Full wwPDB EM Validation Report ⓘ

Dec 16, 2024 – 12:27 PM JST

PDB ID	:	8JTI
EMDB ID	:	EMD-36645
Title	:	Cryo-EM structure of human 26S RP (Eb state) bound to K11/K48-branched ubiquitin (Ub) chain composed of four Ub.
Authors	:	Hsu, S.T.D.; Draczkowski, P.; Wang, Y.S.
Deposited on	:	2023-06-21
Resolution	:	3.80 Å(reported)
Based on initial model	:	6MSB

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

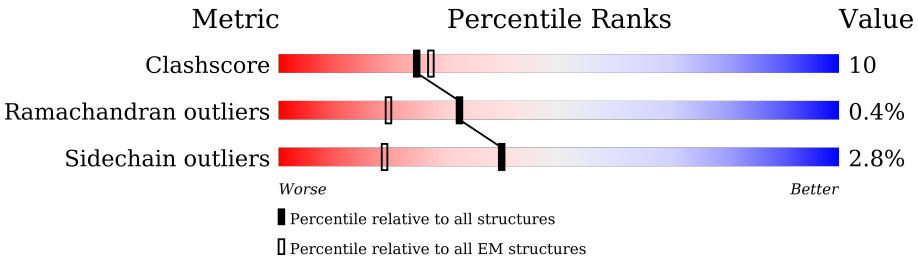
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

1 Overall quality at a glance

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

The reported resolution of this entry is 3.80 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	433	6% 68% 21% • 9%
2	B	440	7% 60% 27% • 13%
3	C	406	8% 63% 25% • 10%
4	D	418	• 65% 24% • 9%
5	E	389	5% 79% 16% • •
6	F	439	5% 74% 15% 10%
7	G	246	78% 20% •
8	H	234	• 85% 14% •

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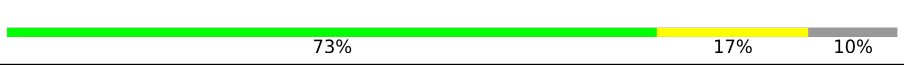
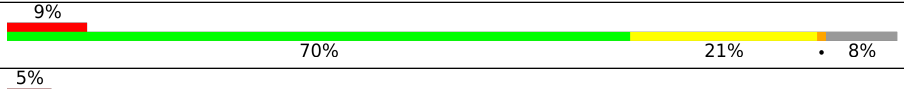
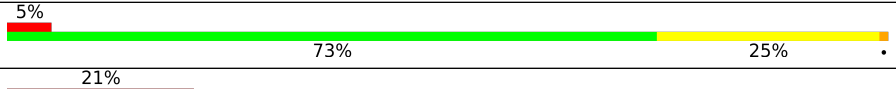
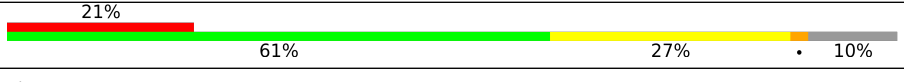
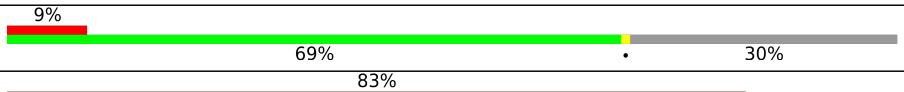
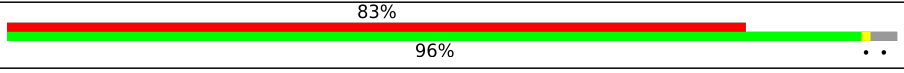
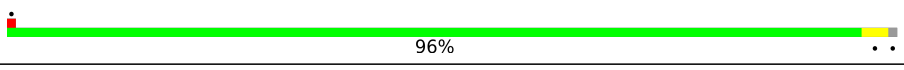
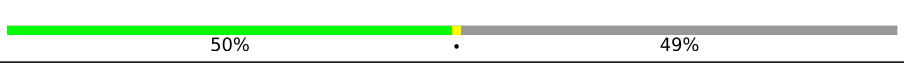
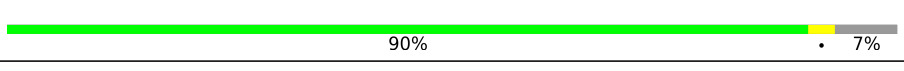
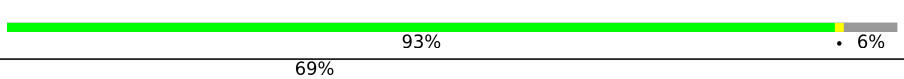
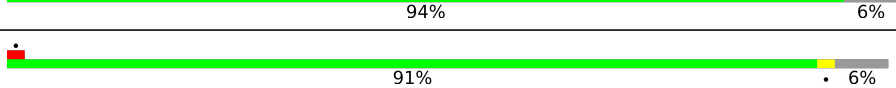
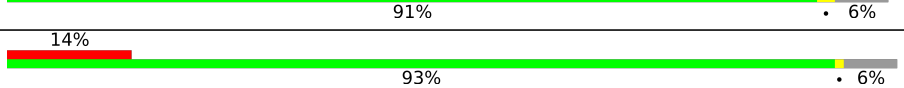
Mol	Chain	Length	Quality of chain
9	I	261	
10	J	248	
11	K	241	
12	L	263	
13	M	255	
14	U	953	
15	V	534	
16	W	456	
17	X	422	
18	Y	389	
19	Z	324	
20	d	350	
21	e	70	
22	f	908	
23	a	376	
24	b	377	
25	c	310	
26	u	81	
26	v	81	
26	w	81	
26	x	81	

2 Entry composition

There are 29 unique types of molecules in this entry. The entry contains 67839 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	394	3096	1951	543	584	18	0	0

- Molecule 2 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	384	3004	1895	515	580	14	0	0

- Molecule 3 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	365	2868	1811	515	526	16	0	0

- Molecule 4 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	380	3039	1923	524	579	13	0	0

- Molecule 5 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	375	2979	1875	529	559	16	0	0

- Molecule 6 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	395	3093	1943	535	598	17	0	0

- Molecule 7 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	240	Total	C	N	O	S	0	0
			1826	1160	305	348	13		

- Molecule 8 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	232	Total	C	N	O	S	0	0
			1708	1081	289	333	5		

- Molecule 9 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	250	Total	C	N	O	S	0	0
			1912	1204	329	371	8		

- Molecule 10 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	239	Total	C	N	O	S	0	0
			1713	1062	311	335	5		

- Molecule 11 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	234	Total	C	N	O	S	0	0
			1759	1102	290	356	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	238	Total	C	N	O	S	0	0
			1850	1159	334	346	11		

- Molecule 13 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	240	Total	C	N	O	S	0	0
			1856	1178	314	353	11		

- Molecule 14 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	U	815	Total	C	N	O	S	0	0
			6361	4040	1083	1194	44		

- Molecule 15 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	493	Total	C	N	O	S	0	0
			3315	2075	622	611	7		

- Molecule 16 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	456	Total	C	N	O	S	0	0
			3292	2064	584	630	14		

- Molecule 17 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	380	Total	C	N	O	S	0	0
			2793	1763	487	534	9		

- Molecule 18 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	378	Total	C	N	O	S	0	0
			3115	1987	533	578	17		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	286	Total	C	N	O	S	0	0
			2281	1457	392	427	5		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	d	257	Total	C	N	O	S	0	0
			2053	1332	336	376	9		

- Molecule 21 is a protein called 26S proteasome complex subunit DSS1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	e	49	Total	C	N	O	S	0	0
			280	171	52	56	1		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	f	880	Total	C	N	O	0	0
			4338	2578	880	880		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	a	373	Total	C	N	O	S	0	0
			2995	1911	510	559	15		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	b	191	Total	C	N	O	S	0	0
			1458	910	261	279	8		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	c	287	Total	C	N	O	S	0	0
			2260	1430	389	422	19		

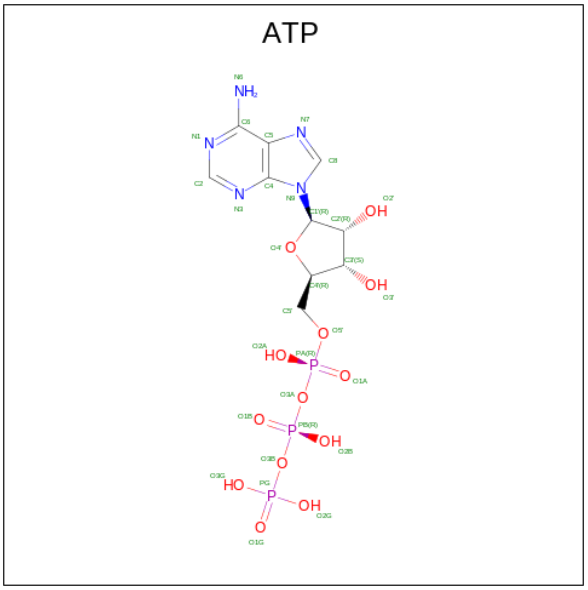
- Molecule 26 is a protein called Polyubiquitin-B.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	v	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
26	u	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
26	x	76	Total	C	N	O	S	0	0
			603	378	107	117	1		
26	w	76	Total	C	N	O	S	0	0
			603	378	107	117	1		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
v	-4	GLY	-	linker	UNP P0CG47
v	-3	SER	-	linker	UNP P0CG47
v	-2	GLY	-	linker	UNP P0CG47
v	-1	GLY	-	linker	UNP P0CG47
v	0	SER	-	linker	UNP P0CG47
v	63	ARG	LYS	engineered mutation	UNP P0CG47
u	-4	GLY	-	linker	UNP P0CG47
u	-3	SER	-	linker	UNP P0CG47
u	-2	GLY	-	linker	UNP P0CG47
u	-1	GLY	-	linker	UNP P0CG47
u	0	SER	-	linker	UNP P0CG47
u	63	ARG	LYS	engineered mutation	UNP P0CG47
x	-4	GLY	-	linker	UNP P0CG47
x	-3	SER	-	linker	UNP P0CG47
x	-2	GLY	-	linker	UNP P0CG47
x	-1	GLY	-	linker	UNP P0CG47
x	0	SER	-	linker	UNP P0CG47
x	63	ARG	LYS	engineered mutation	UNP P0CG47
w	-4	GLY	-	linker	UNP P0CG47
w	-3	SER	-	linker	UNP P0CG47
w	-2	GLY	-	linker	UNP P0CG47
w	-1	GLY	-	linker	UNP P0CG47
w	0	SER	-	linker	UNP P0CG47
w	63	ARG	LYS	engineered mutation	UNP P0CG47

- Molecule 27 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

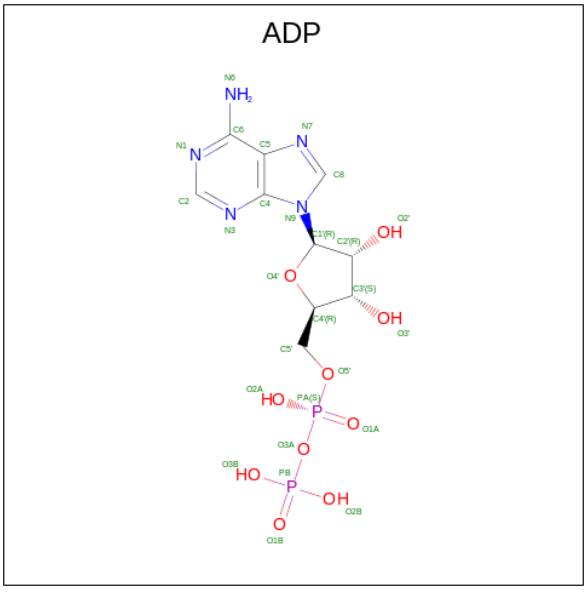


Mol	Chain	Residues	Atoms					AltConf
27	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
27	B	1	Total	C	N	O	P	0
			31	10	5	13	3	
27	D	1	Total	C	N	O	P	0
			31	10	5	13	3	
27	E	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 28 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
28	A	1	Total	Mg	0
			1	1	
28	B	1	Total	Mg	0
			1	1	
28	D	1	Total	Mg	0
			1	1	
28	E	1	Total	Mg	0
			1	1	
28	F	1	Total	Mg	0
			1	1	

- Molecule 29 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



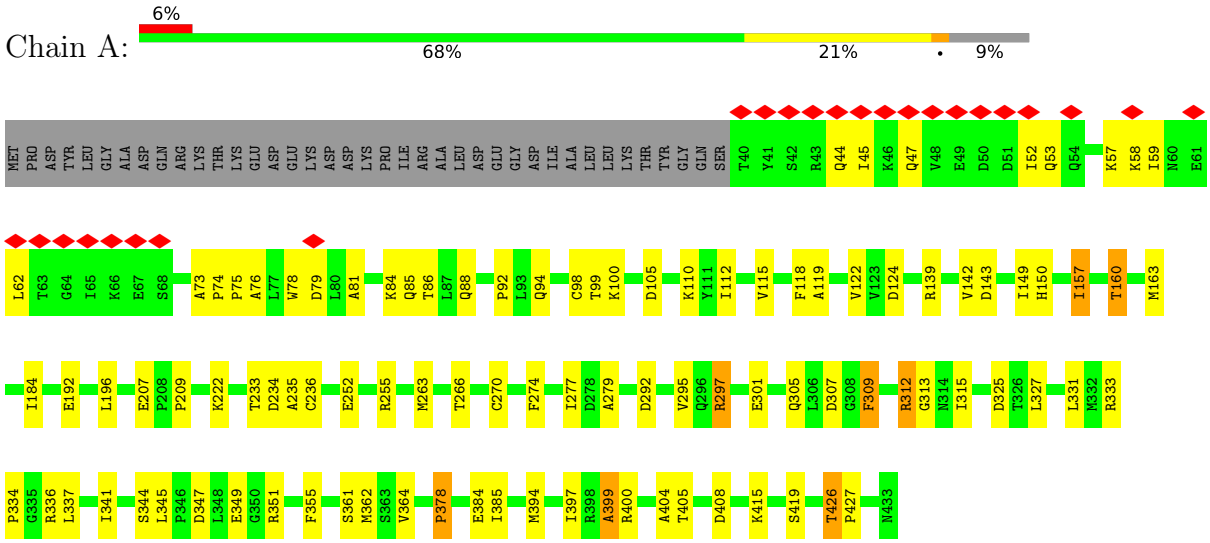
Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
29	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

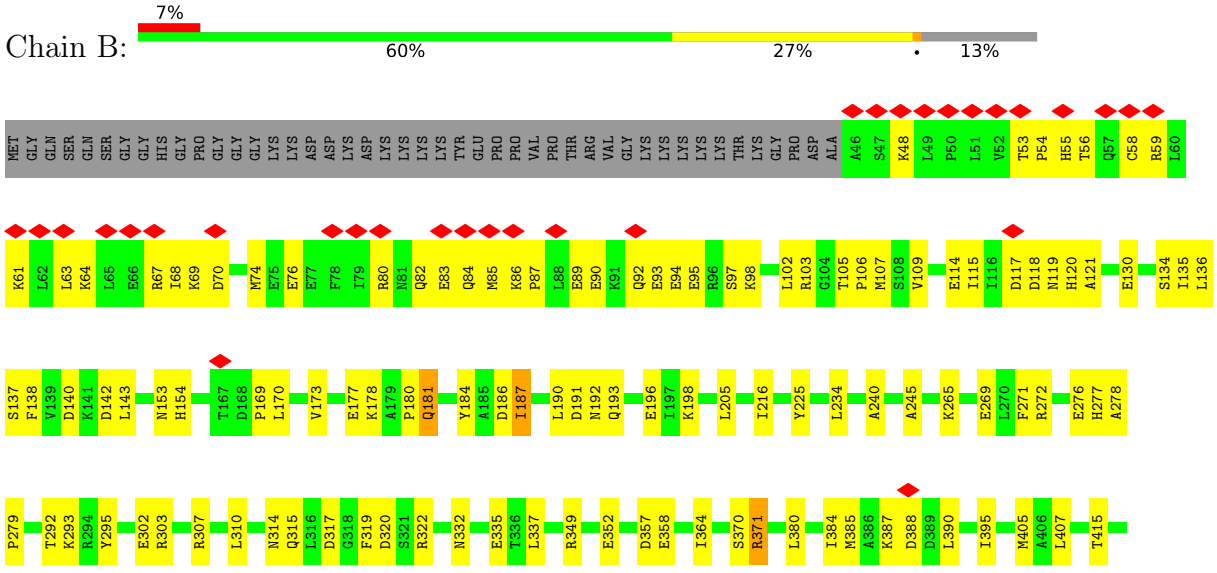
• Molecule 1: 26S protease regulatory subunit 7

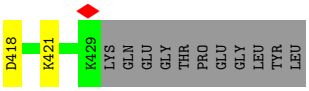
Chain A:



• Molecule 2: 26S protease regulatory subunit 4

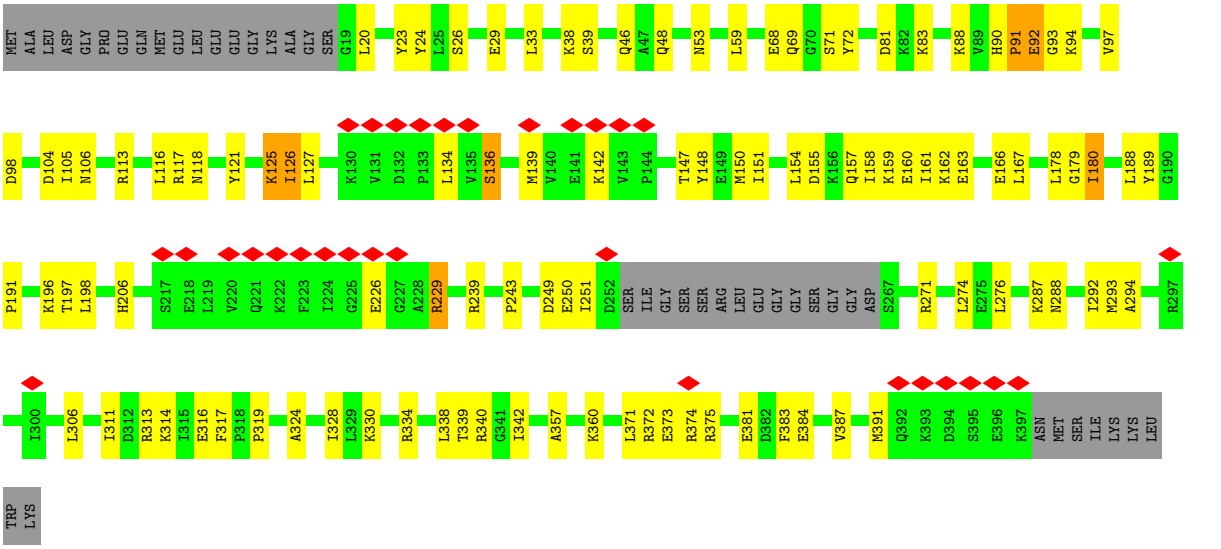
Chain B:





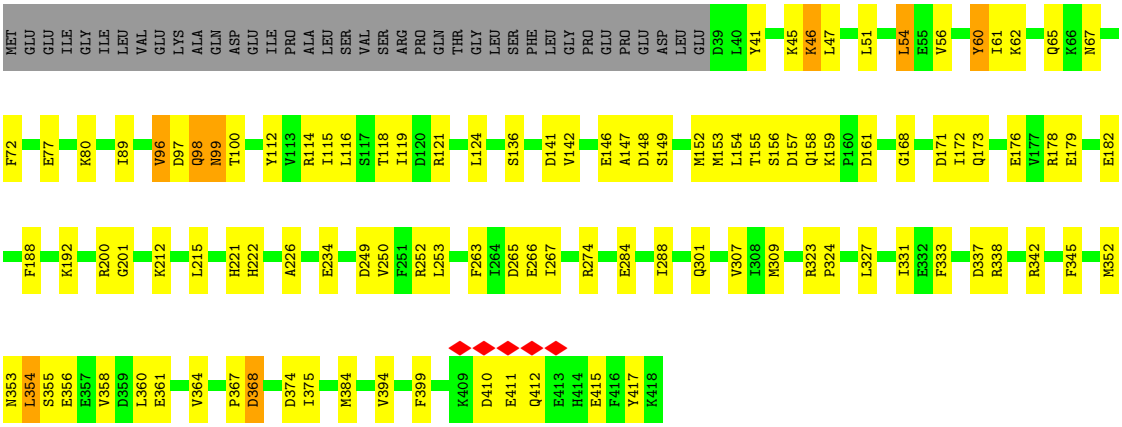
• Molecule 3: 26S protease regulatory subunit 8

