Full wwPDB EM Validation Report (i)

May 19, 2025 – 02:24 pm BST

PDB ID	:	9ESH / pdb_00009esh
EMDB ID	:	EMD-19941
Title	:	Structure of a B-state intermediate committed to discard (Bd-I state)
Authors	:	Soni, K.; Wild, K.; Sinning, I.
Deposited on	:	2024-03-26
Resolution	:	3.20 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 (1)) were used in the production of this report:

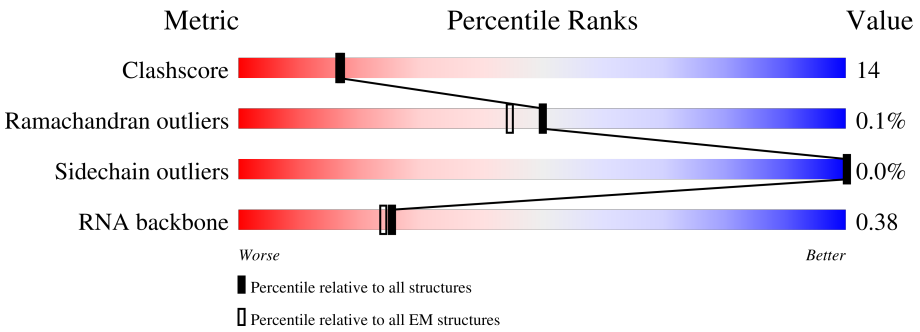
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 3.20 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
RNA backbone	6643	2191

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	1	29	62%; 28%, 48%, 24%
2	2	186	8%; 5%, 6%, •, 87%
3	5	120	•; 54%, 23%, 8%, 15%
4	6	99	37%; 25%, 42%, 25%, 7%
5	A	2363	•; 54%, 19%, 26%
6	B	984	•; 67%, 26%, 7%
7	C	340	9%; 56%, 32%, 11%

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Mol	Chain	Length	Quality of chain
8	D	97	62% 37%
9	E	147	6% 47% 19% 34%
10	F	117	5% 32% 37% 31%
11	G	115	8% 48% 41% 11%
12	H	84	74% 21% 5%
13	I	78	53% 41% 6%
14	J	77	70% 25% 5%
15	K	473	58% 25% 17%
16	L	557	8% 33% 9% 58%
17	M	354	40% 44% 22% 34%
18	N	1284	100% 77% 23%
19	O	146	72% 27%
20	P	388	33% 42% 27% 30%
21	Q	265	29% 5% 66%
22	R	674	53% 58% 31% 11%
23	S	488	27% 18% 9% 73%
23	T	488	26% 15% 12% 73%
23	U	488	86% 70% 18% 12%
23	V	488	27% 20% 7% 73%
24	W	757	38% 47% 22% 31%
25	X	790	81% 56% 27% 17%
26	Y	229	43% 32% 21% 48%
27	Z	187	67% 51% 32% 17%
28	a	558	12% 20% 7% 73%
29	b	293	26% 24% 12% 65%

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Mol	Chain	Length	Quality of chain
30	c	887	14% 9% 77%
31	d	155	45% 57% 43%
32	f	22	86% 100%
33	m	797	10% 8% 90%
34	r	346	17% 17% 81%
35	y	534	20% 23% 12% 65%
36	z	647	80% 66% 31%

2 Entry composition (i)

There are 41 unique types of molecules in this entry. The entry contains 90868 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 RNA chain called pre-mRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	1	29	605	272	91	213	29	0	0

- Molecule 2 is a RNA chain called U2snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
2	2	24	500	224	79	173	24	0	0

- Molecule 3 is a RNA chain called U5snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
3	5	102	2149	963	358	726	102	0	0

- Molecule 4 is a RNA chain called U6snRNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
4	6	92	1970	882	365	631	92	0	0

- Molecule 5 is a protein called Pre-mRNA-splicing factor spp42.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	A	1737	14402	9229	2543	2565	65	0	0

- Molecule 6 is a protein called Pre-mRNA-splicing factor cwf10.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	B	918	7298	4650	1251	1362	35	0	0

- Molecule 7 is a protein called Pre-mRNA-splicing factor cwf17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	C	301	2328	1460	415	442	11	0	0

- Molecule 8 is a protein called Small nuclear ribonucleoprotein Sm D3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
8	D	96	760	470	147	136	7	0	0

- Molecule 9 is a protein called Small nuclear ribonucleoprotein-associated protein B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	E	97	726	462	129	130	5	0	0

- Molecule 10 is a protein called Small nuclear ribonucleoprotein Sm D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
10	F	81	638	407	109	118	4	0	0

- Molecule 11 is a protein called Small nuclear ribonucleoprotein Sm D2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	G	102	819	516	150	149	4	0	0

- Molecule 12 is a protein called Small nuclear ribonucleoprotein E.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
12	H	80	652	422	113	115	2	0	0

- Molecule 13 is a protein called Small nuclear ribonucleoprotein F.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
13	I	73	574	373	95	104	2	0	0

- Molecule 14 is a protein called Small nuclear ribonucleoprotein G.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
14	J	73	573	366	98	108	1	0	0

- Molecule 15 is a protein called Pre-mRNA-splicing factor prp5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
15	K	391	3053	1925	551	563	14	0	0

- Molecule 16 is a protein called Pre-mRNA-processing protein 45.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
16	L	234	1849	1154	345	345	5	0	0

- Molecule 17 is a protein called Pre-mRNA-splicing factor cwf5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
17	M	234	1818	1131	329	343	15	0	0

- Molecule 18 is a protein called Pre-mRNA-splicing factor cwf11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
18	N	1284	10461	6715	1732	1969	45	0	0

- Molecule 19 is a protein called Pre-mRNA-splicing factor cwf14.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
19	O	144	1176	733	216	214	13	0	0

- Molecule 20 is a protein called Pre-mRNA-splicing factor cwf2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
20	P	271	2178	1354	397	416	11	0	0

- Molecule 21 is a protein called Pre-mRNA-splicing factor cwf15.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
21	Q	90	752	467	146	138	1	0	0

- Molecule 22 is a protein called Pre-mRNA-splicing factor cwf4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
22	R	603	5108	3280	892	913	23	0	0

- Molecule 23 is a protein called Pre-mRNA-processing factor 19.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
23	S	132	1055	664	181	207	3	0	0
23	T	134	1069	671	183	212	3	0	0
23	U	430	2870	1806	492	563	9	0	0
23	V	131	1044	655	180	206	3	0	0

- Molecule 24 is a protein called Pre-mRNA-splicing factor cdc5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
24	W	526	4346	2710	792	832	12	0	0

- Molecule 25 is a protein called Pre-mRNA-splicing factor cwf3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
25	X	654	5467	3534	918	996	19	0	0

- Molecule 26 is a protein called Pre-mRNA-splicing factor syf2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
26	Y	120	1049	656	195	198	0	0

- Molecule 27 is a protein called Pre-mRNA-splicing factor cwf7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
27	Z	155	1232	766	220	243	3	0	0

- Molecule 28 is a protein called Pre-mRNA-processing factor 17.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	a	152	1035	644	185	205	1	0	0

- Molecule 29 is a protein called Pre-mRNA-splicing factor cwf21.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
29	b	104	822	503	148	169	2	0	0

- Molecule 30 is a protein called Pre-mRNA-splicing factor cwf22.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
30	c	204	1678	1071	280	315	12	0	0

- Molecule 31 is a protein called Peptidyl-prolyl cis-trans isomerase ppi1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
31	d	154	1179	750	202	223	4	0	0

- Molecule 32 is a protein called UNK1.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
32	f	22	110	66	22	22	0	0

- Molecule 33 is a protein called G-patch domain-containing protein C1486.03.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
33	m	81	649	413	112	122	2	0	0

- Molecule 34 is a protein called UNK2.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
34	r	67	335	201	67	67	0	0

- Molecule 35 is a protein called Uncharacterized protein C20H4.06c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
35	y	185	1480	921	257	298	4	0	0

- Molecule 36 is a protein called Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
36	z	626	4980	3193	835	933	19	0	0

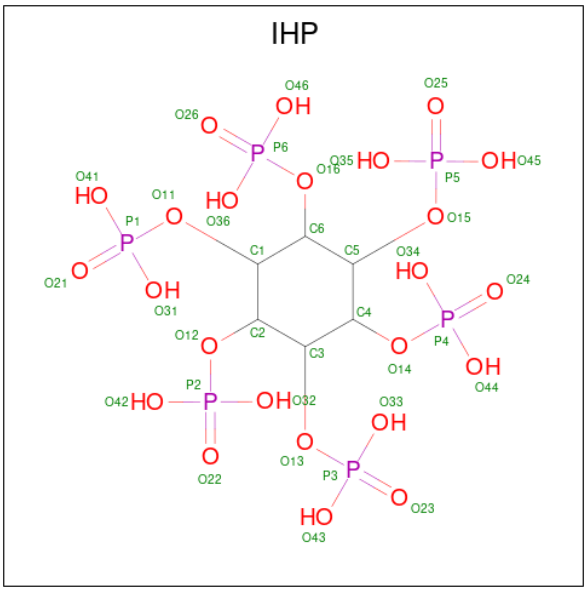
- Molecule 37 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
37	6	3	3	3	0
37	B	1	1	1	0

- Molecule 38 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

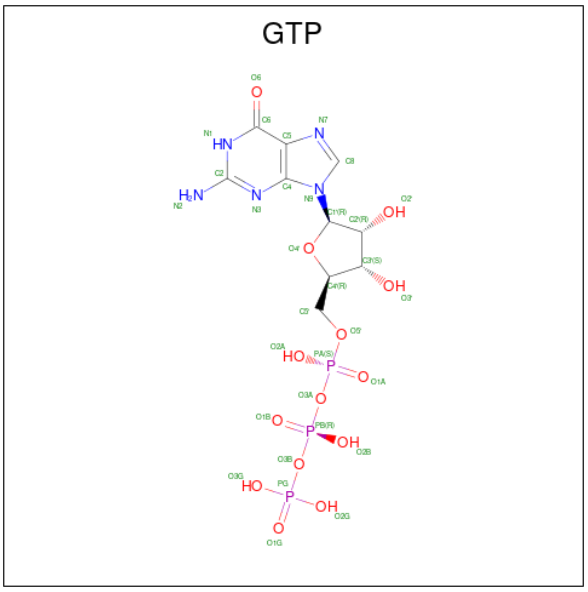
Mol	Chain	Residues	Atoms		AltConf
			Total	K	
38	6	1	1	1	0

- Molecule 39 is INOSITOL HEXAKISPHOSPHATE (CCD ID: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
39	A	1	36	6	24	6	0

- Molecule 40 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
40	B	1	32	10	5	14	3	0

- Molecule 41 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

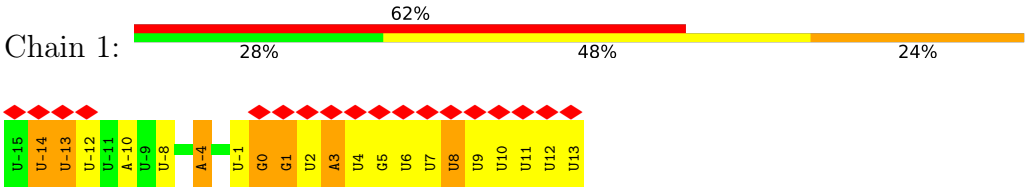
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
41	M	2	2	2	0
41	O	3	3	3	0
41	P	1	1	1	0

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.

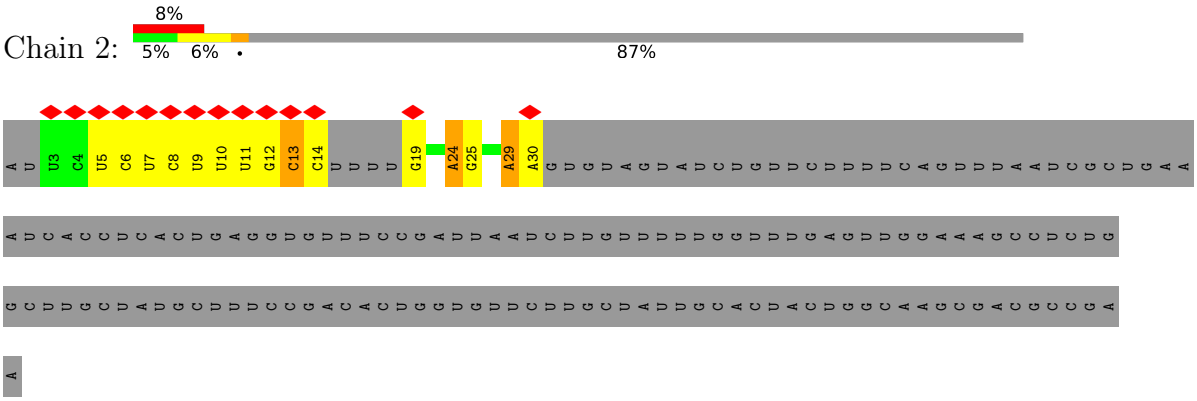
- Molecule 1: pre-mRNA

Chain 1:



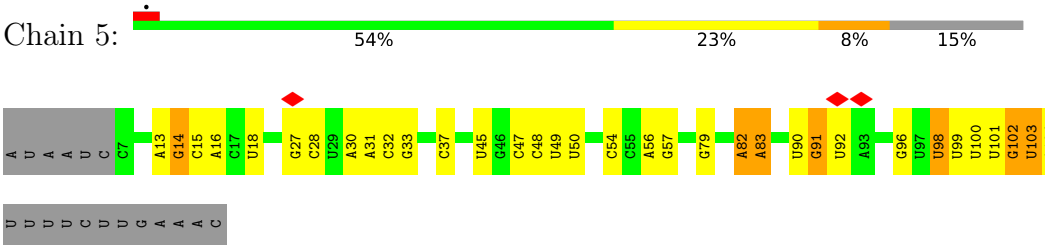
- Molecule 2: U2snRNA

Chain 2:



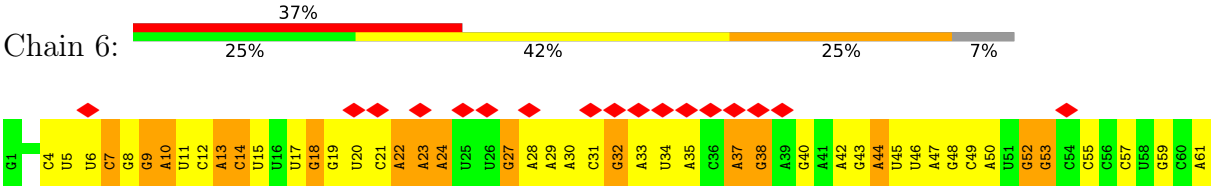
- Molecule 3: U5snRNA

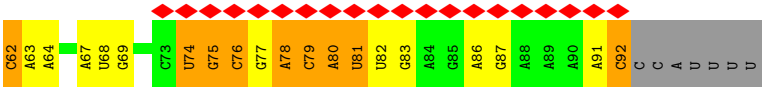
Chain 5:



- Molecule 4: U6snRNA

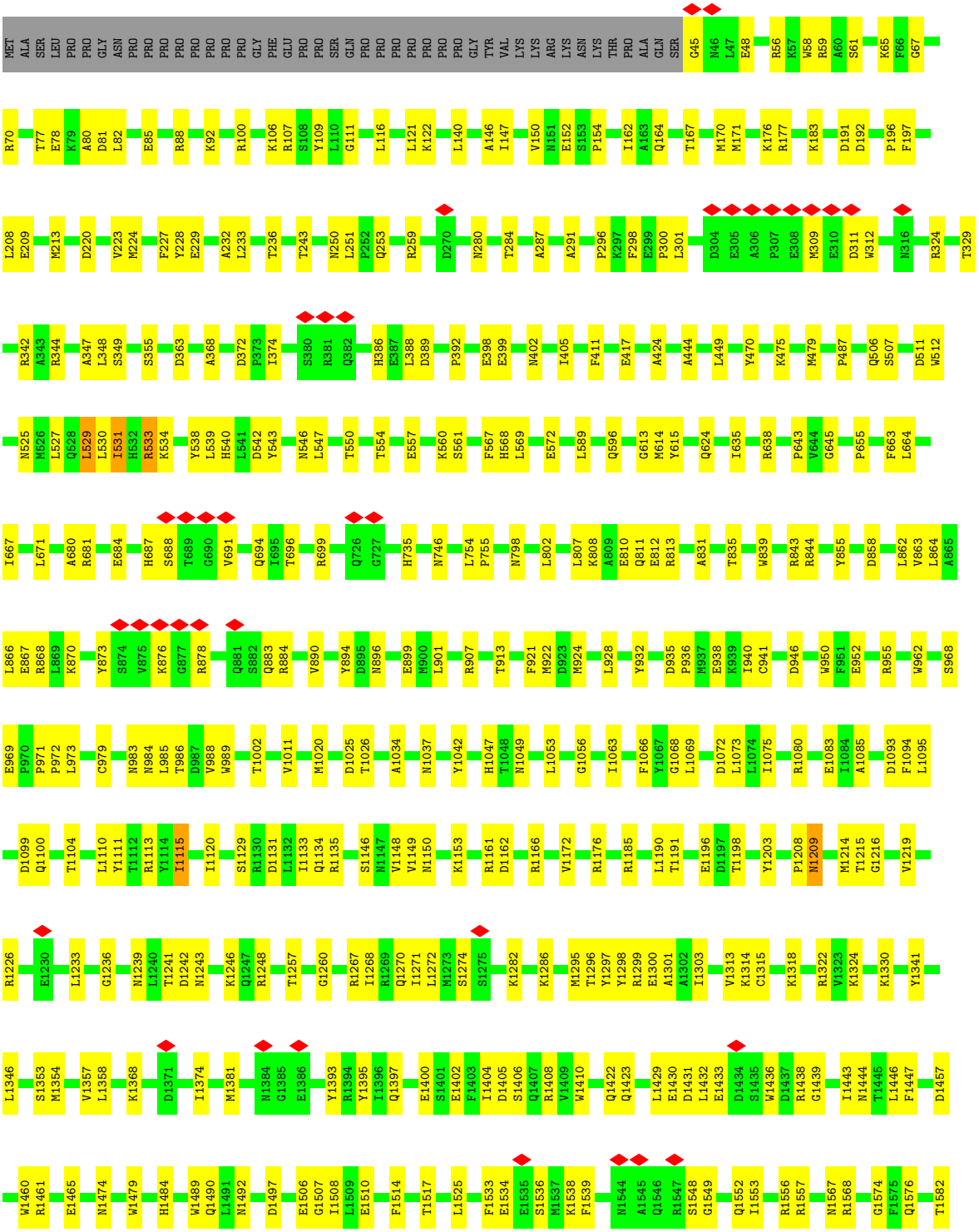
Chain 6:

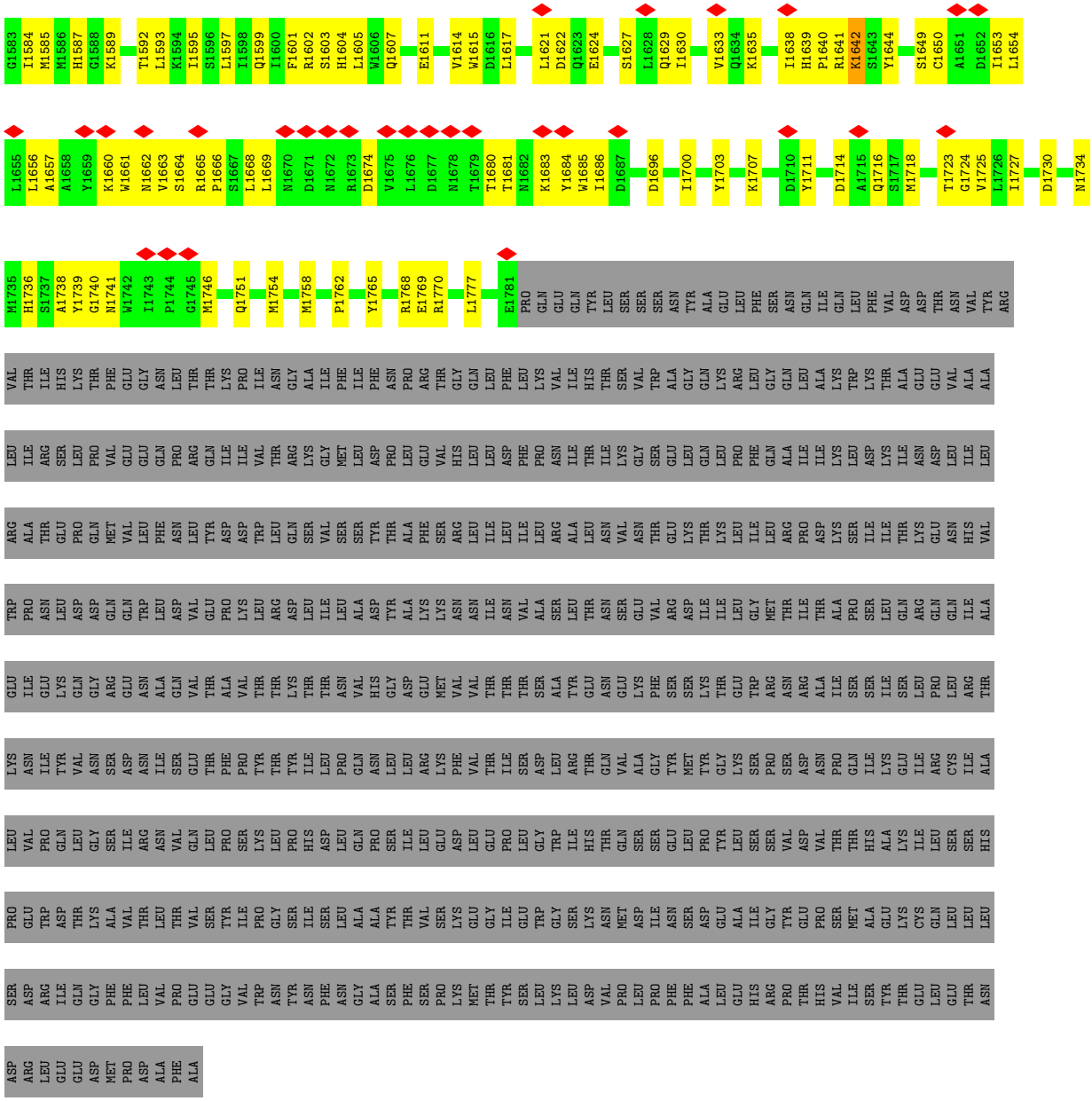




• Molecule 5: Pre-mRNA-splicing factor spp42

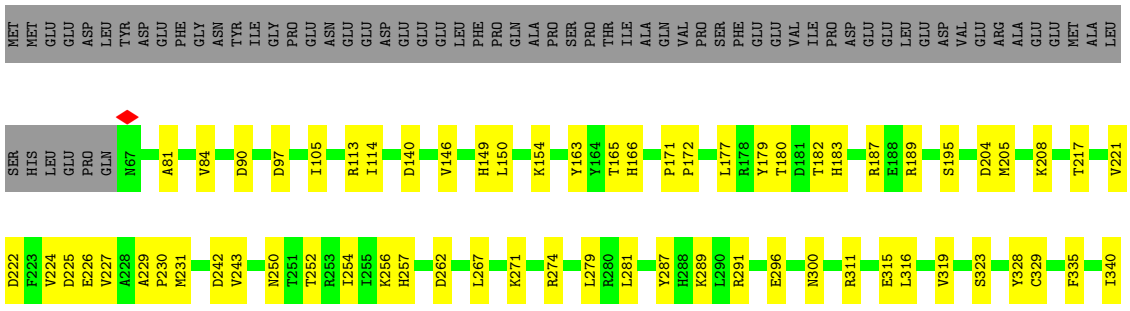
Chain A:

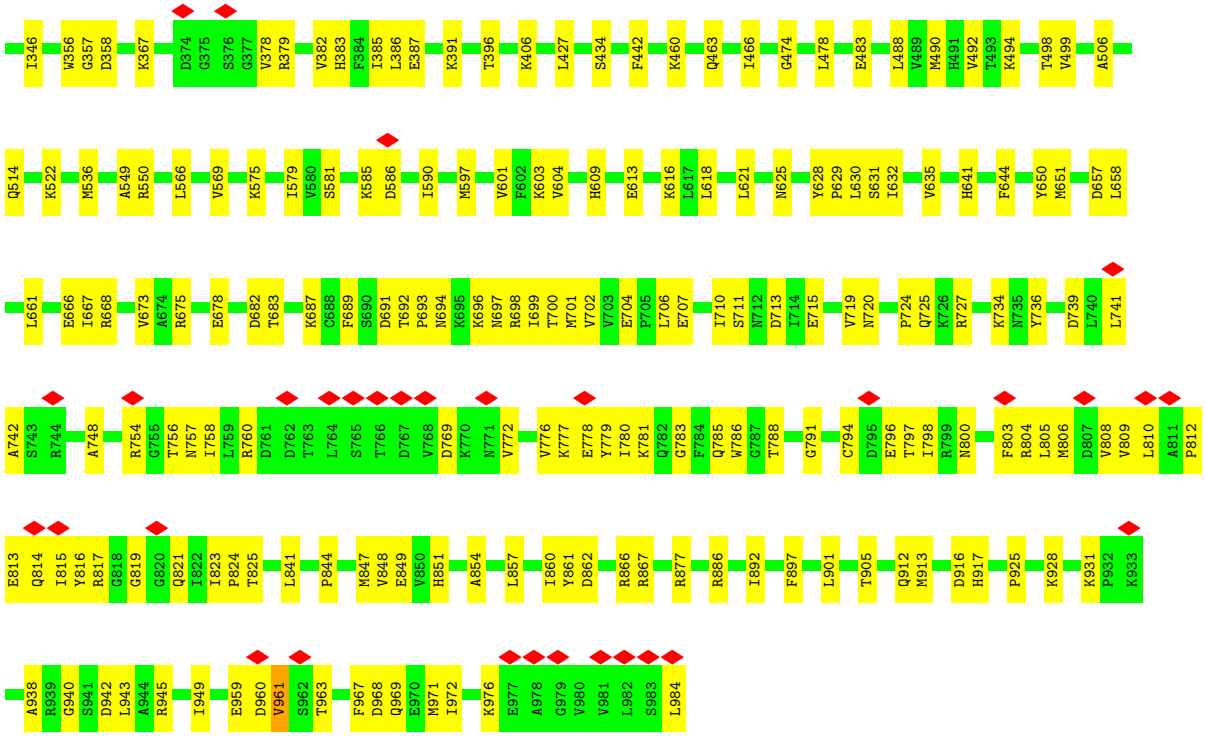




• Molecule 6: Pre-mRNA-splicing factor cwf10

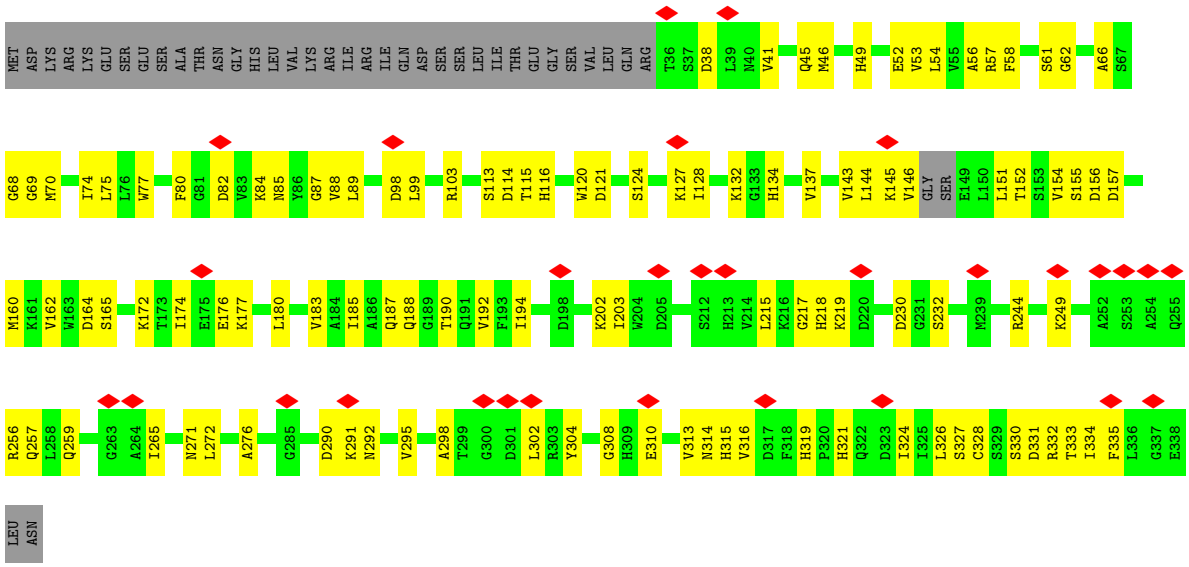
Chain B:





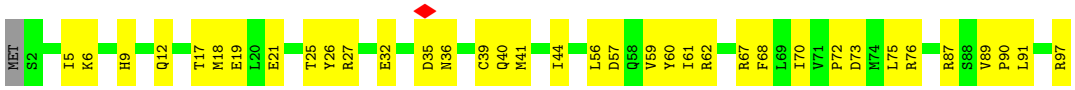
- Molecule 7: Pre-mRNA-splicing factor cwf17

Chain C:



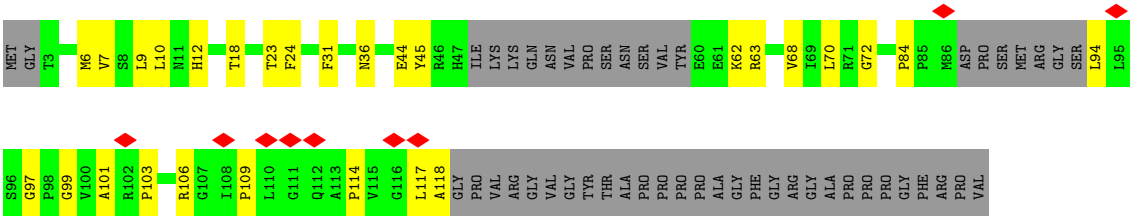
- Molecule 8: Small nuclear ribonucleoprotein Sm D3

Chain D:



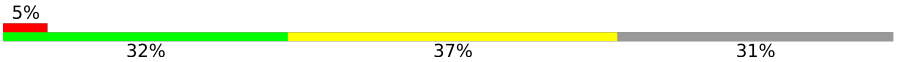
• Molecule 9: Small nuclear ribonucleoprotein-associated protein B

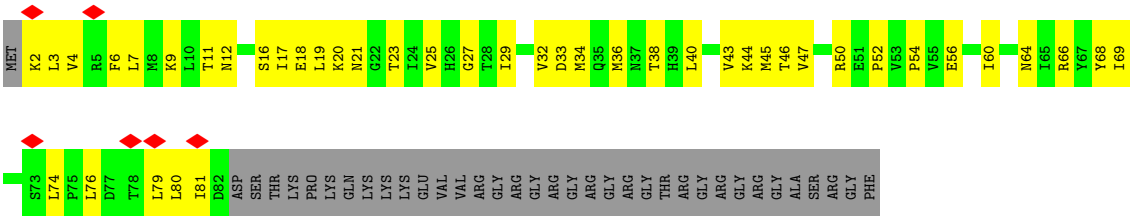
Chain E:



• Molecule 10: Small nuclear ribonucleoprotein Sm D1

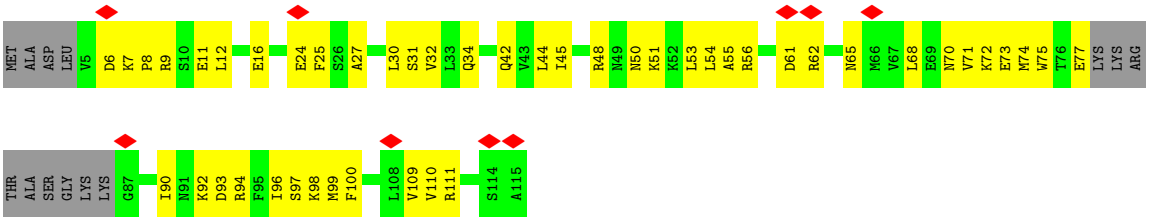
Chain F:





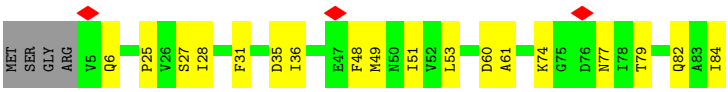
• Molecule 11: Small nuclear ribonucleoprotein Sm D2

Chain G:



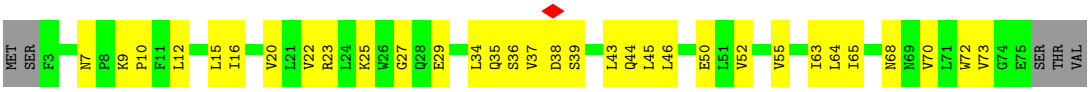
• Molecule 12: Small nuclear ribonucleoprotein E

Chain H:



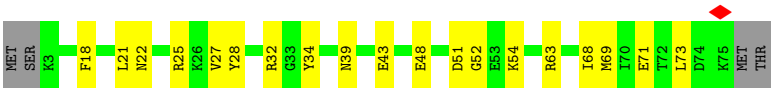
• Molecule 13: Small nuclear ribonucleoprotein F

Chain I:



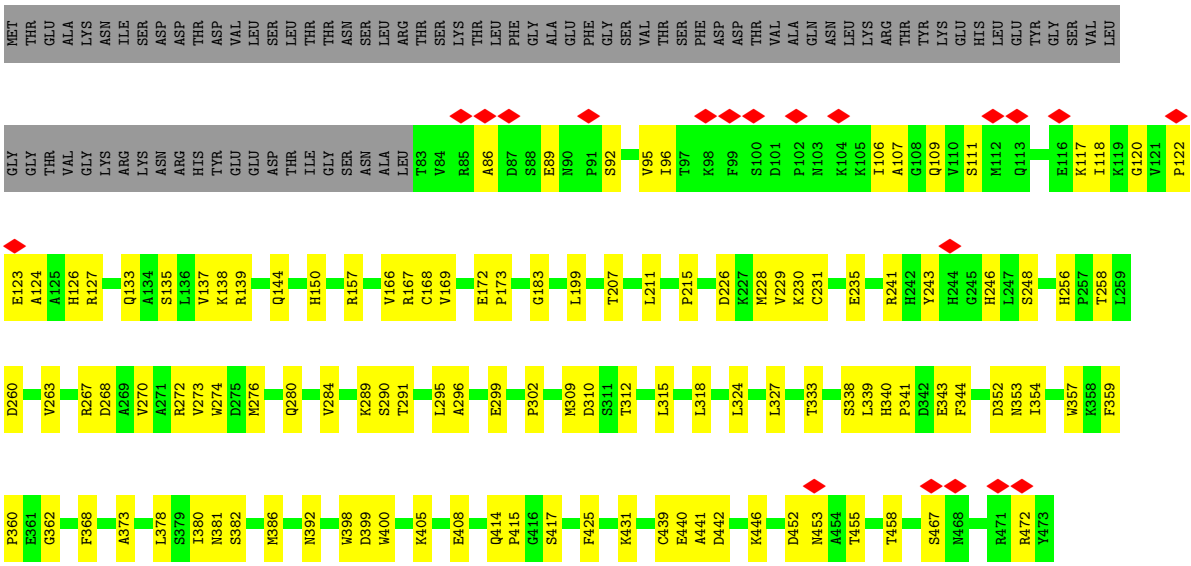
• Molecule 14: Small nuclear ribonucleoprotein G

Chain J: 70% 25% 5%



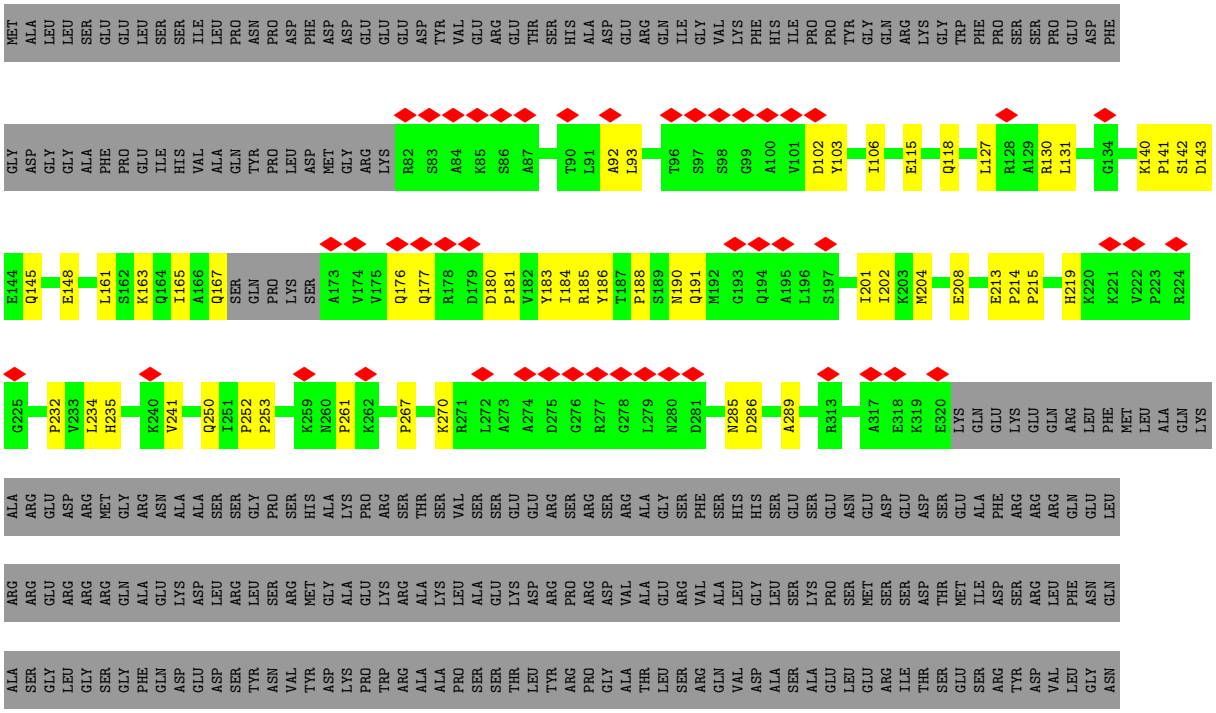
• Molecule 15: Pre-mRNA-splicing factor prp5

Chain K: 58% 25% 17%



• Molecule 16: Pre-mRNA-processing protein 45

Chain L: 8% 33% 9% 58%



ALA HIS LYS LYS PHE LYS GLY SER ASP GLU VAL VAL GLU SER ARG ALA GLY PRO VAL THR PHE GLU LYS ASP ILE ALA ASP PRO PHE GLY VAL ASP THR PHE LEU ASN ASN VAL SER SER LYS LYS THR

- Molecule 17: Pre-mRNA-splicing factor cwf5

Chain M:

MET SER HIS GLY PRO LYS GLY ASP ILE ASN LYS GLN GLU TRP GLU D16 V17 E18 F19 P20 S21 I22 C23 E24 R25 C26 D29 N30 S31 Y32 M35 T36 K37 E38 P39 C44 C47 S48 K49 T52 I53 F54 R55 K58 G61 Q62 K63 Q68 I69 C73 A74

R75 S82 C83 M84 L85 D86 F89 G90 L91 A94 L95 R96 D97 A98 A99 L100 K101 L102 V103 E104 S105 G106 P107 T108 N109 D110 I111 N112 R113 E114 F115 F116 A117 Q118 N119 Q120 Q121 R122 L123 L124 S125 N126 G127 E128 T129 A130 Y131 D132 A136 S137 A138 A139 A140 R141 N142 L143

V144 K145 K146 V147 E148 K149 R150 E151 L152 HIS SER ARG PRO PRO LYS ARG LYS LEU ASP ASP V164 E165 S166 K167 Q168 I169 L170 K171 E172 A173 R174 A175 S176 D177 A178 S179 L180 N181 A182 GLU ARG PRO LEU PHE PRO VAL LYS LYS ILE ILE ASN G195 N196 V197 S198 L199 S200 I201 N202 M203

E204 P205 PRO LYS ASP LYS LYS ILE ALA SER LEU PHE LEU ILE GLY VAL GLU ASP E222 L223 A224 D225 Y226 K227 I228 R229 K230 H231 F232 E233 Q234 Y235 G236 P237 L238 K239 S240 C243 S244 H245 R246 A247 K248 C249 A250 F251 V252 N253 F254 K255 T256 R257 S258 S259 A260 E261 I262 A263 A264

A265 A266 S267 P268 ASP GLY ASN VAL VAL ILE ILE GLU GLY PHE ARG L279 K280 V281 Q282 W283 GLY LYS PRO ARG SER LEU GLY G291 P292 E293 G294 E295 V296 R297 N298 A299 K300 L301 A302 D303 L304 V305 MET ARG GLY SER SER HIS GLY ASN LYS THR SER GLN LYS SER THR ILE LYS ASN ILE

GLU ASN GLU ASP HIS GLU ASN THR LYS SER PRO ALA VAL ALA ILE PRO ILE ASP PRO ASN GLN PRO ARG TYR ARG SER GLN ILE PRO ARG

- Molecule 18: Pre-mRNA-splicing factor cwf11

Chain N:

M1 V2 L3 Y4 K5 N6 K7 K8 K9 Q10 I11 I12 N13 Y14 A15 N16 S17 N18 W19 G20 Q21 N22 E23 G24 V25 E26 F27 Q28 E29 T30 M31 L32 Q33 C34 I35 L36 E37 A38 V39 I40 V41 S42 K43 D44 A45 K46 Q47 V48 L49 S50 L51 L52 H53 E54 L55 K56 L57 F58 E59 N60

F61 L62 W63 Q64 R65 V66 N67 T68 E69 M70 S71 L72 N73 H74 I75 N76 L77 T78 C79 M80 L81 L82 L83 Y84 K85 S86 K87 Y88 E89 Y90 I91 T92 W93 D94 L95 I96 D97 E98 N99 R100 F101 Q102 L103 F104 F105 E106 K107 V108 I109 E110 V111 S112 L113 S114 L115 N116 L117 S118 E119 V120

V121 Y122 M123 I124 Q125 F126 I127 T128 L129 C130 F131 Q132 F133 S134 N135 I136 E137 K138 L139 R140 K141 L142 V143 Y144 Q145 L146 T147 N148 I149 S150 I151 L152 N153 S154 L155 D156 N157 L158 D159 K160 V161 K162 Y163 L164 L165 H166 D167 S168 S169 S170 L171 T172 K173 A174 F175 D176 S177 Y178 K179 E180

K181 R182 P183 S184 I185 V186 E187 K188 F189 P190 L191 H192 N193 L194 L195 S196 R197 W198 I199 H200 S201 L202 L203 I204 K205 S206 I207 S208 Y209 A210 Q211 T212 E213 K214 Q215 E216 A217 K218 V219 T220 P221 L222 L223 A224 T225 I226 N227 M228 S229 L230 V231 L232 L233 S234 A235 F236 P237 T238 R239 R240

F241 A242 H243 P244 V245 I246 E247 D248 S249 C250 F251 Y252 T253 A254 L255 R256 M257 S258 L259 Y260 Y261 D262 S263 N264 E265 L266 F267 K268 K269 M270 T271 D272 D273 L274 N275 Y276 V277 L278 K279 F280 P281 F282 D283 N284 T285 R286 G287 M288 E289 Y290 E291 K292 E293 Q294 K295 I296 R297 N298 D299 E300

L301 V302 Y303 Y304 H305 L306 Q307 L308 T309 L310 F311 S312 D313 F314 Q315 K316 E317 L318 G319 D320 L321 V322 F323 C324 T325 Q326 T327 S328 L329 Q330 Q331 R332 Q333 K334 L335 E336 E337 I338 T339 S340 F341 L342 S343 F344 N345 S346 L347 K348 S349 L350 C351 S352 K353 C354 Y355 L356 R357 T358 S359 F360

P361 E362 K363 Y364 A365 I366 K367 V368 D369 F370 E371 F372 L373 K374 N375 V376 F377 I378 N379 T380 Y381 D382 R383 T384 R385 L386 V387 N388 D389 Y390 D391 E392 I393 I394 N395 F396 T397 L398 K399 D400 V401 L402 G403 E404 R405 S406 V407 M408 D409 Q410 E411 N412 S413 L414 T415 N416 Y417 F418 L419 L420

Q421 N422 T423 A424 I425 Q426 Y427 L428 S429 I430 S431 F432 F433 M434 R435 Q436 Q437 S438 K439 A440 Y441 K442 K443 L444 L445 L446 R447 S448 L449 Y450 A451 E452 L453 L454 N455 F456 S457 E458 Q459 Y460 R461 R462 L463 S464 I465 K466 N467 A468 T469 K470 N471 L472 T473 K474 D475 N476 F477 F478 S479 L480

N481 M482 F483 K484 V485 T486 S487 V488 A489 P490 P491 Q492 I493 G494 Q495 V496 L497 P498 Q499 F500 V501 K502 C503 Q504 M505 G506 L507 S508 R509 P510 G511 P512 F513 H514 S515 A516 L517 R518 D519 L520 K521 N522 S523 I524 K525 S526 P527 F528 L529 C530 L531 I532 Y533 I534 S535 K536 D537 M538 E539 Y540

K541 L542 L543 H544 G545 N546 A547 L548 D549 P550 L551 E552 G553 V554 T555 D556 F557 T558 I559 A560 T561 I562 C563 N564 D565 D566 V567 G568 M569 F570 Q571 S572 D573 M574 Q575 S576 D577 S578 D579 N580 K581 S582 I583 N584 V585 Y586 L587 S588 P589 F590 Y591 Y592 H593 S594 L595 A596 G597 L598 G599 E600

Y601 R602 P603 K604 Q605 L606 K607 F608 N609 F610 A611 L612 V613 L614 S615 P616 E617 A618 N619 K620 Y621 W622 L623 D624 L625 N626 I627 L628 V629 S630 L631 L632 N633 R634 A635 K636 E637 F638 P639 K640 W641 F642 E643 D644 L645 F646 L647 G648 F649 G650 T651 P652 D653 I654 C655 A656 F657 P658 N659 A660

G661 L662 N663 S664 I665 Y666 A667 R668 N669 L670 F671 N672 T673 V674 E675 Q676 L677 Q678 S679 V680 L681 P682 N683 G684 H685 V686 P687 S688 N689 L690 S691 T692 E693 S694 L695 L696 I697 K698 F699 Y700 T701 N702 Q703 N704 K705 I706 S707 A708 D709 V710 T711 A712 S713 D714 R715 H716 F717 L718 L719 P720

S721 N722 R723 L724 Y725 T726 Y727 N728 D729 K730 Q731 L732 E733 S734 I735 L736 R737 G738 S739 Q740 P741 G742 L743 T744 M745 V746 N747 G748 P749 T750 R751 C752 G753 K754 H755 V756 L757 V758 C759 K760 L761 L762 E763 V764 L765 Q766 D767 T768 S769 P770 N771 D772 R773 T774 V775 V776 L777 S778 D779 S780

N781 F782 S783 M784 N785 T786 L787 F788 T789 L790 L791 E792 K793 A794 R795 C796 F797 H798 Q799 G800 H801 L802 L803 Y804 L805 S806 D807 E808 G809 K810 D811 E812 T813 L814 E815 R816 Y817 G818 T819 L820 S821 S822 W823 I824 S825 K826 L827 P828 G829 L830 L831 R832 E833 I834 G835 R836 L837 A838 A839 S840

I841 Q842 A843 P844 G845 S846 H847 D848 A849 S850 P851 D852 T853 A854 L855 Y856 F857 R858 D859 A860 Y861 I862 K863 R864 L865 W866 E867 K868 Y869 L870 N871 T872 V873 D874 D875 K876 D877 S878 V879 D880 A881 Y882 N883 R884 F885 P886 F887 H888 S889 Y890 F891 G892 D893 K894 S895 K896 R897 P898 I899 E900

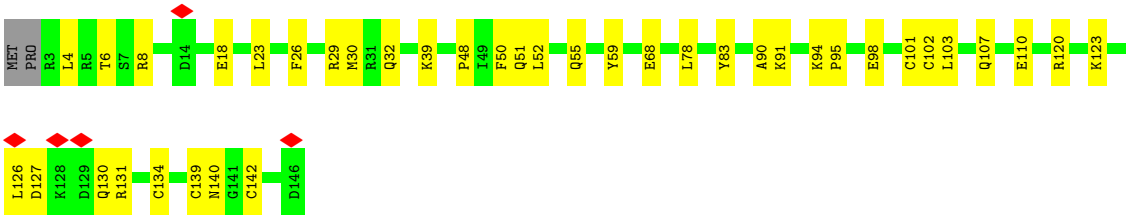
T901 Y902 N903 K904 D905 N906 F907 F908 D909 Y910 A911 T912 K913 L914 Y915 G916 E917 L918 E919 Y920 M921 F922 Q923 Q924 L925 E926 E927 I928 R929 P930 F931 G932 L933 L934 R935 Y936 Y937 E938 D939 Q940 E941 L942 Y943 A944 L945 C946 Q947 Q948 S949 R950 I951 I952 G953 C954 T955 W956 T957 S958 L959 S960

