HD3	2.10	0.51
1:D:349:ARG:NH1	1:g:749:ASP:OD2	2.44	0.51
1:D:630:ARG:HG3	1:D:631:ASN:N	2.25	0.51
1:G:124:PHE:CZ	1:i:432:ARG:HD3	2.45	0.51
1:G:156:ILE:HD13	1:G:252:VAL:HG23	1.93	0.51
1:G:214:PRO:HG2	1:G:286:ALA:HB2	1.91	0.51
1:G:782:ARG:H	1:G:804:LEU:HD21	1.75	0.51
1:I:432:ARG:NH1	1:I:477:ASP:OD2	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:902:THR:HB	1:I:903:PRO:HD3	1.92	0.51
1:X:432:ARG:NE	1:X:477:ASP:OD1	2.33	0.51
1:X:743:LEU:HD13	1:Y:351:PHE:HB2	1.92	0.51
1:g:647:GLU:HG2	1:g:661:TYR:CZ	2.46	0.51
1:g:888:HIS:CD2	1:g:890:PRO:HG3	2.45	0.51
1:h:875:LEU:HD23	1:h:877:VAL:H	1.75	0.51
1:A:656:ASP:HB3	1:A:659:PHE:HB2	1.92	0.51
1:A:801:TYR:OH	1:X:256:GLU:OE2	2.29	0.51
1:D:98:SER:O	1:D:99:THR:OG1	2.24	0.51
4:E:71:SER:HB3	6:M:223:VAL:HG12	1.92	0.51
1:I:57:THR:HG21	1:J:836:SER:HB2	1.91	0.51
1:J:183:GLU:HG2	1:J:185:GLN:OE1	2.10	0.51
1:J:314:VAL:HG12	1:J:544:GLU:HB2	1.93	0.51
1:J:642:ARG:HH21	1:J:869:ILE:HG12	1.76	0.51
1:J:719:SER:HB3	1:J:760:PRO:HB3	1.93	0.51
1:A:799:HIS:HD2	1:X:184:PRO:HB3	1.75	0.51
1:D:373:VAL:HG11	1:D:428:ALA:HA	1.93	0.51
1:F:679:ARG:NH1	1:F:867:ASP:OD1	2.43	0.51
1:F:782:ARG:HB2	1:g:185:GLN:NE2	2.25	0.51
1:G:89:GLY:HA3	1:G:92:ARG:NE	2.20	0.51
1:G:314:VAL:HG12	1:G:323:ASN:ND2	2.26	0.51
1:G:633:ALA:O	1:G:635:PHE:N	2.44	0.51
1:H:16:ALA:HA	1:H:48:PRO:HB3	1.93	0.51
1:H:691:TRP:HH2	1:H:847:LEU:HD22	1.75	0.51
1:I:500:HIS:HA	1:I:558:THR:HG21	1.91	0.51
1:J:801:TYR:O	1:J:803:GLN:NE2	2.43	0.51
1:X:88:VAL:HB	1:X:538:PRO:HA	1.92	0.51
1:X:717:ALA:HA	1:Y:353:MET:HA	1.93	0.51
1:h:432:ARG:NH2	1:h:792:CYS:SG	2.83	0.51
1:i:117:SER:HB3	1:i:291:PRO:HG3	1.91	0.51
1:A:405:ASN:OD1	1:Y:242:ARG:NH2	2.43	0.51
1:F:109:ARG:N	1:F:516:ARG:O	2.36	0.51
1:F:625:LEU:CD2	1:F:863:THR:CG2	2.89	0.51
1:G:112:SER:OG	1:G:561:ASN:ND2	2.43	0.51
1:G:184:PRO:O	1:i:799:HIS:N	2.44	0.51
1:G:305:TYR:CE2	1:G:548:ARG:HA	2.45	0.51
1:H:515:GLY:HA3	1:I:817:ARG:HE	1.76	0.51
5:K:198:GLN:HG2	5:K:198:GLN:O	2.11	0.51
8:V:59:HIS:O	8:V:64:ARG:NH2	2.43	0.51
1:A:421:ALA:HB3	1:X:796:ARG:HE	1.75	0.51
1:A:517:PHE:HB2	1:Y:817:ARG:HD3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:113:PHE:HB2	1:G:294:ILE:HD12	1.92	0.51
1:G:321:GLN:HE21	1:g:631:ASN:CB	2.23	0.51
1:G:321:GLN:NE2	1:g:631:ASN:HB3	2.25	0.51
1:G:850:ASN:OD1	1:G:851:LEU:N	2.43	0.51
1:I:869:ILE:HD11	1:I:873:THR:HG21	1.93	0.51
1:J:116:TYR:OH	1:J:264:ASP:OD1	2.25	0.51
1:J:313:GLY:HA3	1:J:545:TRP:CE3	2.46	0.51
1:Y:608:TYR:O	1:Y:610:SER:N	2.42	0.51
1:Y:887:VAL:HG13	1:Y:897:VAL:HG22	1.91	0.51
1:g:448:LYS:O	1:g:469:ARG:NH1	2.44	0.51
9:j:348:ILE:HD11	9:j:379:LEU:HD13	1.92	0.51
1:D:352:SER:O	1:g:718:GLN:NE2	2.43	0.51
1:D:370:ASN:HB3	1:D:482:ILE:HA	1.92	0.51
1:H:385:SER:OG	1:H:386:GLY:N	2.44	0.51
1:X:674:LEU:O	1:X:677:THR:OG1	2.29	0.51
1:Y:357:ALA:HB3	1:Y:508:ARG:HE	1.75	0.51
1:A:394:HIS:ND1	1:A:410:ASP:OD1	2.42	0.51
1:A:831:ARG:NH1	1:A:880:GLU:OE2	2.43	0.51
1:H:784:THR:HG22	1:J:122:ASN:HA	1.92	0.51
1:I:368:ILE:O	1:I:368:ILE:HG13	2.11	0.51
1:J:290:ARG:HH11	1:J:441:LEU:HB3	1.75	0.51
1:X:117:SER:HB3	1:X:291:PRO:HG3	1.92	0.51
1:X:419:LEU:HD13	1:Y:786:ALA:HB1	1.92	0.51
1:h:102:ASP:N	1:h:576:ASN:O	2.43	0.51
1:h:250:GLU:HG3	1:h:251:THR:HG23	1.93	0.51
1:h:782:ARG:NE	1:h:802:PRO:O	2.29	0.51
1:i:297:ARG:NH2	1:i:552:ASN:O	2.43	0.51
1:i:370:ASN:HB3	1:i:482:ILE:HA	1.93	0.51
9:j:198:LYS:HB3	9:j:230:VAL:HB	1.93	0.51
1:A:113:PHE:CZ	1:A:115:PRO:HG3	2.45	0.51
1:A:188:ILE:HG21	1:A:193:ALA:HB3	1.93	0.51
1:G:189:GLU:HG2	1:i:269:HIS:NE2	2.26	0.51
1:G:615:LEU:HD22	1:G:874:LEU:CD1	2.41	0.51
1:H:419:LEU:HD11	1:J:800:PRO:HD3	1.92	0.51
1:g:548:ARG:HB3	1:g:554:ILE:HD11	1.93	0.51
1:D:16:ALA:HA	1:D:48:PRO:HB3	1.93	0.50
1:D:675:SER:O	1:D:830:TRP:NE1	2.30	0.50
1:G:347:ARG:HD3	1:G:358:MET:SD	2.51	0.50
1:G:484:THR:HA	1:h:510:GLN:HG2	1.92	0.50
1:G:514:ASN:O	1:i:764:GLN:HG3	2.11	0.50
1:H:360:SER:N	1:H:502:ASN:OD1	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:876:TYR:CZ	1:I:878:LEU:HD21	2.46	0.50
1:X:817:ARG:NH2	1:Y:519:ASP:OD1	2.44	0.50
1:Y:473:SER:HB3	1:Y:792:CYS:H	1.75	0.50
1:Y:786:ALA:H	1:Y:798:GLY:HA3	1.75	0.50
1:i:182:PRO:HG2	1:i:205:ARG:HH11	1.76	0.50
1:D:630:ARG:HH21	1:D:905:SER:H	1.58	0.50
1:F:642:ARG:NH1	1:F:867:ASP:O	2.42	0.50
1:G:422:MET:HB2	1:i:383:PRO:HA	1.93	0.50
1:G:426:LEU:O	1:G:427:ALA:C	2.53	0.50
1:H:20:ALA:HA	1:H:23:TYR:CE2	2.47	0.50
1:H:623:THR:HG21	1:H:865:GLU:OE1	2.09	0.50
1:I:355:ASN:HB3	1:I:508:ARG:HD3	1.93	0.50
1:X:250:GLU:OE1	1:Y:416:LYS:NZ	2.37	0.50
1:i:584:MET:HG3	1:i:589:ALA:HB2	1.92	0.50
1:A:154:ALA:HB1	1:A:164:GLN:H	1.76	0.50
1:A:419:LEU:HD13	1:X:786:ALA:HB1	1.93	0.50
1:A:584:MET:HG3	1:A:589:ALA:HB2	1.94	0.50
1:F:680:LYS:HD3	1:F:702:GLU:OE1	2.11	0.50
1:G:18:GLN:HB2	1:G:22:GLU:HG3	1.93	0.50
1:H:181:GLN:O	1:H:183:GLU:N	2.45	0.50
1:J:133:THR:HG23	1:J:210:PRO:HG3	1.93	0.50
1:X:738:TYR:HD2	1:X:839:MET:HE3	1.76	0.50
1:X:902:THR:OG1	1:X:903:PRO:HD3	2.11	0.50
1:Y:451:PRO:HG2	1:Y:454:ILE:HG21	1.93	0.50
1:h:675:SER:O	1:h:830:TRP:NE1	2.28	0.50
1:A:623:THR:HG22	1:A:865:GLU:HA	1.94	0.50
1:A:887:VAL:HG13	1:A:897:VAL:HG22	1.94	0.50
1:F:636:ARG:HH12	2:T:31:HIS:HA	1.76	0.50
1:H:354:TRP:CD1	1:H:525:PRO:HD3	2.46	0.50
1:I:511:LEU:HB3	1:J:718:GLN:OE1	2.12	0.50
1:X:358:MET:SD	1:X:751:THR:HG21	2.52	0.50
1:Y:366:ARG:HD3	1:Y:496:PRO:HB3	1.94	0.50
1:h:163:LEU:HD11	1:h:203:GLY:HA3	1.93	0.50
1:h:352:SER:HB2	1:h:511:LEU:HD21	1.93	0.50
1:h:787:TYR:HE2	1:i:126:PRO:HD3	1.77	0.50
1:i:561:ASN:ND2	1:i:566:ASP:OD2	2.44	0.50
1:D:46:ARG:HD2	1:g:606:ASN:HB3	1.93	0.50
1:D:686:ASP:OD2	1:D:858:HIS:ND1	2.37	0.50
1:F:72:ASP:OD2	1:F:83:ARG:NH2	2.44	0.50
1:G:352:SER:HB2	1:G:511:LEU:HD21	1.93	0.50
1:G:435:LEU:HD21	1:G:476:ILE:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:593:GLU:O	1:G:597:ARG:HG2	2.12	0.50
1:G:679:ARG:HH21	1:G:868:PRO:HD3	1.76	0.50
1:H:149:GLN:HG3	1:J:415:GLY:O	2.10	0.50
1:H:512:LEU:O	1:I:764:GLN:NE2	2.45	0.50
1:H:706:LYS:NZ	1:H:867:ASP:OD2	2.44	0.50
1:I:347:ARG:HB3	1:I:358:MET:SD	2.51	0.50
1:J:888:HIS:HB3	7:N:40:MET:SD	2.51	0.50
5:K:220:VAL:HG11	5:K:256:LEU:HB2	1.94	0.50
1:g:164:GLN:NE2	1:g:166:GLY:O	2.44	0.50
1:h:482:ILE:O	1:i:514:ASN:ND2	2.42	0.50
9:j:63:ILE:HG21	9:j:355:MET:HE1	1.93	0.50
1:D:117:SER:HA	1:D:291:PRO:HG3	1.93	0.50
1:D:734:TYR:HB2	1:D:736:ILE:HG12	1.92	0.50
1:F:818:ASP:N	1:F:818:ASP:OD1	2.42	0.50
1:G:633:ALA:O	1:G:634:ALA:C	2.52	0.50
1:H:665:ILE:O	1:H:669:ASP:CB	2.60	0.50
1:H:855:ASN:HB3	7:R:203:ARG:HB2	1.94	0.50
1:I:61:SER:HA	1:J:694:ASN:HB3	1.92	0.50
1:I:704:GLU:O	1:I:722:THR:OG1	2.25	0.50
1:J:432:ARG:NH1	1:J:477:ASP:OD1	2.45	0.50
1:X:887:VAL:HG13	1:X:897:VAL:HG22	1.93	0.50
1:Y:113:PHE:HB2	1:Y:294:ILE:HD12	1.93	0.50
1:Y:476:ILE:HD12	1:Y:480:VAL:HG21	1.94	0.50
1:h:10:TRP:O	1:h:15:ILE:N	2.42	0.50
9:j:261:VAL:O	9:j:261:VAL:HG12	2.12	0.50
1:A:285:HIS:CG	1:A:793:ARG:HH12	2.29	0.50
1:F:613:ASN:HB3	1:F:876:TYR:HE1	1.77	0.50
1:F:647:GLU:HG2	1:F:661:TYR:CZ	2.46	0.50
1:G:881:VAL:HA	1:G:903:PRO:HG2	1.94	0.50
1:H:347:ARG:HH21	1:H:356:GLN:HA	1.77	0.50
1:I:207:LEU:HD21	1:J:802:PRO:HG2	1.92	0.50
1:J:333:THR:HA	1:J:336:SER:HB2	1.93	0.50
1:J:764:GLN:NE2	1:J:819:PRO:HB3	2.27	0.50
1:Y:328:LEU:O	1:Y:330:ASP:N	2.44	0.50
1:Y:618:ILE:CD1	1:Y:866:MET:HE1	2.37	0.50
1:Y:796:ARG:H	1:Y:796:ARG:HD3	1.77	0.50
1:h:787:TYR:CE2	1:i:125:ALA:HA	2.47	0.50
1:A:441:LEU:HD11	1:Y:376:GLU:HG2	1.94	0.50
1:D:122:ASN:CG	1:g:803:GLN:NE2	2.69	0.50
1:D:297:ARG:HB3	1:D:301:VAL:HG12	1.94	0.50
1:F:182:PRO:HD2	1:F:205:ARG:HH21	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:121:TYR:O	1:I:783:THR:OG1	2.30	0.50
1:X:528:PHE:HD2	1:X:531:ILE:HG12	1.77	0.50
1:Y:290:ARG:HH12	1:Y:441:LEU:HB3	1.75	0.50
1:h:224:ASN:OD1	1:h:228:GLY:N	2.37	0.50
1:A:595:MET:HE3	7:N:190:TYR:HB3	1.93	0.50
1:F:19:ASP:HB2	2:T:14:GLY:HA3	1.94	0.50
1:H:370:ASN:HB2	1:H:482:ILE:HA	1.93	0.50
1:Y:212:GLN:NE2	1:Y:282:LEU:HD23	2.21	0.50
1:Y:721:MET:HE1	1:Y:754:PHE:HZ	1.77	0.50
1:g:635:PHE:HE1	1:g:879:PHE:HB3	1.77	0.50
9:j:239:PHE:HE2	9:j:245:ASN:HB3	1.76	0.50
1:A:62:GLN:O	1:Y:696:ARG:NH1	2.44	0.49
1:D:715:ASN:O	1:D:723:LYS:NZ	2.38	0.49
1:H:165:MET:HE3	1:H:181:GLN:HG3	1.94	0.49
1:H:207:LEU:HD21	1:H:260:VAL:HG21	1.94	0.49
1:J:528:PHE:HD2	1:J:531:ILE:HG12	1.76	0.49
1:Y:447:LEU:HD13	1:Y:475:LEU:HD13	1.94	0.49
1:i:62:GLN:HB2	1:i:92:ARG:HH22	1.76	0.49
1:D:250:GLU:HG3	1:D:251:THR:HG23	1.94	0.49
1:D:678:PHE:HB3	1:D:705:ILE:HD12	1.93	0.49
1:F:179:THR:O	1:F:205:ARG:NH1	2.45	0.49
1:F:643:LEU:HD22	1:F:666:PRO:HB2	1.93	0.49
1:F:887:VAL:HG22	1:F:897:VAL:HG13	1.92	0.49
1:G:721:MET:HE1	1:G:754:PHE:HZ	1.77	0.49
1:I:448:LYS:O	1:I:469:ARG:NH1	2.44	0.49
1:I:724:ASP:OD1	1:I:725:TRP:N	2.45	0.49
1:X:716:VAL:HB	1:X:723:LYS:HA	1.92	0.49
1:i:697:LEU:HD22	1:i:724:ASP:HB2	1.94	0.49
1:F:219:TYR:HD2	1:F:261:LEU:HD21	1.77	0.49
1:F:473:SER:HB2	1:F:792:CYS:H	1.78	0.49
1:J:724:ASP:OD1	1:J:725:TRP:N	2.45	0.49
8:O:63:ALA:HB3	8:O:69:GLN:HB2	1.93	0.49
7:R:31:MET:HG2	1:h:13:MET:HE3	1.94	0.49
1:X:380:TYR:CD2	1:Y:796:ARG:HB3	2.47	0.49
1:Y:610:SER:OG	2:d:30:MET:SD	2.58	0.49
1:g:297:ARG:HG2	1:g:556:GLN:HB2	1.93	0.49
1:h:305:TYR:OH	1:h:654:PRO:O	2.25	0.49
1:h:370:ASN:HB3	1:h:482:ILE:HA	1.94	0.49
1:h:394:HIS:ND1	1:h:410:ASP:OD1	2.37	0.49
1:h:719:SER:HB3	1:h:760:PRO:HB3	1.92	0.49
1:i:177:ASN:OD1	1:i:181:GLN:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:553:MET:HE1	1:i:668:LEU:HD21	1.93	0.49
1:A:369:ASP:HB3	1:A:485:ARG:HB3	1.95	0.49
1:D:551:VAL:HG13	1:D:555:LEU:HD12	1.93	0.49
1:F:819:PRO:HG3	1:g:519:ASP:H	1.76	0.49
1:G:305:TYR:HE1	1:G:654:PRO:HA	1.78	0.49
1:G:371:VAL:HG23	1:h:293:PHE:HZ	1.77	0.49
1:G:709:VAL:HG13	1:G:710:ASP:H	1.78	0.49
1:H:741:TYR:HB2	1:J:354:TRP:CH2	2.48	0.49
1:I:256:GLU:OE2	1:J:801:TYR:OH	2.25	0.49
1:I:366:ARG:NE	1:I:826:ASP:OD2	2.43	0.49
1:J:275:ASP:HA	1:J:278:LYS:HD3	1.94	0.49
1:X:790:ARG:HD3	1:Y:185:GLN:HG3	1.94	0.49
1:Y:112:SER:OG	1:Y:561:ASN:ND2	2.45	0.49
1:Y:627:ILE:CG2	1:Y:860:LEU:O	2.57	0.49
1:g:139:ASN:HD22	1:g:142:HIS:CE1	2.30	0.49
1:g:459:ASN:HB3	1:g:462:THR:OG1	2.12	0.49
1:h:133:THR:HG22	1:h:207:LEU:HD12	1.94	0.49
1:A:582:PHE:CD2	1:A:584:MET:HB3	2.48	0.49
1:A:836:SER:HB2	1:X:57:THR:HG21	1.93	0.49
1:D:695:ASP:HA	1:D:700:PRO:HB3	1.94	0.49
1:F:359:ASP:OD1	1:F:508:ARG:NH2	2.42	0.49
1:H:785:PRO:HG2	1:H:801:TYR:H	1.77	0.49
8:Q:59:HIS:O	8:Q:64:ARG:NH2	2.46	0.49
1:i:563:LEU:HB3	1:i:568:ALA:HB3	1.95	0.49
1:A:735:ASN:HD22	1:A:735:ASN:N	2.11	0.49
1:F:109:ARG:NH1	1:F:513:GLY:O	2.38	0.49
1:G:185:GLN:HG3	1:i:790:ARG:HH11	1.78	0.49
1:I:113:PHE:CZ	1:I:115:PRO:HG3	2.46	0.49
1:J:869:ILE:HD11	1:J:873:THR:HG21	1.93	0.49
5:K:300:THR:HB	5:K:304:ARG:CZ	2.42	0.49
2:L:197:LEU:HD12	2:L:211:LYS:HA	1.95	0.49
1:X:724:ASP:OD1	1:X:725:TRP:N	2.45	0.49
1:h:112:SER:OG	1:h:112:SER:O	2.30	0.49
1:h:438:ASN:ND2	1:h:501:ARG:HE	2.10	0.49
1:i:303:LEU:HD13	1:i:554:ILE:HG12	1.95	0.49
1:i:508:ARG:NH1	1:i:556:GLN:OE1	2.38	0.49
1:A:122:ASN:OD1	1:Y:803:GLN:NE2	2.45	0.49
1:F:245:ASP:OD1	1:g:405:ASN:ND2	2.45	0.49
1:F:419:LEU:HD13	1:g:786:ALA:HB1	1.94	0.49
1:H:98:SER:O	1:H:99:THR:OG1	2.29	0.49
1:H:122:ASN:OD1	1:I:803:GLN:NE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:612:ALA:HB1	1:H:614:MET:HE2	1.94	0.49
1:I:83:ARG:HA	1:I:544:GLU:HB3	1.95	0.49
1:X:799:HIS:NE2	1:Y:205:ARG:O	2.44	0.49
1:X:803:GLN:HE22	1:Y:122:ASN:HD21	1.60	0.49
1:Y:117:SER:HB3	1:Y:291:PRO:HG3	1.94	0.49
1:Y:651:LEU:HD11	1:Y:668:LEU:HD23	1.95	0.49
1:i:621:ASN:HB3	1:i:868:PRO:HB3	1.95	0.49
1:A:609:LEU:HD12	2:b:32:GLY:HA2	1.94	0.49
1:A:817:ARG:NH2	1:X:517:PHE:O	2.46	0.49
1:D:902:THR:OG1	1:D:903:PRO:HD3	2.13	0.49
1:F:767:ASN:O	1:F:769:ALA:N	2.38	0.49
1:F:817:ARG:NH2	1:g:517:PHE:H	1.94	0.49
1:G:231:LYS:HE3	1:G:259:ASP:HB3	1.94	0.49
1:H:251:THR:HG21	1:J:414:ILE:HG21	1.95	0.49
1:H:617:PRO:O	1:H:624:GLN:NE2	2.46	0.49
1:I:109:ARG:NH2	1:I:518:CYS:SG	2.83	0.49
1:I:461:ASN:OD1	1:I:646:ARG:NH1	2.44	0.49
6:M:248:PRO:HB2	6:M:250:HIS:CE1	2.47	0.49
1:h:447:LEU:HD11	1:h:490:VAL:HG11	1.94	0.49
1:A:353:MET:HA	1:Y:717:ALA:HA	1.95	0.49
1:A:631:ASN:HD22	1:J:321:GLN:HB2	1.78	0.49
1:G:113:PHE:CZ	1:G:115:PRO:HB3	2.47	0.49
1:G:427:ALA:O	1:G:428:ALA:C	2.53	0.49
1:I:887:VAL:HG12	1:I:897:VAL:HG22	1.93	0.49
1:X:208:ARG:NH1	1:X:237:GLU:OE1	2.46	0.49
1:g:60:ARG:HD2	1:g:586:HIS:CD2	2.47	0.49
1:h:103:ILE:HD11	1:h:547:PHE:CD1	2.47	0.49
9:j:267:LEU:HD22	9:j:317:TRP:HA	1.94	0.49
1:A:721:MET:HE1	1:A:726:PHE:HD1	1.78	0.49
1:A:852:LEU:HD11	1:X:6:MET:HB2	1.94	0.49
1:D:58:THR:HB	1:D:585:SER:HA	1.95	0.49
1:F:22:GLU:OE2	2:T:16:ARG:NH1	2.46	0.49
1:G:720:ASN:OD1	1:G:822:LYS:HA	2.13	0.49
1:H:613:ASN:H	1:H:613:ASN:HD22	1.61	0.49
1:H:624:GLN:O	1:H:625:LEU:HD23	2.13	0.49
1:I:643:LEU:HD12	1:I:874:LEU:HD11	1.94	0.49
7:R:58:GLN:O	7:R:62:THR:HG22	2.12	0.49
1:Y:212:GLN:HE21	1:Y:281:GLY:C	2.20	0.49
1:g:87:ALA:HA	1:g:540:THR:HA	1.93	0.49
1:h:626:PRO:HB3	1:h:861:ASP:HA	1.94	0.49
1:i:261:LEU:HD12	1:i:263:PRO:HD3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:PHE:CZ	1:g:432:ARG:HD3	2.48	0.48
1:D:208:ARG:NH2	1:D:235:GLN:O	2.41	0.48
1:D:473:SER:HB3	1:D:792:CYS:H	1.78	0.48
1:F:902:THR:HB	1:F:903:PRO:HD3	1.95	0.48
1:G:62:GLN:NE2	1:G:583:PRO:HA	2.28	0.48
1:G:380:TYR:OH	1:h:795:PRO:HB3	2.12	0.48
1:G:783:THR:OG1	1:h:121:TYR:O	2.30	0.48
1:H:306:TYR:HE2	1:H:527:LYS:HD2	1.77	0.48
1:H:881:VAL:HB	1:H:903:PRO:HD2	1.95	0.48
1:J:121:TYR:CE2	1:J:263:PRO:HG2	2.48	0.48
1:J:680:LYS:NZ	1:J:865:GLU:OE1	2.38	0.48
5:K:304:ARG:HH21	5:K:316:LEU:HD11	1.78	0.48
1:Y:88:VAL:HB	1:Y:538:PRO:HA	1.94	0.48
1:Y:95:ASP:HA	1:Y:535:LEU:HA	1.94	0.48
1:Y:286:ALA:O	1:Y:793:ARG:NH2	2.39	0.48
1:Y:582:PHE:CD1	1:Y:584:MET:HB3	2.48	0.48
1:Y:785:PRO:HD2	1:Y:803:GLN:HE21	1.78	0.48
2:c:17:PRO:HB2	2:c:19:LEU:HD13	1.94	0.48
1:g:456:LEU:HD21	1:g:468:GLY:HA3	1.95	0.48
1:i:270:ALA:HA	1:i:284:GLN:HG2	1.94	0.48
1:i:392:ARG:HD2	1:i:411:ASN:HA	1.95	0.48
1:A:426:LEU:HD13	1:X:426:LEU:HD23	1.94	0.48
1:A:526:GLN:OE1	1:A:543:TYR:OH	2.31	0.48
1:D:548:ARG:O	1:D:554:ILE:HD11	2.13	0.48
1:D:647:GLU:HG2	1:D:661:TYR:CZ	2.48	0.48
1:F:651:LEU:HG	1:F:652:GLY:H	1.77	0.48
1:F:716:VAL:HG21	1:F:726:PHE:CD2	2.48	0.48
1:G:122:ASN:OD1	1:i:803:GLN:NE2	2.45	0.48
1:G:294:ILE:HG12	1:G:557:SER:HB3	1.94	0.48
1:I:271:VAL:HG21	1:I:281:GLY:HA2	1.94	0.48
1:J:789:PHE:CD2	1:J:794:ALA:HB3	2.48	0.48
1:Y:720:ASN:HB2	1:Y:822:LYS:HA	1.94	0.48
1:g:792:CYS:O	1:g:793:ARG:HB3	2.12	0.48
1:h:611:ALA:HA	1:h:881:VAL:HG22	1.95	0.48
9:j:208:TYR:OH	9:j:308:ARG:NH2	2.46	0.48
1:A:623:THR:CB	1:A:864:PHE:O	2.60	0.48
1:D:354:TRP:HZ2	1:g:741:TYR:HB2	1.78	0.48
1:D:611:ALA:HA	1:D:881:VAL:HG22	1.95	0.48
1:G:137:GLN:HE21	1:h:411:ASN:HD22	1.60	0.48
1:G:380:TYR:CE1	1:i:384:LEU:HD13	2.48	0.48
1:G:705:ILE:HG23	1:G:725:TRP:CD1	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:371:VAL:HG23	1:J:293:PHE:HZ	1.77	0.48
1:H:630:ARG:HG3	1:H:631:ASN:H	1.77	0.48
1:I:550:ASP:O	1:I:554:ILE:HG12	2.13	0.48
1:J:297:ARG:HD3	1:J:556:GLN:HB2	1.96	0.48
1:X:462:THR:O	1:X:466:MET:HG3	2.13	0.48
1:X:784:THR:HG21	1:Y:124:PHE:HB2	1.94	0.48
1:g:305:TYR:OH	1:g:654:PRO:O	2.24	0.48
1:i:879:PHE:O	1:i:881:VAL:HG13	2.13	0.48
1:A:628:PRO:HG3	1:J:72:ASP:CG	2.38	0.48
1:A:786:ALA:HB2	1:A:798:GLY:C	2.38	0.48
1:D:813:ARG:HH12	1:F:261:LEU:HB3	1.78	0.48
1:F:380:TYR:OH	1:g:795:PRO:HB3	2.13	0.48
1:G:81:LYS:HA	1:G:546:SER:HA	1.95	0.48
1:G:114:LYS:HD2	1:G:289:ASN:HB3	1.93	0.48
1:G:165:MET:HE1	1:G:182:PRO:HA	1.95	0.48
1:H:377:MET:HE1	1:J:432:ARG:HD3	1.95	0.48
1:J:704:GLU:O	1:J:725:TRP:HB2	2.13	0.48
1:X:625:LEU:HD12	1:X:625:LEU:O	2.13	0.48
1:Y:366:ARG:NH1	1:Y:496:PRO:HG3	2.29	0.48
1:g:369:ASP:HB3	1:g:485:ARG:HB3	1.95	0.48
1:A:351:PHE:HB3	1:A:356:GLN:HB2	1.95	0.48
1:F:20:ALA:HA	1:F:23:TYR:CE2	2.49	0.48
1:F:224:ASN:OD1	1:F:228:GLY:N	2.43	0.48
1:H:122:ASN:HB2	1:H:216:TYR:O	2.13	0.48
1:I:248:ASN:OD1	1:I:249:PRO:HD2	2.13	0.48
1:J:242:ARG:HH11	1:J:247:GLY:H	1.62	0.48
1:J:720:ASN:OD1	1:J:822:LYS:HA	2.13	0.48
1:X:246:ASN:OD1	1:X:247:GLY:N	2.47	0.48
1:X:330:ASP:O	1:X:901:ARG:NH1	2.44	0.48
1:Y:846:ASP:OD1	1:Y:847:LEU:N	2.44	0.48
2:Z:12:ARG:HA	2:Z:17:PRO:HA	1.96	0.48
1:g:304:MET:HE2	1:g:524:VAL:HG12	1.95	0.48
1:g:535:LEU:HB3	1:g:603:GLN:HE22	1.77	0.48
1:h:764:GLN:HG3	1:i:514:ASN:O	2.13	0.48
9:j:253:ARG:HD3	9:j:335:LEU:HB3	1.95	0.48
1:A:325:VAL:HG22	1:A:531:ILE:HD11	1.94	0.48
1:D:881:VAL:HG12	1:D:903:PRO:HB2	1.94	0.48
1:F:147:ILE:HG13	1:F:147:ILE:O	2.14	0.48
1:F:149:GLN:HG3	1:g:415:GLY:O	2.12	0.48
1:F:615:LEU:HD22	1:F:874:LEU:CD1	2.44	0.48
1:F:782:ARG:HB3	1:F:804:LEU:HG	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:810:TRP:NE1	1:g:116:TYR:OH	2.45	0.48
1:G:424:ILE:O	1:G:429:ASN:ND2	2.46	0.48
1:H:876:TYR:CE2	1:H:878:LEU:HD11	2.48	0.48
1:J:611:ALA:HA	1:J:881:VAL:HG22	1.94	0.48
7:R:90:GLU:OE2	7:R:155:GLN:NE2	2.46	0.48
1:X:108:ASP:OD2	1:X:516:ARG:NH2	2.40	0.48
1:X:784:THR:N	1:X:803:GLN:HG2	2.25	0.48
1:Y:114:LYS:NZ	1:Y:118:GLY:O	2.46	0.48
1:Y:133:THR:OG1	1:Y:210:PRO:HG3	2.14	0.48
1:Y:302:GLY:O	1:Y:548:ARG:NH1	2.46	0.48
1:g:84:PHE:HZ	1:g:575:VAL:HG12	1.79	0.48
1:i:315:LEU:HD13	1:i:531:ILE:HD12	1.94	0.48
1:i:357:ALA:HB3	1:i:508:ARG:HG3	1.94	0.48
1:A:73:ARG:HG3	1:A:82:THR:HG22	1.96	0.48
1:A:120:ALA:HB2	1:Y:482:ILE:HD13	1.94	0.48
1:A:139:ASN:HD21	1:A:142:HIS:CE1	2.31	0.48
1:A:184:PRO:HB3	1:Y:799:HIS:HB3	1.96	0.48
1:G:109:ARG:HH22	1:G:512:LEU:HG	1.77	0.48
1:G:185:GLN:HG2	1:G:186:LEU:HD12	1.95	0.48
1:G:376:GLU:O	1:h:793:ARG:NH1	2.47	0.48
1:G:583:PRO:HG2	1:i:837:ASN:HB3	1.96	0.48
1:G:680:LYS:HD3	1:G:702:GLU:OE2	2.14	0.48
1:G:900:LEU:HD22	1:h:13:MET:HG3	1.95	0.48
1:H:163:LEU:HD11	1:H:203:GLY:HA3	1.96	0.48
1:J:134:GLN:HG2	1:J:146:THR:HG22	1.95	0.48
1:X:611:ALA:HA	1:X:881:VAL:HG22	1.94	0.48
1:X:790:ARG:HH11	1:X:790:ARG:HG3	1.78	0.48
1:Y:627:ILE:HD11	1:Y:630:ARG:HH21	1.79	0.48
1:D:24:LEU:HD13	1:D:28:LEU:HD23	1.94	0.48
1:D:810:TRP:CZ2	1:F:114:LYS:HG3	2.49	0.48
1:H:381:CYS:SG	1:H:422:MET:HB2	2.54	0.48
1:H:741:TYR:HB2	1:J:354:TRP:CZ3	2.48	0.48
1:I:106:THR:HG22	1:I:519:ASP:OD1	2.13	0.48
1:J:268:VAL:HG13	1:J:285:HIS:CE1	2.49	0.48
1:J:642:ARG:NH2	1:J:869:ILE:HG12	2.28	0.48
1:J:643:LEU:HD22	1:J:666:PRO:HB2	1.96	0.48
1:J:901:ARG:O	1:J:905:SER:HB3	2.13	0.48
1:Y:137:GLN:NE2	1:Y:145:GLN:OE1	2.47	0.48
1:Y:615:LEU:HA	1:Y:875:LEU:O	2.13	0.48
1:Y:783:THR:OG1	1:Y:805:ALA:HB2	2.14	0.48
2:a:16:ARG:HH22	1:h:21:SER:HG	1.57	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:268:VAL:HG23	1:i:285:HIS:CE1	2.49	0.48
1:A:65:GLN:HE21	1:Y:727:LEU:HD22	1.78	0.48
1:A:400:GLN:OE1	1:A:404:GLN:NE2	2.47	0.48
1:A:629:SER:OG	1:A:630:ARG:N	2.45	0.48
1:H:398:ARG:HH21	1:H:401:GLN:HA	1.78	0.48
1:I:328:LEU:O	1:I:329:GLN:HG2	2.13	0.48
1:I:876:TYR:CE2	1:I:878:LEU:HD21	2.49	0.48
1:J:367:VAL:CG1	1:J:761:MET:HE1	2.44	0.48
1:h:299:CYS:HA	1:h:354:TRP:O	2.14	0.48
1:h:808:PRO:HD3	1:i:219:TYR:CZ	2.49	0.48
1:i:881:VAL:HB	1:i:903:PRO:HD2	1.95	0.48
9:j:351:SER:OG	9:j:372:PRO:O	2.21	0.48
1:A:122:ASN:HD21	1:Y:803:GLN:HE22	1.60	0.48
2:B:11:PRO:HA	1:J:52:PRO:HD3	1.95	0.48
1:D:242:ARG:NH1	1:D:247:GLY:O	2.47	0.48
1:G:20:ALA:HA	1:G:23:TYR:CE2	2.48	0.48
1:G:261:LEU:HD13	1:i:813:ARG:HD2	1.95	0.48
1:H:382:PHE:HD1	1:H:383:PRO:HD2	1.79	0.48
1:H:484:THR:HA	1:J:510:GLN:HG2	1.96	0.48
1:J:75:ASP:HB3	1:J:80:TYR:HD1	1.79	0.48
1:J:293:PHE:HB2	1:J:558:THR:HG23	1.95	0.48
1:X:866:MET:HE1	1:X:875:LEU:HD12	1.96	0.48
1:Y:212:GLN:OE1	1:Y:212:GLN:HA	2.14	0.48
1:Y:597:ARG:CZ	1:Y:892:ARG:H	2.27	0.48
1:g:83:ARG:NH1	1:g:544:GLU:OE1	2.47	0.48
1:g:451:PRO:HG2	1:g:454:ILE:HG21	1.95	0.48
1:A:716:VAL:HB	1:A:723:LYS:HA	1.95	0.47
1:D:60:ARG:HD2	1:D:586:HIS:CE1	2.49	0.47
1:D:279:VAL:O	1:D:280:GLU:HG3	2.13	0.47
1:D:398:ARG:NH1	1:D:401:GLN:O	2.47	0.47
1:H:630:ARG:CG	1:H:631:ASN:N	2.76	0.47
1:I:642:ARG:NH1	1:I:867:ASP:O	2.37	0.47
8:P:11:TYR:CD1	8:Q:11:TYR:HB3	2.49	0.47
1:Y:347:ARG:HH21	1:Y:356:GLN:HA	1.78	0.47
1:Y:394:HIS:ND1	1:Y:410:ASP:OD1	2.47	0.47
1:Y:396:VAL:HG22	1:Y:405:ASN:HA	1.96	0.47
1:i:721:MET:HE1	1:i:754:PHE:CZ	2.49	0.47
9:j:205:SER:HB2	9:j:319:LEU:HD13	1.95	0.47
1:A:710:ASP:OD1	1:A:715:ASN:HB2	2.14	0.47
1:D:165:MET:HA	1:D:165:MET:HE3	1.96	0.47
1:G:409:SER:HB2	1:i:143:PRO:HG2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:TRP:CZ2	1:I:634:ALA:HB2	2.50	0.47
1:H:185:GLN:NE2	1:I:782:ARG:HD3	2.29	0.47
1:H:717:ALA:HA	1:J:353:MET:HA	1.96	0.47
1:I:300:PHE:HE2	1:I:354:TRP:HA	1.79	0.47
1:I:517:PHE:HB2	1:J:817:ARG:HB3	1.95	0.47
1:I:602:ASP:OD1	1:I:888:HIS:ND1	2.39	0.47
1:J:279:VAL:HG22	1:J:280:GLU:H	1.78	0.47
7:N:66:ARG:NH1	7:N:180:GLU:OE2	2.47	0.47
1:F:432:ARG:HD3	1:g:124:PHE:CZ	2.49	0.47
1:G:516:ARG:HB2	1:i:810:TRP:HA	1.96	0.47
1:H:623:THR:CG2	1:H:865:GLU:OE2	2.62	0.47
1:I:424:ILE:HG12	1:J:381:CYS:HB3	1.96	0.47
1:I:619:PRO:HB2	8:Q:8:TYR:CE2	2.49	0.47
2:L:199:ALA:HB3	2:L:209:VAL:HG21	1.94	0.47
7:N:63:ALA:HA	7:N:180:GLU:HG3	1.96	0.47
7:N:165:SER:C	7:N:166:ARG:HD2	2.40	0.47
8:V:40:ASN:HA	1:h:868:PRO:HG2	1.96	0.47
1:X:526:GLN:NE2	1:X:543:TYR:OH	2.40	0.47
1:Y:550:ASP:OD2	1:Y:564:ARG:NH2	2.45	0.47
1:i:307:ASN:HA	1:i:327:ASP:HB3	1.96	0.47
1:i:615:LEU:HD23	1:i:876:TYR:HB3	1.97	0.47
1:i:630:ARG:HG3	1:i:631:ASN:H	1.79	0.47
1:A:696:ARG:NH1	1:X:62:GLN:O	2.47	0.47
1:A:796:ARG:HB3	1:Y:380:TYR:CD2	2.50	0.47
1:D:94:LEU:HD12	1:D:581:PHE:CZ	2.49	0.47
1:D:131:ASN:ND2	1:D:213:THR:O	2.48	0.47
1:D:717:ALA:HA	1:F:353:MET:HA	1.96	0.47
1:F:133:THR:OG1	1:F:210:PRO:HG3	2.14	0.47
1:F:809:HIS:HB2	1:F:810:TRP:CE3	2.48	0.47
1:G:108:ASP:O	1:G:568:ALA:HA	2.15	0.47
1:G:795:PRO:HA	1:i:380:TYR:HE2	1.79	0.47