Chain C:



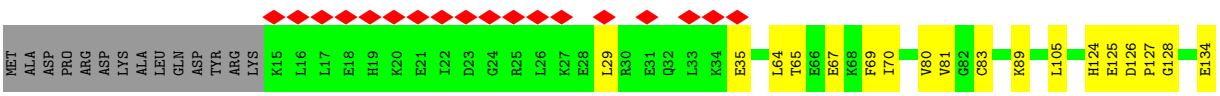
• Molecule 4: 26S protease regulatory subunit 6B

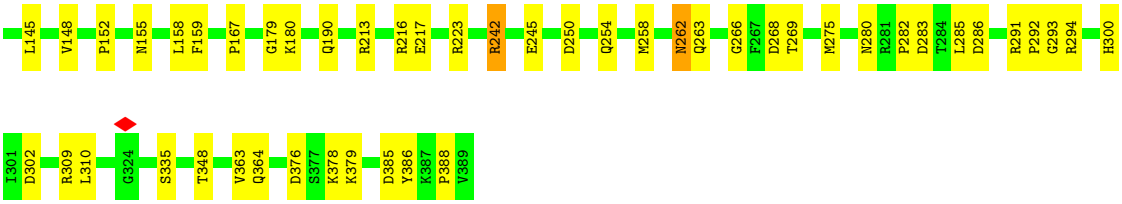
Chain D:



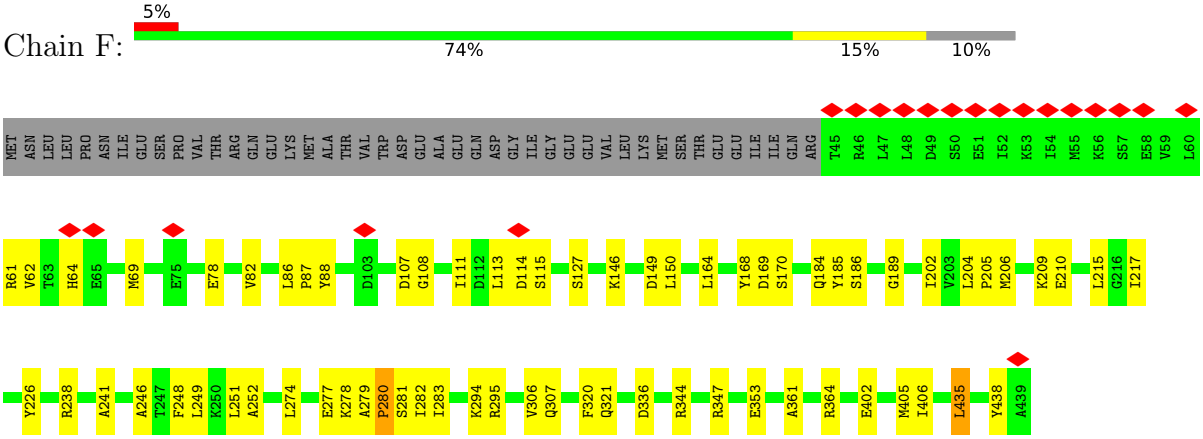
• Molecule 5: 26S protease regulatory subunit 10B

Chain E:

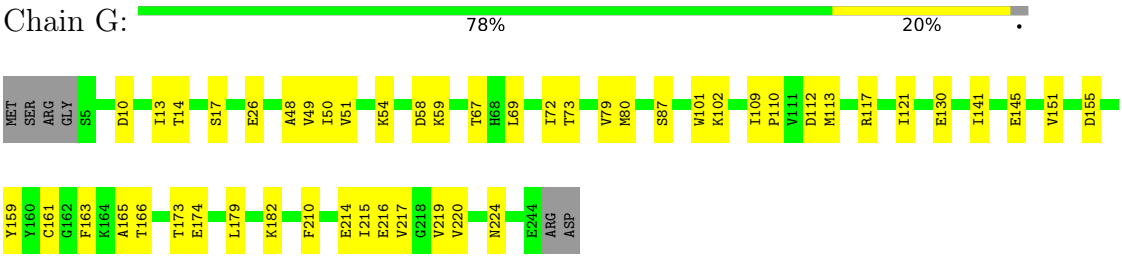




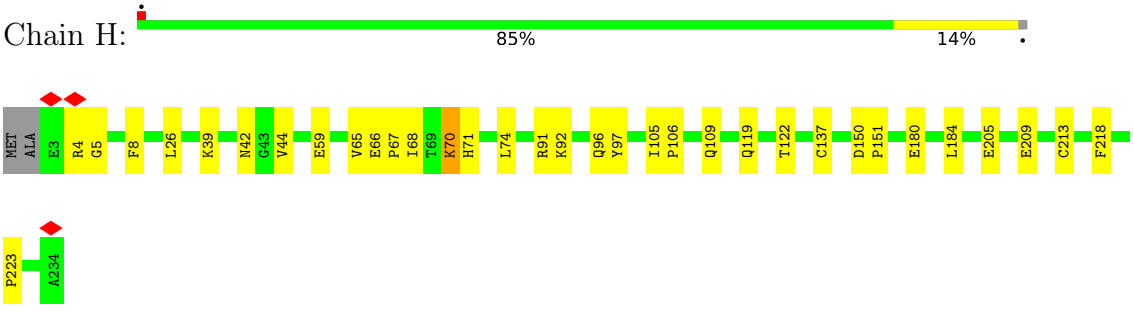
• Molecule 6: 26S protease regulatory subunit 6A



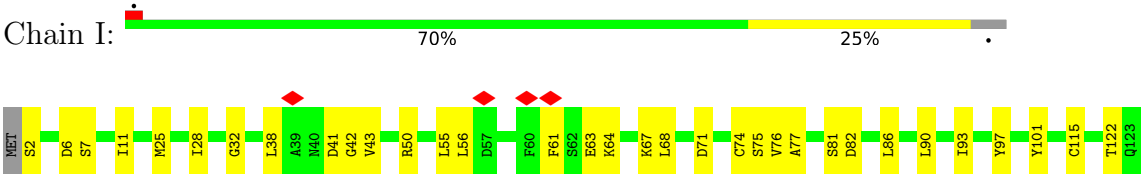
• Molecule 7: Proteasome subunit alpha type-6



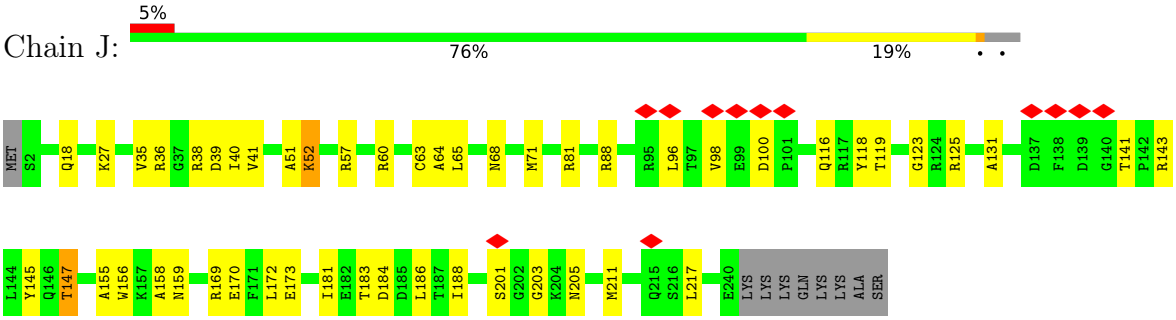
• Molecule 8: Proteasome subunit alpha type-2



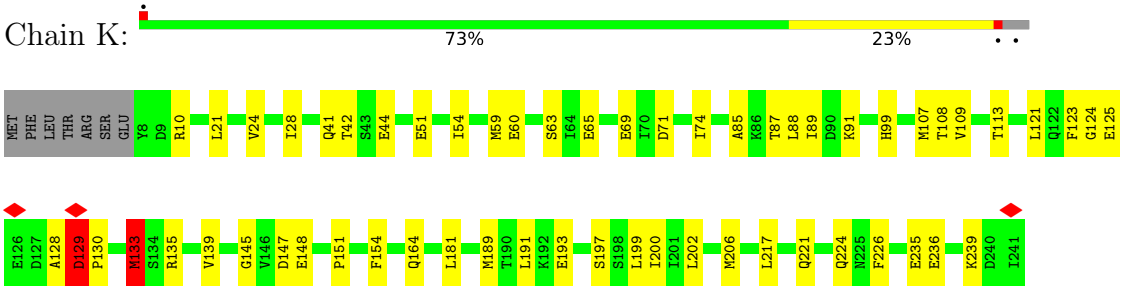
• Molecule 9: Proteasome subunit alpha type-4



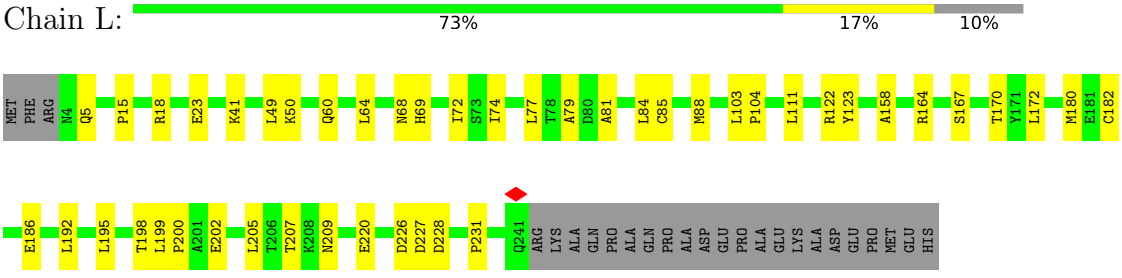
• Molecule 10: Proteasome subunit alpha type-7



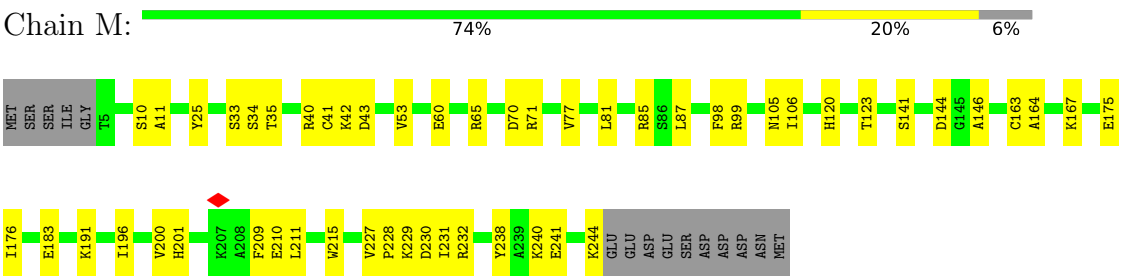
• Molecule 11: Proteasome subunit alpha type-5



• Molecule 12: Proteasome subunit alpha type-1

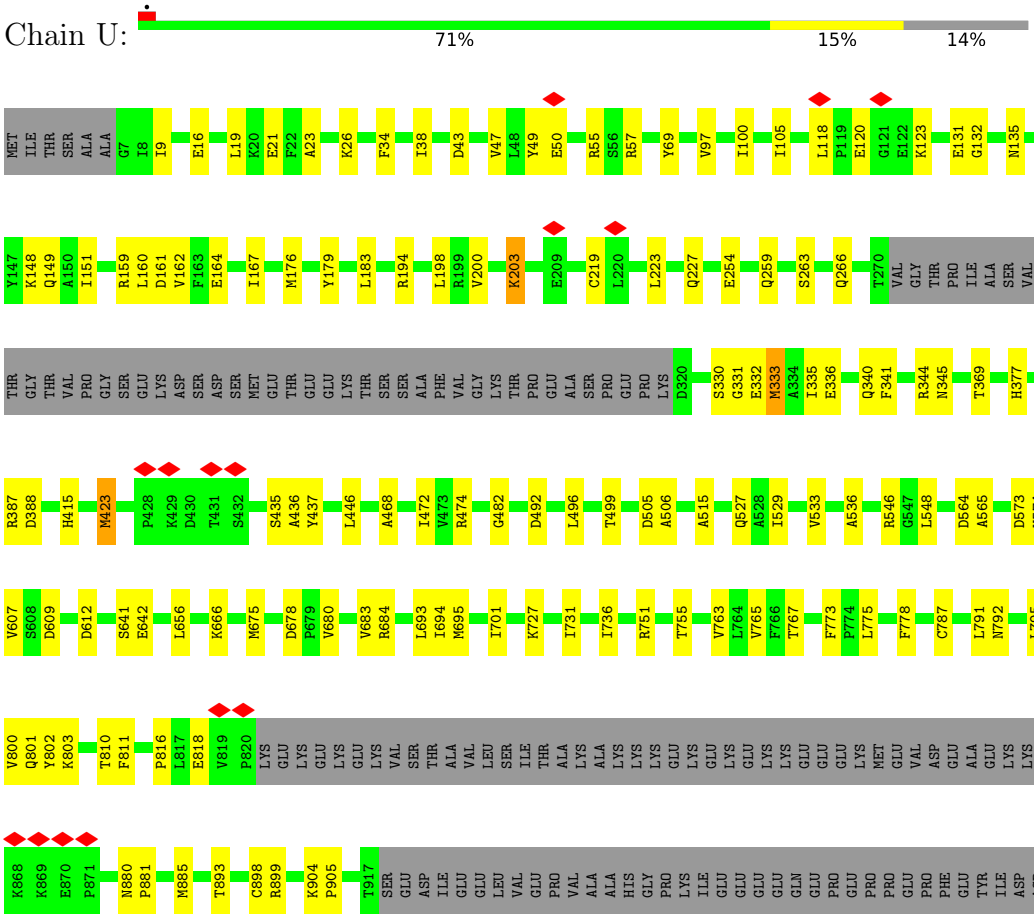


• Molecule 13: Proteasome subunit alpha type-3



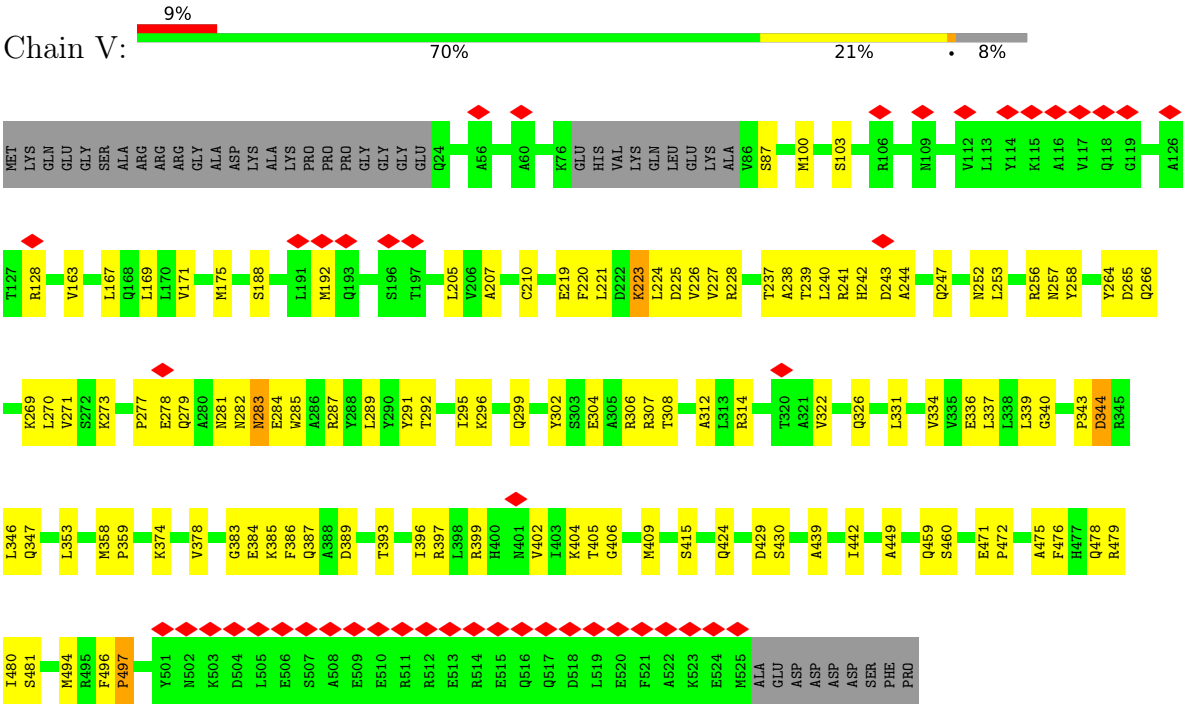
• Molecule 14: 26S proteasome non-ATPase regulatory subunit 1

Chain U:



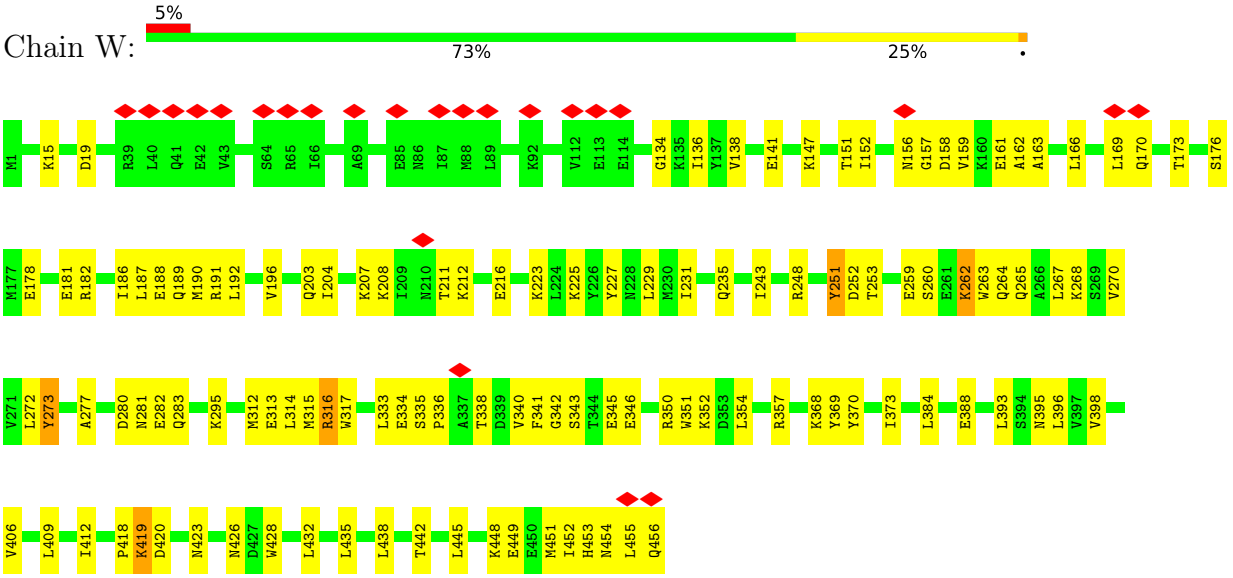
• Molecule 15: 26S proteasome non-ATPase regulatory subunit 3

Chain V:



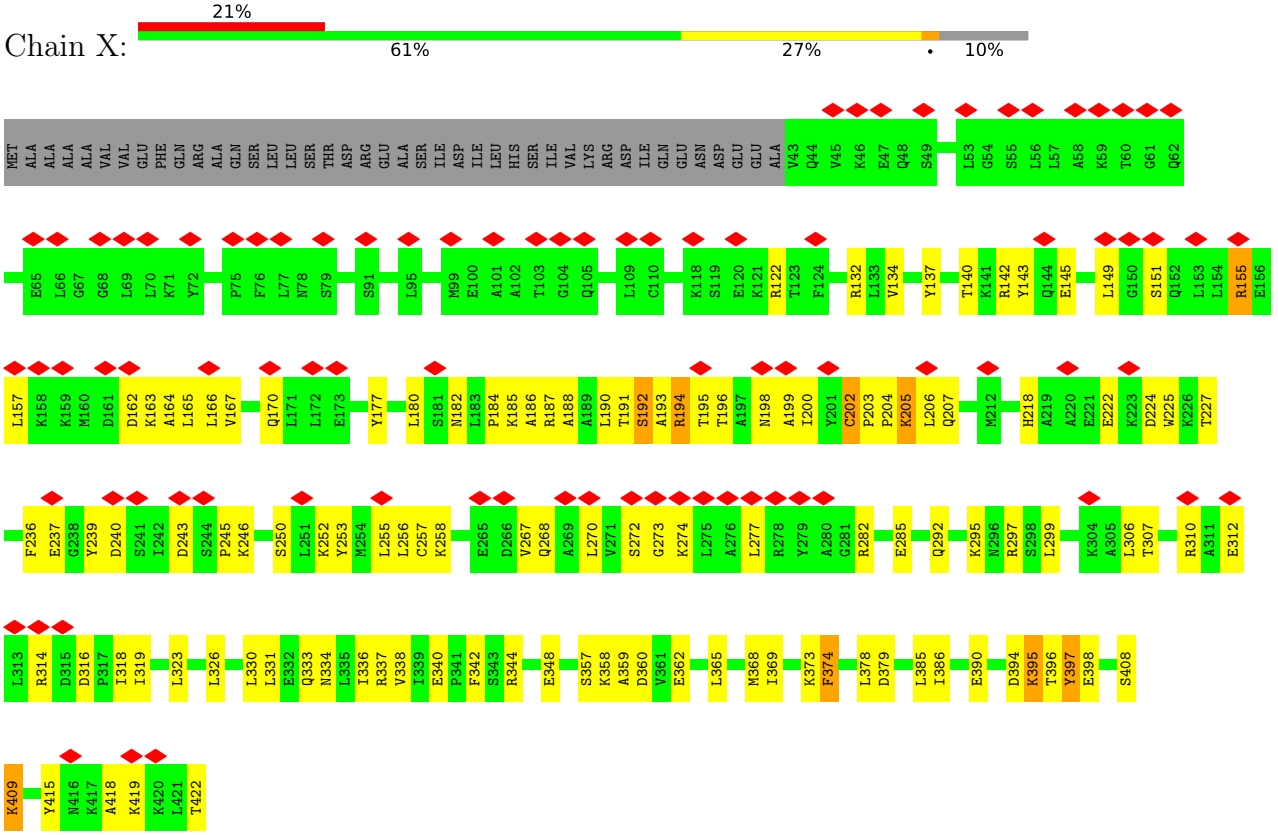
• Molecule 16: 26S proteasome non-ATPase regulatory subunit 12

Chain W:



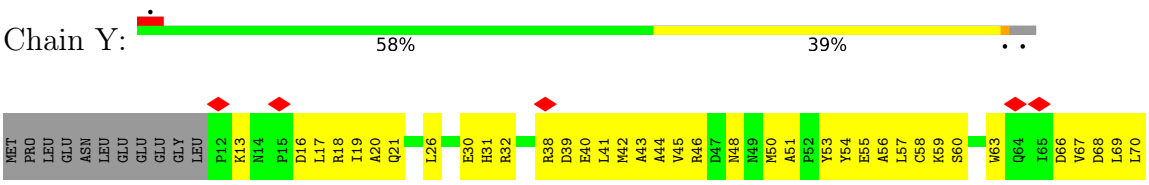
• Molecule 17: 26S proteasome non-ATPase regulatory subunit 11

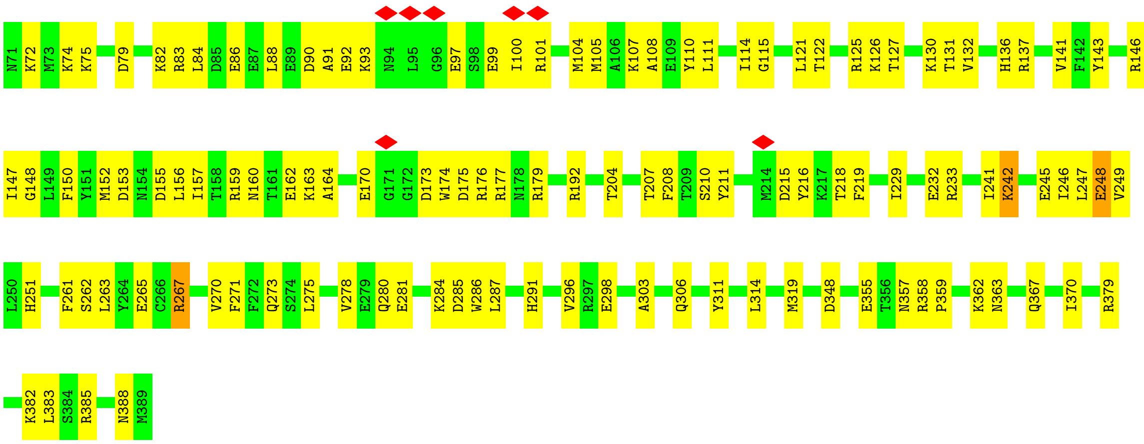
Chain X:



• Molecule 18: 26S proteasome non-ATPase regulatory subunit 6

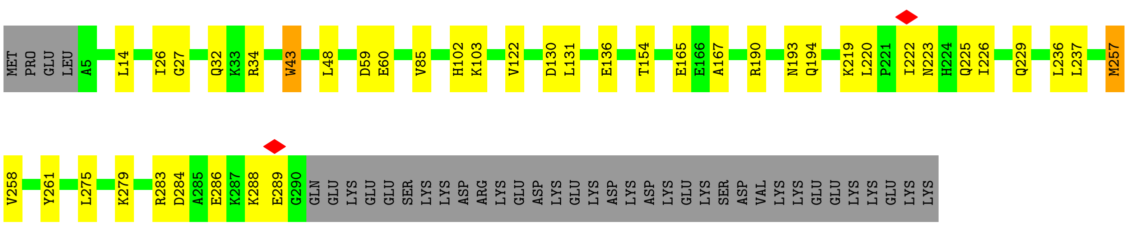
Chain Y:





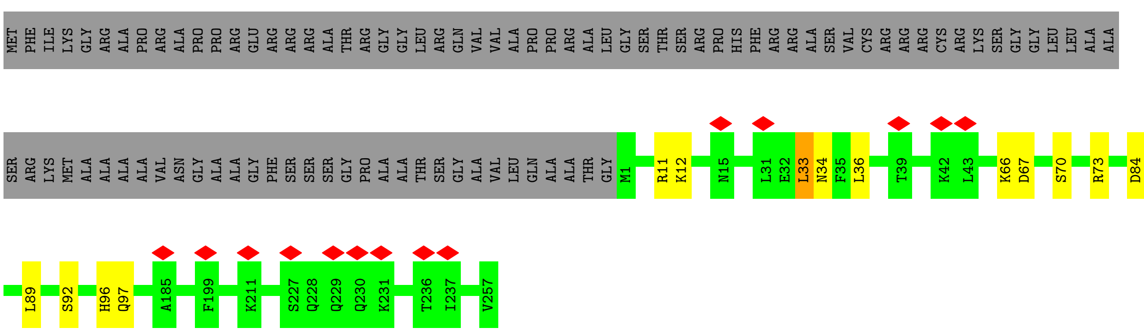
- Molecule 19: 26S proteasome non-ATPase regulatory subunit 7

Chain Z:



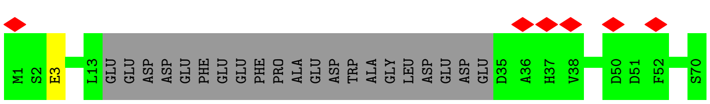
- Molecule 20: 26S proteasome non-ATPase regulatory subunit 8

Chain d:



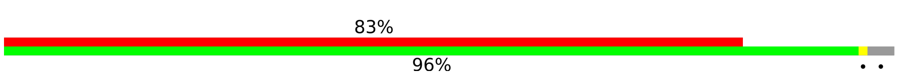
- Molecule 21: 26S proteasome complex subunit DSS1

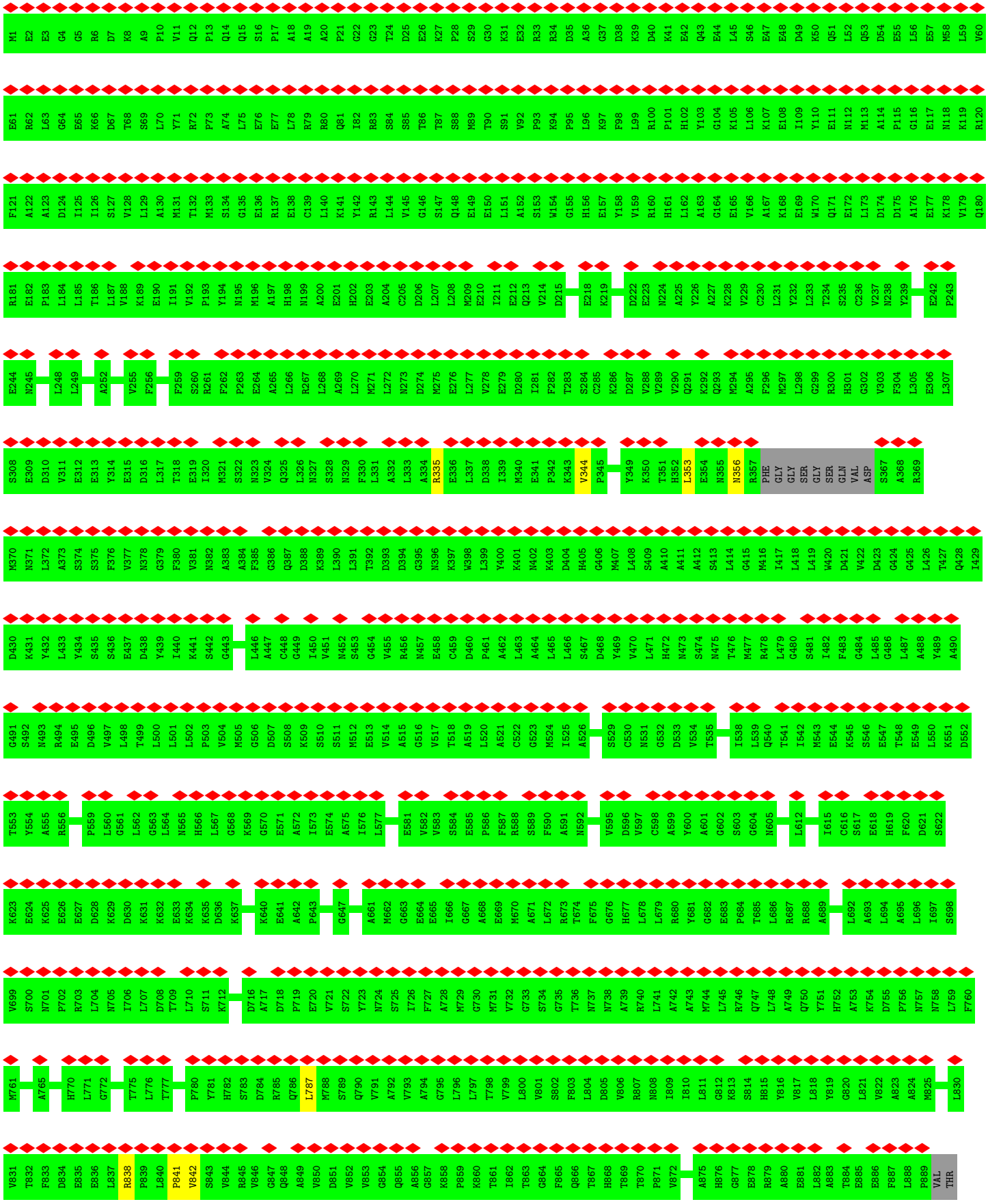
Chain e:



- Molecule 22: 26S proteasome non-ATPase regulatory subunit 2

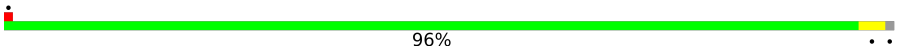
Chain f:

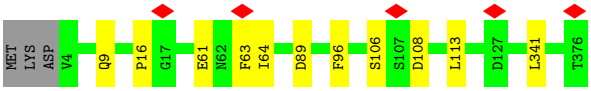



M1 E2 E3 G4 G5 R6 D7 K8 A9 P10 V11 Q12 P13 Q14 Q15 S16 P17 A18 A19 A20 P21 G22 G23 T24 D25 E26 K27 P28 S29 G30 K31 E32 R33 R34 D35 A36 G37 D38 K39 D40 K41 E42 Q43 E44 L45 S46 E47 E48 D49 K50 Q51 L52 Q53 D54 E55 L56 E57 M58 L59 V60
E61 R62 L63 G64 E65 K66 D67 T68 S69 L70 Y71 R72 P73 A74 L75 E76 E77 L78 R79 R80 Q81 I82 R83 S84 S85 T86 T87 S88 M89 T90 S91 V92 P93 K94 P95 L96 K97 F98 L99 R100 P101 H102 Y103 G104 K105 L106 K107 E108 I109 Y110 E111 N112 M113 A114 P115 G116 E117 N118 K119 R120
F121 A122 A123 D124 I125 I126 S127 V128 L129 A130 M131 T132 M133 S134 G135 E136 R137 E138 C139 L140 K141 Y142 R143 L144 V145 G146 S147 Q148 E149 E150 L151 A152 S153 W154 G155 H156 E157 Y158 V159 R160 H161 L162 A163 G164 E165 V166 A167 K168 E169 W170 Q171 E172 L173 D174 D175 A176 E177 K178 V179 Q180
R181 E182 P183 L184 L185 T186 L187 V188 K189 E190 I191 V192 P193 Y194 N195 M196 A197 H198 N199 A200 E201 H202 E203 A204 C205 D206 L207 L208 M209 E210 I211 E212 Q213 V214 D215 E218 K219 D222 E223 N224 A225 Y226 A227 K228 V229 C230 L231 Y232 L233 T234 S235 C236 V237 N238 Y239 E242 P243
E244 N245 L248 L249 A252 V255 F256 F259 S260 R261 F262 P263 E264 A265 L266 R267 L268 A269 L270 M271 L272 N273 D274 M275 E276 L277 V278 E279 D280 I281 F282 T283 S284 C285 K286 D287 V288 V289 V290 Q291 K292 Q293 M294 A295 F296 M297 L298 G299 R300 H301 G302 V303 F304 L305 E306 L307
S308 E309 D310 V311 E312 E313 Y314 E315 D316 L317 T318 E319 I320 M321 S322 N323 V324 Q325 L326 N327 S328 N329 F330 L331 A332 L333 A334 R335 E336 L337 D338 I339 M340 E341 P342 K343 V344 P345 Y349 K350 T351 H352 L353 E354 N355 N356 R357 PHE GLY GLY SER GLY SER GLN VAL ASP S367 A368 R369
M370 N371 L372 A373 S374 S375 F376 V377 N378 G379 F380 V381 N382 A383 A384 F385 G386 Q387 D388 K389 L390 L391 T392 D393 D394 G395 N396 K397 W398 L399 Y400 K401 N402 K403 D404 H405 G406 M407 L408 S409 A410 A411 A412 S413 L414 G415 M416 I417 L418 L419 W420 D421 V422 D423 G424 G425 L426 T427 Q428 I429
D430 K431 Y432 L433 Y434 S435 S436 E437 D438 Y439 I440 K441 S442 G443 L446 A447 C448 G449 I450 V451 N452 S453 G454 V455 R456 N457 E458 C459 D460 P461 A462 L463 A464 L465 L466 S467 D468 Y469 V470 L471 H472 N473 S474 N475 T476 M477 R478 L479 G480 S481 I482 F483 G484 L485 G486 L487 A488 Y489 A490
G491 S492 N493 R494 E495 D496 V497 L498 T499 L500 L501 L502 P503 V504 M505 G506 D507 S508 K509 S510 S511 M512 E513 V514 A515 G516 V517 T518 A519 L520 A521 C522 G523 M524 I525 A526 S529 C530 N531 G532 D533 V534 T535 I538 L539 Q540 T541 I542 M543 E544 K545 S546 E547 T548 E549 L550 K551 D552
T553 Y554 A555 R556 P559 L560 G561 L562 G563 L564 N565 H566 L567 G568 K569 G570 E571 A572 I573 E574 A575 T576 L577 E581 V582 V583 S584 E585 P586 F587 R588 S589 F590 A591 N592 V595 D596 V597 C598 A599 Y600 A601 G602 S603 G604 N605 L612 I615 C616 S617 E618 H619 F620 D621 S622
K623 E624 K625 E626 E627 D628 K629 D630 K631 K632 E633 K634 K635 D636 K637 K640 E641 A642 P643 G647 A661 M662 G663 E664 E665 I666 G667 A668 E669 M670 A671 L672 R673 T674 F675 G676 H677 L678 L679 R680 Y681 G682 E683 P684 T685 L686 R687 R688 A689 L692 A693 L694 A695 L696 I697 S698
V699 S700 N701 P702 R703 L704 N705 I706 L707 D708 T709 L710 S711 K712 D716 A717 D718 P719 E720 V721 S722 Y723 N724 S725 I726 F727 A728 M729 G730 M731 V732 G733 S734 G735 T736 N737 N738 A739 R740 L741 A742 A743 M744 L745 R746 Q747 L748 A749 Q750 Y751 H752 A753 K754 D755 P756 N757 N758 L759 F760
M761 A765 H770 L771 G772 T775 L776 T777 P780 Y781 H782 S783 D784 R785 Q786 L787 M788 S789 Q790 V791 A792 V793 A794 G795 L796 L797 T798 V799 L800 V801 S802 F803 L804 D805 V806 R807 N808 I809 I810 L811 G812 K813 S814 H815 Y816 V817 L818 Y819 G820 L821 V822 A823 A824 M825 L830
V831 T832 F833 D834 E835 E836 L837 R838 P839 L840 P841 V842 S843 V844 R845 V846 G847 Q848 A849 V850 D851 V852 V853 G854 Q855 A856 G857 K858 P859 K860 T861 I862 T863 G864 F865 Q866 T867 H868 T869 T870 P871 V872 A875 H876 G877 E878 R879 A880 E881 L882 A883 T884 E885 E886 F887 L888 P889 VAL THR

• Molecule 23: 26S proteasome non-ATPase regulatory subunit 13

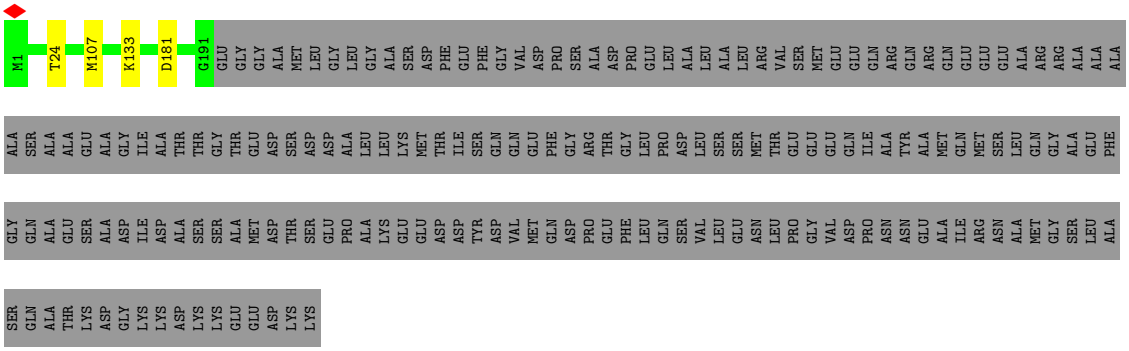
Chain a:





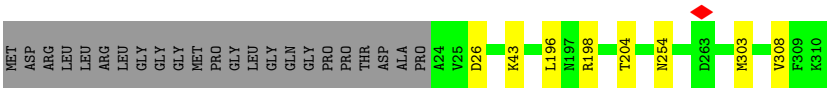
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 4

Chain b:



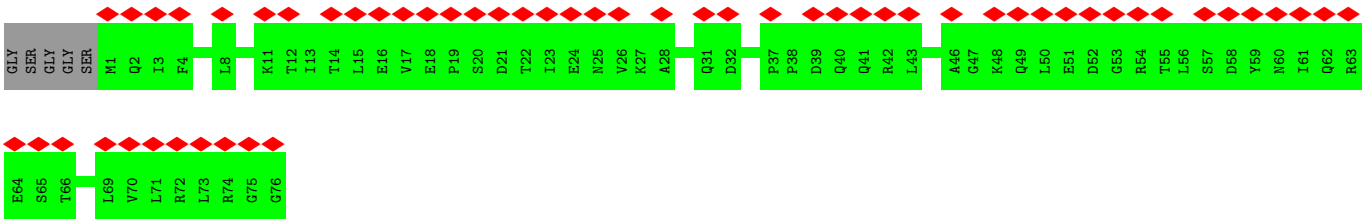
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 14

Chain c:



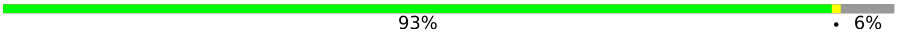
• Molecule 26: Polyubiquitin-B

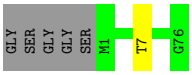
Chain v:



• Molecule 26: Polyubiquitin-B

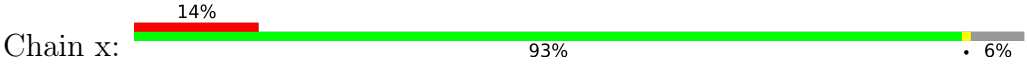
Chain u:

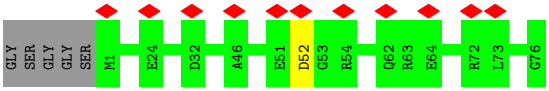




• Molecule 26: Polyubiquitin-B

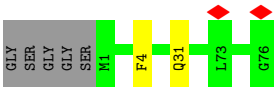
Chain x:





• Molecule 26: Polyubiquitin-B

Chain w:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	52216	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	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	70000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	50.794	Depositor
Minimum map value	-23.427	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	5	Depositor
Map size (Å)	560.0, 560.0, 560.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4, 1.4, 1.4	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ATP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.59	0/3148	0.66	0/4250
2	B	0.49	0/3047	0.63	0/4111
3	C	0.42	0/2905	0.62	0/3910
4	D	0.52	0/3089	0.61	0/4168
5	E	0.57	0/3025	0.69	0/4073
6	F	0.56	0/3134	0.65	0/4225
7	G	0.46	0/1859	0.56	0/2523
8	H	0.43	0/1743	0.53	0/2372
9	I	0.38	0/1942	0.55	0/2628
10	J	0.42	0/1737	0.57	0/2369
11	K	0.41	0/1786	0.56	0/2419
12	L	0.46	0/1885	0.59	0/2552
13	M	0.47	0/1891	0.56	0/2552
14	U	0.51	0/6476	0.62	0/8764
15	V	0.42	0/3360	0.60	0/4587
16	W	0.40	0/3332	0.56	0/4514
17	X	0.35	0/2831	0.53	0/3835
18	Y	0.46	0/3173	0.59	0/4273
19	Z	0.63	0/2324	0.64	0/3150
20	d	0.39	0/2096	0.59	0/2835
21	e	0.29	0/279	0.59	0/379
22	f	0.24	0/4336	0.45	0/6030
23	a	0.39	0/3053	0.58	0/4133
24	b	0.48	0/1478	0.67	0/2001
25	c	0.61	0/2302	0.65	0/3110
26	u	0.51	0/609	0.62	0/819
26	v	0.28	0/609	0.53	0/819
26	w	0.38	0/609	0.64	0/819
26	x	0.29	0/609	0.56	0/819
All	All	0.47	0/68667	0.60	0/93039

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3096	0	3138	78	0
2	B	3004	0	3063	93	0
3	C	2868	0	2964	81	0
4	D	3039	0	3075	80	0
5	E	2979	0	3052	45	0
6	F	3093	0	3165	44	0
7	G	1826	0	1796	35	0
8	H	1708	0	1594	23	0
9	I	1912	0	1851	50	0
10	J	1713	0	1537	39	0
11	K	1759	0	1707	41	0
12	L	1850	0	1822	31	0
13	M	1856	0	1814	34	0
14	U	6361	0	6397	83	0
15	V	3315	0	2757	82	0
16	W	3292	0	2975	100	0
17	X	2793	0	2662	83	0
18	Y	3115	0	3120	129	0
19	Z	2281	0	2312	38	0
20	d	2053	0	2029	0	0
21	e	280	0	190	0	0
22	f	4338	0	2026	0	0
23	a	2995	0	3012	0	0
24	b	1458	0	1505	0	0
25	c	2260	0	2276	0	0
26	u	603	0	629	0	0
26	v	603	0	629	0	0
26	w	603	0	629	0	0
26	x	603	0	629	0	0
27	A	31	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
27	B	31	0	12	0	0
27	D	31	0	12	1	0
27	E	31	0	12	2	0
28	A	1	0	0	0	0
28	B	1	0	0	0	0
28	D	1	0	0	0	0
28	E	1	0	0	0	0
28	F	1	0	0	0	0
29	C	27	0	12	3	0
29	F	27	0	12	1	0
All	All	67839	0	64427	1097	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 10.