T961 R962 L963 G964 T965 L966 K967 E968 K969 G970 F971 C972 F973 N974 N975 L976 I977 V978 M979 N980 S981 Q982 N983 I984 S985 E986 S987 S988 I989 T990 S991 I992 L993 S994 L995 N996 C997 E998 P999 T1000 G1001 F1002 D1003 R1004 L1005 V1006 L1007 L1008 G1009 N1010 Q1011 Y1012 L1013 T1014 S1015 G1016 N1017 Q1018 D1019 I1020

N1021 N1022 T1023 S1024 N1025 G1026 S1027 L1028 F1029 K1030 R1031 L1032 R1033 Y1034 L1035 K1036 S1037 R1038 I1039 I1040 D1041 L1042 N1043 T1044 Q1045 Y1046 N1047 V1048 R1049 E1050 S1051 I1052 S1053 S1054 L1055 C1056 S1057 S1058 I1059 Y1060 P1061 L1062 D1063 I1064 K1065 T1066 V1067 D1068 S1069 S1070 P1071 N1072 K1073 R1074 L1075 D1076 Y1077 G1078 N1079 S1080

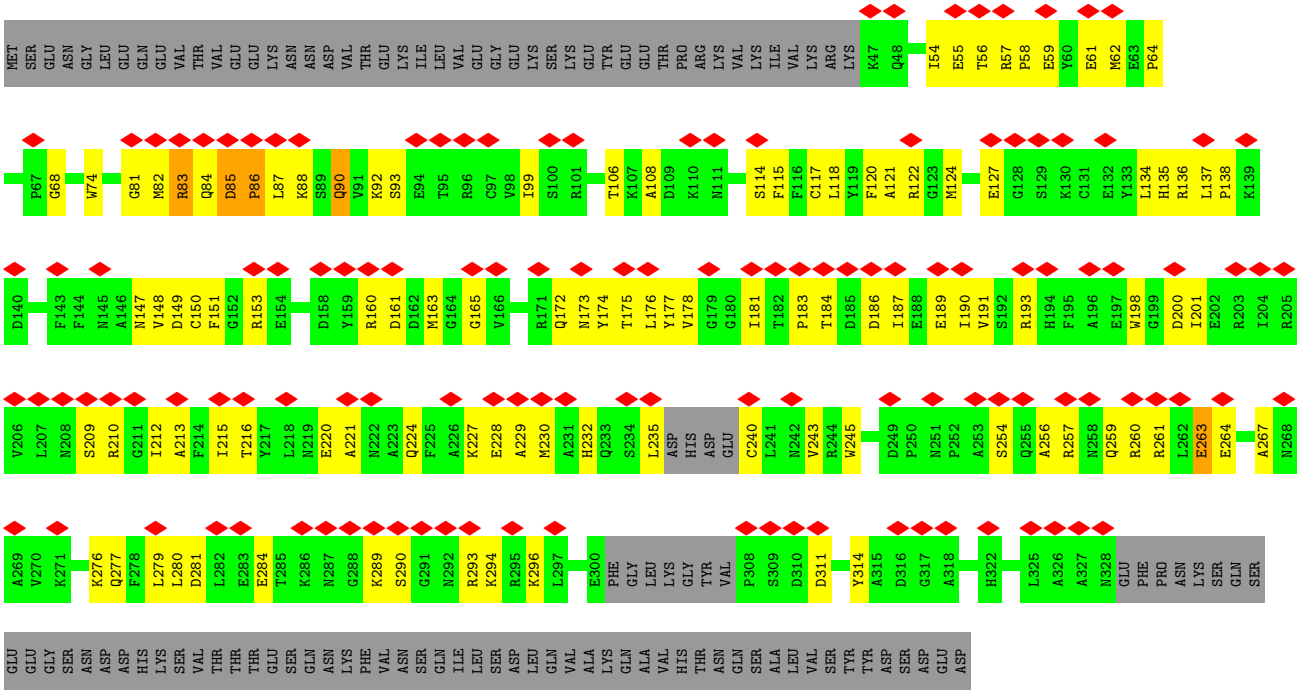
- Molecule 19: Pre-mRNA-splicing factor cwf14

Chain O:



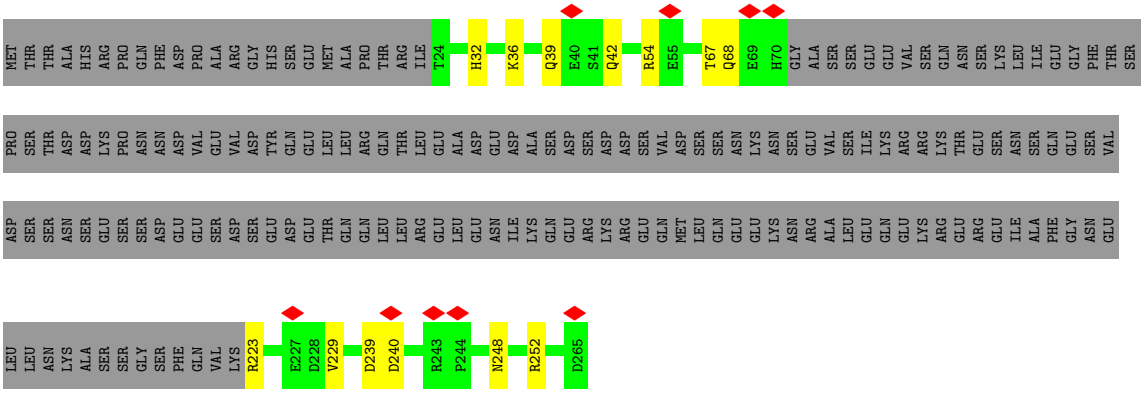
- Molecule 20: Pre-mRNA-splicing factor cwf2

Chain P:



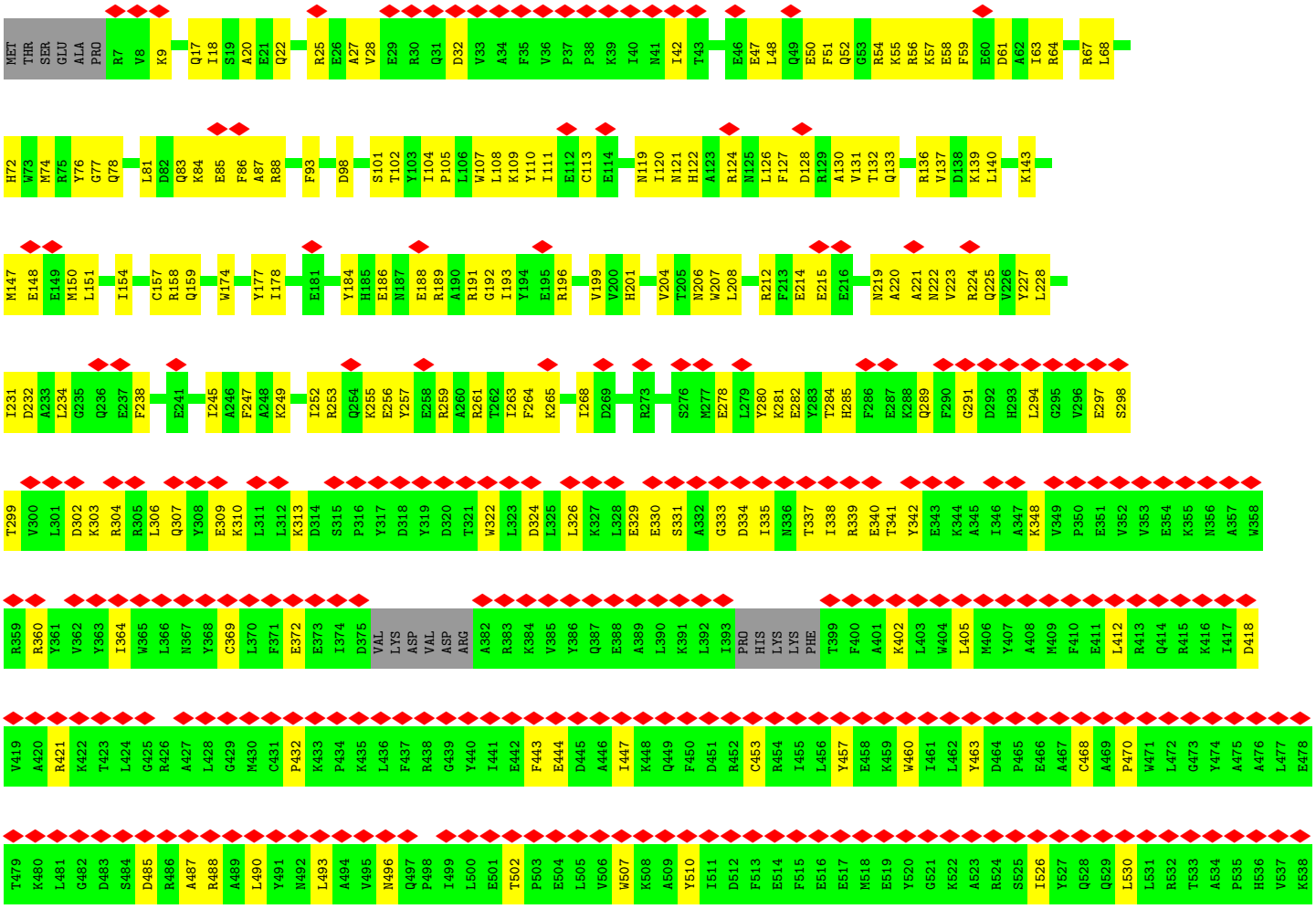
• Molecule 21: Pre-mRNA-splicing factor cwf15

Chain Q:



• Molecule 22: Pre-mRNA-splicing factor cwf4

Chain R:



V539 W540 I541 S542 F543 A544 N545 F546 E547 I548 A549 H550 L551 E552 D553 D554 D555 E556 E557 P558 P559 N560 E561 E562 V563 A564 S565 P566 T567 A568 V569 V570 R571 A572 R573 N574 V575 F576 E577 N578 A579 L580 A581 H582 L583 R584 Q585 Q586 G587 L588 K589 E590 E591 R592 V593 V594 L595 L596 E597 A598

W599 K600 Q601 F602 E603 A604 M605 H606 G607 T608 E609 D610 T611 R612 K613 H614 V615 S616 S617 L618 M619 P620 GLN VAL VAL LYS LYS ARG ARG ARG LEU GLU ASP GLY SER PHE GLU GLU TYR LEU ASP TYR LEU PHE PRO ASP THR ALA THR ASP GLN GLY ASP LYS MET ARG LYS MET LEU GLU

LEU SER ARG LYS TRP LYS GLU GLU MET ALA LYS LYS LYS LEU GLU ALA

- Molecule 23: Pre-mRNA-processing factor 19

Chain S: 27% 18% 9% 73%

M1 F2 C3 S4 I5 S6 G7 E8 T9 P10 K11 E12 P13 V14 I15 S16 R17 V18 S19 G20 N21 V22 Y23 E24 K25 R26 L27 I28 E29 Q30 V31 I32 R33 E34 T35 S36 K37 D38 P39 V40 T41 Q42 Q43 E44 C45 T46 L47 E48 D49 L50 V51 P52 V53 K54 V55 P56 D57 F58 V59 R60

P61 R62 P63 P64 S65 A66 T67 S68 L69 P70 A71 L72 L73 S74 L75 F76 Q77 E78 E79 W80 D81 S82 V83 A84 L85 E86 Q87 F88 E89 L90 R91 R92 N93 L94 T95 E96 T97 K98 Q99 E100 L101 S102 T103 A104 L105 Y106 S107 L108 D109 A110 A111 L112 R113 V114 I115 S116 R117 L118 T119 K120

E121 R122 D123 E124 A125 R126 E127 A128 L129 A130 K131 F132 SER ASP ASN ILE GLY THR VAL SER SER LYS THR ILE GLU VAL GLN GLU VAL GLU MET GLY GLU SER ASP ASP GLN LEU LYS THR SER LEU ARG SER THR VAL GLU LYS THR PHE GLN GLU LEU SER SER LYS ARG LYS ARG THR

LYS LEU GLN PRO LYS TRP ALA THR ASP ASP ALA VAL SER GLN LEU LEU GLN ALA THR PRO SER THR ILE LEU GLU ASN LEU GLU THR GLU SER THR THR SER PHE PHE PRO SER PRO GLU ASN SER SER PHE VAL LEU CYS LEU HIS LYS ASP GLU LEU LEU CYS LEU ASP ILE GLN SER

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

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

GLU THR SER SER GLY ASN GLU LEU THR LYS PHE GLY PRO HIS SER SER PRO VAL LYS THR LEU GLN PHE GLY GLU ASN GLY TYR TRP LEU VAL VAL THR THR ASN ASP ASP SER ASP ILE PHE ILE TRP ASP LEU ARG LYS SER GLU LEU VAL GLN LYS ILE PRO LEU GLN THR LYS VAL

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

ASN GLY ALA ILE LEU ARG LEU GLY

- Molecule 23: Pre-mRNA-processing factor 19

Chain T: 26% 15% 12% 73%

M1 F2 C3 S4 I5 S6 G7 E8 T9 P10 K11 E12 P13 V14 I15 S16 R17 V18 S19 G20 N21 V22 Y23 E24 K25 R26 L27 I28 E29 Q30 V31 I32 R33 E34 T35 S36 K37 D38 P39 V40 T41 Q42 Q43 E44 C45 T46 L47 E48 D49 L50 V51 P52 V53 K54 V55 P56 D57 F58 V59 R60

P61 R62 P63 P64 S65 A66 T67 S68 L69 P70 A71 L72 L73 S74 L75 F76 Q77 E78 E79 W80 D81 S82 V83 A84 L85 E86 Q87 F88 E89 L90 R91 R92 N93 L94 T95 E96 T97 K98 Q99 E100 L101 S102 T103 A104 L105 Y106 S107 L108 D109 A110 A111 L112 R113 V114 I115 S116 R117 L118 T119 K120

E121 R122 D123 E124 A125 R126 E127 A128 L129 A130 K131 F132 S133 D134 ASN ILE GLY THR VAL SER SER LYS THR ILE GLU VAL GLN GLN GLU VAL GLU MET GLY GLU SER ASP ASP GLN LEU LYS THR SER LEU ARG SER THR VAL GLU LYS THR PHE GLN GLU LEU SER SER LYS ARG LYS ARG THR

LYS LEU GLN PRO LYS TRP ALA THR ASP ASP ALA VAL SER GLN LEU LEU GLN ALA THR PRO SER THR ILE LEU GLU ASN LEU GLU THR GLU SER THR THR SER PHE PHE PRO SER PRO GLU ASN SER SER PHE VAL LEU CYS LEU HIS LYS ASP GLU LEU LEU CYS LEU ASP ILE GLN SER

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

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

GLU THR SER SER GLY ASN GLU LEU THR LYS PHE GLY PRO HIS SER SER PRO VAL LYS THR LEU GLN PHE GLY GLU ASN GLY TYR TRP LEU VAL VAL THR THR ASN ASP ASP SER ASP ILE PHE ILE TRP ASP LEU ARG LYS SER GLU LEU VAL GLN LYS ILE PRO LEU GLN THR LYS VAL

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

ASN GLY ALA ILE LEU ARG LEU GLY

- Molecule 23: Pre-mRNA-processing factor 19

Chain U: 86% 70% 18% 12%

M1 F2 C3 S4 I5 S6 G7 E8 T9 P10 K11 E12 P13 V14 I15 S16 R17 V18 S19 G20 N21 V22 Y23 E24 K25 R26 L27 I28 E29 Q30 V31 I32 R33 E34 T35 S36 K37 D38 P39 V40 T41 Q42 Q43 E44 C45 T46 L47 E48 D49 L50 V51 P52 V53 K54 V55 P56 D57 F58 V59 R60

P61 R62 P63 P64 S65 A66 T67 S68 L69 P70 A71 L72 L73 S74 L75 F76 Q77 E78 E79 W80 D81 S82 V83 A84 L85 E86 Q87 F88 E89 L90 R91 R92 N93 L94 T95 E96 T97 K98 Q99 E100 L101 S102 T103 A104 L105 Y106 S107 L108 D109 A110 A111 L112 R113 V114 I115 S116 R117 L118 T119 K120

E121 R122 D123 E124 A125 R126 E127 A128 L129 A130 K131 F132 S133 D134 N135 ILE GLY THR VAL SER SER LYS THR ILE GLU VAL GLN GLU VAL GLU MET GLY GLU SER ASP ASP GLN LEU LYS THR SER LEU ARG SER THR VAL GLU LYS THR PHE GLN GLU L173 S174 S175 K176 R177 K178 R179 T180

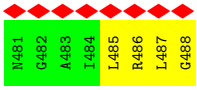
K181 L182 Q183 P184 K185 W186 A187 T188 D189 D190 A191 V192 S193 Q194 L195 L196 Q197 A198 T199 P200 S201 T202 I203 L204 E205 N206 L207 E208 T209 E210 S211 T212 T213 S214 F215 F216 P217 S218 P219 E220 N221 S222 S223 F224 V225 L226 C227 L228 H229 K230 D231 E232 L233 L234 C235 L236 D237 I238 Q239 S240

ASN SER THR LEU LYS ILE PHE E248 G249 S250 A251 L252 A253 C254 C255 W256 L257 T258 S259 S260 K261 I262 A263 V264 A265 T266 A267 D268 A269 I270 S271 I272 F273 E274 F275 P276 V277 S278 S279 S280 G281 L282 Q283 S284 V285 G286 E287 PRO THR SER SER ILE PRO I294 D295 E296 K297 V298 N299 F300

L301 Q302 A303 H304 P305 S306 G307 E308 Y309 L310 L311 A312 A313 S314 N315 E316 K317 C318 Y319 I320 F321 S322 LEU K324 S325 Q326 V327 Y328 N329 I330 T331 V332 A333 Q334 H335 I336 T337 S338 L339 A340 V341 H342 P343 D344 G345 N346 L347 F348 V349 A350 G351 L352 E353 N354 G355 E356 L357 R358 F359 F360

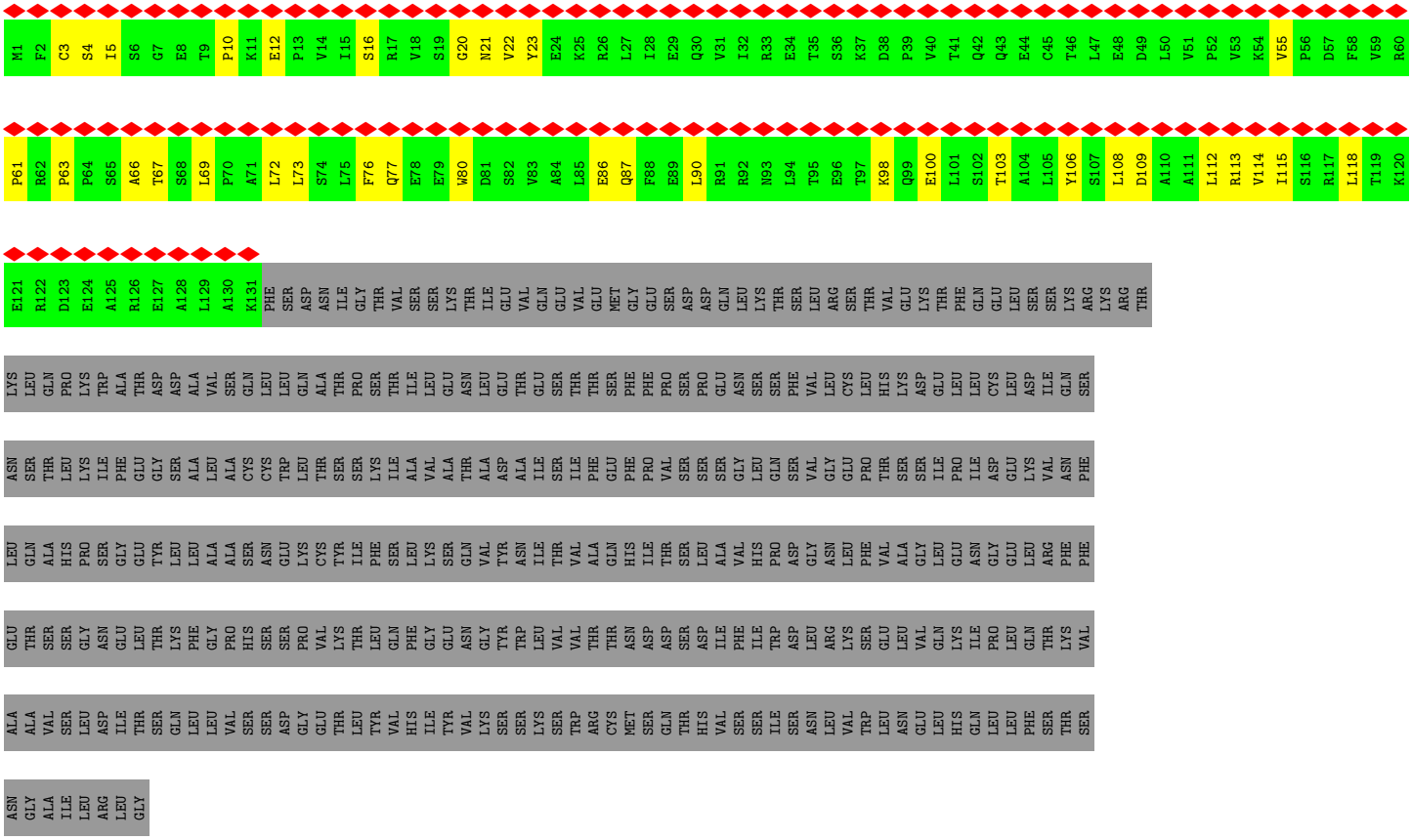
E361 T362 S363 S364 G365 N366 E367 L368 T369 K370 F371 G372 P373 H374 S375 S376 P377 V378 K379 T380 L381 Q382 F383 G384 E385 N386 G387 Y388 W389 L390 V391 V392 T393 T394 N395 ASP ASP S398 D399 I400 F401 I402 W403 D404 L405 R406 K407 S408 E409 L410 V411 Q412 K413 I414 P415 L416 Q417 T418 K419 V420

A421 A422 V423 S424 L425 D426 I427 T428 SER Q430 L431 L432 V433 S434 S435 D436 G437 E438 T439 L440 Y441 V442 H443 I444 Y445 V446 K447 S448 SER LYS SER TRP R453 C454 M455 S456 Q457 T458 H459 V460 S461 S462 I463 S464 N465 L466 V467 W468 L469 N470 E471 L472 H473 Q474 L475 L476 F477 S478 T479 S480



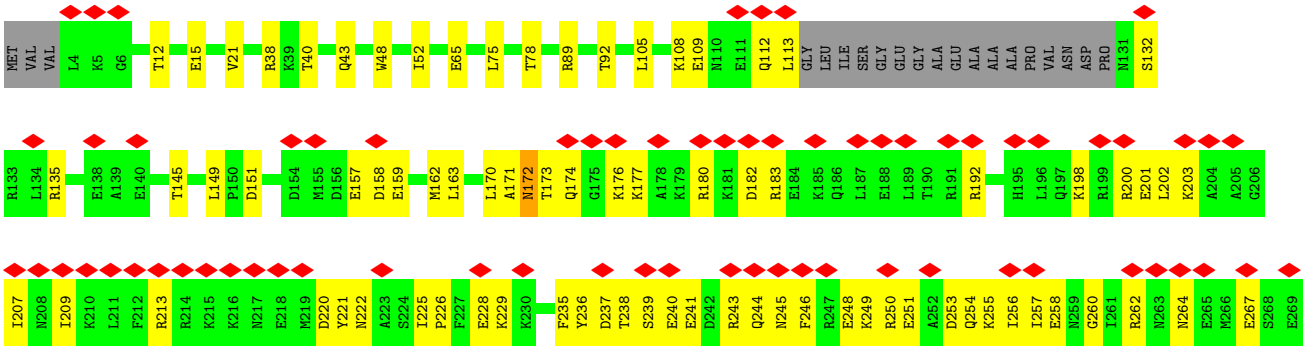
• Molecule 23: Pre-mRNA-processing factor 19

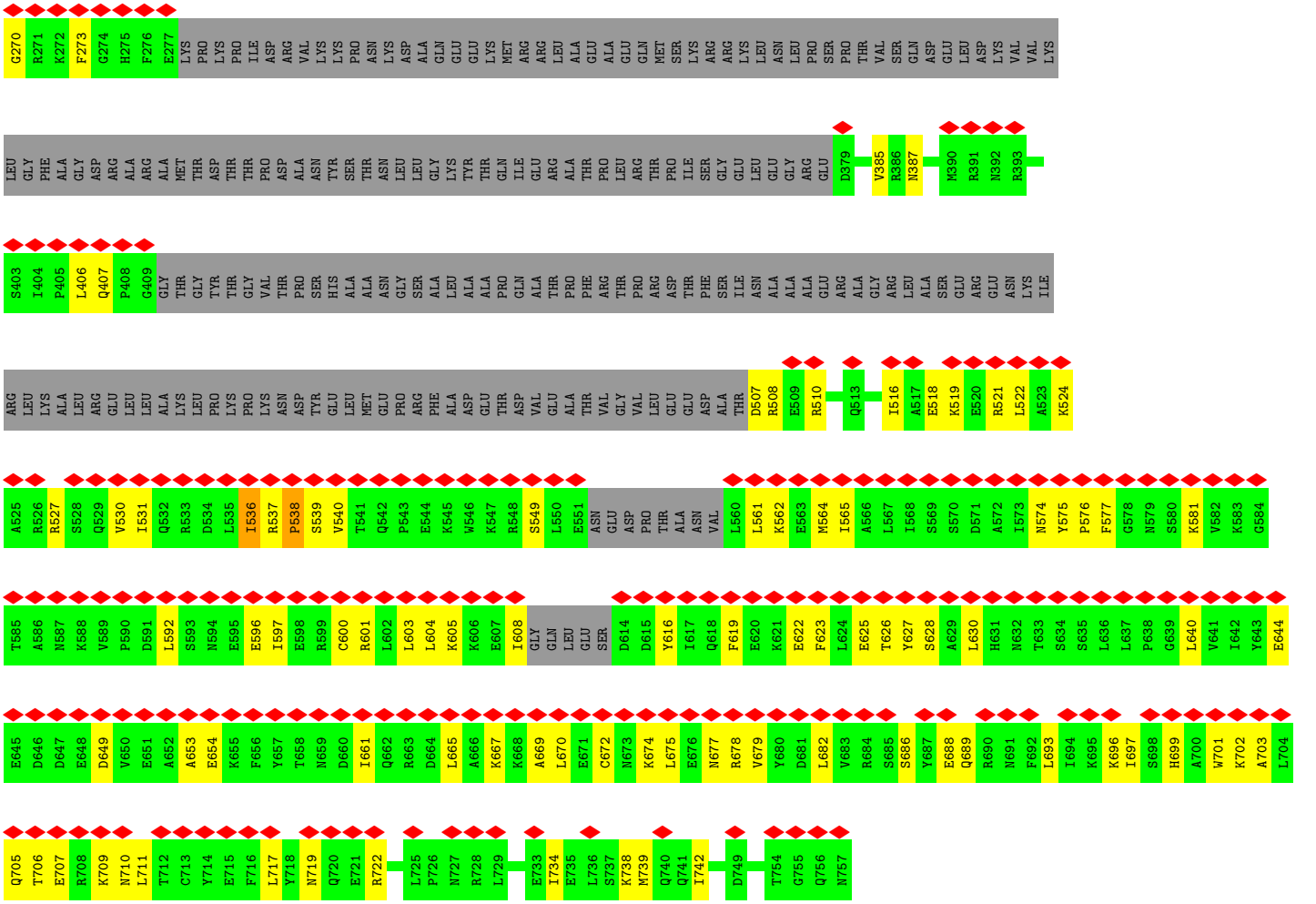
Chain V:



• Molecule 24: Pre-mRNA-splicing factor cdc5

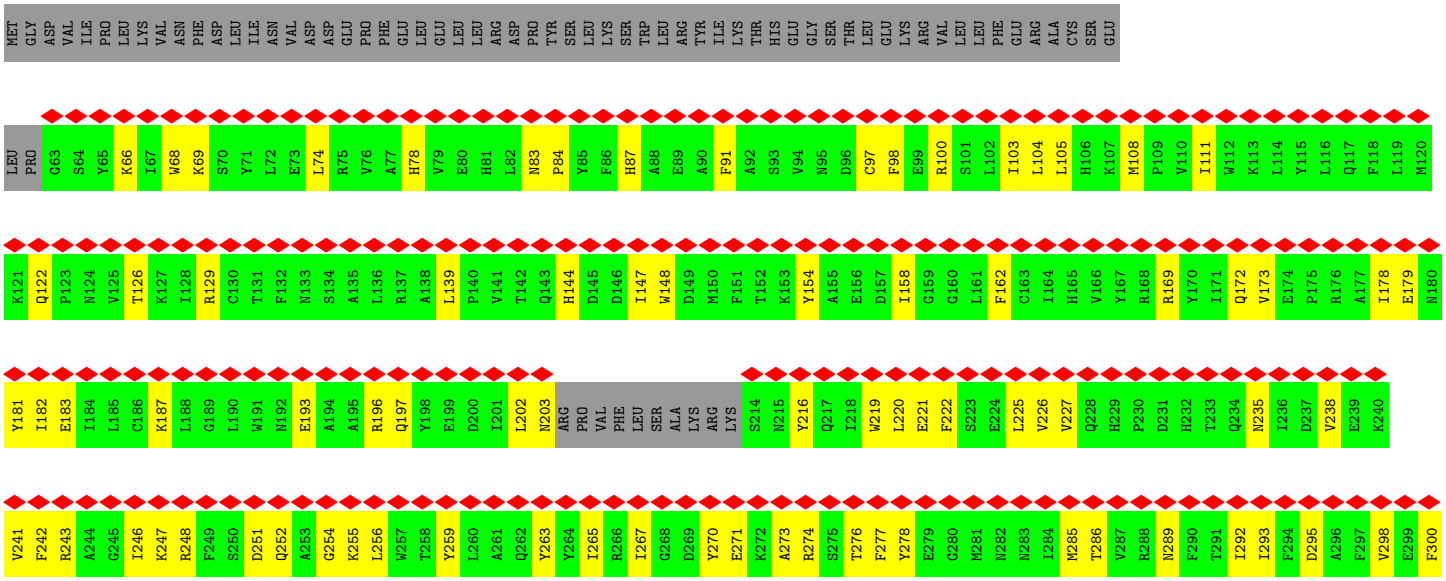
Chain W:





• Molecule 25: Pre-mRNA-splicing factor cwf3

Chain X:



E301 E302 Q303 W304 L305 S306 A307 R308 V309 E310 A311 S312 S313 G314 N315 A316 N317 D318 E319 L320 S321 I322 D323 F324 H325 M326 A327 W328 L329 E330 K331 I332 L333 D334 K335 R336 P337 L338 Y339 I340 N341 D342 V343 L344 L345 R346 GLN ASN I349 N350 N351 V352 D353 E354 W355 L356 R357 R358 V359 K360

F361 L362 E363 D364 D365 S366 E367 K368 V369 V370 Q371 V372 Y373 T374 D375 A376 I377 K378 N379 V380 N381 P382 K383 L384 A385 H386 G387 S388 L389 G390 K391 L392 F393 S394 E395 F396 A397 R398 F399 Y400 E401 N402 F403 D404 D405 L406 E407 Q408 S409 R410 I411 I412 F413 E414 K415 A416 T417 H418 V419 P420

Y421 LYS THR VAL N425 E426 L427 A428 Q429 V430 W431 I432 D433 W434 A435 E436 M437 E438 L439 R440 H441 Q442 N443 F444 D445 A446 A447 R448 K449 L450 I451 G452 D453 A454 V455 H456 A457 P458 R459 K460 S461 H462 I463 S464 F465 F466 D467 E468 S469 L470 S471 P472 Q473 V474 R475 L476 H477 K478 S479 S480

K481 I482 W483 M484 Y485 Y486 L487 D488 L489 E490 E491 S492 V493 G494 T495 I496 E497 T498 T499 R500 K501 L502 Y503 D504 R505 V506 F507 E508 L509 K510 I511 A512 T513 P514 Q515 V516 V517 V518 N519 Y520 A521 N522 L523 L524 E525 E526 N527 A528 Y529 F530 E531 D532 S533 F534 K535 I536 Y537 E538 R539 G540

V541 A542 L543 F544 S545 Y546 P547 V548 A549 F550 E551 L552 W553 N554 L555 Y556 L557 T558 K559 F560 V561 K562 R563 Y564 Q565 G566 T567 H568 M569 E570 R571 T572 R573 D574 L575 F576 E577 Q578 A579 L580 E581 G582 C583 P584 P585 E586 F587 S588 K589 S590 I591 Y592 L593 L594 Y595 A596 D597 F598 E599 E600

K601 F602 G603 K604 A605 K606 R607 S608 I609 S610 I611 L612 E613 K614 A615 A616 D617 K618 V619 K620 T621 A622 D623 R624 L625 A626 I627 Y628 N629 V630 L631 L632 V633 K634 V635 A636 L637 N638 Y639 G640 V641 L642 A643 T644 R645 T646 V647 Y648 E649 K650 A651 I652 E653 S654 L655 SER ASP S658 E659 V660

K661 D662 M663 C664 L665 R666 F667 A668 E669 M670 E671 T672 K673 L674 G675 E676 I677 D678 R679 A680 R681 L682 I683 Y684 I685 H686 G687 S688 Q689 Y690 C691 ASP PRO R694 V695 E696 T697 D698 Y699 W700 K701 A702 W703 Q704 E705 F706 E707 I708 R709 Y710 G711 N712 P713 E714 E715 T716 V717 K718 E719 M720

L721 R722 I723 K724 R725 S726 V727 Q728 T729 K730 F731 S732 T733 D734 S735 LEU HIS ILE ALA LYS ARG ALA ALA LYS ILE GLU SER ALA ALA ALA PRO MET ASP PRO MET GLU GLN LEU GLU MET GLU LYS SER GLU GLY PRO LYS ALA LEU ALA GLY PHE VAL LEU SER LYS SER ASN PRO GLN

GLU THR SER LYS ILE THR GLY GLU GLU ASN

- Molecule 26: Pre-mRNA-splicing factor syf2

Chain Y:

MET ASP SER PRO SER HIS SER ARG GLU ALA ARG VAL GLU LYS LEU LYS LYS LYS ILE ARG GLU GLN MET ARG LYS SER SER HIS GLU ASN ARG LYS GLU VAL VAL GLN GLU HIS SER ARG MET ARG ILE ASP PRO ALA LEU GLU ARG ARG LEU GLU ARG LYS ARG MET GLU ALA GLU GLU GLU

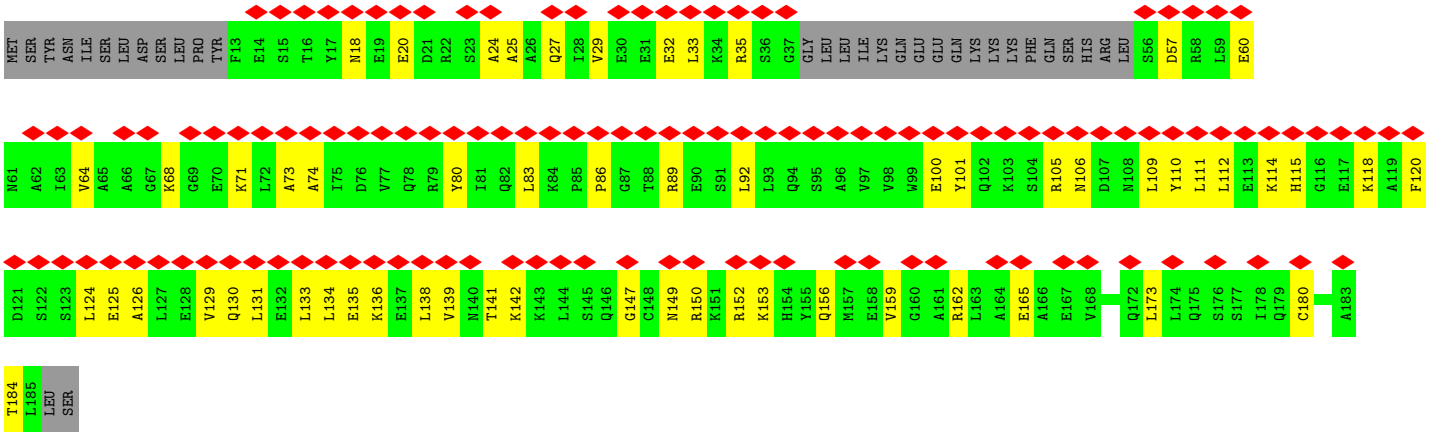
LEU ALA LYS ILE GLU THR GLU GLU GLU GLY GLY ASP PHE GLU ARG ARG ARG ALA TRP ASP TRP THR I83 E84 E85 S86 E87 K88 W89 D90 Q91 R92 L93 R94 K95 K96 K97 Q98 T99 I100 GLN ASN VAL ALA F105 S106 D107 Y108 H109 S110 Q111 K114 D115 Y116 N117 R118 G119 I120

L123 K124 P125 D126 Y127 E128 K129 Y130 D131 K132 D133 K134 K135 E136 E137 K138 S139 K140 S141 R142 S143 V144 A145 L146 Y147 D148 E149 A150 E151 R152 L153 D154 W155 V156 S157 N158 K159 P160 D161 K162 E163 H164 V165 E166 R167 L168 V169 E170 S171 I172 K173 K174 Q175 D176 Q177 R178 R179 L180 K181 N182

T183 K184 ARG ARG GLY THR ASP GLU GLU ASP HIS I194 T195 F196 I197 N198 E199 R200 N201 R202 K203 F204 N205 L206 K207 L208 Q209 R210 F211 Y212 S213 K214 Y215 THR LYS ASP ILE LYS GLU ASP LEU GLU ARG GLY THR ALA LEU

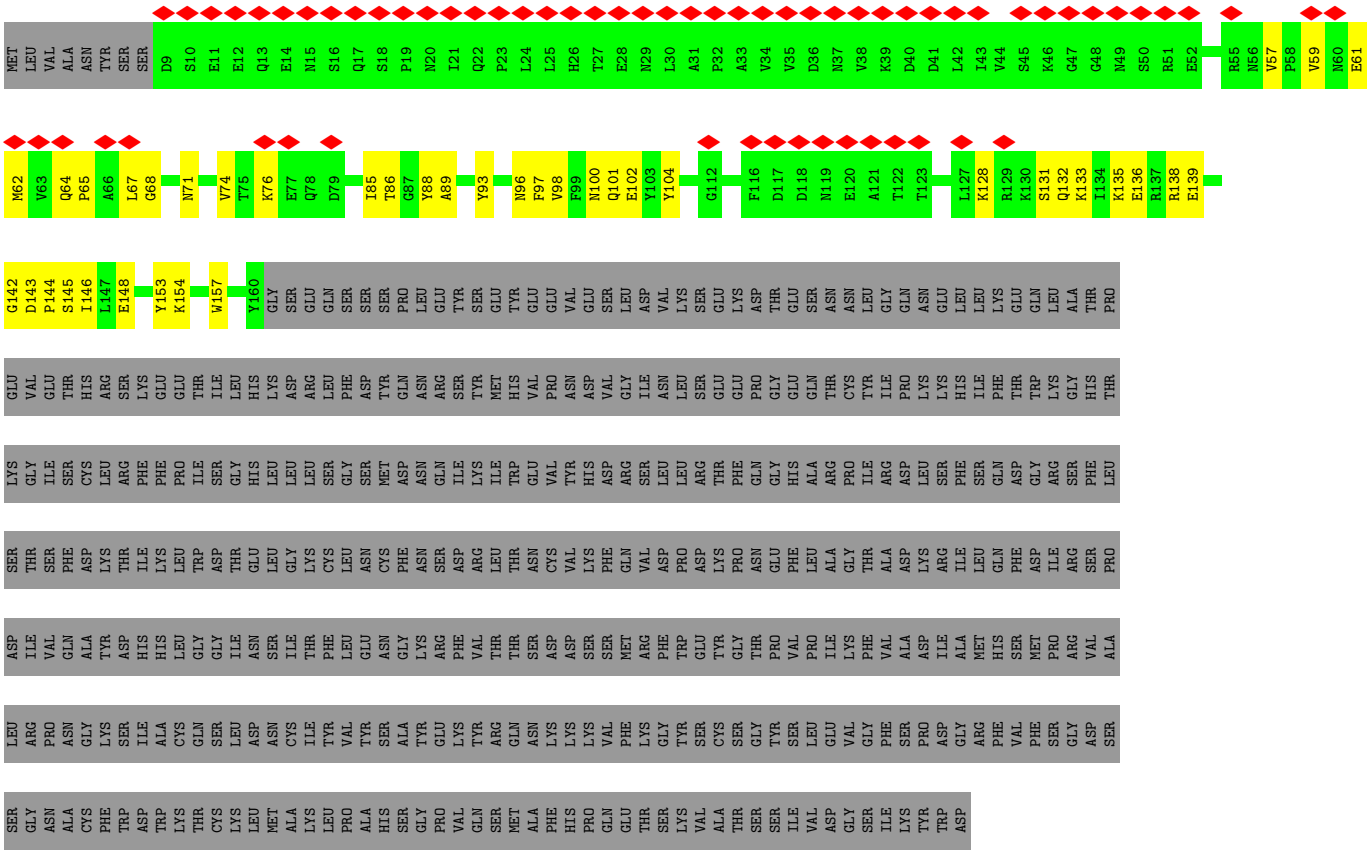
- Molecule 27: Pre-mRNA-splicing factor cwf7

Chain Z:



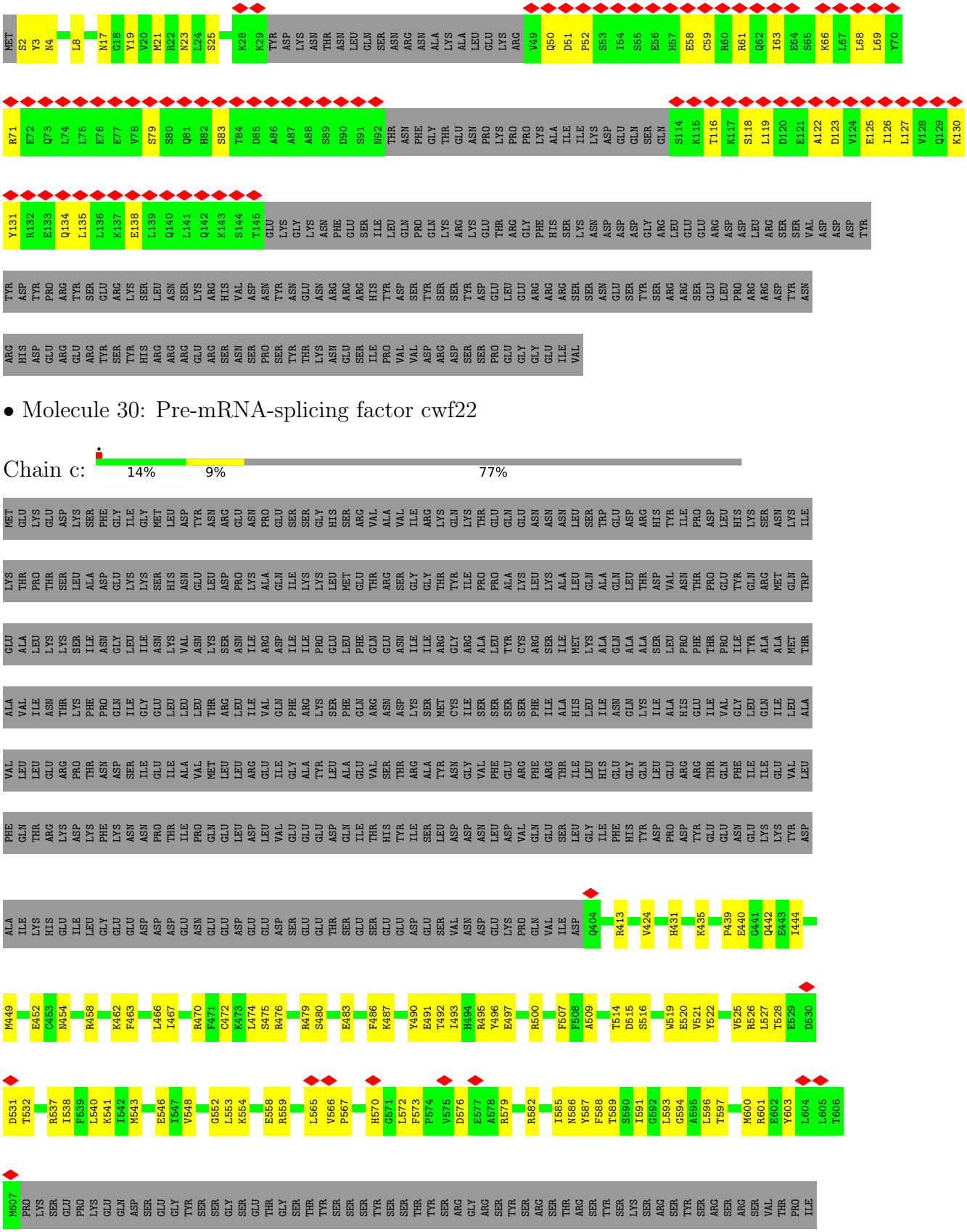
• Molecule 28: Pre-mRNA-processing factor 17

Chain a:



• Molecule 29: Pre-mRNA-splicing factor cwf21

Chain b:



• Molecule 30: Pre-mRNA-splicing factor cwf22

Chain c: 14% 9% 77%

ASN ASN ILE ASN HIS LYS LYS TYR ILE ARG LYS ASP ARG GLU LEU SER PRO ARG GLY ARG GLU ARG SER SER ASN ARG ASN SER TYR SER ASP LEU SER ARG SER SER SER LEU SER ARG GLY ARG SER ARG SER TYR THR PRO GLU GLY ARG LEU ILE GLU SER GLU ASP LYS GLY TYR

ARG SER ARG SER SER PRO ALA SER ARG LYS TYR ARG SER ARG GLN ARG TYR ARG ARG SER TYR ARG GLY SER THR SER ARG GLY ARG SER PHE SER ARG SER PRO SER TYR ARG ARG ARG LEU SER MET SER CYS SER VAL SER TYR SER ARG SER PRO SER PRO ALA ALA ARG PRO

ILE SER ARG SER PRO ALA ARG ASN LYS ARG LEU ARG SER TYR ASP SER LEU SER TYR ASN ARG GLN TYR SER PRO LYS VAL SER ARG LYS ARG SER ASN GLU SER ARG SER PRO SER PRO TYR THR LEU ARG LYS GLN LYS THR TYR HIS LEU ASN LYS ARG ASN GLU ASP PHE VAL VAL LYS MET

ASP LYS LYS GLY SER GLU SER PRO VAL ILE LEU ALA PRO TRP LEU ARG GLU VAL ASP ASP GLY GLU LEU TYR LYS ASP ARG ASN SER GLU SER ASP SER VAL ARG LYS GLN PRO ARG ALA ASP

- Molecule 31: Peptidyl-prolyl cis-trans isomerase ppi1

Chain d: 45% 57% 43%

MET A2 E5 L6 Q7 T8 S9 L10 G11 K12 I13 L14 I15 E16 L17 Y18 T19 E20 H21 A22 P23 K24 Q27 N28 F29 Y30 T31 L32 A33 K34 E35 G36 Y37 Y38 D39 I42 F43 H44 R45 V46 I47 P48 D49 F50 V51 I52 Q53 G54 G55 D56 P57 T58 G59 T60 G61 R62 G63

G64 T65 G69 D70 D73 D74 H77 S78 D79 H82 T83 G84 A85 L88 S89 M90 A91 N92 A93 G94 P95 N96 T97 N98 S99 S100 Q101 F102 F103 L106 A107 P108 W111 L112 D113 G114 K115 H116 T117 G120 V123 S124 G125 V128 C129 K130 R131 M132 G133 L134

I135 R136 T137 D138 S139 S140 D141 E145 P146 L147 K148 I149 I150 K151 A152 V153 A154 L155

- Molecule 32: UNK1

Chain f: 86% 100%

X1 X2 X3 X4 X5 X6 X7 X8 X9 X10 X11 X12 X13 X14 X15 X16 X17 X18 X19 X20 X21 X22

- Molecule 33: G-patch domain-containing protein C1486.03

Chain m: 10% 8% 90%

MET GLN ASN GLU TYR VAL ASP MET ASN SER SER SER GLU ASP SER ASP GLY ASP SER ILE LEU GLU GLU GLY ARG LEU ARG PRO SER PHE ARG GLY GLN GLN LYS GLU ARG ASP MET LEU GLY ILE PHE GLY GLU GLU ASP GLU ASP GLY PHE HIS ASN SER GLY ILE GLY SER ALA ARG