1:H:691:TRP:CH2	1:H:847:LEU:HD22	2.49	0.47
1:H:819:PRO:HG3	1:J:519:ASP:H	1.79	0.47
1:I:88:VAL:HB	1:I:538:PRO:HA	1.96	0.47
1:J:212:GLN:NE2	1:J:282:LEU:HD23	2.27	0.47
1:J:304:MET:HB3	1:J:545:TRP:HE1	1.80	0.47
1:X:76:THR:HG22	1:X:77:GLN:OE1	2.14	0.47
1:g:396:VAL:HG22	1:g:405:ASN:HA	1.96	0.47
1:h:648:THR:HB	1:h:874:LEU:HD21	1.95	0.47
9:j:359:PRO:HG2	9:j:362:PHE:HD2	1.79	0.47
1:A:886:ARG:NH1	1:X:12:TYR:O	2.46	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:665:ILE:HD11	1:D:668:LEU:HD11	1.97	0.47
1:F:611:ALA:HA	1:F:881:VAL:HG22	1.96	0.47
1:H:290:ARG:NH1	1:H:466:MET:O	2.47	0.47
1:I:270:ALA:HA	1:I:284:GLN:HG2	1.96	0.47
5:K:248:LEU:HD23	5:K:248:LEU:H	1.80	0.47
8:P:63:ALA:HB3	8:P:69:GLN:HB2	1.96	0.47
8:Q:16:LEU:HD12	8:Q:17:PRO:HD2	1.96	0.47
7:R:186:TYR:CZ	7:R:198:PRO:HG3	2.49	0.47
1:X:777:GLY:O	1:X:781:HIS:ND1	2.47	0.47
1:X:804:LEU:HD12	1:Y:222:PRO:HB3	1.96	0.47
1:Y:181:GLN:O	1:Y:183:GLU:N	2.46	0.47
1:Y:610:SER:OG	1:Y:610:SER:O	2.33	0.47
2:a:16:ARG:NH2	1:h:21:SER:OG	2.33	0.47
1:h:79:SER:HB3	1:h:305:TYR:HE2	1.79	0.47
1:i:181:GLN:O	1:i:183:GLU:N	2.47	0.47
1:A:156:ILE:HG22	1:A:161:ASN:HB3	1.96	0.47
1:A:366:ARG:HH11	1:A:496:PRO:HG3	1.79	0.47
1:A:764:GLN:NE2	1:X:513:GLY:HA3	2.29	0.47
1:F:340:LEU:O	1:F:344:THR:HG23	2.14	0.47
1:G:145:GLN:HG2	1:h:411:ASN:HB2	1.97	0.47
1:G:628:PRO:HD3	1:g:318:GLN:O	2.14	0.47
1:I:314:VAL:O	1:I:314:VAL:HG12	2.14	0.47
1:I:648:THR:HG21	1:I:874:LEU:HD21	1.96	0.47
1:X:697:LEU:HD23	1:X:697:LEU:H	1.79	0.47
1:Y:789:PHE:HB3	1:Y:794:ALA:HB3	1.95	0.47
1:A:109:ARG:HD2	1:A:113:PHE:CD2	2.49	0.47
1:A:463:TYR:CE2	1:Y:810:TRP:HZ2	2.32	0.47
1:A:499:HIS:CD2	1:A:501:ARG:H	2.24	0.47
1:D:132:ASN:OD1	1:g:799:HIS:CE1	2.68	0.47
1:D:556:GLN:HG3	1:D:663:GLY:HA2	1.96	0.47
4:E:11:LEU:HD12	6:M:260:LEU:HD12	1.96	0.47
1:F:786:ALA:HB2	1:F:798:GLY:C	2.40	0.47
1:H:81:LYS:HA	1:H:546:SER:HA	1.97	0.47
1:H:803:GLN:HG2	1:J:121:TYR:HD1	1.80	0.47
1:I:109:ARG:HH22	1:I:512:LEU:HG	1.80	0.47
1:I:796:ARG:HH21	1:J:421:ALA:HB3	1.79	0.47
1:J:784:THR:H	1:J:803:GLN:HG2	1.79	0.47
5:K:86:ARG:O	9:j:38:ARG:NH2	2.47	0.47
1:X:584:MET:HG3	1:X:589:ALA:HB2	1.95	0.47
1:X:634:ALA:HB2	1:Y:10:TRP:HZ2	1.79	0.47
1:X:783:THR:HA	1:X:803:GLN:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:366:ARG:NH1	1:Y:826:ASP:OD2	2.48	0.47
1:h:109:ARG:NH2	1:h:513:GLY:O	2.41	0.47
1:h:377:MET:HE1	1:i:432:ARG:HE	1.79	0.47
1:h:615:LEU:HD22	1:h:874:LEU:HD13	1.97	0.47
9:j:50:ARG:NH1	9:j:108:ASP:OD1	2.41	0.47
1:A:149:GLN:O	1:Y:799:HIS:ND1	2.47	0.47
1:A:370:ASN:ND2	1:A:480:VAL:O	2.47	0.47
1:D:380:TYR:CD2	1:F:796:ARG:HD2	2.48	0.47
1:F:143:PRO:HG2	1:g:409:SER:HB2	1.96	0.47
1:G:109:ARG:HD2	1:G:113:PHE:CG	2.50	0.47
1:G:306:TYR:CE2	1:G:527:LYS:HB2	2.50	0.47
1:H:436:TYR:HE2	1:I:376:GLU:HB3	1.80	0.47
1:H:692:PRO:HB2	1:H:697:LEU:HD23	1.96	0.47
1:J:619:PRO:O	1:J:621:ASN:N	2.44	0.47
1:X:388:GLN:HB2	1:X:420:PRO:HG3	1.96	0.47
1:g:262:THR:O	1:g:262:THR:OG1	2.33	0.47
1:h:902:THR:HB	1:h:903:PRO:HD3	1.96	0.47
1:A:687:SER:OG	1:F:630:ARG:NH1	2.48	0.47
1:G:451:PRO:HG2	1:G:454:ILE:HG21	1.96	0.47
1:G:537:LEU:HB3	1:G:597:ARG:HH21	1.80	0.47
1:H:66:LEU:HD13	1:H:581:PHE:CD1	2.50	0.47
1:I:13:MET:HG3	1:J:900:LEU:HD22	1.96	0.47
1:I:62:GLN:HE21	1:I:583:PRO:HA	1.80	0.47
1:I:796:ARG:NH2	1:J:419:LEU:O	2.47	0.47
1:J:354:TRP:HD1	1:J:525:PRO:HD3	1.79	0.47
1:J:866:MET:HE1	1:J:875:LEU:HD13	1.96	0.47
8:Q:56:ASP:N	8:Q:56:ASP:OD1	2.48	0.47
1:Y:724:ASP:OD1	1:Y:725:TRP:N	2.47	0.47
1:g:609:LEU:HD11	1:g:878:LEU:HD11	1.96	0.47
1:i:132:ASN:ND2	1:i:206:VAL:HA	2.30	0.47
1:A:451:PRO:HG2	1:A:454:ILE:HD12	1.96	0.47
1:A:550:ASP:OD2	1:A:564:ARG:NH2	2.39	0.47
1:D:817:ARG:HG3	1:D:818:ASP:H	1.81	0.47
1:F:143:PRO:O	1:F:145:GLN:NE2	2.48	0.47
1:G:376:GLU:HG3	1:h:437:SER:HB2	1.96	0.47
1:H:623:THR:CG2	1:H:865:GLU:CD	2.84	0.47
1:H:627:ILE:HD11	1:H:632:TRP:CZ2	2.50	0.47
1:I:95:ASP:OD1	1:I:95:ASP:N	2.48	0.47
1:I:303:LEU:HD13	1:I:554:ILE:HD12	1.97	0.47
1:Y:367:VAL:HG21	1:Y:759:ILE:HG21	1.97	0.47
1:h:20:ALA:HA	1:h:23:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:357:ALA:HB3	1:h:508:ARG:HG3	1.97	0.47
1:h:380:TYR:OH	1:i:795:PRO:HA	2.14	0.47
1:A:697:LEU:O	1:X:63:ARG:NH1	2.48	0.46
1:G:24:LEU:HD22	1:G:28:LEU:HD23	1.96	0.46
1:H:704:GLU:O	1:H:725:TRP:HB2	2.14	0.46
8:V:67:GLU:N	8:V:67:GLU:OE2	2.48	0.46
1:X:482:ILE:HD13	1:Y:120:ALA:HB2	1.96	0.46
1:X:610:SER:HB2	1:X:883:ASP:H	1.80	0.46
1:X:738:TYR:CD2	1:X:839:MET:HE3	2.49	0.46
1:Y:294:ILE:HG12	1:Y:557:SER:HB3	1.97	0.46
1:Y:500:HIS:HA	1:Y:558:THR:HG21	1.97	0.46
1:Y:719:SER:HB3	1:Y:760:PRO:HB3	1.97	0.46
1:g:93:VAL:HG22	1:g:538:PRO:HD3	1.97	0.46
1:h:526:GLN:NE2	1:h:543:TYR:OH	2.32	0.46
1:h:764:GLN:HB3	1:h:817:ARG:CZ	2.45	0.46
9:j:200:ASP:OD2	9:j:202:ARG:NH2	2.48	0.46
9:j:352:LEU:HD23	9:j:354:ASP:H	1.80	0.46
1:A:764:GLN:CD	1:A:817:ARG:NH2	2.74	0.46
1:D:261:LEU:HD12	1:D:263:PRO:HD3	1.95	0.46
1:D:679:ARG:NH1	1:D:867:ASP:OD1	2.48	0.46
1:D:837:ASN:HD21	1:D:841:MET:HE1	1.79	0.46
1:G:422:MET:SD	1:h:422:MET:HE1	2.55	0.46
1:G:680:LYS:HB3	1:G:865:GLU:HG2	1.97	0.46
1:G:709:VAL:HG13	1:G:710:ASP:N	2.30	0.46
1:G:881:VAL:HG11	1:G:904:PHE:HB2	1.95	0.46
1:H:550:ASP:CG	1:H:564:ARG:HH21	2.22	0.46
1:I:678:PHE:HB3	1:I:705:ILE:HD12	1.96	0.46
1:J:716:VAL:HG11	1:J:726:PHE:CB	2.39	0.46
1:Y:619:PRO:O	1:Y:621:ASN:N	2.44	0.46
1:Y:785:PRO:CD	1:Y:803:GLN:HE21	2.27	0.46
1:Y:801:TYR:CG	1:Y:802:PRO:HD2	2.50	0.46
1:g:164:GLN:HE22	1:g:173:PRO:HA	1.81	0.46
1:g:463:TYR:HB2	1:g:561:ASN:HD22	1.79	0.46
9:j:221:THR:HG22	9:j:223:GLU:HG2	1.97	0.46
1:A:19:ASP:OD1	1:A:20:ALA:N	2.48	0.46
1:A:556:GLN:NE2	1:A:664:THR:HG22	2.31	0.46
1:D:139:ASN:HB3	1:D:142:HIS:CD2	2.51	0.46
1:D:290:ARG:HD2	1:D:441:LEU:HB3	1.98	0.46
1:F:788:TRP:HA	1:F:796:ARG:HA	1.98	0.46
1:F:801:TYR:OH	1:g:256:GLU:OE2	2.25	0.46
1:G:370:ASN:HB3	1:G:482:ILE:HA	1.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:314:VAL:HA	1:H:323:ASN:ND2	2.30	0.46
1:I:536:LEU:HD21	1:I:541:TYR:CD1	2.51	0.46
1:I:615:LEU:HD11	1:I:667:TYR:CE1	2.50	0.46
1:h:844:LEU:HD13	1:i:16:ALA:HB2	1.98	0.46
1:D:335:LEU:O	1:D:339:MET:HG3	2.16	0.46
1:G:479:TYR:HB2	1:G:806:LEU:HD21	1.97	0.46
1:G:595:MET:O	1:G:601:ASN:ND2	2.42	0.46
1:G:790:ARG:NH1	1:h:185:GLN:HB2	2.30	0.46
1:G:882:PHE:CD1	1:h:15:ILE:HD12	2.49	0.46
1:H:279:VAL:C	1:H:281:GLY:H	2.23	0.46
1:J:75:ASP:HB3	1:J:80:TYR:CD1	2.50	0.46
1:Y:716:VAL:HB	1:Y:723:LYS:HG2	1.98	0.46
1:h:279:VAL:O	1:h:279:VAL:HG13	2.16	0.46
1:h:281:GLY:HA2	1:h:284:GLN:HG3	1.97	0.46
1:h:537:LEU:HD12	1:h:593:GLU:HG3	1.98	0.46
1:h:803:GLN:HE22	1:i:122:ASN:ND2	2.13	0.46
1:A:43:ASN:HA	2:d:27:THR:HG21	1.98	0.46
1:A:302:GLY:O	1:A:548:ARG:NH1	2.43	0.46
1:A:644:LYS:HA	1:A:873:THR:HG22	1.97	0.46
1:A:718:GLN:HB2	1:X:511:LEU:HD22	1.97	0.46
1:F:380:TYR:CD2	1:g:796:ARG:HB3	2.50	0.46
1:F:696:ARG:HH12	1:g:62:GLN:H	1.64	0.46
1:G:211:THR:O	1:G:276:ARG:NH1	2.49	0.46
1:G:219:TYR:O	1:G:261:LEU:N	2.47	0.46
1:H:88:VAL:HB	1:H:538:PRO:HA	1.97	0.46
1:H:240:TYR:CD1	1:H:252:VAL:HG22	2.51	0.46
1:H:451:PRO:HG2	1:H:454:ILE:HG21	1.97	0.46
1:H:797:GLU:OE2	1:J:189:GLU:HA	2.16	0.46
1:I:53:THR:HG21	5:K:317:GLN:HG2	1.97	0.46
6:M:299:LEU:HD12	6:M:303:ASP:HB3	1.96	0.46
8:O:108:LEU:O	8:O:112:VAL:HG23	2.15	0.46
1:g:112:SER:O	1:g:292:ASN:ND2	2.28	0.46
1:g:135:PHE:HB2	1:g:278:LYS:O	2.16	0.46
1:h:644:LYS:HE3	1:h:674:LEU:HD11	1.97	0.46
1:i:721:MET:HE1	1:i:754:PHE:HZ	1.81	0.46
1:A:665:ILE:HD11	1:A:668:LEU:HD11	1.98	0.46
1:D:6:MET:HG2	1:D:9:GLN:HB2	1.97	0.46
1:D:278:LYS:HE2	1:D:278:LYS:HB3	1.77	0.46
1:D:330:ASP:HB2	1:D:901:ARG:HH12	1.81	0.46
1:D:414:ILE:HD13	1:g:253:PHE:HE2	1.80	0.46
1:D:684:GLN:HB3	1:D:861:ASP:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:434:PHE:HD1	1:F:435:LEU:HD12	1.80	0.46
1:F:534:LEU:HD21	1:F:887:VAL:HG21	1.97	0.46
1:F:810:TRP:O	1:F:810:TRP:CD1	2.69	0.46
1:G:626:PRO:HB2	1:G:627:ILE:HG12	1.96	0.46
1:G:811:ASP:HB2	1:G:812:PRO:HD2	1.98	0.46
1:H:513:GLY:HA3	1:I:764:GLN:HE21	1.80	0.46
1:H:626:PRO:CG	1:H:861:ASP:HA	2.46	0.46
1:I:297:ARG:NH2	1:I:663:GLY:O	2.48	0.46
1:J:616:TYR:HB3	1:J:624:GLN:HE22	1.81	0.46
6:M:295:LYS:HA	6:M:295:LYS:HD3	1.76	0.46
1:g:19:ASP:OD1	1:g:20:ALA:N	2.48	0.46
1:i:388:GLN:HB2	1:i:420:PRO:HG3	1.97	0.46
1:i:640:LEU:HD22	1:i:864:PHE:HE2	1.80	0.46
1:A:95:ASP:HB3	1:A:535:LEU:HD13	1.97	0.46
1:A:626:PRO:HD3	1:A:862:MET:O	2.15	0.46
1:D:229:ILE:HG13	1:D:229:ILE:O	2.16	0.46
1:D:351:PHE:HB3	1:D:356:GLN:HB2	1.97	0.46
1:F:782:ARG:HB2	1:g:185:GLN:HE21	1.81	0.46
1:H:261:LEU:HD23	1:H:261:LEU:H	1.80	0.46
1:H:265:THR:OG1	1:H:287:ALA:O	2.23	0.46
1:H:625:LEU:HB3	1:H:626:PRO:CD	2.44	0.46
1:I:181:GLN:O	1:I:183:GLU:N	2.49	0.46
1:I:665:ILE:O	1:I:669:ASP:CB	2.64	0.46
1:J:313:GLY:HA3	1:J:545:TRP:CZ3	2.50	0.46
7:N:64:THR:OG1	7:N:180:GLU:OE2	2.27	0.46
8:Q:35:VAL:HG13	8:Q:66:PRO:HA	1.97	0.46
1:X:382:PHE:CE2	1:Y:787:TYR:HD1	2.33	0.46
1:X:697:LEU:HB2	1:X:724:ASP:HB2	1.97	0.46
1:g:619:PRO:O	1:g:621:ASN:N	2.44	0.46
1:h:206:VAL:HB	1:h:255:THR:HG22	1.97	0.46
1:h:716:VAL:HG12	1:h:721:MET:O	2.15	0.46
1:h:734:TYR:HB2	1:h:736:ILE:HD12	1.98	0.46
1:i:305:TYR:OH	1:i:654:PRO:O	2.22	0.46
1:i:659:PHE:HZ	1:i:665:ILE:HG21	1.79	0.46
1:i:724:ASP:OD1	1:i:725:TRP:N	2.49	0.46
9:j:458:ARG:HE	9:j:460:ARG:NH1	2.14	0.46
1:A:416:LYS:NZ	1:Y:250:GLU:OE1	2.42	0.46
1:A:508:ARG:NH1	1:A:556:GLN:OE1	2.43	0.46
1:A:741:TYR:HB2	1:X:354:TRP:HZ2	1.81	0.46
1:D:716:VAL:HB	1:D:723:LYS:HA	1.97	0.46
1:F:380:TYR:HE2	1:g:795:PRO:C	2.24	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:625:LEU:HD13	1:H:628:PRO:HG3	1.97	0.46
1:H:242:ARG:NH1	1:H:247:GLY:H	2.13	0.46
1:H:486:TRP:CZ2	1:H:822:LYS:HE3	2.50	0.46
1:I:446:ASN:OD1	1:I:447:LEU:HD22	2.16	0.46
1:J:20:ALA:HA	1:J:23:TYR:CE2	2.50	0.46
1:J:354:TRP:CD1	1:J:525:PRO:HD3	2.51	0.46
7:R:172:ILE:HG23	7:R:176:GLN:OE1	2.15	0.46
1:X:76:THR:HG22	1:X:77:GLN:H	1.81	0.46
1:Y:122:ASN:HB2	1:Y:216:TYR:O	2.16	0.46
1:g:354:TRP:O	1:g:356:GLN:N	2.48	0.46
1:g:550:ASP:OD2	1:g:564:ARG:NH2	2.48	0.46
1:h:705:ILE:HG23	1:h:725:TRP:CD1	2.51	0.46
1:i:20:ALA:HA	1:i:23:TYR:CE2	2.51	0.46
1:i:593:GLU:OE2	1:i:597:ARG:NH1	2.47	0.46
1:A:783:THR:HB	1:A:805:ALA:HB2	1.98	0.46
1:D:382:PHE:HZ	1:F:796:ARG:HG3	1.81	0.46
1:G:628:PRO:HG3	1:g:319:SER:HA	1.97	0.46
1:H:70:PRO:HG2	1:H:73:ARG:NH2	2.31	0.46
1:H:208:ARG:NH2	1:H:235:GLN:O	2.36	0.46
1:H:796:ARG:HG3	1:I:382:PHE:CE1	2.51	0.46
1:J:758:PHE:CZ	1:J:760:PRO:HG3	2.51	0.46
6:M:297:LEU:O	6:M:297:LEU:HD23	2.16	0.46
1:X:96:MET:HB2	1:X:531:ILE:O	2.16	0.46
1:g:118:GLY:HA2	1:g:288:PRO:HG2	1.98	0.46
1:g:294:ILE:HD13	1:g:563:LEU:HD11	1.97	0.46
1:i:887:VAL:HG13	1:i:897:VAL:HG22	1.97	0.46
1:G:550:ASP:CG	1:G:564:ARG:HH21	2.22	0.46
1:H:109:ARG:NH2	1:H:513:GLY:O	2.44	0.46
1:H:216:TYR:HB3	1:H:286:ALA:HB3	1.97	0.46
1:I:553:MET:HE3	1:I:553:MET:HB3	1.80	0.46
1:I:584:MET:HE2	1:I:588:THR:HG23	1.98	0.46
1:I:763:ARG:HG2	1:I:764:GLN:N	2.31	0.46
8:O:24:GLN:HE21	8:O:40:ASN:ND2	2.14	0.46
8:P:25:ASP:OD1	8:P:40:ASN:ND2	2.41	0.46
1:X:271:VAL:HG11	1:X:280:GLU:HG3	1.98	0.46
1:Y:614:MET:HE1	9:j:99:GLU:OE2	2.15	0.46
1:g:373:VAL:HG11	1:g:428:ALA:HA	1.98	0.46
1:g:438:ASN:HD21	1:g:501:ARG:HH11	1.62	0.46
1:g:615:LEU:HB3	1:g:874:LEU:HD13	1.98	0.46
1:i:715:ASN:ND2	1:i:720:ASN:O	2.49	0.46
1:A:75:ASP:OD1	1:A:75:ASP:N	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:PHE:HZ	1:Y:371:VAL:HG23	1.81	0.45
1:A:615:LEU:HD22	1:A:874:LEU:CD1	2.46	0.45
1:D:8:PRO:HB2	7:R:41:ILE:HD13	1.97	0.45
1:D:185:GLN:NE2	1:g:782:ARG:HB2	2.30	0.45
1:D:248:ASN:OD1	1:D:249:PRO:HD2	2.15	0.45
1:F:107:LEU:HB3	1:F:570:VAL:HG23	1.98	0.45
1:F:328:LEU:HD23	1:F:328:LEU:H	1.81	0.45
1:F:380:TYR:CE2	1:g:796:ARG:HB3	2.51	0.45
1:G:251:THR:HG21	1:h:414:ILE:HG21	1.99	0.45
1:H:343:ASN:ND2	1:H:608:TYR:OH	2.37	0.45
1:H:429:ASN:ND2	1:I:379:ASN:HD22	2.14	0.45
1:H:482:ILE:HD13	1:J:120:ALA:HB2	1.98	0.45
1:I:128:SER:HB3	1:I:285:HIS:HB3	1.97	0.45
1:I:240:TYR:HD1	1:I:252:VAL:HG22	1.81	0.45
1:I:764:GLN:HB2	1:I:817:ARG:NH2	2.31	0.45
1:I:810:TRP:CD1	1:I:810:TRP:H	2.34	0.45
1:X:19:ASP:OD1	1:X:20:ALA:N	2.49	0.45
2:a:13:GLN:NE2	2:a:18:MET:SD	2.86	0.45
1:h:155:THR:OG1	1:h:164:GLN:OE1	2.34	0.45
1:i:301:VAL:HG22	1:i:668:LEU:HD13	1.97	0.45
1:i:456:LEU:HD22	1:i:465:TYR:HA	1.98	0.45
1:D:432:ARG:HD3	1:F:124:PHE:CZ	2.51	0.45
1:D:536:LEU:HD11	1:D:895:ILE:HD11	1.98	0.45
1:F:557:SER:OG	1:F:559:LEU:O	2.25	0.45
1:G:683:ILE:HG23	1:G:860:LEU:HD11	1.99	0.45
1:H:297:ARG:NH2	1:H:663:GLY:O	2.49	0.45
1:I:716:VAL:HG12	1:I:721:MET:O	2.17	0.45
1:Y:272:PRO:HD3	1:Y:453:ASN:HD22	1.80	0.45
1:g:785:PRO:CD	1:g:803:GLN:HE21	2.28	0.45
1:i:385:SER:OG	1:i:386:GLY:N	2.50	0.45
1:i:462:THR:O	1:i:466:MET:HG3	2.16	0.45
1:A:817:ARG:HH22	1:X:518:CYS:CA	2.30	0.45
1:F:240:TYR:HD1	1:F:252:VAL:HG22	1.81	0.45
1:I:716:VAL:HB	1:I:723:LYS:HA	1.99	0.45
1:X:783:THR:HB	1:X:805:ALA:HB2	1.97	0.45
1:Y:732:ALA:HB2	1:Y:833:PRO:HD3	1.97	0.45
1:h:88:VAL:O	1:h:88:VAL:HG12	2.17	0.45
1:h:705:ILE:HG12	1:h:725:TRP:CD2	2.51	0.45
1:i:122:ASN:HB3	1:i:125:ALA:HB3	1.98	0.45
1:i:554:ILE:HG22	1:i:555:LEU:HG	1.98	0.45
9:j:250:ILE:HD13	9:j:260:PHE:HZ	1.80	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ARG:NH2	1:X:518:CYS:HA	2.30	0.45
1:D:33:GLN:HB2	2:S:20:SER:HB3	1.99	0.45
1:D:122:ASN:CA	1:g:784:THR:HG22	2.41	0.45
1:D:550:ASP:CG	1:D:564:ARG:HH21	2.24	0.45
1:D:634:ALA:HB2	1:F:10:TRP:CZ2	2.50	0.45
1:F:781:HIS:HA	1:F:804:LEU:HD11	1.98	0.45
1:G:111:ALA:HB1	1:i:812:PRO:HD3	1.98	0.45
1:G:716:VAL:HG12	1:G:721:MET:O	2.16	0.45
1:H:128:SER:HB3	1:H:285:HIS:HB3	1.99	0.45
1:H:627:ILE:HB	1:H:628:PRO:HD2	1.98	0.45
7:R:204:HIS:ND1	7:R:204:HIS:O	2.47	0.45
1:X:482:ILE:O	1:Y:514:ASN:ND2	2.44	0.45
1:X:634:ALA:HB2	1:Y:10:TRP:CZ2	2.51	0.45
1:g:749:ASP:OD1	1:g:756:HIS:HB2	2.16	0.45
1:h:245:ASP:OD1	1:h:245:ASP:N	2.46	0.45
1:h:339:MET:HE1	1:h:609:LEU:HD13	1.98	0.45
1:i:412:ASN:HB3	1:i:414:ILE:HD12	1.98	0.45
9:j:178:VAL:O	9:j:182:LEU:HG	2.16	0.45
9:j:395:GLN:NE2	9:j:418:ARG:HE	2.14	0.45
1:A:132:ASN:OD1	1:A:148:ALA:HA	2.17	0.45
1:A:632:TRP:CH2	1:A:860:LEU:HD13	2.51	0.45
1:A:817:ARG:HH22	1:X:518:CYS:CB	2.29	0.45
1:D:721:MET:SD	1:D:725:TRP:HD1	2.40	0.45
1:D:810:TRP:CH2	1:F:114:LYS:HG3	2.51	0.45
1:D:811:ASP:OD2	1:F:263:PRO:HA	2.17	0.45
1:H:855:ASN:ND2	7:R:203:ARG:O	2.41	0.45
1:H:860:LEU:HD21	1:H:862:MET:HG3	1.99	0.45
1:I:183:GLU:HB3	1:I:185:GLN:OE1	2.16	0.45
1:I:307:ASN:ND2	1:I:327:ASP:OD2	2.49	0.45
1:I:736:ILE:O	1:I:740:GLY:O	2.34	0.45
1:J:154:ALA:HB3	1:J:163:LEU:HD22	1.98	0.45
7:N:37:GLY:O	7:N:41:ILE:HG12	2.17	0.45
2:S:11:PRO:HA	1:g:52:PRO:HD3	1.97	0.45
1:X:314:VAL:HG12	1:X:323:ASN:ND2	2.31	0.45
1:X:725:TRP:HZ2	1:X:830:TRP:HB3	1.81	0.45
1:g:380:TYR:CE1	1:g:423:GLU:HG2	2.51	0.45
1:g:584:MET:HG3	1:g:589:ALA:HB2	1.98	0.45
1:h:442:TYR:OH	1:h:500:HIS:ND1	2.37	0.45
1:h:869:ILE:HD11	1:h:873:THR:HG21	1.99	0.45
1:h:886:ARG:NH1	1:i:12:TYR:O	2.46	0.45
1:D:36:GLU:OE1	2:S:20:SER:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:TYR:CE2	1:D:263:PRO:HG2	2.51	0.45
1:G:903:PRO:O	7:R:28:SER:OG	2.28	0.45
1:H:537:LEU:HD23	1:H:889:GLN:NE2	2.31	0.45
1:H:630:ARG:CG	1:H:631:ASN:H	2.29	0.45
1:I:630:ARG:O	1:I:632:TRP:NE1	2.50	0.45
6:M:214:ASN:HB3	1:g:60:ARG:NH2	2.26	0.45
8:V:19:TRP:NE1	1:h:865:GLU:OE1	2.50	0.45
1:X:114:LYS:NZ	1:X:289:ASN:O	2.50	0.45
1:X:847:LEU:HA	1:X:850:ASN:HB2	1.98	0.45
1:Y:616:TYR:HB3	1:Y:624:GLN:NE2	2.30	0.45
1:i:70:PRO:HG2	1:i:73:ARG:HE	1.81	0.45
1:i:610:SER:HB2	1:i:883:ASP:H	1.81	0.45
1:i:784:THR:HG1	1:i:788:TRP:NE1	2.12	0.45
9:j:384:ARG:NE	9:j:429:GLU:OE2	2.45	0.45
1:A:610:SER:HB2	1:A:883:ASP:H	1.82	0.45
1:G:263:PRO:HA	1:i:811:ASP:OD2	2.16	0.45
1:G:422:MET:CB	1:i:383:PRO:HA	2.47	0.45
1:G:764:GLN:HE21	1:G:819:PRO:HG3	1.81	0.45
1:G:789:PHE:HE1	1:h:186:LEU:HD13	1.81	0.45
1:H:518:CYS:HB2	1:I:764:GLN:HE22	1.82	0.45
1:I:551:VAL:HG13	1:I:555:LEU:HD12	1.99	0.45
1:J:84:PHE:HZ	1:J:575:VAL:HG12	1.82	0.45
1:X:99:THR:HB	1:X:577:LEU:HD11	1.99	0.45
1:X:447:LEU:HD11	1:X:490:VAL:HG11	1.99	0.45
1:Y:103:ILE:HG12	1:Y:575:VAL:HG22	1.97	0.45
1:Y:557:SER:OG	1:Y:559:LEU:O	2.26	0.45
1:Y:793:ARG:O	1:Y:793:ARG:HD3	2.16	0.45
2:c:30:MET:HG3	2:c:30:MET:O	2.15	0.45
1:i:720:ASN:HB2	1:i:822:LYS:HA	1.99	0.45
1:D:642:ARG:NH1	1:D:867:ASP:O	2.42	0.45
1:D:720:ASN:HB2	1:D:822:LYS:HA	1.99	0.45
1:F:373:VAL:O	1:F:427:ALA:HB1	2.17	0.45
1:G:380:TYR:CE1	1:G:423:GLU:HG2	2.52	0.45
1:I:163:LEU:HD11	1:I:252:VAL:HB	1.98	0.45
1:I:328:LEU:HD11	1:I:901:ARG:CZ	2.46	0.45
1:J:640:LEU:HD22	1:J:864:PHE:CE2	2.48	0.45
1:X:113:PHE:CE2	1:X:115:PRO:HG3	2.52	0.45
1:X:817:ARG:HG2	1:X:819:PRO:HD3	1.97	0.45
1:Y:60:ARG:HD2	1:Y:586:HIS:CD2	2.52	0.45
1:Y:767:ASN:O	1:Y:769:ALA:N	2.45	0.45
1:i:122:ASN:HB2	1:i:216:TYR:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:i:609:LEU:HG	1:i:609:LEU:O	2.17	0.45
1:i:629:SER:HA	1:i:859:ALA:HA	1.98	0.45
1:A:111:ALA:HB2	1:A:516:ARG:HH21	1.82	0.45
1:A:116:TYR:CD1	1:Y:482:ILE:HG12	2.51	0.45
1:A:568:ALA:O	1:A:569:THR:OG1	2.28	0.45
1:D:419:LEU:O	1:F:796:ARG:NH2	2.49	0.45
1:F:384:LEU:HD11	1:g:380:TYR:CE1	2.52	0.45
1:F:562:ASP:HB3	1:F:565:VAL:HG22	1.99	0.45
1:F:619:PRO:O	1:F:621:ASN:N	2.44	0.45
1:G:422:MET:HB2	1:i:382:PHE:O	2.17	0.45
1:G:881:VAL:HB	1:G:903:PRO:HD2	1.99	0.45
1:H:84:PHE:HZ	1:H:575:VAL:HG12	1.82	0.45
1:H:231:LYS:HZ1	1:H:259:ASP:HB3	1.82	0.45
1:H:253:PHE:HE2	1:J:414:ILE:HG12	1.81	0.45
1:H:387:VAL:HG11	1:I:149:GLN:HB2	1.99	0.45
1:H:424:ILE:HG12	1:I:381:CYS:HB3	1.99	0.45
1:J:181:GLN:O	1:J:183:GLU:N	2.50	0.45
1:J:297:ARG:HB3	1:J:301:VAL:HG12	1.99	0.45
1:J:782:ARG:HG2	1:J:804:LEU:HD23	1.99	0.45
1:X:107:LEU:HD12	1:X:555:LEU:HD11	1.99	0.45
1:g:215:CYS:O	1:g:218:SER:OG	2.27	0.45
1:g:534:LEU:HA	1:g:605:PHE:CZ	2.51	0.45
1:g:665:ILE:HG13	1:g:665:ILE:O	2.17	0.45
1:h:651:LEU:HD23	1:h:651:LEU:H	1.82	0.45
1:i:17:GLY:H	1:i:48:PRO:HB3	1.80	0.45
1:i:817:ARG:HD2	1:i:819:PRO:HD3	1.99	0.45
1:F:535:LEU:HB3	1:F:603:GLN:HE22	1.81	0.45
1:F:821:ARG:NH2	1:g:519:ASP:O	2.48	0.45
1:I:561:ASN:ND2	1:I:566:ASP:OD2	2.50	0.45
1:X:373:VAL:HG11	1:X:428:ALA:HA	1.99	0.45
1:X:456:LEU:HD21	1:X:468:GLY:HA3	1.98	0.45
1:X:659:PHE:HZ	1:X:665:ILE:HG21	1.81	0.45
1:Y:114:LYS:HD2	1:Y:289:ASN:HB2	1.98	0.45
1:Y:716:VAL:HB	1:Y:723:LYS:HA	1.99	0.45
1:Y:881:VAL:HB	1:Y:903:PRO:HD2	1.98	0.45
1:g:163:LEU:HD13	1:g:254:TYR:HE1	1.82	0.45
1:g:789:PHE:CG	1:g:790:ARG:N	2.85	0.45
1:i:242:ARG:HA	1:i:250:GLU:HG2	1.99	0.45
1:A:306:TYR:HE2	1:A:527:LYS:HE3	1.82	0.44
1:D:677:THR:HB	1:D:867:ASP:HB2	1.98	0.44
1:F:153:VAL:HG21	1:F:188:ILE:HD13	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:352:SER:HB2	1:F:511:LEU:HD21	1.98	0.44
1:H:373:VAL:HG11	1:H:428:ALA:HA	1.99	0.44
1:H:517:PHE:O	1:I:817:ARG:HG2	2.16	0.44
1:H:804:LEU:HD11	1:J:227:GLY:HA2	1.98	0.44
1:I:98:SER:O	1:I:99:THR:OG1	2.27	0.44
1:I:841:MET:HE3	1:I:841:MET:HB2	1.93	0.44
1:J:96:MET:HB2	1:J:531:ILE:O	2.17	0.44
1:J:99:THR:HG22	1:J:579:ALA:HA	1.99	0.44
1:J:212:GLN:HG2	1:J:276:ARG:O	2.18	0.44
1:J:789:PHE:HA	1:J:797:GLU:OE1	2.17	0.44
1:X:901:ARG:O	1:X:905:SER:OG	2.28	0.44
1:Y:825:CYS:HG	1:Y:828:THR:HG1	1.47	0.44
1:g:343:ASN:HA	1:g:750:ARG:HD2	1.98	0.44
1:g:432:ARG:NH2	1:g:792:CYS:SG	2.90	0.44
1:g:693:GLY:HA3	1:g:696:ARG:HG3	1.99	0.44
1:h:177:ASN:HB3	1:h:181:GLN:HB2	1.98	0.44
1:h:301:VAL:HG23	1:h:334:GLU:OE1	2.18	0.44
1:i:147:ILE:O	1:i:147:ILE:HG22	2.16	0.44
1:A:293:PHE:HB2	1:A:558:THR:HG23	1.99	0.44
1:A:528:PHE:HD2	1:A:531:ILE:HG13	1.83	0.44
1:A:764:GLN:CG	1:A:817:ARG:CZ	2.95	0.44
1:F:537:LEU:HD12	1:F:593:GLU:HG3	1.98	0.44
1:G:229:ILE:HG12	1:i:782:ARG:HH22	1.82	0.44
1:G:803:GLN:OE1	1:G:803:GLN:N	2.50	0.44
1:H:126:PRO:HB2	1:H:129:ALA:HB2	1.99	0.44
1:H:264:ASP:HA	1:I:810:TRP:CH2	2.51	0.44
1:I:18:GLN:HG3	1:I:23:TYR:HB3	1.99	0.44
1:J:10:TRP:NE1	7:R:16:GLN:HB3	2.33	0.44
1:J:177:ASN:HB3	1:J:181:GLN:HB2	2.00	0.44
1:J:272:PRO:HD3	1:J:453:ASN:ND2	2.32	0.44
5:K:107:ILE:HG23	5:K:111:GLU:HG3	1.98	0.44
1:X:716:VAL:HG12	1:X:721:MET:O	2.17	0.44
1:Y:139:ASN:HD21	1:Y:142:HIS:CE1	2.35	0.44
1:Y:297:ARG:NH1	1:Y:663:GLY:O	2.43	0.44
1:i:134:GLN:HG3	1:i:146:THR:HG22	1.98	0.44
1:i:890:PRO:HG2	1:i:894:VAL:HG13	1.98	0.44
9:j:293:ASP:OD1	9:j:294:PRO:HD2	2.17	0.44
1:A:635:PHE:HE1	1:A:879:PHE:HB3	1.81	0.44
1:D:432:ARG:HB3	1:g:377:MET:HE1	1.99	0.44
1:F:99:THR:HA	1:F:578:TYR:O	2.18	0.44
1:G:177:ASN:H	1:G:181:GLN:HG3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:803:GLN:N	1:G:803:GLN:CD	2.76	0.44
1:H:116:TYR:CD1	1:I:482:ILE:HG12	2.53	0.44
1:H:492:ASP:OD2	1:H:822:LYS:NZ	2.27	0.44
1:H:695:ASP:HA	1:H:700:PRO:HB3	1.98	0.44
1:I:109:ARG:HD2	1:I:113:PHE:CD2	2.52	0.44
1:I:352:SER:OG	1:J:760:PRO:HG2	2.18	0.44
5:K:108:ARG:NH1	5:K:110:ASP:OD1	2.50	0.44
7:N:20:ALA:HB2	7:N:177:PHE:HE1	1.83	0.44
2:S:32:GLY:HA2	1:g:609:LEU:HD12	1.98	0.44
1:Y:335:LEU:HG	1:Y:609:LEU:CD2	2.47	0.44
1:Y:627:ILE:HD12	1:Y:628:PRO:HD2	2.00	0.44
1:h:12:TYR:HD2	1:h:13:MET:HE2	1.83	0.44
1:h:561:ASN:ND2	1:h:566:ASP:OD2	2.50	0.44
1:i:268:VAL:HG12	1:i:470:ILE:HD11	2.00	0.44
1:i:400:GLN:NE2	1:i:402:GLN:HE21	2.15	0.44
1:i:627:ILE:HG13	1:i:628:PRO:HD2	2.00	0.44
1:A:107:LEU:HD23	1:A:107:LEU:H	1.83	0.44
1:A:167:VAL:HG13	1:A:171:GLN:HA	1.99	0.44
1:D:269:HIS:ND1	1:D:269:HIS:O	2.50	0.44
1:D:339:MET:SD	1:D:609:LEU:HD12	2.57	0.44
1:D:817:ARG:HH11	1:D:819:PRO:HD2	1.82	0.44
1:G:109:ARG:NH2	1:G:512:LEU:HG	2.32	0.44
1:G:164:GLN:HE21	1:G:173:PRO:HB3	1.81	0.44
1:G:411:ASN:HB3	1:i:145:GLN:HG2	2.00	0.44
1:H:131:ASN:ND2	1:I:802:PRO:HG3	2.33	0.44
1:H:882:PHE:O	1:H:901:ARG:HA	2.17	0.44
1:J:716:VAL:HB	1:J:723:LYS:HG2	1.99	0.44
7:N:80:LYS:NZ	7:N:179:GLU:OE1	2.51	0.44