All (1097) 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)
4:D:60:TYR:HB2	14:U:603:LEU:HD21	1.51	0.93
9:I:42:GLY:HA2	9:I:216:LEU:O	1.70	0.92
7:G:50:ILE:HG21	7:G:79:VAL:HG21	1.50	0.91
15:V:270:LEU:HD12	15:V:271:VAL:HG13	1.54	0.88
6:F:111:ILE:HG22	6:F:113:LEU:H	1.37	0.88
3:C:20:LEU:HD13	14:U:149:GLN:HG2	1.63	0.78
16:W:260:SER:HA	16:W:263:TRP:HB3	1.65	0.78
1:A:85:GLN:HE22	2:B:136:LEU:HD13	1.47	0.78
17:X:202:CYS:H	17:X:203:PRO:HD3	1.50	0.77
5:E:282:PRO:HB2	5:E:388:PRO:HB3	1.67	0.75
15:V:242:HIS:NE2	15:V:244:ALA:O	2.19	0.75
12:L:74:ILE:HD13	12:L:81:ALA:HB1	1.68	0.75
2:B:105:THR:HG23	2:B:106:PRO:HD3	1.69	0.74
1:A:52:ILE:HD13	2:B:69:LYS:HD2	1.68	0.74
14:U:135:ASN:HA	14:U:138:PHE:HD2	1.53	0.73
15:V:266:GLN:OE1	15:V:299:GLN:NE2	2.20	0.73
3:C:125:LYS:NZ	3:C:126:ILE:O	2.18	0.73
1:A:309:PHE:H	6:F:238:ARG:HH21	1.36	0.73
10:J:63:CYS:SG	10:J:88:ARG:NH2	2.61	0.73
1:A:295:VAL:HG21	2:B:307:ARG:HH22	1.53	0.73
4:D:141:ASP:OD1	4:D:142:VAL:N	2.22	0.72
8:H:68:ILE:HD11	8:H:74:LEU:HB2	1.70	0.72
16:W:216:GLU:HB3	16:W:223:LYS:HB2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:287:LYS:HE3	3:C:288:ASN:H	1.53	0.72
3:C:371:LEU:O	3:C:374:ARG:NH1	2.23	0.72
2:B:80:ARG:HG2	2:B:84:GLN:HE22	1.56	0.71
5:E:64:LEU:HD23	5:E:65:THR:HG23	1.71	0.71
18:Y:101:ARG:NH2	18:Y:126:LYS:O	2.24	0.71
9:I:218:ARG:NH1	9:I:219:GLU:O	2.23	0.71
16:W:449:GLU:HB3	19:Z:222:ILE:HG12	1.73	0.71
13:M:141:SER:HB3	13:M:144:ASP:HB2	1.71	0.71
16:W:173:THR:O	16:W:182:ARG:NH1	2.23	0.71
13:M:215:TRP:HE3	13:M:227:VAL:HG12	1.55	0.71
18:Y:107:LYS:HZ1	18:Y:110:TYR:HD2	1.37	0.71
19:Z:223:ASN:OD1	19:Z:225:GLN:N	2.23	0.70
4:D:274:ARG:NH1	5:E:245:GLU:OE2	2.25	0.70
18:Y:241:ILE:HD11	18:Y:261:PHE:HE1	1.56	0.70
14:U:468:ALA:O	14:U:474:ARG:NH2	2.23	0.70
2:B:269:GLU:OE2	2:B:272:ARG:NH2	2.25	0.70
16:W:451:MET:SD	19:Z:103:LYS:NZ	2.62	0.70
16:W:452:ILE:HA	19:Z:103:LYS:HZ3	1.57	0.70
18:Y:192:ARG:HD3	18:Y:291:HIS:CG	2.26	0.70
1:A:351:ARG:NH1	1:A:378:PRO:O	2.25	0.69
2:B:364:ILE:HG22	2:B:395:ILE:HG21	1.75	0.69
11:K:124:GLY:H	11:K:133:MET:HG2	1.57	0.69
12:L:192:LEU:HD12	12:L:205:LEU:HD21	1.75	0.69
16:W:203:GLN:OE1	16:W:207:LYS:NZ	2.26	0.69
2:B:405:MET:SD	2:B:421:LYS:NZ	2.62	0.68
18:Y:121:LEU:HG	18:Y:125:ARG:HH12	1.58	0.68
1:A:84:LYS:O	1:A:88:GLN:NE2	2.26	0.68
13:M:34:SER:OG	13:M:65:ARG:NH1	2.25	0.68
4:D:384:MET:HE1	5:E:167:PRO:HD3	1.74	0.68
10:J:65:LEU:HB2	10:J:71:MET:HE3	1.76	0.68
18:Y:39:ASP:OD1	18:Y:40:GLU:N	2.26	0.68
10:J:131:ALA:H	10:J:147:THR:HG22	1.59	0.68
13:M:201:HIS:O	13:M:201:HIS:ND1	2.26	0.68
3:C:53:ASN:ND2	14:U:642:GLU:O	2.28	0.67
18:Y:358:ARG:HD2	18:Y:359:PRO:HD2	1.74	0.67
3:C:189:TYR:CE1	3:C:316:GLU:HG2	2.29	0.67
11:K:221:GLN:OE1	11:K:224:GLN:NE2	2.27	0.67
4:D:67:ASN:ND2	14:U:607:VAL:O	2.27	0.67
1:A:207:GLU:OE1	1:A:207:GLU:N	2.27	0.67
16:W:452:ILE:HA	19:Z:103:LYS:NZ	2.10	0.67
5:E:127:PRO:HD3	6:F:321:GLN:HG2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:266:GLU:OE2	5:E:258:MET:HB2	1.95	0.66
13:M:65:ARG:NH2	13:M:77:VAL:O	2.24	0.66
16:W:338:THR:O	16:W:342:GLY:N	2.22	0.66
2:B:89:GLU:HB2	2:B:94:GLU:HG2	1.78	0.66
8:H:105:ILE:HD11	8:H:109:GLN:HB2	1.78	0.66
15:V:171:VAL:O	15:V:175:MET:N	2.24	0.66
8:H:213:CYS:HB2	8:H:218:PHE:HD1	1.60	0.66
16:W:169:LEU:HD11	16:W:189:GLN:HG3	1.77	0.66
4:D:374:ASP:OD1	5:E:292:PRO:HG2	1.96	0.66
15:V:399:ARG:O	15:V:402:VAL:HB	1.95	0.66
1:A:274:PHE:HB3	1:A:277:ILE:HD11	1.77	0.66
16:W:272:LEU:HD21	16:W:340:VAL:HG21	1.77	0.66
17:X:218:HIS:NE2	17:X:227:THR:OG1	2.29	0.66
15:V:384:GLU:HA	15:V:387:GLN:HE21	1.62	0.65
4:D:173:GLN:HG2	4:D:333:PHE:CE1	2.31	0.65
17:X:397:TYR:HE1	19:Z:258:VAL:HG11	1.62	0.65
7:G:173:THR:OG1	7:G:174:GLU:OE1	2.15	0.65
14:U:120:GLU:HA	14:U:123:LYS:HE3	1.78	0.65
16:W:189:GLN:HA	16:W:192:LEU:HD13	1.78	0.65
18:Y:130:LYS:NZ	18:Y:131:THR:OG1	2.29	0.65
7:G:174:GLU:OE1	7:G:174:GLU:N	2.26	0.65
16:W:280:ASP:OD1	16:W:281:ASN:N	2.30	0.65
16:W:453:HIS:CD2	19:Z:219:LYS:HD2	2.31	0.65
17:X:282:ARG:NH1	17:X:312:GLU:OE1	2.30	0.65
1:A:86:THR:HB	2:B:102:LEU:HD11	1.79	0.65
10:J:40:ILE:HA	10:J:211:MET:O	1.96	0.65
19:Z:219:LYS:HD3	19:Z:220:LEU:H	1.62	0.65
14:U:678:ASP:O	14:U:684:ARG:NH1	2.30	0.64
3:C:48:GLN:HB3	4:D:65:GLN:HE22	1.62	0.64
3:C:147:THR:OG1	3:C:206:HIS:NE2	2.30	0.64
2:B:357:ASP:OD1	2:B:358:GLU:N	2.30	0.64
4:D:89:ILE:HD11	5:E:80:VAL:HG23	1.77	0.64
14:U:536:ALA:HB2	14:U:548:LEU:HD23	1.78	0.64
15:V:322:VAL:O	15:V:326:GLN:NE2	2.22	0.64
18:Y:53:TYR:HD2	18:Y:57:LEU:HD13	1.61	0.64
16:W:452:ILE:HG13	16:W:453:HIS:ND1	2.12	0.64
12:L:164:ARG:HH22	12:L:200:PRO:HD3	1.62	0.64
13:M:163:CYS:SG	13:M:164:ALA:N	2.71	0.63
15:V:289:LEU:HB3	15:V:312:ALA:HB2	1.80	0.63
5:E:268:ASP:OD1	5:E:269:THR:N	2.30	0.63
2:B:371:ARG:NH2	3:C:178:LEU:O	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:234:GLU:OE2	5:E:216:ARG:NH1	2.31	0.63
18:Y:84:LEU:HD21	18:Y:107:LYS:HG2	1.78	0.63
17:X:256:LEU:HD22	17:X:319:ILE:HD11	1.79	0.63
3:C:38:LYS:HB3	4:D:54:LEU:HD22	1.79	0.63
3:C:197:THR:N	29:C:501:ADP:O2A	2.30	0.63
16:W:189:GLN:N	16:W:189:GLN:OE1	2.31	0.63
6:F:279:ALA:HB3	6:F:280:PRO:HD3	1.79	0.62
17:X:323:LEU:HD23	17:X:326:LEU:HD21	1.81	0.62
17:X:222:GLU:OE2	17:X:225:TRP:NE1	2.31	0.62
1:A:115:VAL:HG21	1:A:118:PHE:HB2	1.80	0.62
16:W:163:ALA:HA	16:W:166:LEU:HD13	1.82	0.62
1:A:100:LYS:HD3	1:A:139:ARG:HH12	1.65	0.62
9:I:90:LEU:HA	9:I:93:ILE:HD12	1.80	0.62
3:C:159:LYS:O	3:C:162:LYS:HG2	2.00	0.62
7:G:80:MET:HG2	7:G:87:SER:HB3	1.81	0.62
17:X:307:THR:HG23	17:X:310:ARG:HH22	1.64	0.62
1:A:307:ASP:OD2	1:A:333:ARG:NH2	2.33	0.62
15:V:281:ASN:C	15:V:283:ASN:H	2.03	0.62
15:V:494:MET:HB3	19:Z:275:LEU:HD11	1.79	0.62
18:Y:13:LYS:HG3	18:Y:146:ARG:HD2	1.82	0.62
5:E:262:ASN:ND2	5:E:266:GLY:HA3	2.15	0.61
14:U:880:ASN:HB3	14:U:881:PRO:HD3	1.81	0.61
16:W:176:SER:O	16:W:182:ARG:NH2	2.32	0.61
17:X:252:LYS:NZ	17:X:316:ASP:OD2	2.25	0.61
18:Y:13:LYS:HE2	18:Y:146:ARG:HB3	1.82	0.61
18:Y:208:PHE:O	18:Y:210:SER:N	2.33	0.61
16:W:260:SER:O	16:W:264:GLN:HG2	2.00	0.61
15:V:314:ARG:O	18:Y:382:LYS:NZ	2.34	0.61
16:W:136:ILE:O	16:W:138:VAL:N	2.34	0.61
9:I:122:THR:O	10:J:125:ARG:NH2	2.32	0.61
11:K:107:MET:SD	11:K:107:MET:N	2.73	0.61
17:X:306:LEU:HD21	17:X:314:ARG:HH22	1.65	0.61
6:F:107:ASP:OD1	6:F:108:GLY:N	2.33	0.60
6:F:209:LYS:H	6:F:209:LYS:HD3	1.65	0.60
15:V:242:HIS:CE1	15:V:244:ALA:HB3	2.37	0.60
15:V:476:PHE:HB3	19:Z:257:MET:HE1	1.83	0.60
1:A:44:GLN:O	1:A:47:GLN:HG2	2.02	0.60
11:K:44:GLU:OE1	11:K:191:LEU:N	2.35	0.60
18:Y:38:ARG:O	18:Y:41:LEU:HB3	2.01	0.60
12:L:5:GLN:OE1	12:L:5:GLN:N	2.31	0.60
9:I:176:LYS:NZ	10:J:51:ALA:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:43:ASP:OD1	13:M:43:ASP:N	2.34	0.60
16:W:445:LEU:HD23	19:Z:226:ILE:HG13	1.84	0.60
4:D:146:GLU:O	4:D:252:ARG:NH2	2.35	0.59
17:X:237:GLU:HA	17:X:240:ASP:HB2	1.83	0.59
18:Y:53:TYR:CD2	18:Y:57:LEU:HD13	2.37	0.59
1:A:59:ILE:HA	1:A:62:LEU:HB2	1.83	0.59
4:D:147:ALA:HB3	4:D:253:LEU:HD12	1.84	0.59
14:U:492:ASP:OD1	14:U:492:ASP:N	2.35	0.59
16:W:187:LEU:HA	16:W:190:MET:HG3	1.83	0.59
4:D:173:GLN:HG2	4:D:333:PHE:HE1	1.68	0.59
12:L:158:ALA:HB1	12:L:172:LEU:HD23	1.83	0.59
14:U:693:LEU:HD23	14:U:736:ILE:HG21	1.84	0.59
15:V:264:TYR:HB2	15:V:266:GLN:NE2	2.18	0.59
18:Y:285:ASP:OD1	18:Y:286:TRP:N	2.36	0.59
5:E:67:GLU:OE2	5:E:89:LYS:NZ	2.35	0.59
17:X:422:THR:OG1	19:Z:279:LYS:NZ	2.32	0.59
10:J:63:CYS:HG	10:J:88:ARG:HH21	1.48	0.59
16:W:265:GLN:OE1	16:W:265:GLN:N	2.31	0.59
14:U:333:MET:O	14:U:336:GLU:HG2	2.03	0.59
16:W:178:GLU:OE1	16:W:181:GLU:N	2.31	0.59
16:W:211:THR:HG23	16:W:212:LYS:HD3	1.85	0.59
17:X:368:MET:SD	17:X:373:LYS:HB3	2.43	0.59
9:I:154:GLY:O	10:J:81:ARG:NH2	2.33	0.58
18:Y:53:TYR:HA	18:Y:56:ALA:HB3	1.84	0.58
14:U:564:ASP:OD1	14:U:565:ALA:N	2.37	0.58
7:G:49:VAL:HG22	7:G:219:VAL:HG12	1.85	0.58
4:D:77:GLU:O	4:D:80:LYS:HG2	2.03	0.58
11:K:41:GLN:NE2	11:K:151:PRO:O	2.37	0.58
13:M:241:GLU:HA	13:M:244:LYS:HZ3	1.67	0.58
18:Y:101:ARG:HH21	18:Y:127:THR:HA	1.69	0.58
4:D:212:LYS:HG2	4:D:333:PHE:CD2	2.38	0.58
17:X:134:VAL:HB	17:X:149:LEU:HD23	1.85	0.58
10:J:39:ASP:OD1	10:J:39:ASP:N	2.34	0.58
18:Y:42:MET:HB2	18:Y:46:ARG:NH2	2.17	0.58
17:X:225:TRP:HE3	17:X:257:CYS:HG	1.50	0.58
18:Y:101:ARG:HA	18:Y:104:MET:HG3	1.85	0.58
8:H:66:GLU:OE2	8:H:91:ARG:NH2	2.37	0.57
2:B:415:THR:OG1	2:B:418:ASP:OD1	2.22	0.57
14:U:49:TYR:HD1	14:U:57:ARG:HG2	1.68	0.57
1:A:143:ASP:OD1	1:A:143:ASP:N	2.38	0.57
14:U:436:ALA:HB3	14:U:472:ILE:HD11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:224:ASP:OD1	17:X:225:TRP:N	2.38	0.57
17:X:255:LEU:HD22	17:X:267:VAL:HG13	1.86	0.57
4:D:116:LEU:HD23	4:D:118:THR:H	1.70	0.57
9:I:241:GLU:O	9:I:244:GLU:HG2	2.05	0.57
2:B:80:ARG:O	2:B:84:GLN:NE2	2.37	0.57
3:C:88:LYS:HB3	3:C:94:LYS:HG3	1.86	0.57
15:V:306:ARG:NH2	15:V:336:GLU:OE2	2.36	0.57
1:A:142:VAL:HG12	1:A:149:ILE:HA	1.87	0.57
3:C:387:VAL:O	3:C:391:MET:HG2	2.05	0.57
4:D:345:PHE:CE2	4:D:375:ILE:HD12	2.39	0.57
11:K:99:HIS:ND1	11:K:107:MET:SD	2.78	0.57
16:W:169:LEU:HD22	16:W:186:ILE:HA	1.87	0.57
16:W:455:LEU:HD13	19:Z:103:LYS:HG2	1.87	0.57
9:I:32:GLY:H	9:I:50:ARG:HH21	1.51	0.57
10:J:35:VAL:HG23	10:J:158:ALA:HB2	1.86	0.56
15:V:393:THR:O	15:V:396:ILE:HG22	2.04	0.56
18:Y:13:LYS:HB2	18:Y:16:ASP:OD2	2.05	0.56
18:Y:20:ALA:HB2	18:Y:150:PHE:CE1	2.40	0.56
2:B:83:GLU:N	2:B:83:GLU:OE1	2.37	0.56
2:B:120:HIS:HA	2:B:135:ILE:HG13	1.86	0.56
7:G:67:THR:HG22	7:G:69:LEU:H	1.69	0.56
2:B:225:TYR:CZ	2:B:352:GLU:HB3	2.40	0.56
3:C:72:TYR:HE1	3:C:118:ASN:HA	1.70	0.56
9:I:234:GLU:OE1	9:I:234:GLU:N	2.29	0.56
14:U:811:PHE:HE1	14:U:885:MET:H	1.53	0.56
14:U:148:LYS:O	14:U:151:ILE:HG22	2.06	0.56
14:U:773:PHE:O	14:U:775:LEU:N	2.39	0.56
3:C:198:LEU:HD23	29:C:501:ADP:H2'	1.88	0.56
5:E:376:ASP:O	5:E:379:LYS:NZ	2.38	0.56
18:Y:67:VAL:HA	18:Y:70:LEU:HD12	1.87	0.56
11:K:123:PHE:HB2	11:K:133:MET:HE2	1.87	0.56
11:K:85:ALA:HB2	11:K:139:VAL:HG11	1.88	0.56
1:A:45:ILE:HD11	2:B:61:LYS:HB3	1.87	0.56
2:B:53:THR:O	2:B:55:HIS:ND1	2.38	0.56
2:B:184:TYR:CE2	2:B:198:LYS:HE2	2.40	0.56
3:C:69:GLN:OE1	3:C:69:GLN:N	2.34	0.56
4:D:178:ARG:O	4:D:182:GLU:HG2	2.06	0.56
9:I:38:LEU:HD12	9:I:43:VAL:HB	1.87	0.56
16:W:152:ILE:O	16:W:156:ASN:N	2.39	0.56
13:M:33:SER:O	13:M:167:LYS:HG3	2.05	0.56
14:U:765:VAL:HG11	14:U:778:PHE:CD2	2.40	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:25:MET:O	9:I:28:ILE:HG22	2.05	0.55
17:X:273:GLY:O	17:X:277:LEU:HG	2.06	0.55
18:Y:13:LYS:HE3	18:Y:147:ILE:HG13	1.88	0.55
16:W:282:GLU:HG2	16:W:283:GLN:N	2.20	0.55
2:B:109:VAL:HG21	3:C:94:LYS:HE2	1.89	0.55
9:I:161:ALA:HB1	9:I:175:LEU:HD13	1.88	0.55
9:I:216:LEU:HD13	9:I:225:ILE:HG12	1.88	0.55
14:U:482:GLY:HA3	14:U:515:ALA:HB1	1.89	0.55
15:V:223:LYS:HZ3	15:V:226:VAL:HB	1.71	0.55
18:Y:97:GLU:HG3	18:Y:99:GLU:OE2	2.07	0.55
2:B:130:GLU:OE1	2:B:130:GLU:N	2.39	0.55
11:K:147:ASP:OD1	11:K:148:GLU:N	2.34	0.55
7:G:101:TRP:CD2	7:G:109:ILE:HD13	2.41	0.55
9:I:63:GLU:OE1	9:I:64:LYS:HG3	2.06	0.55
14:U:341:PHE:CE2	14:U:787:CYS:HB3	2.42	0.55
16:W:420:ASP:HB3	16:W:423:ASN:HB2	1.89	0.55
14:U:21:GLU:OE1	14:U:55:ARG:NH1	2.40	0.55
16:W:452:ILE:HG22	19:Z:103:LYS:HZ1	1.71	0.55
18:Y:16:ASP:HA	18:Y:19:ILE:HD12	1.89	0.55
18:Y:92:GLU:HB3	18:Y:100:ILE:HD11	1.87	0.55
18:Y:275:LEU:HD21	18:Y:296:VAL:HG22	1.89	0.55
9:I:140:ASP:OD2	9:I:146:GLN:NE2	2.39	0.55
15:V:383:GLY:O	15:V:387:GLN:HG3	2.07	0.55
15:V:384:GLU:OE1	15:V:384:GLU:N	2.32	0.55
17:X:333:GLN:O	17:X:336:ILE:HG22	2.07	0.55
19:Z:59:ASP:OD1	19:Z:60:GLU:N	2.40	0.55
6:F:86:LEU:O	6:F:88:TYR:N	2.38	0.55
15:V:270:LEU:CD1	15:V:271:VAL:HG13	2.31	0.55
18:Y:51:ALA:HA	18:Y:54:TYR:CE2	2.42	0.55
18:Y:281:GLU:OE1	18:Y:284:LYS:NZ	2.30	0.55
5:E:179:GLY:N	27:E:401:ATP:O2B	2.33	0.55
15:V:478:GLN:O	15:V:481:SER:OG	2.23	0.55
18:Y:26:LEU:HD13	18:Y:32:ARG:O	2.07	0.55
7:G:163:PHE:HD2	7:G:166:THR:HG1	1.55	0.54
14:U:797:MET:SD	14:U:880:ASN:ND2	2.80	0.54
4:D:154:LEU:HD11	4:D:157:ASP:OD1	2.06	0.54
4:D:155:THR:HG23	4:D:159:LYS:HE2	1.89	0.54
4:D:355:SER:HB3	4:D:394:VAL:O	2.07	0.54
3:C:158:ILE:HA	3:C:161:ILE:HG22	1.90	0.54
13:M:191:LYS:HB3	13:M:238:TYR:CE2	2.42	0.54
17:X:415:TYR:OH	18:Y:383:LEU:HD22	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:270:VAL:HA	18:Y:273:GLN:HG2	1.88	0.54
1:A:399:ALA:O	1:A:400:ARG:HD2	2.08	0.54
2:B:48:LYS:HD3	2:B:68:ILE:HG21	1.90	0.54
11:K:197:SER:HA	11:K:200:ILE:HD12	1.88	0.54
16:W:395:ASN:HA	16:W:398:VAL:HG22	1.89	0.54
17:X:243:ASP:OD1	17:X:245:PRO:HD2	2.07	0.54
19:Z:26:ILE:HD12	19:Z:27:GLY:N	2.23	0.54