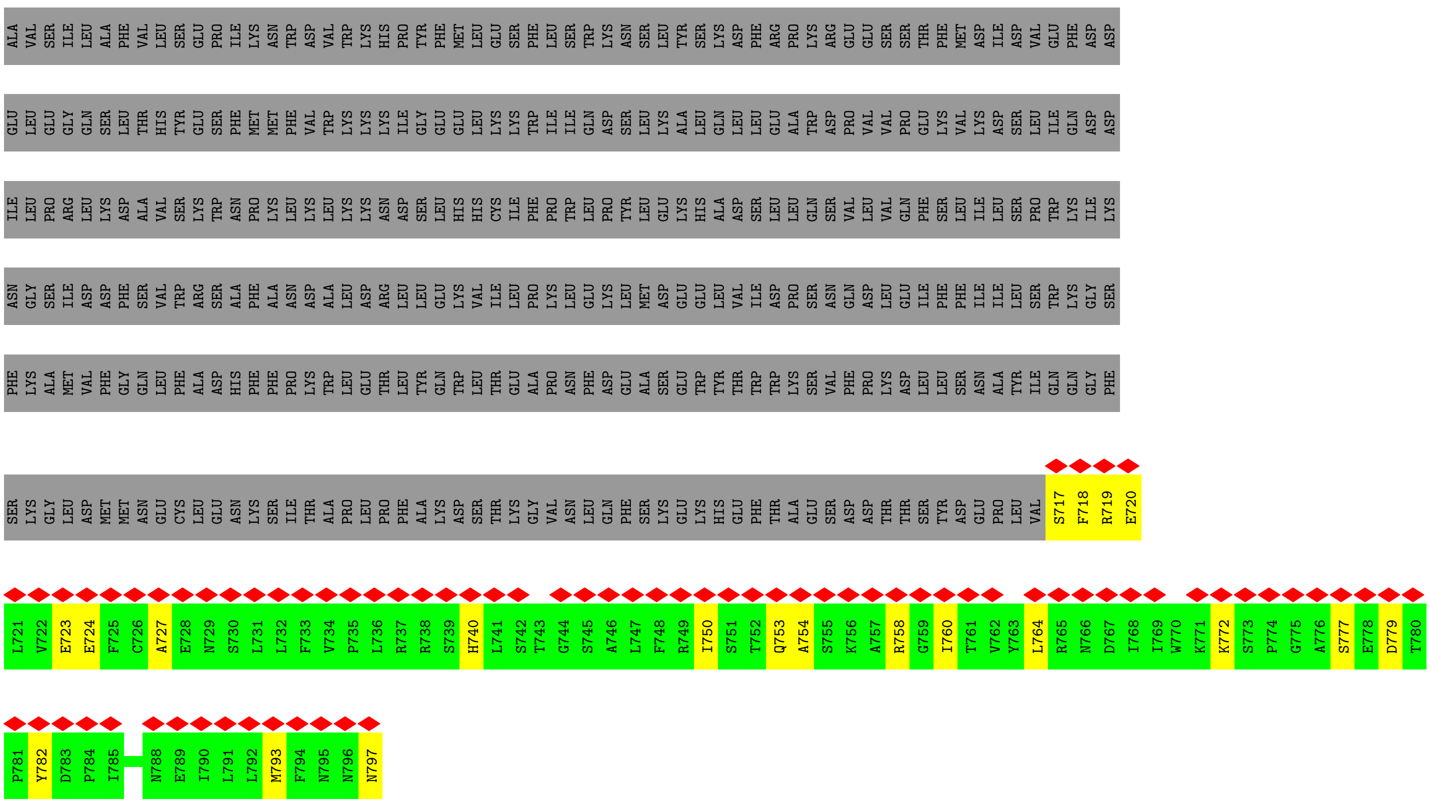
LEU ARG ARG LYS ASN ILE SER PHE VAL GLU LYS SER GLU GLN VAL LYS ALA ASN LYS GLN VAL THR ALA ASP ASP LEU LEU GLU ALA HIS SER ILE PRO GLN LEU LYS ASN LYS ASN ASP GLU VAL SER GLN ALA LYS ASN ILE PRO LYS MET LYS PHE ASN THR THR GLY PHE GLY ALA

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

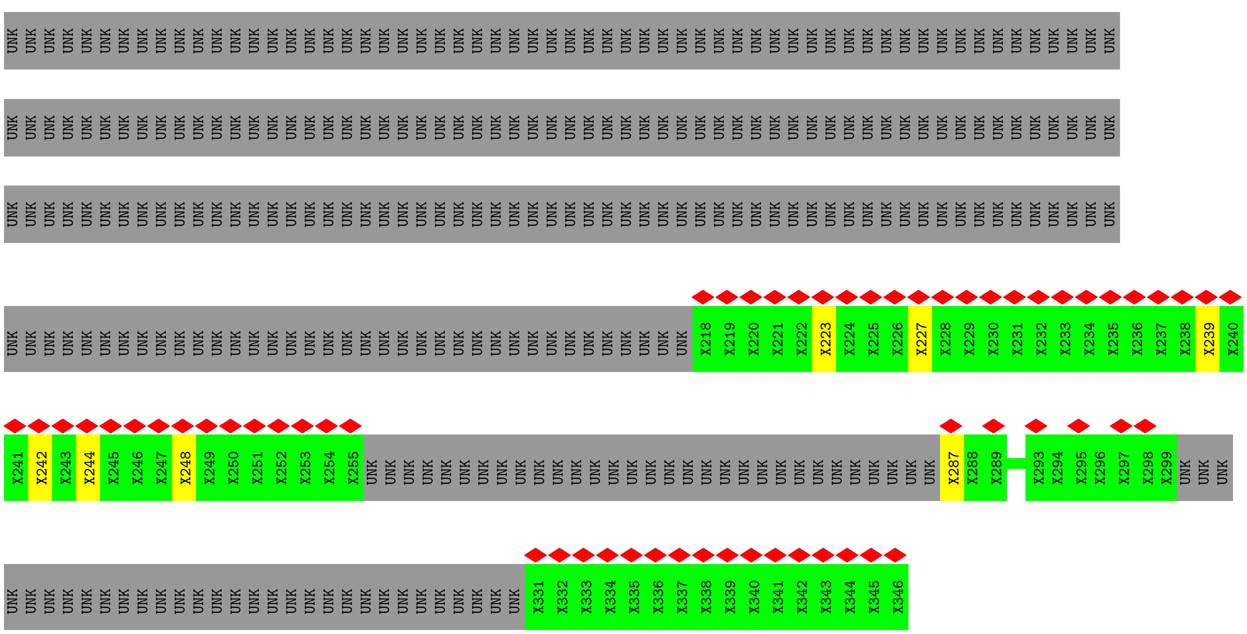
ASP GLU LYS HIS THR VAL LYS GLN LYS PRO LEU ARG GLU LYS LYS LYS PRO LEU LYS SER SER GLU GLU ILE SER LYS ASP MET GLY SER TYR ASN LEU PRO ARG PHE LEU ALA SER LEU ILE ASP ALA SER LEU ASN ASP THR LYS GLU ILE GLU PHE VAL THR SER ASN LYS GLU

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

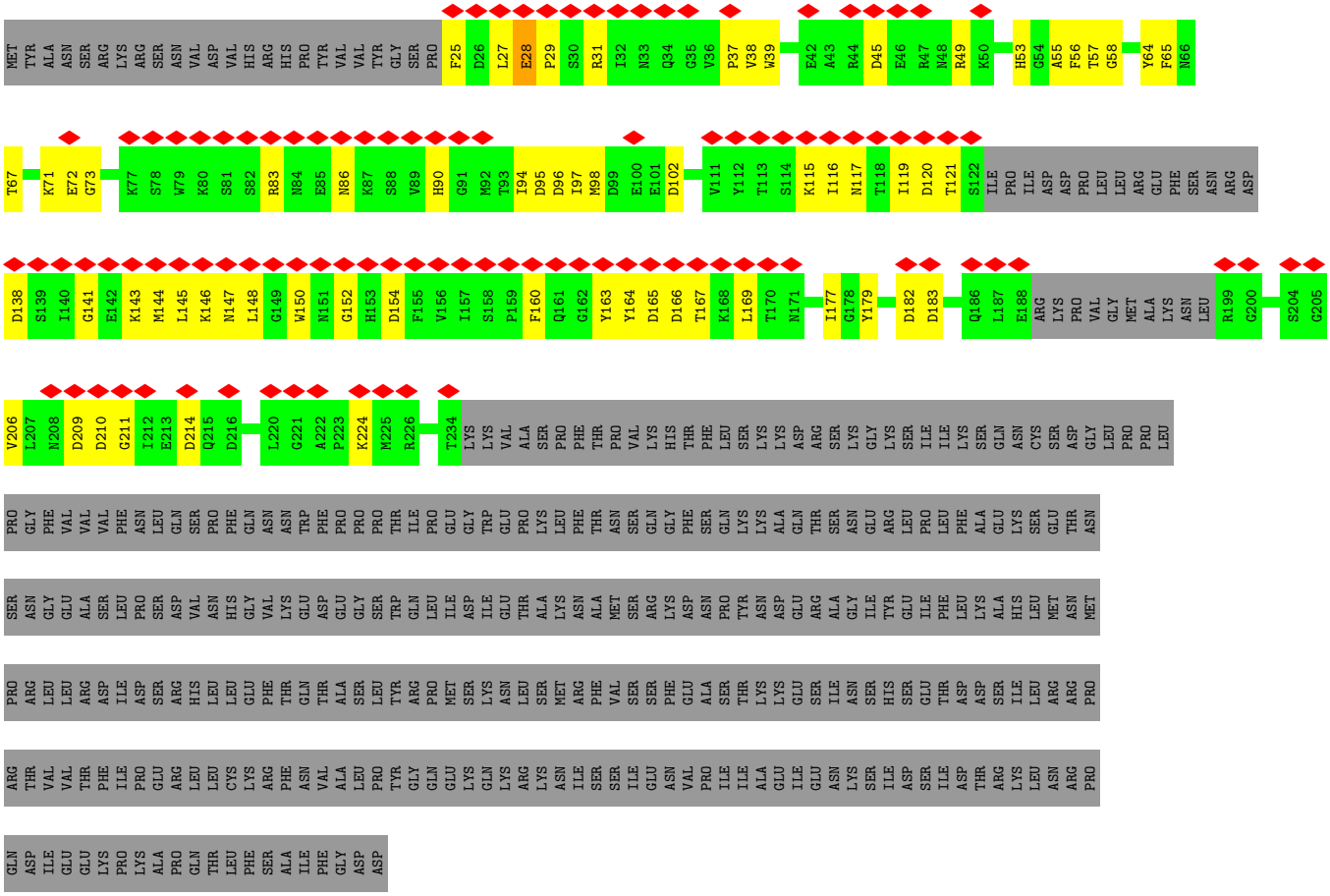
SER ARG LEU GLU LYS LEU LEU GLY LYS VAL MET GLU VAL LYS SER ARG SER MET GLU PHE THR VAL PRO GLU ALA GLU ILE ASP VAL ILE GLU LYS ARG LEU GLN PRO LEU ASN ASN LEU ILE GLU THR LEU PRO VAL GLU PHE SER GLU ALA SER MET HIS PHE GLU LEU ASP SER VAL



• Molecule 34: UNK2

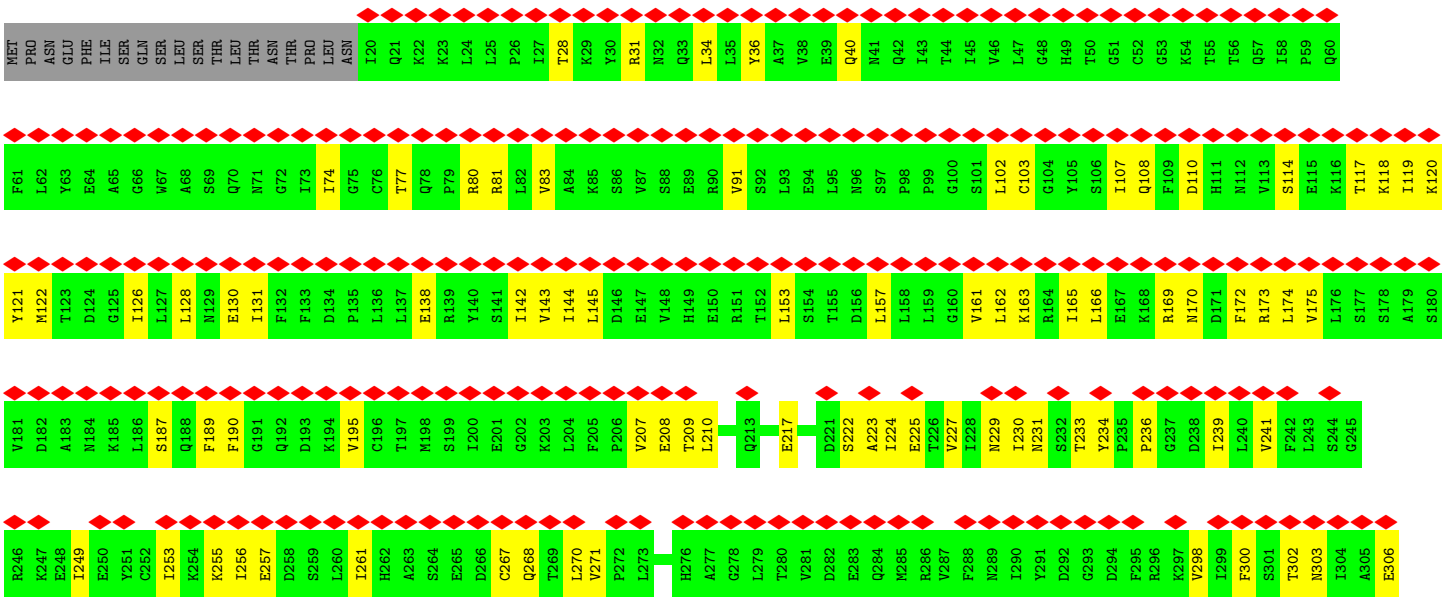


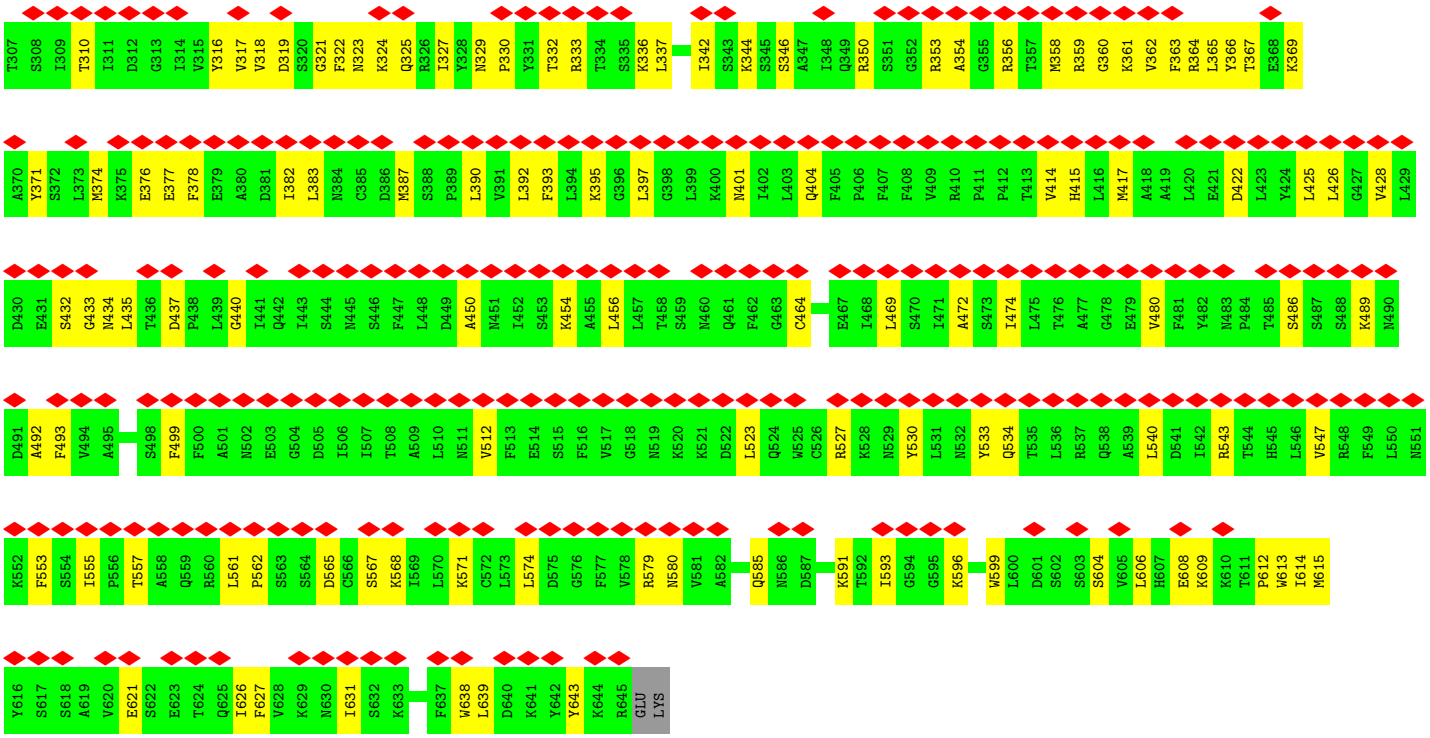
• Molecule 35: Uncharacterized protein C20H4.06c



• Molecule 36: Putative pre-mRNA-splicing factor ATP-dependent RNA helicase C20H4.09

Chain z:




T307 S308 I309 T310 I311 D312 G313 I314 V315 Y316 V317 V318 D319 S320 G321 F322 N323 K324 Q325 R326 I327 Y328 N329 P330 Y331 T332 R333 T334 S335 K336 L337 I342 S343 K344 S345 S346 A347 I348 Q349 R350 S351 G352 R353 A354 G355 R356 T357 M358 R359 G360 K361 V362 F363 R364 L365 Y366 T367 E368 K369
A370 Y371 S372 L373 M374 K375 E376 E377 F378 E379 A380 D381 I382 L383 N384 C385 D386 M387 S388 P389 L390 V391 L392 F393 L394 K395 G396 L397 G398 L399 K400 N401 I402 L403 Q404 F405 P406 F407 F408 V409 R410 P411 P412 T413 V414 H415 L416 M417 A418 A419 L420 E421 D422 L423 Y424 L425 L426 G427 V428 L429
D430 E431 S432 G433 N434 L435 T436 D437 P438 L439 G440 I441 Q442 I443 S444 N445 S446 F447 L448 D449 A450 N451 I452 S453 K454 A455 L456 L457 T458 S459 N460 Q461 F462 G463 C464 E467 I468 L469 S470 I471 A472 S473 I474 L475 T476 A477 G478 E479 V480 F481 Y482 N483 P484 T485 S486 S487 S488 K489 N490
D491 A492 F493 V494 A495 S498 F499 F500 A501 N502 E503 G504 D505 I506 I507 T508 A509 L510 N511 V512 F513 E514 S515 F516 V517 G518 N519 K520 K521 D522 L523 Q524 W525 C526 R527 K528 N529 Y530 L531 N532 Y533 Q534 T535 L536 R537 Q538 A539 L540 D541 I542 R543 T544 H545 L546 V547 R548 F549 L550 N551
K552 F553 S554 I555 P556 T557 A558 Q559 R560 L561 P562 S563 S564 D565 C566 S567 K568 I569 L570 K571 C572 L573 L574 D575 G576 F577 V578 R579 N580 V581 A582 Q585 N586 D587 K591 T592 I593 G594 G595 K596 W599 L600 D601 S602 S603 S604 V605 L606 H607 E608 K609 K610 T611 P612 W613 I614 M615
Y616 S617 S618 A619 V620 E621 S622 E623 T624 Q625 I626 F627 V628 K629 N630 I631 S632 K633 F637 W638 L639 D640 K641 Y642 Y643 K644 R645 GLU LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	49.4	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	37.729	Depositor
Minimum map value	-20.085	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.902	Depositor
Recommended contour level	3.55	Depositor
Map size (Å)	460.32, 460.32, 460.32	wwPDB
Map dimensions	560, 560, 560	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ZN, K, GTP, IHP

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	1	0.17	0/673	0.40	0/1043
2	2	0.12	0/554	0.24	0/856
3	5	0.18	0/2397	0.25	0/3727
4	6	0.14	0/2207	0.35	0/3438
5	A	0.24	0/14793	0.43	5/20040 (0.0%)
6	B	0.22	0/7459	0.43	0/10117
7	C	0.18	0/2376	0.48	0/3216
8	D	0.21	0/772	0.43	0/1038
9	E	0.17	0/737	0.43	0/993
10	F	0.22	0/646	0.57	0/875
11	G	0.23	0/829	0.66	0/1111
12	H	0.16	0/662	0.44	0/894
13	I	0.16	0/585	0.48	0/794
14	J	0.19	0/578	0.48	0/774
15	K	0.23	0/3130	0.47	0/4251
16	L	0.19	0/1885	0.43	0/2545
17	M	0.19	0/1841	0.47	0/2468
18	N	0.12	0/10690	0.33	0/14463
19	O	0.24	0/1199	0.49	0/1609
20	P	0.28	0/2222	0.58	3/2991 (0.1%)
21	Q	0.16	0/767	0.35	0/1028
22	R	0.19	0/5235	0.48	1/7067 (0.0%)
23	S	0.21	0/1072	0.47	0/1453
23	T	0.23	0/1086	0.61	0/1472
23	U	0.14	0/2897	0.42	1/3914 (0.0%)
23	V	0.19	0/1060	0.48	0/1437
24	W	0.20	0/4407	0.50	3/5907 (0.1%)
25	X	0.16	0/5599	0.40	0/7566
26	Y	0.17	0/1065	0.50	0/1413
27	Z	0.17	0/1244	0.43	0/1667
28	a	0.18	0/1055	0.45	0/1443
29	b	0.17	0/829	0.38	0/1111

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
30	c	0.20	0/1711	0.46	0/2312
31	d	0.20	0/1206	0.50	0/1636
33	m	0.14	0/663	0.38	0/895
35	y	0.18	0/1511	0.52	0/2032
36	z	0.16	0/5079	0.41	0/6875
All	All	0.19	0/92721	0.44	13/126471 (0.0%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	531	ILE	N-CA-C	-6.22	105.65	112.80
24	W	626	THR	CA-C-N	-5.86	112.92	120.65
24	W	626	THR	C-N-CA	-5.86	112.92	120.65
5	A	533	ARG	N-CA-C	-5.85	106.38	112.93
23	U	118	LEU	CA-CB-CG	5.68	136.19	116.30
22	R	596	LEU	CA-CB-CG	5.55	135.71	116.30
5	A	1642	LYS	N-CA-C	-5.53	106.43	114.12
5	A	529	LEU	O-C-N	-5.29	116.04	122.22
24	W	220	ASP	N-CA-CB	-5.24	108.20	114.17
20	P	263	GLU	N-CA-CB	5.12	117.74	110.16
20	P	83	ARG	N-CA-C	-5.06	105.28	111.75
5	A	534	LYS	O-C-N	5.03	128.13	122.20
20	P	85	ASP	CB-CA-C	-5.01	100.30	110.17

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	1	605	0	302	12	0
2	2	500	0	257	14	0
3	5	2149	0	1085	23	0
4	6	1970	0	994	53	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	14402	0	14306	361	0
6	B	7298	0	7336	189	0
7	C	2328	0	2276	89	0
8	D	760	0	776	28	0
9	E	726	0	750	24	0
10	F	638	0	682	37	0
11	G	819	0	845	49	0
12	H	652	0	680	14	0
13	I	574	0	591	28	0
14	J	573	0	602	14	0
15	K	3053	0	3011	92	0
16	L	1849	0	1879	55	0
17	M	1818	0	1822	74	0
18	N	10461	0	10412	198	0
19	O	1176	0	1167	37	0
20	P	2178	0	2101	108	0
21	Q	752	0	729	15	0
22	R	5108	0	5024	185	0
23	S	1055	0	1075	61	0
23	T	1069	0	1084	74	0
23	U	2870	0	2403	85	0
23	V	1044	0	1066	47	0
24	W	4346	0	4375	184	0
25	X	5467	0	5372	163	0
26	Y	1049	0	1052	54	0
27	Z	1232	0	1242	59	0
28	a	1035	0	837	40	0
29	b	822	0	820	28	0
30	c	1678	0	1659	63	0
31	d	1179	0	1169	60	0
32	f	110	0	29	0	0
33	m	649	0	641	16	0
34	r	335	0	77	8	0
35	y	1480	0	1379	62	0
36	z	4980	0	5047	153	0
37	6	3	0	0	0	0
37	B	1	0	0	0	0
38	6	1	0	0	0	0
39	A	36	0	6	0	0
40	B	32	0	12	3	0
41	M	2	0	0	0	0
41	O	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	P	1	0	0	0	0
All	All	90868	0	86972	2460	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 14.