7:N:186:TYR:CE2	7:N:189:PRO:HA	2.52	0.44
9:j:70:SER:HB3	9:j:87:THR:HG22	1.99	0.44
1:A:20:ALA:HA	1:A:23:TYR:CE2	2.53	0.44
1:A:519:ASP:HB2	1:Y:819:PRO:HG2	2.00	0.44
1:D:887:VAL:HG22	1:D:897:VAL:HG12	1.99	0.44
1:F:682:ALA:HB2	1:F:702:GLU:HG2	1.99	0.44
1:G:706:LYS:NZ	1:G:867:ASP:OD2	2.41	0.44
1:G:715:ASN:HB2	1:h:521:HIS:CE1	2.53	0.44
1:G:789:PHE:HB2	1:G:797:GLU:HG2	1.99	0.44
1:H:382:PHE:CE2	1:J:787:TYR:HD1	2.36	0.44
1:I:359:ASP:OD1	1:I:556:GLN:NE2	2.35	0.44
1:I:785:PRO:CD	1:I:803:GLN:HE21	2.28	0.44
5:K:186:VAL:O	5:K:190:LYS:HG3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:84:PHE:HZ	1:X:575:VAL:HG12	1.82	0.44
1:g:49:THR:O	1:g:49:THR:HG22	2.16	0.44
1:g:487:SER:H	1:g:761:MET:HE3	1.81	0.44
1:g:719:SER:HB3	1:g:760:PRO:HB3	2.00	0.44
1:g:782:ARG:HB3	1:g:804:LEU:HD23	1.98	0.44
1:i:266:HIS:HB3	1:i:289:ASN:ND2	2.32	0.44
1:A:269:HIS:O	1:A:269:HIS:CG	2.71	0.44
1:D:218:SER:H	1:D:262:THR:HG22	1.82	0.44
1:D:695:ASP:O	1:F:63:ARG:HD3	2.17	0.44
1:D:804:LEU:HB2	1:F:222:PRO:HD3	1.99	0.44
1:D:882:PHE:O	1:D:901:ARG:HA	2.17	0.44
1:H:382:PHE:O	1:J:423:GLU:N	2.51	0.44
1:H:803:GLN:N	1:J:218:SER:O	2.47	0.44
1:H:813:ARG:HD2	1:J:261:LEU:HD13	1.99	0.44
1:H:814:HIS:CD2	1:J:517:PHE:HE2	2.35	0.44
1:I:234:THR:HG21	1:I:257:GLU:HB3	1.99	0.44
1:I:354:TRP:CH2	1:J:741:TYR:HB2	2.52	0.44
1:J:535:LEU:HB3	1:J:603:GLN:NE2	2.30	0.44
1:X:368:ILE:HG13	1:X:368:ILE:O	2.17	0.44
1:Y:137:GLN:HG3	1:Y:142:HIS:HB2	1.98	0.44
1:g:436:TYR:HE2	1:g:793:ARG:HH21	1.65	0.44
1:g:680:LYS:HD3	1:g:702:GLU:HG2	1.99	0.44
1:h:463:TYR:HB2	1:h:561:ASN:HD22	1.83	0.44
1:h:745:PRO:HG2	1:h:748:LYS:HB2	1.99	0.44
1:i:278:LYS:HG3	1:i:279:VAL:H	1.82	0.44
1:i:328:LEU:HD23	1:i:328:LEU:H	1.83	0.44
1:i:611:ALA:HA	1:i:881:VAL:HG22	1.99	0.44
1:A:521:HIS:CE1	1:Y:715:ASN:HB2	2.52	0.44
1:D:396:VAL:HG11	1:D:403:TRP:HB3	1.99	0.44
1:F:240:TYR:CD1	1:F:252:VAL:HG22	2.53	0.44
1:F:242:ARG:HA	1:F:250:GLU:HG2	1.98	0.44
1:F:776:LEU:HD21	1:g:227:GLY:HA2	2.00	0.44
1:G:181:GLN:O	1:G:183:GLU:N	2.50	0.44
1:G:804:LEU:HD23	1:G:804:LEU:H	1.83	0.44
1:H:176:ALA:HB1	1:H:181:GLN:HB3	2.00	0.44
1:H:422:MET:HG2	1:I:383:PRO:HA	1.99	0.44
1:H:534:LEU:HA	1:H:605:PHE:CZ	2.53	0.44
1:H:549:LYS:HA	1:H:554:ILE:HD11	1.99	0.44
1:H:721:MET:HE1	1:H:754:PHE:CZ	2.43	0.44
1:I:622:ALA:HB2	8:Q:8:TYR:HD2	1.82	0.44
1:J:768:PRO:HA	1:J:773:TYR:CD2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:636:ARG:NH1	3:f:21:TYR:O	2.49	0.44
1:X:636:ARG:NH2	1:X:880:GLU:HB3	2.33	0.44
1:X:881:VAL:HB	1:X:903:PRO:HD2	2.00	0.44
1:Y:113:PHE:HD1	1:Y:294:ILE:H	1.65	0.44
1:Y:290:ARG:HH21	1:Y:559:LEU:HD22	1.81	0.44
1:Y:686:ASP:N	1:Y:859:ALA:O	2.47	0.44
1:h:287:ALA:HB2	1:h:793:ARG:HD3	2.00	0.44
1:h:396:VAL:CG1	1:h:403:TRP:HB3	2.48	0.44
1:i:314:VAL:HG23	1:i:323:ASN:HA	2.00	0.44
9:j:292:GLU:OE1	9:j:297:ARG:N	2.50	0.44
1:A:553:MET:HE3	1:A:553:MET:HB3	1.80	0.44
1:D:368:ILE:HD11	1:D:439:VAL:HG11	1.99	0.44
1:D:400:GLN:HG2	1:D:401:GLN:N	2.33	0.44
1:D:419:LEU:HD13	1:F:786:ALA:HB1	2.00	0.44
1:G:131:ASN:HD22	1:i:802:PRO:HG3	1.82	0.44
1:G:296:PHE:O	1:G:508:ARG:NH1	2.49	0.44
1:G:597:ARG:NH1	1:G:892:ARG:H	2.15	0.44
1:H:222:PRO:HD3	1:I:804:LEU:HB2	1.99	0.44
1:H:278:LYS:HG3	1:H:279:VAL:H	1.81	0.44
1:H:306:TYR:CE2	1:H:527:LYS:HB2	2.52	0.44
1:J:647:GLU:HG2	1:J:661:TYR:CZ	2.53	0.44
1:Y:636:ARG:HD3	2:d:30:MET:HE1	2.00	0.44
1:g:616:TYR:HA	1:g:617:PRO:HD3	1.88	0.44
1:g:703:PHE:HE1	1:g:728:VAL:HG21	1.83	0.44
1:h:721:MET:HE1	1:h:754:PHE:HZ	1.82	0.44
1:h:784:THR:HG22	1:i:122:ASN:HA	2.00	0.44
1:G:615:LEU:HB3	1:G:874:LEU:HD13	1.99	0.44
1:G:696:ARG:NH1	1:h:62:GLN:O	2.42	0.44
1:I:156:ILE:HD13	1:I:252:VAL:HG23	2.00	0.44
1:I:176:ALA:HB1	1:I:181:GLN:HB3	2.00	0.44
7:N:36:ALA:HB1	7:N:40:MET:HB2	2.00	0.44
1:X:293:PHE:HB2	1:X:558:THR:HG23	2.00	0.44
1:g:354:TRP:HB2	1:g:356:GLN:HG3	2.00	0.44
1:g:639:SER:O	1:g:878:LEU:HD23	2.18	0.44
1:h:214:PRO:HG2	1:h:286:ALA:HB2	2.00	0.44
1:h:473:SER:HB3	1:h:792:CYS:N	2.31	0.44
1:i:231:LYS:O	1:i:234:THR:OG1	2.30	0.44
1:i:313:GLY:HA3	1:i:545:TRP:CE3	2.53	0.44
1:i:882:PHE:O	1:i:901:ARG:HA	2.17	0.44
9:j:262:ILE:O	9:j:262:ILE:HG13	2.18	0.44
1:A:879:PHE:O	1:A:881:VAL:HG13	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:380:TYR:CG	1:F:796:ARG:HD2	2.53	0.43
1:F:357:ALA:HB3	1:F:508:ARG:HH11	1.83	0.43
1:G:734:TYR:OH	1:G:753:SER:HB3	2.17	0.43
1:H:796:ARG:NH2	1:I:419:LEU:O	2.51	0.43
1:J:627:ILE:HD12	1:J:628:PRO:HD2	2.00	0.43
1:J:716:VAL:HB	1:J:723:LYS:HA	2.00	0.43
2:T:7:ALA:HB1	2:T:17:PRO:HG2	2.00	0.43
2:T:17:PRO:HB2	2:T:19:LEU:HD13	2.00	0.43
1:X:88:VAL:HG13	1:X:581:PHE:HE2	1.82	0.43
1:Y:130:PRO:HB3	1:Y:282:LEU:HB3	2.00	0.43
1:Y:643:LEU:HD12	1:Y:874:LEU:HD11	1.99	0.43
1:h:114:LYS:NZ	1:h:289:ASN:O	2.51	0.43
1:h:353:MET:HE3	1:h:353:MET:HB3	1.80	0.43
1:h:365:VAL:HG21	1:h:501:ARG:HD2	1.98	0.43
1:h:392:ARG:NH1	1:h:411:ASN:OD1	2.47	0.43
1:A:396:VAL:HG12	1:A:403:TRP:HE3	1.83	0.43
1:A:724:ASP:OD1	1:A:725:TRP:N	2.51	0.43
1:D:120:ALA:HB2	1:g:482:ILE:HD13	1.99	0.43
1:D:156:ILE:HD13	1:D:252:VAL:HG23	1.99	0.43
1:D:466:MET:HE2	1:D:559:LEU:HB3	2.00	0.43
1:F:548:ARG:O	1:F:554:ILE:HD11	2.17	0.43
1:F:675:SER:O	1:F:830:TRP:NE1	2.46	0.43
1:F:862:MET:HG3	1:F:864:PHE:CE1	2.53	0.43
1:G:56:VAL:O	1:G:584:MET:HA	2.17	0.43
1:G:109:ARG:HD2	1:G:113:PHE:CD2	2.53	0.43
1:G:482:ILE:HG12	1:h:116:TYR:CD2	2.53	0.43
1:J:645:GLN:HA	1:J:874:LEU:HD22	1.99	0.43
1:g:615:LEU:HD22	1:g:874:LEU:CD1	2.47	0.43
1:h:704:GLU:OE2	1:h:707:ILE:HG12	2.17	0.43
1:A:616:TYR:HB3	1:A:624:GLN:HE22	1.82	0.43
1:D:60:ARG:HD2	1:D:586:HIS:ND1	2.33	0.43
1:D:343:ASN:HA	1:D:750:ARG:HD2	1.99	0.43
1:D:536:LEU:HD12	1:D:536:LEU:HA	1.88	0.43
1:F:114:LYS:NZ	1:F:289:ASN:O	2.32	0.43
1:F:388:GLN:HB2	1:F:420:PRO:HG3	1.99	0.43
1:G:256:GLU:OE2	1:i:801:TYR:OH	2.28	0.43
1:G:297:ARG:HG2	1:G:556:GLN:HB2	1.99	0.43
1:H:108:ASP:OD1	1:H:516:ARG:HG2	2.19	0.43
1:H:124:PHE:CZ	1:I:429:ASN:HA	2.53	0.43
1:H:627:ILE:HG12	1:H:860:LEU:HB3	2.00	0.43
1:I:240:TYR:CD1	1:I:252:VAL:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:651:LEU:HD23	1:I:651:LEU:H	1.82	0.43
1:J:587:ASN:OD1	6:M:216:ASP:HA	2.18	0.43
1:X:283:SER:HA	1:Y:191:TRP:NE1	2.33	0.43
1:X:629:SER:HB2	1:X:859:ALA:HB2	2.00	0.43
1:X:792:CYS:SG	1:X:793:ARG:N	2.91	0.43
1:X:799:HIS:N	1:Y:184:PRO:O	2.51	0.43
1:X:802:PRO:HD3	1:Y:207:LEU:HD11	2.00	0.43
1:Y:396:VAL:HG11	1:Y:403:TRP:HB3	2.00	0.43
1:Y:782:ARG:HG3	1:Y:785:PRO:HG3	2.00	0.43
1:h:107:LEU:HD22	1:h:520:PHE:CD1	2.53	0.43
1:h:496:PRO:HG2	1:h:497:PHE:CD1	2.53	0.43
1:h:787:TYR:CE2	1:i:126:PRO:HD3	2.51	0.43
1:i:597:ARG:HD2	1:i:891:HIS:HA	2.00	0.43
9:j:245:ASN:OD1	9:j:245:ASN:N	2.52	0.43
1:A:396:VAL:HG11	1:A:403:TRP:HB3	2.01	0.43
1:A:422:MET:HB3	1:Y:382:PHE:O	2.18	0.43
1:A:764:GLN:HB3	1:A:817:ARG:HD2	1.99	0.43
1:D:279:VAL:HG22	1:D:280:GLU:H	1.83	0.43
1:D:636:ARG:NH2	3:U:21:TYR:O	2.27	0.43
1:F:84:PHE:HZ	1:F:575:VAL:HG12	1.82	0.43
1:F:431:TRP:CE2	1:F:435:LEU:HD11	2.53	0.43
1:G:810:TRP:HB2	1:h:113:PHE:O	2.19	0.43
1:H:112:SER:O	1:H:292:ASN:ND2	2.43	0.43
1:H:114:LYS:CG	1:H:291:PRO:HA	2.49	0.43
1:H:132:ASN:HD21	1:I:799:HIS:HB2	1.81	0.43
1:H:206:VAL:HB	1:H:255:THR:HG22	2.01	0.43
1:H:416:LYS:NZ	1:I:199:ILE:O	2.45	0.43
1:I:268:VAL:HG13	1:I:285:HIS:CE1	2.54	0.43
1:J:475:LEU:O	1:J:480:VAL:HG11	2.18	0.43
6:M:266:VAL:HG22	6:M:269:ARG:HH21	1.83	0.43
8:P:8:TYR:CD2	8:P:9:VAL:HG23	2.52	0.43
1:X:207:LEU:HD21	1:X:260:VAL:HG11	1.99	0.43
1:X:564:ARG:HH21	1:X:660:THR:H	1.67	0.43
1:Y:489:ASP:OD1	1:Y:763:ARG:NH2	2.51	0.43
1:Y:582:PHE:HD1	1:Y:584:MET:HB3	1.83	0.43
1:Y:602:ASP:HB2	1:Y:886:ARG:NH2	2.33	0.43
1:Y:672:PHE:O	1:Y:827:ARG:N	2.41	0.43
1:g:591:THR:O	1:g:595:MET:HG3	2.19	0.43
1:g:630:ARG:HB2	1:g:631:ASN:H	1.69	0.43
1:h:135:PHE:HB3	1:h:282:LEU:HD11	1.99	0.43
1:h:328:LEU:O	1:h:329:GLN:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:644:LYS:HG2	1:h:873:THR:HG22	1.99	0.43
1:i:643:LEU:HD21	1:i:876:TYR:HE1	1.84	0.43
9:j:213:GLN:HB3	9:j:308:ARG:HH21	1.83	0.43
1:A:360:SER:N	1:A:502:ASN:OD1	2.51	0.43
1:A:366:ARG:NH1	1:A:496:PRO:HG3	2.33	0.43
1:F:292:ASN:OD1	1:F:557:SER:HB2	2.18	0.43
1:G:189:GLU:HG2	1:i:269:HIS:CD2	2.53	0.43
1:H:64:LEU:HD11	1:H:583:PRO:HG3	2.00	0.43
1:H:314:VAL:HA	1:H:323:ASN:HD21	1.83	0.43
1:H:619:PRO:O	1:H:621:ASN:N	2.44	0.43
1:H:765:VAL:O	1:H:818:ASP:HB3	2.18	0.43
1:I:165:MET:HE3	1:I:176:ALA:HB2	2.00	0.43
1:X:371:VAL:HG13	1:Y:293:PHE:HZ	1.84	0.43
1:X:636:ARG:CZ	1:X:880:GLU:HB3	2.48	0.43
1:Y:340:LEU:HD13	1:Y:608:TYR:CD1	2.53	0.43
1:Y:397:GLN:HE21	1:Y:404:GLN:HE21	1.67	0.43
1:Y:734:TYR:OH	1:Y:749:ASP:OD1	2.29	0.43
1:A:253:PHE:HE2	1:X:414:ILE:HD13	1.83	0.43
1:A:810:TRP:HE3	1:A:811:ASP:HB3	1.83	0.43
1:D:147:ILE:HD12	1:F:413:TYR:HB2	2.01	0.43
1:F:553:MET:HE3	1:F:553:MET:HB3	1.92	0.43
1:F:809:HIS:HB3	1:g:515:GLY:HA2	2.01	0.43
1:F:817:ARG:HH22	1:g:516:ARG:HB3	1.78	0.43
1:G:205:ARG:HH11	1:G:256:GLU:CD	2.26	0.43
1:G:614:MET:HE3	1:g:321:GLN:HB3	2.01	0.43
1:G:722:THR:OG1	1:G:724:ASP:OD1	2.22	0.43
1:H:423:GLU:OE2	1:J:127:LYS:HG3	2.19	0.43
1:H:639:SER:HA	1:H:830:TRP:O	2.18	0.43
1:I:683:ILE:HG23	1:I:860:LEU:HD11	2.01	0.43
1:I:685:PHE:CE2	1:I:691:TRP:HB2	2.54	0.43
1:I:895:ILE:HG22	1:I:897:VAL:HG23	2.00	0.43
1:J:292:ASN:OD1	1:J:557:SER:HB2	2.18	0.43
1:J:475:LEU:HB2	1:J:778:ILE:HD11	1.99	0.43
1:X:133:THR:OG1	1:X:210:PRO:HG3	2.19	0.43
1:X:778:ILE:HA	1:X:781:HIS:HD1	1.84	0.43
1:Y:193:ALA:HA	1:Y:197:ALA:HB3	2.00	0.43
1:Y:234:THR:HG21	1:Y:257:GLU:HG2	2.01	0.43
1:Y:690:THR:HG21	1:Y:701:ASN:HB2	2.00	0.43
1:g:690:THR:HB	1:g:692:PRO:HD2	2.00	0.43
1:i:375:ASP:HB3	1:i:427:ALA:HB3	2.01	0.43
1:A:114:LYS:HB3	1:A:291:PRO:HA	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:519:ASP:OD1	1:Y:817:ARG:NH2	2.49	0.43
1:F:495:ASN:HD21	1:F:664:THR:HG23	1.84	0.43
1:F:887:VAL:HG13	1:F:897:VAL:HG22	2.00	0.43
1:G:786:ALA:HB2	1:G:798:GLY:C	2.44	0.43
1:I:76:THR:HG23	1:I:79:SER:H	1.83	0.43
1:I:764:GLN:HB2	1:I:817:ARG:CZ	2.49	0.43
1:I:770:THR:HG23	1:I:816:LEU:HD13	1.99	0.43
1:J:269:HIS:O	1:J:269:HIS:CG	2.72	0.43
1:J:290:ARG:NH1	1:J:441:LEU:HB3	2.34	0.43
1:J:394:HIS:ND1	1:J:410:ASP:OD1	2.38	0.43
1:X:240:TYR:CD2	1:X:252:VAL:HG22	2.54	0.43
1:X:343:ASN:HA	1:X:750:ARG:HD3	2.00	0.43
1:Y:134:GLN:HG2	1:Y:146:THR:HG22	1.99	0.43
1:Y:153:VAL:HG12	1:Y:202:ALA:HB2	2.00	0.43
1:Y:396:VAL:HG12	1:Y:403:TRP:HE3	1.84	0.43
1:Y:627:ILE:HG21	1:Y:860:LEU:HB3	2.01	0.43
1:h:665:ILE:O	1:h:669:ASP:HB2	2.19	0.43
1:i:179:THR:O	1:i:205:ARG:NH2	2.50	0.43
1:i:451:PRO:HG2	1:i:454:ILE:HB	2.00	0.43
1:A:83:ARG:CG	1:A:544:GLU:HB2	2.48	0.43
1:A:519:ASP:O	1:Y:821:ARG:NH2	2.48	0.43
1:A:615:LEU:HA	1:A:875:LEU:O	2.19	0.43
1:A:627:ILE:HD12	1:A:628:PRO:HD2	2.00	0.43
1:A:716:VAL:HG12	1:A:721:MET:O	2.19	0.43
1:F:282:LEU:HD12	1:g:196:MET:HE1	2.00	0.43
1:G:881:VAL:HG21	1:G:901:ARG:HH21	1.84	0.43
1:H:179:THR:O	1:H:205:ARG:NH1	2.49	0.43
1:I:297:ARG:HE	1:I:556:GLN:HB2	1.84	0.43
1:J:75:ASP:OD1	1:J:75:ASP:N	2.51	0.43
1:J:464:GLU:N	1:J:464:GLU:OE2	2.49	0.43
7:N:80:LYS:HD3	7:N:176:GLN:HB2	2.00	0.43
1:X:564:ARG:NH2	1:X:660:THR:H	2.17	0.43
1:Y:447:LEU:HD22	1:Y:475:LEU:HD11	2.00	0.43
1:g:322:LEU:HD12	1:g:322:LEU:HA	1.75	0.43
1:h:716:VAL:HG21	1:h:726:PHE:CD2	2.54	0.43
1:i:176:ALA:HB1	1:i:182:PRO:HD3	2.01	0.43
9:j:385:SER:HA	9:j:426:SER:HA	2.00	0.43
1:A:878:LEU:HD12	1:A:878:LEU:O	2.19	0.43
1:F:76:THR:HG22	1:F:78:TYR:H	1.83	0.43
1:F:219:TYR:CD2	1:F:261:LEU:HD21	2.54	0.43
1:F:535:LEU:HD12	1:F:535:LEU:HA	1.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:758:PHE:CE2	1:F:760:PRO:HG3	2.53	0.43
1:F:797:GLU:HG2	1:g:188:ILE:O	2.19	0.43
1:G:321:GLN:HE21	1:g:631:ASN:CG	2.26	0.43
1:G:902:THR:HB	1:G:903:PRO:HD3	2.00	0.43
1:H:382:PHE:N	1:J:423:GLU:O	2.43	0.43
1:I:541:TYR:CZ	1:I:893:GLY:HA2	2.54	0.43
1:J:586:HIS:H	6:M:216:ASP:HB2	1.83	0.43
1:J:783:THR:HA	1:J:803:GLN:HG2	2.00	0.43
5:K:28:GLY:HA3	5:K:37:GLN:HG2	2.00	0.43
7:R:203:ARG:HH21	1:g:892:ARG:HH11	1.65	0.43
1:X:18:GLN:HG2	1:X:22:GLU:HG2	2.00	0.43
1:X:371:VAL:HG22	1:Y:510:GLN:HE22	1.84	0.43
1:X:552:ASN:HD21	1:X:661:TYR:N	2.16	0.43
1:X:808:PRO:HD3	1:Y:219:TYR:CZ	2.54	0.43
1:Y:30:GLN:O	1:Y:33:GLN:HG3	2.18	0.43
1:Y:128:SER:HB3	1:Y:285:HIS:HB3	1.99	0.43
1:g:550:ASP:O	1:g:554:ILE:HG12	2.19	0.43
1:h:132:ASN:OD1	1:h:206:VAL:HG22	2.18	0.43
1:i:789:PHE:HB2	1:i:797:GLU:HG2	2.00	0.43
3:C:21:TYR:CG	1:H:339:MET:HE1	2.54	0.43
1:D:354:TRP:HB2	1:D:356:GLN:HG3	2.01	0.43
1:D:705:ILE:HG23	1:D:725:TRP:CD1	2.54	0.43
1:F:207:LEU:HD21	1:F:260:VAL:HG21	2.01	0.43
1:G:283:SER:HB3	1:h:192:THR:HG23	2.01	0.43
1:G:328:LEU:O	1:g:322:LEU:HD11	2.19	0.43
1:G:477:ASP:OD1	1:G:478:THR:N	2.49	0.43
1:G:492:ASP:CG	1:G:822:LYS:HZ3	2.25	0.43
1:J:499:HIS:ND1	1:J:501:ARG:HG2	2.34	0.43
1:J:551:VAL:HG13	1:J:555:LEU:HD12	2.01	0.43
7:N:26:ASP:OD2	7:N:29:THR:OG1	2.36	0.43
1:X:613:ASN:HB3	1:X:876:TYR:HE1	1.83	0.43
1:Y:58:THR:O	1:Y:59:GLU:HG3	2.19	0.43
1:Y:62:GLN:HE21	1:Y:583:PRO:HA	1.84	0.43
1:g:126:PRO:HB2	1:g:129:ALA:HB2	2.00	0.43
1:g:636:ARG:NH1	1:g:881:VAL:O	2.51	0.43
1:h:665:ILE:HD11	1:h:668:LEU:HD11	2.01	0.43
1:A:283:SER:HB3	1:X:192:THR:HG23	2.01	0.42
1:A:651:LEU:HD12	1:A:667:TYR:HE2	1.84	0.42
1:D:800:PRO:HD3	1:g:419:LEU:HD11	2.00	0.42
1:G:52:PRO:HD3	2:c:11:PRO:HA	2.00	0.42
1:G:306:TYR:HE2	1:G:527:LYS:HD2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:185:GLN:NE2	1:J:782:ARG:HD3	2.34	0.42
1:I:269:HIS:O	1:I:269:HIS:CG	2.72	0.42
1:J:505:LEU:HD22	1:J:556:GLN:HE21	1.83	0.42
8:P:42:GLN:OE1	8:P:42:GLN:HA	2.19	0.42
1:Y:180:TYR:CG	1:Y:226:HIS:HB3	2.53	0.42
1:Y:712:GLU:OE1	1:Y:712:GLU:N	2.52	0.42
1:Y:808:PRO:O	1:Y:814:HIS:HB2	2.20	0.42
1:Y:879:PHE:O	1:Y:881:VAL:HG13	2.18	0.42
1:g:114:LYS:HD3	1:g:289:ASN:HB2	1.99	0.42
1:h:680:LYS:NZ	1:h:865:GLU:OE2	2.36	0.42
1:i:412:ASN:HB3	1:i:414:ILE:CD1	2.49	0.42
9:j:348:ILE:HG21	9:j:454:LEU:HD23	2.01	0.42
1:A:151:SER:OG	1:A:152:TYR:N	2.52	0.42
1:A:787:TYR:HD1	1:Y:382:PHE:CE2	2.37	0.42
1:A:803:GLN:HE21	1:X:121:TYR:HB3	1.84	0.42
1:D:306:TYR:HE2	1:D:527:LYS:HE2	1.84	0.42
1:D:376:GLU:O	1:F:793:ARG:HG3	2.19	0.42
4:E:76:ALA:HA	6:M:228:MET:HB2	2.00	0.42
1:F:687:SER:HB2	1:J:69:VAL:HG22	2.01	0.42
1:F:790:ARG:HG2	1:F:790:ARG:NH1	2.34	0.42
1:G:499:HIS:ND1	1:G:501:ARG:HG2	2.34	0.42
1:H:130:PRO:HD2	1:J:386:GLY:H	1.84	0.42
1:I:22:GLU:OE2	2:Z:16:ARG:NH1	2.52	0.42
1:I:881:VAL:HG12	1:I:903:PRO:HB2	2.00	0.42
1:J:670:GLY:HA2	1:J:672:PHE:CE1	2.54	0.42
1:X:593:GLU:O	1:X:597:ARG:HG3	2.19	0.42
1:Y:462:THR:HG23	1:Y:465:TYR:H	1.82	0.42
1:g:94:LEU:HD22	1:g:581:PHE:CE2	2.53	0.42
1:g:339:MET:SD	1:g:609:LEU:HD13	2.59	0.42
1:h:58:THR:OG1	1:h:586:HIS:NE2	2.51	0.42
1:i:156:ILE:HD12	1:i:201:GLN:HG2	2.01	0.42
1:i:208:ARG:HG3	1:i:257:GLU:HG2	2.00	0.42
1:i:548:ARG:O	1:i:554:ILE:HD11	2.19	0.42
1:i:704:GLU:O	1:i:725:TRP:HB2	2.20	0.42
1:D:162:ASP:OD1	1:D:238:LYS:NZ	2.42	0.42
1:D:691:TRP:CH2	1:D:847:LEU:HD22	2.54	0.42
1:D:731:LEU:HD22	1:D:839:MET:HG3	2.02	0.42
1:F:208:ARG:O	1:F:257:GLU:HG2	2.19	0.42
1:F:322:LEU:HD23	1:F:322:LEU:HA	1.85	0.42
1:G:16:ALA:HA	1:G:48:PRO:HB3	2.01	0.42
1:H:49:THR:HG21	2:Z:28:HIS:CG	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:103:ILE:HG12	1:H:575:VAL:HG22	1.99	0.42
1:H:738:TYR:HD2	1:H:839:MET:HE3	1.84	0.42
1:H:788:TRP:HA	1:H:796:ARG:HA	2.01	0.42
1:I:58:THR:HG22	1:I:60:ARG:N	2.33	0.42
1:I:289:ASN:OD1	1:I:467:ASN:ND2	2.51	0.42
1:I:680:LYS:HB3	1:I:680:LYS:HE2	1.80	0.42
1:J:106:THR:HG22	1:J:519:ASP:OD1	2.19	0.42
1:J:112:SER:O	1:J:292:ASN:ND2	2.41	0.42
1:J:265:THR:OG1	1:J:287:ALA:O	2.29	0.42
1:J:330:ASP:O	1:J:613:ASN:ND2	2.26	0.42
1:J:380:TYR:CE1	1:J:423:GLU:HG2	2.54	0.42
1:J:782:ARG:NH2	1:J:802:PRO:O	2.52	0.42
1:J:902:THR:HB	1:J:903:PRO:HD3	2.00	0.42
5:K:257:LEU:HA	5:K:260:ILE:HG22	2.01	0.42
7:R:186:TYR:CE2	7:R:189:PRO:HA	2.55	0.42
1:X:290:ARG:NH2	1:X:441:LEU:O	2.45	0.42
1:X:784:THR:HB	1:X:788:TRP:NE1	2.32	0.42
1:Y:289:ASN:O	1:Y:290:ARG:C	2.57	0.42
1:Y:625:LEU:HA	1:Y:862:MET:O	2.19	0.42
1:g:782:ARG:NE	1:g:802:PRO:O	2.41	0.42
1:i:624:GLN:NE2	1:i:875:LEU:HD13	2.34	0.42
9:j:67:ASP:OD2	9:j:467:LYS:HA	2.19	0.42
9:j:252:LYS:HG2	9:j:260:PHE:HD1	1.84	0.42
1:D:444:PRO:HB2	1:D:446:ASN:OD1	2.20	0.42
1:D:597:ARG:HD3	1:D:889:GLN:O	2.19	0.42
1:D:764:GLN:OE1	1:F:513:GLY:HA3	2.19	0.42
1:D:815:ALA:O	1:D:816:LEU:HB2	2.19	0.42
1:F:446:ASN:OD1	1:F:447:LEU:HG	2.19	0.42
1:G:310:GLY:HA3	1:g:328:LEU:HA	1.99	0.42
1:G:534:LEU:HD11	1:G:895:ILE:HD11	2.01	0.42
1:G:616:TYR:OH	1:G:627:ILE:HD11	2.19	0.42
1:G:783:THR:HA	1:G:803:GLN:CG	2.48	0.42
1:G:808:PRO:HB3	1:h:121:TYR:OH	2.20	0.42
1:I:84:PHE:HZ	1:I:575:VAL:HG12	1.84	0.42
1:I:126:PRO:HB2	1:I:129:ALA:HB2	2.00	0.42
5:K:184:ALA:HB3	5:K:269:ILE:HD13	2.01	0.42
8:O:11:TYR:CD1	8:P:11:TYR:HB3	2.55	0.42
7:R:199:ASP:C	7:R:201:PHE:H	2.27	0.42
1:X:759:ILE:HG13	1:X:759:ILE:O	2.19	0.42
1:Y:13:MET:O	1:Y:15:ILE:N	2.52	0.42
1:Y:325:VAL:HG13	1:Y:528:PHE:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:g:875:LEU:HG	1:g:877:VAL:HG23	2.01	0.42
1:h:479:TYR:CD1	1:h:783:THR:HG21	2.54	0.42
1:h:723:LYS:HE3	1:i:578:TYR:CZ	2.55	0.42
1:i:111:ALA:HA	1:i:516:ARG:HD2	2.01	0.42
1:i:368:ILE:O	1:i:368:ILE:HG13	2.19	0.42
9:j:212:THR:HG23	9:j:214:LEU:H	1.83	0.42
1:A:217:GLY:HA3	1:A:262:THR:HB	2.01	0.42
1:A:387:VAL:HG21	1:Y:149:GLN:HB3	2.02	0.42
1:A:760:PRO:HG3	1:X:352:SER:HB2	2.01	0.42
1:D:405:ASN:OD1	1:g:242:ARG:NH2	2.53	0.42
1:F:741:TYR:O	1:g:354:TRP:NE1	2.29	0.42
1:G:351:PHE:HB3	1:G:356:GLN:HB2	2.01	0.42
1:G:882:PHE:HD1	1:h:15:ILE:HD12	1.84	0.42
1:H:613:ASN:HB3	1:H:876:TYR:HE1	1.85	0.42
1:I:46:ARG:HH12	1:J:606:ASN:ND2	2.17	0.42
1:I:624:GLN:HE21	8:Q:13:THR:HB	1.85	0.42
1:J:156:ILE:HD13	1:J:252:VAL:HG23	2.01	0.42
1:J:306:TYR:CE2	1:J:527:LYS:HB2	2.55	0.42
5:K:39:LEU:O	5:K:43:GLN:HB2	2.19	0.42
5:K:276:GLY:O	5:K:280:THR:HG23	2.18	0.42
6:M:210:ARG:NH2	2:S:5:ASN:O	2.52	0.42
7:N:185:VAL:HG12	7:N:187:LEU:HD22	2.02	0.42
1:X:13:MET:O	1:X:15:ILE:N	2.52	0.42
1:X:283:SER:HB3	1:Y:192:THR:HG23	2.01	0.42
1:g:328:LEU:HD11	1:g:901:ARG:CZ	2.49	0.42
1:g:379:ASN:OD1	1:g:424:ILE:O	2.38	0.42
1:g:497:PHE:HE2	1:g:827:ARG:HH21	1.66	0.42
1:i:635:PHE:HE1	1:i:879:PHE:HB3	1.84	0.42
1:A:719:SER:HB3	1:A:760:PRO:HB3	2.01	0.42
1:A:777:GLY:O	1:A:781:HIS:ND1	2.45	0.42
1:F:52:PRO:HD3	2:T:11:PRO:HA	2.02	0.42
1:F:290:ARG:HH11	1:F:441:LEU:HD22	1.84	0.42
1:F:336:SER:OG	1:F:609:LEU:HB3	2.19	0.42
1:F:371:VAL:HG21	1:g:506:ARG:HD3	2.00	0.42
1:F:381:CYS:SG	1:g:422:MET:CE	3.07	0.42
1:G:85:GLN:HB2	1:G:318:GLN:HE21	1.84	0.42
1:H:353:MET:HA	1:I:717:ALA:HA	2.01	0.42
1:H:777:GLY:O	1:H:781:HIS:NE2	2.52	0.42
1:H:789:PHE:CE1	1:J:186:LEU:HA	2.55	0.42
1:H:810:TRP:HE1	1:J:116:TYR:HE2	1.67	0.42
1:H:900:LEU:HD22	1:J:13:MET:HG3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:216:TYR:HB3	1:I:286:ALA:HB3	2.01	0.42
1:I:422:MET:HE1	1:J:422:MET:SD	2.60	0.42
1:I:796:ARG:HD2	1:I:796:ARG:C	2.44	0.42
5:K:82:VAL:HG12	5:K:83:VAL:HG23	2.01	0.42
1:X:290:ARG:HH21	1:X:441:LEU:C	2.28	0.42
1:X:374:GLU:OE1	1:Y:438:ASN:ND2	2.53	0.42
1:X:704:GLU:OE1	1:X:707:ILE:HG12	2.20	0.42
1:Y:74:GLU:OE2	1:Y:81:LYS:HE2	2.20	0.42
1:Y:96:MET:HE2	1:Y:96:MET:HB3	1.88	0.42
1:Y:400:GLN:HG2	1:Y:401:GLN:H	1.83	0.42
1:Y:505:LEU:HD22	1:Y:556:GLN:NE2	2.33	0.42
1:Y:537:LEU:HD12	1:Y:889:GLN:HB2	2.00	0.42
1:Y:790:ARG:HG2	1:Y:790:ARG:NH1	2.31	0.42
1:g:205:ARG:HH11	1:g:256:GLU:CD	2.27	0.42
1:g:679:ARG:HB2	1:g:865:GLU:HG2	2.02	0.42
1:h:422:MET:HE2	1:i:422:MET:SD	2.60	0.42
1:i:18:GLN:HG2	1:i:22:GLU:HG3	2.00	0.42
1:i:635:PHE:CE1	1:i:879:PHE:HB3	2.55	0.42
1:A:318:GLN:H	1:A:318:GLN:HG3	1.70	0.42
1:F:399:ASN:OD1	1:F:400:GLN:N	2.51	0.42
1:G:72:ASP:OD2	1:g:628:PRO:HG3	2.19	0.42
1:G:548:ARG:O	1:G:554:ILE:HD11	2.19	0.42
1:G:795:PRO:HA	1:i:380:TYR:CE2	2.55	0.42
1:H:131:ASN:HD22	1:I:802:PRO:HG3	1.85	0.42
1:H:593:GLU:O	1:H:597:ARG:HG2	2.19	0.42
1:H:613:ASN:N	1:H:613:ASN:ND2	2.67	0.42
1:J:128:SER:HB3	1:J:285:HIS:HB3	2.00	0.42
1:J:379:ASN:OD1	1:J:426:LEU:N	2.33	0.42
1:J:767:ASN:HD22	1:J:816:LEU:HD23	1.84	0.42
7:R:190:TYR:CD1	1:g:595:MET:HG2	2.55	0.42
1:g:99:THR:HG22	1:g:579:ALA:HA	2.02	0.42
1:h:176:ALA:HB1	1:h:182:PRO:HD3	2.02	0.42
1:h:719:SER:HB2	1:h:823:PHE:HB3	2.00	0.42
1:i:83:ARG:HA	1:i:544:GLU:HB3	2.01	0.42
1:i:242:ARG:NH1	1:i:247:GLY:H	2.18	0.42
1:A:698:LEU:HG	1:X:65:GLN:HB2	2.02	0.42
1:D:300:PHE:CZ	1:D:522:ILE:HB	2.55	0.42
1:D:341:LEU:HD23	1:D:341:LEU:HA	1.90	0.42
1:F:627:ILE:HG13	1:F:628:PRO:N	2.35	0.42
1:G:633:ALA:O	1:G:903:PRO:HG3	2.19	0.42
1:H:313:GLY:C	1:H:315:LEU:H	2.28	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:625:LEU:CB	1:H:626:PRO:HD3	2.50	0.42
1:H:786:ALA:HB1	1:I:419:LEU:HG	2.00	0.42
1:H:887:VAL:HG13	1:H:897:VAL:HG22	2.02	0.42
1:I:95:ASP:HA	1:I:535:LEU:HA	2.01	0.42
1:J:357:ALA:HB1	1:J:504:GLY:HA2	2.00	0.42
7:R:7:THR:HG21	7:R:30:ARG:HD3	2.02	0.42
1:Y:147:ILE:HG13	1:Y:147:ILE:O	2.20	0.42
1:Y:304:MET:HG2	1:Y:547:PHE:CD1	2.55	0.42
1:Y:499:HIS:ND1	1:Y:501:ARG:HG2	2.35	0.42
1:g:147:ILE:HG13	1:g:147:ILE:O	2.20	0.42
1:g:292:ASN:O	1:g:558:THR:OG1	2.33	0.42
1:i:621:ASN:CB	1:i:868:PRO:HB3	2.50	0.42
1:i:684:GLN:O	1:i:861:ASP:N	2.49	0.42
9:j:219:VAL:HG13	9:j:414:GLN:HE22	1.85	0.42
1:A:366:ARG:HH21	1:A:492:ASP:HA	1.84	0.42
1:A:383:PRO:HG2	1:A:386:GLY:O	2.20	0.42
1:A:695:ASP:O	1:X:63:ARG:HG2	2.20	0.42
1:G:353:MET:HA	1:i:717:ALA:HA	2.01	0.42
1:G:379:ASN:OD1	1:G:426:LEU:HG	2.19	0.42
1:H:488:PRO:HB2	1:H:491:MET:HB2	2.02	0.42
7:R:194:PRO:HA	7:R:197:TYR:CG	2.54	0.42
1:X:382:PHE:CE1	1:Y:796:ARG:HG3	2.55	0.42
1:X:475:LEU:HG	1:X:778:ILE:HD12	2.01	0.42
1:Y:75:ASP:OD1	1:Y:75:ASP:N	2.52	0.42
1:Y:548:ARG:HG2	1:Y:550:ASP:H	1.85	0.42