1:A:405:THR:N	1:A:408:ASP:OD2	2.31	0.54
18:Y:21:GLN:HE22	18:Y:286:TRP:H	1.56	0.54
4:D:212:LYS:HG2	4:D:333:PHE:HD2	1.72	0.54
4:D:411:GLU:HG2	4:D:412:GLN:N	2.21	0.54
5:E:348:THR:HA	6:F:217:ILE:HD11	1.89	0.54
16:W:334:GLU:OE1	16:W:334:GLU:N	2.40	0.54
1:A:73:ALA:HB3	1:A:78:TRP:HD1	1.72	0.54
3:C:113:ARG:HB2	3:C:127:LEU:HB2	1.89	0.54
18:Y:170:GLU:N	18:Y:170:GLU:OE1	2.40	0.54
2:B:64:LYS:HG3	2:B:67:ARG:HH21	1.72	0.53
2:B:407:LEU:HD12	3:C:178:LEU:HD12	1.90	0.53
18:Y:66:ASP:O	18:Y:70:LEU:N	2.27	0.53
18:Y:122:THR:HA	18:Y:125:ARG:HG2	1.89	0.53
2:B:54:PRO:HB2	2:B:61:LYS:HG3	1.91	0.53
2:B:118:ASP:N	2:B:118:ASP:OD1	2.39	0.53
11:K:71:ASP:OD1	11:K:74:ILE:N	2.40	0.53
13:M:200:VAL:HG22	13:M:201:HIS:H	1.74	0.53
16:W:138:VAL:HA	16:W:141:GLU:OE2	2.08	0.53
5:E:300:HIS:NE2	5:E:302:ASP:OD1	2.40	0.53
15:V:282:ASN:HD22	18:Y:385:ARG:HG2	1.73	0.53
14:U:369:THR:HG22	14:U:731:ILE:HD11	1.91	0.53
15:V:266:GLN:O	15:V:269:LYS:HG2	2.09	0.53
18:Y:90:ASP:O	18:Y:93:LYS:HG2	2.09	0.53
3:C:226:GLU:OE2	3:C:229:ARG:NH1	2.42	0.53
4:D:155:THR:HA	4:D:159:LYS:NZ	2.24	0.53
14:U:377:HIS:O	14:U:380:THR:HG22	2.08	0.53
16:W:15:LYS:O	16:W:19:ASP:N	2.38	0.53
17:X:163:LYS:HA	17:X:166:LEU:HD23	1.91	0.53
5:E:262:ASN:ND2	5:E:262:ASN:O	2.41	0.53
9:I:41:ASP:N	9:I:41:ASP:OD1	2.41	0.53
17:X:157:LEU:HG	17:X:166:LEU:HD22	1.91	0.53
17:X:274:LYS:HA	17:X:277:LEU:HD12	1.90	0.53
19:Z:193:ASN:O	19:Z:194:GLN:NE2	2.42	0.53
2:B:85:MET:HG3	2:B:86:LYS:HD3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:THR:CG2	2:B:106:PRO:HD3	2.38	0.53
11:K:236:GLU:OE1	11:K:236:GLU:N	2.42	0.53
14:U:680:VAL:O	14:U:683:VAL:HG12	2.08	0.53
6:F:168:TYR:CD2	6:F:274:LEU:HD12	2.44	0.53
15:V:475:ALA:O	15:V:479:ARG:NH1	2.41	0.53
18:Y:39:ASP:O	18:Y:42:MET:HG3	2.09	0.53
1:A:192:GLU:OE2	1:A:196:LEU:HD12	2.09	0.53
2:B:295:TYR:CE2	3:C:271:ARG:HD2	2.44	0.53
4:D:188:PHE:CZ	4:D:192:LYS:HE2	2.44	0.53
11:K:129:ASP:HB2	11:K:130:PRO:HD2	1.89	0.53
18:Y:204:THR:O	18:Y:216:TYR:OH	2.26	0.53
16:W:281:ASN:OD1	16:W:282:GLU:N	2.41	0.52
17:X:360:ASP:OD1	17:X:360:ASP:N	2.40	0.52
18:Y:281:GLU:HA	18:Y:284:LYS:HZ2	1.73	0.52
9:I:71:ASP:HB3	9:I:223:THR:HG21	1.91	0.52
14:U:816:PRO:HB2	14:U:818:GLU:OE1	2.09	0.52
17:X:422:THR:OXT	19:Z:283:ARG:NH1	2.40	0.52
18:Y:303:ALA:O	18:Y:306:GLN:HB3	2.09	0.52
1:A:100:LYS:HD3	1:A:139:ARG:NH1	2.23	0.52
1:A:331:LEU:O	1:A:337:LEU:HD23	2.09	0.52
6:F:249:LEU:HB2	6:F:283:ILE:HG22	1.91	0.52
14:U:161:ASP:OD1	14:U:162:VAL:N	2.40	0.52
1:A:361:SER:O	1:A:361:SER:OG	2.25	0.52
9:I:232:GLU:O	9:I:235:GLN:NE2	2.38	0.52
3:C:160:GLU:HA	3:C:163:GLU:HG2	1.91	0.52
5:E:291:ARG:HH21	5:E:294:ARG:NH1	2.08	0.52
11:K:42:THR:HG23	11:K:189:MET:HB3	1.91	0.52
18:Y:215:ASP:O	18:Y:218:THR:OG1	2.26	0.52
4:D:263:PHE:CE2	4:D:265:ASP:HB2	2.45	0.52
15:V:439:ALA:HA	15:V:442:ILE:HD12	1.92	0.52
4:D:176:GLU:OE2	4:D:331:ILE:HD13	2.09	0.52
12:L:84:LEU:O	12:L:88:MET:HG2	2.10	0.52
15:V:302:TYR:OH	15:V:397:ARG:NH1	2.40	0.52
18:Y:121:LEU:HG	18:Y:125:ARG:NH1	2.23	0.52
6:F:344:ARG:HH11	6:F:347:ARG:NH1	2.08	0.52
14:U:818:GLU:OE1	14:U:818:GLU:N	2.36	0.52
18:Y:111:LEU:O	18:Y:115:GLY:N	2.36	0.52
1:A:234:ASP:OD1	1:A:235:ALA:N	2.42	0.52
1:A:426:THR:HG22	1:A:427:PRO:HD3	1.91	0.52
3:C:249:ASP:OD1	3:C:249:ASP:N	2.43	0.52
8:H:180:GLU:N	8:H:180:GLU:OE1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:57:ARG:HA	10:J:60:ARG:HE	1.75	0.52
16:W:186:ILE:O	16:W:189:GLN:NE2	2.38	0.52
2:B:337:LEU:HD23	2:B:337:LEU:H	1.73	0.52
9:I:82:ASP:O	9:I:86:LEU:HG	2.10	0.52
15:V:480:ILE:HD11	19:Z:261:TYR:HA	1.90	0.52
16:W:235:GLN:OE1	16:W:350:ARG:NH2	2.42	0.52
2:B:387:LYS:HB3	2:B:390:LEU:HB3	1.93	0.51
1:A:81:ALA:HA	1:A:85:GLN:HB3	1.91	0.51
15:V:269:LYS:HD3	15:V:295:ILE:HD11	1.92	0.51
16:W:141:GLU:OE1	16:W:141:GLU:N	2.25	0.51
1:A:312:ARG:HG3	1:A:315:ILE:HB	1.91	0.51
9:I:115:CYS:HB3	10:J:81:ARG:HH22	1.75	0.51
16:W:448:LYS:HE3	19:Z:154:THR:CG2	2.40	0.51
17:X:195:THR:HA	17:X:198:ASN:HD21	1.75	0.51
17:X:348:GLU:OE1	17:X:348:GLU:N	2.41	0.51
4:D:156:SER:OG	4:D:157:ASP:N	2.41	0.51
15:V:415:SER:HB3	18:Y:348:ASP:OD1	2.11	0.51
16:W:169:LEU:O	16:W:173:THR:HG23	2.10	0.51
1:A:384:GLU:OE1	1:A:384:GLU:HA	2.10	0.51
2:B:114:GLU:O	2:B:121:ALA:HB1	2.10	0.51
5:E:242:ARG:NE	5:E:286:ASP:OD2	2.37	0.51
14:U:773:PHE:C	14:U:775:LEU:H	2.14	0.51
14:U:435:SER:O	14:U:437:TYR:N	2.44	0.51
2:B:320:ASP:OD1	2:B:320:ASP:N	2.39	0.51
4:D:323:ARG:HE	4:D:324:PRO:HD2	1.75	0.51
4:D:417:TYR:OH	7:G:26:GLU:OE2	2.21	0.51
9:I:71:ASP:OD1	9:I:71:ASP:N	2.43	0.51
11:K:109:VAL:HG11	11:K:145:GLY:HA3	1.93	0.51
16:W:251:TYR:HE1	16:W:267:LEU:HD21	1.75	0.51
17:X:306:LEU:HD21	17:X:314:ARG:HH12	1.76	0.51
18:Y:40:GLU:O	18:Y:44:ALA:N	2.43	0.51
18:Y:379:ARG:O	18:Y:383:LEU:HG	2.10	0.51
2:B:120:HIS:HB3	2:B:134:SER:HA	1.93	0.51
18:Y:91:ALA:HB1	18:Y:99:GLU:HB2	1.93	0.51
19:Z:130:ASP:OD1	19:Z:131:LEU:N	2.44	0.51
1:A:327:LEU:HD12	1:A:331:LEU:HD22	1.93	0.51
5:E:280:ASN:ND2	5:E:280:ASN:O	2.43	0.51
11:K:87:THR:HB	11:K:91:LYS:NZ	2.25	0.51
17:X:306:LEU:HD11	17:X:314:ARG:HH12	1.76	0.51
18:Y:60:SER:HB3	18:Y:63:TRP:HZ3	1.75	0.51
9:I:124:PHE:HB2	10:J:123:GLY:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:131:THR:HG21	18:Y:136:HIS:HB2	1.93	0.51
3:C:196:LYS:N	29:C:501:ADP:O2A	2.44	0.50
12:L:228:ASP:O	12:L:231:PRO:HD2	2.11	0.50
15:V:353:LEU:HD12	15:V:353:LEU:O	2.11	0.50
17:X:415:TYR:HD1	17:X:418:ALA:HB3	1.76	0.50
18:Y:97:GLU:N	18:Y:99:GLU:OE2	2.44	0.50
9:I:174:MET:SD	9:I:196:VAL:HG22	2.51	0.50
18:Y:68:ASP:OD1	18:Y:68:ASP:N	2.40	0.50
1:A:124:ASP:OD1	1:A:124:ASP:N	2.44	0.50
2:B:153:ASN:OD1	2:B:154:HIS:N	2.44	0.50
16:W:216:GLU:OE1	16:W:223:LYS:HE2	2.11	0.50
18:Y:13:LYS:HZ3	18:Y:143:TYR:HD1	1.60	0.50
2:B:335:GLU:OE1	2:B:335:GLU:N	2.36	0.50
3:C:162:LYS:O	3:C:166:GLU:HG2	2.11	0.50
15:V:239:THR:H	15:V:247:GLN:HE21	1.58	0.50
15:V:281:ASN:HB2	15:V:284:GLU:OE1	2.11	0.50
3:C:20:LEU:O	3:C:24:TYR:HB3	2.11	0.50
4:D:361:GLU:HA	4:D:364:VAL:HG22	1.94	0.50
12:L:50:LYS:HG2	12:L:60:GLN:O	2.12	0.50
16:W:335:SER:OG	16:W:336:PRO:HD3	2.12	0.50
3:C:178:LEU:HB3	3:C:180:ILE:HD13	1.94	0.50
15:V:264:TYR:HB2	15:V:266:GLN:HE22	1.75	0.50
18:Y:363:ASN:O	18:Y:367:GLN:HG2	2.12	0.50
19:Z:43:TRP:HB3	19:Z:48:LEU:HA	1.93	0.50
2:B:388:ASP:N	2:B:388:ASP:OD1	2.43	0.50
3:C:381:GLU:HA	3:C:384:GLU:HG3	1.94	0.50
14:U:904:LYS:HE3	14:U:905:PRO:HD2	1.94	0.50
16:W:343:SER:HB2	16:W:346:GLU:HB3	1.93	0.50
18:Y:263:LEU:HB2	18:Y:271:PHE:CE1	2.47	0.50
18:Y:379:ARG:NH1	18:Y:383:LEU:HD21	2.27	0.50
19:Z:165:GLU:HG2	19:Z:167:ALA:H	1.77	0.50
9:I:75:SER:OG	9:I:76:VAL:N	2.45	0.50
18:Y:42:MET:HA	18:Y:45:VAL:HG22	1.93	0.50
2:B:140:ASP:O	2:B:142:ASP:N	2.42	0.50
3:C:340:ARG:HD3	18:Y:207:THR:O	2.12	0.50
4:D:171:ASP:OD1	4:D:172:ILE:N	2.45	0.50
16:W:159:VAL:HG12	16:W:196:VAL:HG22	1.94	0.50
17:X:194:ARG:O	17:X:198:ASN:ND2	2.45	0.50
10:J:183:THR:H	10:J:186:LEU:HD12	1.76	0.49
15:V:169:LEU:CB	15:V:221:LEU:HD11	2.42	0.49
15:V:205:LEU:O	15:V:207:ALA:N	2.41	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:239:TYR:CZ	17:X:246:LYS:HD2	2.47	0.49
18:Y:173:ASP:HB3	18:Y:176:ARG:HB2	1.94	0.49
18:Y:179:ARG:HG2	18:Y:208:PHE:CE1	2.47	0.49
2:B:90:GLU:HG3	2:B:92:GLN:HB2	1.94	0.49
6:F:246:ALA:HB1	6:F:280:PRO:O	2.12	0.49
13:M:53:VAL:HG23	13:M:209:PHE:HA	1.93	0.49
16:W:453:HIS:HB3	19:Z:219:LYS:HZ2	1.77	0.49
1:A:292:ASP:OD2	2:B:303:ARG:HD3	2.13	0.49
15:V:424:GLN:N	15:V:424:GLN:OE1	2.44	0.49
17:X:419:LYS:O	17:X:422:THR:HG22	2.11	0.49
3:C:20:LEU:O	3:C:24:TYR:CB	2.60	0.49
4:D:212:LYS:HA	4:D:333:PHE:HE2	1.78	0.49
9:I:68:LEU:HD22	9:I:90:LEU:HD11	1.93	0.49
9:I:115:CYS:HB3	10:J:81:ARG:NH2	2.27	0.49
11:K:123:PHE:HA	11:K:133:MET:HA	1.95	0.49
13:M:201:HIS:O	13:M:201:HIS:CG	2.64	0.49
14:U:164:GLU:OE2	14:U:203:LYS:NZ	2.28	0.49
18:Y:79:ASP:O	18:Y:82:LYS:HG2	2.12	0.49
3:C:23:TYR:CZ	14:U:105:ILE:HD11	2.47	0.49
7:G:210:PHE:CD1	7:G:215:ILE:HD13	2.48	0.49
12:L:122:ARG:HG3	12:L:123:TYR:H	1.77	0.49
14:U:332:GLU:OE1	14:U:332:GLU:N	2.41	0.49
17:X:299:LEU:HD21	17:X:331:LEU:HA	1.95	0.49
1:A:347:ASP:OD1	1:A:347:ASP:N	2.31	0.49
2:B:63:LEU:HB3	2:B:67:ARG:NH1	2.28	0.49
3:C:90:HIS:HB3	3:C:91:PRO:HD3	1.95	0.49
5:E:262:ASN:HD22	5:E:266:GLY:HA3	1.77	0.49
7:G:109:ILE:HD12	7:G:110:PRO:HD2	1.94	0.49
14:U:573:ASP:OD1	14:U:574:LYS:N	2.45	0.49
19:Z:286:GLU:HA	19:Z:289:GLU:OE2	2.13	0.49
5:E:152:PRO:HB3	5:E:159:PHE:CE2	2.47	0.49
7:G:51:VAL:HG22	7:G:217:VAL:HG22	1.95	0.49
15:V:346:LEU:O	15:V:347:GLN:HG2	2.13	0.49
17:X:253:TYR:CE1	17:X:318:ILE:HD11	2.47	0.49
3:C:148:TYR:H	3:C:206:HIS:HE2	1.59	0.49
18:Y:69:LEU:HA	18:Y:72:LYS:HE3	1.95	0.49
1:A:277:ILE:O	1:A:279:ALA:N	2.45	0.49
2:B:196:GLU:OE1	2:B:349:ARG:NH2	2.46	0.49
9:I:166:ASN:OD1	9:I:167:ASN:N	2.46	0.49
1:A:160:THR:O	1:A:163:MET:HG2	2.14	0.48
2:B:93:GLU:O	2:B:97:SER:N	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:114:ASP:OD1	6:F:115:SER:N	2.45	0.48
9:I:74:CYS:HB2	9:I:135:LEU:O	2.13	0.48
13:M:230:ASP:N	13:M:230:ASP:OD1	2.45	0.48
14:U:132:GLY:HA2	14:U:135:ASN:HD21	1.78	0.48
16:W:277:ALA:O	16:W:283:GLN:NE2	2.45	0.48
3:C:330:LYS:O	3:C:334:ARG:NH1	2.40	0.48
5:E:363:VAL:HG22	5:E:364:GLN:H	1.78	0.48
9:I:235:GLN:HA	9:I:238:LYS:HG2	1.95	0.48
14:U:131:GLU:OE2	14:U:159:ARG:NH2	2.44	0.48
14:U:792:ASN:HD21	14:U:798:PRO:HB3	1.78	0.48
16:W:393:LEU:HA	16:W:396:LEU:HD12	1.95	0.48
17:X:218:HIS:NE2	17:X:224:ASP:HB3	2.28	0.48
18:Y:385:ARG:NH2	18:Y:388:ASN:O	2.46	0.48
8:H:119:GLN:O	8:H:122:THR:HG22	2.14	0.48
15:V:296:LYS:HG2	15:V:304:GLU:OE2	2.13	0.48
18:Y:107:LYS:NZ	18:Y:110:TYR:HD2	2.08	0.48
19:Z:283:ARG:HG3	19:Z:284:ASP:N	2.28	0.48
1:A:105:ASP:OD1	1:A:105:ASP:N	2.45	0.48
3:C:104:ASP:OD1	3:C:105:ILE:N	2.46	0.48
3:C:311:ILE:HG21	3:C:314:LYS:HE2	1.96	0.48
15:V:252:ASN:ND2	15:V:287:ARG:HG3	2.29	0.48
16:W:454:ASN:OD1	19:Z:219:LYS:HE3	2.13	0.48
17:X:365:LEU:O	17:X:369:ILE:HG22	2.14	0.48
18:Y:280:GLN:OE1	18:Y:280:GLN:HA	2.13	0.48
1:A:81:ALA:HB3	2:B:137:SER:HB2	1.95	0.48
4:D:98:GLN:H	4:D:98:GLN:HG2	1.48	0.48
6:F:61:ARG:O	6:F:64:HIS:ND1	2.47	0.48
6:F:204:LEU:C	6:F:206:MET:H	2.17	0.48
6:F:226:TYR:CZ	6:F:353:GLU:HB3	2.48	0.48
11:K:51:GLU:OE2	11:K:202:LEU:HD22	2.14	0.48
15:V:277:PRO:O	15:V:278:GLU:HB2	2.13	0.48
17:X:258:LYS:HB3	17:X:267:VAL:HG22	1.95	0.48
18:Y:46:ARG:C	18:Y:48:ASN:H	2.16	0.48
5:E:385:ASP:OD1	5:E:386:TYR:N	2.43	0.48
6:F:402:GLU:O	6:F:406:ILE:HG12	2.13	0.48
7:G:112:ASP:OD1	7:G:113:MET:N	2.47	0.48
7:G:141:ILE:HG22	7:G:151:VAL:HG22	1.96	0.48
1:A:44:GLN:OE1	1:A:47:GLN:NE2	2.46	0.48
6:F:150:LEU:HD23	6:F:164:LEU:HD23	1.96	0.48
14:U:198:LEU:HG	14:U:219:CYS:SG	2.54	0.48
15:V:100:MET:H	15:V:103:SER:CB	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:LEU:O	2:B:191:ASP:HB2	2.13	0.48
4:D:249:ASP:OD1	4:D:250:VAL:N	2.46	0.48
11:K:60:GLU:OE1	11:K:63:SER:N	2.47	0.48
14:U:546:ARG:HA	14:U:577:ILE:HD11	1.95	0.48
18:Y:51:ALA:HA	18:Y:54:TYR:CZ	2.49	0.48
2:B:142:ASP:OD1	2:B:143:LEU:N	2.47	0.48
3:C:339:THR:H	3:C:342:ILE:HD11	1.78	0.48
13:M:40:ARG:HD2	13:M:146:ALA:HB3	1.96	0.48
15:V:87:SER:CB	15:V:128:ARG:H	2.27	0.48
16:W:334:GLU:O	16:W:338:THR:N	2.42	0.48
16:W:370:TYR:CD2	16:W:373:ILE:HD12	2.49	0.48
1:A:355:PHE:CE1	1:A:385:ILE:HD12	2.49	0.48
2:B:271:PHE:HD2	2:B:322:ARG:HH12	1.60	0.48
6:F:361:ALA:O	6:F:364:ARG:N	2.46	0.48
10:J:201:SER:OG	10:J:205:ASN:HB2	2.13	0.48
15:V:340:GLY:HA2	15:V:405:THR:OG1	2.14	0.48
15:V:386:PHE:HA	15:V:389:ASP:OD2	2.14	0.48
16:W:216:GLU:OE1	16:W:216:GLU:N	2.44	0.48
18:Y:55:GLU:HG3	18:Y:59:LYS:HG3	1.95	0.48
4:D:161:ASP:HA	4:D:221:HIS:ND1	2.29	0.47
4:D:221:HIS:HD2	4:D:222:HIS:CD2	2.31	0.47
5:E:213:ARG:NH1	5:E:217:GLU:OE2	2.47	0.47
7:G:10:ASP:OD2	7:G:17:SER:HA	2.14	0.47
17:X:167:VAL:HG11	17:X:206:LEU:HD13	1.95	0.47
18:Y:88:LEU:HD22	18:Y:100:ILE:HG23	1.96	0.47
4:D:267:ILE:HG13	4:D:267:ILE:O	2.13	0.47
14:U:529:ILE:O	14:U:533:VAL:HG13	2.14	0.47
18:Y:148:GLY:O	18:Y:152:MET:N	2.47	0.47
18:Y:281:GLU:HA	18:Y:284:LYS:NZ	2.28	0.47
3:C:338:LEU:HB2	3:C:342:ILE:HD11	1.96	0.47
4:D:342:ARG:HG2	4:D:364:VAL:HG11	1.96	0.47
13:M:34:SER:O	13:M:35:THR:OG1	2.20	0.47
13:M:81:LEU:HB3	13:M:85:ARG:NH1	2.29	0.47
17:X:143:TYR:HD1	17:X:180:LEU:HD22	1.79	0.47
17:X:202:CYS:N	17:X:203:PRO:HD3	2.22	0.47
19:Z:85:VAL:HG12	19:Z:85:VAL:O	2.14	0.47
1:A:349:GLU:OE1	1:A:349:GLU:N	2.46	0.47
2:B:115:ILE:HA	2:B:121:ALA:HB1	1.96	0.47
3:C:243:PRO:HB3	3:C:288:ASN:HD21	1.80	0.47
15:V:256:ARG:HD3	15:V:291:TYR:OH	2.15	0.47
15:V:374:LYS:O	15:V:378:VAL:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:180:LYS:HZ3	27:E:401:ATP:PB	2.36	0.47