All (2460) 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)
5:A:1642:LYS:HD3	5:A:1650:CYS:SG	1.36	1.62
5:A:1642:LYS:CD	5:A:1650:CYS:SG	2.14	1.34
5:A:1638:ILE:CD1	5:A:1642:LYS:HE3	1.73	1.18
4:6:32:G:N2	20:P:82:MET:HG2	1.57	1.17
4:6:32:G:N2	20:P:82:MET:CG	2.07	1.16
4:6:32:G:H21	20:P:82:MET:CG	1.57	1.15
5:A:1638:ILE:HD12	5:A:1642:LYS:HE3	1.14	1.13
4:6:32:G:H21	20:P:82:MET:HG2	0.91	1.08
15:K:117:LYS:HG3	22:R:225:GLN:HE21	1.22	1.01
5:A:1638:ILE:HG21	5:A:1642:LYS:HE2	1.44	0.96
5:A:1642:LYS:HD3	5:A:1650:CYS:HG	1.33	0.93
15:K:86:ALA:O	22:R:259:ARG:NH2	2.01	0.92
36:z:169:ARG:HE	36:z:172:PHE:HB2	1.33	0.91
5:A:1576:GLN:HB3	5:A:1585:MET:HE3	1.55	0.88
4:6:32:G:N2	20:P:82:MET:SD	2.47	0.87
36:z:323:ASN:HD22	36:z:342:ILE:HG22	1.40	0.87
16:L:204:MET:HE3	17:M:37:LYS:HD3	1.55	0.86
23:V:98:LYS:HE3	24:W:537:ARG:HA	1.58	0.85
20:P:149:ASP:OD1	20:P:224:GLN:NE2	2.08	0.85
22:R:78:GLN:NE2	22:R:113:CYS:SG	2.49	0.85
10:F:27:GLY:HA3	10:F:43:VAL:HG12	1.58	0.84
5:A:1639:HIS:CE1	5:A:1718:MET:HE1	2.11	0.84
36:z:208:GLU:HG2	36:z:361:LYS:HG3	1.59	0.84
26:Y:94:ARG:O	26:Y:98:GLN:NE2	2.10	0.84
5:A:922:MET:HE3	5:A:924:MET:HE2	1.59	0.84
22:R:191:ARG:NH1	22:R:214:GLU:OE2	2.10	0.84
11:G:94:ARG:HE	11:G:96:ILE:HD11	1.41	0.83
5:A:866:LEU:HD12	5:A:890:VAL:HG13	1.60	0.83
6:B:195:SER:HB3	6:B:226:GLU:HB3	1.59	0.83
7:C:271:ASN:ND2	7:C:314:ASN:OD1	2.12	0.83
5:A:1601:PHE:HA	5:A:1605:LEU:HD12	1.60	0.83
23:S:73:LEU:HD23	23:S:76:PHE:HD2	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:281:ASP:HA	20:P:284:GLU:HG2	1.61	0.82
20:P:160:ARG:HH12	20:P:165:GLY:H	1.28	0.82
5:A:1642:LYS:HD2	5:A:1650:CYS:SG	2.19	0.81
7:C:87:GLY:HA3	9:E:94:LEU:HD23	1.62	0.81
15:K:343:GLU:OE1	15:K:400:TRP:NE1	2.12	0.81
18:N:70:MET:HG3	18:N:74:HIS:HD1	1.44	0.81
24:W:653:ALA:HB1	27:Z:92:LEU:HD11	1.63	0.81
36:z:547:VAL:HG22	36:z:557:THR:HG21	1.61	0.81
7:C:45:GLN:NE2	7:C:333:THR:HB	1.95	0.81
4:6:55:C:OP2	22:R:64:ARG:NH2	2.14	0.81
11:G:45:ILE:HB	11:G:53:LEU:HB2	1.63	0.81
27:Z:153:LYS:HE3	27:Z:156:GLN:HE22	1.45	0.81
5:A:1638:ILE:CD1	5:A:1642:LYS:CE	2.58	0.80
36:z:568:LYS:HA	36:z:571:LYS:HG2	1.64	0.80
24:W:561:LEU:HA	24:W:564:MET:HE2	1.62	0.80
24:W:507:ASP:OD2	25:X:563:ARG:NH1	2.14	0.80
25:X:490:GLU:HG2	25:X:494:GLY:HA3	1.63	0.80
11:G:42:GLN:HG2	11:G:56:ARG:HH22	1.47	0.80
10:F:16:SER:HB3	10:F:69:ILE:HB	1.64	0.80
5:A:1429:LEU:HD12	5:A:1430:GLU:H	1.47	0.79
11:G:32:VAL:O	11:G:111:ARG:NH2	2.16	0.79
3:5:91:G:N7	8:D:97:ARG:NH1	2.31	0.79
23:T:94:LEU:HD12	23:U:90:LEU:HD11	1.64	0.79
23:T:122:ARG:NH1	23:U:118:LEU:O	2.16	0.79
27:Z:153:LYS:HE3	27:Z:156:GLN:NE2	1.98	0.78
24:W:672:CYS:HA	24:W:675:LEU:HG	1.65	0.78
36:z:142:ILE:HG22	36:z:173:ARG:HB2	1.65	0.78
36:z:395:LYS:NZ	36:z:433:GLY:O	2.15	0.78
17:M:239:LYS:HD2	17:M:253:ASN:HD22	1.49	0.78
20:P:293:ARG:HB2	20:P:296:LYS:HE2	1.64	0.78
23:V:12:GLU:HA	23:V:55:VAL:HG11	1.66	0.78
28:a:62:MET:HA	28:a:64:GLN:HE21	1.49	0.78
18:N:1188:SER:OG	18:N:1216:ASN:ND2	2.16	0.78
24:W:258:GLU:HB3	24:W:262:ARG:HH12	1.49	0.77
22:R:280:TYR:HB3	22:R:306:LEU:HD11	1.65	0.77
15:K:263:VAL:HG12	15:K:295:LEU:HD21	1.66	0.77
16:L:191:GLN:NE2	17:M:24:GLU:OE1	2.15	0.77
25:X:585:PRO:HG2	25:X:620:LYS:HE2	1.66	0.77
23:S:72:LEU:HG	23:S:76:PHE:CZ	2.19	0.77
8:D:17:THR:HG22	8:D:27:ARG:HD2	1.67	0.76
18:N:737:ARG:HD3	18:N:1040:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:798:HIS:HE1	18:N:924:GLN:HG2	1.50	0.76
31:d:15:ILE:HG12	31:d:88:LEU:HD22	1.68	0.75
5:A:1615:TRP:NE1	35:y:90:HIS:O	2.19	0.75
7:C:203:ILE:HD11	7:C:215:LEU:HG	1.68	0.75
4:6:42:A:H5"	24:W:176:LYS:HG3	1.69	0.75
5:A:1400:GLU:OE1	30:c:462:LYS:NZ	2.20	0.75
4:6:22:A:OP2	17:M:63:LYS:NZ	2.19	0.75
16:L:183:TYR:OH	28:a:96:ASN:OD1	2.05	0.75
15:K:440:GLU:OE1	15:K:446:LYS:NZ	2.20	0.75
18:N:306:LEU:HD23	18:N:329:LEU:HD21	1.68	0.75
25:X:719:GLU:O	25:X:722:ARG:HG2	1.87	0.75
4:6:81:U:H5"	26:Y:178:ARG:HH21	1.52	0.75
23:S:62:ARG:HH21	23:S:64:PRO:HA	1.52	0.75
23:T:86:GLU:OE2	23:U:91:ARG:NH2	2.20	0.75
18:N:1136:CYS:HA	18:N:1167:GLY:O	1.87	0.74
23:U:383:PHE:HD1	23:U:390:LEU:HD22	1.52	0.74
17:M:38:GLU:OE2	17:M:55:ARG:NH1	2.19	0.74
17:M:47:CYS:SG	17:M:121:GLN:NE2	2.60	0.74
27:Z:126:ALA:O	27:Z:130:GLN:NE2	2.20	0.74
20:P:165:GLY:O	20:P:227:LYS:NZ	2.21	0.74
10:F:76:LEU:HD11	11:G:98:LYS:HZ2	1.53	0.74
20:P:150:CYS:SG	20:P:224:GLN:NE2	2.61	0.74
20:P:198:TRP:NE1	20:P:230:MET:SD	2.59	0.74
23:S:63:PRO:HB3	24:W:693:LEU:HD21	1.67	0.74
36:z:371:TYR:HA	36:z:374:MET:HE2	1.67	0.74
23:V:108:LEU:HD11	24:W:604:LEU:HB2	1.69	0.74
5:A:1665:ARG:HE	5:A:1666:PRO:HD2	1.53	0.74
7:C:145:LYS:HE2	7:C:187:GLN:HE21	1.53	0.74
10:F:40:LEU:HB3	10:F:43:VAL:HG11	1.70	0.74
24:W:537:ARG:HD2	24:W:577:PHE:CG	2.23	0.74
3:5:105:A:O2'	11:G:50:ASN:OD1	2.06	0.74
5:A:1639:HIS:HE1	5:A:1718:MET:HE1	1.53	0.74
22:R:151:LEU:HD22	26:Y:168:LEU:HD11	1.69	0.74
5:A:1185:ARG:HD2	21:Q:229:VAL:HG11	1.70	0.73
5:A:1209:ASN:HD22	5:A:1209:ASN:C	1.96	0.73
36:z:169:ARG:HG2	36:z:172:PHE:H	1.53	0.73
22:R:78:GLN:NE2	22:R:109:LYS:HE2	2.03	0.73
22:R:121:ASN:ND2	24:W:237:ASP:O	2.22	0.73
4:6:80:A:O5'	26:Y:111:GLN:NE2	2.22	0.73
4:6:75:G:N7	26:Y:200:ARG:NH1	2.35	0.73
23:T:90:LEU:HD21	23:U:90:LEU:HB3	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:122:ARG:NH1	23:U:122:ARG:HB2	2.02	0.73
36:z:318:VAL:HG12	36:z:363:PHE:HB2	1.71	0.73
22:R:264:PHE:O	22:R:268:ILE:HG12	1.89	0.73
23:V:87:GLN:HE22	34:r:239:UNK:H	1.37	0.72
15:K:107:ALA:HB1	22:R:238:PHE:HE2	1.52	0.72
23:S:90:LEU:HB2	23:V:90:LEU:HD11	1.69	0.72
7:C:217:GLY:O	7:C:219:LYS:NZ	2.21	0.72
11:G:25:PHE:HB3	11:G:34:GLN:HE21	1.54	0.72
24:W:575:TYR:CG	24:W:576:PRO:HD2	2.25	0.72
18:N:830:LEU:O	18:N:834:ILE:HG13	1.88	0.72
7:C:46:MET:HB3	7:C:334:ILE:HG13	1.71	0.72
5:A:1635:LYS:HB2	5:A:1653:ILE:HG22	1.71	0.72
5:A:1723:THR:OG1	5:A:1741:ASN:OD1	2.05	0.72
15:K:117:LYS:HG3	22:R:225:GLN:NE2	2.03	0.72
6:B:739:ASP:HB3	29:b:66:LYS:HG2	1.71	0.72
9:E:45:TYR:HE1	9:E:62:LYS:HE2	1.54	0.72
22:R:84:LYS:NZ	22:R:87:ALA:HB3	2.04	0.71
23:U:59:VAL:HG23	23:U:61:PRO:HD3	1.72	0.71
23:U:76:PHE:HE2	23:V:72:LEU:HD22	1.55	0.71
36:z:131:ILE:HG21	36:z:161:VAL:HG11	1.71	0.71
13:I:25:LYS:NZ	13:I:68:ASN:O	2.22	0.71
5:A:59:ARG:HH12	7:C:156:ASP:HB3	1.54	0.71
19:O:30:MET:HG2	19:O:52:LEU:HD23	1.73	0.71
24:W:387:ASN:HD22	24:W:406:LEU:HD22	1.55	0.71
20:P:90:GLN:HB3	20:P:240:CYS:SG	2.31	0.71
36:z:229:ASN:O	36:z:233:THR:OG1	2.07	0.71
5:A:1582:THR:HG22	5:A:1584:ILE:H	1.54	0.71
24:W:112:GLN:HG2	24:W:113:LEU:HD12	1.73	0.71
26:Y:93:LEU:HA	26:Y:96:LYS:HE2	1.71	0.71
24:W:516:ILE:HA	24:W:519:LYS:HE2	1.73	0.71
10:F:9:LYS:NZ	10:F:81:ILE:O	2.24	0.71
23:U:71:ALA:HB1	23:V:63:PRO:HD3	1.72	0.71
23:T:62:ARG:HH21	23:T:66:ALA:H	1.38	0.70
6:B:585:LYS:NZ	6:B:586:ASP:O	2.24	0.70
17:M:39:PRO:HA	17:M:52:THR:HG22	1.73	0.70
22:R:17:GLN:NE2	24:W:151:ASP:OD1	2.23	0.70
15:K:120:GLY:HA2	22:R:191:ARG:HD2	1.72	0.70
15:K:455:THR:OG1	15:K:458:THR:OG1	2.08	0.70
30:c:565:LEU:HB3	30:c:567:PRO:HD2	1.72	0.70
36:z:225:GLU:OE2	36:z:229:ASN:ND2	2.25	0.70
6:B:713:ASP:OD2	6:B:736:TYR:OH	2.09	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:38:GLU:HG2	17:M:53:ILE:HB	1.74	0.70
20:P:232:HIS:HA	20:P:240:CYS:HB2	1.74	0.70
6:B:114:ILE:HG21	6:B:661:LEU:HD11	1.74	0.69
13:I:15:LEU:HD21	13:I:20:VAL:HG11	1.74	0.69
18:N:209:TYR:HB3	18:N:222:LEU:HD21	1.73	0.69
24:W:507:ASP:N	25:X:529:TYR:O	2.25	0.69
23:S:73:LEU:HA	23:S:76:PHE:CD2	2.27	0.69
5:A:1630:ILE:O	35:y:83:ARG:NH2	2.26	0.69
23:T:118:LEU:HA	23:T:121:GLU:HG2	1.74	0.69
7:C:74:ILE:HB	7:C:89:LEU:HB2	1.75	0.69
23:V:112:LEU:HD13	24:W:596:GLU:HG2	1.74	0.69
23:T:119:THR:HA	23:T:122:ARG:HG2	1.75	0.69
22:R:294:LEU:HD23	22:R:297:GLU:HB2	1.74	0.69
22:R:418:ASP:OD1	22:R:421:ARG:NH1	2.25	0.69
18:N:93:TRP:O	18:N:138:LYS:NZ	2.25	0.69
15:K:310:ASP:HB2	15:K:312:THR:HG22	1.74	0.69
19:O:140:ASN:O	28:a:138:ARG:NH2	2.26	0.69
25:X:668:ALA:HB2	25:X:683:ILE:HD11	1.74	0.69
30:c:487:LYS:NZ	30:c:491:GLU:OE2	2.26	0.68
36:z:74:ILE:HG23	36:z:119:ILE:HA	1.75	0.68
6:B:848:VAL:HG12	6:B:913:MET:HG2	1.76	0.68
6:B:492:VAL:HG21	6:B:506:ALA:HB1	1.75	0.68
19:O:120:ARG:HH11	19:O:142:CYS:HB3	1.57	0.68
15:K:290:SER:HB3	15:K:309:MET:HE2	1.76	0.68
23:S:69:LEU:HD23	23:U:80:TRP:HB2	1.74	0.68
23:S:43:GLN:NE2	23:S:44:GLU:OE1	2.25	0.68
25:X:105:LEU:HD12	25:X:108:MET:HB2	1.76	0.68
35:y:28:GLU:HG2	35:y:29:PRO:HD2	1.74	0.68
11:G:6:ASP:OD1	11:G:7:LYS:NZ	2.25	0.68
18:N:1183:PHE:HB3	18:N:1213:VAL:HG22	1.74	0.68
11:G:61:ASP:OD1	11:G:62:ARG:N	2.26	0.68
23:T:69:LEU:HD12	23:T:70:PRO:HD2	1.74	0.68
23:U:191:ALA:HB3	23:U:485:LEU:HB3	1.76	0.68
30:c:520:GLU:HA	30:c:567:PRO:HG3	1.76	0.68
33:m:758:ARG:NH2	33:m:793:MET:O	2.23	0.68
7:C:155:SER:OG	7:C:157:ASP:OD1	2.12	0.68
20:P:160:ARG:NH1	20:P:165:GLY:H	1.91	0.68
25:X:472:PRO:HA	25:X:475:ARG:HB2	1.76	0.68
5:A:1638:ILE:HD13	5:A:1642:LYS:HE3	1.74	0.67
11:G:93:ASP:OD1	11:G:94:ARG:N	2.27	0.67
22:R:485:ASP:OD1	22:R:488:ARG:NH1	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:105:LEU:HD22	24:W:385:VAL:HG12	1.76	0.67
5:A:1429:LEU:O	5:A:1430:GLU:HG3	1.94	0.67
3:5:101:U:H3	11:G:65:ASN:HD21	1.41	0.67
30:c:439:PRO:HB2	30:c:442:GLN:NE2	2.10	0.67
24:W:203:LYS:HA	24:W:207:ILE:HB	1.76	0.67
35:y:177:ILE:HD11	36:z:321:GLY:HA3	1.76	0.67
36:z:540:LEU:HD23	36:z:543:ARG:HD3	1.75	0.67
36:z:162:LEU:HA	36:z:165:ILE:HG22	1.75	0.67
6:B:140:ASP:OD2	6:B:208:LYS:NZ	2.28	0.67
6:B:812:PRO:HG2	6:B:817:ARG:HH12	1.57	0.67
5:A:1602:ARG:HE	5:A:1770:ARG:HH11	1.42	0.67
23:V:3:CYS:HB2	23:V:10:PRO:HD3	1.77	0.67
4:6:32:G:N2	20:P:82:MET:CB	2.58	0.67
17:M:141:ARG:NH2	20:P:314:TYR:O	2.28	0.67
23:S:118:LEU:O	23:S:122:ARG:HD3	1.95	0.67
24:W:132:SER:OG	24:W:135:ARG:NH2	2.28	0.67
2:2:30:A:C6	35:y:37:PRO:HD2	2.29	0.67
7:C:41:VAL:HG21	9:E:103:PRO:HB3	1.76	0.67
13:I:22:VAL:HG12	13:I:73:VAL:HG12	1.75	0.67
24:W:518:GLU:HA	24:W:521:ARG:HE	1.58	0.67
26:Y:153:LEU:HD22	31:d:131:ARG:HH12	1.59	0.67
30:c:515:ASP:OD2	30:c:559:ARG:NH1	2.23	0.67
5:A:107:ARG:NH1	16:L:213:GLU:OE2	2.27	0.67
18:N:529:LEU:HD11	18:N:611:ALA:HB1	1.76	0.67
24:W:172:ASN:O	24:W:173:THR:HG22	1.94	0.67
10:F:17:ILE:HD12	10:F:40:LEU:HD11	1.76	0.66
18:N:207:ILE:HG21	18:N:360:PHE:HE2	1.60	0.66
17:M:24:GLU:OE1	17:M:24:GLU:N	2.28	0.66
22:R:603:GLU:HG3	22:R:615:VAL:HG21	1.77	0.66
23:T:94:LEU:O	23:T:98:LYS:HD3	1.96	0.66
5:A:694:GLN:O	5:A:699:ARG:NH2	2.25	0.66
18:N:697:ILE:HD11	18:N:708:ALA:HB1	1.78	0.66
19:O:127:ASP:O	19:O:131:ARG:NE	2.28	0.66
4:6:47:A:H5"	4:6:47:A:H8	1.59	0.66
5:A:1267:ARG:HH11	5:A:1270:GLN:HE21	1.43	0.66
5:A:1663:VAL:HG11	5:A:1741:ASN:HB3	1.77	0.66
6:B:227:VAL:HG11	6:B:254:ILE:HD12	1.77	0.66
6:B:267:LEU:HB3	6:B:319:VAL:HG22	1.78	0.66
22:R:545:ASN:HA	22:R:548:ILE:HD12	1.77	0.66
11:G:55:ALA:HB2	11:G:71:VAL:HA	1.78	0.66
22:R:289:GLN:HE22	25:X:538:GLU:HB2	1.61	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:T:73:LEU:HA	23:T:76:PHE:HD2	1.60	0.66
36:z:169:ARG:NE	36:z:172:PHE:HB2	2.09	0.66
4:6:32:G:C2	20:P:82:MET:HG2	2.31	0.66
5:A:952:GLU:OE2	5:A:955:ARG:NH2	2.29	0.66
17:M:227:LYS:HD3	17:M:230:LYS:HZ3	1.61	0.66
18:N:922:PHE:HA	18:N:925:LEU:HD12	1.77	0.66
22:R:48:LEU:HD11	22:R:52:GLN:HE22	1.61	0.66
23:U:336:ILE:HA	23:U:352:LEU:HA	1.78	0.66
17:M:86:ASP:OD1	17:M:90:GLY:N	2.29	0.65
24:W:510:ARG:HH21	25:X:531:GLU:HG2	1.62	0.65
31:d:58:THR:HG23	31:d:60:THR:H	1.60	0.65
5:A:250:ASN:HB2	5:A:253:GLN:HG3	1.78	0.65
23:V:76:PHE:HB3	23:V:80:TRP:HZ3	1.59	0.65
24:W:246:PHE:HA	24:W:249:LYS:HG2	1.78	0.65
24:W:696:LYS:HG3	27:Z:131:LEU:HD12	1.77	0.65
17:M:237:PRO:HB2	17:M:255:LYS:HD3	1.77	0.65
22:R:593:VAL:HA	22:R:596:LEU:HD22	1.77	0.65
5:A:1602:ARG:HH21	5:A:1770:ARG:HD3	1.62	0.65
6:B:628:TYR:OH	6:B:657:ASP:OD2	2.13	0.65
22:R:285:HIS:O	22:R:289:GLN:HG2	1.97	0.65
23:T:62:ARG:NH2	23:T:66:ALA:H	1.95	0.65
25:X:139:LEU:HD13	25:X:147:ILE:HG23	1.79	0.65
5:A:810:GLU:OE2	5:A:813:ARG:NH2	2.29	0.65
18:N:694:SER:HB3	18:N:713:SER:HB3	1.78	0.65
20:P:160:ARG:HH22	20:P:165:GLY:N	1.94	0.65
22:R:256:GLU:HB3	22:R:259:ARG:HH11	1.61	0.65
25:X:439:LEU:HD11	25:X:489:LEU:HD11	1.79	0.65
30:c:472:CYS:SG	30:c:516:SER:HB3	2.36	0.65
5:A:1020:MET:HG2	5:A:1066:PHE:HZ	1.62	0.65
5:A:1025:ASP:OD1	5:A:1026:THR:N	2.30	0.65
7:C:217:GLY:O	7:C:244:ARG:NH1	2.29	0.65
15:K:109:GLN:HA	15:K:133:GLN:NE2	2.12	0.65
16:L:186:TYR:HD1	28:a:89:ALA:HB2	1.61	0.65
23:S:69:LEU:N	23:T:79:GLU:OE2	2.30	0.65
7:C:188:GLN:HE22	7:C:190:THR:H	1.45	0.65
23:U:180:THR:O	23:U:184:PRO:CG	2.45	0.65
26:Y:167:ARG:HA	26:Y:170:GLU:HG2	1.78	0.65
5:A:1115:ILE:HD11	5:A:1465:GLU:HG2	1.79	0.64
18:N:803:LEU:HD21	18:N:945:LEU:HD23	1.79	0.64
20:P:134:LEU:HD23	20:P:136:ARG:HE	1.61	0.64
23:T:6:SER:HB3	23:U:84:ALA:HB1	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:105:LEU:O	24:W:109:GLU:HG2	1.97	0.64
25:X:87:HIS:HB2	25:X:91:PHE:HE1	1.63	0.64
5:A:873:TYR:CE1	5:A:883:GLN:NE2	2.65	0.64
5:A:899:GLU:OE1	5:A:899:GLU:N	2.29	0.64
18:N:378:ILE:O	18:N:382:ASP:N	2.28	0.64
28:a:57:VAL:HG22	28:a:61:GLU:OE2	1.98	0.64
36:z:126:ILE:O	36:z:130:GLU:HG2	1.97	0.64
5:A:58:TRP:HH2	7:C:272:LEU:HD11	1.63	0.64
17:M:227:LYS:O	17:M:231:HIS:ND1	2.29	0.64
5:A:164:GLN:NE2	5:A:227:PHE:O	2.23	0.64
5:A:1438:ARG:NH2	30:c:458:ARG:O	2.30	0.64
20:P:190:ILE:HG22	20:P:193:ARG:HH22	1.62	0.64
25:X:243:ARG:HA	25:X:246:ILE:HG12	1.78	0.64
26:Y:159:LYS:NZ	26:Y:160:PRO:O	2.30	0.64
27:Z:18:ASN:ND2	27:Z:20:GLU:HG3	2.12	0.64
5:A:1298:TYR:HB3	5:A:1301:ALA:HB3	1.78	0.64
18:N:390:TYR:HE1	18:N:632:LEU:HD11	1.61	0.64
25:X:500:ARG:NH1	25:X:532:ASP:OD2	2.28	0.64
5:A:45:GLY:N	5:A:48:GLU:OE2	2.31	0.64
16:L:163:LYS:O	16:L:167:GLN:NE2	2.30	0.64
20:P:118:LEU:HA	20:P:151:PHE:CZ	2.32	0.64
33:m:777:SER:OG	33:m:779:ASP:OD1	2.12	0.64
23:V:98:LYS:HD2	24:W:536:ILE:HG13	1.79	0.64
5:A:1185:ARG:HH11	21:Q:229:VAL:HG11	1.63	0.64
10:F:46:THR:HG22	10:F:52:PRO:HB3	1.80	0.64
28:a:133:LYS:HA	28:a:136:GLU:HG3	1.79	0.64
36:z:346:SER:HB3	36:z:378:PHE:HE2	1.62	0.64
6:B:644:PHE:CE2	6:B:675:ARG:HD2	2.32	0.64
7:C:45:GLN:HE22	7:C:333:THR:HB	1.60	0.64
18:N:1179:ASN:HA	18:N:1208:SER:HB2	1.79	0.64
24:W:597:ILE:O	24:W:601:ARG:HG2	1.98	0.64
35:y:210:ASP:OD1	35:y:211:GLY:N	2.32	0.64
4:6:34:U:H2'	4:6:35:A:H8	1.62	0.63
5:A:1432:LEU:HD12	5:A:1447:PHE:HZ	1.63	0.63
6:B:90:ASP:OD2	15:K:157:ARG:NH1	2.31	0.63
17:M:267:SER:HB2	17:M:282:GLN:HE21	1.63	0.63
5:A:1430:GLU:HA	5:A:1433:GLU:HG2	1.81	0.63
7:C:244:ARG:HB3	7:C:257:GLN:HE22	1.64	0.63
18:N:460:TYR:HD1	18:N:472:LEU:HD21	1.61	0.63
19:O:101:CYS:SG	19:O:102:CYS:N	2.71	0.63
15:K:122:PRO:HA	15:K:126:HIS:HB2	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:243:CYS:SG	17:M:244:SER:N	2.72	0.63
25:X:458:PRO:HG2	25:X:461:SER:HB3	1.80	0.63
36:z:249:ILE:O	36:z:253:ILE:HG12	1.98	0.63
2:2:19:G:H22	4:6:50:A:H2	1.47	0.63
5:A:251:LEU:HD21	5:A:424:ALA:HB2	1.79	0.63
5:A:839:TRP:CZ2	5:A:843:ARG:HD2	2.33	0.63
23:T:121:GLU:HA	23:T:124:GLU:CD	2.24	0.63
23:T:122:ARG:HD3	23:U:122:ARG:HH21	1.64	0.63
25:X:84:PRO:HG2	25:X:122:GLN:HG2	1.79	0.63
25:X:538:GLU:HA	25:X:541:VAL:HG22	1.79	0.63
6:B:692:THR:HA	6:B:825:THR:HG21	1.80	0.63
7:C:327:SER:HB2	7:C:335:PHE:HB2	1.81	0.63
19:O:98:GLU:OE1	19:O:98:GLU:N	2.30	0.63
24:W:207:ILE:HG12	24:W:209:ILE:H	1.61	0.63
5:A:1296:THR:HG21	5:A:1489:TRP:CE3	2.34	0.63
7:C:183:VAL:HG12	7:C:194:ILE:HG22	1.81	0.63
24:W:250:ARG:HH11	24:W:254:GLN:HG3	1.62	0.63
5:A:986:THR:HG21	5:A:1100:GLN:HG2	1.80	0.63
5:A:1374:ILE:O	29:b:23:ASN:ND2	2.32	0.63
5:A:1669:LEU:HD23	5:A:1751:GLN:HG2	1.80	0.63
7:C:185:ILE:HG13	7:C:192:VAL:HG12	1.81	0.63
23:S:88:PHE:O	23:S:92:ARG:HG2	1.98	0.63
24:W:251:GLU:HB2	24:W:255:LYS:HZ3	1.63	0.63
25:X:554:ASN:O	25:X:558:THR:HG23	1.98	0.63
5:A:1303:ILE:HD12	30:c:424:VAL:HG13	1.79	0.62
30:c:548:VAL:HG13	30:c:553:LEU:HB2	1.80	0.62
5:A:1153:LYS:HE3	5:A:1196:GLU:HA	1.81	0.62
5:A:1765:TYR:O	5:A:1769:GLU:HG2	1.98	0.62
6:B:488:LEU:HD21	6:B:490:MET:HE3	1.81	0.62
7:C:145:LYS:HE2	7:C:187:GLN:NE2	2.13	0.62
23:T:118:LEU:HD12	23:U:122:ARG:NH2	2.14	0.62
4:6:42:A:OP1	24:W:176:LYS:NZ	2.27	0.62
5:A:140:LEU:HD12	5:A:506:GLN:O	1.99	0.62
6:B:613:GLU:OE1	6:B:616:LYS:NZ	2.30	0.62
16:L:127:LEU:HA	16:L:130:ARG:HG3	1.82	0.62
16:L:127:LEU:HD23	16:L:130:ARG:HG3	1.80	0.62
19:O:123:LYS:HD2	19:O:131:ARG:HD2	1.81	0.62
36:z:606:LEU:HA	36:z:609:LYS:HG2	1.80	0.62
6:B:777:LYS:HA	6:B:780:ILE:HG22	1.81	0.62
17:M:82:SER:O	20:P:147:ASN:ND2	2.32	0.62
18:N:533:TYR:HB3	18:N:556:ASP:HB2	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1639:HIS:CE1	5:A:1650:CYS:HB3	2.34	0.62
23:S:62:ARG:HD3	23:T:8:GLU:HA	1.82	0.62
23:U:118:LEU:HG	23:U:122:ARG:NH2	2.15	0.62
24:W:200:ARG:HA	24:W:203:LYS:HG2	1.80	0.62
26:Y:199:GLU:HG3	26:Y:202:ARG:HH12	1.64	0.62
28:a:61:GLU:O	28:a:62:MET:HE2	1.98	0.62
19:O:127:ASP:OD2	19:O:130:GLN:NE2	2.32	0.62
22:R:48:LEU:HD22	24:W:257:ILE:HG23	1.80	0.62
23:U:115:ILE:HD13	23:U:118:LEU:HD23	1.80	0.62
27:Z:89:ARG:HA	27:Z:92:LEU:HD13	1.79	0.62
30:c:439:PRO:HB2	30:c:442:GLN:HE21	1.64	0.62
5:A:1405:ASP:OD1	5:A:1408:ARG:NH2	2.31	0.62
15:K:150:HIS:CE1	15:K:399:ASP:OD2	2.53	0.62
15:K:172:GLU:HG2	15:K:173:PRO:HD2	1.81	0.62
17:M:109:ASN:OD1	17:M:112:ASN:HB2	1.98	0.62
18:N:7:LYS:HA	18:N:10:GLN:HG2	1.81	0.62
23:U:90:LEU:HD12	23:U:93:ASN:HB2	1.81	0.62
23:V:77:GLN:NE2	27:Z:101:TYR:OH	2.32	0.62
5:A:1629:GLN:HA	5:A:1657:ALA:HA	1.80	0.62
6:B:715:GLU:O	6:B:754:ARG:NH1	2.32	0.62
20:P:209:SER:OG	20:P:210:ARG:NH1	2.32	0.62
22:R:329:GLU:HG3	22:R:330:GLU:OE2	1.99	0.62
26:Y:178:ARG:O	26:Y:182:ASN:ND2	2.33	0.62
36:z:120:LYS:HE2	36:z:122:MET:HE2	1.81	0.62
36:z:306:GLU:O	36:z:353:ARG:NH2	2.33	0.62
2:2:29:A:OP1	5:A:884:ARG:NH2	2.33	0.62
23:V:76:PHE:HB3	23:V:80:TRP:CZ3	2.34	0.62
36:z:608:GLU:N	36:z:608:GLU:OE1	2.33	0.62
4:6:10:A:OP1	5:A:56:ARG:NH1	2.27	0.62
5:A:1638:ILE:HD13	5:A:1642:LYS:CE	2.29	0.62
6:B:204:ASP:OD1	6:B:205:MET:N	2.31	0.62
23:S:88:PHE:HB3	23:S:92:ARG:NH2	2.15	0.62
24:W:689:GLN:O	24:W:693:LEU:HB2	2.00	0.62
7:C:62:GLY:O	7:C:319:HIS:NE2	2.32	0.61
18:N:357:ARG:HH21	18:N:361:PRO:HD3	1.65	0.61
18:N:741:PRO:HA	18:N:1004:ARG:HG2	1.81	0.61
18:N:772:ASP:OD1	18:N:950:ARG:NH1	2.33	0.61
22:R:61:ASP:HA	22:R:64:ARG:HG2	1.82	0.61
3:5:103:U:OP2	13:I:68:ASN:ND2	2.33	0.61
7:C:77:TRP:CZ3	7:C:85:ASN:HB3	2.35	0.61
27:Z:111:LEU:HA	27:Z:114:LYS:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:a:64:GLN:OE1	31:d:62:ARG:NH1	2.31	0.61
36:z:28:THR:HG23	36:z:31:ARG:HH21	1.65	0.61
22:R:84:LYS:HZ3	22:R:87:ALA:HB3	1.65	0.61
36:z:456:LEU:HD21	36:z:472:ALA:HB2	1.82	0.61
7:C:58:PHE:CE1	7:C:326:LEU:HD22	2.35	0.61
24:W:157:GLU:OE1	24:W:157:GLU:N	2.33	0.61
5:A:1209:ASN:O	5:A:1209:ASN:ND2	2.24	0.61
5:A:1660:LYS:HZ1	5:A:1680:THR:C	2.08	0.61
5:A:1660:LYS:NZ	5:A:1661:TRP:O	2.33	0.61
6:B:769:ASP:HB2	6:B:772:VAL:HB	1.81	0.61
22:R:67:ARG:HG3	22:R:68:LEU:HD22	1.82	0.61
5:A:921:PHE:HD2	5:A:928:LEU:HB3	1.65	0.61
5:A:1072:ASP:OD1	5:A:1111:TYR:OH	2.18	0.61
15:K:268:ASP:OD2	15:K:272:ARG:NH1	2.33	0.61
23:U:299:ASN:N	23:U:313:ALA:O	2.30	0.61
25:X:286:THR:HG21	25:X:289:ASN:HB2	1.83	0.61
5:A:287:ALA:HA	5:A:301:LEU:HD23	1.82	0.61
25:X:295:ASP:HA	25:X:298:VAL:HG12	1.83	0.61
35:y:144:MET:HE2	35:y:144:MET:HA	1.82	0.61
5:A:1020:MET:HG2	5:A:1066:PHE:CZ	2.36	0.61
6:B:154:LYS:NZ	40:B:1001:GTP:O2G	2.34	0.61
6:B:860:ILE:HG12	6:B:901:LEU:HD11	1.81	0.61
8:D:21:GLU:HA	8:D:67:ARG:HE	1.65	0.61
15:K:302:PRO:HG3	15:K:315:LEU:HD23	1.83	0.61
18:N:778:SER:HB2	18:N:979:MET:HG3	1.82	0.61
23:T:129:LEU:HD22	23:U:129:LEU:HD12	1.81	0.61
5:A:1534:GLU:OE2	5:A:1557:ARG:NH2	2.34	0.61
6:B:706:LEU:HD12	6:B:710:ILE:HD13	1.83	0.61
7:C:188:GLN:NE2	7:C:190:THR:H	1.98	0.61
18:N:113:LEU:O	18:N:205:LYS:NZ	2.34	0.61
24:W:198:LYS:HE3	24:W:198:LYS:HA	1.83	0.61
18:N:307:GLN:NE2	18:N:324:CYS:O	2.33	0.60
35:y:148:LEU:O	36:z:401:ASN:ND2	2.34	0.60
36:z:303:ASN:HD21	36:z:323:ASN:HB2	1.66	0.60
36:z:492:ALA:HB2	36:z:530:TYR:HD2	1.65	0.60
12:H:49:MET:HE2	14:J:63:ARG:HD2	1.84	0.60
5:A:1215:THR:OG1	5:A:1216:GLY:N	2.33	0.60
6:B:488:LEU:HD12	6:B:514:GLN:O	2.02	0.60
6:B:678:GLU:OE2	6:B:791:GLY:HA3	2.01	0.60
6:B:146:VAL:O	6:B:217:THR:OG1	2.18	0.60
15:K:231:CYS:HB3	15:K:241:ARG:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:160:ARG:HH22	20:P:165:GLY:H	1.49	0.60
5:A:870:LYS:NZ	5:A:894:TYR:OH	2.34	0.60
5:A:1190:LEU:HD12	5:A:1191:THR:HG22	1.84	0.60
5:A:1633:VAL:HA	5:A:1654:LEU:O	2.00	0.60
18:N:18:ASN:HA	18:N:25:VAL:HG21	1.84	0.60
18:N:836:ARG:NH2	18:N:890:TYR:O	2.33	0.60
22:R:326:LEU:HD23	22:R:329:GLU:OE2	2.01	0.60
23:U:357:LEU:O	23:U:370:LYS:HA	2.02	0.60
31:d:45:ARG:HE	31:d:47:ILE:HD11	1.65	0.60
5:A:1239:ASN:HB3	5:A:1248:ARG:HD3	1.83	0.60
22:R:214:GLU:HB3	22:R:223:VAL:HG22	1.83	0.60
23:S:73:LEU:HD23	23:S:76:PHE:CD2	2.32	0.60
5:A:1622:ASP:OD2	35:y:86:ASN:ND2	2.35	0.60
22:R:219:ASN:ND2	22:R:222:ASN:HB2	2.16	0.60
22:R:593:VAL:HA	22:R:596:LEU:CD2	2.31	0.60
23:T:90:LEU:HD23	23:U:90:LEU:HD23	1.83	0.60
4:6:18:G:N1	16:L:208:GLU:O	2.30	0.60
5:A:533:ARG:HG2	5:A:533:ARG:O	2.02	0.60
5:A:746:ASN:OD1	5:A:808:LYS:NZ	2.35	0.60
5:A:1685:TRP:O	5:A:1725:VAL:N	2.31	0.60
5:A:1762:PRO:HB3	35:y:94:ILE:HD13	1.83	0.60
25:X:139:LEU:HD22	25:X:147:ILE:HG12	1.83	0.60
5:A:1700:ILE:HD12	5:A:1730:ASP:HB2	1.82	0.60
30:c:454:ASN:ND2	30:c:507:PHE:HB2	2.17	0.60
35:y:53:HIS:O	35:y:57:THR:OG1	2.18	0.60
4:6:52:G:H2'	4:6:53:G:C8	2.37	0.59
6:B:229:ALA:HB3	6:B:494:LYS:NZ	2.16	0.59
18:N:430:ILE:HG22	18:N:434:MET:HE2	1.83	0.59
18:N:628:LEU:HD11	18:N:987:SER:HB3	1.83	0.59
15:K:92:SER:HA	15:K:95:VAL:HG12	1.83	0.59
15:K:417:SER:OG	21:Q:248:ASN:ND2	2.35	0.59
25:X:400:TYR:HD2	25:X:409:SER:HB2	1.67	0.59
28:a:98:VAL:HA	28:a:101:GLN:HE21	1.67	0.59
13:I:45:LEU:HB2	13:I:63:ILE:HB	1.83	0.59
15:K:235:GLU:OE2	21:Q:42:GLN:NE2	2.35	0.59
17:M:44:CYS:SG	17:M:47:CYS:HB2	2.42	0.59
24:W:270:GLY:HA2	24:W:273:PHE:HB3	1.84	0.59
25:X:129:ARG:HD2	25:X:169:ARG:HH22	1.66	0.59
9:E:12:HIS:CE1	9:E:84:PRO:HD3	2.38	0.59
10:F:23:THR:HG22	10:F:47:VAL:HA	1.83	0.59
9:E:44:GLU:OE1	9:E:63:ARG:NE	2.31	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:824:ILE:HD11	18:N:940:GLN:HE22	1.68	0.59
22:R:110:TYR:CE2	22:R:126:LEU:HD13	2.37	0.59
15:K:168:CYS:SG	15:K:211:LEU:HG	2.42	0.59
16:L:188:PRO:HB3	17:M:24:GLU:OE2	2.02	0.59
23:U:383:PHE:CD1	23:U:390:LEU:HD22	2.36	0.59
24:W:258:GLU:HB3	24:W:262:ARG:NH1	2.18	0.59
25:X:337:PRO:HA	25:X:340:ILE:HG12	1.84	0.59
5:A:635:ILE:HD11	5:A:655:PRO:HG2	1.84	0.59
5:A:1295:MET:HG3	5:A:1354:MET:SD	2.42	0.59
10:F:33:ASP:OD1	10:F:34:MET:N	2.36	0.59
23:T:40:VAL:HG22	23:U:92:ARG:HH22	1.68	0.59
23:U:342:HIS:HD2	23:U:344:ASP:HB2	1.68	0.59
23:V:67:THR:C	23:V:69:LEU:H	2.10	0.59
24:W:203:LYS:HB3	24:W:207:ILE:HD12	1.85	0.59
25:X:512:ALA:HB2	26:Y:83:ILE:HG13	1.85	0.59
25:X:671:GLU:HA	25:X:674:LEU:HD12	1.85	0.59
5:A:664:LEU:HA	5:A:667:ILE:HG22	1.84	0.59
6:B:704:GLU:OE2	6:B:804:ARG:NH2	2.35	0.59
10:F:6:PHE:CE1	10:F:80:LEU:HD22	2.37	0.59
17:M:235:TYR:HB3	17:M:263:ALA:HB2	1.83	0.59
22:R:20:ALA:N	24:W:15:GLU:OE1	2.35	0.59
22:R:487:ALA:HA	22:R:490:LEU:HD12	1.82	0.59
23:S:103:THR:HA	23:S:106:TYR:CE2	2.38	0.59
11:G:44:LEU:HB3	11:G:110:VAL:HG23	1.85	0.59
31:d:88:LEU:HB3	31:d:120:GLY:HA3	1.83	0.59
1:1:3:A:N6	4:6:38:G:O2'	2.36	0.59
6:B:250:ASN:O	6:B:254:ILE:HG12	2.02	0.59
7:C:328:CYS:HA	7:C:334:ILE:HG22	1.84	0.59
19:O:18:GLU:OE1	19:O:18:GLU:N	2.32	0.59
23:T:132:PHE:CZ	23:U:132:PHE:HB3	2.38	0.59
25:X:679:ARG:HA	25:X:682:LEU:HD12	1.85	0.59
6:B:242:ASP:OD1	6:B:271:LYS:HD2	2.03	0.58
6:B:631:SER:HA	6:B:644:PHE:O	2.03	0.58
18:N:778:SER:HB3	18:N:784:MET:HE3	1.85	0.58
24:W:705:GLN:O	24:W:709:LYS:HG2	2.03	0.58
31:d:128:VAL:O	31:d:132:MET:HG2	2.03	0.58
5:A:177:ARG:HD3	5:A:643:PRO:HB2	1.85	0.58
5:A:539:LEU:HD11	5:A:561:SER:HB2	1.83	0.58
6:B:601:VAL:HB	6:B:844:PRO:HG3	1.85	0.58
7:C:57:ARG:HG2	7:C:57:ARG:HH11	1.68	0.58
36:z:612:PRO:HD2	36:z:613:TRP:H	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:F:32:VAL:HG23	10:F:38:THR:HG22	1.84	0.58
11:G:98:LYS:O	11:G:99:MET:HE2	2.04	0.58
15:K:229:VAL:HB	15:K:243:TYR:HB2	1.86	0.58
22:R:121:ASN:HA	22:R:124:ARG:HD3	1.84	0.58
24:W:521:ARG:HA	24:W:524:LYS:HD3	1.86	0.58
36:z:143:VAL:HB	36:z:172:PHE:HZ	1.69	0.58
6:B:916:ASP:OD2	6:B:917:HIS:ND1	2.32	0.58
16:L:250:GLN:HG2	26:Y:211:PHE:HE1	1.68	0.58
23:S:122:ARG:HE	23:V:114:VAL:HG22	1.68	0.58
23:T:1:MET:SD	27:Z:130:GLN:HG2	2.44	0.58
5:A:1638:ILE:CG2	5:A:1642:LYS:HE2	2.27	0.58
9:E:45:TYR:CE1	9:E:62:LYS:HE2	2.38	0.58
10:F:7:LEU:HB3	10:F:32:VAL:HG11	1.83	0.58
16:L:184:ILE:HG21	17:M:19:PHE:CE1	2.38	0.58
18:N:25:VAL:O	18:N:65:ARG:NH2	2.37	0.58
18:N:945:LEU:HD13	18:N:966:LEU:HD21	1.86	0.58
23:T:62:ARG:HH11	27:Z:112:LEU:HD22	1.67	0.58
25:X:624:ARG:NH1	25:X:654:SER:O	2.36	0.58
31:d:89:SER:HG	31:d:116:HIS:CE1	2.20	0.58
15:K:352:ASP:OD1	15:K:353:ASN:N	2.36	0.58
23:U:71:ALA:HB2	23:V:61:PRO:HG2	1.84	0.58
25:X:637:LEU:HD23	25:X:638:ASN:H	1.69	0.58
30:c:509:ALA:HB1	30:c:546:GLU:OE1	2.03	0.58
5:A:1576:GLN:HG2	5:A:1587:HIS:CE1	2.38	0.58
24:W:149:LEU:HD13	36:z:261:ILE:HG21	1.84	0.58
25:X:252:GLN:OE1	25:X:255:LYS:NZ	2.37	0.58
36:z:474:ILE:HD12	36:z:480:VAL:HG11	1.86	0.58
1:1:-4:A:H5'	5:A:1589:LYS:HG3	1.86	0.58
18:N:664:SER:HB2	18:N:696:LEU:HD11	1.86	0.58
5:A:1063:ILE:HA	5:A:1066:PHE:CE1	2.38	0.58
6:B:146:VAL:HG12	6:B:154:LYS:HB2	1.85	0.58
7:C:308:GLY:HA3	9:E:106:ARG:HG2	1.85	0.58
20:P:121:ALA:HB1	20:P:229:ALA:HB2	1.86	0.58
22:R:333:GLY:O	22:R:337:THR:OG1	2.21	0.58
25:X:685:ILE:HD11	25:X:723:ILE:HG21	1.85	0.58
29:b:68:LEU:HG	29:b:127:LEU:HD11	1.86	0.58
5:A:1111:TYR:HD1	5:A:1120:ILE:HG12	1.69	0.57
6:B:221:VAL:HG21	6:B:912:GLN:HB3	1.86	0.57
18:N:117:LEU:HD11	18:N:205:LYS:HB3	1.85	0.57
18:N:872:THR:O	18:N:884:ARG:NH1	2.37	0.57
22:R:86:PHE:HE1	22:R:119:ASN:HD21	1.50	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:71:ALA:HB2	23:T:60:ARG:HH21	1.69	0.57
23:V:106:TYR:CE2	24:W:564:MET:HB3	2.39	0.57
25:X:337:PRO:O	25:X:341:ASN:ND2	2.36	0.57
25:X:394:SER:O	25:X:398:ARG:HG3	2.03	0.57
1:1:-1:U:H5'	1:1:0:G:H5"	1.86	0.57
5:A:1642:LYS:HG2	5:A:1642:LYS:O	2.04	0.57
6:B:378:VAL:HG13	6:B:383:HIS:HB2	1.86	0.57
6:B:741:LEU:HB3	29:b:66:LYS:HE3	1.84	0.57
18:N:809:GLY:HA2	18:N:814:LEU:HD12	1.86	0.57
5:A:1236:GLY:HA2	5:A:1300:GLU:HG3	1.86	0.57
6:B:658:LEU:HD22	6:B:667:ILE:HD13	1.84	0.57
5:A:863:VAL:O	5:A:867:GLU:HG3	2.03	0.57
20:P:201:ILE:HD13	20:P:215:ILE:HD11	1.85	0.57
25:X:560:PHE:HZ	25:X:571:ARG:HD2	1.69	0.57
5:A:1638:ILE:HG21	5:A:1642:LYS:CE	2.28	0.57
7:C:121:ASP:HB2	7:C:128:ILE:HD11	1.87	0.57
7:C:259:GLN:NE2	7:C:298:ALA:O	2.36	0.57
19:O:126:LEU:O	19:O:131:ARG:NH2	2.37	0.57
23:U:118:LEU:HG	23:U:122:ARG:HH22	1.67	0.57
25:X:524:LEU:HD21	25:X:532:ASP:HB2	1.86	0.57
25:X:552:LEU:HD23	25:X:555:LEU:HD21	1.87	0.57
5:A:154:PRO:O	5:A:444:ALA:N	2.37	0.57
5:A:1568:ARG:NH2	5:A:1696:ASP:OD1	2.32	0.57
24:W:510:ARG:NH2	25:X:531:GLU:HG2	2.20	0.57
25:X:543:LEU:HD13	26:Y:83:ILE:HD11	1.86	0.57
15:K:344:PHE:CE2	15:K:360:PRO:HG3	2.40	0.57
23:U:83:VAL:HG22	23:U:87:GLN:HE21	1.70	0.57
35:y:65:PHE:H	35:y:67:THR:HG22	1.68	0.57
36:z:187:SER:HA	36:z:195:VAL:HG11	1.87	0.57
5:A:968:SER:HB2	5:A:969:GLU:OE1	2.03	0.57
9:E:23:THR:HB	9:E:45:TYR:HB2	1.86	0.57
19:O:29:ARG:O	19:O:32:GLN:HG2	2.05	0.57
25:X:532:ASP:HA	25:X:535:LYS:HB2	1.85	0.57
5:A:1669:LEU:HD13	5:A:1738:ALA:HB3	1.86	0.57
15:K:118:ILE:HG13	22:R:225:GLN:NE2	2.19	0.57
18:N:149:ILE:HG13	18:N:152:LEU:HD12	1.87	0.57
18:N:527:PRO:O	18:N:562:ILE:N	2.25	0.57
18:N:562:ILE:HA	18:N:585:VAL:HG22	1.87	0.57
22:R:104:ILE:HD13	22:R:137:VAL:HG21	1.86	0.57
23:T:118:LEU:HD12	23:U:122:ARG:CZ	2.35	0.57
5:A:368:ALA:H	5:A:417:GLU:CD	2.12	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:983:ASN:ND2	5:A:1241:THR:O	2.38	0.57
15:K:386:MET:HB3	15:K:398:TRP:HB2	1.85	0.57
16:L:204:MET:HE1	17:M:54:PHE:HE2	1.69	0.57
20:P:289:LYS:O	20:P:293:ARG:NH1	2.37	0.57
23:T:21:ASN:HB2	23:T:23:TYR:CE2	2.39	0.57
25:X:321:SER:O	25:X:325:HIS:ND1	2.35	0.57
15:K:381:ASN:OD1	15:K:382:SER:N	2.38	0.56
31:d:6:LEU:HB2	31:d:13:ILE:HB	1.86	0.56
36:z:387:MET:HE2	36:z:415:HIS:HB3	1.87	0.56
3:5:102:G:N7	11:G:48:ARG:HD3	2.19	0.56
5:A:811:GLN:HG2	5:A:1047:HIS:HB3	1.87	0.56
5:A:1268:ILE:HG21	5:A:1315:CYS:HB2	1.86	0.56
5:A:1736:HIS:ND1	5:A:1758:MET:SD	2.78	0.56
6:B:886:ARG:HG3	6:B:886:ARG:HH11	1.70	0.56
20:P:87:LEU:O	20:P:88:LYS:C	2.47	0.56
5:A:402:ASN:HA	6:B:367:LYS:HE3	1.88	0.56
6:B:897:PHE:HB3	6:B:913:MET:HE1	1.87	0.56
7:C:265:ILE:HD11	7:C:290:ASP:HB3	1.86	0.56
11:G:12:LEU:HB3	11:G:16:GLU:HG2	1.87	0.56
15:K:256:HIS:HD1	15:K:258:THR:H	1.53	0.56
23:T:25:LYS:O	23:T:29:GLU:HG2	2.06	0.56
23:U:405:LEU:HG	23:U:406:ARG:HD2	1.87	0.56
24:W:38:ARG:NH2	24:W:158:ASP:OD2	2.38	0.56
24:W:244:GLN:HG2	24:W:245:ASN:HD22	1.71	0.56
5:A:1641:ARG:HB3	5:A:1644:TYR:CZ	2.41	0.56
24:W:678:ARG:HD2	27:Z:109:LEU:HD22	1.86	0.56
25:X:400:TYR:CD2	25:X:409:SER:HB2	2.41	0.56
25:X:551:GLU:HA	25:X:554:ASN:HD22	1.70	0.56
3:5:103:U:O5'	11:G:48:ARG:NH2	2.38	0.56
5:A:312:TRP:H	5:A:312:TRP:HE3	1.53	0.56
17:M:102:LEU:HD11	17:M:136:ALA:HA	1.88	0.56
18:N:299:ASP:HB3	18:N:383:ARG:HH12	1.71	0.56
18:N:1049:ARG:HE	18:N:1075:LEU:HA	1.70	0.56
22:R:261:ARG:O	22:R:265:LYS:HG2	2.05	0.56
23:T:85:LEU:HA	23:T:88:PHE:HD2	1.70	0.56
25:X:684:TYR:HB3	25:X:703:TRP:CZ3	2.41	0.56
18:N:70:MET:HG3	18:N:74:HIS:ND1	2.19	0.56
7:C:82:ASP:OD2	7:C:84:LYS:HD3	2.06	0.56
8:D:19:GLU:HB3	8:D:25:THR:HG22	1.88	0.56
25:X:661:LYS:HA	25:X:664:CYS:HB2	1.87	0.56
5:A:1639:HIS:HE1	5:A:1650:CYS:HB3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:93:SER:N	20:P:232:HIS:O	2.39	0.56
20:P:176:LEU:HD22	20:P:227:LYS:HB2	1.87	0.56
23:U:388:TYR:HA	23:U:405:LEU:HD22	1.87	0.56
25:X:581:GLU:OE1	25:X:581:GLU:N	2.39	0.56
26:Y:140:LYS:HB3	26:Y:142:ARG:HH11	1.71	0.56
31:d:73:ASP:OD1	31:d:96:ASN:ND2	2.33	0.56
1:1:8:U:OP1	24:W:213:ARG:NH2	2.39	0.56
5:A:1069:LEU:O	5:A:1073:LEU:HD13	2.06	0.56
7:C:103:ARG:HD3	7:C:145:LYS:HA	1.88	0.56
18:N:396:PHE:HE1	18:N:442:LYS:HG3	1.70	0.56
18:N:460:TYR:CD1	18:N:472:LEU:HD21	2.40	0.56
22:R:604:ALA:O	22:R:612:ARG:NH2	2.39	0.56
23:S:61:PRO:HB3	23:T:2:PHE:HB3	1.87	0.56
28:a:67:LEU:HA	31:d:93:ALA:HB2	1.87	0.56
35:y:147:ASN:ND2	36:z:432:SER:O	2.39	0.56
36:z:319:ASP:OD1	36:z:350:ARG:NH1	2.33	0.56
36:z:358:MET:SD	36:z:359:ARG:N	2.79	0.56
16:L:190:ASN:ND2	28:a:76:LYS:HB2	2.21	0.56
18:N:1223:THR:HB	18:N:1226:LEU:HD12	1.87	0.56
22:R:83:GLN:HG2	22:R:84:LYS:N	2.21	0.56
23:T:1:MET:HE1	24:W:696:LYS:NZ	2.21	0.56
28:a:61:GLU:OE1	28:a:61:GLU:N	2.38	0.56
35:y:25:PHE:CE2	35:y:27:LEU:HA	2.40	0.56
5:A:309:MET:HG2	5:A:311:ASP:H	1.70	0.55
23:T:87:GLN:OE1	23:U:87:GLN:NE2	2.32	0.55
24:W:202:LEU:HG	24:W:207:ILE:HA	1.86	0.55
25:X:395:GLU:OE1	25:X:398:ARG:NH1	2.38	0.55
26:Y:174:LYS:HD2	26:Y:174:LYS:O	2.06	0.55
4:6:74:U:H4'	4:6:75:G:OP1	2.06	0.55
5:A:542:ASP:OD2	5:A:546:ASN:ND2	2.30	0.55
6:B:396:THR:HG23	6:B:427:LEU:HG	1.87	0.55
6:B:862:ASP:OD1	6:B:866:ARG:NH2	2.40	0.55
7:C:113:SER:HA	7:C:137:VAL:HG13	1.88	0.55
7:C:218:HIS:CE1	7:C:244:ARG:HG3	2.40	0.55
12:H:35:ASP:OD1	12:H:36:ILE:N	2.40	0.55
15:K:344:PHE:HE2	15:K:360:PRO:HG3	1.71	0.55
22:R:63:ILE:HG22	22:R:72:HIS:HB3	1.89	0.55
23:V:98:LYS:NZ	24:W:530:VAL:HG13	2.21	0.55
24:W:238:THR:HG23	24:W:241:GLU:HB3	1.86	0.55
25:X:103:ILE:HG22	25:X:104:LEU:HD22	1.88	0.55
5:A:812:GLU:OE2	21:Q:252:ARG:NH2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:230:PRO:HD3	6:B:494:LYS:HZ1	1.71	0.55
10:F:44:LYS:NZ	10:F:54:PRO:HB3	2.20	0.55
11:G:44:LEU:HA	11:G:53:LEU:O	2.06	0.55
18:N:860:ALA:HA	25:X:103:ILE:HG12	1.86	0.55
23:V:98:LYS:HE3	24:W:537:ARG:CA	2.33	0.55
24:W:575:TYR:CD1	24:W:576:PRO:HD2	2.41	0.55
5:A:220:ASP:O	5:A:224:MET:HG2	2.07	0.55
5:A:1684:TYR:HB2	5:A:1724:GLY:HA2	1.87	0.55
22:R:110:TYR:HE2	22:R:126:LEU:HD22	1.71	0.55
23:T:73:LEU:HD22	23:V:73:LEU:HD22	1.89	0.55
5:A:80:ALA:HB2	19:O:103:LEU:HD23	1.88	0.55
18:N:680:VAL:HG12	18:N:681:LEU:HG	1.88	0.55
18:N:1151:SER:HA	18:N:1155:SER:HB3	1.87	0.55
22:R:547:GLU:O	22:R:568:ALA:HB1	2.07	0.55
24:W:717:LEU:HB3	27:Z:152:ARG:HH22	1.71	0.55
8:D:21:GLU:HA	8:D:67:ARG:NE	2.22	0.55
18:N:267:PHE:HA	18:N:270:MET:HG3	1.87	0.55
22:R:9:LYS:NZ	36:z:257:GLU:OE2	2.40	0.55
24:W:173:THR:HG23	24:W:174:GLN:N	2.22	0.55
30:c:579:ARG:HA	30:c:582:ARG:NH2	2.22	0.55
5:A:1507:GLY:O	5:A:1510:GLU:HG2	2.06	0.55
24:W:686:SER:HB2	27:Z:120:PHE:HE2	1.72	0.55
25:X:274:ARG:HG2	25:X:278:TYR:CE2	2.42	0.55
4:6:78:A:C8	22:R:105:PRO:HG3	2.42	0.55
5:A:1553:ILE:HD11	35:y:58:GLY:N	2.22	0.55
15:K:373:ALA:HB1	15:K:392:ASN:HD21	1.72	0.55
19:O:68:GLU:N	19:O:68:GLU:OE1	2.40	0.55
25:X:560:PHE:CZ	25:X:571:ARG:HD2	2.41	0.55
27:Z:180:CYS:O	27:Z:184:THR:HG23	2.07	0.55
36:z:163:LYS:NZ	36:z:189:PHE:O	2.40	0.55
36:z:604:SER:HB2	36:z:631:ILE:HD13	1.88	0.55
5:A:67:GLY:HA3	5:A:70:ARG:HD2	1.89	0.55
5:A:109:TYR:CE1	5:A:146:ALA:HA	2.42	0.55
5:A:1461:ARG:NH1	5:A:1479:TRP:O	2.40	0.55
16:L:241:VAL:HG22	26:Y:107:ASP:OD1	2.06	0.55
22:R:460:TRP:CE2	22:R:470:PRO:HG3	2.41	0.55
25:X:637:LEU:HD23	25:X:638:ASN:N	2.22	0.55
26:Y:153:LEU:HB3	31:d:131:ARG:HH22	1.71	0.55
34:r:242:UNK:O	34:r:244:UNK:N	2.40	0.55
5:A:176:LYS:NZ	5:A:645:GLY:O	2.40	0.55
22:R:120:ILE:HG22	22:R:124:ARG:HD2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:654:GLU:HG2	27:Z:86:PRO:HB3	1.88	0.55
30:c:522:TYR:O	30:c:525:VAL:HG12	2.06	0.55
5:A:935:ASP:HB3	5:A:938:GLU:HG3	1.89	0.54
6:B:358:ASP:H	6:B:379:ARG:NH1	2.04	0.54
20:P:99:ILE:HG12	20:P:137:LEU:HB2	1.87	0.54
25:X:243:ARG:HD2	25:X:246:ILE:HD11	1.88	0.54
25:X:503:TYR:HD1	25:X:507:PHE:HE2	1.54	0.54
36:z:395:LYS:NZ	36:z:434:ASN:HA	2.22	0.54
18:N:253:THR:HG21	18:N:376:VAL:HA	1.89	0.54
25:X:238:VAL:O	25:X:242:PHE:HB2	2.08	0.54
25:X:273:ALA:O	25:X:276:THR:OG1	2.22	0.54
30:c:594:GLY:O	30:c:597:THR:HG22	2.05	0.54
18:N:950:ARG:HG2	18:N:951:ILE:HG13	1.89	0.54
20:P:160:ARG:HH12	20:P:165:GLY:N	2.01	0.54
26:Y:199:GLU:HG3	26:Y:202:ARG:NH1	2.21	0.54
36:z:614:ILE:HD11	36:z:631:ILE:HG23	1.89	0.54
4:6:53:G:O2'	4:6:55:C:OP1	2.22	0.54
6:B:725:GLN:N	6:B:725:GLN:OE1	2.36	0.54
14:J:21:LEU:HB2	14:J:25:ARG:HB2	1.87	0.54
17:M:75:ARG:HG2	17:M:75:ARG:HH11	1.73	0.54
22:R:177:TYR:CE2	22:R:193:ILE:HD13	2.41	0.54
22:R:204:VAL:O	22:R:208:LEU:HG	2.07	0.54
29:b:68:LEU:HD21	29:b:131:TYR:HE1	1.72	0.54
36:z:144:ILE:HG12	36:z:175:VAL:HB	1.88	0.54
5:A:1714:ASP:OD2	5:A:1716:GLN:NE2	2.40	0.54
6:B:604:VAL:HB	6:B:651:MET:HE2	1.89	0.54
18:N:32:LEU:HD22	18:N:77:LEU:HD11	1.89	0.54
22:R:337:THR:OG1	22:R:342:TYR:OH	2.15	0.54
23:T:9:THR:HB	23:T:58:PHE:CD2	2.42	0.54
5:A:1605:LEU:HD11	5:A:1770:ARG:NH2	2.23	0.54
5:A:1725:VAL:HA	5:A:1740:GLY:HA3	1.89	0.54
7:C:244:ARG:HD3	7:C:257:GLN:NE2	2.23	0.54
24:W:239:SER:OG	24:W:240:GLU:N	2.38	0.54
25:X:68:TRP:HE1	25:X:104:LEU:HD23	1.72	0.54
31:d:44:HIS:HD2	31:d:54:GLY:HA2	1.73	0.54
31:d:89:SER:OG	31:d:117:THR:O	2.26	0.54
6:B:434:SER:O	8:D:87:ARG:NH2	2.40	0.54
18:N:736:LEU:O	18:N:740:GLN:HG3	2.07	0.54
20:P:160:ARG:NH2	20:P:165:GLY:H	2.06	0.54
24:W:703:ALA:O	24:W:707:GLU:HG2	2.08	0.54
5:A:862:LEU:HD12	5:A:901:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:971:PRO:HB3	5:A:1215:THR:HG21	1.88	0.54
5:A:1267:ARG:CZ	5:A:1474:ASN:HD21	2.20	0.54
5:A:1629:GLN:HG3	5:A:1657:ALA:HB2	1.90	0.54
5:A:1641:ARG:HG2	5:A:1644:TYR:OH	2.08	0.54
10:F:11:THR:HA	10:F:29:ILE:HD11	1.90	0.54
29:b:119:LEU:HD13	29:b:122:ALA:HB3	1.90	0.54
3:5:98:U:C2	8:D:36:ASN:HB3	2.43	0.54
5:A:932:TYR:HB2	5:A:1056:GLY:HA3	1.90	0.54
7:C:75:LEU:HD13	7:C:88:VAL:HG12	1.90	0.54
12:H:25:PRO:HG2	12:H:84:ILE:HG12	1.90	0.54
15:K:414:GLN:HB2	15:K:415:PRO:HD2	1.88	0.54
21:Q:68:GLN:N	21:Q:68:GLN:OE1	2.41	0.54
23:U:310:LEU:H	23:U:322:SER:HB3	1.71	0.54
6:B:609:HIS:O	6:B:668:ARG:NH2	2.40	0.54
6:B:819:GLY:O	6:B:823:ILE:HG13	2.08	0.54
7:C:265:ILE:HD12	9:E:114:PRO:HG3	1.90	0.54
8:D:17:THR:HA	8:D:26:TYR:O	2.08	0.54
22:R:219:ASN:OD1	22:R:220:ALA:N	2.40	0.54
27:Z:149:ASN:O	27:Z:153:LYS:HG2	2.08	0.54
27:Z:162:ARG:O	27:Z:165:GLU:HG3	2.08	0.54
36:z:376:GLU:HB2	36:z:377:GLU:OE1	2.08	0.54
1:1:0:G:H1'	1:1:1:G:OP2	2.08	0.53
6:B:711:SER:HG	6:B:800:ASN:HD22	1.54	0.53
10:F:2:LYS:NZ	11:G:62:ARG:HH22	2.06	0.53
23:U:371:PHE:HE1	27:Z:35:ARG:HA	1.73	0.53
30:c:470:ARG:O	30:c:474:LEU:HG	2.08	0.53
3:5:18:U:OP1	5:A:243:THR:OG1	2.22	0.53
16:L:145:GLN:HA	16:L:148:GLU:HG2	1.90	0.53
17:M:123:LEU:HA	17:M:126:ASN:OD1	2.08	0.53
23:S:122:ARG:HD2	23:V:118:LEU:HB2	1.90	0.53
25:X:572:THR:O	25:X:575:LEU:HG	2.08	0.53
30:c:486:PHE:CD2	30:c:521:VAL:HB	2.43	0.53
6:B:315:GLU:HG2	6:B:316:LEU:HD12	1.90	0.53
20:P:150:CYS:SG	20:P:221:ALA:HA	2.49	0.53
36:z:80:ARG:HB2	36:z:83:VAL:HB	1.91	0.53
5:A:1422:GLN:NE2	5:A:1423:GLN:HE21	2.07	0.53
5:A:1621:LEU:HD11	5:A:1746:MET:HE1	1.89	0.53
5:A:1666:PRO:HD3	5:A:1741:ASN:HD21	1.72	0.53
5:A:1762:PRO:HB3	35:y:94:ILE:HA	1.90	0.53
6:B:821:GLN:HG3	33:m:727:ALA:HB1	1.91	0.53
7:C:98:ASP:OD1	7:C:99:LEU:N	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:163:MET:HB3	20:P:245:TRP:HB2	1.90	0.53
22:R:121:ASN:HB3	24:W:241:GLU:OE1	2.08	0.53
22:R:306:LEU:O	22:R:310:LYS:HG2	2.08	0.53
30:c:538:ILE:HA	30:c:541:LYS:HG2	1.91	0.53
36:z:367:THR:HG22	36:z:369:LYS:H	1.73	0.53
5:A:969:GLU:HB2	5:A:973:LEU:HB3	1.90	0.53
6:B:696:LYS:HZ1	6:B:816:TYR:HB3	1.72	0.53
6:B:854:ALA:HA	6:B:857:LEU:HD23	1.89	0.53
15:K:340:HIS:CD2	15:K:380:ILE:HG21	2.44	0.53
18:N:505:MET:HE1	18:N:585:VAL:HG21	1.90	0.53
20:P:122:ARG:HB3	20:P:124:MET:HE1	1.90	0.53
24:W:540:VAL:HG11	24:W:581:LYS:HB3	1.89	0.53
24:W:688:GLU:OE1	24:W:688:GLU:N	2.41	0.53
24:W:706:THR:O	24:W:710:ASN:ND2	2.42	0.53
33:m:772:LYS:HB3	33:m:782:TYR:CE1	2.44	0.53
36:z:428:VAL:HG23	36:z:440:GLY:HA2	1.91	0.53
5:A:1429:LEU:C	5:A:1431:ASP:H	2.16	0.53
7:C:249:LYS:O	7:C:256:ARG:NH2	2.37	0.53