1:Y:620:PRO:HB3	1:Y:870:ASN:O	2.20	0.42
1:g:114:LYS:NZ	1:g:116:TYR:O	2.49	0.42
1:g:319:SER:CB	1:g:894:VAL:HG22	2.49	0.42
1:g:718:GLN:HB3	1:g:821:ARG:HH12	1.84	0.42
1:i:512:LEU:HD23	1:i:512:LEU:H	1.85	0.42
1:i:734:TYR:OH	1:i:753:SER:HB3	2.20	0.42
9:j:63:ILE:HG23	9:j:89:ILE:HG23	2.01	0.42
1:A:88:VAL:HG12	1:A:88:VAL:O	2.20	0.42
1:A:307:ASN:HD21	1:A:333:THR:H	1.67	0.42
1:D:336:SER:OG	1:D:609:LEU:HB3	2.20	0.42
1:D:382:PHE:CZ	1:F:796:ARG:HG3	2.54	0.42
1:D:665:ILE:HG13	1:D:665:ILE:O	2.20	0.42
1:F:66:LEU:HD23	1:F:66:LEU:HA	1.85	0.42
1:G:332:ASN:HB2	1:G:613:ASN:OD1	2.19	0.42
1:H:120:ALA:HB2	1:I:482:ILE:HD13	2.02	0.42
1:H:124:PHE:HB2	1:I:784:THR:HG21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:279:VAL:C	1:I:281:GLY:H	2.27	0.42
1:J:548:ARG:O	1:J:554:ILE:HD11	2.20	0.42
1:J:553:MET:HE3	1:J:553:MET:HB3	1.81	0.42
5:K:126:TYR:O	5:K:131:VAL:HG21	2.20	0.42
6:M:208:LYS:HG2	6:M:209:ARG:N	2.35	0.42
8:O:43:ALA:HB1	8:O:59:HIS:CE1	2.55	0.42
1:X:432:ARG:HH21	1:X:477:ASP:CG	2.28	0.42
1:X:776:LEU:HD21	1:Y:227:GLY:HA2	2.01	0.42
1:Y:333:THR:HA	1:Y:336:SER:HB2	2.02	0.42
1:g:290:ARG:HE	1:g:441:LEU:HB3	1.84	0.42
1:g:314:VAL:HG23	1:g:323:ASN:CG	2.45	0.42
1:g:582:PHE:CE2	1:g:584:MET:HB3	2.55	0.42
1:h:185:GLN:HG2	1:h:186:LEU:HD22	2.01	0.42
1:h:235:GLN:H	1:h:235:GLN:CD	2.28	0.42
1:h:887:VAL:HG13	1:h:897:VAL:HG22	2.02	0.42
1:h:902:THR:HG23	1:i:6:MET:HE2	2.02	0.42
1:i:6:MET:HE3	1:i:6:MET:HB3	1.84	0.42
1:i:350:TYR:HD1	1:i:357:ALA:HA	1.85	0.42
9:j:429:GLU:C	9:j:430:ASN:HD22	2.28	0.42
1:A:10:TRP:HD1	1:Y:853:TYR:CZ	2.38	0.41
1:A:132:ASN:ND2	1:Y:799:HIS:NE2	2.67	0.41
1:A:241:TYR:HB2	1:A:251:THR:OG1	2.20	0.41
1:A:487:SER:H	1:A:761:MET:HE3	1.85	0.41
1:D:12:TYR:CD1	7:R:34:PHE:HZ	2.38	0.41
1:D:650:ALA:N	1:D:656:ASP:OD2	2.51	0.41
1:F:672:PHE:O	1:F:827:ARG:N	2.26	0.41
1:G:442:TYR:HH	1:G:500:HIS:HB3	1.84	0.41
1:G:777:GLY:O	1:G:781:HIS:ND1	2.50	0.41
1:H:58:THR:HA	1:H:585:SER:HA	2.02	0.41
1:H:85:GLN:O	1:H:85:GLN:HG3	2.19	0.41
1:I:18:GLN:H	2:Z:15:SER:HB3	1.85	0.41
1:I:107:LEU:HD23	1:I:520:PHE:CD1	2.55	0.41
1:I:121:TYR:CE2	1:I:263:PRO:HG2	2.54	0.41
1:I:315:LEU:HD23	1:I:531:ILE:HD12	2.02	0.41
8:O:83:LEU:HD13	8:P:83:LEU:HD23	2.02	0.41
1:X:162:ASP:HB2	1:X:254:TYR:OH	2.19	0.41
1:X:585:SER:HB3	1:X:588:THR:HG22	2.01	0.41
1:Y:551:VAL:HG13	1:Y:555:LEU:HD12	2.02	0.41
1:Y:618:ILE:HD13	1:Y:866:MET:CE	2.46	0.41
1:h:137:GLN:HG3	1:h:145:GLN:OE1	2.20	0.41
1:h:401:GLN:OE1	1:h:401:GLN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:551:VAL:HG21	1:h:568:ALA:O	2.19	0.41
1:h:755:LEU:HD23	1:h:755:LEU:HA	1.84	0.41
1:i:95:ASP:OD1	1:i:95:ASP:N	2.49	0.41
1:A:242:ARG:NH1	1:A:247:GLY:H	2.18	0.41
1:D:131:ASN:HB3	1:D:215:CYS:HA	2.02	0.41
1:D:396:VAL:CG1	1:D:403:TRP:HB3	2.49	0.41
1:D:477:ASP:HB3	1:D:479:TYR:CE1	2.55	0.41
4:E:54:LEU:C	4:E:57:PRO:HD2	2.45	0.41
1:F:451:PRO:HG2	1:F:454:ILE:HG21	2.01	0.41
1:G:62:GLN:OE1	1:G:92:ARG:HD2	2.19	0.41
1:G:768:PRO:HA	1:G:773:TYR:CD2	2.55	0.41
1:G:837:ASN:HB3	1:h:583:PRO:HG2	2.02	0.41
1:H:143:PRO:O	1:H:145:GLN:NE2	2.53	0.41
1:H:156:ILE:HD13	1:H:252:VAL:HG23	2.02	0.41
1:H:354:TRP:HZ3	1:I:741:TYR:O	2.02	0.41
1:H:634:ALA:HB2	1:J:10:TRP:CZ2	2.54	0.41
1:H:787:TYR:HD1	1:I:382:PHE:CE2	2.39	0.41
1:I:182:PRO:HD2	1:I:205:ARG:HH21	1.85	0.41
1:I:328:LEU:HD23	1:I:328:LEU:H	1.83	0.41
1:J:240:TYR:CD2	1:J:252:VAL:HG22	2.55	0.41
1:J:560:GLY:O	1:J:646:ARG:NH2	2.53	0.41
1:X:216:TYR:HD2	1:X:265:THR:HG21	1.84	0.41
1:X:710:ASP:N	1:X:710:ASP:OD1	2.53	0.41
1:Y:114:LYS:HD3	1:Y:289:ASN:O	2.21	0.41
1:Y:176:ALA:HB1	1:Y:181:GLN:HB3	2.01	0.41
1:Y:217:GLY:HA3	1:Y:262:THR:HG22	2.02	0.41
1:Y:675:SER:O	1:Y:830:TRP:NE1	2.34	0.41
1:Y:833:PRO:HG2	1:Y:838:PHE:HA	2.02	0.41
1:g:560:GLY:O	1:g:646:ARG:NH2	2.51	0.41
1:g:615:LEU:HD12	1:g:651:LEU:HD11	2.01	0.41
1:g:691:TRP:N	1:g:692:PRO:HD2	2.35	0.41
1:h:183:GLU:HB2	1:h:186:LEU:HD23	2.02	0.41
1:h:369:ASP:HA	1:h:485:ARG:HA	2.01	0.41
1:h:419:LEU:HG	1:i:786:ALA:HB1	2.01	0.41
1:h:548:ARG:O	1:h:554:ILE:HD11	2.20	0.41
1:i:325:VAL:HG13	1:i:528:PHE:CE2	2.55	0.41
1:i:636:ARG:CZ	1:i:880:GLU:HB3	2.49	0.41
1:i:786:ALA:H	1:i:798:GLY:HA3	1.85	0.41
9:j:252:LYS:HB3	9:j:252:LYS:HE2	1.71	0.41
1:A:308:SER:OG	1:A:309:GLY:N	2.53	0.41
1:A:354:TRP:HH2	1:Y:741:TYR:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:665:ILE:O	1:A:669:ASP:HB2	2.21	0.41
1:A:735:ASN:N	1:A:735:ASN:ND2	2.68	0.41
1:A:782:ARG:O	1:A:803:GLN:HB2	2.21	0.41
1:A:802:PRO:HD3	1:X:131:ASN:HB2	2.01	0.41
1:D:881:VAL:CG1	1:D:903:PRO:HB2	2.50	0.41
1:F:56:VAL:O	1:F:584:MET:HA	2.21	0.41
1:F:316:ALA:HB2	1:F:323:ASN:HA	2.02	0.41
1:F:705:ILE:HG23	1:F:725:TRP:CD1	2.56	0.41
1:H:416:LYS:HE2	1:I:199:ILE:HG13	2.01	0.41
1:H:625:LEU:CD2	1:H:626:PRO:HD3	2.49	0.41
1:H:765:VAL:O	1:H:767:ASN:N	2.49	0.41
1:H:811:ASP:OD1	1:H:812:PRO:HD2	2.19	0.41
1:J:8:PRO:HB3	7:R:18:GLY:HA3	2.02	0.41
1:X:608:TYR:HE2	3:f:19:LYS:HG2	1.86	0.41
1:Y:122:ASN:ND2	1:Y:215:CYS:O	2.54	0.41
1:Y:785:PRO:HB2	1:Y:799:HIS:O	2.19	0.41
1:g:290:ARG:HD2	1:g:441:LEU:HD22	2.01	0.41
9:j:365:SER:OG	9:j:370:ASN:HB3	2.20	0.41
1:A:149:GLN:HG2	1:X:419:LEU:HD12	2.02	0.41
1:A:199:ILE:O	1:X:416:LYS:NZ	2.41	0.41
1:A:370:ASN:CB	1:A:482:ILE:HA	2.50	0.41
1:A:636:ARG:CZ	1:A:880:GLU:HB3	2.50	0.41
1:D:306:TYR:CZ	1:D:527:LYS:HB2	2.55	0.41
1:D:803:GLN:HE22	1:F:122:ASN:HD21	1.68	0.41
1:G:191:TRP:HB3	1:G:384:LEU:HD23	2.02	0.41
1:G:321:GLN:NE2	1:g:631:ASN:ND2	2.66	0.41
1:H:477:ASP:OD1	1:H:478:THR:N	2.43	0.41
1:H:783:THR:OG1	1:H:803:GLN:NE2	2.42	0.41
1:I:47:ASN:HA	1:I:48:PRO:HD3	1.92	0.41
1:I:882:PHE:O	1:I:901:ARG:HA	2.20	0.41
1:J:609:LEU:O	1:J:609:LEU:HD23	2.20	0.41
7:R:200:GLN:NE2	7:R:207:VAL:HG22	2.34	0.41
1:Y:19:ASP:OD1	2:d:14:GLY:HA3	2.20	0.41
1:Y:68:PHE:HB2	1:Y:577:LEU:HD21	2.01	0.41
1:Y:278:LYS:HG3	1:Y:279:VAL:H	1.84	0.41
1:g:240:TYR:CD2	1:g:252:VAL:HG22	2.55	0.41
1:g:318:GLN:NE2	1:g:540:THR:HG22	2.36	0.41
1:g:370:ASN:CB	1:g:482:ILE:HA	2.50	0.41
1:g:512:LEU:HD23	1:g:512:LEU:H	1.85	0.41
1:g:642:ARG:NH1	1:g:867:ASP:O	2.31	0.41
1:g:816:LEU:HB3	1:g:817:ARG:H	1.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:782:ARG:CZ	1:h:804:LEU:HD22	2.50	0.41
1:i:195:SER:HB3	1:i:389:ILE:HG21	2.02	0.41
9:j:293:ASP:HB3	9:j:297:ARG:H	1.84	0.41
1:A:133:THR:HG22	1:A:207:LEU:HB2	2.02	0.41
1:A:292:ASN:HD21	1:A:561:ASN:HD21	1.69	0.41
1:F:396:VAL:HG12	1:F:405:ASN:HA	2.01	0.41
1:G:482:ILE:HD13	1:h:120:ALA:HB2	2.03	0.41
1:G:582:PHE:CD2	1:G:584:MET:HB3	2.55	0.41
1:G:821:ARG:NH2	1:h:519:ASP:O	2.54	0.41
1:I:219:TYR:CZ	1:J:808:PRO:HD3	2.55	0.41
1:I:499:HIS:ND1	1:I:501:ARG:HG2	2.36	0.41
1:I:627:ILE:HG12	1:I:861:ASP:HA	2.01	0.41
1:J:473:SER:OG	1:J:791:PHE:N	2.40	0.41
1:X:19:ASP:HB3	1:X:22:GLU:CD	2.46	0.41
1:X:132:ASN:OD1	1:X:148:ALA:HA	2.21	0.41
1:g:261:LEU:HD23	1:g:261:LEU:H	1.85	0.41
1:g:396:VAL:HG11	1:g:403:TRP:HB3	2.01	0.41
1:h:486:TRP:CD1	1:h:763:ARG:HD3	2.55	0.41
1:h:550:ASP:CG	1:h:564:ARG:HH21	2.28	0.41
1:i:56:VAL:O	1:i:584:MET:HA	2.21	0.41
9:j:456:ASP:OD1	9:j:457:ALA:N	2.48	0.41
1:G:684:GLN:NE2	1:H:906:ALA:HB3	2.35	0.41
1:H:618:ILE:CD1	1:H:866:MET:HE1	2.51	0.41
1:J:343:ASN:HA	1:J:750:ARG:HD2	2.02	0.41
8:P:93:SER:O	8:P:97:LEU:HD23	2.21	0.41
1:X:315:LEU:HD23	1:X:531:ILE:HD12	2.01	0.41
1:X:451:PRO:O	1:X:454:ILE:HG22	2.21	0.41
1:Y:366:ARG:HH11	1:Y:496:PRO:HG3	1.84	0.41
1:g:156:ILE:HD13	1:g:252:VAL:HG23	2.01	0.41
1:g:298:ASP:OD1	1:g:347:ARG:NH2	2.51	0.41
1:g:547:PHE:CE2	1:g:575:VAL:HG11	2.55	0.41
1:g:627:ILE:HA	1:g:628:PRO:HD3	1.94	0.41
1:g:811:ASP:HB2	1:g:812:PRO:HD2	2.03	0.41
1:h:88:VAL:HB	1:h:538:PRO:HA	2.03	0.41
1:h:626:PRO:CB	1:h:861:ASP:HA	2.50	0.41
1:i:39:PHE:CE2	1:i:41:ILE:HD11	2.56	0.41
1:A:354:TRP:O	1:A:356:GLN:N	2.52	0.41
1:A:370:ASN:HB3	1:A:482:ILE:HA	2.02	0.41
1:D:551:VAL:HG11	1:D:568:ALA:HB3	2.02	0.41
1:D:721:MET:HE1	1:D:754:PHE:CZ	2.56	0.41
1:F:330:ASP:HB2	1:F:901:ARG:HH12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:648:THR:HG22	1:F:649:PRO:O	2.20	0.41
1:G:182:PRO:HD2	1:G:205:ARG:HH21	1.85	0.41
1:G:790:ARG:H	1:G:790:ARG:HG2	1.64	0.41
1:G:888:HIS:HB3	7:R:40:MET:SD	2.61	0.41
1:H:165:MET:HG3	1:H:181:GLN:HG3	2.03	0.41
1:H:396:VAL:CG1	1:H:403:TRP:HB3	2.50	0.41
1:H:743:LEU:HD23	1:H:743:LEU:HA	1.83	0.41
1:I:46:ARG:HH12	1:J:606:ASN:HD22	1.68	0.41
1:I:721:MET:HE3	1:I:726:PHE:HD1	1.85	0.41
1:J:500:HIS:HA	1:J:558:THR:HG21	2.01	0.41
7:R:203:ARG:NH2	1:g:892:ARG:HH11	2.18	0.41
1:h:83:ARG:HA	1:h:544:GLU:HA	2.02	0.41
1:h:814:HIS:CG	1:i:517:PHE:HE1	2.39	0.41
1:i:205:ARG:HH21	1:i:256:GLU:CD	2.29	0.41
1:i:240:TYR:CD1	1:i:252:VAL:HG22	2.50	0.41
1:i:369:ASP:O	1:i:371:VAL:N	2.50	0.41
1:A:38:TYR:HB2	1:X:839:MET:SD	2.61	0.41
1:A:266:HIS:CD2	1:A:287:ALA:HB3	2.56	0.41
1:D:66:LEU:HD13	1:D:581:PHE:CE1	2.56	0.41
1:F:819:PRO:HG2	1:g:519:ASP:HB2	2.02	0.41
1:G:153:VAL:HG21	1:G:188:ILE:HB	2.03	0.41
1:G:245:ASP:OD1	1:h:405:ASN:ND2	2.50	0.41
1:I:120:ALA:HB2	1:J:482:ILE:HD13	2.02	0.41
1:I:298:ASP:O	1:I:301:VAL:HG23	2.21	0.41
1:I:389:ILE:HD11	1:J:147:ILE:HD11	2.03	0.41
1:I:613:ASN:ND2	1:I:878:LEU:HD22	2.35	0.41
1:J:908:ASN:HB2	7:N:33:TRP:CE2	2.56	0.41
5:K:26:SER:HB3	5:K:37:GLN:NE2	2.35	0.41
6:M:212:ALA:O	7:R:211:SER:HA	2.21	0.41
1:Y:532:ARG:NH2	1:Y:533:ASN:OD1	2.54	0.41
1:g:20:ALA:HA	1:g:23:TYR:CE2	2.55	0.41
1:g:43:ASN:OD1	1:g:44:LYS:HD2	2.21	0.41
1:g:165:MET:SD	1:g:181:GLN:HG3	2.60	0.41
1:g:321:GLN:O	1:g:321:GLN:HG2	2.21	0.41
1:g:623:THR:HG22	1:g:865:GLU:HA	2.02	0.41
1:g:786:ALA:H	1:g:798:GLY:HA3	1.86	0.41
1:h:557:SER:OG	1:h:559:LEU:O	2.31	0.41
1:i:353:MET:HG2	1:i:354:TRP:CD2	2.55	0.41
9:j:285:LYS:HA	9:j:285:LYS:HD3	1.84	0.41
9:j:321:TYR:CE2	9:j:335:LEU:HA	2.53	0.41
1:A:145:GLN:HE21	1:X:409:SER:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:THR:HA	1:A:864:PHE:O	2.21	0.41
1:A:626:PRO:CD	1:A:862:MET:O	2.69	0.41
1:A:749:ASP:OD2	1:X:349:ARG:NH1	2.54	0.41
1:D:216:TYR:HE2	1:D:288:PRO:HG3	1.85	0.41
1:D:245:ASP:OD1	1:F:405:ASN:ND2	2.52	0.41
1:D:382:PHE:CE2	1:F:787:TYR:HD1	2.39	0.41
1:D:512:LEU:HD23	1:D:512:LEU:H	1.86	0.41
1:D:647:GLU:HG2	1:D:661:TYR:CE2	2.56	0.41
1:F:105:GLY:HA2	1:F:573:THR:HG22	2.03	0.41
1:F:139:ASN:HB3	1:F:142:HIS:ND1	2.36	0.41
1:F:290:ARG:NH1	1:F:441:LEU:HB3	2.35	0.41
1:F:496:PRO:HG2	1:F:497:PHE:CD1	2.56	0.41
1:F:534:LEU:HD23	1:F:605:PHE:CE2	2.56	0.41
1:G:615:LEU:HD23	1:G:876:TYR:CD1	2.56	0.41
1:G:623:THR:HG22	1:G:865:GLU:HB3	2.02	0.41
1:G:627:ILE:HB	1:G:860:LEU:O	2.21	0.41
1:H:231:LYS:NZ	1:H:259:ASP:HB3	2.36	0.41
1:H:381:CYS:HB3	1:J:424:ILE:HG12	2.02	0.41
1:H:479:TYR:HB2	1:H:806:LEU:HD22	2.03	0.41
1:I:62:GLN:NE2	1:I:583:PRO:HA	2.36	0.41
1:I:293:PHE:HB2	1:I:558:THR:HG23	2.02	0.41
1:I:302:GLY:O	1:I:548:ARG:NH1	2.48	0.41
1:I:794:ALA:HA	1:I:795:PRO:HD3	1.84	0.41
1:J:183:GLU:HA	1:J:184:PRO:HD3	1.88	0.41
1:J:294:ILE:HG12	1:J:557:SER:HB3	2.03	0.41
1:J:761:MET:N	1:J:822:LYS:O	2.53	0.41
5:K:221:ASN:HB3	5:K:252:ASN:ND2	2.36	0.41
2:L:216:PHE:CD1	7:R:192:GLY:HA2	2.56	0.41
8:Q:57:ASN:OD1	8:Q:58:LEU:N	2.54	0.41
8:V:47:GLU:HB2	1:h:720:ASN:OD1	2.20	0.41
1:X:396:VAL:HG11	1:X:403:TRP:HB3	2.02	0.41
1:X:564:ARG:NH2	1:X:659:PHE:HB3	2.32	0.41
1:Y:153:VAL:HA	1:Y:202:ALA:HA	2.03	0.41
1:Y:163:LEU:HD21	1:Y:203:GLY:HA3	2.02	0.41
1:Y:354:TRP:CH2	1:Y:525:PRO:HB3	2.56	0.41
1:Y:631:ASN:O	1:Y:632:TRP:HB2	2.20	0.41
1:g:19:ASP:HB3	1:g:22:GLU:HG2	2.02	0.41
1:g:103:ILE:HG12	1:g:575:VAL:HG22	2.03	0.41
1:g:116:TYR:OH	1:g:264:ASP:OD2	2.36	0.41
1:g:315:LEU:HD13	1:g:531:ILE:HD12	2.03	0.41
1:g:743:LEU:HD12	1:g:744:PRO:HD2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:19:ASP:OD1	1:h:20:ALA:N	2.54	0.41
1:i:289:ASN:O	1:i:290:ARG:O	2.39	0.41
1:i:642:ARG:HD3	1:i:677:THR:OG1	2.21	0.41
1:i:682:ALA:O	1:i:862:MET:HA	2.21	0.41
9:j:198:LYS:HD2	9:j:198:LYS:HA	1.94	0.41
9:j:412:GLU:H	9:j:412:GLU:CD	2.29	0.41
9:j:451:ARG:HG2	9:j:453:THR:HG23	2.03	0.41
1:A:186:LEU:HD13	1:Y:789:PHE:CE1	2.56	0.41
1:A:304:MET:HB3	1:A:545:TRP:HE1	1.85	0.41
1:A:723:LYS:NZ	1:X:102:ASP:OD2	2.51	0.41
1:A:852:LEU:HD22	1:X:10:TRP:CZ3	2.56	0.41
1:D:57:THR:HA	1:D:584:MET:HA	2.01	0.41
1:F:83:ARG:HG3	1:F:544:GLU:HB3	2.03	0.41
1:G:456:LEU:HD21	1:G:468:GLY:HA3	2.02	0.41
1:G:491:MET:HE3	1:G:491:MET:HB3	2.00	0.41
1:G:512:LEU:HD23	1:G:512:LEU:H	1.85	0.41
1:H:259:ASP:OD1	1:H:259:ASP:N	2.53	0.41
1:H:816:LEU:HG	1:H:817:ARG:H	1.86	0.41
1:H:902:THR:HG21	1:J:10:TRP:HE1	1.85	0.41
1:I:185:GLN:HB2	1:I:186:LEU:HD12	2.03	0.41
1:I:583:PRO:HG2	1:J:837:ASN:HB3	2.03	0.41
1:J:66:LEU:HD23	1:J:66:LEU:HA	1.89	0.41
1:J:108:ASP:OD1	1:J:516:ARG:HG2	2.21	0.41
1:J:259:ASP:OD1	1:J:259:ASP:N	2.53	0.41
1:J:306:TYR:CZ	1:J:527:LYS:HB2	2.56	0.41
8:O:87:MET:HE1	8:P:87:MET:CE	2.51	0.41
1:X:155:THR:OG1	1:X:164:GLN:OE1	2.39	0.41
1:X:200:ASP:OD1	1:X:201:GLN:N	2.55	0.41
1:X:635:PHE:HE2	1:X:638:TRP:CE2	2.39	0.41
1:X:760:PRO:HG2	1:Y:352:SER:OG	2.21	0.41
1:X:790:ARG:HG3	1:X:790:ARG:NH1	2.35	0.41
1:Y:114:LYS:HB3	1:Y:291:PRO:HA	2.03	0.41
1:g:298:ASP:O	1:g:301:VAL:HG23	2.21	0.41
1:h:75:ASP:HB3	1:h:80:TYR:CD1	2.56	0.41
1:h:366:ARG:NH1	1:h:496:PRO:HG3	2.36	0.41
1:h:624:GLN:HG3	1:h:875:LEU:HD13	2.03	0.41
1:i:639:SER:HA	1:i:830:TRP:O	2.21	0.41
9:j:264:TYR:C	9:j:266:ASP:H	2.28	0.41
9:j:379:LEU:O	9:j:381:LEU:N	2.52	0.41
1:A:598:ASN:OD1	1:A:599:ASP:N	2.54	0.40
1:D:28:LEU:HD22	1:g:601:ASN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:767:ASN:CB	1:D:816:LEU:HD23	2.51	0.40
1:D:777:GLY:O	1:D:781:HIS:HB2	2.21	0.40
1:D:811:ASP:OD1	1:D:812:PRO:HD2	2.21	0.40
1:F:211:THR:HG22	1:F:276:ARG:NH1	2.36	0.40
1:F:723:LYS:HE3	1:g:578:TYR:CE1	2.56	0.40
1:G:743:LEU:HD21	1:h:349:ARG:HB3	2.03	0.40
1:H:19:ASP:HB3	1:H:22:GLU:HG2	2.03	0.40
1:I:101:PHE:HB2	1:I:524:VAL:HG22	2.03	0.40
1:I:112:SER:OG	1:I:561:ASN:ND2	2.54	0.40
1:I:614:MET:HB2	1:I:877:VAL:HG13	2.03	0.40
1:I:658:TYR:CZ	8:Q:39:PRO:HD3	2.57	0.40
1:I:880:GLU:C	1:I:881:VAL:HG13	2.46	0.40
1:J:308:SER:OG	1:J:311:ASN:O	2.40	0.40
1:J:639:SER:O	1:J:878:LEU:HD23	2.21	0.40
1:X:181:GLN:O	1:X:183:GLU:N	2.54	0.40
1:Y:31:PHE:O	1:Y:35:THR:HG22	2.22	0.40
1:Y:290:ARG:HH21	1:Y:559:LEU:CD2	2.34	0.40
1:Y:611:ALA:HA	1:Y:881:VAL:HG22	2.03	0.40
1:g:177:ASN:HB3	1:g:181:GLN:HB2	2.03	0.40
1:g:511:LEU:HD23	1:g:511:LEU:HA	1.87	0.40
1:i:473:SER:OG	1:i:792:CYS:N	2.54	0.40
1:A:124:PHE:CZ	1:Y:429:ASN:HA	2.55	0.40
1:A:343:ASN:HA	1:A:750:ARG:HD2	2.03	0.40
1:A:351:PHE:CE2	1:A:353:MET:HB3	2.56	0.40
1:A:438:ASN:O	1:A:499:HIS:HE1	2.04	0.40
4:E:15:VAL:HG12	6:M:240:ILE:HA	2.04	0.40
4:E:63:ILE:HD11	6:M:260:LEU:HD21	2.03	0.40
1:F:367:VAL:HG13	1:F:367:VAL:O	2.22	0.40
1:F:377:MET:HE1	1:g:432:ARG:HB3	2.03	0.40
1:F:431:TRP:CZ2	1:F:435:LEU:HD11	2.56	0.40
1:F:459:ASN:HB3	1:F:462:THR:OG1	2.21	0.40
1:G:63:ARG:HH21	1:i:695:ASP:HB3	1.87	0.40
1:G:369:ASP:O	1:G:371:VAL:N	2.52	0.40
1:G:424:ILE:HG13	1:i:381:CYS:SG	2.61	0.40
1:G:615:LEU:HD22	1:G:874:LEU:HD13	2.02	0.40
1:H:212:GLN:HG2	1:H:276:ARG:O	2.21	0.40
1:H:768:PRO:HA	1:H:773:TYR:CD2	2.57	0.40
1:I:117:SER:H	1:J:372:GLY:HA3	1.85	0.40
1:I:122:ASN:OD1	1:J:784:THR:HA	2.21	0.40
1:I:192:THR:HG23	1:J:283:SER:HB3	2.03	0.40
1:I:537:LEU:HB3	1:I:597:ARG:HH21	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:890:PRO:HB2	1:I:891:HIS:ND1	2.36	0.40
1:J:200:ASP:OD1	1:J:200:ASP:N	2.47	0.40
1:J:467:ASN:C	1:J:467:ASN:HD22	2.26	0.40
1:J:675:SER:O	1:J:830:TRP:NE1	2.39	0.40
1:J:764:GLN:HE21	1:J:819:PRO:HB3	1.85	0.40
1:X:679:ARG:NH2	1:X:867:ASP:HA	2.35	0.40
1:X:801:TYR:CD1	1:X:802:PRO:HD2	2.57	0.40
1:Y:366:ARG:HA	1:Y:366:ARG:HD2	1.89	0.40
1:h:242:ARG:HA	1:h:250:GLU:HG2	2.03	0.40
1:i:300:PHE:CG	1:i:524:VAL:HG12	2.56	0.40
1:i:314:VAL:HG23	1:i:323:ASN:CG	2.46	0.40
1:i:785:PRO:CD	1:i:803:GLN:HE21	2.33	0.40
1:A:13:MET:O	1:A:15:ILE:N	2.53	0.40
1:A:94:LEU:HB2	1:A:581:PHE:CE2	2.56	0.40
1:A:259:ASP:OD1	1:A:259:ASP:N	2.45	0.40
1:A:328:LEU:C	1:A:330:ASP:H	2.28	0.40
1:A:611:ALA:HA	1:A:881:VAL:HG22	2.03	0.40
1:D:635:PHE:HE1	1:D:879:PHE:HB3	1.86	0.40
1:G:62:GLN:HE22	1:G:583:PRO:HA	1.85	0.40
1:G:438:ASN:OD1	1:G:500:HIS:NE2	2.53	0.40
1:G:553:MET:HE3	1:G:553:MET:HB3	1.82	0.40
1:H:13:MET:HG3	1:I:900:LEU:HD22	2.04	0.40
1:H:369:ASP:OD1	1:H:369:ASP:N	2.53	0.40
1:H:482:ILE:HG12	1:J:116:TYR:CD2	2.55	0.40
1:H:723:LYS:HB2	1:H:723:LYS:HE3	1.73	0.40
1:I:20:ALA:HA	1:I:23:TYR:CE2	2.56	0.40
1:I:147:ILE:HG13	1:I:147:ILE:O	2.21	0.40
1:I:222:PRO:HB3	1:J:804:LEU:HD12	2.04	0.40
1:I:512:LEU:HD23	1:I:512:LEU:H	1.86	0.40
1:I:551:VAL:HG21	1:I:568:ALA:O	2.20	0.40
1:I:786:ALA:HB1	1:J:419:LEU:HD13	2.03	0.40
1:J:398:ARG:HD3	1:J:403:TRP:CE2	2.56	0.40
1:J:731:LEU:HD23	1:J:737:GLY:H	1.86	0.40
5:K:264:THR:HG23	5:K:283:ARG:NH2	2.37	0.40
7:N:172:ILE:HG23	7:N:176:GLN:HB3	2.04	0.40
1:X:127:LYS:HB2	1:X:285:HIS:CE1	2.56	0.40
1:X:336:SER:OG	1:X:609:LEU:HB3	2.22	0.40
1:Y:67:ARG:HD2	1:Y:578:TYR:OH	2.21	0.40
1:Y:194:GLY:HA2	1:Y:199:ILE:HG21	2.03	0.40
1:Y:242:ARG:NH1	1:Y:247:GLY:H	2.19	0.40
1:Y:328:LEU:O	1:Y:328:LEU:HG	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:366:ARG:NH2	1:Y:824:LEU:HD11	2.36	0.40
1:Y:630:ARG:HG2	1:Y:631:ASN:H	1.87	0.40
1:h:307:ASN:ND2	1:h:327:ASP:OD2	2.55	0.40
1:h:630:ARG:HA	1:h:630:ARG:HD3	1.92	0.40
9:j:124:ASN:HA	9:j:430:ASN:OD1	2.22	0.40
9:j:213:GLN:OE1	9:j:308:ARG:NE	2.51	0.40
9:j:413:ASN:HB3	9:j:416:LEU:HB2	2.03	0.40
1:A:207:LEU:HD12	1:Y:801:TYR:CE1	2.57	0.40
1:A:600:THR:HG21	7:N:189:PRO:HG2	2.03	0.40
1:D:12:TYR:CE2	1:G:909:ALA:HB3	2.54	0.40
1:D:409:SER:HA	1:g:145:GLN:HE21	1.86	0.40
1:D:505:LEU:HD22	1:D:556:GLN:NE2	2.37	0.40
4:E:55:LEU:O	4:E:59:ILE:HG12	2.22	0.40
1:F:399:ASN:CG	1:F:400:GLN:H	2.29	0.40
1:F:782:ARG:HD2	1:F:785:PRO:HG3	2.04	0.40
1:G:114:LYS:CD	1:G:289:ASN:HB3	2.51	0.40
1:G:658:TYR:HE2	1:g:81:LYS:HE3	1.85	0.40
1:H:514:ASN:ND2	1:I:482:ILE:O	2.40	0.40
1:I:267:LEU:HD23	1:I:267:LEU:HA	1.97	0.40
1:I:306:TYR:HE2	1:I:527:LYS:HE2	1.86	0.40
1:I:435:LEU:HD12	1:I:435:LEU:HA	1.94	0.40
1:I:877:VAL:C	1:I:878:LEU:HD23	2.46	0.40
1:J:109:ARG:NH2	1:J:512:LEU:HG	2.36	0.40
1:J:273:ALA:HA	1:J:276:ARG:HB2	2.02	0.40
1:J:431:TRP:CD1	1:J:478:THR:HG1	2.39	0.40
6:M:181:VAL:HG13	6:M:182:THR:HG23	2.04	0.40
8:O:16:LEU:HD12	8:O:17:PRO:HD2	2.02	0.40
2:T:28:HIS:O	2:T:28:HIS:ND1	2.52	0.40
1:Y:377:MET:HE2	1:Y:377:MET:HB3	1.90	0.40
1:Y:550:ASP:O	1:Y:554:ILE:HG12	2.21	0.40
1:Y:734:TYR:HB2	1:Y:736:ILE:HG12	2.03	0.40
1:Y:784:THR:N	1:Y:785:PRO:HD3	2.36	0.40
1:h:145:GLN:HG2	1:i:411:ASN:HB2	2.03	0.40
1:h:797:GLU:OE1	1:i:187:GLY:N	2.54	0.40
1:h:847:LEU:HD23	1:h:853:TYR:CE2	2.57	0.40
1:i:553:MET:HE3	1:i:553:MET:HB3	1.82	0.40
1:A:891:HIS:O	1:A:894:VAL:HG12	2.21	0.40
1:D:477:ASP:O	1:D:480:VAL:HG22	2.21	0.40
1:D:630:ARG:NH2	1:D:905:SER:H	2.19	0.40
1:F:176:ALA:HB1	1:F:181:GLN:HB3	2.03	0.40
1:F:789:PHE:CD1	1:F:790:ARG:N	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:77:GLN:HG3	1:G:78:TYR:CD1	2.56	0.40
1:G:121:TYR:O	1:i:783:THR:OG1	2.38	0.40
1:G:382:PHE:CD2	1:h:787:TYR:HD2	2.39	0.40
1:G:479:TYR:HB2	1:G:806:LEU:HD11	2.04	0.40
1:G:683:ILE:HG13	1:G:862:MET:HE3	2.02	0.40
1:G:809:HIS:ND1	1:G:809:HIS:O	2.54	0.40
1:I:109:ARG:HB2	1:I:294:ILE:HG21	2.02	0.40
1:I:684:GLN:O	1:I:860:LEU:HD12	2.22	0.40
1:I:874:LEU:HD12	1:I:874:LEU:O	2.21	0.40
1:J:369:ASP:HB3	1:J:485:ARG:HG2	2.04	0.40
1:J:512:LEU:H	1:J:512:LEU:HD23	1.87	0.40
8:P:24:GLN:HG3	8:P:40:ASN:ND2	2.36	0.40
1:X:716:VAL:HG11	1:X:726:PHE:CB	2.46	0.40
1:X:799:HIS:HA	1:Y:149:GLN:NE2	2.36	0.40
1:Y:681:VAL:O	1:Y:703:PHE:N	2.49	0.40
1:Y:758:PHE:CE2	1:Y:760:PRO:HG3	2.57	0.40
1:g:337:TYR:CD2	1:g:527:LYS:HD3	2.57	0.40
1:g:627:ILE:HG21	1:g:860:LEU:HB2	2.03	0.40
1:h:366:ARG:CZ	1:h:824:LEU:HD21	2.52	0.40
1:h:686:ASP:OD2	1:h:858:HIS:ND1	2.34	0.40
1:i:491:MET:HE3	1:i:491:MET:HB3	1.92	0.40
9:j:244:LEU:HD13	9:j:247:LEU:HD21	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	896/911 (98%)	800 (89%)	89 (10%)	7 (1%)	16 46
1	D	901/911 (99%)	810 (90%)	90 (10%)	1 (0%)	48 76
1	F	903/911 (99%)	811 (90%)	91 (10%)	1 (0%)	48 76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	905/911 (99%)	811 (90%)	91 (10%)	3 (0%)	37	66
1	H	899/911 (99%)	803 (89%)	93 (10%)	3 (0%)	37	66
1	I	895/911 (98%)	813 (91%)	80 (9%)	2 (0%)	44	71
1	J	907/911 (100%)	818 (90%)	86 (10%)	3 (0%)	37	66
1	X	902/911 (99%)	828 (92%)	72 (8%)	2 (0%)	44	71
1	Y	902/911 (99%)	801 (89%)	97 (11%)	4 (0%)	30	61
1	g	903/911 (99%)	818 (91%)	79 (9%)	6 (1%)	19	50
1	h	903/911 (99%)	818 (91%)	83 (9%)	2 (0%)	44	71
1	i	902/911 (99%)	821 (91%)	79 (9%)	2 (0%)	44	71
2	B	16/263 (6%)	11 (69%)	5 (31%)	0	100	100
2	L	48/263 (18%)	45 (94%)	3 (6%)	0	100	100
2	S	31/263 (12%)	30 (97%)	1 (3%)	0	100	100
2	T	24/263 (9%)	22 (92%)	2 (8%)	0	100	100
2	Z	20/263 (8%)	18 (90%)	2 (10%)	0	100	100
2	a	23/263 (9%)	22 (96%)	1 (4%)	0	100	100
2	b	28/263 (11%)	27 (96%)	1 (4%)	0	100	100
2	c	22/263 (8%)	22 (100%)	0	0	100	100
2	d	12/263 (5%)	10 (83%)	2 (17%)	0	100	100
3	C	6/171 (4%)	5 (83%)	1 (17%)	0	100	100
3	U	6/171 (4%)	5 (83%)	1 (17%)	0	100	100
3	e	6/171 (4%)	6 (100%)	0	0	100	100
3	f	6/171 (4%)	6 (100%)	0	0	100	100
4	E	34/80 (42%)	33 (97%)	1 (3%)	0	100	100
5	K	250/568 (44%)	239 (96%)	11 (4%)	0	100	100
6	M	102/410 (25%)	91 (89%)	9 (9%)	2 (2%)	6	28
7	N	174/216 (81%)	161 (92%)	12 (7%)	1 (1%)	22	53
7	R	174/216 (81%)	162 (93%)	12 (7%)	0	100	100
8	O	109/125 (87%)	105 (96%)	3 (3%)	1 (1%)	14	44
8	P	109/125 (87%)	105 (96%)	4 (4%)	0	100	100
8	Q	109/125 (87%)	106 (97%)	1 (1%)	2 (2%)	7	30
8	V	109/125 (87%)	107 (98%)	1 (1%)	1 (1%)	14	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	j	437/482 (91%)	401 (92%)	36 (8%)	0	100	100
All	All	12673/16455 (77%)	11491 (91%)	1139 (9%)	43 (0%)	38	66