14:U:701:ILE:HG21	14:U:810:THR:HG22	1.95	0.47
17:X:258:LYS:HE3	17:X:270:LEU:HD13	1.97	0.47
18:Y:108:ALA:HA	18:Y:111:LEU:HD12	1.95	0.47
1:A:236:CYS:O	1:A:270:CYS:HB2	2.14	0.47
1:A:415:LYS:O	1:A:419:SER:HB3	2.14	0.47
3:C:72:TYR:CE1	3:C:118:ASN:HA	2.48	0.47
4:D:148:ASP:CG	4:D:149:SER:H	2.18	0.47
9:I:135:LEU:HD21	9:I:164:ILE:HD11	1.97	0.47
15:V:243:ASP:HA	15:V:247:GLN:NE2	2.28	0.47
17:X:357:SER:OG	17:X:358:LYS:N	2.48	0.47
18:Y:31:HIS:H	18:Y:31:HIS:CD2	2.31	0.47
18:Y:153:ASP:O	18:Y:157:ILE:HG12	2.14	0.47
1:A:53:GLN:HG3	1:A:57:LYS:NZ	2.30	0.47
2:B:59:ARG:HH11	2:B:63:LEU:HD12	1.80	0.47
2:B:87:PRO:C	2:B:89:GLU:H	2.18	0.47
3:C:118:ASN:OD1	3:C:118:ASN:N	2.47	0.47
7:G:161:CYS:HB3	7:G:163:PHE:HE1	1.80	0.47
13:M:98:PHE:CD2	13:M:106:ILE:HB	2.49	0.47
15:V:269:LYS:HG3	15:V:270:LEU:N	2.30	0.47
18:Y:101:ARG:HH21	18:Y:127:THR:CA	2.28	0.47
18:Y:265:GLU:HB2	18:Y:267:ARG:NE	2.29	0.47
18:Y:275:LEU:HA	18:Y:278:VAL:HG12	1.96	0.47
4:D:176:GLU:HA	4:D:179:GLU:HG2	1.95	0.47
5:E:155:ASN:HB3	5:E:158:LEU:HD13	1.97	0.47
7:G:165:ALA:HB1	7:G:179:LEU:HD13	1.97	0.47
10:J:211:MET:HE3	10:J:217:LEU:HA	1.97	0.47
12:L:64:LEU:HD13	12:L:74:ILE:HD12	1.95	0.47
15:V:284:GLU:OE1	15:V:284:GLU:N	2.46	0.47
17:X:184:PRO:HA	17:X:187:ARG:CZ	2.45	0.47
17:X:268:GLN:O	17:X:272:SER:OG	2.28	0.47
8:H:59:GLU:H	8:H:59:GLU:CD	2.18	0.47
11:K:154:PHE:CE1	11:K:164:GLN:HB2	2.50	0.47
14:U:802:TYR:HE1	14:U:880:ASN:HA	1.80	0.47
17:X:142:ARG:HD3	17:X:145:GLU:OE2	2.14	0.47
18:Y:107:LYS:O	18:Y:111:LEU:HG	2.14	0.47
1:A:99:THR:HG22	1:A:115:VAL:HG12	1.97	0.47
2:B:135:ILE:HG22	2:B:136:LEU:O	2.15	0.47
9:I:38:LEU:HD11	9:I:145:PHE:HB3	1.97	0.47
14:U:227:GLN:OE1	14:U:227:GLN:N	2.48	0.47
14:U:380:THR:HG23	14:U:382:SER:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:273:LYS:O	15:V:273:LYS:HG3	2.14	0.47
2:B:265:LYS:HE3	2:B:265:LYS:HB2	1.73	0.46
3:C:373:GLU:HG3	3:C:375:ARG:HG3	1.97	0.46
11:K:133:MET:O	11:K:135:ARG:N	2.47	0.46
12:L:72:ILE:HD11	12:L:85:CYS:SG	2.54	0.46
13:M:228:PRO:HD2	13:M:231:ILE:HD12	1.96	0.46
17:X:299:LEU:HD23	17:X:334:ASN:HD22	1.80	0.46
1:A:98:CYS:SG	2:B:130:GLU:HG2	2.55	0.46
3:C:24:TYR:OH	4:D:41:TYR:HD1	1.99	0.46
11:K:108:THR:HA	11:K:147:ASP:OD2	2.15	0.46
12:L:68:ASN:O	12:L:220:GLU:HG2	2.15	0.46
13:M:99:ARG:NH2	13:M:105:ASN:OD1	2.48	0.46
14:U:254:GLU:OE2	14:U:751:ARG:NH1	2.46	0.46
14:U:818:GLU:O	14:U:818:GLU:HG2	2.15	0.46
18:Y:60:SER:HB3	18:Y:63:TRP:CZ3	2.50	0.46
19:Z:34:ARG:HH21	19:Z:102:HIS:CE1	2.33	0.46
3:C:324:ALA:O	3:C:328:ILE:HG12	2.14	0.46
14:U:9:ILE:HD12	14:U:9:ILE:H	1.81	0.46
14:U:135:ASN:HA	14:U:138:PHE:CD2	2.41	0.46
16:W:263:TRP:HZ2	16:W:295:LYS:HD3	1.79	0.46
16:W:406:VAL:O	17:X:342:PHE:HB2	2.15	0.46
17:X:162:ASP:OD1	17:X:164:ALA:N	2.49	0.46
18:Y:122:THR:HA	18:Y:125:ARG:HH11	1.80	0.46
1:A:394:MET:HA	1:A:397:ILE:HG22	1.98	0.46
2:B:302:GLU:OE1	2:B:302:GLU:N	2.48	0.46
4:D:124:LEU:HD12	4:D:124:LEU:O	2.16	0.46
4:D:263:PHE:HE2	4:D:265:ASP:HB2	1.80	0.46
6:F:146:LYS:N	6:F:149:ASP:OD2	2.39	0.46
6:F:241:ALA:HB2	6:F:248:PHE:CE2	2.50	0.46
10:J:41:VAL:CG2	10:J:211:MET:HB2	2.45	0.46
2:B:82:GLN:O	2:B:86:LYS:N	2.42	0.46
2:B:245:ALA:HB1	2:B:279:PRO:O	2.14	0.46
3:C:142:LYS:HD2	4:D:323:ARG:HG2	1.97	0.46
3:C:357:ALA:O	3:C:360:LYS:HG2	2.16	0.46
11:K:24:VAL:O	11:K:28:ILE:HG12	2.16	0.46
14:U:331:GLY:O	14:U:335:ILE:HG12	2.15	0.46
15:V:281:ASN:O	15:V:283:ASN:N	2.48	0.46
18:Y:48:ASN:O	18:Y:114:ILE:HD12	2.16	0.46
3:C:150:MET:SD	3:C:150:MET:N	2.89	0.46
3:C:157:GLN:HG2	3:C:317:PHE:CE1	2.51	0.46
6:F:336:ASP:OD1	6:F:336:ASP:N	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:97:TYR:CZ	9:I:101:TYR:HD2	2.34	0.46
14:U:49:TYR:CE2	14:U:50:GLU:HG3	2.51	0.46
15:V:223:LYS:NZ	15:V:226:VAL:HB	2.30	0.46
16:W:384:LEU:HD13	16:W:388:GLU:HB3	1.98	0.46
16:W:428:TRP:O	16:W:432:LEU:HD23	2.15	0.46
4:D:212:LYS:HE3	4:D:212:LYS:HB3	3.97	0.46
4:D:307:VAL:HG12	4:D:309:MET:HG3	1.98	0.46
5:E:283:ASP:N	5:E:283:ASP:OD1	2.49	0.46
7:G:58:ASP:OD1	7:G:59:LYS:N	2.47	0.46
15:V:449:ALA:HA	15:V:460:SER:HA	1.96	0.46
16:W:243:ILE:HD12	16:W:273:TYR:CE2	2.50	0.46
16:W:251:TYR:CE1	16:W:267:LEU:HD11	2.50	0.46
2:B:332:ASN:N	2:B:332:ASN:OD1	2.48	0.46
4:D:46:LYS:HB3	4:D:46:LYS:HE2	1.36	0.46
8:H:65:VAL:N	8:H:209:GLU:OE2	2.27	0.46
18:Y:16:ASP:OD1	18:Y:17:LEU:HD12	2.16	0.46
3:C:104:ASP:OD2	3:C:106:ASN:ND2	2.49	0.46
6:F:295:ARG:HA	6:F:307:GLN:NE2	2.31	0.46
11:K:125:GLU:HA	11:K:133:MET:SD	2.56	0.46
15:V:479:ARG:CZ	18:Y:370:ILE:HD11	2.46	0.46
17:X:282:ARG:HA	17:X:285:GLU:OE1	2.15	0.46
17:X:415:TYR:HA	17:X:418:ALA:HB3	1.97	0.46
19:Z:190:ARG:HB3	19:Z:190:ARG:CZ	2.45	0.46
1:A:92:PRO:O	1:A:94:GLN:NE2	2.40	0.46
4:D:116:LEU:HB3	4:D:119:ILE:CD1	2.46	0.45
16:W:170:GLN:HA	16:W:173:THR:HG23	1.98	0.45
18:Y:132:VAL:HA	18:Y:137:ARG:NH2	2.31	0.45
1:A:325:ASP:OD1	1:A:325:ASP:N	2.47	0.45
14:U:160:LEU:HD23	14:U:200:VAL:HG21	1.98	0.45
17:X:157:LEU:HD21	17:X:165:LEU:HB3	1.97	0.45
18:Y:156:LEU:O	18:Y:160:ASN:ND2	2.49	0.45
9:I:38:LEU:O	9:I:179:TYR:OH	2.35	0.45
11:K:181:LEU:HD12	11:K:181:LEU:HA	1.79	0.45
14:U:97:VAL:HA	14:U:100:ILE:HG12	1.97	0.45
15:V:163:VAL:O	15:V:167:LEU:CB	2.65	0.45
17:X:204:PRO:HA	17:X:207:GLN:HE22	1.80	0.45
3:C:26:SER:HA	3:C:29:GLU:HG3	1.99	0.45
3:C:68:GLU:O	4:D:136:SER:OG	2.33	0.45
5:E:69:PHE:CE1	5:E:83:CYS:HB2	2.51	0.45
8:H:105:ILE:HD12	8:H:106:PRO:HD2	1.98	0.45
15:V:281:ASN:C	15:V:283:ASN:N	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:263:TRP:CZ2	16:W:295:LYS:HD3	2.52	0.45
19:Z:122:VAL:HA	19:Z:136:GLU:O	2.16	0.45
2:B:187:ILE:HD13	2:B:234:LEU:HD22	1.99	0.45
3:C:97:VAL:HG21	3:C:121:TYR:O	2.16	0.45
3:C:189:TYR:CZ	3:C:316:GLU:HG2	2.51	0.45
10:J:65:LEU:HD12	10:J:88:ARG:HG3	1.98	0.45
10:J:169:ARG:O	10:J:172:LEU:N	2.49	0.45
12:L:18:ARG:NH1	12:L:23:GLU:OE2	2.49	0.45
17:X:170:GLN:HB3	17:X:193:ALA:HB2	1.99	0.45
18:Y:141:VAL:HG11	18:Y:164:ALA:HB2	1.97	0.45
1:A:252:GLU:OE1	1:A:255:ARG:NH1	2.48	0.45
1:A:279:ALA:HB2	2:B:310:LEU:HD13	1.98	0.45
5:E:124:HIS:ND1	5:E:125:GLU:OE2	2.44	0.45
9:I:28:ILE:HD11	9:I:77:ALA:O	2.16	0.45
15:V:292:THR:HA	15:V:295:ILE:HG12	1.99	0.45
7:G:214:GLU:C	7:G:215:ILE:HD12	2.37	0.45
10:J:201:SER:O	10:J:203:GLY:N	2.46	0.45
14:U:496:LEU:O	14:U:499:THR:HG22	2.16	0.45
16:W:268:LYS:HZ1	16:W:336:PRO:HB2	1.81	0.45
18:Y:42:MET:SD	18:Y:43:ALA:N	2.89	0.45
2:B:371:ARG:HE	2:B:371:ARG:HB2	1.56	0.45
2:B:380:LEU:HD23	2:B:380:LEU:H	1.82	0.45
3:C:81:ASP:OD1	3:C:81:ASP:N	2.45	0.45
5:E:64:LEU:HD12	5:E:70:ILE:HD11	1.97	0.45
6:F:114:ASP:CG	6:F:115:SER:H	2.20	0.45
10:J:184:ASP:O	10:J:188:ILE:HG12	2.17	0.45
1:A:362:MET:SD	2:B:216:ILE:HD11	2.57	0.45
2:B:70:ASP:O	2:B:74:MET:HG2	2.16	0.45
4:D:323:ARG:HG3	4:D:324:PRO:HD2	1.98	0.45
6:F:86:LEU:HA	6:F:88:TYR:CE1	2.52	0.45
14:U:423:MET:HG2	14:U:446:LEU:HD11	1.99	0.45
15:V:406:GLY:O	15:V:409:MET:HG3	2.17	0.45
16:W:134:GLY:C	16:W:136:ILE:H	2.20	0.45
18:Y:175:ASP:OD1	18:Y:176:ARG:N	2.48	0.45
1:A:336:ARG:C	1:A:337:LEU:HD22	2.37	0.45
2:B:278:ALA:HB1	2:B:279:PRO:HD2	1.99	0.45
3:C:46:GLN:HA	4:D:61:ILE:HD11	1.99	0.45
3:C:188:LEU:HD11	3:C:292:ILE:HD11	1.99	0.45
4:D:354:LEU:HD21	4:D:399:PHE:CZ	2.51	0.45
11:K:65:GLU:N	11:K:65:GLU:OE1	2.50	0.45
14:U:16:GLU:HG3	14:U:19:LEU:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:316:ARG:HE	16:W:316:ARG:HB2	1.54	0.45
18:Y:130:LYS:HG3	18:Y:131:THR:N	2.32	0.45
18:Y:242:LYS:HD2	18:Y:242:LYS:HA	1.77	0.45
2:B:143:LEU:H	2:B:143:LEU:HD23	1.81	0.44
4:D:152:MET:O	4:D:153:MET:HB3	2.17	0.44
5:E:69:PHE:HE1	5:E:83:CYS:HB2	1.83	0.44
5:E:155:ASN:HB3	5:E:158:LEU:CD1	2.47	0.44
12:L:68:ASN:OD1	12:L:69:HIS:N	2.50	0.44
15:V:277:PRO:HB3	15:V:285:TRP:HH2	1.82	0.44
3:C:274:LEU:HD12	3:C:274:LEU:HA	1.83	0.44
4:D:96:VAL:HG23	4:D:97:ASP:H	1.82	0.44
5:E:126:ASP:OD1	5:E:128:GLY:N	2.49	0.44
16:W:409:LEU:HD23	17:X:344:ARG:HH21	1.82	0.44
18:Y:31:HIS:ND1	18:Y:32:ARG:HG2	2.32	0.44
1:A:362:MET:HB3	1:A:364:VAL:HG13	1.98	0.44
2:B:117:ASP:O	2:B:119:ASN:N	2.46	0.44
9:I:11:ILE:HD11	10:J:18:GLN:CD	2.37	0.44
10:J:211:MET:HE3	10:J:217:LEU:HD13	1.98	0.44
16:W:248:ARG:HG3	16:W:270:VAL:HG21	1.99	0.44
16:W:368:LYS:HZ2	16:W:369:TYR:HE1	1.66	0.44
3:C:313:ARG:HD2	3:C:313:ARG:HA	1.80	0.44
10:J:38:ARG:NH2	10:J:181:ILE:O	2.50	0.44
14:U:138:PHE:O	14:U:142:LEU:HG	2.18	0.44
1:A:75:PRO:HA	1:A:78:TRP:CE2	2.53	0.44
4:D:99:ASN:O	4:D:114:ARG:HD3	2.16	0.44
7:G:155:ASP:OD1	7:G:159:TYR:N	2.47	0.44
13:M:240:LYS:HA	13:M:240:LYS:HD3	1.77	0.44
15:V:257:ASN:OD1	15:V:258:TYR:N	2.51	0.44
15:V:358:MET:HB3	15:V:359:PRO:HD3	2.00	0.44
16:W:419:LYS:HB3	16:W:419:LYS:HE3	1.51	0.44
16:W:453:HIS:HD2	19:Z:219:LYS:HD2	1.81	0.44
17:X:192:SER:O	17:X:195:THR:HB	2.18	0.44
17:X:359:ALA:HA	17:X:362:GLU:OE2	2.18	0.44
17:X:386:ILE:HD12	17:X:386:ILE:H	1.83	0.44
2:B:276:GLU:OE1	2:B:277:HIS:ND1	2.50	0.44
4:D:51:LEU:HD12	4:D:51:LEU:HA	1.82	0.44
5:E:216:ARG:HG2	5:E:263:GLN:NE2	2.33	0.44
6:F:189:GLY:H	29:F:501:ADP:N6	2.15	0.44
6:F:438:TYR:CE1	12:L:77:LEU:HB3	2.52	0.44
11:K:235:GLU:OE1	11:K:235:GLU:N	2.29	0.44
15:V:339:LEU:O	15:V:404:LYS:HD2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:368:MET:HG3	17:X:374:PHE:HD2	1.82	0.44
18:Y:311:TYR:HD2	18:Y:314:LEU:HD22	1.82	0.44
6:F:438:TYR:HE1	12:L:77:LEU:HB3	1.82	0.44
7:G:161:CYS:HB3	7:G:163:PHE:CE1	2.53	0.44
9:I:198:ASN:HA	9:I:206:LEU:HD21	2.00	0.44
1:A:99:THR:CG2	1:A:115:VAL:HG12	2.48	0.44
4:D:41:TYR:CE2	14:U:183:LEU:HD11	2.53	0.44
7:G:13:ILE:HG22	7:G:14:THR:H	1.83	0.44
8:H:205:GLU:OE1	8:H:223:PRO:HB3	2.18	0.44
14:U:505:ASP:OD1	14:U:506:ALA:N	2.51	0.44
15:V:188:SER:O	15:V:192:MET:N	2.51	0.44
3:C:98:ASP:OD1	3:C:98:ASP:N	2.48	0.44
8:H:4:ARG:HD3	8:H:5:GLY:O	2.18	0.44
8:H:150:ASP:OD1	8:H:151:PRO:HD2	2.17	0.44
9:I:238:LYS:HA	9:I:241:GLU:OE1	2.18	0.44
15:V:238:ALA:C	15:V:240:LEU:H	2.21	0.44
15:V:277:PRO:C	15:V:279:GLN:H	2.21	0.44
16:W:203:GLN:NE2	16:W:204:ILE:HG13	2.33	0.44
17:X:378:LEU:HD12	17:X:379:ASP:H	1.83	0.44
1:A:119:ALA:CB	6:F:127:SER:HB2	2.48	0.43
3:C:151:ILE:CG2	3:C:154:LEU:HB2	2.48	0.43
3:C:191:PRO:HG2	3:C:319:PRO:HG3	2.00	0.43
5:E:250:ASP:OD2	5:E:254:GLN:NE2	2.46	0.43
7:G:182:LYS:HE2	7:G:182:LYS:HB2	1.71	0.43
8:H:44:VAL:HG21	8:H:137:CYS:HB2	1.99	0.43
8:H:105:ILE:HG13	8:H:106:PRO:O	2.18	0.43
9:I:25:MET:HA	9:I:28:ILE:HG22	1.99	0.43
12:L:182:CYS:HB2	12:L:186:GLU:CG	2.48	0.43
13:M:176:ILE:HD13	13:M:196:ILE:HD13	2.00	0.43
16:W:448:LYS:HE2	16:W:448:LYS:HB2	1.61	0.43
4:D:153:MET:SD	4:D:158:GLN:HB3	2.58	0.43
4:D:415:GLU:N	4:D:415:GLU:OE1	2.50	0.43
6:F:204:LEU:O	6:F:206:MET:N	2.52	0.43
9:I:6:ASP:OD1	9:I:7:SER:N	2.48	0.43
16:W:357:ARG:HA	16:W:357:ARG:HD3	1.77	0.43
18:Y:75:LYS:HE2	18:Y:79:ASP:OD1	2.18	0.43
4:D:115:ILE:HD11	4:D:121:ARG:NH2	2.33	0.43
8:H:119:GLN:HG3	9:I:81:SER:HB2	2.00	0.43
11:K:109:VAL:O	11:K:113:THR:OG1	2.25	0.43
15:V:219:GLU:HG2	15:V:224:LEU:HD21	1.99	0.43
18:Y:160:ASN:HA	18:Y:163:LYS:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Y:248:GLU:O	18:Y:251:HIS:HB3	2.18	0.43
18:Y:314:LEU:HD21	18:Y:319:MET:SD	2.58	0.43
3:C:155:ASP:N	3:C:155:ASP:OD1	2.51	0.43
7:G:54:LYS:HD3	7:G:216:GLU:OE2	2.19	0.43
8:H:8:PHE:CE2	9:I:6:ASP:HA	2.53	0.43
12:L:15:PRO:HA	13:M:25:TYR:CD1	2.53	0.43
15:V:429:ASP:OD1	15:V:430:SER:N	2.51	0.43
16:W:252:ASP:HB3	16:W:253:THR:H	1.63	0.43
18:Y:176:ARG:HA	18:Y:179:ARG:HD2	1.99	0.43
2:B:180:PRO:HG2	2:B:240:ALA:HB3	2.00	0.43
9:I:240:HIS:NE2	9:I:244:GLU:OE1	2.50	0.43
10:J:116:GLN:O	10:J:119:THR:OG1	2.35	0.43
12:L:167:SER:O	12:L:170:THR:OG1	2.30	0.43
14:U:898:CYS:SG	14:U:899:ARG:N	2.92	0.43
16:W:423:ASN:O	16:W:426:ASN:HB2	2.18	0.43
16:W:449:GLU:CB	19:Z:222:ILE:HG12	2.46	0.43
17:X:140:THR:O	17:X:142:ARG:NH1	2.52	0.43
5:E:376:ASP:HB2	5:E:379:LYS:HZ1	1.83	0.43
6:F:294:LYS:HB2	6:F:294:LYS:HE3	1.77	0.43
10:J:141:THR:O	10:J:143:ARG:HG2	2.19	0.43
11:K:206:MET:HE2	11:K:206:MET:HB3	1.78	0.43
16:W:173:THR:HG21	16:W:208:LYS:CE	2.49	0.43
16:W:231:ILE:O	16:W:235:GLN:HB2	2.18	0.43
6:F:184:GLN:OE1	6:F:186:SER:N	2.41	0.43
10:J:145:TYR:CE1	10:J:155:ALA:HB2	2.54	0.43
12:L:84:LEU:HD23	12:L:84:LEU:HA	1.83	0.43
16:W:158:ASP:OD2	16:W:161:GLU:HG2	2.19	0.43
18:Y:146:ARG:HD3	18:Y:211:TYR:HE2	1.84	0.43
18:Y:174:TRP:HA	18:Y:177:ARG:HB3	2.01	0.43
1:A:209:PRO:HD3	6:F:405:MET:CE	2.48	0.43
1:A:397:ILE:HD13	1:A:397:ILE:HG21	1.83	0.43
2:B:120:HIS:CB	2:B:134:SER:HA	2.49	0.43
4:D:161:ASP:OD1	4:D:221:HIS:ND1	2.50	0.43
7:G:102:LYS:HD2	7:G:102:LYS:HA	1.84	0.43
11:K:54:ILE:HG23	11:K:59:MET:HG3	2.01	0.43