15:K:144:GLN:HE22	15:K:467:SER:H	1.57	0.53
20:P:172:GLN:OE1	20:P:172:GLN:N	2.40	0.53
23:U:114:VAL:HG13	23:U:117:ARG:NH2	2.24	0.53
23:V:108:LEU:HD12	24:W:600:CYS:SG	2.49	0.53
5:A:1129:SER:O	5:A:1133:ILE:HG13	2.09	0.53
5:A:1341:TYR:CE1	5:A:1353:SER:HB2	2.43	0.53
17:M:264:ALA:O	17:M:282:GLN:NE2	2.42	0.53
20:P:293:ARG:O	20:P:296:LYS:HG2	2.09	0.53
22:R:333:GLY:O	22:R:342:TYR:OH	2.27	0.53
23:U:255:CYS:HB3	23:U:264:VAL:HG23	1.90	0.53
24:W:531:ILE:HG12	24:W:537:ARG:NH2	2.23	0.53
24:W:686:SER:HB2	27:Z:120:PHE:CE2	2.44	0.53
25:X:178:ILE:HA	25:X:181:TYR:CE1	2.43	0.53
36:z:392:LEU:HD11	36:z:450:ALA:HB2	1.90	0.53
4:6:27:G:C2	20:P:160:ARG:HG3	2.43	0.53
6:B:222:ASP:HB3	6:B:650:TYR:HB2	1.90	0.53
6:B:575:LYS:NZ	6:B:625:ASN:O	2.42	0.53
7:C:46:MET:HE2	7:C:77:TRP:CZ3	2.44	0.53
15:K:280:GLN:HG3	16:L:165:ILE:HD11	1.90	0.53
17:M:26:CYS:HA	17:M:58:LYS:NZ	2.24	0.53
20:P:186:ASP:O	20:P:189:GLU:HG3	2.09	0.53
25:X:98:PHE:HD1	25:X:111:ILE:HG23	1.74	0.53
36:z:143:VAL:HB	36:z:172:PHE:CZ	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:z:425:LEU:HD12	36:z:579:ARG:NH2	2.24	0.53
36:z:456:LEU:HD11	36:z:469:LEU:HA	1.89	0.53
5:A:121:LEU:HD13	5:A:664:LEU:HB3	1.91	0.53
5:A:530:LEU:HG	5:A:530:LEU:O	2.07	0.53
5:A:681:ARG:HH11	5:A:681:ARG:HG2	1.74	0.53
15:K:183:GLY:HA2	15:K:207:THR:HG23	1.91	0.53
18:N:966:LEU:HD22	18:N:971:PHE:HB2	1.91	0.53
20:P:68:GLY:O	20:P:81:GLY:HA3	2.09	0.53
22:R:154:ILE:HA	22:R:157:CYS:SG	2.49	0.53
22:R:322:TRP:HH2	22:R:348:LYS:HG3	1.74	0.53
22:R:326:LEU:HA	22:R:329:GLU:HG2	1.91	0.53
23:S:90:LEU:HD13	23:V:86:GLU:HG2	1.90	0.53
24:W:640:LEU:O	24:W:644:GLU:N	2.40	0.53
24:W:678:ARG:CZ	27:Z:109:LEU:HB3	2.38	0.53
5:A:1267:ARG:NH1	5:A:1474:ASN:HD21	2.07	0.53
17:M:201:ILE:HG22	17:M:203:MET:CE	2.39	0.53
27:Z:71:LYS:HE3	27:Z:73:ALA:HB2	1.89	0.53
35:y:116:ILE:O	35:y:119:ILE:HG12	2.09	0.53
5:A:1649:SER:H	5:A:1711:TYR:HE2	1.57	0.52
7:C:89:LEU:HD12	7:C:120:TRP:CD2	2.45	0.52
27:Z:114:LYS:NZ	34:r:248:UNK:O	2.39	0.52
30:c:585:ILE:HD12	30:c:601:ARG:HH12	1.74	0.52
36:z:114:SER:HG	36:z:117:THR:HG1	1.53	0.52
5:A:913:THR:HG21	24:W:92:THR:HG22	1.91	0.52
5:A:1514:PHE:O	5:A:1517:THR:OG1	2.27	0.52
5:A:1584:ILE:HD13	5:A:1597:LEU:HD13	1.91	0.52
5:A:1668:LEU:HD23	5:A:1739:TYR:HD1	1.74	0.52
22:R:338:ILE:O	22:R:341:THR:HG22	2.08	0.52
23:T:122:ARG:HD2	23:U:122:ARG:HE	1.74	0.52
25:X:445:ASP:OD1	25:X:446:ALA:N	2.42	0.52
28:a:139:GLU:OE1	28:a:139:GLU:N	2.37	0.52
31:d:32:LEU:HD11	31:d:37:TYR:HE1	1.73	0.52
36:z:323:ASN:ND2	36:z:342:ILE:HG22	2.16	0.52
5:A:896:ASN:ND2	5:A:899:GLU:OE2	2.42	0.52
10:F:29:ILE:HA	10:F:40:LEU:HD23	1.90	0.52
17:M:68:GLN:CD	20:P:147:ASN:HD21	2.17	0.52
17:M:91:LEU:HD12	17:M:95:LEU:HD22	1.91	0.52
18:N:777:LEU:HD23	18:N:984:ILE:HD13	1.91	0.52
20:P:177:TYR:HE1	20:P:212:ILE:HG23	1.73	0.52
22:R:221:ALA:O	22:R:225:GLN:HB2	2.09	0.52
35:y:116:ILE:H	36:z:643:TYR:HH	1.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:5:104:A:O2'	11:G:48:ARG:HG2	2.09	0.52
5:A:171:MET:HE2	5:A:213:MET:HA	1.90	0.52
6:B:757:ASN:OD1	6:B:788:THR:OG1	2.24	0.52
16:L:184:ILE:HG21	17:M:19:PHE:HE1	1.74	0.52
23:S:118:LEU:HD22	23:S:122:ARG:HH22	1.74	0.52
24:W:719:ASN:O	24:W:722:ARG:HG3	2.09	0.52
30:c:576:ASP:HB3	30:c:603:TYR:CZ	2.44	0.52
35:y:138:ASP:CG	35:y:141:GLY:HA3	2.34	0.52
6:B:335:PHE:CD2	6:B:385:ILE:HG12	2.45	0.52
6:B:692:THR:HG22	6:B:693:PRO:HD2	1.92	0.52
24:W:40:THR:OG1	24:W:43:GLN:OE1	2.23	0.52
24:W:245:ASN:HB2	24:W:248:GLU:HG2	1.91	0.52
36:z:31:ARG:O	36:z:34:LEU:HG	2.10	0.52
36:z:103:CYS:HA	36:z:119:ILE:O	2.09	0.52
1:1:-10:A:C2	29:b:3:TYR:HB3	2.45	0.52
5:A:962:TRP:HZ3	5:A:1085:ALA:HB2	1.75	0.52
9:E:117:LEU:O	16:L:185:ARG:NH2	2.27	0.52
15:K:302:PRO:HD2	15:K:359:PHE:CE2	2.45	0.52
20:P:82:MET:C	20:P:84:GLN:N	2.66	0.52
22:R:159:GLN:HE22	26:Y:155:TRP:CD1	2.28	0.52
23:T:27:LEU:O	23:T:30:GLN:HG2	2.09	0.52
26:Y:131:ASP:HA	26:Y:134:LYS:HG2	1.92	0.52
13:I:23:ARG:HH12	13:I:27:GLY:HA2	1.72	0.52
18:N:1014:THR:HG21	18:N:1030:LYS:HE3	1.90	0.52
23:T:18:VAL:HG11	23:T:41:THR:HG21	1.91	0.52
5:A:363:ASP:N	5:A:363:ASP:OD1	2.42	0.52
6:B:960:ASP:OD1	6:B:961:VAL:N	2.43	0.52
7:C:162:VAL:HG12	7:C:172:LYS:HB3	1.91	0.52
18:N:223:LEU:HD12	18:N:270:MET:HE3	1.91	0.52
18:N:318:LEU:HD21	18:N:342:LEU:HG	1.92	0.52
25:X:557:LEU:HD22	25:X:576:PHE:HE1	1.75	0.52
28:a:100:ASN:O	28:a:104:TYR:HD1	1.93	0.52
35:y:117:ASN:HD22	36:z:593:ILE:HG13	1.74	0.52
35:y:147:ASN:ND2	36:z:433:GLY:HA3	2.24	0.52
36:z:364:ARG:HB3	36:z:366:TYR:CE1	2.44	0.52
1:1:8:U:H5"	24:W:213:ARG:NH2	2.24	0.52
17:M:20:PRO:HG3	17:M:54:PHE:CG	2.45	0.52
19:O:23:LEU:HD23	19:O:83:TYR:CD1	2.45	0.52
23:T:116:SER:O	23:T:120:LYS:HG2	2.10	0.52
23:V:16:SER:H	23:V:20:GLY:HA2	1.75	0.52
24:W:537:ARG:C	24:W:539:SER:H	2.18	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:251:ASP:OD1	25:X:251:ASP:N	2.43	0.52
30:c:492:THR:HB	30:c:495:ARG:NH1	2.25	0.52
36:z:81:ARG:HG2	36:z:107:ILE:HB	1.91	0.52
5:A:1324:LYS:HB3	5:A:1330:LYS:HA	1.92	0.52
6:B:928:LYS:O	6:B:931:LYS:NZ	2.32	0.52
13:I:16:ILE:HG23	13:I:35:GLN:HA	1.91	0.52
19:O:90:ALA:O	19:O:94:LYS:NZ	2.42	0.52
20:P:92:LYS:O	20:P:93:SER:C	2.52	0.52
20:P:149:ASP:N	20:P:153:ARG:O	2.38	0.52
21:Q:239:ASP:N	21:Q:239:ASP:OD1	2.43	0.52
23:S:122:ARG:NE	23:V:114:VAL:HG22	2.25	0.52
23:T:122:ARG:HH11	23:U:122:ARG:CZ	2.22	0.52
24:W:627:TYR:O	24:W:630:LEU:N	2.43	0.52
6:B:781:LYS:O	6:B:785:GLN:HG2	2.10	0.51
7:C:160:MET:HE3	7:C:174:ILE:HD13	1.92	0.51
8:D:57:ASP:OD1	8:D:57:ASP:N	2.41	0.51
17:M:238:LEU:O	17:M:255:LYS:NZ	2.42	0.51
18:N:699:PHE:CZ	18:N:736:LEU:HD21	2.46	0.51
20:P:174:TYR:CE1	20:P:220:GLU:HG2	2.46	0.51
22:R:47:GLU:HA	22:R:50:GLU:HG3	1.92	0.51
24:W:251:GLU:CB	24:W:255:LYS:HZ3	2.22	0.51
24:W:623:PHE:CE1	24:W:627:TYR:CE1	2.98	0.51
27:Z:64:VAL:O	27:Z:68:LYS:HG2	2.10	0.51
35:y:64:TYR:OH	35:y:71:LYS:HG3	2.11	0.51
5:A:985:LEU:HB2	5:A:988:VAL:HB	1.91	0.51
6:B:224:VAL:HB	6:B:597:MET:HE3	1.92	0.51
8:D:73:ASP:OD1	8:D:76:ARG:NH2	2.43	0.51
17:M:141:ARG:NH1	20:P:311:ASP:OD1	2.43	0.51
18:N:498:PRO:HG2	18:N:589:PRO:HB3	1.92	0.51
24:W:537:ARG:NH1	24:W:577:PHE:HB2	2.25	0.51
36:z:153:LEU:HD12	36:z:382:ILE:HG13	1.92	0.51
5:A:61:SER:OG	5:A:65:LYS:NZ	2.42	0.51
5:A:296:PRO:HB3	5:A:475:LYS:HB2	1.91	0.51
5:A:1111:TYR:CD1	5:A:1120:ILE:HG12	2.44	0.51
13:I:43:LEU:HD11	13:I:65:ILE:HD12	1.91	0.51
18:N:1059:ILE:HG21	18:N:1201:TYR:HB2	1.92	0.51
18:N:1107:LYS:NZ	18:N:1187:GLU:OE2	2.35	0.51
24:W:158:ASP:OD1	24:W:159:GLU:N	2.43	0.51
25:X:444:PHE:O	25:X:448:ARG:HG2	2.10	0.51
26:Y:155:TRP:HA	26:Y:158:ASN:OD1	2.10	0.51
27:Z:29:VAL:O	27:Z:32:GLU:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:569:LEU:HD23	5:A:671:LEU:HD21	1.93	0.51
7:C:54:LEU:HD21	7:C:70:MET:HE2	1.93	0.51
17:M:100:LEU:HD22	17:M:143:LEU:HD13	1.93	0.51
20:P:54:ILE:HD13	20:P:124:MET:HB2	1.92	0.51
23:S:76:PHE:CE1	23:T:72:LEU:HG	2.45	0.51
23:S:89:GLU:OE2	23:S:93:ASN:ND2	2.44	0.51
23:U:276:PRO:HG2	23:U:279:SER:HB2	1.92	0.51
15:K:169:VAL:HB	15:K:439:CYS:SG	2.50	0.51
15:K:296:ALA:HB1	15:K:339:LEU:HD11	1.93	0.51
21:Q:240:ASP:N	21:Q:240:ASP:OD1	2.44	0.51
25:X:179:GLU:HA	25:X:182:ILE:HG22	1.93	0.51
4:6:37:A:O2'	4:6:38:G:OP1	2.29	0.51
5:A:280:ASN:HB2	5:A:349:SER:HB3	1.93	0.51
6:B:113:ARG:HE	6:B:499:VAL:HG11	1.74	0.51
6:B:225:ASP:OD1	6:B:630:LEU:HG	2.11	0.51
11:G:90:ILE:HG13	11:G:92:LYS:HZ1	1.76	0.51
18:N:396:PHE:CE1	18:N:442:LYS:HG3	2.46	0.51
23:V:73:LEU:HD11	23:V:77:GLN:HE21	1.76	0.51
29:b:59:CYS:O	29:b:63:ILE:HG23	2.10	0.51
35:y:147:ASN:HD22	36:z:433:GLY:HA3	1.76	0.51
24:W:248:GLU:HA	24:W:251:GLU:HG2	1.91	0.51
33:m:718:PHE:HE2	33:m:764:LEU:HD22	1.75	0.51
4:6:92:C:H5'	26:Y:92:ARG:HH22	1.74	0.51
5:A:1274:SER:OG	5:A:1286:LYS:NZ	2.44	0.51
7:C:302:LEU:HD22	28:a:59:VAL:HG21	1.93	0.51
10:F:18:GLU:HG3	10:F:66:ARG:HB3	1.93	0.51
15:K:109:GLN:HA	15:K:133:GLN:HE22	1.74	0.51
15:K:327:LEU:HD23	15:K:357:TRP:CE2	2.46	0.51
17:M:47:CYS:HB3	17:M:49:LYS:HB2	1.93	0.51
18:N:687:PRO:HD2	18:N:690:LEU:HD12	1.93	0.51
18:N:751:ARG:NH1	18:N:1207:CYS:O	2.44	0.51
20:P:254:SER:HA	20:P:257:ARG:HG2	1.92	0.51
23:U:99:GLN:HA	24:W:709:LYS:HZ1	1.75	0.51
25:X:667:PHE:CE2	25:X:683:ILE:HD13	2.46	0.51
4:6:47:A:H5"	4:6:47:A:C8	2.43	0.51
5:A:972:PRO:HD3	5:A:1297:TYR:HE1	1.75	0.51
11:G:68:LEU:HB2	11:G:99:MET:HB2	1.93	0.51
15:K:135:SER:O	15:K:139:ARG:HG3	2.11	0.51
22:R:150:MET:SD	26:Y:168:LEU:HD12	2.50	0.51
23:T:67:THR:HB	27:Z:105:ARG:HA	1.93	0.51
26:Y:159:LYS:HD2	26:Y:160:PRO:HD2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:Z:159:VAL:HG12	27:Z:162:ARG:HH22	1.75	0.51
30:c:440:GLU:OE1	30:c:440:GLU:N	2.39	0.51
35:y:141:GLY:HA2	35:y:144:MET:HB2	1.93	0.51
3:5:96:G:N2	13:I:39:SER:O	2.39	0.51
5:A:936:PRO:O	5:A:940:ILE:HG12	2.11	0.51
7:C:164:ASP:OD1	7:C:165:SER:N	2.43	0.51
15:K:106:ILE:HG21	15:K:137:VAL:HA	1.91	0.51
18:N:536:LYS:HA	18:N:539:GLU:HG3	1.93	0.51
22:R:83:GLN:HA	24:W:256:ILE:HD13	1.92	0.51
22:R:147:MET:O	22:R:151:LEU:HD23	2.11	0.51
23:S:105:LEU:HD13	24:W:625:GLU:CD	2.36	0.51
31:d:8:THR:HG23	31:d:11:GLY:H	1.75	0.51
20:P:173:ASN:OD1	20:P:175:THR:HG22	2.11	0.50
23:T:3:CYS:N	23:T:8:GLU:O	2.28	0.50
6:B:229:ALA:HB3	6:B:494:LYS:HZ1	1.74	0.50
6:B:711:SER:OG	6:B:800:ASN:ND2	2.39	0.50
11:G:42:GLN:HE21	11:G:56:ARG:HH12	1.60	0.50
16:L:184:ILE:HB	16:L:202:ILE:HG22	1.93	0.50
18:N:494:GLY:HA2	25:X:241:VAL:HA	1.91	0.50
18:N:844:PRO:O	18:N:847:HIS:NE2	2.45	0.50
22:R:490:LEU:HA	22:R:493:LEU:HD12	1.93	0.50
28:a:143:ASP:HB3	28:a:146:ILE:HD13	1.93	0.50
4:6:15:U:C2	28:a:104:TYR:CE2	3.00	0.50
5:A:1272:LEU:O	5:A:1322:ARG:NH2	2.44	0.50
7:C:194:ILE:HG13	7:C:202:LYS:HB2	1.93	0.50
13:I:7:ASN:HB2	13:I:10:PRO:HD2	1.92	0.50
20:P:59:GLU:OE2	20:P:61:GLU:HG3	2.11	0.50
22:R:107:TRP:O	22:R:111:ILE:HG12	2.12	0.50
23:T:90:LEU:HD11	23:U:91:ARG:HG3	1.93	0.50
5:A:1567:ASN:HB2	5:A:1593:LEU:HD21	1.94	0.50
6:B:252:THR:O	6:B:256:LYS:HG2	2.10	0.50
18:N:139:LEU:O	18:N:143:VAL:HG23	2.12	0.50
18:N:407:VAL:HG13	18:N:419:LEU:HD13	1.94	0.50
18:N:443:LYS:HE2	18:N:447:ARG:HH21	1.76	0.50
22:R:261:ARG:NH2	22:R:291:GLY:O	2.43	0.50
23:S:90:LEU:CD1	23:V:86:GLU:HG2	2.41	0.50
24:W:177:LYS:HB3	24:W:180:ARG:HH12	1.77	0.50
27:Z:134:LEU:O	27:Z:138:LEU:HD23	2.11	0.50
5:A:1533:PHE:O	5:A:1536:SER:OG	2.23	0.50
5:A:1611:GLU:O	5:A:1615:TRP:HB2	2.11	0.50
15:K:166:VAL:HG12	15:K:439:CYS:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:666:TYR:HB2	18:N:768:THR:HA	1.93	0.50
22:R:83:GLN:HG2	22:R:84:LYS:H	1.75	0.50
23:T:61:PRO:HB2	27:Z:120:PHE:CZ	2.46	0.50
30:c:537:ARG:HG2	30:c:587:TYR:CE2	2.47	0.50
31:d:9:SER:HB3	31:d:148:LYS:O	2.12	0.50
31:d:103:PHE:HE1	31:d:116:HIS:CE1	2.29	0.50
36:z:162:LEU:HD23	36:z:174:LEU:HD22	1.94	0.50
36:z:523:LEU:O	36:z:527:ARG:HG2	2.12	0.50
5:A:1657:ALA:O	5:A:1683:LYS:NZ	2.45	0.50
14:J:32:ARG:HG3	14:J:43:GLU:HG3	1.92	0.50
17:M:26:CYS:HA	17:M:58:LYS:HZ3	1.77	0.50
18:N:772:ASP:HB2	18:N:974:ASN:HB2	1.94	0.50
18:N:1049:ARG:NH2	18:N:1077:TYR:O	2.44	0.50
23:U:389:TRP:O	23:U:390:LEU:HD23	2.12	0.50
31:d:47:ILE:HB	31:d:50:PHE:HB3	1.94	0.50
36:z:344:LYS:HD2	36:z:376:GLU:CD	2.36	0.50
6:B:632:ILE:O	6:B:644:PHE:HD1	1.94	0.50
6:B:796:GLU:HG3	6:B:797:THR:N	2.27	0.50
6:B:824:PRO:HG3	33:m:723:GLU:OE1	2.11	0.50
22:R:186:GLU:HG3	22:R:189:ARG:HG2	1.93	0.50
22:R:212:ARG:O	22:R:215:GLU:HG3	2.12	0.50
23:T:94:LEU:HD12	23:U:90:LEU:CD1	2.39	0.50
23:U:99:GLN:HA	24:W:709:LYS:NZ	2.27	0.50
25:X:550:PHE:CE1	25:X:587:PHE:HB3	2.47	0.50
33:m:718:PHE:CE2	33:m:764:LEU:HD22	2.47	0.50
5:A:109:TYR:OH	5:A:525:ASN:HB2	2.12	0.50
15:K:302:PRO:O	15:K:359:PHE:HZ	1.94	0.50
17:M:69:ILE:HD11	17:M:84:MET:SD	2.51	0.50
18:N:12:ILE:HG13	18:N:51:LEU:HD21	1.94	0.50
18:N:15:ALA:O	18:N:20:GLY:N	2.45	0.50
18:N:528:PHE:HE2	18:N:623:LEU:HD21	1.77	0.50
18:N:753:GLY:O	18:N:757:LEU:HD23	2.12	0.50
22:R:59:PHE:HD2	22:R:76:TYR:HD1	1.59	0.50
22:R:84:LYS:NZ	22:R:88:ARG:HG2	2.27	0.50
23:U:126:ARG:HG2	23:U:126:ARG:HH11	1.77	0.50
24:W:600:CYS:HA	24:W:603:LEU:HB2	1.93	0.50
35:y:150:TRP:CE2	35:y:152:GLY:HA3	2.47	0.50
4:6:49:C:H2'	4:6:50:A:O4'	2.12	0.50
5:A:291:ALA:N	29:b:2:SER:O	2.41	0.50
15:K:341:PRO:O	16:L:140:LYS:NZ	2.34	0.50
17:M:73:CYS:C	17:M:75:ARG:H	2.18	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:75:ARG:HH12	17:M:124:LEU:CD2	2.24	0.50
18:N:226:ILE:HG21	18:N:270:MET:HE1	1.94	0.50
5:A:197:PHE:CE2	5:A:589:LEU:HD21	2.46	0.49
5:A:1313:VAL:HG13	5:A:1381:MET:HG3	1.94	0.49
5:A:1410:TRP:CH2	5:A:1446:LEU:HD21	2.47	0.49
15:K:235:GLU:OE1	21:Q:36:LYS:NZ	2.45	0.49
17:M:264:ALA:HA	17:M:282:GLN:HE22	1.76	0.49
22:R:151:LEU:HD21	26:Y:168:LEU:HD21	1.94	0.49
23:S:62:ARG:HH12	23:S:71:ALA:HB2	1.77	0.49
24:W:159:GLU:HA	24:W:162:MET:HG3	1.94	0.49
5:A:405:ILE:HG22	6:B:346:ILE:HD13	1.93	0.49
5:A:907:ARG:HD2	5:A:941:CYS:SG	2.52	0.49
9:E:9:LEU:HA	9:E:12:HIS:CD2	2.47	0.49
18:N:748:GLY:HA3	18:N:1042:LEU:HD12	1.93	0.49
22:R:278:GLU:HA	22:R:281:LYS:HG2	1.94	0.49
22:R:310:LYS:O	22:R:313:LYS:HG2	2.12	0.49
25:X:549:ALA:O	25:X:553:TRP:HD1	1.95	0.49
36:z:565:ASP:OD1	36:z:567:SER:OG	2.27	0.49
5:A:989:TRP:O	5:A:1203:TYR:OH	2.26	0.49
5:A:1649:SER:N	5:A:1711:TYR:HE2	2.10	0.49
6:B:701:MET:SD	6:B:803:PHE:HB3	2.53	0.49
6:B:972:ILE:HG22	6:B:976:LYS:HE3	1.94	0.49
15:K:138:LYS:HD3	16:L:131:LEU:HA	1.94	0.49
18:N:1185:THR:O	18:N:1187:GLU:N	2.43	0.49
20:P:290:SER:O	20:P:294:LYS:HG2	2.12	0.49
22:R:56:ARG:NH1	24:W:222:ASN:OD1	2.45	0.49
33:m:717:SER:OG	33:m:718:PHE:N	2.45	0.49
36:z:393:PHE:O	36:z:397:LEU:HG	2.12	0.49
4:6:32:G:N2	20:P:82:MET:HB3	2.25	0.49
5:A:342:ARG:HD2	5:A:344:ARG:NH1	2.27	0.49
10:F:17:ILE:HG12	10:F:68:TYR:CE1	2.46	0.49
11:G:7:LYS:N	11:G:8:PRO:HD3	2.28	0.49
12:H:60:ASP:OD1	12:H:61:ALA:N	2.39	0.49
23:S:87:GLN:HA	23:S:90:LEU:HG	1.95	0.49
23:U:24:GLU:HB3	23:U:27:LEU:HD12	1.94	0.49
28:a:128:LYS:O	28:a:132:GLN:HG2	2.13	0.49
2:2:12:G:H2'	2:2:13:C:H4'	1.94	0.49
12:H:27:SER:H	12:H:82:GLN:HB3	1.77	0.49
15:K:263:VAL:HG22	15:K:273:VAL:HG22	1.94	0.49
22:R:228:LEU:HA	22:R:231:ILE:HG12	1.94	0.49
23:S:73:LEU:HD22	23:U:73:LEU:HD12	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:216:TYR:CZ	25:X:220:LEU:HD21	2.47	0.49
27:Z:147:GLY:O	27:Z:150:ARG:HG2	2.12	0.49
36:z:231:ASN:OD1	36:z:267:CYS:HB3	2.13	0.49
5:A:107:ARG:NH2	16:L:215:PRO:O	2.37	0.49
5:A:398:GLU:CD	12:H:6:GLN:HE22	2.21	0.49
5:A:613:GLY:HA2	5:A:615:TYR:CE2	2.48	0.49
5:A:1669:LEU:CD1	5:A:1738:ALA:HB3	2.41	0.49
6:B:742:ALA:HB1	6:B:760:ARG:HH11	1.77	0.49
18:N:751:ARG:NH2	18:N:1206:ALA:O	2.45	0.49
18:N:769:SER:OG	18:N:772:ASP:OD2	2.18	0.49
24:W:241:GLU:C	24:W:245:ASN:HD21	2.20	0.49
24:W:616:TYR:HA	24:W:619:PHE:HD2	1.78	0.49
26:Y:180:LEU:O	26:Y:184:LYS:NZ	2.43	0.49
27:Z:25:ALA:O	27:Z:29:VAL:HG23	2.12	0.49
5:A:85:GLU:HG2	19:O:30:MET:HE3	1.95	0.49
5:A:527:LEU:O	5:A:531:ILE:HG13	2.12	0.49
5:A:1209:ASN:C	5:A:1209:ASN:ND2	2.69	0.49
7:C:49:HIS:HE1	7:C:68:GLY:HA2	1.78	0.49
18:N:453:LEU:HB3	18:N:551:LEU:HD11	1.95	0.49
18:N:788:PHE:CD1	18:N:791:LEU:HD12	2.48	0.49
24:W:738:LYS:HD3	24:W:738:LYS:N	2.27	0.49
25:X:246:ILE:HG13	25:X:247:LYS:N	2.27	0.49
25:X:289:ASN:HA	25:X:292:ILE:HG22	1.93	0.49
26:Y:175:GLN:HE21	26:Y:179:ARG:HG2	1.77	0.49
7:C:114:ASP:OD1	7:C:116:HIS:HD2	1.96	0.49
15:K:354:ILE:HB	15:K:368:PHE:HB2	1.95	0.49
16:L:267:PRO:HG2	16:L:270:LYS:HD2	1.93	0.49
18:N:411:GLU:HG3	18:N:419:LEU:HD12	1.95	0.49
19:O:39:LYS:HD2	19:O:39:LYS:O	2.13	0.49
22:R:22:GLN:HA	22:R:25:ARG:HG2	1.93	0.49
22:R:338:ILE:HG13	22:R:340:GLU:H	1.78	0.49
24:W:531:ILE:HG12	24:W:537:ARG:HH21	1.78	0.49
29:b:50:GLN:NE2	29:b:52:PRO:O	2.38	0.49
7:C:54:LEU:HD11	7:C:70:MET:HE2	1.95	0.49
9:E:36:ASN:OD1	9:E:72:GLY:N	2.46	0.49
15:K:120:GLY:CA	22:R:191:ARG:HD2	2.42	0.49
18:N:533:TYR:HB2	18:N:608:PHE:HA	1.95	0.49
18:N:534:ILE:HG12	18:N:554:VAL:HA	1.95	0.49
22:R:108:LEU:HD11	22:R:139:LYS:HG2	1.95	0.49
22:R:294:LEU:O	22:R:298:SER:OG	2.24	0.49
30:c:490:TYR:HE1	30:c:540:LEU:HD21	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:z:325:GLN:O	36:z:337:LEU:HA	2.11	0.49
8:D:18:MET:HE1	8:D:39:CYS:HB2	1.93	0.49
22:R:78:GLN:HE21	22:R:109:LYS:HE2	1.78	0.49
30:c:538:ILE:O	30:c:541:LYS:HG2	2.13	0.49
36:z:107:ILE:HG13	36:z:110:ASP:HB3	1.94	0.49
5:A:572:GLU:HB3	5:A:614:MET:HB2	1.94	0.48
5:A:979:CYS:SG	5:A:1219:VAL:HG11	2.53	0.48
5:A:1131:ASP:O	5:A:1134:GLN:HG2	2.13	0.48
6:B:474:GLY:O	6:B:478:LEU:HD23	2.13	0.48
18:N:410:GLN:O	18:N:413:SER:OG	2.29	0.48
22:R:566:PRO:O	22:R:570:VAL:HG23	2.13	0.48
23:V:80:TRP:CD1	27:Z:100:GLU:HB3	2.47	0.48
31:d:141:ASP:OD1	31:d:141:ASP:N	2.44	0.48
33:m:758:ARG:NH1	33:m:797:ASN:HB2	2.28	0.48
5:A:862:LEU:HD23	5:A:866:LEU:HD23	1.95	0.48
5:A:1548:SER:O	5:A:1552:GLN:HG2	2.13	0.48
20:P:122:ARG:HG3	20:P:228:GLU:OE2	2.13	0.48
22:R:304:ARG:HE	22:R:335:ILE:HD13	1.78	0.48
22:R:583:LEU:HD12	22:R:595:LEU:HD22	1.96	0.48
25:X:534:PHE:HA	25:X:537:TYR:HD2	1.78	0.48
25:X:574:ASP:HA	25:X:577:GLU:CD	2.38	0.48
26:Y:152:ARG:O	26:Y:155:TRP:NE1	2.44	0.48
36:z:366:TYR:HE2	36:z:371:TYR:HB2	1.78	0.48
6:B:905:THR:O	6:B:905:THR:HG22	2.13	0.48
8:D:9:HIS:O	8:D:12:GLN:HG2	2.12	0.48
18:N:73:ASN:O	18:N:77:LEU:HG	2.12	0.48
18:N:504:GLN:HA	18:N:583:ILE:O	2.13	0.48
22:R:61:ASP:O	22:R:64:ARG:HG2	2.14	0.48
22:R:306:LEU:O	22:R:309:GLU:HG3	2.12	0.48
23:S:104:ALA:HB1	23:V:100:GLU:HG2	1.95	0.48
25:X:496:ILE:O	25:X:500:ARG:HG2	2.13	0.48
27:Z:139:VAL:HA	27:Z:142:LYS:HG2	1.94	0.48
29:b:51:ASP:HB2	29:b:52:PRO:HD3	1.95	0.48
35:y:28:GLU:HG2	35:y:29:PRO:CD	2.43	0.48
36:z:163:LYS:HD2	36:z:166:LEU:HD11	1.95	0.48
36:z:241:VAL:HG21	36:z:300:PHE:HD1	1.77	0.48
5:A:843:ARG:O	5:A:844:ARG:C	2.56	0.48
6:B:699:ILE:HG13	6:B:808:VAL:HG22	1.96	0.48
6:B:849:GLU:OE2	6:B:851:HIS:NE2	2.43	0.48
11:G:61:ASP:HB3	11:G:65:ASN:HB2	1.96	0.48
17:M:202:ASN:C	17:M:203:MET:HE2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:P:122:ARG:CB	20:P:124:MET:HE1	2.43	0.48
23:V:112:LEU:O	23:V:115:ILE:HG22	2.12	0.48
30:c:588:PHE:HD2	30:c:596:LEU:HD21	1.79	0.48
35:y:163:TYR:HB3	36:z:327:ILE:HD12	1.95	0.48
36:z:317:VAL:HG23	36:z:354:ALA:HB2	1.94	0.48
4:6:59:G:N2	4:6:62:C:OP2	2.39	0.48
5:A:81:ASP:OD1	5:A:507:SER:OG	2.25	0.48
5:A:324:ARG:HG3	6:B:892:ILE:HG13	1.96	0.48
5:A:1148:VAL:HG12	5:A:1172:VAL:HG11	1.96	0.48
5:A:1654:LEU:HD21	5:A:1656:LEU:HG	1.95	0.48
18:N:14:TYR:O	18:N:18:ASN:ND2	2.47	0.48
18:N:58:PHE:HA	18:N:62:LEU:HG	1.96	0.48
18:N:209:TYR:OH	18:N:218:LYS:HD3	2.13	0.48
23:T:5:ILE:HA	23:U:88:PHE:CD1	2.48	0.48
31:d:42:ILE:HD11	31:d:146:PRO:HA	1.95	0.48
36:z:231:ASN:HD22	36:z:270:LEU:HD12	1.78	0.48
4:6:23:A:N6	20:P:127:GLU:OE1	2.47	0.48
5:A:109:TYR:CD1	5:A:146:ALA:HA	2.49	0.48
5:A:1432:LEU:HD12	5:A:1447:PHE:CZ	2.45	0.48
20:P:85:ASP:CG	20:P:88:LYS:HB3	2.38	0.48
24:W:251:GLU:HB2	24:W:255:LYS:NZ	2.29	0.48
24:W:706:THR:O	24:W:709:LYS:HB2	2.13	0.48
24:W:734:ILE:HG23	24:W:738:LYS:HE2	1.96	0.48
35:y:179:TYR:CZ	36:z:217:GLU:HG3	2.48	0.48
5:A:1490:GLN:NE2	5:A:1492:ASN:HD22	2.11	0.48
7:C:291:LYS:HD2	9:E:109:PRO:HG3	1.95	0.48
7:C:319:HIS:HB2	7:C:324:ILE:HB	1.95	0.48
14:J:51:ASP:OD1	14:J:52:GLY:N	2.47	0.48
17:M:110:ASP:N	17:M:110:ASP:OD1	2.44	0.48
23:T:109:ASP:O	23:T:113:ARG:HG3	2.13	0.48
24:W:674:LYS:O	24:W:678:ARG:HG3	2.14	0.48
30:c:527:LEU:HD11	30:c:572:LEU:HD12	1.96	0.48
30:c:579:ARG:HA	30:c:582:ARG:CZ	2.43	0.48
35:y:138:ASP:OD2	36:z:417:MET:HE3	2.14	0.48
36:z:553:PHE:HB2	36:z:555:ILE:HG12	1.95	0.48
5:A:1315:CYS:HA	5:A:1318:LYS:HG2	1.96	0.48
16:L:204:MET:HE1	17:M:54:PHE:CE2	2.47	0.48
17:M:75:ARG:HH22	17:M:124:LEU:HD23	1.78	0.48
18:N:90:TYR:OH	18:N:1224:ARG:NH2	2.33	0.48
24:W:65:GLU:OE2	24:W:89:ARG:NH2	2.46	0.48
25:X:624:ARG:O	25:X:627:ILE:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:c:493:ILE:HD12	30:c:496:TYR:HD2	1.78	0.48
31:d:70:ASP:OD1	31:d:70:ASP:N	2.46	0.48
31:d:88:LEU:HD11	31:d:102:PHE:CD2	2.49	0.48
36:z:153:LEU:HD13	36:z:382:ILE:HA	1.95	0.48
4:6:13:A:O2'	4:6:14:C:OP1	2.27	0.48
4:6:44:A:H2'	4:6:45:U:C6	2.49	0.48
5:A:80:ALA:CB	19:O:103:LEU:HD23	2.43	0.48
6:B:105:ILE:HD11	15:K:199:LEU:CD2	2.44	0.48
6:B:498:THR:HG22	6:B:499:VAL:H	1.79	0.48
6:B:786:TRP:HZ2	33:m:719:ARG:HH21	1.62	0.48
11:G:73:GLU:OE2	11:G:94:ARG:HB3	2.14	0.48
16:L:185:ARG:HA	16:L:201:ILE:HG22	1.96	0.48
17:M:145:LYS:O	17:M:148:GLU:HG3	2.14	0.48
22:R:101:SER:OG	22:R:133:GLN:OE1	2.25	0.48
30:c:586:ASN:HA	30:c:589:THR:HG22	1.95	0.48
35:y:138:ASP:OD1	35:y:141:GLY:HA3	2.14	0.48
2:2:24:A:H5'	2:2:25:G:H5"	1.96	0.48
10:F:3:LEU:HD13	11:G:61:ASP:HB2	1.95	0.48
18:N:321:LEU:HD13	18:N:338:ILE:HA	1.96	0.48
18:N:830:LEU:HB3	18:N:925:LEU:HD21	1.95	0.48
18:N:850:SER:O	18:N:853:THR:OG1	2.29	0.48
24:W:207:ILE:HG12	24:W:209:ILE:N	2.29	0.48
25:X:503:TYR:HA	25:X:506:VAL:HG22	1.94	0.48
25:X:513:THR:H	25:X:544:PHE:HZ	1.61	0.48
25:X:703:TRP:NE1	25:X:724:LYS:HE2	2.28	0.48
26:Y:153:LEU:HD22	31:d:131:ARG:NH1	2.28	0.48
31:d:7:GLN:CD	31:d:12:LYS:HZ3	2.22	0.48
36:z:383:LEU:O	36:z:383:LEU:HD23	2.13	0.48
6:B:498:THR:HG22	6:B:499:VAL:N	2.29	0.47
8:D:17:THR:CG2	8:D:27:ARG:HD2	2.40	0.47
18:N:727:TYR:HE1	18:N:756:VAL:HG12	1.78	0.47
22:R:9:LYS:HD2	36:z:271:VAL:HG22	1.96	0.47
22:R:299:THR:O	22:R:303:LYS:HG2	2.14	0.47
23:U:361:GLU:HB3	23:U:364:SER:OG	2.14	0.47
23:V:66:ALA:HB1	27:Z:60:GLU:HG3	1.95	0.47
24:W:682:LEU:HD11	27:Z:120:PHE:CZ	2.49	0.47
25:X:178:ILE:HG22	25:X:181:TYR:HE1	1.79	0.47
30:c:582:ARG:HA	30:c:585:ILE:HG12	1.96	0.47
31:d:10:LEU:HD12	31:d:131:ARG:HD3	1.95	0.47
5:A:1161:ARG:HD3	5:A:1368:LYS:NZ	2.30	0.47
6:B:814:GLN:HA	6:B:817:ARG:HD3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:963:THR:OG1	6:B:984:LEU:OXT	2.32	0.47
9:E:118:ALA:N	17:M:32:TYR:OH	2.44	0.47
17:M:75:ARG:HH12	17:M:124:LEU:HD21	1.79	0.47
18:N:788:PHE:HZ	18:N:953:GLY:HA3	1.79	0.47
23:U:264:VAL:HA	23:U:274:GLU:HA	1.95	0.47
23:V:87:GLN:NE2	34:r:239:UNK:H	2.10	0.47
24:W:682:LEU:HG	24:W:686:SER:HB3	1.96	0.47
6:B:165:THR:OG1	6:B:166:HIS:ND1	2.44	0.47
18:N:942:LEU:HB3	18:N:969:LYS:HD2	1.95	0.47
20:P:261:ARG:O	20:P:264:GLU:HG3	2.14	0.47
22:R:83:GLN:HA	24:W:256:ILE:HG21	1.95	0.47
22:R:259:ARG:O	22:R:263:ILE:HG23	2.13	0.47
22:R:281:LYS:O	22:R:284:THR:OG1	2.26	0.47
23:T:112:LEU:HA	23:T:115:ILE:HG12	1.96	0.47
23:U:188:THR:N	23:U:487:LEU:O	2.40	0.47
30:c:514:THR:OG1	30:c:516:SER:OG	2.27	0.47
5:A:862:LEU:O	5:A:866:LEU:HD23	2.14	0.47
8:D:68:PHE:HB3	9:E:70:LEU:HD13	1.96	0.47
14:J:27:VAL:HG12	14:J:28:TYR:O	2.14	0.47
16:L:232:PRO:HB2	16:L:234:LEU:CD1	2.45	0.47
25:X:608:SER:O	25:X:612:LEU:HD23	2.14	0.47
5:A:1406:SER:HA	5:A:1439:GLY:HA2	1.97	0.47
6:B:81:ALA:HA	6:B:84:VAL:HG12	1.96	0.47
7:C:45:GLN:OE1	7:C:335:PHE:CE1	2.68	0.47
13:I:29:GLU:OE1	13:I:29:GLU:N	2.47	0.47
18:N:480:LEU:HD23	18:N:608:PHE:O	2.15	0.47
21:Q:39:GLN:OE1	21:Q:39:GLN:HA	2.14	0.47
23:S:122:ARG:CD	23:V:118:LEU:HB2	2.44	0.47
25:X:549:ALA:O	25:X:553:TRP:CD1	2.68	0.47
36:z:224:ILE:HG13	36:z:255:LYS:HE2	1.96	0.47
6:B:490:MET:CG	6:B:579:ILE:HB	2.44	0.47
7:C:58:PHE:CZ	7:C:326:LEU:HB2	2.50	0.47
20:P:177:TYR:CE1	20:P:212:ILE:HG23	2.50	0.47
23:S:122:ARG:NH1	23:V:118:LEU:HD22	2.29	0.47
24:W:675:LEU:O	24:W:679:VAL:HG22	2.15	0.47
3:5:56:A:O2'	3:5:57:G:H5"	2.15	0.47
5:A:191:ASP:OD1	5:A:192:ASP:N	2.48	0.47
5:A:1099:ASP:N	5:A:1099:ASP:OD1	2.47	0.47
6:B:644:PHE:CD2	6:B:675:ARG:HD2	2.49	0.47
6:B:867:ARG:HD2	6:B:897:PHE:HD1	1.80	0.47
10:F:20:LYS:HB2	10:F:64:ASN:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:G:11:GLU:C	11:G:12:LEU:HD12	2.40	0.47
12:H:31:PHE:HA	12:H:79:THR:OG1	2.14	0.47
15:K:338:SER:OG	15:K:380:ILE:HD12	2.15	0.47
15:K:398:TRP:CZ3	15:K:405:LYS:HB2	2.49	0.47
22:R:184:TYR:HB3	26:Y:130:TYR:CE2	2.49	0.47
22:R:278:GLU:O	22:R:282:GLU:HG2	2.14	0.47
23:U:110:ALA:O	23:U:114:VAL:HG23	2.15	0.47
23:V:80:TRP:HD1	27:Z:100:GLU:HB3	1.79	0.47
24:W:245:ASN:HB2	24:W:248:GLU:CG	2.45	0.47
24:W:549:SER:OG	24:W:562:LYS:HB2	2.14	0.47
25:X:382:PRO:HA	25:X:389:LEU:HD21	1.96	0.47
5:A:1358:LEU:HD22	29:b:21:MET:HE1	1.96	0.47
17:M:165:GLU:O	17:M:168:GLN:NE2	2.48	0.47
18:N:737:ARG:HA	18:N:740:GLN:NE2	2.30	0.47
18:N:931:PHE:HD1	18:N:940:GLN:HG3	1.79	0.47
23:S:38:ASP:N	23:S:43:GLN:O	2.48	0.47
23:S:62:ARG:HD3	23:T:9:THR:H	1.80	0.47
24:W:518:GLU:O	24:W:522:LEU:HG	2.15	0.47
25:X:350:ASN:HD22	25:X:384:LEU:C	2.23	0.47
5:A:220:ASP:OD1	5:A:259:ARG:NH2	2.42	0.47
5:A:531:ILE:HG22	5:A:531:ILE:O	2.15	0.47
5:A:1214:MET:HE3	5:A:1214:MET:HB2	1.86	0.47
15:K:467:SER:O	15:K:467:SER:OG	2.32	0.47
18:N:534:ILE:HG23	18:N:553:GLY:O	2.15	0.47
22:R:57:LYS:HA	24:W:221:TYR:CE2	2.50	0.47
22:R:84:LYS:HZ1	22:R:87:ALA:HB3	1.77	0.47
23:T:127:GLU:O	23:T:131:LYS:HG2	2.14	0.47
24:W:253:ASP:OD1	24:W:257:ILE:HD11	2.15	0.47
24:W:627:TYR:O	24:W:628:SER:C	2.57	0.47
5:A:1460:TRP:CD1	5:A:1460:TRP:H	2.32	0.47
5:A:1703:TYR:O	5:A:1707:LYS:HG2	2.15	0.47
10:F:21:ASN:OD1	10:F:23:THR:HG23	2.15	0.47
10:F:50:ARG:NH1	10:F:50:ARG:HG2	2.30	0.47
11:G:9:ARG:O	11:G:9:ARG:HD3	2.15	0.47
18:N:8:LYS:HG3	18:N:51:LEU:HD22	1.97	0.47
19:O:107:GLN:HE21	19:O:110:GLU:HG3	1.79	0.47
22:R:444:GLU:HA	22:R:447:ILE:HG22	1.97	0.47
23:U:14:VAL:HG12	23:U:51:VAL:HB	1.97	0.47
30:c:452:GLU:OE1	30:c:500:ARG:NH2	2.48	0.47
30:c:480:SER:HA	30:c:483:GLU:HG2	1.96	0.47
30:c:509:ALA:HB2	30:c:543:MET:HG3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
36:z:163:LYS:HD3	36:z:190:PHE:CD1	2.50	0.47
36:z:210:LEU:HD23	36:z:363:PHE:CD1	2.50	0.47
36:z:574:LEU:HD21	36:z:639:LEU:HA	1.97	0.47
4:6:6:U:O2'	4:6:7:C:O5'	2.30	0.46
5:A:688:SER:O	5:A:691:VAL:HG22	2.15	0.46
5:A:1400:GLU:O	5:A:1404:ILE:HG12	2.14	0.46
6:B:628:TYR:O	6:B:631:SER:OG	2.31	0.46
6:B:813:GLU:HG2	6:B:815:ILE:H	1.79	0.46
7:C:46:MET:SD	9:E:101:ALA:HB2	2.55	0.46
18:N:1184:THR:HG22	18:N:1214:LEU:HD12	1.97	0.46
22:R:143:LYS:HE2	22:R:143:LYS:HB2	1.79	0.46
24:W:524:LYS:O	24:W:527:ARG:NE	2.48	0.46
25:X:246:ILE:HA	25:X:256:LEU:HD12	1.96	0.46
2:2:30:A:C6	35:y:39:TRP:CE2	3.03	0.46
5:A:88:ARG:HG2	5:A:92:LYS:HE3	1.97	0.46
6:B:460:LYS:HD2	6:B:460:LYS:HA	1.73	0.46
14:J:48:GLU:HG2	14:J:54:LYS:HE3	1.96	0.46
16:L:235:HIS:O	22:R:136:ARG:HG3	2.15	0.46
17:M:226:TYR:HB3	20:P:200:ASP:OD1	2.15	0.46
22:R:249:LYS:O	22:R:253:ARG:NE	2.46	0.46
23:S:79:GLU:OE2	23:T:68:SER:HB2	2.15	0.46
25:X:179:GLU:O	25:X:182:ILE:HG22	2.15	0.46
33:m:753:GLN:CD	33:m:754:ALA:H	2.23	0.46
36:z:36:TYR:CZ	36:z:40:GLN:HG3	2.50	0.46
36:z:434:ASN:OD1	36:z:435:LEU:N	2.48	0.46
3:5:100:U:H4'	3:5:101:U:H5'	1.97	0.46
4:6:86:A:H2'	4:6:87:G:C8	2.50	0.46
5:A:122:LYS:NZ	5:A:152:GLU:O	2.40	0.46
5:A:1075:ILE:HA	5:A:1185:ARG:HG2	1.96	0.46
6:B:697:ASN:HA	6:B:809:VAL:O	2.15	0.46
7:C:144:LEU:HG	7:C:146:VAL:H	1.79	0.46
17:M:31:SER:O	17:M:32:TYR:CD1	2.68	0.46
21:Q:67:THR:OG1	21:Q:68:GLN:OE1	2.31	0.46
24:W:605:LYS:HA	24:W:608:ILE:HG22	1.97	0.46
25:X:604:LYS:HE2	25:X:606:LYS:HB2	1.97	0.46
35:y:120:ASP:HB2	36:z:425:LEU:HD11	1.98	0.46
36:z:621:GLU:HG2	36:z:626:ILE:HG13	1.96	0.46
5:A:162:ILE:HG12	5:A:449:LEU:HD23	1.95	0.46
6:B:113:ARG:HG3	6:B:113:ARG:HH11	1.81	0.46
8:D:72:PRO:HG2	8:D:75:LEU:HD13	1.98	0.46
15:K:173:PRO:HA	15:K:431:LYS:HE3	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:18:ILE:O	24:W:15:GLU:HG3	2.15	0.46
22:R:289:GLN:NE2	25:X:538:GLU:HB2	2.30	0.46
23:V:112:LEU:HG	24:W:600:CYS:HB2	1.97	0.46
24:W:198:LYS:O	24:W:201:GLU:HG3	2.16	0.46
24:W:682:LEU:HD12	24:W:682:LEU:HA	1.64	0.46
25:X:97:CYS:SG	25:X:100:ARG:NH2	2.88	0.46
25:X:624:ARG:HD3	25:X:628:TYR:OH	2.15	0.46
25:X:705:GLU:OE2	25:X:709:ARG:NH2	2.49	0.46
26:Y:209:GLN:OE1	26:Y:213:SER:HB3	2.15	0.46
36:z:128:LEU:HB3	36:z:393:PHE:CE1	2.51	0.46
36:z:236:PRO:HG3	36:z:268:GLN:HE22	1.81	0.46
36:z:499:PHE:HD2	36:z:512:VAL:HG22	1.80	0.46
5:A:831:ALA:O	5:A:835:THR:HG23	2.16	0.46
18:N:70:MET:HE2	18:N:75:ILE:HA	1.98	0.46
20:P:160:ARG:CZ	20:P:165:GLY:H	2.28	0.46
22:R:121:ASN:OD1	24:W:236:TYR:HB3	2.15	0.46
23:T:70:PRO:HG2	27:Z:80:TYR:HD2	1.80	0.46
23:U:304:HIS:HB2	23:U:309:TYR:HD2	1.81	0.46
5:A:59:ARG:HG2	5:A:59:ARG:HH11	1.80	0.46
9:E:68:VAL:HG12	9:E:70:LEU:HD22	1.98	0.46
15:K:106:ILE:HG12	15:K:109:GLN:HG2	1.96	0.46
22:R:196:ARG:HA	22:R:199:VAL:HG12	1.98	0.46
23:S:62:ARG:NH1	23:S:68:SER:HB3	2.30	0.46
23:T:68:SER:OG	23:T:69:LEU:N	2.48	0.46
23:U:28:ILE:O	23:U:32:ILE:HG12	2.15	0.46
26:Y:131:ASP:N	26:Y:131:ASP:OD1	2.48	0.46
30:c:449:MET:O	30:c:449:MET:HG3	2.15	0.46
35:y:45:ASP:HB3	35:y:49:ARG:N	2.31	0.46
35:y:120:ASP:O	35:y:121:THR:HG23	2.14	0.46
5:A:411:PHE:HB2	6:B:391:LYS:HD2	1.97	0.46
5:A:1506:GLU:CD	5:A:1506:GLU:H	2.23	0.46
6:B:387:GLU:O	6:B:391:LYS:HG3	2.16	0.46
8:D:32:GLU:HB2	8:D:40:GLN:HG3	1.96	0.46
12:H:74:LYS:HG3	13:I:70:VAL:HG23	1.98	0.46
16:L:289:ALA:HA	24:W:75:LEU:HD22	1.98	0.46
22:R:302:ASP:O	22:R:306:LEU:HD23	2.16	0.46
23:S:69:LEU:HD23	23:U:80:TRP:CD1	2.51	0.46
25:X:289:ASN:O	25:X:292:ILE:HG22	2.15	0.46
25:X:573:ARG:O	25:X:577:GLU:OE1	2.34	0.46
25:X:606:LYS:HZ2	34:r:287:UNK:C	2.29	0.46
36:z:464:CYS:SG	36:z:568:LYS:HD2	2.55	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:298:PHE:HE1	5:A:479:MET:HG2	1.80	0.46
5:A:1135:ARG:HD2	21:Q:223:ARG:CZ	2.46	0.46
5:A:1282:LYS:NZ	35:y:214:ASP:OD2	2.37	0.46
10:F:50:ARG:HG2	10:F:50:ARG:HH11	1.79	0.46
11:G:51:LYS:HD3	11:G:75:TRP:HB3	1.98	0.46
11:G:54:LEU:HD23	11:G:72:LYS:O	2.16	0.46
12:H:28:ILE:HD12	12:H:53:LEU:HD11	1.97	0.46
15:K:267:ARG:HG3	15:K:291:THR:HG22	1.97	0.46
20:P:117:CYS:HB2	20:P:120:PHE:HB2	1.97	0.46
25:X:172:GLN:NE2	25:X:173:VAL:HG13	2.31	0.46
36:z:302:THR:HB	36:z:324:LYS:NZ	2.31	0.46
36:z:599:TRP:O	36:z:627:PHE:HA	2.16	0.46
6:B:700:THR:HG23	6:B:806:MET:HB2	1.98	0.46
6:B:938:ALA:HB3	6:B:943:LEU:HD23	1.96	0.46
7:C:38:ASP:HB3	7:C:80:PHE:CE1	2.51	0.46
9:E:9:LEU:HA	9:E:12:HIS:HD2	1.80	0.46
15:K:96:ILE:HG21	22:R:228:LEU:HB3	1.97	0.46
20:P:117:CYS:SG	20:P:135:HIS:HD2	2.22	0.46
22:R:57:LYS:HA	24:W:221:TYR:HE2	1.80	0.46
22:R:510:TYR:CE2	22:R:526:ILE:HG21	2.50	0.46
23:U:378:VAL:HA	23:U:394:THR:HA	1.98	0.46
25:X:517:VAL:HG21	25:X:544:PHE:HE2	1.80	0.46
25:X:523:LEU:O	25:X:526:GLU:HG2	2.16	0.46
30:c:476:ARG:NH1	30:c:479:ARG:HH11	2.13	0.46
31:d:56:ASP:HB3	31:d:101:GLN:NE2	2.31	0.46
36:z:241:VAL:CG2	36:z:300:PHE:HA	2.46	0.46
36:z:571:LYS:HE2	36:z:638:TRP:CD2	2.51	0.46
36:z:580:ASN:O	36:z:615:MET:HG2	2.15	0.46
7:C:121:ASP:OD2	7:C:124:SER:OG	2.34	0.46
15:K:226:ASP:OD1	15:K:228:MET:HE2	2.16	0.46
15:K:270:VAL:HG11	15:K:284:VAL:HG13	1.97	0.46
17:M:111:ILE:O	17:M:114:GLU:HG3	2.16	0.46
17:M:143:LEU:HD21	20:P:263:GLU:O	2.16	0.46
24:W:697:ILE:HG23	24:W:701:TRP:CD1	2.51	0.46
31:d:45:ARG:HB3	31:d:53:GLN:HB3	1.98	0.46
35:y:154:ASP:OD1	35:y:154:ASP:N	2.49	0.46
2:2:14:C:H2'	4:6:76:C:C4	2.51	0.45
5:A:1556:ARG:HG2	5:A:1592:THR:HG23	1.98	0.45
6:B:382:VAL:HG22	6:B:386:LEU:HD12	1.98	0.45
7:C:77:TRP:HH2	9:E:99:GLY:HA3	1.81	0.45
8:D:17:THR:OG1	8:D:70:ILE:HB	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:309:MET:HA	15:K:333:THR:OG1	2.15	0.45
19:O:6:THR:HG21	19:O:8:ARG:NH1	2.32	0.45
20:P:183:PRO:HD2	20:P:187:ILE:HG22	1.97	0.45
21:Q:54:ARG:HE	21:Q:54:ARG:HB2	1.59	0.45
22:R:412:LEU:HD13	22:R:443:PHE:HE1	1.81	0.45
23:S:5:ILE:HD11	23:S:39:PRO:HG3	1.97	0.45
23:V:21:ASN:HB3	23:V:23:TYR:CE2	2.51	0.45
23:V:98:LYS:HZ1	24:W:530:VAL:HG13	1.81	0.45
28:a:131:SER:O	28:a:135:LYS:HG3	2.16	0.45
35:y:143:LYS:HA	35:y:146:LYS:HD2	1.98	0.45
4:6:57:C:H4'	5:A:560:LYS:NZ	2.32	0.45
5:A:284:THR:OG1	5:A:347:ALA:O	2.34	0.45
5:A:329:THR:HG23	29:b:4:ASN:H	1.81	0.45
6:B:490:MET:HG3	6:B:579:ILE:HB	1.98	0.45
7:C:188:GLN:OE1	7:C:190:THR:HG22	2.17	0.45
18:N:45:ALA:O	18:N:48:VAL:HG12	2.16	0.45
23:T:73:LEU:HA	23:T:76:PHE:CD2	2.45	0.45
23:T:87:GLN:HE21	23:T:91:ARG:HG2	1.81	0.45
23:T:122:ARG:CZ	23:U:118:LEU:HD12	2.46	0.45
24:W:48:TRP:HA	24:W:52:ILE:HB	1.97	0.45
24:W:537:ARG:O	24:W:539:SER:N	2.49	0.45
25:X:183:GLU:O	25:X:187:LYS:HG2	2.16	0.45
29:b:135:LEU:O	29:b:138:GLU:HG3	2.16	0.45
31:d:18:TYR:HB3	31:d:21:HIS:HB2	1.98	0.45
31:d:147:LEU:HD12	31:d:147:LEU:HA	1.66	0.45
36:z:157:LEU:HD22	36:z:390:LEU:HG	1.97	0.45
36:z:492:ALA:HB2	36:z:530:TYR:CD2	2.48	0.45
2:2:12:G:H1	4:6:77:G:H21	1.65	0.45
5:A:1299:ARG:HD3	5:A:1397:GLN:O	2.16	0.45
5:A:1479:TRP:CD1	5:A:1479:TRP:H	2.34	0.45
18:N:193:ASN:OD1	18:N:194:LEU:N	2.49	0.45
18:N:668:ARG:NH1	18:N:720:PRO:HA	2.32	0.45
23:T:73:LEU:O	23:T:76:PHE:HB2	2.17	0.45
5:A:969:GLU:HB3	5:A:973:LEU:HD22	1.98	0.45
11:G:90:ILE:HG13	11:G:92:LYS:NZ	2.32	0.45
11:G:97:SER:OG	11:G:98:LYS:N	2.49	0.45
13:I:12:LEU:HD22	13:I:37:VAL:HG21	1.96	0.45
15:K:405:LYS:HD3	15:K:408:GLU:HG3	1.97	0.45
18:N:665:ILE:HD11	18:N:740:GLN:HG2	1.98	0.45
19:O:59:TYR:CE1	28:a:145:SER:HB3	2.52	0.45
20:P:68:GLY:O	20:P:81:GLY:CA	2.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:51:PHE:HA	22:R:54:ARG:HG2	1.98	0.45
23:S:85:LEU:HA	23:S:88:PHE:HD2	1.82	0.45
23:U:83:VAL:HG22	23:U:87:GLN:NE2	2.31	0.45
23:V:3:CYS:HA	23:V:22:VAL:HG11	1.98	0.45
30:c:475:SER:OG	30:c:476:ARG:N	2.50	0.45
36:z:540:LEU:O	36:z:543:ARG:HG2	2.17	0.45
5:A:109:TYR:HD2	5:A:529:LEU:HD12	1.82	0.45
5:A:312:TRP:HB3	5:A:1161:ARG:NH1	2.31	0.45
5:A:389:ASP:N	5:A:389:ASP:OD1	2.48	0.45
6:B:707:GLU:HB2	6:B:710:ILE:HD12	1.98	0.45
7:C:152:THR:OG1	7:C:160:MET:SD	2.75	0.45
17:M:75:ARG:HG3	28:a:85:ILE:HD11	1.97	0.45
18:N:798:HIS:NE2	18:N:927:GLU:OE1	2.49	0.45
23:S:117:ARG:O	23:S:121:GLU:HG2	2.17	0.45
24:W:240:GLU:HA	24:W:243:ARG:HG3	1.99	0.45
24:W:264:ASN:HA	24:W:267:GLU:HG2	1.97	0.45
24:W:507:ASP:HA	24:W:510:ARG:NE	2.32	0.45
24:W:507:ASP:HB3	24:W:508:ARG:HH21	1.82	0.45
25:X:219:TRP:HE1	25:X:256:LEU:HD22	1.82	0.45
29:b:83:SER:HB3	29:b:116:THR:HG22	1.98	0.45
30:c:526:ARG:NH2	30:c:570:HIS:O	2.50	0.45
36:z:561:LEU:HD12	36:z:562:PRO:HD2	1.98	0.45
5:A:386:HIS:CE1	6:B:311:ARG:HG3	2.52	0.45
5:A:1272:LEU:HA	5:A:1272:LEU:HD23	1.81	0.45
5:A:1660:LYS:HZ1	5:A:1681:THR:N	2.15	0.45
6:B:271:LYS:HG2	40:B:1001:GTP:C6	2.52	0.45
11:G:109:VAL:HG22	13:I:64:LEU:HB3	1.99	0.45
13:I:50:GLU:OE1	13:I:50:GLU:N	2.43	0.45
17:M:32:TYR:CE2	28:a:102:GLU:OE1	2.70	0.45
18:N:587:LEU:O	18:N:589:PRO:HD3	2.17	0.45
20:P:106:THR:HG23	20:P:108:ALA:H	1.82	0.45
23:S:102:SER:OG	24:W:622:GLU:OE2	2.27	0.45
29:b:122:ALA:HA	29:b:125:GLU:OE1	2.16	0.45
31:d:82:HIS:O	31:d:108:PRO:HA	2.16	0.45
3:5:101:U:H3	11:G:65:ASN:ND2	2.13	0.45
5:A:399:GLU:OE2	12:H:6:GLN:NE2	2.50	0.45
5:A:984:ASN:ND2	5:A:1243:ASN:OD1	2.50	0.45
5:A:1295:MET:HE2	5:A:1393:TYR:HB2	1.99	0.45
6:B:183:HIS:O	6:B:187:ARG:HG2	2.17	0.45
18:N:48:VAL:O	18:N:52:LEU:HG	2.17	0.45
18:N:506:GLY:HA2	18:N:581:LYS:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:493:LEU:HA	22:R:496:ASN:ND2	2.32	0.45
23:U:21:ASN:HB3	23:U:23:TYR:CZ	2.52	0.45
25:X:277:PHE:HZ	25:X:300:PHE:CD2	2.35	0.45
25:X:524:LEU:HD11	25:X:529:TYR:HD2	1.82	0.45
25:X:673:LYS:HA	25:X:673:LYS:HD2	1.85	0.45
30:c:593:LEU:HB3	30:c:596:LEU:CD2	2.47	0.45
35:y:177:ILE:HG13	36:z:322:PHE:CE2	2.52	0.45
2:2:7:U:H2'	2:2:8:C:C6	2.51	0.45
3:5:15:C:H2'	3:5:16:A:C8	2.52	0.45
5:A:111:GLY:HA3	16:L:214:PRO:HD3	1.98	0.45
6:B:97:ASP:OD2	15:K:199:LEU:HA	2.17	0.45
6:B:490:MET:SD	6:B:566:LEU:HD11	2.57	0.45
6:B:689:PHE:HB2	6:B:698:ARG:HD2	1.99	0.45
7:C:53:VAL:HA	7:C:69:GLY:HA3	1.99	0.45
11:G:45:ILE:HD13	11:G:109:VAL:HG12	1.98	0.45
18:N:620:LYS:HE2	18:N:956:TRP:CD1	2.52	0.45
18:N:751:ARG:NH1	18:N:1208:SER:OG	2.50	0.45
18:N:859:ASP:OD1	18:N:860:ALA:N	2.50	0.45
22:R:507:TRP:CD2	22:R:530:LEU:HD13	2.52	0.45
23:S:17:ARG:NH2	23:S:48:GLU:O	2.42	0.45
23:S:38:ASP:OD2	23:S:41:THR:OG1	2.32	0.45
25:X:98:PHE:CD1	25:X:111:ILE:HG23	2.52	0.45
25:X:634:LYS:HA	25:X:634:LYS:HD2	1.85	0.45
28:a:144:PRO:O	28:a:145:SER:OG	2.32	0.45
30:c:576:ASP:HB3	30:c:603:TYR:CE1	2.51	0.45
30:c:585:ILE:HG13	30:c:586:ASN:N	2.32	0.45
31:d:7:GLN:O	31:d:150:ILE:HG12	2.17	0.45
31:d:34:LYS:HE2	31:d:154:ALA:HB3	1.98	0.45
4:6:57:C:H4'	5:A:560:LYS:HZ2	1.82	0.45
5:A:855:TYR:HB3	5:A:858:ASP:OD2	2.17	0.45
5:A:1093:ASP:OD1	5:A:1094:PHE:N	2.46	0.45
13:I:23:ARG:HD3	13:I:72:TRP:NE1	2.32	0.45
16:L:253:PRO:O	26:Y:212:TYR:OH	2.20	0.45
22:R:570:VAL:HA	22:R:573:ARG:HD2	1.99	0.45
23:S:76:PHE:HE1	23:T:72:LEU:HG	1.81	0.45
23:T:75:LEU:HD12	23:T:75:LEU:HA	1.72	0.45
24:W:92:THR:HG21	24:W:145:THR:HG21	1.98	0.45
24:W:260:GLY:O	24:W:264:ASN:ND2	2.50	0.45
27:Z:136:LYS:O	27:Z:139:VAL:HG12	2.17	0.45
28:a:97:PHE:O	28:a:101:GLN:HG3	2.16	0.45
33:m:750:ILE:HB	33:m:760:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:y:145:LEU:HD13	35:y:148:LEU:HD12	1.98	0.45
36:z:224:ILE:HG13	36:z:255:LYS:CE	2.47	0.45
5:A:1080:ARG:NH1	5:A:1083:GLU:OE1	2.40	0.45
6:B:857:LEU:O	6:B:861:TYR:HD1	2.00	0.45
13:I:34:LEU:H	13:I:34:LEU:HD23	1.82	0.45
19:O:51:GLN:HE21	28:a:157:TRP:CG	2.35	0.45
20:P:172:GLN:O	20:P:172:GLN:HG2	2.17	0.45
22:R:28:VAL:HG23	26:Y:197:ILE:O	2.17	0.45
22:R:303:LYS:O	22:R:307:GLN:HG2	2.17	0.45
23:T:122:ARG:O	23:T:126:ARG:HG2	2.17	0.45
24:W:537:ARG:HG2	24:W:538:PRO:HD2	1.98	0.45
36:z:162:LEU:HA	36:z:165:ILE:CG2	2.46	0.45
5:A:372:ASP:CG	5:A:374:ILE:HG22	2.43	0.44
5:A:1257:THR:HG23	5:A:1260:GLY:H	1.82	0.44
6:B:179:TYR:O	6:B:180:THR:OG1	2.28	0.44
7:C:46:MET:HB3	7:C:334:ILE:CG1	2.43	0.44
8:D:41:MET:HB2	8:D:59:VAL:HG22	1.98	0.44
17:M:150:ARG:O	17:M:150:ARG:HD3	2.16	0.44
18:N:378:ILE:HG13	18:N:379:ASN:N	2.33	0.44
18:N:825:SER:O	18:N:828:PRO:HD2	2.16	0.44
18:N:970:GLY:HA2	18:N:997:CYS:SG	2.58	0.44
22:R:54:ARG:NH2	24:W:192:ARG:NH2	2.65	0.44
22:R:58:GLU:HA	22:R:61:ASP:OD1	2.16	0.44
22:R:453:CYS:HB3	22:R:457:TYR:CE2	2.52	0.44
23:T:77:GLN:OE1	27:Z:74:ALA:HB3	2.17	0.44
23:T:114:VAL:O	23:T:118:LEU:HD23	2.17	0.44
25:X:277:PHE:HZ	25:X:300:PHE:HD2	1.65	0.44
30:c:519:TRP:N	30:c:519:TRP:CD1	2.84	0.44
31:d:112:LEU:HD23	31:d:112:LEU:O	2.17	0.44
36:z:230:ILE:HA	36:z:234:TYR:HD2	1.81	0.44
36:z:330:PRO:HG3	36:z:415:HIS:NE2	2.32	0.44
3:5:15:C:H2'	3:5:16:A:H8	1.82	0.44