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	634	ALA
1	H	626	PRO
1	H	827	ARG
1	I	796	ARG
1	J	355	ASN
6	M	290	ALA
1	X	355	ASN
1	Y	630	ARG
1	g	626	PRO
1	g	811	ASP
1	i	795	PRO
1	A	9	GLN
1	A	630	ARG
1	F	628	PRO
1	J	608	TYR
7	N	150	SER
1	g	288	PRO
1	g	628	PRO
1	A	627	ILE
1	G	627	ILE
1	J	627	ILE
1	X	627	ILE
1	Y	627	ILE
1	h	380	TYR
1	i	290	ARG
1	A	199	ILE
1	G	427	ALA
6	M	168	VAL
8	O	76	VAL
8	Q	76	VAL
8	V	76	VAL
1	g	795	PRO
1	A	380	TYR
1	A	628	PRO
1	g	627	ILE
1	Y	628	PRO

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Mol	Chain	Res	Type
1	D	811	ASP
1	H	628	PRO
1	I	881	VAL
1	h	795	PRO
8	Q	7	ILE
1	A	794	ALA
1	Y	199	ILE

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	777/786 (99%)	775 (100%)	2 (0%)	91	94
1	D	780/786 (99%)	779 (100%)	1 (0%)	92	96
1	F	782/786 (100%)	781 (100%)	1 (0%)	92	96
1	G	782/786 (100%)	782 (100%)	0	100	100
1	H	778/786 (99%)	774 (100%)	4 (0%)	86	91
1	I	776/786 (99%)	774 (100%)	2 (0%)	91	94
1	J	783/786 (100%)	782 (100%)	1 (0%)	92	96
1	X	781/786 (99%)	780 (100%)	1 (0%)	92	96
1	Y	781/786 (99%)	780 (100%)	1 (0%)	92	96
1	g	782/786 (100%)	780 (100%)	2 (0%)	91	94
1	h	782/786 (100%)	781 (100%)	1 (0%)	92	96
1	i	781/786 (99%)	781 (100%)	0	100	100
2	B	14/210 (7%)	14 (100%)	0	100	100
2	L	42/210 (20%)	42 (100%)	0	100	100
2	S	25/210 (12%)	25 (100%)	0	100	100
2	T	21/210 (10%)	21 (100%)	0	100	100
2	Z	16/210 (8%)	16 (100%)	0	100	100
2	a	19/210 (9%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	22/210 (10%)	22 (100%)	0	100	100
2	c	19/210 (9%)	19 (100%)	0	100	100
2	d	11/210 (5%)	11 (100%)	0	100	100
3	C	6/127 (5%)	6 (100%)	0	100	100
3	U	6/127 (5%)	6 (100%)	0	100	100
3	e	6/127 (5%)	6 (100%)	0	100	100
3	f	6/127 (5%)	6 (100%)	0	100	100
4	E	27/55 (49%)	27 (100%)	0	100	100
5	K	222/474 (47%)	221 (100%)	1 (0%)	86	91
6	M	98/345 (28%)	98 (100%)	0	100	100
7	N	151/179 (84%)	151 (100%)	0	100	100
7	R	151/179 (84%)	151 (100%)	0	100	100
8	O	93/103 (90%)	93 (100%)	0	100	100
8	P	93/103 (90%)	93 (100%)	0	100	100
8	Q	93/103 (90%)	92 (99%)	1 (1%)	70	82
8	V	93/103 (90%)	93 (100%)	0	100	100
9	j	394/432 (91%)	394 (100%)	0	100	100
All	All	10993/13906 (79%)	10975 (100%)	18 (0%)	91	95

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	614	MET
1	A	735	ASN
1	D	132	ASN
1	F	694	ASN
1	H	615	LEU
1	H	627	ILE
1	H	875	LEU
1	H	877	VAL
1	I	736	ILE
1	I	878	LEU
1	J	609	LEU
5	K	105	GLN
8	Q	48	THR
1	X	735	ASN

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Mol	Chain	Res	Type
1	Y	609	LEU
1	g	426	LEU
1	g	627	ILE
1	h	523	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (211) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	GLN
1	A	33	GLN
1	A	65	GLN
1	A	91	ASN
1	A	122	ASN
1	A	161	ASN
1	A	185	GLN
1	A	266	HIS
1	A	307	ASN
1	A	343	ASN
1	A	397	GLN
1	A	438	ASN
1	A	467	ASN
1	A	499	HIS
1	A	523	GLN
1	A	561	ASN
1	A	624	GLN
1	A	735	ASN
1	A	799	HIS
2	B	31	HIS
1	D	122	ASN
1	D	226	HIS
1	D	266	HIS
1	D	453	ASN
1	D	459	ASN
1	D	461	ASN
1	D	715	ASN
1	D	803	GLN
1	F	9	GLN
1	F	122	ASN
1	F	142	HIS
1	F	185	GLN
1	F	226	HIS
1	F	289	ASN