5:A:1295:MET:SD	5:A:1354:MET:HE1	2.57	0.44
5:A:1553:ILE:HD11	35:y:58:GLY:H	1.80	0.44
5:A:1666:PRO:HD3	5:A:1741:ASN:ND2	2.32	0.44
5:A:1686:ILE:HG12	5:A:1725:VAL:HB	1.98	0.44
6:B:356:TRP:CG	6:B:357:GLY:H	2.35	0.44
6:B:632:ILE:HB	6:B:644:PHE:HB2	1.98	0.44
6:B:776:VAL:HA	6:B:779:TYR:CZ	2.52	0.44
6:B:959:GLU:O	6:B:961:VAL:HG23	2.17	0.44
7:C:61:SER:O	7:C:321:HIS:NE2	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:230:ASP:OD1	7:C:232:SER:N	2.50	0.44
22:R:249:LYS:HA	22:R:252:ILE:HG12	1.99	0.44
23:S:114:VAL:O	23:S:118:LEU:HG	2.18	0.44
23:T:72:LEU:HD23	23:T:76:PHE:HE2	1.82	0.44
25:X:285:MET:HG3	25:X:285:MET:O	2.17	0.44
25:X:589:LYS:NZ	25:X:623:ASP:O	2.48	0.44
25:X:703:TRP:HZ2	25:X:720:MET:CG	2.30	0.44
36:z:327:ILE:HG23	36:z:336:LYS:HG3	2.00	0.44
5:A:196:PRO:HD3	5:A:543:TYR:CE1	2.52	0.44
5:A:342:ARG:HD3	6:B:666:GLU:OE2	2.17	0.44
6:B:689:PHE:HB3	6:B:700:THR:HB	1.98	0.44
6:B:724:PRO:HG2	6:B:727:ARG:HG3	1.98	0.44
8:D:6:LYS:HD2	8:D:90:PRO:HG2	1.99	0.44
18:N:773:ARG:HG2	18:N:950:ARG:HA	2.00	0.44
22:R:569:VAL:HG13	22:R:602:PHE:CZ	2.51	0.44
23:S:34:GLU:OE2	23:S:35:THR:HG22	2.17	0.44
23:S:118:LEU:HD22	23:S:122:ARG:NH2	2.32	0.44
24:W:739:MET:HE3	27:Z:173:LEU:HD22	1.99	0.44
25:X:222:PHE:O	25:X:226:VAL:HG23	2.18	0.44
25:X:270:TYR:CE2	25:X:304:TRP:HB2	2.53	0.44
25:X:500:ARG:HH12	25:X:532:ASP:CG	2.24	0.44
25:X:537:TYR:O	25:X:541:VAL:HG13	2.17	0.44
25:X:554:ASN:O	25:X:557:LEU:HG	2.17	0.44
29:b:58:GLU:HA	29:b:61:ARG:HD2	1.99	0.44
36:z:486:SER:O	36:z:489:LYS:HG2	2.17	0.44
5:A:1095:LEU:HD22	5:A:1110:LEU:HD22	1.98	0.44
6:B:698:ARG:HB3	6:B:809:VAL:CG2	2.48	0.44
11:G:27:ALA:O	13:I:36:SER:OG	2.31	0.44
18:N:256:ARG:HD3	18:N:379:ASN:ND2	2.33	0.44
18:N:697:ILE:HD13	18:N:710:VAL:HG22	2.00	0.44
18:N:918:LEU:O	18:N:921:MET:HG2	2.16	0.44
23:U:90:LEU:HD12	23:U:90:LEU:HA	1.71	0.44
26:Y:202:ARG:O	26:Y:206:LEU:HD23	2.17	0.44
31:d:128:VAL:O	31:d:131:ARG:HG3	2.18	0.44
35:y:98:MET:HE3	35:y:102:ASP:HB3	1.98	0.44
5:A:170:MET:SD	5:A:213:MET:HE1	2.58	0.44
5:A:183:LYS:O	5:A:596:GLN:NE2	2.51	0.44
5:A:1402:GLU:CD	30:c:458:ARG:HH22	2.26	0.44
5:A:1639:HIS:O	5:A:1640:PRO:C	2.59	0.44
6:B:243:VAL:O	6:B:289:LYS:HE3	2.18	0.44
6:B:406:LYS:HE3	6:B:406:LYS:HB3	1.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:289:LYS:HB2	15:K:310:ASP:OD2	2.18	0.44
18:N:751:ARG:HH21	18:N:1178:VAL:H	1.66	0.44
20:P:99:ILE:HD11	20:P:137:LEU:HD13	1.99	0.44
22:R:127:PHE:O	22:R:131:VAL:HG22	2.18	0.44
27:Z:131:LEU:O	27:Z:135:GLU:HG2	2.17	0.44
30:c:552:GLY:C	30:c:554:LYS:H	2.25	0.44
35:y:144:MET:O	35:y:148:LEU:HG	2.17	0.44
5:A:754:LEU:HD12	5:A:755:PRO:HD2	1.99	0.44
6:B:748:ALA:HB2	6:B:781:LYS:HD3	2.00	0.44
6:B:810:LEU:HD12	6:B:817:ARG:NE	2.32	0.44
17:M:99:ALA:HB1	20:P:263:GLU:HA	1.99	0.44
19:O:134:CYS:HB3	19:O:139:CYS:H	1.83	0.44
20:P:57:ARG:HD3	20:P:58:PRO:HD2	1.99	0.44
20:P:62:MET:SD	20:P:64:PRO:HD3	2.58	0.44
22:R:207:TRP:CD1	22:R:234:LEU:HD11	2.53	0.44
22:R:360:ARG:O	22:R:364:ILE:HG12	2.17	0.44
25:X:154:TYR:O	25:X:158:ILE:HG22	2.17	0.44
25:X:216:TYR:O	25:X:220:LEU:HD23	2.17	0.44
25:X:427:LEU:HD11	25:X:472:PRO:HB2	2.00	0.44
25:X:439:LEU:HD21	25:X:489:LEU:CD2	2.47	0.44
27:Z:29:VAL:O	27:Z:33:LEU:HD23	2.17	0.44
30:c:573:PHE:HA	30:c:600:MET:HE1	1.99	0.44
31:d:90:MET:HE3	31:d:99:SER:O	2.17	0.44
36:z:414:VAL:HA	36:z:417:MET:HG2	1.99	0.44
4:6:32:G:C2	20:P:82:MET:CB	3.00	0.44
5:A:167:THR:HG21	5:A:228:TYR:OH	2.18	0.44
5:A:229:GLU:HB2	5:A:232:ALA:HA	1.99	0.44
5:A:300:PRO:O	5:A:301:LEU:HB3	2.16	0.44
6:B:603:LYS:HE2	6:B:644:PHE:CZ	2.52	0.44
6:B:778:GLU:OE2	6:B:779:TYR:HD2	2.01	0.44
7:C:116:HIS:ND1	7:C:132:LYS:HG2	2.32	0.44
11:G:77:GLU:OE2	11:G:92:LYS:NZ	2.40	0.44
13:I:23:ARG:HD3	13:I:72:TRP:CE2	2.52	0.44
20:P:114:SER:OG	20:P:134:LEU:HD11	2.18	0.44
22:R:324:ASP:OD1	22:R:324:ASP:N	2.46	0.44
23:U:298:VAL:HA	23:U:314:SER:HA	1.99	0.44
25:X:144:HIS:HB2	25:X:148:TRP:NE1	2.33	0.44
25:X:639:TYR:HA	34:r:287:UNK:H2	1.81	0.44
25:X:648:TYR:CE2	25:X:667:PHE:HB2	2.53	0.44
27:Z:24:ALA:O	27:Z:27:GLN:HG2	2.17	0.44
27:Z:139:VAL:HG21	31:d:35:GLU:OE2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:30:TYR:O	31:d:34:LYS:HG2	2.17	0.44
36:z:239:ILE:O	36:z:298:VAL:HA	2.18	0.44
5:A:1162:ASP:C	5:A:1162:ASP:OD1	2.60	0.44
6:B:182:THR:O	6:B:183:HIS:ND1	2.51	0.44
6:B:692:THR:OG1	6:B:697:ASN:HB2	2.17	0.44
11:G:70:ASN:N	11:G:97:SER:O	2.41	0.44
14:J:73:LEU:H	14:J:73:LEU:HD23	1.83	0.44
17:M:256:THR:HG23	17:M:259:SER:H	1.83	0.44
20:P:115:PHE:CZ	20:P:148:VAL:HG11	2.53	0.44
22:R:59:PHE:HD2	22:R:76:TYR:CD1	2.35	0.44
23:S:122:ARG:HG2	23:V:114:VAL:HG22	1.99	0.44
24:W:132:SER:HG	24:W:135:ARG:HH21	1.61	0.44
31:d:89:SER:OG	31:d:90:MET:N	2.50	0.44
5:A:470:TYR:OH	5:A:638:ARG:NH1	2.50	0.44
5:A:1346:LEU:HD23	5:A:1508:ILE:HG21	2.00	0.44
6:B:231:MET:HE1	6:B:257:HIS:ND1	2.31	0.44
6:B:847:MET:HB2	6:B:916:ASP:HB2	2.00	0.44
7:C:176:GLU:HG3	7:C:177:LYS:H	1.83	0.44
8:D:26:TYR:HD2	8:D:44:ILE:HG21	1.81	0.44
10:F:19:LEU:HD21	10:F:60:ILE:HD12	1.99	0.44
15:K:167:ARG:HA	15:K:167:ARG:HD2	1.75	0.44
17:M:282:GLN:OE1	17:M:282:GLN:HA	2.17	0.44
18:N:686:VAL:HG13	18:N:690:LEU:HD13	2.00	0.44
18:N:804:TYR:HE2	18:N:816:ARG:HH11	1.65	0.44
19:O:30:MET:CG	19:O:52:LEU:HD23	2.44	0.44
19:O:51:GLN:NE2	28:a:157:TRP:CG	2.86	0.44
20:P:85:ASP:OD2	20:P:88:LYS:N	2.51	0.44
20:P:181:ILE:HG13	20:P:183:PRO:HD3	1.99	0.44
22:R:111:ILE:HG21	22:R:127:PHE:CZ	2.52	0.44
23:S:59:VAL:HG22	23:S:60:ARG:H	1.83	0.44
31:d:10:LEU:CD2	31:d:147:LEU:HD11	2.48	0.44
36:z:138:GLU:HA	36:z:169:ARG:HH12	1.83	0.44
5:A:1666:PRO:HB3	5:A:1740:GLY:C	2.43	0.43
5:A:1686:ILE:HA	5:A:1725:VAL:O	2.18	0.43
6:B:657:ASP:O	6:B:661:LEU:HB2	2.18	0.43
15:K:226:ASP:OD1	15:K:228:MET:HG2	2.18	0.43
16:L:184:ILE:HD13	17:M:19:PHE:HE1	1.83	0.43
17:M:17:VAL:O	17:M:17:VAL:HG12	2.18	0.43
18:N:798:HIS:HD2	18:N:801:HIS:H	1.65	0.43
20:P:175:THR:HB	20:P:216:THR:HG23	2.00	0.43
22:R:77:GLY:HA3	22:R:93:PHE:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:192:ARG:CZ	24:W:192:ARG:HB2	2.47	0.43
24:W:537:ARG:HH11	24:W:577:PHE:HB2	1.83	0.43
29:b:71:ARG:NH1	29:b:130:LYS:HD3	2.33	0.43
30:c:527:LEU:HD13	30:c:572:LEU:HA	1.99	0.43
36:z:102:LEU:O	36:z:118:LYS:N	2.43	0.43
5:A:1603:SER:O	5:A:1605:LEU:N	2.51	0.43
6:B:967:PHE:HB2	6:B:971:MET:HG2	1.99	0.43
7:C:310:GLU:HB2	7:C:331:ASP:OD2	2.19	0.43
8:D:5:ILE:HG21	8:D:35:ASP:HA	2.00	0.43
16:L:252:PRO:HB2	26:Y:212:TYR:OH	2.18	0.43
18:N:204:ILE:HA	18:N:207:ILE:HD12	2.00	0.43
20:P:178:VAL:HG13	20:P:213:ALA:HB3	2.00	0.43
22:R:280:TYR:CD2	22:R:309:GLU:HG2	2.54	0.43
23:T:64:PRO:HG3	24:W:682:LEU:HD23	2.00	0.43
26:Y:153:LEU:HB3	31:d:131:ARG:NH2	2.34	0.43
29:b:17:ASN:OD1	29:b:17:ASN:N	2.49	0.43
5:A:106:LYS:HB3	20:P:74:TRP:CZ3	2.53	0.43
5:A:969:GLU:CB	5:A:973:LEU:HD22	2.48	0.43
5:A:1068:GLY:O	5:A:1113:ARG:NE	2.51	0.43
9:E:10:LEU:HD21	9:E:31:PHE:CE1	2.53	0.43
11:G:45:ILE:CD1	11:G:109:VAL:HG12	2.48	0.43
16:L:252:PRO:HB2	26:Y:212:TYR:CZ	2.53	0.43
18:N:313:ASP:OD1	18:N:353:LYS:NZ	2.51	0.43
18:N:528:PHE:CE2	18:N:623:LEU:HD21	2.54	0.43
18:N:863:LYS:O	18:N:867:GLU:HG3	2.19	0.43
19:O:120:ARG:NH1	19:O:142:CYS:HB3	2.28	0.43
20:P:86:PRO:CD	20:P:87:LEU:H	2.31	0.43
20:P:227:LYS:HE2	20:P:245:TRP:CE2	2.53	0.43
22:R:339:ARG:HA	22:R:342:TYR:HD2	1.83	0.43
30:c:497:GLU:OE1	30:c:497:GLU:N	2.38	0.43
36:z:302:THR:OG1	36:z:303:ASN:N	2.47	0.43
2:2:9:U:H2'	2:2:10:U:H6	1.82	0.43
5:A:116:LEU:HA	5:A:147:ILE:HD11	1.99	0.43
5:A:624:GLN:HG2	5:A:663:PHE:HB2	1.99	0.43
5:A:1037:ASN:ND2	5:A:1049:ASN:O	2.45	0.43
6:B:687:LYS:NZ	6:B:806:MET:HG3	2.33	0.43
6:B:788:THR:HA	6:B:798:ILE:HD12	2.00	0.43
16:L:202:ILE:HD11	17:M:35:MET:HE3	1.99	0.43
18:N:559:ILE:HG21	18:N:622:TRP:HE1	1.83	0.43
22:R:201:HIS:O	22:R:206:ASN:ND2	2.49	0.43
22:R:245:ILE:O	22:R:249:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:S:68:SER:O	23:S:72:LEU:N	2.36	0.43
23:T:80:TRP:HZ2	23:U:76:PHE:CD1	2.36	0.43
24:W:574:ASN:OD1	24:W:575:TYR:N	2.52	0.43
25:X:503:TYR:O	25:X:507:PHE:HD2	2.01	0.43
25:X:598:PHE:HA	25:X:601:LYS:HD3	2.00	0.43
27:Z:153:LYS:O	27:Z:156:GLN:HG2	2.18	0.43
28:a:148:GLU:OE1	28:a:148:GLU:HA	2.18	0.43
35:y:164:TYR:O	35:y:167:THR:OG1	2.18	0.43
4:6:15:U:N3	28:a:104:TYR:CE2	2.87	0.43
4:6:24:A:C4	5:A:100:ARG:HD2	2.53	0.43
5:A:511:ASP:OD1	5:A:512:TRP:N	2.51	0.43
5:A:811:GLN:HG2	5:A:1047:HIS:CB	2.49	0.43
5:A:1657:ALA:HB1	5:A:1661:TRP:HE1	1.82	0.43
10:F:25:VAL:HG12	10:F:45:MET:HA	1.99	0.43
15:K:362:GLY:O	16:L:118:GLN:NE2	2.41	0.43
16:L:285:ASN:OD1	16:L:286:ASP:N	2.51	0.43
18:N:266:LEU:HD11	18:N:419:LEU:HD11	1.99	0.43
18:N:655:CYS:C	18:N:660:ALA:HB2	2.44	0.43
20:P:277:GLN:HA	20:P:280:LEU:HG	2.01	0.43
22:R:51:PHE:O	22:R:55:LYS:HG2	2.18	0.43
22:R:130:ALA:HB1	22:R:140:LEU:HD13	1.99	0.43
22:R:158:ARG:HB3	26:Y:149:GLU:OE1	2.18	0.43
22:R:225:GLN:HA	22:R:228:LEU:HD12	2.01	0.43
23:S:105:LEU:HA	23:V:100:GLU:OE2	2.17	0.43
23:T:111:ALA:HA	23:T:114:VAL:HG12	1.99	0.43
23:U:403:TRP:CD1	23:U:410:LEU:HA	2.53	0.43
25:X:221:GLU:O	25:X:225:LEU:HG	2.17	0.43
26:Y:174:LYS:HD2	26:Y:174:LYS:C	2.44	0.43
30:c:532:THR:HG23	30:c:537:ARG:HH12	1.83	0.43
31:d:96:ASN:OD1	31:d:96:ASN:N	2.51	0.43
35:y:117:ASN:ND2	36:z:593:ILE:HG23	2.33	0.43
36:z:207:VAL:HG23	36:z:360:GLY:O	2.19	0.43
5:A:1549:GLY:O	5:A:1553:ILE:HG12	2.19	0.43
6:B:569:VAL:O	6:B:569:VAL:HG13	2.19	0.43
13:I:52:VAL:O	13:I:55:VAL:HG22	2.17	0.43
15:K:123:GLU:O	15:K:127:ARG:HD3	2.19	0.43
18:N:502:LYS:HE2	18:N:586:TYR:HE1	1.83	0.43
22:R:227:TYR:CD2	22:R:247:PHE:HD1	2.36	0.43
23:S:63:PRO:CB	24:W:693:LEU:HD21	2.44	0.43
23:T:91:ARG:NH2	23:U:86:GLU:OE2	2.50	0.43
23:U:59:VAL:HG12	23:V:4:SER:HA	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:W:12:THR:HB	24:W:163:LEU:HD21	2.01	0.43
24:W:536:ILE:O	24:W:537:ARG:HB2	2.18	0.43
25:X:683:ILE:HG13	25:X:684:TYR:N	2.32	0.43
25:X:726:SER:O	25:X:730:LYS:HG2	2.18	0.43
28:a:142:GLY:HA3	28:a:153:TYR:HA	2.01	0.43
30:c:476:ARG:HH12	30:c:479:ARG:HH11	1.67	0.43
5:A:540:HIS:HB2	5:A:550:THR:HG23	2.01	0.43
5:A:1640:PRO:HD2	5:A:1641:ARG:HH12	1.83	0.43
8:D:56:LEU:HD22	14:J:71:GLU:CD	2.44	0.43
10:F:17:ILE:HG12	10:F:68:TYR:CD1	2.53	0.43
11:G:74:MET:N	11:G:74:MET:SD	2.92	0.43
13:I:35:GLN:NE2	13:I:46:LEU:HD21	2.33	0.43
15:K:173:PRO:HG3	15:K:215:PRO:HA	2.00	0.43
16:L:103:TYR:HA	24:W:235:PHE:HE2	1.82	0.43
18:N:326:GLN:HG3	25:X:271:GLU:HG2	2.00	0.43
22:R:188:GLU:O	22:R:191:ARG:HG2	2.19	0.43
22:R:255:LYS:HG2	22:R:257:TYR:OH	2.18	0.43
24:W:170:LEU:O	26:Y:197:ILE:HD13	2.18	0.43
26:Y:165:VAL:O	26:Y:169:VAL:HG23	2.18	0.43
31:d:90:MET:O	31:d:116:HIS:HE1	2.02	0.43
36:z:393:PHE:CE2	36:z:397:LEU:HD11	2.54	0.43
6:B:296:GLU:O	6:B:300:ASN:ND2	2.39	0.43
6:B:329:CYS:SG	6:B:442:PHE:HB2	2.58	0.43
6:B:466:ILE:HG12	6:B:590:ILE:O	2.19	0.43
6:B:702:VAL:HG13	6:B:804:ARG:HE	1.84	0.43
6:B:805:LEU:O	6:B:806:MET:HE2	2.19	0.43
15:K:248:SER:HB2	15:K:267:ARG:HB3	2.00	0.43
18:N:1138:LEU:HG	18:N:1183:PHE:HZ	1.83	0.43
19:O:30:MET:SD	19:O:52:LEU:HD23	2.58	0.43
22:R:54:ARG:O	22:R:57:LYS:HG2	2.18	0.43
22:R:88:ARG:HB3	24:W:225:ILE:HG12	2.00	0.43
24:W:689:GLN:HB2	27:Z:124:LEU:HD11	1.99	0.43
24:W:702:LYS:O	24:W:706:THR:HG23	2.19	0.43
31:d:17:LEU:HD11	31:d:29:PHE:HD2	1.82	0.43
31:d:90:MET:O	31:d:116:HIS:CE1	2.72	0.43
33:m:720:GLU:O	33:m:724:GLU:HG3	2.19	0.43
4:6:5:U:H1'	4:6:9:G:N2	2.34	0.43
4:6:75:G:C8	26:Y:200:ARG:NH1	2.87	0.43
5:A:82:LEU:HD22	19:O:50:PHE:HE1	1.84	0.43
5:A:1034:ALA:HB2	24:W:78:THR:HB	2.01	0.43
6:B:262:ASP:OD2	6:B:463:GLN:NE2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:C:82:ASP:OD2	7:C:84:LYS:CD	2.67	0.43
7:C:154:VAL:HB	7:C:180:LEU:HB2	2.01	0.43
8:D:40:GLN:HG2	8:D:60:TYR:CD2	2.54	0.43
16:L:176:GLN:OE1	16:L:177:GLN:N	2.52	0.43
18:N:171:LEU:HD23	18:N:171:LEU:HA	1.85	0.43
20:P:259:GLN:O	20:P:263:GLU:OE1	2.35	0.43
22:R:18:ILE:H	22:R:18:ILE:HD12	1.84	0.43
22:R:32:ASP:OD1	22:R:32:ASP:N	2.52	0.43
22:R:56:ARG:NH1	24:W:221:TYR:O	2.51	0.43
23:U:420:VAL:HG23	23:U:438:GLU:HB2	2.00	0.43
23:U:460:VAL:HG12	23:U:486:ARG:HB2	2.00	0.43
25:X:254:GLY:CA	25:X:293:ILE:HD11	2.49	0.43
26:Y:118:ARG:NH2	26:Y:175:GLN:OE1	2.51	0.43
28:a:64:GLN:HA	31:d:62:ARG:CZ	2.49	0.43
28:a:65:PRO:HD2	31:d:62:ARG:NE	2.34	0.43
31:d:77:HIS:HD2	31:d:79:ASP:OD1	2.02	0.43
36:z:585:GLN:CD	36:z:591:LYS:HB2	2.44	0.43
3:5:32:C:C5	5:A:487:PRO:HB2	2.54	0.43
5:A:554:THR:OG1	5:A:557:GLU:OE1	2.35	0.43
6:B:217:THR:HB	6:B:227:VAL:HG22	2.01	0.43
10:F:18:GLU:HG3	10:F:66:ARG:HD2	2.00	0.43
14:J:18:PHE:HE2	14:J:73:LEU:HB3	1.84	0.43
15:K:302:PRO:CG	15:K:315:LEU:HD23	2.47	0.43
16:L:93:LEU:HD12	31:d:9:SER:HB2	2.00	0.43
18:N:480:LEU:HD11	18:N:505:MET:HB3	2.00	0.43
18:N:668:ARG:HH12	18:N:720:PRO:HA	1.84	0.43
19:O:95:PRO:HA	19:O:98:GLU:OE2	2.17	0.43
22:R:590:GLU:O	22:R:594:VAL:HG23	2.18	0.43
24:W:711:LEU:HD11	27:Z:141:THR:HB	2.00	0.43
25:X:66:LYS:HA	25:X:69:LYS:HG2	2.00	0.43
26:Y:159:LYS:HZ3	26:Y:160:PRO:HG2	1.84	0.43
30:c:558:GLU:N	30:c:558:GLU:OE1	2.49	0.43
31:d:39:ASP:OD1	31:d:151:LYS:HA	2.18	0.43
35:y:72:GLU:HG2	35:y:73:GLY:N	2.34	0.43
4:6:13:A:HO2'	4:6:14:C:P	2.42	0.42
6:B:776:VAL:HA	6:B:779:TYR:CE1	2.53	0.42
16:L:141:PRO:O	16:L:145:GLN:HB2	2.19	0.42
17:M:267:SER:HB2	17:M:282:GLN:NE2	2.33	0.42
18:N:80:MET:HE3	18:N:122:TYR:HE1	1.84	0.42
18:N:375:ASN:HA	18:N:378:ILE:HG12	2.01	0.42
18:N:745:MET:N	18:N:745:MET:SD	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:931:PHE:CD1	18:N:940:GLN:HG3	2.54	0.42
22:R:227:TYR:CG	22:R:247:PHE:HD1	2.37	0.42
22:R:331:SER:HA	22:R:334:ASP:OD2	2.19	0.42
22:R:468:CYS:SG	22:R:502:THR:OG1	2.60	0.42
24:W:159:GLU:O	24:W:163:LEU:HD23	2.19	0.42
30:c:573:PHE:HZ	30:c:596:LEU:HD12	1.83	0.42
35:y:182:ASP:OD1	35:y:183:ASP:N	2.51	0.42
36:z:144:ILE:HG23	36:z:175:VAL:HB	2.01	0.42
36:z:241:VAL:HG12	36:z:318:VAL:CG2	2.49	0.42
5:A:798:ASN:O	5:A:802:LEU:HD23	2.19	0.42
5:A:855:TYR:HB3	5:A:858:ASP:CG	2.44	0.42
5:A:1622:ASP:CG	35:y:86:ASN:HD22	2.26	0.42
5:A:1630:ILE:HD12	5:A:1630:ILE:HA	1.91	0.42
5:A:1684:TYR:HA	5:A:1723:THR:O	2.19	0.42
6:B:618:LEU:HD21	6:B:641:HIS:CE1	2.54	0.42
6:B:841:LEU:HG	6:B:925:PRO:HG3	2.01	0.42
12:H:31:PHE:O	14:J:22:ASN:ND2	2.42	0.42
15:K:302:PRO:HB3	15:K:324:LEU:HD12	2.00	0.42
15:K:452:ASP:OD1	15:K:453:ASN:N	2.52	0.42
16:L:232:PRO:HB2	16:L:234:LEU:HD12	2.02	0.42
18:N:120:VAL:HG23	18:N:124:ILE:HD12	2.01	0.42
25:X:126:THR:HG22	25:X:162:PHE:HZ	1.83	0.42
25:X:652:ILE:HD13	25:X:686:HIS:CE1	2.54	0.42
27:Z:111:LEU:HD12	27:Z:114:LYS:HE2	2.02	0.42
27:Z:129:VAL:O	27:Z:133:LEU:HG	2.19	0.42
35:y:224:LYS:HA	35:y:224:LYS:HD3	1.83	0.42
36:z:77:THR:OG1	36:z:145:LEU:HA	2.19	0.42
36:z:557:THR:O	36:z:557:THR:HG22	2.18	0.42
5:A:388:LEU:HD22	5:A:392:PRO:HD3	2.01	0.42
5:A:1604:HIS:HB3	5:A:1607:GLN:HE21	1.84	0.42
6:B:783:GLY:HA2	6:B:823:ILE:HG23	2.01	0.42
6:B:968:ASP:O	6:B:972:ILE:HG13	2.19	0.42
15:K:89:GLU:OE2	22:R:259:ARG:NE	2.50	0.42
16:L:131:LEU:HA	16:L:131:LEU:HD23	1.92	0.42
18:N:993:LEU:HD23	18:N:993:LEU:HA	1.91	0.42
18:N:1084:HIS:HB2	18:N:1087:GLN:HE21	1.84	0.42
20:P:83:ARG:CZ	20:P:83:ARG:HB3	2.47	0.42
22:R:432:PRO:HG2	22:R:463:TYR:CZ	2.53	0.42
23:S:63:PRO:HB3	24:W:693:LEU:CD2	2.45	0.42
23:T:87:GLN:CD	23:U:87:GLN:HE22	2.23	0.42
25:X:630:VAL:O	25:X:634:LYS:HG2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:667:PHE:CD2	25:X:683:ILE:HD13	2.54	0.42
36:z:170:ASN:O	36:z:173:ARG:NH1	2.51	0.42
36:z:395:LYS:HZ1	36:z:434:ASN:HA	1.84	0.42
5:A:864:LEU:HD22	5:A:1457:ASP:HB2	2.02	0.42
5:A:1457:ASP:OD2	5:A:1484:HIS:NE2	2.46	0.42
5:A:1602:ARG:NE	5:A:1770:ARG:HH11	2.14	0.42
6:B:488:LEU:HB3	6:B:581:SER:HB2	2.00	0.42
8:D:44:ILE:HB	8:D:56:LEU:HB2	2.01	0.42
10:F:3:LEU:HD23	10:F:3:LEU:O	2.20	0.42
15:K:425:PHE:CE2	15:K:441:ALA:HB2	2.54	0.42
18:N:59:GLU:OE1	18:N:85:LYS:NZ	2.52	0.42
18:N:1240:LEU:HD23	18:N:1263:ILE:HG13	2.01	0.42
20:P:92:LYS:HE2	20:P:240:CYS:N	2.34	0.42
20:P:184:THR:O	20:P:187:ILE:HG23	2.19	0.42
20:P:227:LYS:HG2	20:P:243:VAL:HG12	2.00	0.42
23:U:309:TYR:CE2	23:U:311:LEU:HD11	2.54	0.42
25:X:434:TRP:O	25:X:438:GLU:HG2	2.18	0.42
26:Y:118:ARG:HD2	26:Y:118:ARG:C	2.44	0.42
27:Z:115:HIS:HB3	27:Z:118:LYS:HE3	2.02	0.42
30:c:591:ILE:HG23	30:c:593:LEU:H	1.85	0.42
36:z:234:TYR:HB3	36:z:316:TYR:HE2	1.84	0.42
3:5:47:C:H2'	3:5:48:C:O4'	2.19	0.42
5:A:1208:PRO:HB3	5:A:1226:ARG:CZ	2.50	0.42
5:A:1539:PHE:HB2	35:y:38:VAL:HG12	2.01	0.42
5:A:1599:GLN:HG2	35:y:56:PHE:CD2	2.55	0.42
6:B:741:LEU:H	29:b:66:LYS:HG3	1.84	0.42
7:C:53:VAL:O	7:C:314:ASN:ND2	2.51	0.42
7:C:85:ASN:OD1	9:E:97:GLY:N	2.53	0.42
11:G:30:LEU:HD23	13:I:64:LEU:HD11	2.01	0.42
13:I:12:LEU:HD21	13:I:37:VAL:HG11	2.01	0.42
13:I:15:LEU:O	13:I:15:LEU:HD23	2.20	0.42
15:K:228:MET:HE3	15:K:230:LYS:HZ1	1.84	0.42
15:K:414:GLN:HG2	15:K:442:ASP:OD1	2.20	0.42
16:L:161:LEU:O	16:L:165:ILE:HG12	2.20	0.42
17:M:22:ILE:O	28:a:86:THR:HG21	2.19	0.42
18:N:946:CYS:SG	18:N:969:LYS:HD3	2.59	0.42
19:O:26:PHE:CD1	19:O:52:LEU:HD11	2.54	0.42
22:R:256:GLU:HB3	22:R:259:ARG:NH1	2.32	0.42
22:R:402:LYS:O	22:R:405:LEU:HG	2.19	0.42
23:U:114:VAL:O	23:U:118:LEU:HB2	2.19	0.42
24:W:739:MET:HA	24:W:742:ILE:HG12	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:507:PHE:CZ	25:X:536:ILE:HD11	2.55	0.42
25:X:550:PHE:CD1	25:X:587:PHE:HB3	2.55	0.42
36:z:210:LEU:HD23	36:z:363:PHE:HD1	1.85	0.42
36:z:236:PRO:HG3	36:z:268:GLN:NE2	2.34	0.42
1:1:-10:A:O2'	29:b:19:TYR:HA	2.19	0.42
5:A:946:ASP:OD1	5:A:950:TRP:HD1	2.02	0.42
5:A:1624:GLU:OE2	5:A:1627:SER:OG	2.37	0.42
6:B:945:ARG:O	6:B:949:ILE:HG12	2.20	0.42
11:G:53:LEU:HD23	11:G:73:GLU:HB3	2.01	0.42
15:K:111:SER:OG	22:R:232:ASP:OD1	2.27	0.42
15:K:472:ARG:HD2	15:K:472:ARG:HA	1.83	0.42
18:N:62:LEU:HB2	18:N:74:HIS:NE2	2.34	0.42
18:N:267:PHE:HA	18:N:270:MET:CG	2.48	0.42
18:N:728:ASN:OD1	18:N:1046:TYR:OH	2.13	0.42
20:P:85:ASP:CB	20:P:88:LYS:HB3	2.50	0.42
23:T:30:GLN:OE1	23:U:81:ASP:HB3	2.19	0.42
24:W:677:ASN:OD1	24:W:678:ARG:N	2.53	0.42
25:X:227:VAL:HG21	25:X:259:TYR:HD1	1.84	0.42
25:X:265:ILE:HG12	25:X:270:TYR:CE1	2.55	0.42
25:X:520:TYR:HD2	25:X:536:ILE:HG12	1.84	0.42
29:b:8:LEU:H	29:b:8:LEU:HD23	1.84	0.42
29:b:69:LEU:HD23	29:b:69:LEU:HA	1.82	0.42
3:5:107:C:O2'	3:5:108:U:H5'	2.19	0.42
5:A:896:ASN:ND2	5:A:899:GLU:CD	2.78	0.42
5:A:1011:VAL:HG11	5:A:1053:LEU:HD12	2.02	0.42
5:A:1268:ILE:HD13	5:A:1271:ILE:HD12	2.02	0.42
7:C:89:LEU:HD12	7:C:120:TRP:CE3	2.55	0.42
18:N:53:HIS:ND1	18:N:85:LYS:HE2	2.35	0.42
18:N:63:TRP:CZ2	18:N:96:ILE:HG23	2.55	0.42
18:N:277:VAL:HA	18:N:280:PHE:HD2	1.85	0.42
18:N:303:TYR:CD2	18:N:329:LEU:HD23	2.55	0.42
18:N:792:GLU:OE1	18:N:817:TYR:HB2	2.19	0.42
18:N:1017:ASN:ND2	18:N:1170:GLU:OE2	2.36	0.42
19:O:91:LYS:HD3	19:O:91:LYS:HA	1.81	0.42
20:P:115:PHE:CE2	20:P:148:VAL:HG11	2.54	0.42
22:R:249:LYS:O	22:R:252:ILE:HG12	2.19	0.42
22:R:299:THR:O	22:R:302:ASP:OD1	2.37	0.42
22:R:493:LEU:HA	22:R:496:ASN:HD21	1.84	0.42
24:W:254:GLN:HA	24:W:257:ILE:HD12	2.01	0.42
24:W:387:ASN:ND2	24:W:406:LEU:HD22	2.28	0.42
24:W:678:ARG:O	24:W:682:LEU:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:X:398:ARG:HG3	25:X:398:ARG:H	1.73	0.42
25:X:426:GLU:HG2	25:X:427:LEU:N	2.35	0.42
36:z:91:VAL:HG21	36:z:121:TYR:OH	2.19	0.42
36:z:310:THR:HA	36:z:356:ARG:HH12	1.85	0.42
2:2:5:U:H2'	2:2:6:C:C6	2.55	0.42
4:6:67:A:OP1	4:6:69:G:O2'	2.38	0.42
5:A:1242:ASP:O	5:A:1246:LYS:N	2.51	0.42
5:A:1730:ASP:O	5:A:1734:ASN:N	2.53	0.42
6:B:812:PRO:HD2	6:B:817:ARG:HH22	1.85	0.42
7:C:120:TRP:HH2	7:C:127:LYS:HE3	1.85	0.42
10:F:74:LEU:HG	10:F:76:LEU:HG	2.01	0.42
14:J:68:ILE:HG22	14:J:69:MET:HG3	2.01	0.42
17:M:68:GLN:OE1	20:P:147:ASN:ND2	2.53	0.42
17:M:141:ARG:HA	17:M:144:VAL:HG12	2.02	0.42
18:N:150:SER:HA	18:N:178:TYR:CZ	2.55	0.42
18:N:410:GLN:HB3	18:N:416:ASN:ND2	2.33	0.42
18:N:492:GLN:HG3	18:N:499:GLN:CD	2.44	0.42
18:N:500:PHE:HE2	18:N:502:LYS:HB2	1.85	0.42
22:R:148:GLU:HG2	22:R:157:CYS:HB3	2.02	0.42
22:R:159:GLN:HE22	26:Y:155:TRP:CG	2.38	0.42
22:R:192:GLY:O	22:R:196:ARG:HG3	2.20	0.42
23:S:71:ALA:CB	23:T:60:ARG:HH21	2.33	0.42
23:U:441:TYR:HA	23:U:455:MET:O	2.20	0.42
24:W:699:HIS:HA	24:W:702:LYS:HE2	2.00	0.42
24:W:738:LYS:O	24:W:742:ILE:HG23	2.20	0.42
33:m:750:ILE:HB	33:m:760:ILE:CG2	2.49	0.42
5:A:922:MET:HE3	5:A:924:MET:CE	2.39	0.42
5:A:1357:VAL:HG11	30:c:424:VAL:HG23	2.01	0.42
5:A:1436:TRP:CE2	5:A:1444:ASN:ND2	2.88	0.42
6:B:635:VAL:HG22	6:B:641:HIS:ND1	2.34	0.42
7:C:290:ASP:OD1	7:C:292:ASN:HB2	2.20	0.42
9:E:18:THR:HG21	9:E:24:PHE:HE1	1.84	0.42
10:F:17:ILE:HB	10:F:25:VAL:HG23	2.02	0.42
14:J:22:ASN:O	14:J:25:ARG:HD3	2.20	0.42
15:K:414:GLN:NE2	21:Q:248:ASN:HB2	2.35	0.42
17:M:112:ASN:ND2	24:W:226:PRO:O	2.53	0.42
20:P:83:ARG:HH22	20:P:86:PRO:HA	1.85	0.42
23:U:476:LEU:H	23:U:488:GLY:C	2.28	0.42
25:X:448:ARG:HH22	25:X:489:LEU:HD23	1.85	0.42
25:X:585:PRO:HB2	25:X:620:LYS:HG3	2.02	0.42
29:b:23:ASN:C	29:b:25:SER:H	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:d:23:PRO:O	31:d:27:GLN:HG3	2.20	0.42
36:z:80:ARG:HD2	36:z:83:VAL:HG21	2.02	0.42
36:z:166:LEU:HD21	36:z:190:PHE:HE1	1.84	0.42
36:z:329:ASN:O	36:z:333:ARG:N	2.53	0.42
2:2:8:C:H2'	2:2:9:U:C6	2.55	0.42
5:A:223:VAL:O	5:A:227:PHE:HB2	2.19	0.42
5:A:539:LEU:HB3	5:A:547:LEU:HD11	2.02	0.42
5:A:687:HIS:NE2	16:L:219:HIS:HB2	2.35	0.42
5:A:864:LEU:O	5:A:868:ARG:HG2	2.20	0.42
5:A:907:ARG:NH1	5:A:907:ARG:HB2	2.35	0.42
5:A:1443:ILE:HA	5:A:1446:LEU:HD23	2.02	0.42
6:B:163:TYR:CE1	6:B:177:LEU:HD22	2.55	0.42
6:B:279:LEU:HG	6:B:281:LEU:HG	2.01	0.42
7:C:58:PHE:HE1	7:C:326:LEU:HD22	1.81	0.42
7:C:313:VAL:HG13	7:C:313:VAL:O	2.20	0.42
9:E:6:MET:HE2	9:E:6:MET:HB2	1.89	0.42
11:G:25:PHE:O	11:G:31:SER:HB3	2.19	0.42
18:N:629:VAL:HA	18:N:632:LEU:HD23	2.02	0.42
20:P:55:GLU:HG3	20:P:56:THR:HG23	2.02	0.42
20:P:118:LEU:HA	20:P:151:PHE:HZ	1.83	0.42
22:R:81:LEU:HD12	22:R:85:GLU:HA	2.02	0.42
25:X:74:LEU:O	25:X:78:HIS:ND1	2.36	0.42
25:X:384:LEU:HD23	25:X:384:LEU:H	1.84	0.42
27:Z:83:LEU:HD23	27:Z:83:LEU:O	2.20	0.42
27:Z:125:GLU:O	27:Z:129:VAL:HG23	2.20	0.42
30:c:566:VAL:HG13	30:c:567:PRO:HD3	2.02	0.42
31:d:149:ILE:O	31:d:149:ILE:HG13	2.20	0.42
35:y:95:ASP:OD1	35:y:96:ASP:N	2.53	0.42
1:1:0:G:O2'	1:1:1:G:OP1	2.32	0.41
2:2:19:G:H5'	16:L:261:PRO:HG2	2.02	0.41
5:A:735:HIS:HE1	16:L:252:PRO:O	2.03	0.41
5:A:876:LYS:HB2	35:y:209:ASP:HB3	2.01	0.41
5:A:1166:ARG:HH11	5:A:1166:ARG:HG3	1.84	0.41
5:A:1233:LEU:O	30:c:466:LEU:HD11	2.19	0.41
5:A:1490:GLN:NE2	5:A:1492:ASN:ND2	2.68	0.41
5:A:1525:LEU:HD13	5:A:1777:LEU:HD21	2.02	0.41
6:B:271:LYS:HG2	40:B:1001:GTP:C5	2.55	0.41
6:B:678:GLU:OE1	6:B:678:GLU:N	2.53	0.41
6:B:734:LYS:O	6:B:734:LYS:HD3	2.20	0.41
10:F:4:VAL:HG11	10:F:34:MET:O	2.20	0.41
10:F:20:LYS:HA	10:F:20:LYS:HD2	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:I:9:LYS:HB3	13:I:10:PRO:HD3	2.02	0.41
15:K:246:HIS:CE1	15:K:274:TRP:HZ2	2.38	0.41
18:N:214:LYS:HE3	18:N:259:LEU:HD12	2.02	0.41
18:N:841:ILE:HD11	18:N:857:PHE:CE1	2.55	0.41
23:U:435:SER:OG	23:U:441:TYR:O	2.26	0.41
23:V:4:SER:H	23:V:22:VAL:CG1	2.32	0.41
24:W:661:ILE:O	24:W:665:LEU:HG	2.20	0.41
25:X:341:ASN:O	25:X:345:LEU:HG	2.20	0.41
25:X:467:ASP:O	25:X:475:ARG:NH2	2.53	0.41
30:c:413:ARG:HD3	30:c:449:MET:HE2	2.01	0.41
1:1:-1:U:H6	1:1:-1:U:H5"	1.85	0.41
2:2:6:C:H2'	2:2:7:U:C6	2.55	0.41
5:A:1617:LEU:O	5:A:1621:LEU:HD23	2.20	0.41
6:B:180:THR:HG22	6:B:549:ALA:HB2	2.01	0.41
6:B:691:ASP:OD1	6:B:698:ARG:NE	2.36	0.41
15:K:124:ALA:HA	15:K:127:ARG:HD3	2.01	0.41
18:N:836:ARG:HH22	18:N:894:LYS:HB2	1.85	0.41
20:P:82:MET:O	20:P:83:ARG:C	2.63	0.41
22:R:184:TYR:HB3	26:Y:130:TYR:HE2	1.85	0.41
24:W:182:ASP:OD1	24:W:183:ARG:N	2.53	0.41
24:W:649:ASP:OD1	24:W:649:ASP:N	2.50	0.41
26:Y:140:LYS:O	26:Y:142:ARG:HD3	2.19	0.41
29:b:68:LEU:HD21	29:b:131:TYR:CE1	2.52	0.41
33:m:740:HIS:NE2	33:m:782:TYR:CE2	2.87	0.41
33:m:758:ARG:HE	33:m:758:ARG:HB2	1.58	0.41
35:y:144:MET:HE1	36:z:433:GLY:CA	2.51	0.41
36:z:344:LYS:HD2	36:z:376:GLU:OE1	2.20	0.41
36:z:346:SER:HB3	36:z:378:PHE:CE2	2.49	0.41
5:A:807:LEU:HD11	5:A:1042:TYR:HB3	2.02	0.41
5:A:1422:GLN:HE21	5:A:1423:GLN:HE21	1.67	0.41
6:B:149:HIS:CG	6:B:150:LEU:H	2.38	0.41
6:B:689:PHE:H	6:B:971:MET:HE1	1.85	0.41
6:B:969:GLN:HA	6:B:972:ILE:HD12	2.01	0.41
11:G:51:LYS:HD3	11:G:51:LYS:HA	1.93	0.41
12:H:49:MET:O	12:H:51:ILE:HG13	2.21	0.41
14:J:34:TYR:HA	14:J:39:ASN:O	2.20	0.41
15:K:89:GLU:OE1	22:R:259:ARG:HG2	2.20	0.41
17:M:75:ARG:HG3	28:a:85:ILE:HG13	2.03	0.41
17:M:147:VAL:HG21	20:P:267:ALA:HB2	2.03	0.41
18:N:18:ASN:HB2	18:N:19:TRP:HE3	1.85	0.41
18:N:690:LEU:HD11	18:N:710:VAL:CG1	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:R:42:ILE:H	24:W:264:ASN:CG	2.28	0.41
23:S:103:THR:HA	23:S:106:TYR:CZ	2.54	0.41
25:X:564:TYR:O	25:X:567:THR:OG1	2.31	0.41
5:A:1080:ARG:HA	5:A:1080:ARG:HD2	1.78	0.41
5:A:1314:LYS:HE3	5:A:1314:LYS:HB2	1.81	0.41
5:A:1662:ASN:OD1	5:A:1680:THR:HG22	2.20	0.41
5:A:1758:MET:O	5:A:1768:ARG:NH2	2.51	0.41
6:B:179:TYR:CE1	6:B:550:ARG:HD2	2.55	0.41
6:B:603:LYS:HB3	6:B:673:VAL:HG13	2.03	0.41
8:D:89:VAL:HG12	8:D:91:LEU:HG	2.03	0.41
10:F:68:TYR:HB2	11:G:100:PHE:HB3	2.02	0.41
15:K:378:LEU:HD22	15:K:386:MET:HE2	2.02	0.41
15:K:453:ASN:O	15:K:455:THR:HG23	2.20	0.41
19:O:52:LEU:HD12	19:O:52:LEU:HA	1.79	0.41
20:P:137:LEU:HD12	20:P:138:PRO:HD2	2.02	0.41
20:P:224:GLN:HG2	20:P:245:TRP:CH2	2.55	0.41
22:R:102:THR:O	22:R:102:THR:HG22	2.20	0.41
22:R:593:VAL:O	22:R:596:LEU:HD23	2.20	0.41
23:S:69:LEU:HD23	23:U:80:TRP:CB	2.47	0.41
23:S:80:TRP:HH2	23:U:70:PRO:HG3	1.85	0.41
23:T:122:ARG:HH11	23:U:122:ARG:NH2	2.18	0.41
23:V:103:THR:HG23	24:W:565:ILE:HD11	2.02	0.41
23:V:106:TYR:OH	23:V:113:ARG:NH2	2.54	0.41
24:W:225:ILE:HG22	24:W:228:GLU:H	1.84	0.41
25:X:263:TYR:CZ	25:X:267:ILE:HD11	2.55	0.41
26:Y:151:GLU:OE1	31:d:12:LYS:HG2	2.20	0.41
31:d:47:ILE:HD12	31:d:51:VAL:HG22	2.03	0.41
35:y:160:PHE:CE2	36:z:415:HIS:CE1	3.08	0.41
36:z:209:THR:HA	36:z:362:VAL:HG12	2.03	0.41
36:z:426:LEU:HG	36:z:454:LYS:HD2	2.02	0.41
1:1:0:G:HO2'	1:1:1:G:P	2.44	0.41
3:5:14:G:H2'	3:5:15:C:C6	2.56	0.41
4:6:64:A:OP1	5:A:696:THR:OG1	2.27	0.41
5:A:348:LEU:HD22	6:B:189:ARG:NH2	2.34	0.41
5:A:1595:ILE:HG12	35:y:55:ALA:HB2	2.02	0.41
5:A:1641:ARG:H	5:A:1641:ARG:HG3	1.58	0.41
6:B:171:PRO:HA	6:B:172:PRO:HD3	1.94	0.41
6:B:628:TYR:HB3	6:B:650:TYR:OH	2.20	0.41
6:B:760:ARG:HH21	6:B:804:ARG:CD	2.34	0.41
6:B:794:CYS:O	6:B:796:GLU:N	2.54	0.41
7:C:115:THR:O	7:C:115:THR:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:56:LEU:HD13	8:D:59:VAL:HG11	2.02	0.41
11:G:24:GLU:HG2	13:I:38:ASP:HB2	2.03	0.41
18:N:315:GLN:HA	18:N:322:VAL:HG21	2.02	0.41
18:N:798:HIS:CD2	18:N:801:HIS:H	2.37	0.41
18:N:841:ILE:HD11	18:N:857:PHE:CZ	2.55	0.41
20:P:276:LYS:HA	20:P:279:LEU:HD12	2.03	0.41
22:R:580:LEU:HD13	22:R:599:TRP:HZ3	1.85	0.41
23:T:70:PRO:O	23:T:73:LEU:HG	2.20	0.41
23:U:409:GLU:HB3	27:Z:35:ARG:HH21	1.85	0.41
23:V:3:CYS:SG	23:V:5:ILE:HG22	2.60	0.41
24:W:667:LYS:HA	24:W:670:LEU:HG	2.03	0.41
25:X:606:LYS:NZ	34:r:287:UNK:O	2.54	0.41
27:Z:57:ASP:OD1	27:Z:57:ASP:N	2.50	0.41
30:c:431:HIS:O	30:c:435:LYS:HG2	2.20	0.41
30:c:541:LYS:HA	30:c:591:ILE:CD1	2.50	0.41
35:y:166:ASP:HA	35:y:169:LEU:HG	2.02	0.41
36:z:333:ARG:NH2	36:z:422:ASP:OD1	2.43	0.41
36:z:401:ASN:HB3	36:z:404:GLN:OE1	2.21	0.41
3:5:98:U:H5”	8:D:62:ARG:NH2	2.34	0.41
4:6:79:C:C5	26:Y:183:THR:HA	2.56	0.41
5:A:355:SER:O	6:B:274:ARG:NH2	2.53	0.41
5:A:1629:GLN:HE22	5:A:1661:TRP:CD1	2.38	0.41
6:B:291:ARG:HH21	6:B:357:GLY:HA3	1.85	0.41
6:B:719:VAL:HG12	6:B:720:ASN:N	2.36	0.41
6:B:940:GLY:C	6:B:942:ASP:H	2.29	0.41
15:K:241:ARG:HE	21:Q:32:HIS:HB3	1.85	0.41
18:N:1081:GLY:HA2	18:N:1243:THR:HB	2.03	0.41
20:P:86:PRO:C	20:P:87:LEU:HD12	2.46	0.41
22:R:74:MET:HE3	22:R:109:LYS:HZ2	1.86	0.41
22:R:224:ARG:O	22:R:228:LEU:HG	2.19	0.41
23:V:109:ASP:OD2	24:W:592:LEU:HD21	2.20	0.41
25:X:551:GLU:HA	25:X:554:ASN:ND2	2.35	0.41
25:X:668:ALA:HA	25:X:671:GLU:HB2	2.02	0.41
27:Z:106:ASN:ND2	27:Z:110:TYR:OH	2.53	0.41
36:z:222:SER:HB3	36:z:365:LEU:HD22	2.01	0.41
4:6:33:A:H2’	4:6:34:U:C6	2.56	0.41
5:A:1538:LYS:HB3	35:y:206:VAL:HG22	2.03	0.41
6:B:279:LEU:HD12	6:B:279:LEU:HA	1.87	0.41
6:B:287:TYR:OH	6:B:357:GLY:HA2	2.21	0.41
6:B:682:ASP:OD1	6:B:683:THR:N	2.53	0.41
13:I:44:GLN:HA	13:I:63:ILE:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:260:ASP:O	15:K:276:MET:HB2	2.21	0.41
16:L:115:GLU:H	16:L:115:GLU:CD	2.29	0.41
18:N:639:PRO:HG2	18:N:993:LEU:HD13	2.03	0.41
20:P:256:ALA:HB1	20:P:260:ARG:HH12	1.84	0.41
22:R:122:HIS:H	24:W:241:GLU:CD	2.29	0.41
24:W:21:VAL:HG11	24:W:48:TRP:CH2	2.56	0.41
24:W:407:GLN:H	24:W:407:GLN:CD	2.23	0.41
24:W:537:ARG:CG	24:W:538:PRO:CD	2.99	0.41
25:X:193:GLU:O	25:X:197:GLN:HG2	2.20	0.41
25:X:196:ARG:HH12	25:X:235:ASN:HB2	1.85	0.41
25:X:448:ARG:HE	25:X:486:TYR:HE1	1.69	0.41
35:y:31:ARG:HA	36:z:493:PHE:HE2	1.86	0.41
36:z:533:TYR:CZ	36:z:534:GLN:NE2	2.88	0.41
3:5:96:G:C5	12:H:48:PHE:HE2	2.38	0.41
5:A:122:LYS:HE3	5:A:150:VAL:O	2.21	0.41
5:A:208:LEU:HG	5:A:209:GLU:H	1.86	0.41
8:D:61:ILE:HG12	14:J:69:MET:HG2	2.02	0.41
10:F:56:GLU:OE1	10:F:56:GLU:N	2.30	0.41
16:L:180:ASP:HA	16:L:181:PRO:HD3	1.93	0.41
16:L:186:TYR:HA	28:a:88:TYR:O	2.21	0.41
17:M:258:SER:O	17:M:261:GLU:HG2	2.21	0.41
18:N:117:LEU:HA	18:N:120:VAL:HG22	2.03	0.41
18:N:425:ILE:HA	18:N:1031:ARG:HD2	2.02	0.41
22:R:128:ASP:O	22:R:132:THR:HG22	2.21	0.41
23:U:415:PRO:C	23:U:416:LEU:HD22	2.46	0.41
28:a:68:GLY:HA3	31:d:45:ARG:NH1	2.35	0.41
30:c:444:ILE:HD12	30:c:444:ILE:HA	1.95	0.41
34:r:223:UNK:O	34:r:227:UNK:N	2.54	0.41
36:z:332:THR:HB	36:z:596:LYS:HE3	2.03	0.41
5:A:807:LEU:HD23	5:A:807:LEU:HA	1.94	0.41
5:A:1146:SER:O	5:A:1149:VAL:HG12	2.21	0.41
5:A:1395:TYR:OH	5:A:1497:ASP:OD2	2.33	0.41
6:B:195:SER:O	6:B:195:SER:OG	2.33	0.41
6:B:323:SER:HB3	6:B:328:TYR:CZ	2.56	0.41
6:B:340:ILE:HD13	6:B:340:ILE:HA	1.84	0.41
6:B:483:GLU:OE1	6:B:483:GLU:N	2.40	0.41
6:B:522:LYS:CG	6:B:536:MET:HG2	2.50	0.41
10:F:11:THR:HG23	10:F:12:ASN:OD1	2.21	0.41
12:H:77:ASN:OD1	13:I:25:LYS:HE3	2.20	0.41
15:K:267:ARG:HG3	15:K:291:THR:CG2	2.51	0.41
16:L:142:SER:OG	16:L:143:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:110:ASP:CG	17:M:111:ILE:HD12	2.46	0.41
18:N:131:PHE:HB3	18:N:231:VAL:HG11	2.03	0.41
18:N:160:LYS:NZ	18:N:355:TYR:O	2.51	0.41
18:N:434:MET:HE1	18:N:635:ALA:HB2	2.01	0.41
18:N:996:ASN:ND2	18:N:998:GLU:O	2.54	0.41
19:O:78:LEU:HD23	19:O:78:LEU:HA	1.85	0.41
22:R:27:ALA:HB1	24:W:171:ALA:HB2	2.02	0.41
22:R:174:TRP:O	22:R:178:ILE:HG12	2.20	0.41
22:R:369:CYS:HA	22:R:372:GLU:HG2	2.02	0.41
22:R:569:VAL:HG12	22:R:573:ARG:NE	2.36	0.41
23:S:14:VAL:HG11	23:S:28:ILE:HG21	2.01	0.41
23:S:121:GLU:HB2	23:S:122:ARG:HH11	1.86	0.41
23:T:81:ASP:O	23:T:85:LEU:HG	2.21	0.41
24:W:158:ASP:OD1	24:W:159:GLU:HG3	2.21	0.41
25:X:355:TRP:O	25:X:359:VAL:HG23	2.20	0.41
25:X:684:TYR:HE2	25:X:706:PHE:CG	2.39	0.41
31:d:28:ASN:OD1	31:d:29:PHE:N	2.54	0.41
36:z:108:GLN:HA	36:z:126:ILE:HD11	2.03	0.41
36:z:122:MET:SD	36:z:126:ILE:HB	2.60	0.41
4:6:32:G:C2	20:P:82:MET:HB3	2.56	0.41
5:A:233:LEU:HB3	5:A:236:THR:OG1	2.21	0.41
5:A:680:ALA:O	5:A:684:GLU:HB2	2.21	0.41
5:A:1002:THR:HB	5:A:1198:THR:HG23	2.03	0.41
5:A:1104:THR:O	5:A:1104:THR:HG22	2.21	0.41
5:A:1605:LEU:HD11	5:A:1770:ARG:CZ	2.51	0.41
5:A:1727:ILE:HD12	5:A:1754:MET:HE2	2.02	0.41
7:C:56:ALA:HA	7:C:66:ALA:O	2.21	0.41
10:F:6:PHE:CE1	10:F:79:LEU:HG	2.56	0.41
22:R:122:HIS:O	22:R:126:LEU:HG	2.20	0.41
23:S:24:GLU:OE2	23:S:27:LEU:N	2.46	0.41
24:W:162:MET:SD	24:W:163:LEU:HD22	2.60	0.41
24:W:669:ALA:HA	24:W:672:CYS:SG	2.61	0.41
28:a:154:LYS:HB3	28:a:154:LYS:HE3	1.84	0.41
31:d:145:GLU:OE2	31:d:147:LEU:HD13	2.21	0.41
35:y:165:ASP:O	35:y:169:LEU:HG	2.21	0.41
36:z:166:LEU:HD21	36:z:190:PHE:CE1	2.57	0.41
5:A:1429:LEU:C	5:A:1431:ASP:N	2.79	0.40
6:B:706:LEU:HD11	6:B:758:ILE:HD12	2.02	0.40
6:B:851:HIS:HE1	6:B:877:ARG:NE	2.19	0.40
7:C:295:VAL:HB	7:C:304:TYR:HB2	2.03	0.40
10:F:36:MET:HE2	10:F:36:MET:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:N:449:LEU:HD13	18:N:557:PHE:HZ	1.85	0.40
18:N:493:ILE:HD13	25:X:248:ARG:NH1	2.36	0.40
18:N:899:ILE:HG21	18:N:907:PHE:HE1	1.86	0.40
20:P:160:ARG:HB3	20:P:161:ASP:H	1.77	0.40
22:R:98:ASP:OD2	24:W:229:LYS:NZ	2.40	0.40
22:R:284:THR:HG21	22:R:306:LEU:HG	2.02	0.40
23:U:322:SER:O	23:U:324:LYS:N	2.54	0.40
25:X:362:LEU:HD23	25:X:362:LEU:HA	1.89	0.40
29:b:123:ASP:HA	29:b:126:ILE:HG22	2.03	0.40
29:b:134:GLN:NE2	29:b:135:LEU:HG	2.36	0.40
30:c:528:THR:OG1	30:c:531:ASP:OD1	2.37	0.40
3:5:104:A:HO2'	11:G:48:ARG:HG2	1.84	0.40
4:6:32:G:N3	20:P:82:MET:HA	2.37	0.40
5:A:615:TYR:OH	5:A:1574:GLY:HA2	2.21	0.40
16:L:106:ILE:HD12	16:L:106:ILE:H	1.85	0.40
16:L:270:LYS:HD3	26:Y:208:LEU:HD13	2.03	0.40
18:N:333:GLN:O	18:N:336:GLU:HG2	2.21	0.40
18:N:668:ARG:O	18:N:760:LYS:NZ	2.52	0.40
18:N:784:MET:HE1	18:N:954:CYS:C	2.46	0.40
18:N:1138:LEU:HG	18:N:1183:PHE:CZ	2.55	0.40
19:O:4:LEU:H	19:O:4:LEU:HD23	1.86	0.40
19:O:48:PRO:O	19:O:51:GLN:HB3	2.21	0.40
20:P:191:VAL:HG12	20:P:235:LEU:HD21	2.02	0.40
22:R:189:ARG:O	22:R:193:ILE:HG13	2.20	0.40
23:S:72:LEU:HG	23:S:76:PHE:CE1	2.57	0.40
23:U:80:TRP:HA	23:U:83:VAL:HG12	2.03	0.40
24:W:105:LEU:HA	24:W:108:LYS:HG2	2.03	0.40
24:W:251:GLU:OE1	24:W:255:LYS:NZ	2.54	0.40
31:d:5:GLU:HG3	31:d:7:GLN:OE1	2.21	0.40
35:y:31:ARG:HA	36:z:493:PHE:CE2	2.56	0.40
36:z:223:ALA:O	36:z:227:VAL:HG23	2.21	0.40
1:1:-14:U:H3'	1:1:-13:U:H5"	2.03	0.40
5:A:527:LEU:HD22	5:A:567:PHE:CE1	2.56	0.40
5:A:538:TYR:O	5:A:550:THR:OG1	2.28	0.40
5:A:1611:GLU:HA	5:A:1614:VAL:HG22	2.03	0.40
5:A:1664:SER:O	5:A:1741:ASN:ND2	2.54	0.40
6:B:692:THR:HB	6:B:694:ASN:OD1	2.21	0.40
7:C:143:VAL:HG12	7:C:151:LEU:HD22	2.03	0.40
7:C:145:LYS:HB2	7:C:187:GLN:HG3	2.04	0.40
7:C:176:GLU:HG3	7:C:177:LYS:N	2.36	0.40
9:E:7:VAL:O	9:E:10:LEU:HD23	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:K:299:GLU:OE1	15:K:299:GLU:N	2.51	0.40
16:L:186:TYR:CD1	28:a:89:ALA:HB2	2.49	0.40
18:N:956:TRP:O	18:N:960:SER:HB3	2.21	0.40
20:P:175:THR:HA	20:P:216:THR:HA	2.02	0.40
24:W:640:LEU:O	24:W:644:GLU:HG3	2.21	0.40
24:W:697:ILE:O	24:W:701:TRP:HB2	2.21	0.40
24:W:701:TRP:CH2	27:Z:134:LEU:HD21	2.57	0.40
25:X:202:LEU:O	25:X:203:ASN:ND2	2.54	0.40
25:X:428:ALA:O	25:X:432:ILE:HG23	2.21	0.40
25:X:450:LEU:O	25:X:454:ALA:HB2	2.20	0.40
27:Z:139:VAL:HA	27:Z:142:LYS:CG	2.51	0.40
30:c:463:PHE:CZ	30:c:467:ILE:HD11	2.56	0.40
31:d:28:ASN:O	31:d:32:LEU:HB2	2.20	0.40
5:A:77:THR:HG22	5:A:78:GLU:N	2.37	0.40
5:A:1150:ASN:O	5:A:1176:ARG:NH2	2.54	0.40
5:A:1762:PRO:HB2	35:y:97:ILE:HD11	2.03	0.40
6:B:225:ASP:HB3	6:B:629:PRO:HG2	2.04	0.40
6:B:621:LEU:HD23	6:B:621:LEU:HA	1.93	0.40
6:B:756:THR:HG22	6:B:756:THR:O	2.22	0.40
16:L:92:ALA:HB1	16:L:102:ASP:H	1.86	0.40
18:N:116:ASN:O	18:N:120:VAL:HG13	2.22	0.40
18:N:858:ARG:HB2	18:N:922:PHE:CZ	2.55	0.40
19:O:55:GLN:HG3	28:a:153:TYR:CD2	2.57	0.40
22:R:186:GLU:HG3	22:R:186:GLU:O	2.21	0.40
23:T:122:ARG:HH12	23:U:122:ARG:HB2	1.84	0.40
27:Z:159:VAL:HG12	27:Z:162:ARG:NH2	2.36	0.40
36:z:256:ILE:HG13	36:z:300:PHE:HZ	1.85	0.40
3:5:82:A:HO2'	3:5:83:A:H8	1.66	0.40
5:A:208:LEU:O	19:O:8:ARG:NH1	2.55	0.40
5:A:568:HIS:O	5:A:572:GLU:HG2	2.22	0.40
5:A:878:ARG:NH1	35:y:209:ASP:OD1	2.55	0.40
5:A:1674:ASP:OD1	5:A:1674:ASP:N	2.47	0.40
6:B:689:PHE:N	6:B:971:MET:HE1	2.37	0.40
7:C:52:GLU:HB3	7:C:330:SER:HB2	2.04	0.40
7:C:57:ARG:HH21	7:C:315:HIS:CE1	2.39	0.40
7:C:134:HIS:ND1	7:C:155:SER:OG	2.39	0.40
7:C:162:VAL:CG1	7:C:172:LYS:HB3	2.51	0.40
7:C:276:ALA:HB2	7:C:316:VAL:O	2.22	0.40
7:C:332:ARG:NH2	28:a:93:TYR:HE2	2.20	0.40
11:G:71:VAL:HG12	11:G:96:ILE:O	2.21	0.40
15:K:318:LEU:HD23	15:K:318:LEU:HA	1.97	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:M:89:PHE:HZ	17:M:136:ALA:HB1	1.85	0.40
17:M:168:GLN:NE2	17:M:169:ILE:HG23	2.37	0.40
24:W:675:LEU:HD11	27:Z:105:ARG:HH21	1.86	0.40
25:X:533:SER:O	25:X:536:ILE:HG22	2.21	0.40
25:X:535:LYS:HA	25:X:538:GLU:OE2	2.22	0.40
26:Y:164:HIS:O	26:Y:167:ARG:HG2	2.22	0.40
28:a:71:ASN:O	28:a:74:VAL:HG22	2.22	0.40
29:b:79:SER:HA	29:b:118:SER:HB2	2.03	0.40
31:d:30:TYR:CZ	31:d:34:LYS:HE3	2.57	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	
5	A	1735/2363 (73%)	1635 (94%)	99 (6%)	1 (0%)	48	80
6	B	916/984 (93%)	866 (94%)	49 (5%)	1 (0%)	48	80
7	C	297/340 (87%)	274 (92%)	23 (8%)	0	100	100
8	D	94/97 (97%)	92 (98%)	2 (2%)	0	100	100
9	E	91/147 (62%)	85 (93%)	6 (7%)	0	100	100
10	F	79/117 (68%)	73 (92%)	6 (8%)	0	100	100
11	G	98/115 (85%)	93 (95%)	5 (5%)	0	100	100
12	H	78/84 (93%)	77 (99%)	1 (1%)	0	100	100
13	I	71/78 (91%)	70 (99%)	1 (1%)	0	100	100
14	J	71/77 (92%)	66 (93%)	5 (7%)	0	100	100
15	K	389/473 (82%)	357 (92%)	32 (8%)	0	100	100
16	L	230/557 (41%)	211 (92%)	19 (8%)	0	100	100
17	M	222/354 (63%)	214 (96%)	8 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
18	N	1282/1284 (100%)	1260 (98%)	22 (2%)	0	100	100
19	O	142/146 (97%)	135 (95%)	7 (5%)	0	100	100
20	P	265/388 (68%)	244 (92%)	19 (7%)	2 (1%)	16	51
21	Q	86/265 (32%)	77 (90%)	9 (10%)	0	100	100
22	R	597/674 (89%)	588 (98%)	9 (2%)	0	100	100
23	S	130/488 (27%)	122 (94%)	8 (6%)	0	100	100
23	T	132/488 (27%)	123 (93%)	9 (7%)	0	100	100
23	U	414/488 (85%)	394 (95%)	20 (5%)	0	100	100
23	V	129/488 (26%)	118 (92%)	11 (8%)	0	100	100
24	W	514/757 (68%)	479 (93%)	32 (6%)	3 (1%)	22	57
25	X	642/790 (81%)	610 (95%)	31 (5%)	1 (0%)	44	75
26	Y	114/229 (50%)	108 (95%)	5 (4%)	1 (1%)	14	49
27	Z	151/187 (81%)	144 (95%)	7 (5%)	0	100	100
28	a	150/558 (27%)	140 (93%)	10 (7%)	0	100	100
29	b	98/293 (33%)	94 (96%)	4 (4%)	0	100	100
30	c	202/887 (23%)	192 (95%)	10 (5%)	0	100	100
31	d	152/155 (98%)	137 (90%)	15 (10%)	0	100	100
33	m	79/797 (10%)	78 (99%)	1 (1%)	0	100	100
35	y	179/534 (34%)	154 (86%)	23 (13%)	2 (1%)	12	44
36	z	624/647 (96%)	611 (98%)	12 (2%)	1 (0%)	44	75
All	All	10453/16329 (64%)	9921 (95%)	520 (5%)	12 (0%)	50	80