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Mol	Chain	Res	Type
1	F	307	ASN
1	F	318	GLN
1	F	355	ASN
1	F	356	GLN
1	F	401	GLN
1	F	402	GLN
1	F	461	ASN
1	F	467	ASN
1	F	495	ASN
1	F	498	ASN
1	F	715	ASN
1	F	733	ASN
1	F	739	GLN
1	F	803	GLN
1	F	809	HIS
1	G	47	ASN
1	G	122	ASN
1	G	137	GLN
1	G	142	HIS
1	G	226	HIS
1	G	292	ASN
1	G	318	GLN
1	G	321	GLN
1	G	402	GLN
1	G	467	ASN
1	G	493	ASN
1	G	624	GLN
1	G	684	GLN
1	G	757	ASN
1	G	799	HIS
1	G	803	GLN
1	H	43	ASN
1	H	62	GLN
1	H	122	ASN
1	H	132	ASN
1	H	139	ASN
1	H	140	ASN
1	H	142	HIS
1	H	164	GLN
1	H	181	GLN
1	H	226	HIS
1	H	266	HIS

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Mol	Chain	Res	Type
1	H	284	GLN
1	H	292	ASN
1	H	318	GLN
1	H	411	ASN
1	H	429	ASN
1	H	467	ASN
1	H	613	ASN
1	H	631	ASN
1	H	715	ASN
1	H	756	HIS
1	I	47	ASN
1	I	164	GLN
1	I	292	ASN
1	I	343	ASN
1	I	355	ASN
1	I	613	ASN
1	I	624	GLN
1	I	739	GLN
1	I	757	ASN
1	I	764	GLN
1	I	803	GLN
1	J	33	GLN
1	J	77	GLN
1	J	132	ASN
1	J	139	ASN
1	J	284	GLN
1	J	292	ASN
1	J	307	ASN
1	J	405	ASN
1	J	425	ASN
1	J	453	ASN
1	J	495	ASN
1	J	624	GLN
1	J	803	GLN
1	J	908	ASN
5	K	48	GLN
5	K	51	HIS
5	K	91	HIS
5	K	105	GLN
5	K	130	ASN
5	K	165	ASN
2	L	194	GLN

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Mol	Chain	Res	Type
2	L	201	GLN
6	M	250	HIS
6	M	265	GLN
7	N	100	HIS
7	N	210	ASN
8	O	40	ASN
8	O	113	GLN
7	R	16	GLN
7	R	88	HIS
1	X	9	GLN
1	X	43	ASN
1	X	132	ASN
1	X	139	ASN
1	X	142	HIS
1	X	248	ASN
1	X	292	ASN
1	X	307	ASN
1	X	397	GLN
1	X	402	GLN
1	X	404	GLN
1	X	493	ASN
1	X	803	GLN
1	X	849	GLN
1	Y	122	ASN
1	Y	131	ASN
1	Y	161	ASN
1	Y	226	HIS
1	Y	269	HIS
1	Y	284	GLN
1	Y	292	ASN
1	Y	343	ASN
1	Y	404	GLN
1	Y	411	ASN
1	Y	429	ASN
1	Y	452	HIS
1	Y	556	GLN
1	Y	613	ASN
1	Y	631	ASN
1	Y	715	ASN
1	Y	733	ASN
1	Y	781	HIS
1	Y	803	GLN

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Mol	Chain	Res	Type
2	b	13	GLN
1	g	54	HIS
1	g	139	ASN
1	g	226	HIS
1	g	289	ASN
1	g	343	ASN
1	g	370	ASN
1	g	401	GLN
1	g	402	GLN
1	g	404	GLN
1	g	452	HIS
1	g	453	ASN
1	g	467	ASN
1	g	586	HIS
1	g	598	ASN
1	g	631	ASN
1	g	733	ASN
1	g	757	ASN
1	g	803	GLN
1	h	122	ASN
1	h	139	ASN
1	h	292	ASN
1	h	338	GLN
1	h	388	GLN
1	h	408	ASN
1	h	425	ASN
1	h	438	ASN
1	h	523	GLN
1	h	576	ASN
1	h	603	GLN
1	h	613	ASN
1	i	122	ASN
1	i	181	GLN
1	i	226	HIS
1	i	266	HIS
1	i	289	ASN
1	i	292	ASN
1	i	370	ASN
1	i	402	GLN
1	i	429	ASN
1	i	461	ASN
1	i	467	ASN

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Mol	Chain	Res	Type
1	i	576	ASN
1	i	631	ASN
1	i	733	ASN
1	i	756	HIS
1	i	757	ASN
1	i	803	GLN
9	j	102	ASN
9	j	370	ASN
9	j	430	ASN

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.

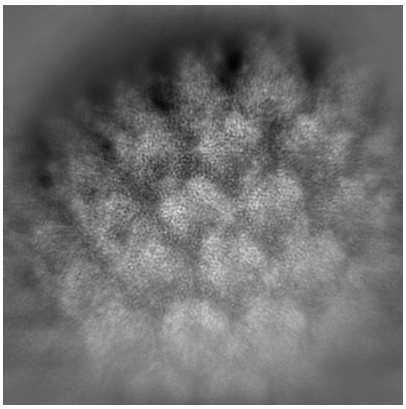
6 Map visualisation (i)

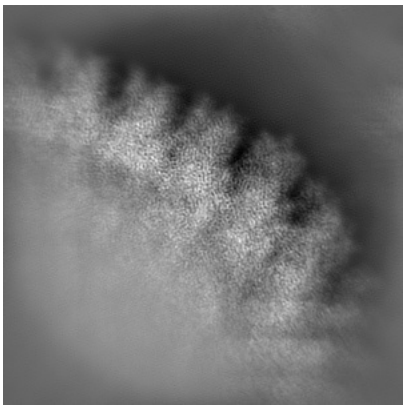
This section contains visualisations of the EMDB entry EMD-63322. These allow visual inspection of the internal detail of the map and identification of artifacts.

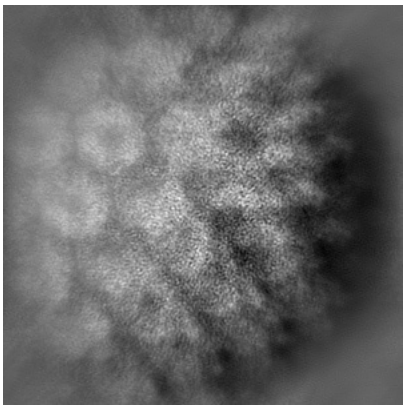
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

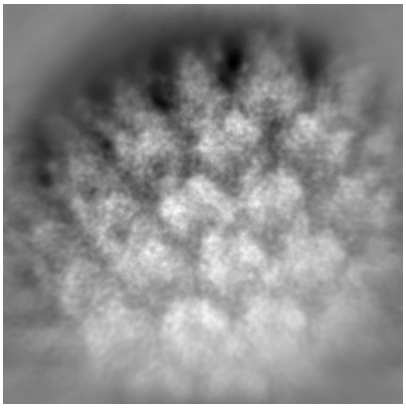
6.1.1 Primary map

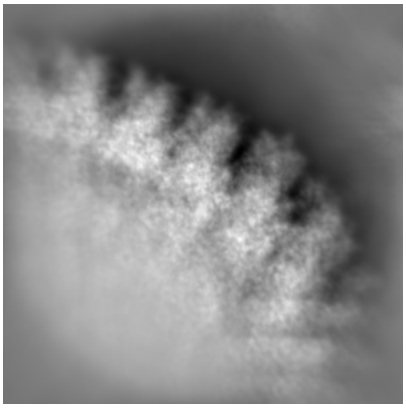

X

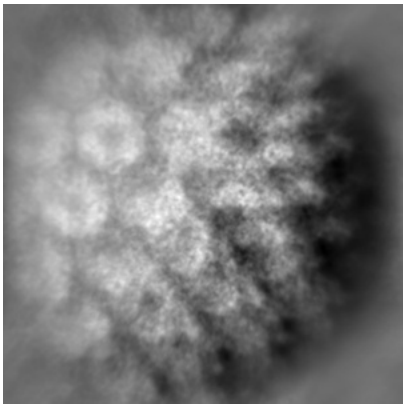

Y


Z

6.1.2 Raw map


X

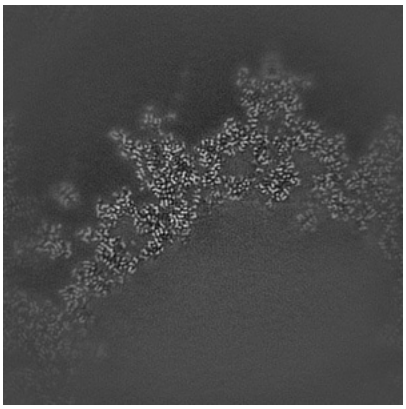

Y

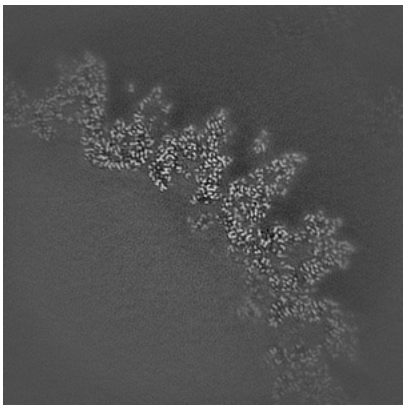

Z

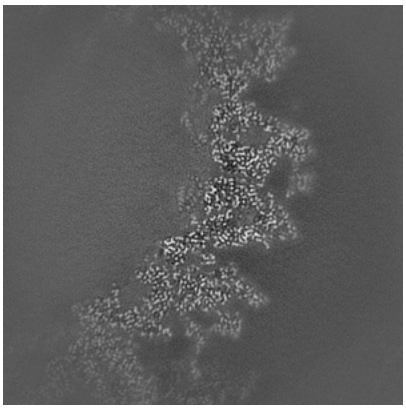
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

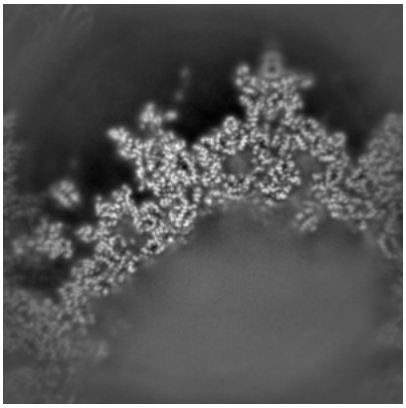
6.2.1 Primary map

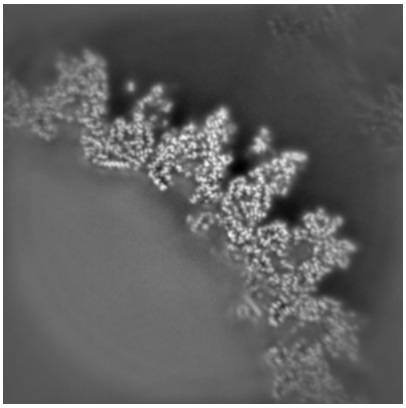

X Index: 184

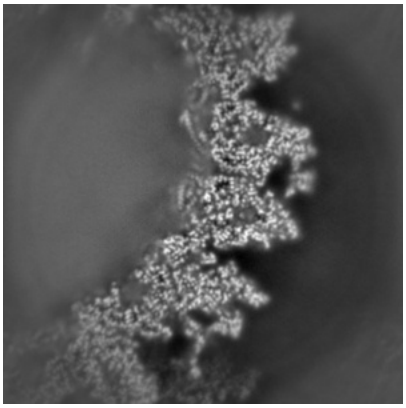

Y Index: 184


Z Index: 184

6.2.2 Raw map


X Index: 184

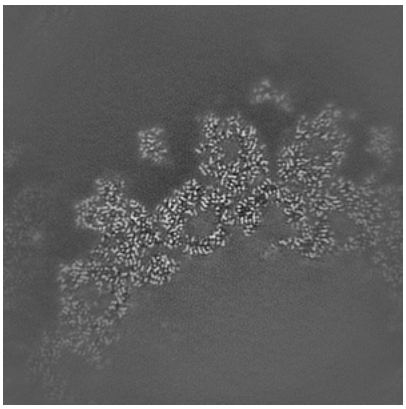

Y Index: 184


Z Index: 184

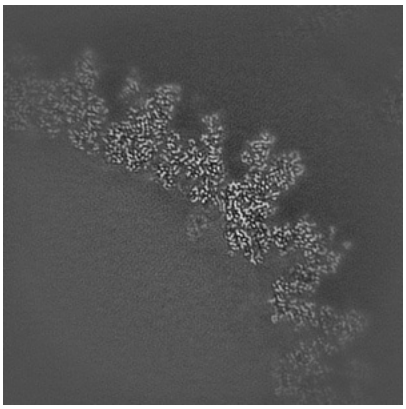
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

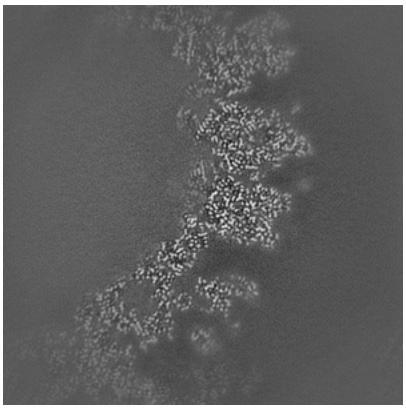
6.3.1 Primary map



X Index: 205

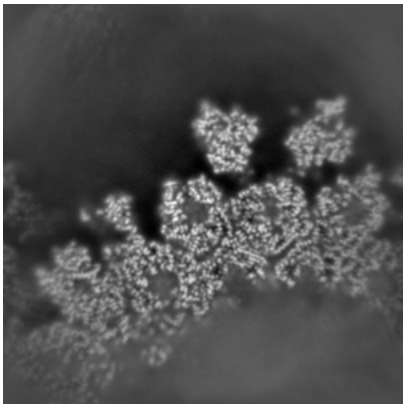


Y Index: 192

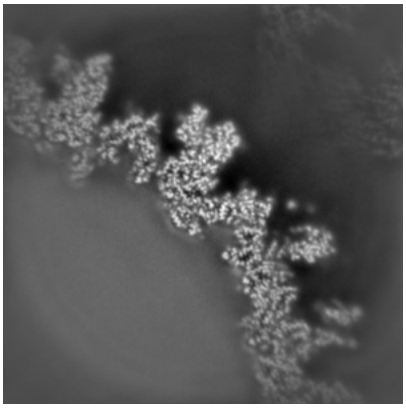


Z Index: 190

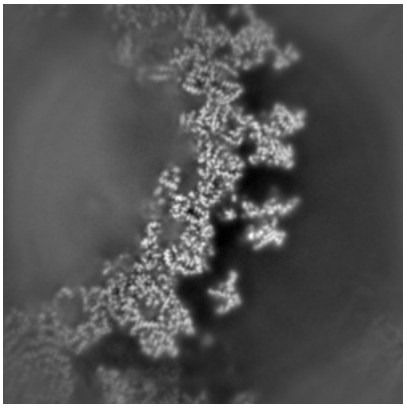
6.3.2 Raw map



X Index: 223



Y Index: 157

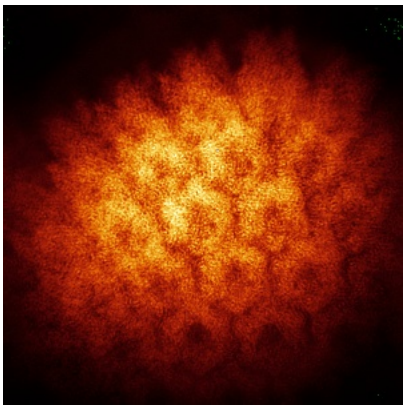


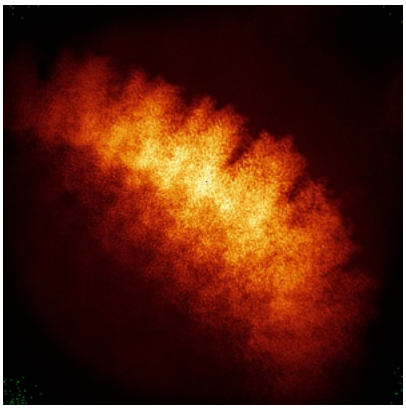
Z Index: 206

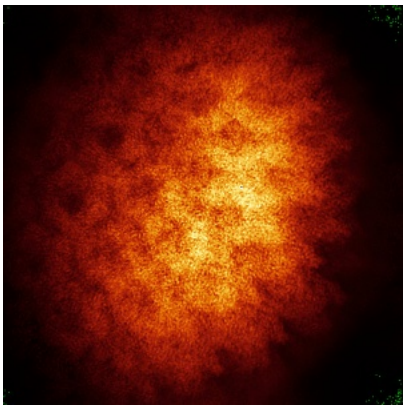
The images above show the largest variance slices of the map in three orthogonal directions.