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
20	P	90	GLN
24	W	536	ILE
35	y	115	LYS
5	A	1115	ILE
26	Y	144	VAL
20	P	86	PRO
36	z	437	ASP
24	W	172	ASN
24	W	538	PRO
6	B	961	VAL

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Mol	Chain	Res	Type
25	X	83	ASN
35	y	28	GLU

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	
5	A	1570/2138 (73%)	1569 (100%)	1 (0%)	92	98
6	B	821/881 (93%)	821 (100%)	0	100	100
7	C	257/292 (88%)	257 (100%)	0	100	100
8	D	85/86 (99%)	85 (100%)	0	100	100
9	E	80/118 (68%)	80 (100%)	0	100	100
10	F	76/102 (74%)	76 (100%)	0	100	100
11	G	91/101 (90%)	91 (100%)	0	100	100
12	H	73/76 (96%)	73 (100%)	0	100	100
13	I	64/69 (93%)	64 (100%)	0	100	100
14	J	63/67 (94%)	63 (100%)	0	100	100
15	K	333/405 (82%)	333 (100%)	0	100	100
16	L	200/477 (42%)	200 (100%)	0	100	100
17	M	198/306 (65%)	198 (100%)	0	100	100
18	N	1188/1188 (100%)	1188 (100%)	0	100	100
19	O	130/132 (98%)	130 (100%)	0	100	100
20	P	231/340 (68%)	231 (100%)	0	100	100
21	Q	79/240 (33%)	79 (100%)	0	100	100
22	R	532/597 (89%)	532 (100%)	0	100	100
23	S	121/443 (27%)	121 (100%)	0	100	100
23	T	123/443 (28%)	123 (100%)	0	100	100
23	U	223/443 (50%)	223 (100%)	0	100	100
23	V	120/443 (27%)	120 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	W	469/656 (72%)	469 (100%)	0	100	100
25	X	586/707 (83%)	586 (100%)	0	100	100
26	Y	116/214 (54%)	116 (100%)	0	100	100
27	Z	132/163 (81%)	132 (100%)	0	100	100
28	a	79/496 (16%)	79 (100%)	0	100	100
29	b	95/275 (34%)	95 (100%)	0	100	100
30	c	188/816 (23%)	188 (100%)	0	100	100
31	d	128/129 (99%)	128 (100%)	0	100	100
33	m	72/719 (10%)	72 (100%)	0	100	100
35	y	158/478 (33%)	158 (100%)	0	100	100
36	z	564/585 (96%)	564 (100%)	0	100	100
All	All	9245/14625 (63%)	9244 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	A	1209	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (100) such sidechains are listed below:

Mol	Chain	Res	Type
5	A	62	GLN
5	A	86	HIS
5	A	256	ASN
5	A	402	ASN
5	A	471	GLN
5	A	586	GLN
5	A	591	ASN
5	A	602	HIS
5	A	694	GLN
5	A	815	HIS
5	A	896	ASN
5	A	898	HIS
5	A	984	ASN
5	A	1027	ASN
5	A	1047	HIS
5	A	1065	GLN

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Mol	Chain	Res	Type
5	A	1184	ASN
5	A	1270	GLN
5	A	1387	HIS
5	A	1423	GLN
5	A	1444	ASN
5	A	1474	ASN
5	A	1490	GLN
5	A	1492	ASN
5	A	1511	HIS
5	A	1544	ASN
5	A	1607	GLN
6	B	821	GLN
6	B	969	GLN
7	C	45	GLN
7	C	116	HIS
7	C	188	GLN
7	C	209	ASN
7	C	241	ASN
8	D	22	ASN
9	E	12	HIS
11	G	34	GLN
13	I	44	GLN
15	K	244	HIS
15	K	303	GLN
15	K	376	ASN
16	L	113	HIS
16	L	250	GLN
17	M	120	GLN
17	M	253	ASN
17	M	282	GLN
18	N	132	GLN
18	N	379	ASN
18	N	659	ASN
18	N	740	GLN
18	N	798	HIS
18	N	947	GLN
18	N	1216	ASN
20	P	147	ASN
20	P	224	GLN
20	P	268	ASN
20	P	287	ASN
20	P	324	GLN

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Mol	Chain	Res	Type
21	Q	248	ASN
22	R	119	ASN
22	R	159	GLN
22	R	225	GLN
22	R	367	ASN
22	R	497	GLN
23	S	43	GLN
23	T	42	GLN
23	U	342	HIS
23	V	21	ASN
23	V	77	GLN
23	V	87	GLN
24	W	245	ASN
24	W	387	ASN
24	W	710	ASN
24	W	747	GLN
25	X	143	GLN
25	X	283	ASN
25	X	350	ASN
25	X	462	HIS
25	X	554	ASN
25	X	686	HIS
25	X	689	GLN
26	Y	182	ASN
27	Z	130	GLN
27	Z	146	GLN
27	Z	156	GLN
28	a	101	GLN
30	c	442	GLN
30	c	561	HIS
31	d	7	GLN
35	y	90	HIS
35	y	117	ASN
35	y	147	ASN
35	y	208	ASN
36	z	33	GLN
36	z	41	ASN
36	z	108	GLN
36	z	231	ASN
36	z	268	GLN
36	z	303	ASN
36	z	384	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	28/29 (96%)	19 (67%)	2 (7%)
2	2	22/186 (11%)	4 (18%)	0
3	5	101/120 (84%)	23 (22%)	2 (1%)
4	6	91/99 (91%)	44 (48%)	7 (7%)
All	All	242/434 (55%)	90 (37%)	11 (4%)

All (90) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	-14	U
1	1	-13	U
1	1	-12	U
1	1	-8	U
1	1	-4	A
1	1	0	G
1	1	1	G
1	1	2	U
1	1	3	A
1	1	4	U
1	1	5	G
1	1	6	U
1	1	7	U
1	1	8	U
1	1	9	U
1	1	10	U
1	1	11	U
1	1	12	U
1	1	13	U
2	2	11	U
2	2	13	C
2	2	24	A
2	2	29	A
3	5	13	A
3	5	14	G
3	5	27	G
3	5	28	C
3	5	30	A
3	5	31	A
3	5	33	G
3	5	37	C
3	5	45	U

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Mol	Chain	Res	Type
3	5	50	U
3	5	54	C
3	5	79	G
3	5	82	A
3	5	83	A
3	5	90	U
3	5	91	G
3	5	92	U
3	5	98	U
3	5	99	U
3	5	102	G
3	5	103	U
3	5	105	A
3	5	108	U
4	6	4	C
4	6	7	C
4	6	8	G
4	6	9	G
4	6	10	A
4	6	11	U
4	6	12	C
4	6	14	C
4	6	18	G
4	6	19	G
4	6	20	U
4	6	21	C
4	6	22	A
4	6	23	A
4	6	24	A
4	6	27	G
4	6	28	A
4	6	29	A
4	6	30	A
4	6	31	C
4	6	32	G
4	6	38	G
4	6	40	G
4	6	43	G
4	6	44	A
4	6	46	U
4	6	48	G
4	6	52	G

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Mol	Chain	Res	Type
4	6	53	G
4	6	61	A
4	6	62	C
4	6	63	A
4	6	68	U
4	6	74	U
4	6	75	G
4	6	76	C
4	6	78	A
4	6	79	C
4	6	80	A
4	6	81	U
4	6	82	U
4	6	83	G
4	6	91	A
4	6	92	C

All (11) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	0	G
1	1	1	G
3	5	27	G
3	5	49	U
4	6	13	A
4	6	17	U
4	6	29	A
4	6	30	A
4	6	37	A
4	6	52	G
4	6	74	U

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)

Of 13 ligands modelled in this entry, 11 are monoatomic - leaving 2 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
39	IHP	A	2401	-	36,36,36	1.39	13 (36%)	54,60,60	1.47	9 (16%)
40	GTP	B	1001	37	26,34,34	1.22	2 (7%)	32,54,54	1.69	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	IHP	A	2401	-	-	5/30/54/54	0/1/1/1
40	GTP	B	1001	37	-	0/18/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	B	1001	GTP	C5-C6	-4.21	1.38	1.47
39	A	2401	IHP	P6-O46	-2.42	1.45	1.54
39	A	2401	IHP	P1-O31	-2.19	1.46	1.54
39	A	2401	IHP	P1-O11	2.18	1.63	1.59
39	A	2401	IHP	P5-O45	-2.11	1.46	1.54
39	A	2401	IHP	P6-O36	-2.10	1.46	1.54
39	A	2401	IHP	P4-O44	-2.09	1.46	1.54
39	A	2401	IHP	P3-O43	-2.09	1.46	1.54
39	A	2401	IHP	P3-O33	-2.07	1.46	1.54
39	A	2401	IHP	P4-O34	-2.05	1.46	1.54
39	A	2401	IHP	P2-O32	-2.05	1.46	1.54
40	B	1001	GTP	C2-N3	2.05	1.38	1.33
39	A	2401	IHP	P2-O42	-2.03	1.47	1.54
39	A	2401	IHP	P5-O35	-2.02	1.47	1.54
39	A	2401	IHP	P1-O41	-2.02	1.47	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	B	1001	GTP	PB-O3B-PG	-4.73	116.59	132.83
40	B	1001	GTP	C5-C6-N1	3.36	119.88	113.95
40	B	1001	GTP	O4'-C1'-C2'	-3.25	102.18	106.93
39	A	2401	IHP	O11-P1-O21	-3.17	97.15	109.39
39	A	2401	IHP	C5-C6-C1	3.15	117.30	110.41
40	B	1001	GTP	C8-N7-C5	3.06	108.83	102.99
40	B	1001	GTP	PA-O3A-PB	-3.06	122.32	132.83
40	B	1001	GTP	C2-N1-C6	-3.01	119.55	125.10
39	A	2401	IHP	C6-C1-C2	2.81	116.56	110.41
39	A	2401	IHP	O41-P1-O31	2.68	117.89	107.64
39	A	2401	IHP	C6-C5-C4	2.36	115.59	110.41
40	B	1001	GTP	O6-C6-C5	-2.25	119.97	124.37
39	A	2401	IHP	O12-P2-O22	-2.22	100.83	109.39
39	A	2401	IHP	O41-P1-O21	2.09	118.86	110.68
39	A	2401	IHP	O15-P5-O25	-2.05	101.48	109.39
39	A	2401	IHP	O42-P2-O32	2.02	115.36	107.64

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
39	A	2401	IHP	C6-O16-P6-O26
39	A	2401	IHP	C1-O11-P1-O41
39	A	2401	IHP	C6-O16-P6-O36
39	A	2401	IHP	C5-O15-P5-O35
39	A	2401	IHP	C5-O15-P5-O45

There are no ring outliers.

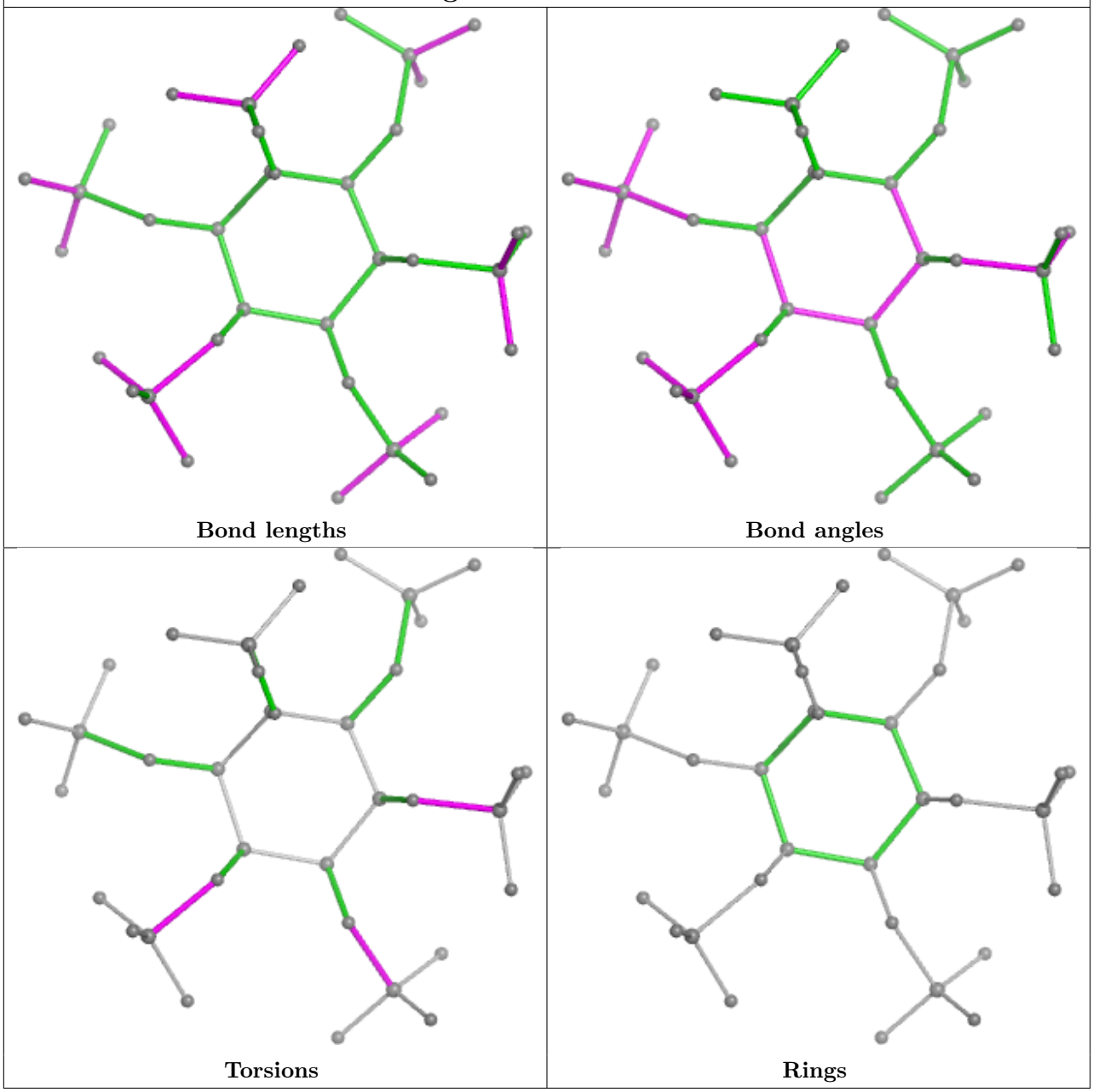
1 monomer is involved in 3 short contacts:

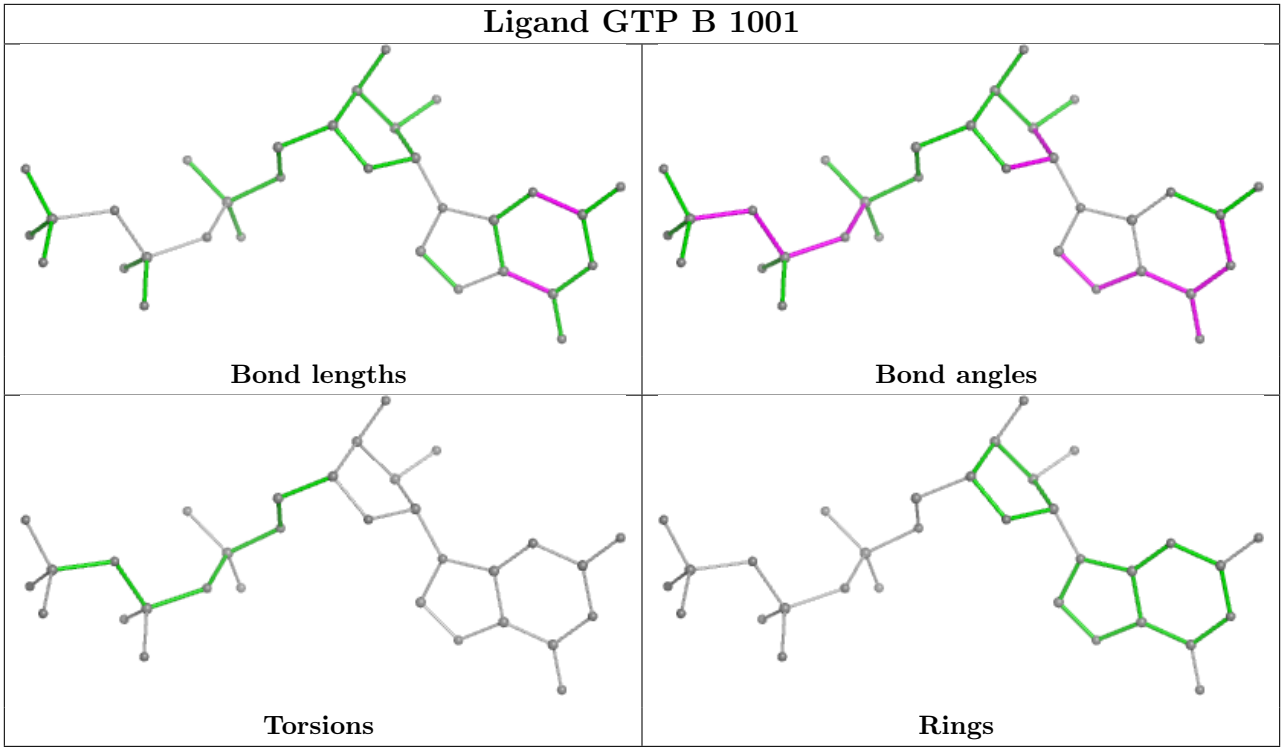
Mol	Chain	Res	Type	Clashes	Symm-Clashes
40	B	1001	GTP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the

average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand IHP A 2401





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.

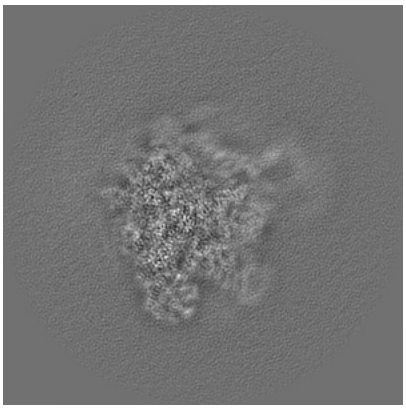
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-19941. These allow visual inspection of the internal detail of the map and identification of artifacts.

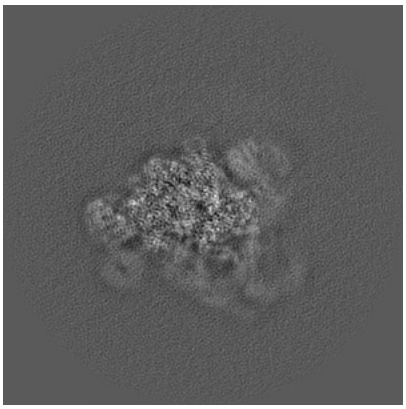
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections (i)

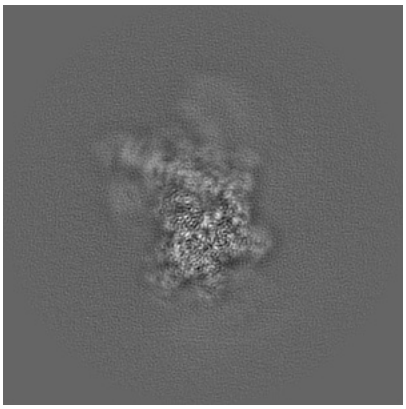
6.1.1 Primary map



X

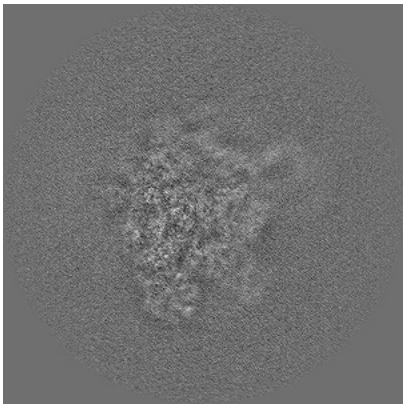


Y

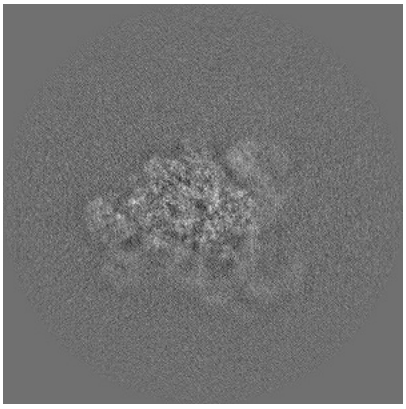


Z

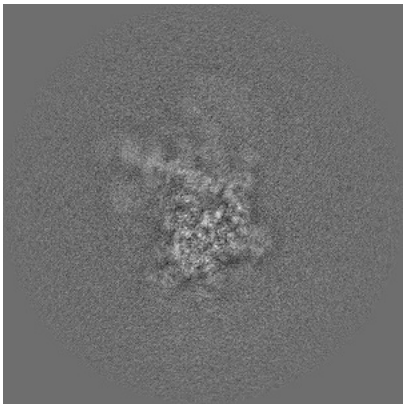
6.1.2 Raw map



X



Y

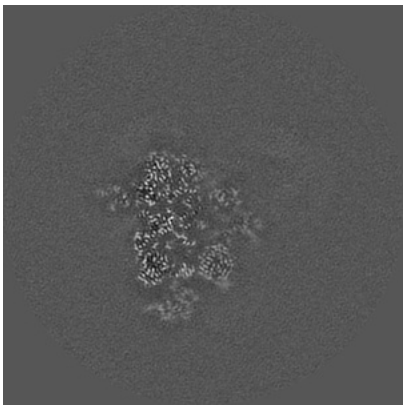


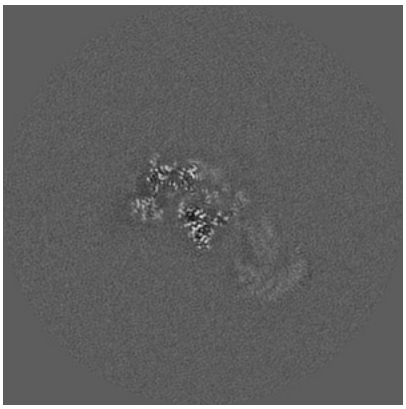
Z

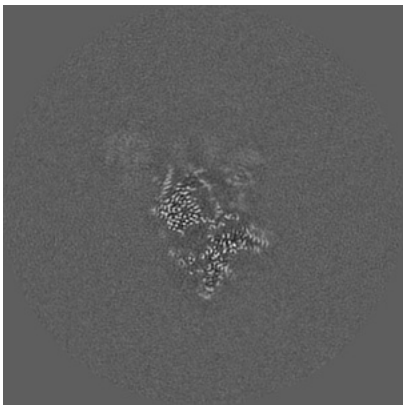
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

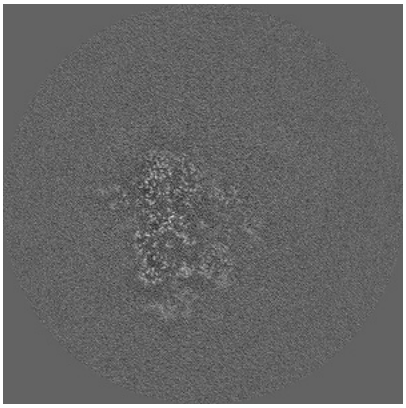
6.2.1 Primary map

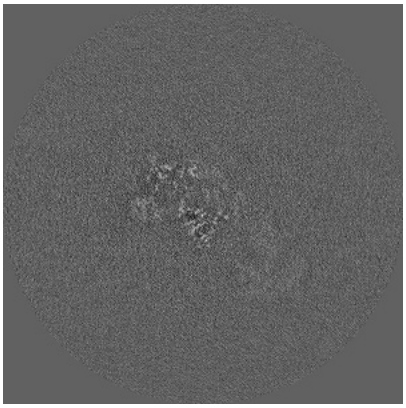

X Index: 280

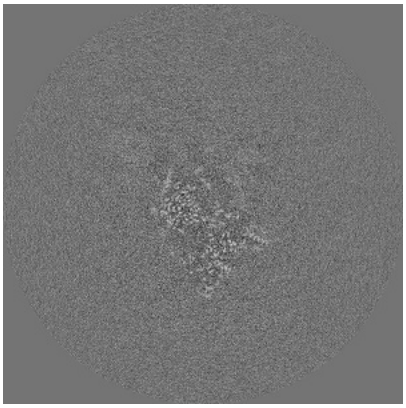

Y Index: 280


Z Index: 280

6.2.2 Raw map


X Index: 280

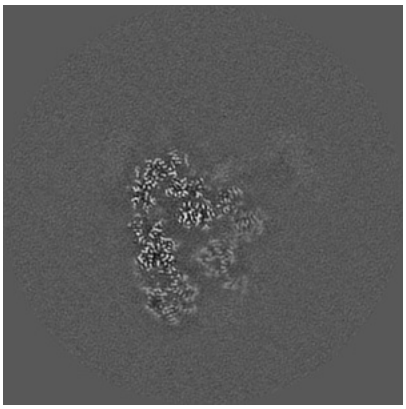

Y Index: 280

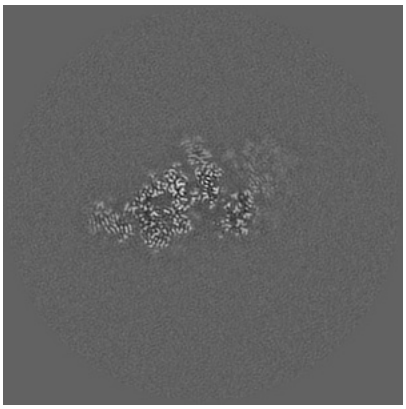

Z Index: 280

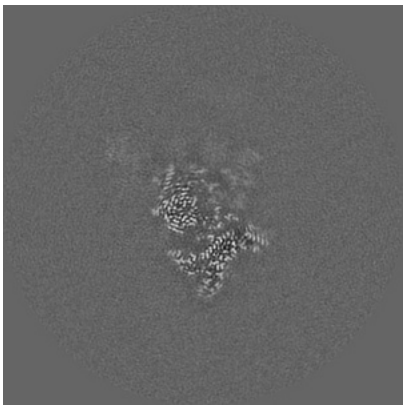
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

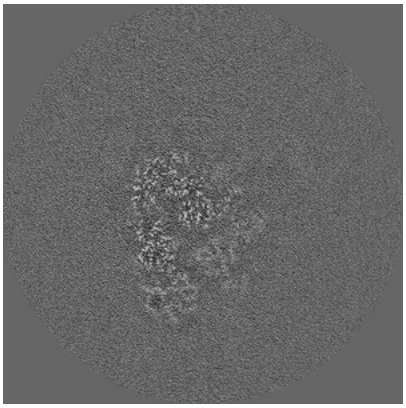
6.3.1 Primary map

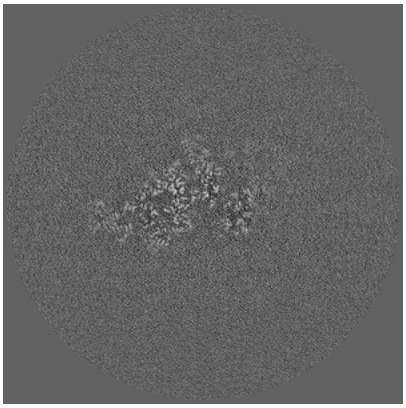

X Index: 263

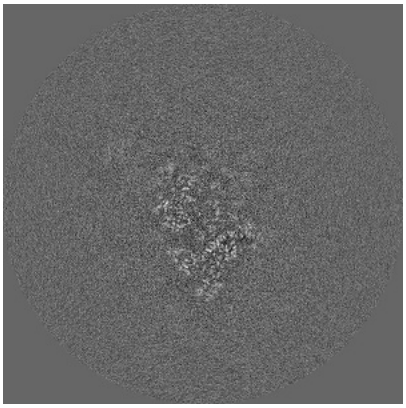

Y Index: 220


Z Index: 282

6.3.2 Raw map


X Index: 263

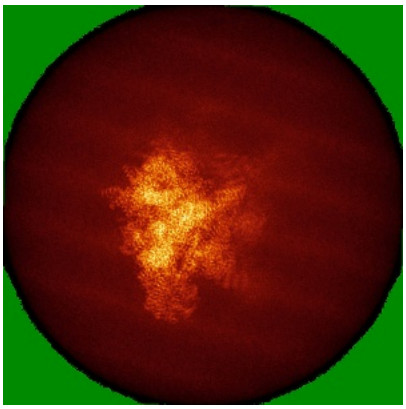

Y Index: 220

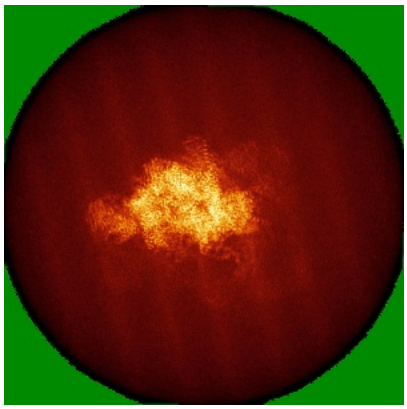

Z Index: 284

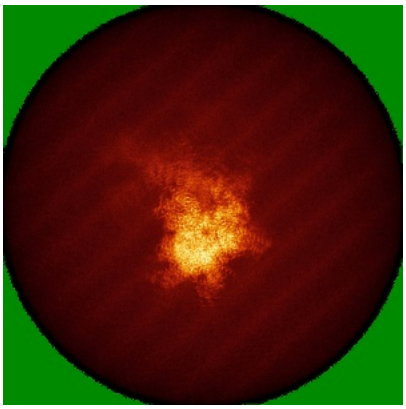
The images above show the largest variance slices of the map in three orthogonal directions.

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

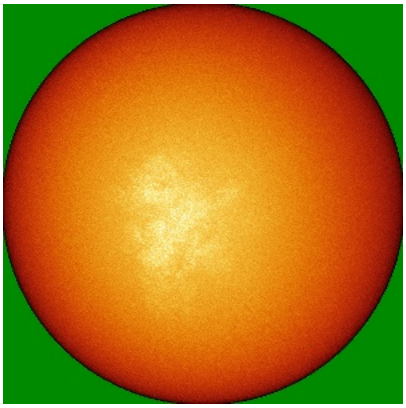
6.4.1 Primary map

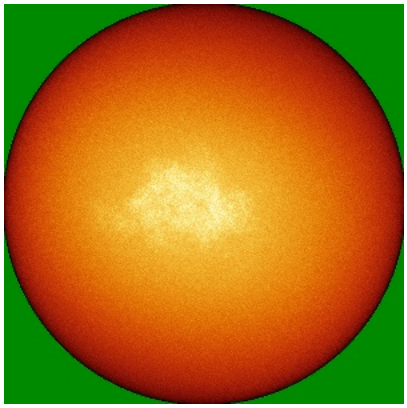

X

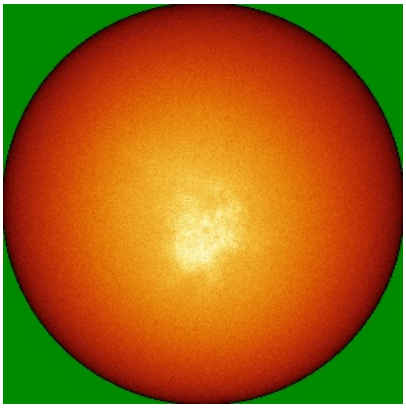

Y


Z

6.4.2 Raw map


X


Y


Z

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

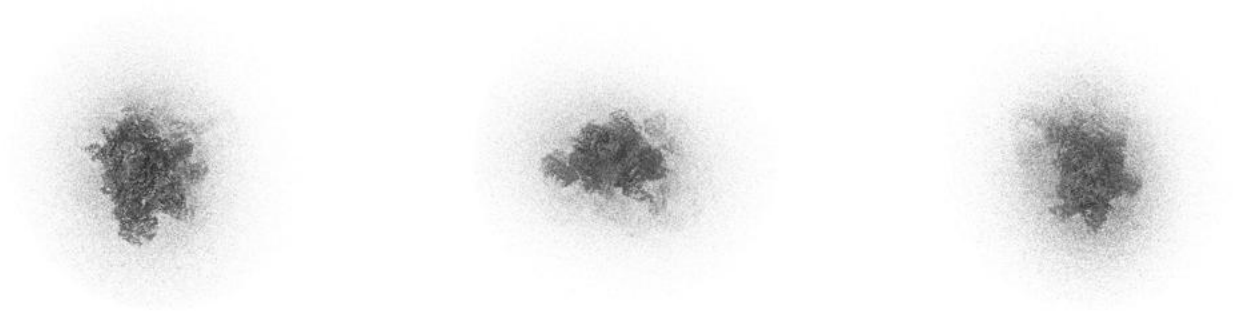
6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 3.55. 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.

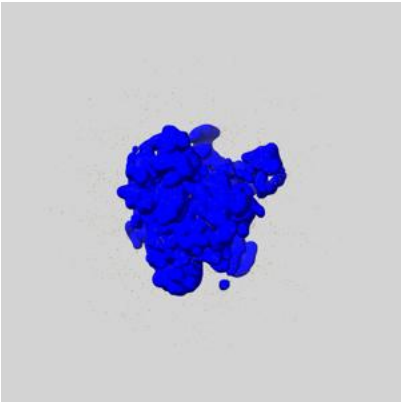
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

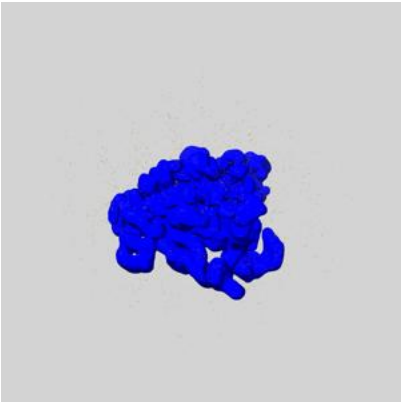
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

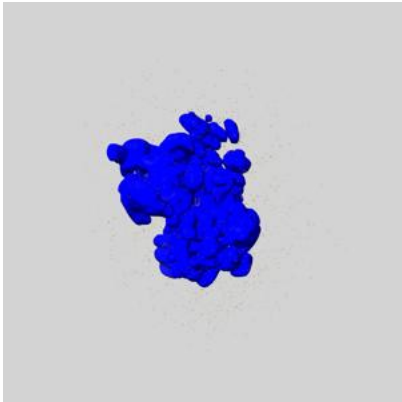
6.6.1 emd_19941_msk_1.map (i)



X



Y

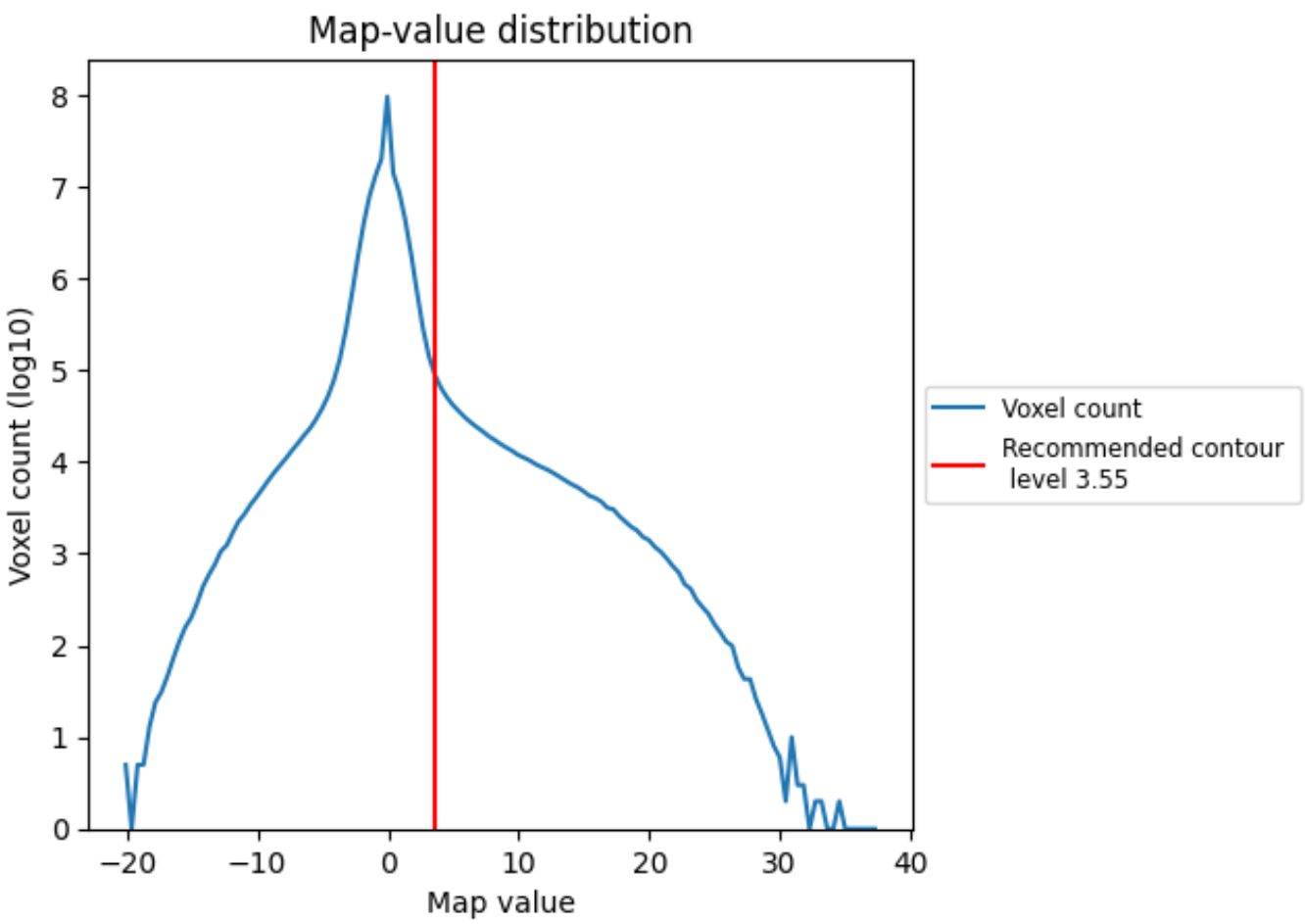


Z

7 Map analysis (i)

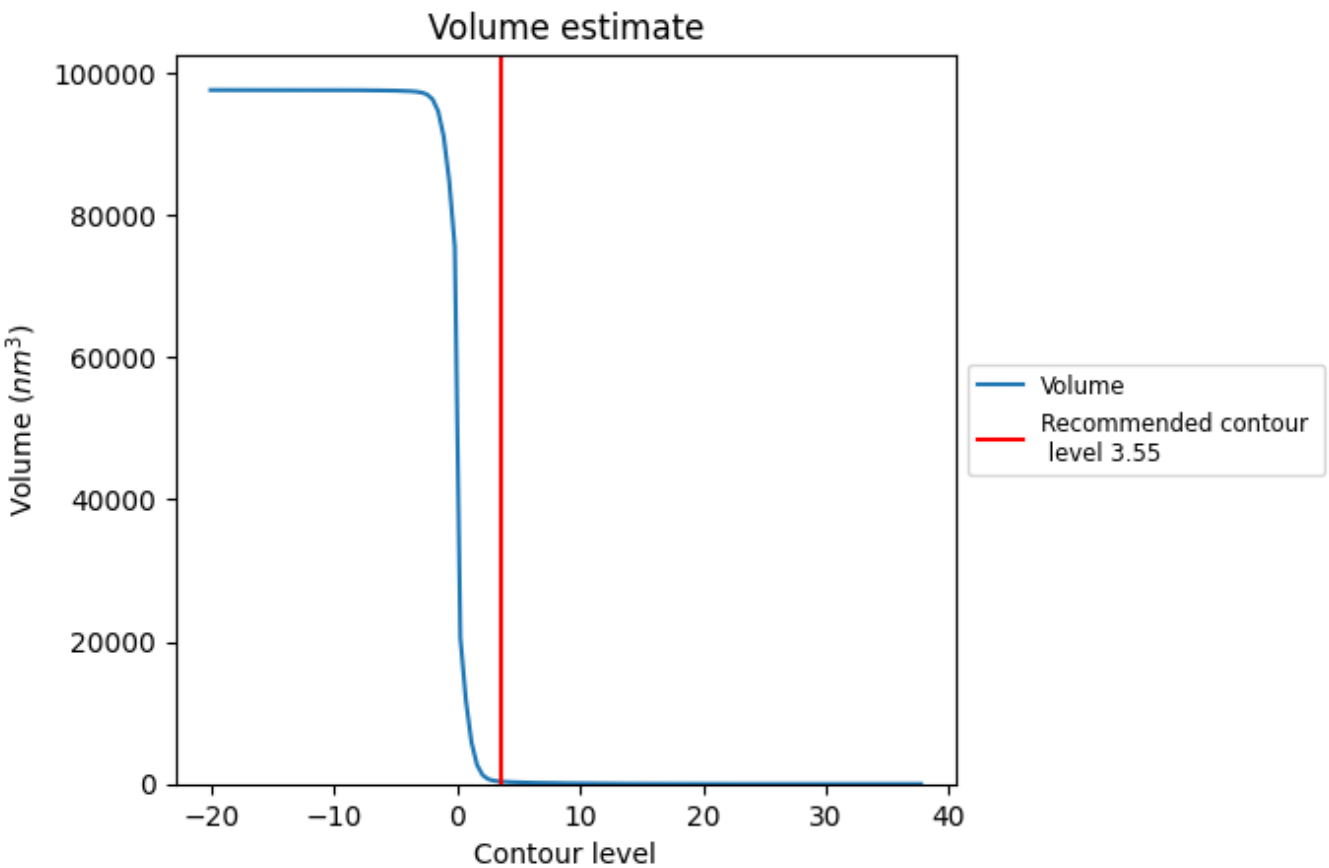
This section contains the results of statistical analysis of the map.

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.

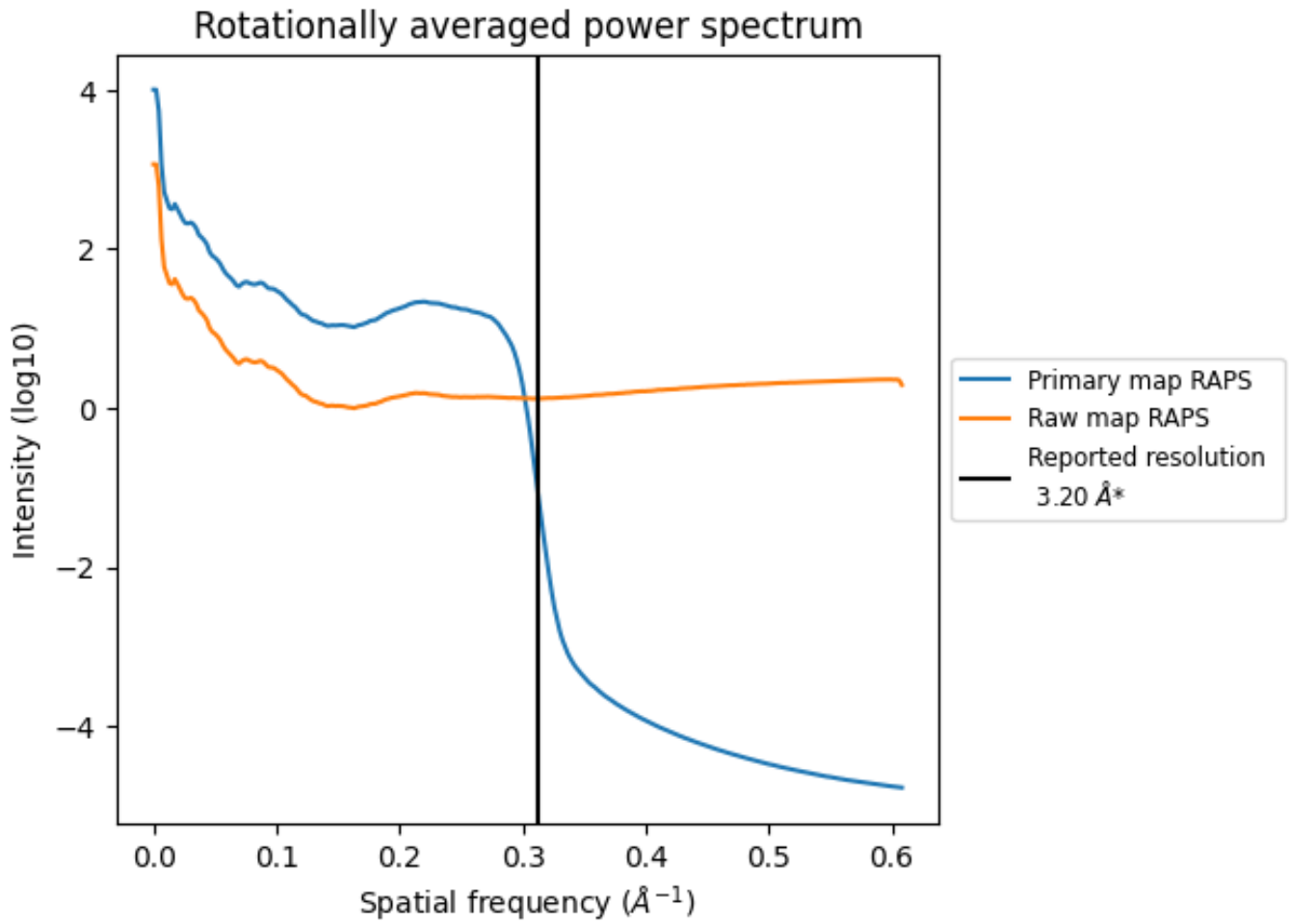
7.2 Volume estimate (i)



The volume at the recommended contour level is 341 nm^3; this corresponds to an approximate mass of 308 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)

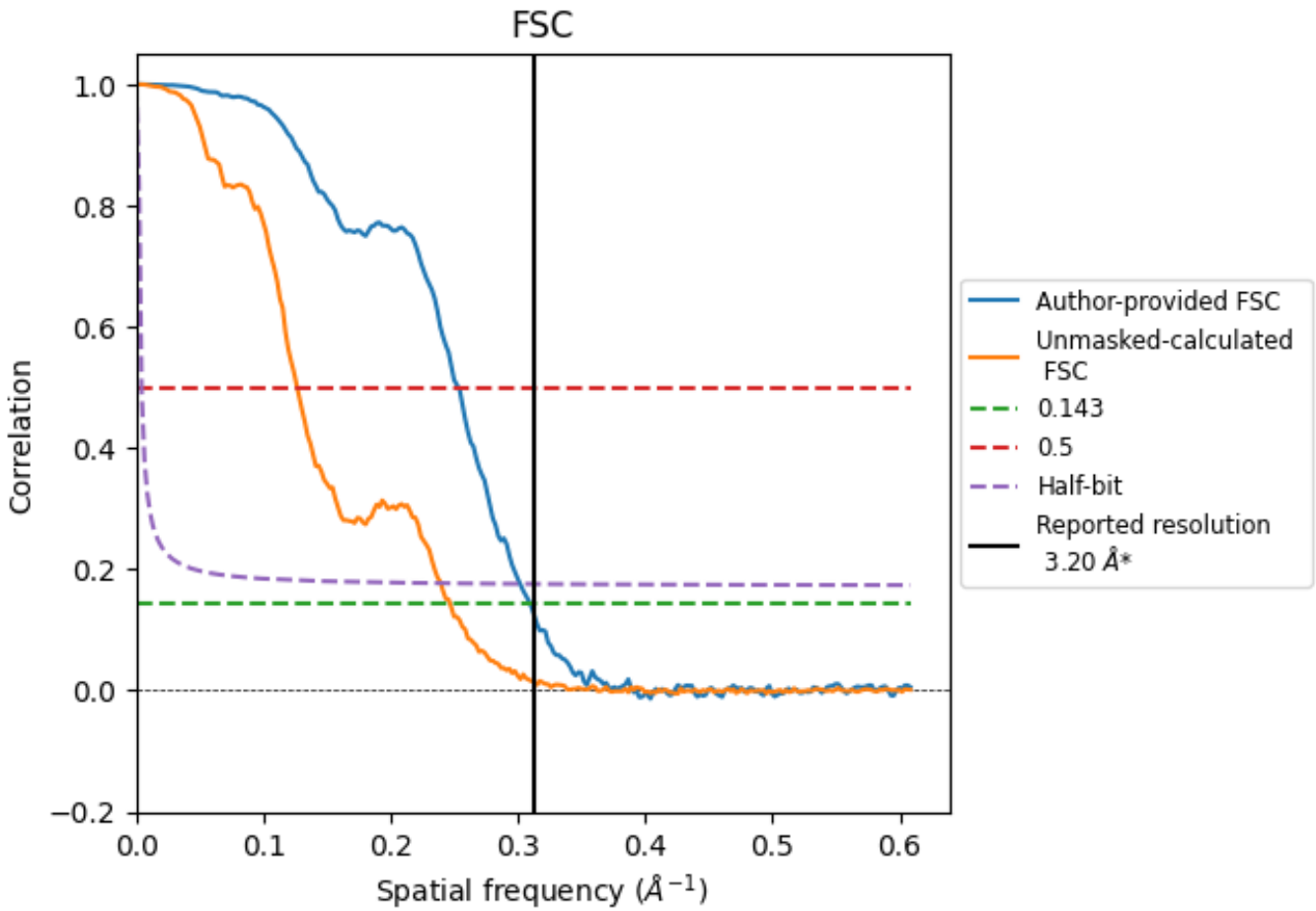


*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

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 0.312 Å^{-1}

8.2 Resolution estimates (i)

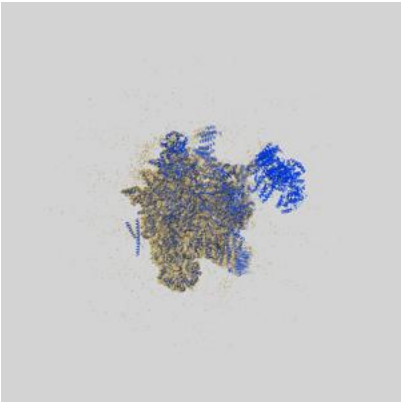
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	3.23	3.95	3.31
Unmasked-calculated*	4.06	7.91	4.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.06 differs from the reported value 3.2 by more than 10 %

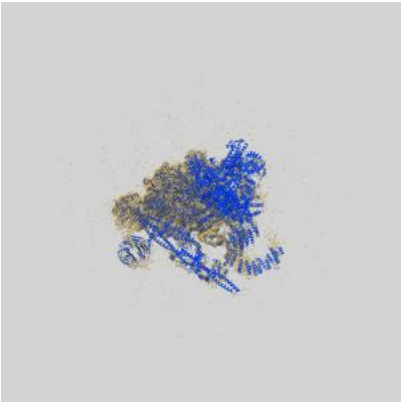
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-19941 and PDB model 9ESH. Per-residue inclusion information can be found in section 3 on page 13.

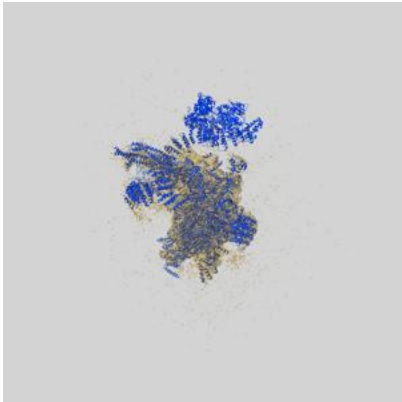
9.1 Map-model overlay (i)



X



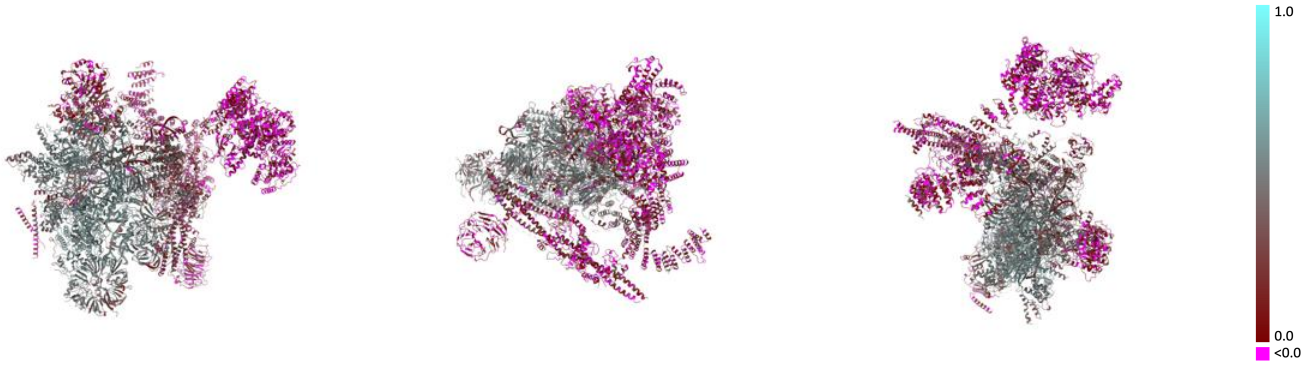
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

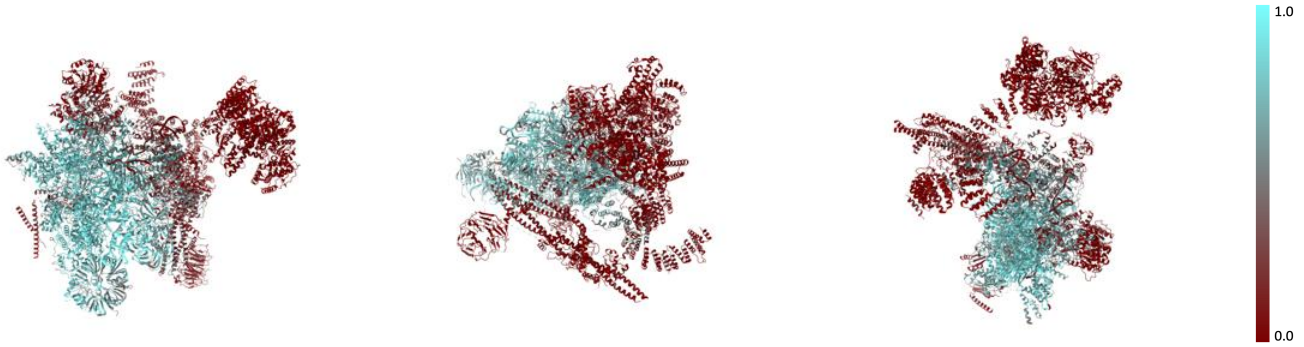
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

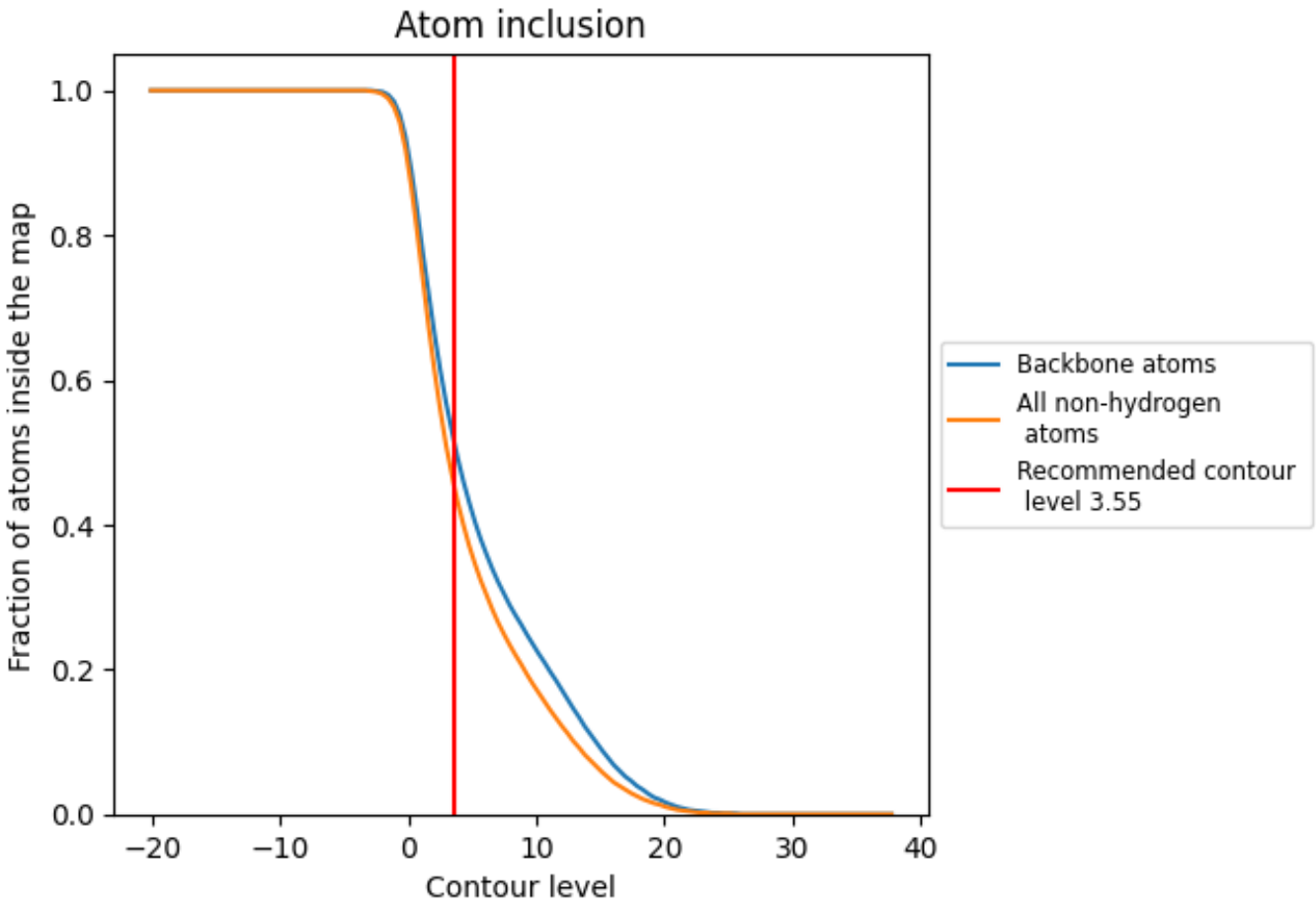
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (3.55).

9.4 Atom inclusion (i)



At the recommended contour level, 52% of all backbone atoms, 46% 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 (3.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4560	0.3240
1	0.4260	0.3460
2	0.4240	0.3160
5	0.8960	0.5180
6	0.5250	0.3510
A	0.8180	0.5270
B	0.8010	0.5140
C	0.6820	0.4410
D	0.8140	0.5290
E	0.7040	0.4790
F	0.6540	0.4320
G	0.6130	0.3800
H	0.7050	0.4650
I	0.7230	0.4510
J	0.7460	0.5120
K	0.8210	0.5120
L	0.6500	0.4400
M	0.3530	0.3180
N	0.0010	0.0390
O	0.7960	0.5120
P	0.4460	0.3400
Q	0.7420	0.5080
R	0.3340	0.2400
S	0.0210	0.0950
T	0.0830	0.1130
U	0.0550	0.1060
V	0.0350	0.0900
W	0.3780	0.2880
X	0.0550	0.0880
Y	0.2010	0.2840
Z	0.1880	0.1880
a	0.5000	0.3400
b	0.2540	0.2530
c	0.7340	0.4730
d	0.4530	0.3460

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Chain	Atom inclusion	Q-score
f	0.2270	0.2320
m	0.1690	0.3020
r	0.1580	0.1660
y	0.3800	0.2950
z	0.1960	0.1910