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

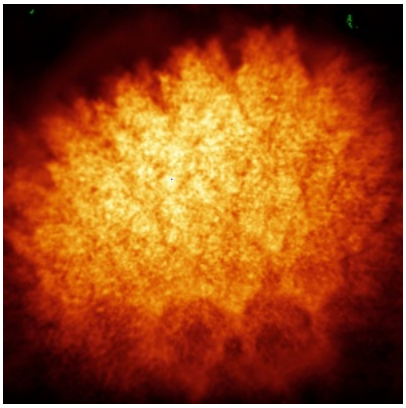
6.4.1 Primary map

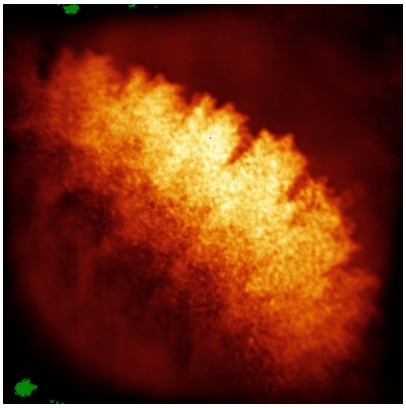

X

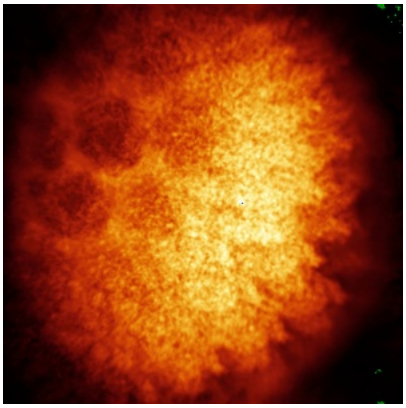

Y


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 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

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

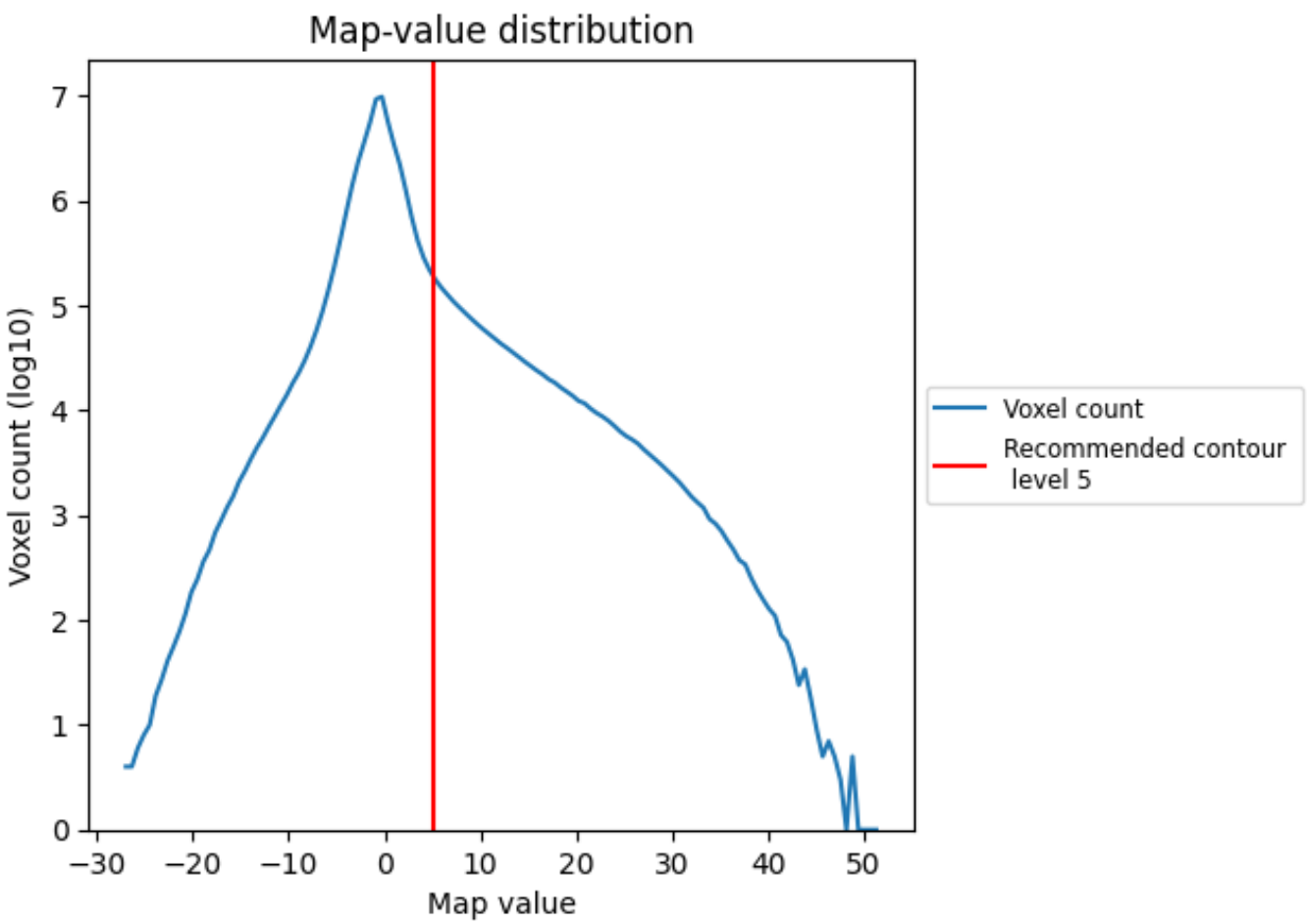
6.6 Mask visualisation (i)

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

7 Map analysis (i)

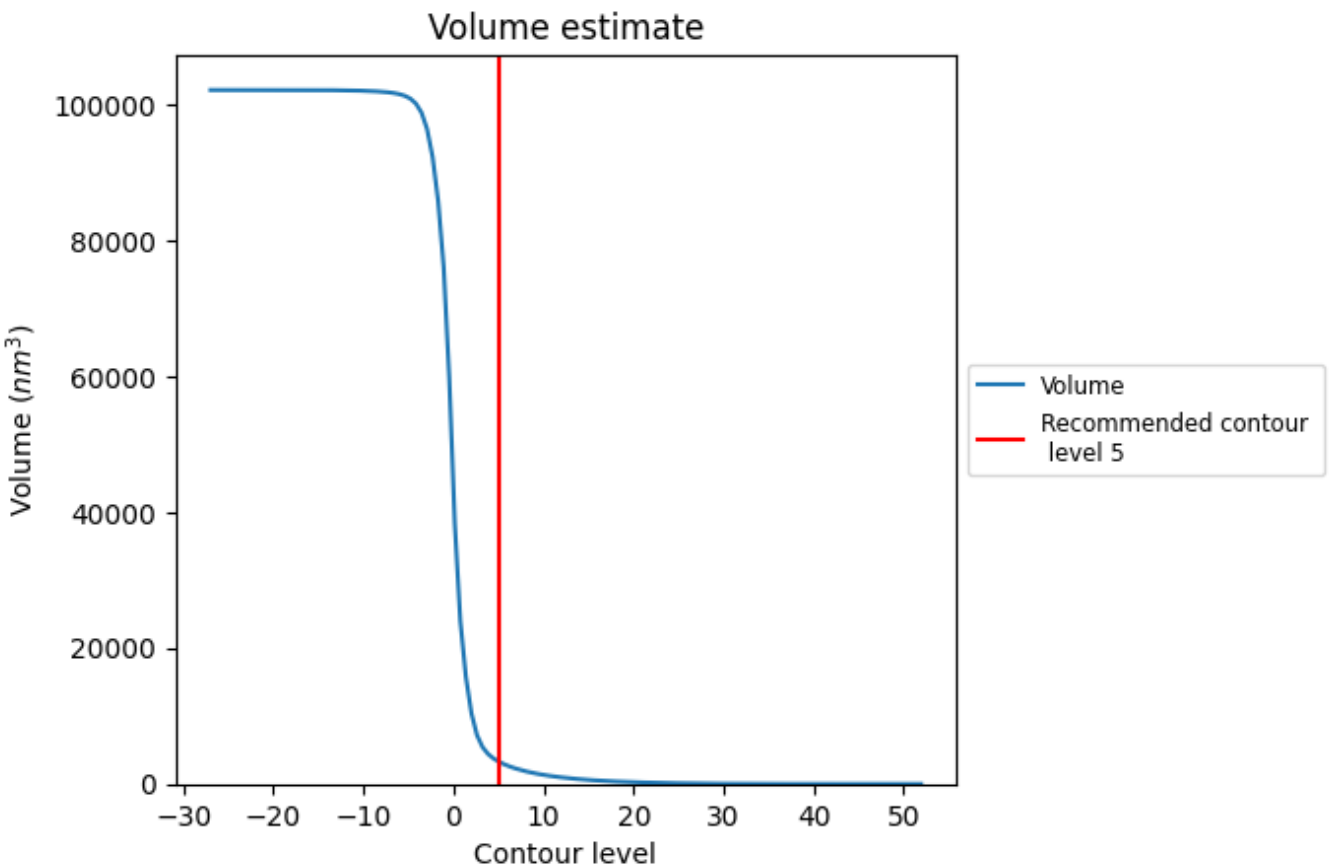
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

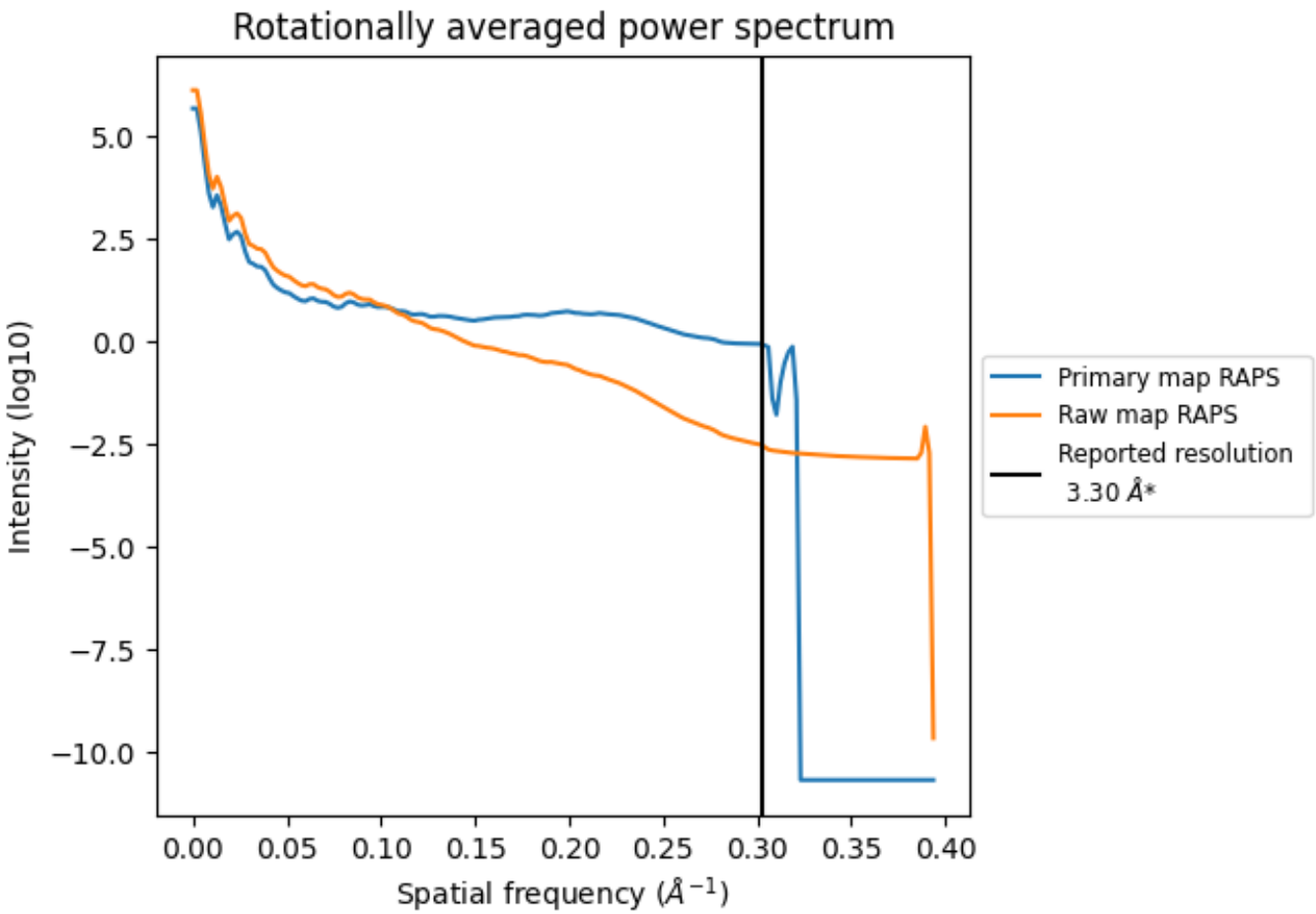
7.2 Volume estimate (i)



The volume at the recommended contour level is 3310 nm^3; this corresponds to an approximate mass of 2990 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)

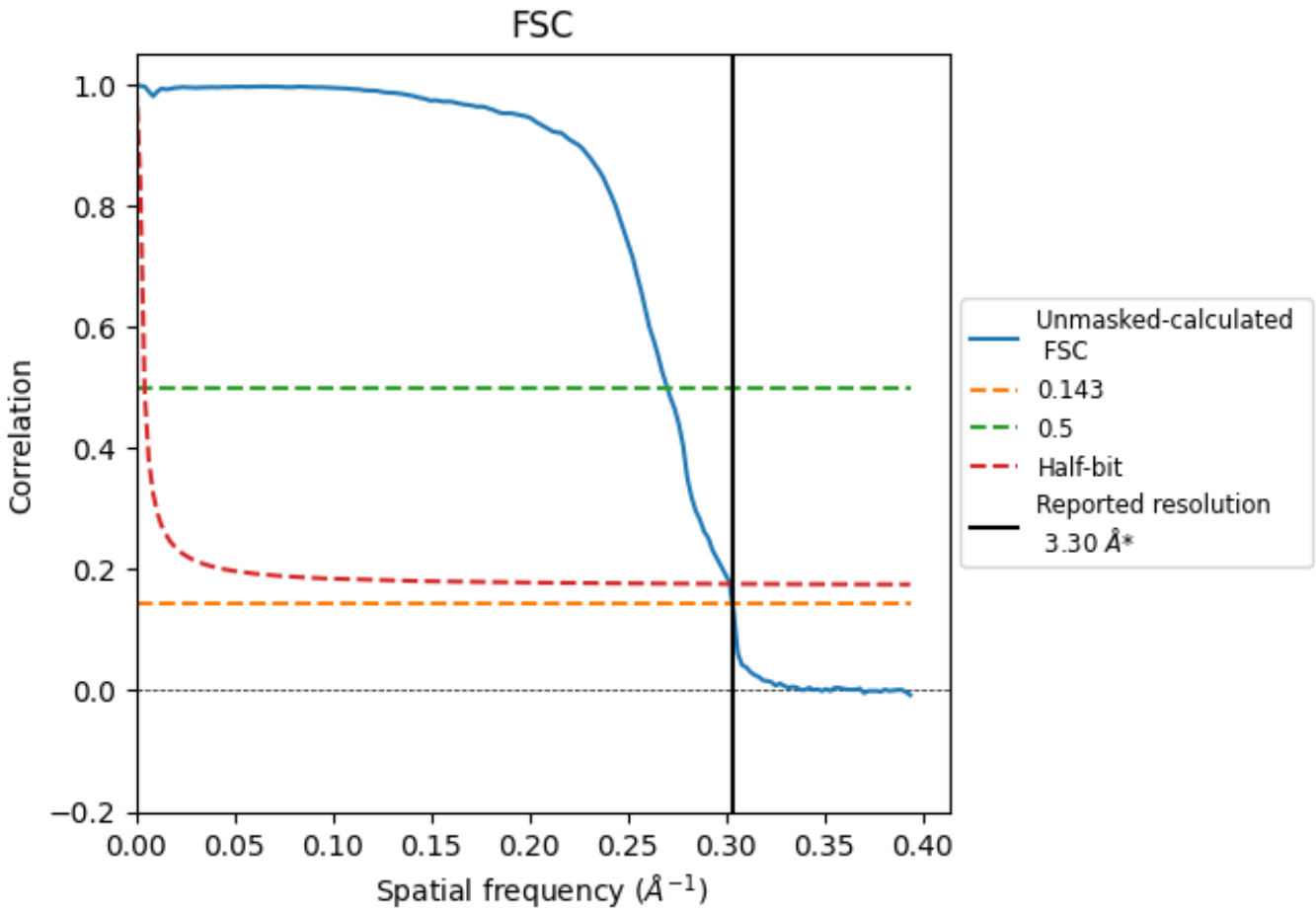


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation (i)

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

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

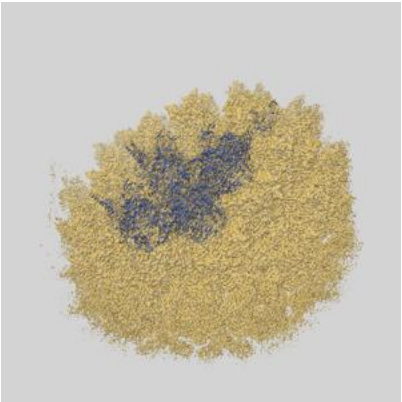
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.30	3.70	3.31

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

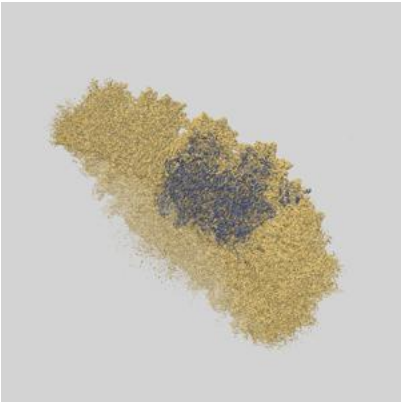
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-63322 and PDB model 9LR9. Per-residue inclusion information can be found in section 3 on page 8.

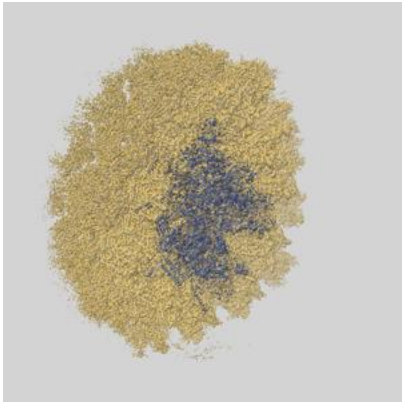
9.1 Map-model overlay (i)



X



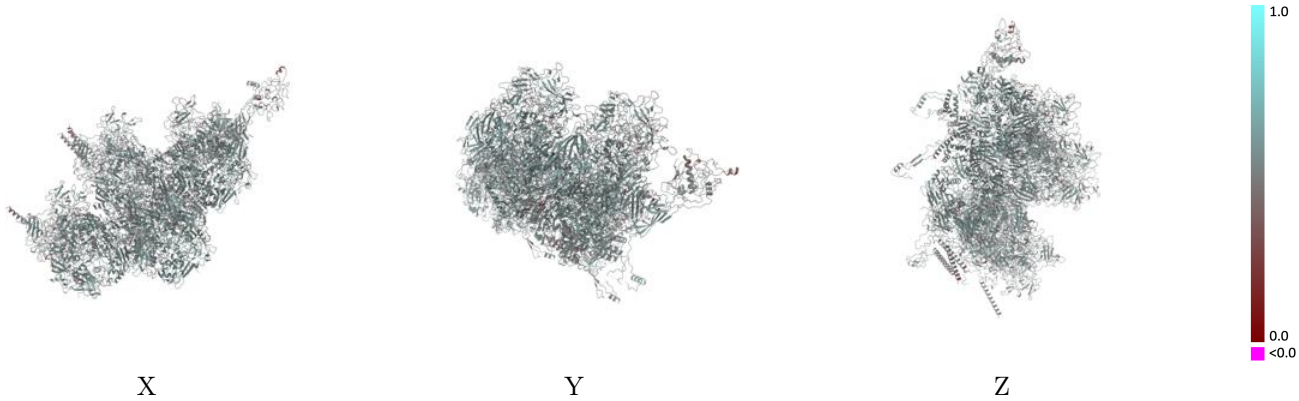
Y



Z

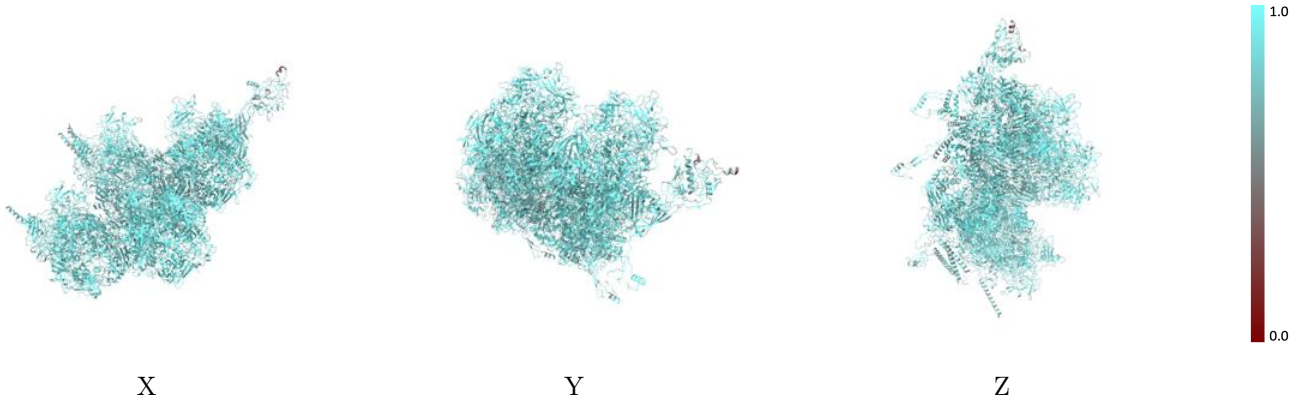
The images above show the 3D surface view of the map at the recommended contour level 5.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



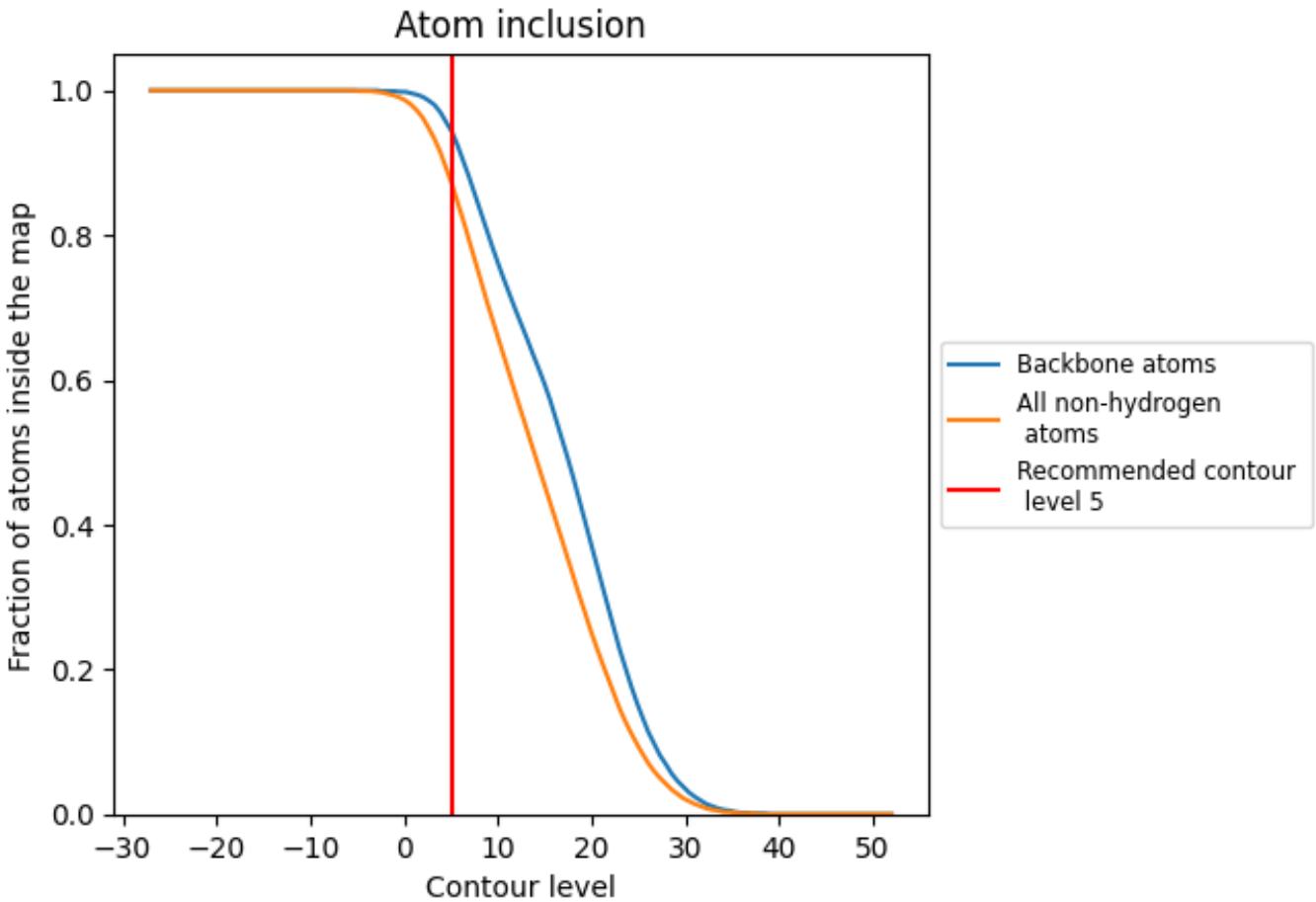
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (5).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8740	0.5200
A	0.8940	0.5200
B	0.5810	0.4520
C	0.7930	0.5350
D	0.9010	0.5280
E	0.6880	0.4750
F	0.9100	0.5310
G	0.8870	0.5280
H	0.8980	0.5240
I	0.8910	0.5260
J	0.9010	0.5260
K	0.7930	0.4950
L	0.6650	0.5110
M	0.7280	0.4800
N	0.8740	0.5390
O	0.7510	0.4970
P	0.7880	0.4900
Q	0.7890	0.4990
R	0.8840	0.5370
S	0.8220	0.5240
T	0.7070	0.4970
U	0.8100	0.5160
V	0.7480	0.4810
X	0.8960	0.5220
Y	0.8710	0.5120
Z	0.4260	0.4150
a	0.6030	0.5000
b	0.8380	0.5280
c	0.5950	0.5050
d	0.4030	0.4390
e	0.8280	0.5670
f	0.7240	0.5150
g	0.9050	0.5280
h	0.8800	0.5260
i	0.8630	0.5170
j	0.7650	0.4910