14:U:641:SER:HB2	14:U:675:MET:CE	2.49	0.43
18:Y:355:GLU:OE1	18:Y:357:ASN:N	2.51	0.43
1:A:59:ILE:HG21	2:B:76:GLU:HB2	2.00	0.43
2:B:95:GLU:HA	2:B:98:LYS:NZ	2.34	0.43
2:B:292:THR:HG23	2:B:293:LYS:HG2	2.01	0.43
3:C:243:PRO:HB3	3:C:288:ASN:ND2	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:154:LEU:HG	4:D:158:GLN:HG2	2.01	0.43
14:U:694:ILE:HG23	14:U:695:MET:HG3	2.01	0.43
14:U:791:LEU:HG	14:U:795:LEU:HA	2.01	0.43
15:V:285:TRP:CD1	15:V:289:LEU:HD13	2.54	0.43
2:B:95:GLU:HA	2:B:98:LYS:HZ3	1.84	0.43
6:F:226:TYR:CE1	6:F:353:GLU:HB3	2.54	0.43
8:H:92:LYS:O	8:H:96:GLN:HG2	2.18	0.43
13:M:229:LYS:HA	13:M:232:ARG:HE	1.83	0.43
17:X:306:LEU:HD11	17:X:314:ARG:NH1	2.34	0.43
17:X:334:ASN:O	17:X:338:VAL:HG23	2.19	0.43
18:Y:175:ASP:OD1	18:Y:175:ASP:N	2.51	0.43
2:B:90:GLU:C	2:B:92:GLN:H	2.21	0.42
3:C:92:GLU:HB3	3:C:93:GLY:H	1.58	0.42
6:F:184:GLN:OE1	6:F:185:TYR:N	2.52	0.42
6:F:210:GLU:OE1	6:F:210:GLU:N	2.40	0.42
9:I:135:LEU:HD11	9:I:164:ILE:HD11	2.00	0.42
14:U:146:LYS:HG3	14:U:149:GLN:OE1	2.18	0.42
18:Y:262:SER:HA	18:Y:267:ARG:HH21	1.84	0.42
1:A:263:MET:O	1:A:266:THR:OG1	2.33	0.42
3:C:155:ASP:O	3:C:158:ILE:HG12	2.19	0.42
5:E:385:ASP:O	5:E:386:TYR:HB2	2.19	0.42
11:K:51:GLU:OE1	11:K:51:GLU:N	2.51	0.42
14:U:656:LEU:HD12	14:U:656:LEU:HA	1.89	0.42
15:V:347:GLN:HG3	15:V:347:GLN:O	2.19	0.42
17:X:297:ARG:NH1	17:X:337:ARG:HB2	2.33	0.42
18:Y:152:MET:N	18:Y:152:MET:SD	2.93	0.42
1:A:341:ILE:HD12	1:A:341:ILE:HG23	1.82	0.42
5:E:29:LEU:HB3	6:F:62:VAL:HG11	2.01	0.42
8:H:26:LEU:HA	8:H:26:LEU:HD23	1.72	0.42
16:W:151:THR:HG23	16:W:161:GLU:HB3	2.01	0.42
17:X:151:SER:O	17:X:155:ARG:NH1	2.53	0.42
17:X:336:ILE:O	17:X:340:GLU:HB2	2.18	0.42
18:Y:55:GLU:OE2	18:Y:58:CYS:HB2	2.19	0.42
1:A:88:GLN:O	1:A:92:PRO:HG2	2.19	0.42
2:B:384:ILE:HG22	2:B:385:MET:SD	2.59	0.42
3:C:276:LEU:HD23	3:C:276:LEU:HA	1.74	0.42
3:C:340:ARG:NH2	18:Y:216:TYR:OH	2.53	0.42
4:D:62:LYS:HE3	4:D:62:LYS:HB2	1.83	0.42
4:D:410:ASP:OD1	4:D:410:ASP:N	2.52	0.42
5:E:291:ARG:HG2	5:E:293:GLY:H	1.83	0.42
7:G:69:LEU:HD22	7:G:79:VAL:HG22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:117:ARG:O	7:G:121:ILE:HG12	2.20	0.42
7:G:145:GLU:CD	7:G:145:GLU:H	2.23	0.42
8:H:97:TYR:CG	8:H:105:ILE:HD13	2.54	0.42
10:J:156:TRP:CG	10:J:159:ASN:ND2	2.87	0.42
13:M:70:ASP:CG	13:M:71:ARG:H	2.21	0.42
14:U:198:LEU:HD23	14:U:223:LEU:HD22	2.01	0.42
18:Y:104:MET:SD	18:Y:105:MET:N	2.92	0.42
1:A:333:ARG:HG2	1:A:334:PRO:O	2.19	0.42
2:B:109:VAL:HG21	3:C:94:LYS:HB2	2.02	0.42
4:D:157:ASP:OD1	4:D:157:ASP:N	2.38	0.42
8:H:70:LYS:HD2	8:H:71:HIS:HB3	2.01	0.42
9:I:55:LEU:O	9:I:56:LEU:HD22	2.20	0.42
17:X:330:LEU:HA	17:X:330:LEU:HD23	1.77	0.42
2:B:371:ARG:NE	3:C:179:GLY:HA3	2.35	0.42
3:C:178:LEU:HD23	3:C:178:LEU:HA	1.86	0.42
14:U:148:LYS:HA	14:U:151:ILE:HG22	2.01	0.42
14:U:763:VAL:O	14:U:767:THR:HG23	2.19	0.42
15:V:253:LEU:O	15:V:256:ARG:HB3	2.20	0.42
16:W:352:LYS:HA	16:W:352:LYS:HD3	1.84	0.42
17:X:177:TYR:CB	17:X:186:ALA:HB2	2.49	0.42
17:X:185:LYS:HB2	17:X:185:LYS:HE2	1.58	0.42
17:X:395:LYS:HE3	17:X:395:LYS:HB2	1.35	0.42
18:Y:155:ASP:OD1	18:Y:156:LEU:N	2.50	0.42
18:Y:159:ARG:O	18:Y:162:GLU:HG3	2.20	0.42
18:Y:229:ILE:HD11	18:Y:298:GLU:HG2	2.01	0.42
1:A:277:ILE:HD13	1:A:277:ILE:HA	1.86	0.42
2:B:82:GLN:HA	2:B:85:MET:HG2	2.01	0.42
5:E:81:VAL:HG13	5:E:105:LEU:O	2.20	0.42
6:F:202:ILE:HD13	6:F:202:ILE:HA	1.86	0.42
8:H:65:VAL:HG23	8:H:209:GLU:HG2	2.02	0.42
13:M:10:SER:OG	13:M:11:ALA:N	2.52	0.42
13:M:87:LEU:HD23	13:M:87:LEU:HA	1.64	0.42
16:W:170:GLN:HA	16:W:173:THR:CG2	2.49	0.42
16:W:259:GLU:HB2	16:W:262:LYS:HE3	2.01	0.42
17:X:292:GLN:HA	17:X:295:LYS:NZ	2.35	0.42
17:X:409:LYS:HB3	17:X:409:LYS:HE3	1.50	0.42
18:Y:245:GLU:O	18:Y:249:VAL:HG23	2.20	0.42
1:A:364:VAL:HG12	1:A:404:ALA:HB3	2.02	0.42
2:B:63:LEU:HD13	2:B:67:ARG:HH12	1.84	0.42
6:F:169:ASP:OD1	6:F:170:SER:N	2.53	0.42
7:G:48:ALA:HB3	7:G:220:VAL:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:41:VAL:HG22	10:J:211:MET:HB2	2.02	0.42
10:J:68:ASN:N	10:J:68:ASN:OD1	2.53	0.42
14:U:167:ILE:HA	14:U:176:MET:HE1	2.01	0.42
14:U:340:GLN:O	14:U:344:ARG:HG2	2.19	0.42
16:W:354:LEU:HA	16:W:354:LEU:HD12	1.80	0.42
16:W:370:TYR:CE2	16:W:373:ILE:HD12	2.54	0.42
16:W:435:LEU:HB2	19:Z:236:LEU:CD2	2.50	0.42
18:Y:68:ASP:O	18:Y:72:LYS:HG2	2.20	0.42
1:A:112:ILE:HD13	1:A:122:VAL:HG22	2.02	0.42
3:C:136:SER:HA	3:C:139:MET:HG3	2.02	0.42
4:D:201:GLY:HA3	4:D:327:LEU:HD13	2.02	0.42
7:G:72:ILE:HG22	7:G:73:THR:OG1	2.20	0.42
11:K:87:THR:HB	11:K:91:LYS:HZ1	1.85	0.42
12:L:41:LYS:HD2	12:L:180:MET:HA	2.02	0.42
12:L:111:LEU:HA	12:L:111:LEU:HD23	1.76	0.42
12:L:192:LEU:HD13	12:L:192:LEU:HA	1.87	0.42
15:V:331:LEU:HA	15:V:334:VAL:HG12	2.02	0.42
18:Y:367:GLN:O	18:Y:370:ILE:HG22	2.19	0.42
3:C:59:LEU:HD13	4:D:72:PHE:HE1	1.83	0.42
7:G:67:THR:HG22	7:G:69:LEU:N	2.35	0.42
9:I:61:PHE:CZ	9:I:227:VAL:HB	2.55	0.42
12:L:202:GLU:N	12:L:202:GLU:OE1	2.52	0.42
1:A:344:SER:OG	1:A:345:LEU:N	2.53	0.41
2:B:103:ARG:HB2	2:B:107:MET:CE	2.49	0.41
3:C:306:LEU:HD23	3:C:306:LEU:HA	1.82	0.41
10:J:36:ARG:HA	10:J:41:VAL:HG12	2.01	0.41
10:J:211:MET:CE	10:J:217:LEU:HA	2.50	0.41
11:K:69:GLU:HB3	11:K:226:PHE:CD2	2.55	0.41
11:K:224:GLN:OE1	11:K:224:GLN:N	2.51	0.41
12:L:49:LEU:HD21	12:L:199:LEU:HD21	2.02	0.41
12:L:103:LEU:HD12	12:L:104:PRO:HD2	2.01	0.41
16:W:333:LEU:N	16:W:334:GLU:OE1	2.52	0.41
17:X:365:LEU:HG	17:X:385:LEU:HD21	2.02	0.41
18:Y:241:ILE:HD11	18:Y:261:PHE:CE1	2.47	0.41
19:Z:32:GLN:H	19:Z:32:GLN:HG2	1.62	0.41
1:A:312:ARG:HG2	1:A:313:GLY:N	2.34	0.41
2:B:371:ARG:CZ	3:C:179:GLY:HA3	2.49	0.41
8:H:42:ASN:HD21	8:H:184:LEU:H	1.68	0.41
16:W:282:GLU:HG2	16:W:283:GLN:H	1.84	0.41
18:Y:18:ARG:HD2	18:Y:18:ARG:HA	1.69	0.41
19:Z:14:LEU:HD12	19:Z:14:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:LYS:O	1:A:62:LEU:HD23	2.20	0.41
2:B:63:LEU:HD23	2:B:63:LEU:HA	1.88	0.41
5:E:378:LYS:HE3	5:E:378:LYS:HB2	1.92	0.41
7:G:130:GLU:OE1	7:G:130:GLU:N	2.53	0.41
7:G:155:ASP:OD2	7:G:159:TYR:HB3	2.20	0.41
9:I:176:LYS:HD3	10:J:52:LYS:HE3	2.02	0.41
11:K:88:LEU:HD23	11:K:88:LEU:HA	1.85	0.41
12:L:200:PRO:HB2	12:L:202:GLU:OE1	2.19	0.41
15:V:384:GLU:HG2	15:V:385:LYS:N	2.36	0.41
16:W:147:LYS:O	16:W:151:THR:HG22	2.20	0.41
17:X:205:LYS:HB2	17:X:205:LYS:HE3	1.33	0.41
18:Y:84:LEU:O	18:Y:88:LEU:HG	2.20	0.41
1:A:76:ALA:HA	1:A:79:ASP:OD2	2.21	0.41
4:D:168:GLY:H	27:D:501:ATP:HN61	1.67	0.41
14:U:472:ILE:HD13	14:U:472:ILE:HG21	1.81	0.41
15:V:225:ASP:O	15:V:228:ARG:N	2.52	0.41
15:V:237:THR:O	15:V:241:ARG:NH2	2.53	0.41
15:V:496:PHE:N	15:V:497:PRO:CD	2.83	0.41
17:X:236:PHE:HB2	17:X:250:SER:OG	2.21	0.41
1:A:301:GLU:OE2	1:A:305:GLN:HG2	2.21	0.41
9:I:38:LEU:HB2	9:I:43:VAL:HG23	2.02	0.41
9:I:238:LYS:O	9:I:242:GLU:HG2	2.21	0.41
13:M:210:GLU:HG2	13:M:211:LEU:H	1.84	0.41
16:W:152:ILE:HG23	16:W:157:GLY:HA2	2.02	0.41
16:W:227:TYR:HD1	16:W:227:TYR:HA	1.78	0.41
16:W:456:GLN:OE1	16:W:456:GLN:N	2.53	0.41
2:B:64:LYS:CG	2:B:67:ARG:HH21	2.33	0.41
4:D:200:ARG:HH22	4:D:301:GLN:H	1.66	0.41
14:U:800:VAL:HG22	14:U:801:GLN:N	2.35	0.41
16:W:251:TYR:CE1	16:W:267:LEU:HD21	2.54	0.41
16:W:316:ARG:O	16:W:317:TRP:HB3	2.20	0.41
17:X:202:CYS:N	17:X:203:PRO:CD	2.84	0.41
18:Y:30:GLU:H	18:Y:30:GLU:CD	2.22	0.41
18:Y:286:TRP:O	18:Y:287:LEU:HG	2.21	0.41
18:Y:362:LYS:HD2	18:Y:362:LYS:HA	1.81	0.41
1:A:184:ILE:HD13	1:A:184:ILE:HA	1.74	0.41
1:A:297:ARG:HH12	6:F:306:VAL:HG21	1.86	0.41
2:B:102:LEU:HD13	2:B:102:LEU:HA	1.82	0.41
2:B:319:PHE:CG	2:B:319:PHE:O	2.73	0.41
3:C:163:GLU:HA	3:C:167:LEU:HD13	2.02	0.41
4:D:45:LYS:HA	4:D:45:LYS:HD2	1.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:70:ASP:OD2	13:M:71:ARG:N	2.51	0.41
15:V:224:LEU:O	15:V:227:VAL:HB	2.21	0.41
16:W:188:GLU:O	16:W:191:ARG:HG2	2.21	0.41
2:B:205:LEU:HD23	2:B:205:LEU:HA	1.88	0.41
3:C:188:LEU:O	3:C:294:ALA:HA	2.21	0.41
5:E:282:PRO:HA	5:E:285:LEU:HD23	2.02	0.41
9:I:150:SER:OG	9:I:151:ASP:N	2.54	0.41
11:K:191:LEU:HD12	11:K:191:LEU:HA	1.85	0.41
16:W:346:GLU:OE2	16:W:350:ARG:NE	2.53	0.41
17:X:122:ARG:HE	17:X:122:ARG:HB2	1.76	0.41
17:X:397:TYR:HD1	17:X:397:TYR:HA	1.72	0.41
18:Y:13:LYS:CE	18:Y:146:ARG:HB3	2.50	0.41
18:Y:83:ARG:HA	18:Y:86:GLU:OE1	2.20	0.41
2:B:56:THR:HG23	2:B:58:CYS:H	1.86	0.41
4:D:215:LEU:HA	4:D:215:LEU:HD23	1.86	0.41
4:D:337:ASP:OD1	4:D:338:ARG:N	2.46	0.41
5:E:145:LEU:O	5:E:148:VAL:HG12	2.20	0.41
6:F:78:GLU:O	6:F:82:VAL:HG13	2.21	0.41
9:I:2:SER:N	12:L:123:TYR:HH	2.18	0.41
10:J:63:CYS:SG	10:J:64:ALA:N	2.93	0.41
11:K:189:MET:CE	11:K:193:GLU:HG3	2.51	0.41
16:W:162:ALA:HA	16:W:192:LEU:HD23	2.01	0.41
16:W:438:LEU:HD12	16:W:438:LEU:HA	1.76	0.41
18:Y:45:VAL:HG23	18:Y:46:ARG:HD3	2.03	0.41
18:Y:241:ILE:HD12	18:Y:241:ILE:HA	1.95	0.41
18:Y:311:TYR:CD2	18:Y:314:LEU:HD22	2.56	0.41
2:B:80:ARG:CG	2:B:84:GLN:HE22	2.31	0.41
4:D:284:GLU:O	4:D:288:ILE:HG13	2.21	0.41
10:J:71:MET:HE2	10:J:71:MET:HB2	1.91	0.41
11:K:199:LEU:HD21	11:K:217:LEU:HD21	2.03	0.41
13:M:60:GLU:H	13:M:60:GLU:CD	2.24	0.41
14:U:132:GLY:HA2	14:U:135:ASN:ND2	2.35	0.41
14:U:727:LYS:O	14:U:731:ILE:HG22	2.19	0.41
1:A:53:GLN:HG3	1:A:57:LYS:HZ1	1.86	0.40
1:A:78:TRP:CG	2:B:138:PHE:HB3	2.56	0.40
1:A:233:THR:OG1	1:A:234:ASP:N	2.54	0.40
4:D:156:SER:OG	4:D:157:ASP:OD1	2.38	0.40
4:D:355:SER:OG	4:D:356:GLU:N	2.52	0.40
5:E:309:ARG:NE	5:E:335:SER:O	2.54	0.40
6:F:435:LEU:HD22	6:F:435:LEU:HA	1.88	0.40
8:H:67:PRO:HB3	8:H:218:PHE:CE2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:K:121:LEU:HD12	12:L:79:ALA:HB3	2.03	0.40
13:M:42:LYS:HE2	13:M:183:GLU:O	2.20	0.40
14:U:34:PHE:O	14:U:38:ILE:HG12	2.21	0.40
15:V:264:TYR:CD2	15:V:265:ASP:N	2.89	0.40
15:V:471:GLU:N	15:V:472:PRO:HD2	2.36	0.40
19:Z:219:LYS:HD3	19:Z:220:LEU:N	2.33	0.40
1:A:74:PRO:HA	1:A:75:PRO:HD3	1.96	0.40
2:B:216:ILE:HD13	2:B:216:ILE:HA	1.72	0.40
3:C:116:LEU:HD23	3:C:117:ARG:O	2.21	0.40
6:F:251:LEU:HD12	6:F:252:ALA:H	1.86	0.40
14:U:43:ASP:O	14:U:47:VAL:HG23	2.20	0.40
14:U:330:SER:OG	14:U:332:GLU:OE1	2.33	0.40
14:U:333:MET:HA	14:U:336:GLU:OE2	2.21	0.40
14:U:803:LYS:C	14:U:893:THR:HB	2.41	0.40
15:V:307:ARG:HG3	15:V:308:THR:N	2.36	0.40
16:W:225:LYS:O	16:W:229:LEU:HG	2.21	0.40
17:X:137:TYR:O	17:X:140:THR:OG1	2.31	0.40
18:Y:204:THR:HG22	18:Y:219:PHE:HE2	1.85	0.40
1:A:222:LYS:H	1:A:222:LYS:HG2	1.71	0.40
2:B:170:LEU:HD12	2:B:173:VAL:HG21	2.02	0.40
6:F:114:ASP:OD1	6:F:114:ASP:N	2.55	0.40
11:K:85:ALA:O	11:K:89:ILE:HG12	2.21	0.40
11:K:236:GLU:HA	11:K:239:LYS:NZ	2.36	0.40
13:M:120:HIS:O	13:M:123:THR:HG22	2.22	0.40
15:V:343:PRO:O	15:V:344:ASP:HB2	2.22	0.40
16:W:345:GLU:H	16:W:345:GLU:CD	2.23	0.40
16:W:442:THR:HA	19:Z:229:GLN:OE1	2.21	0.40
17:X:132:ARG:HA	17:X:132:ARG:HE	1.86	0.40
18:Y:70:LEU:HB3	18:Y:74:LYS:NZ	2.35	0.40
3:C:83:LYS:HA	3:C:105:ILE:HD11	2.03	0.40
7:G:216:GLU:N	7:G:216:GLU:OE1	2.54	0.40
12:L:49:LEU:HD12	12:L:209:ASN:O	2.21	0.40
13:M:241:GLU:O	13:M:244:LYS:HG2	2.20	0.40
14:U:23:ALA:O	14:U:26:LYS:HG2	2.22	0.40
15:V:415:SER:O	15:V:459:GLN:HA	2.22	0.40
17:X:162:ASP:O	17:X:163:LYS:HD3	2.22	0.40
18:Y:155:ASP:OD1	18:Y:155:ASP:N	2.54	0.40
2:B:94:GLU:HG3	2:B:98:LYS:NZ	2.36	0.40
3:C:71:SER:OG	4:D:112:TYR:HD2	2.04	0.40
4:D:152:MET:HE1	4:D:226:ALA:HB1	2.03	0.40
7:G:224:ASN:N	7:G:224:ASN:OD1	2.53	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:51:ALA:O	10:J:52:LYS:HG3	2.21	0.40
10:J:170:GLU:HA	10:J:173:GLU:OE2	2.21	0.40
10:J:183:THR:N	10:J:186:LEU:HD12	2.36	0.40
12:L:195:LEU:O	12:L:198:THR:HG22	2.22	0.40
13:M:175:GLU:N	13:M:175:GLU:OE1	2.55	0.40
14:U:263:SER:O	14:U:266:GLN:HG3	2.22	0.40
15:V:337:LEU:HA	15:V:337:LEU:HD13	1.89	0.40
17:X:132:ARG:HA	17:X:132:ARG:NE	2.37	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	392/433 (90%)	337 (86%)	51 (13%)	4 (1%)	13 44
2	B	382/440 (87%)	337 (88%)	42 (11%)	3 (1%)	16 49
3	C	361/406 (89%)	328 (91%)	32 (9%)	1 (0%)	37 69
4	D	378/418 (90%)	335 (89%)	41 (11%)	2 (0%)	25 58
5	E	373/389 (96%)	342 (92%)	31 (8%)	0	100 100
6	F	393/439 (90%)	358 (91%)	32 (8%)	3 (1%)	16 49
7	G	238/246 (97%)	224 (94%)	14 (6%)	0	100 100
8	H	230/234 (98%)	216 (94%)	14 (6%)	0	100 100
9	I	248/261 (95%)	227 (92%)	21 (8%)	0	100 100
10	J	237/248 (96%)	217 (92%)	19 (8%)	1 (0%)	30 63
11	K	232/241 (96%)	210 (90%)	19 (8%)	3 (1%)	10 39
12	L	236/263 (90%)	214 (91%)	22 (9%)	0	100 100
13	M	238/255 (93%)	219 (92%)	19 (8%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
14	U	809/953 (85%)	750 (93%)	59 (7%)	0	100	100
15	V	489/534 (92%)	423 (86%)	65 (13%)	1 (0%)	44	74
16	W	454/456 (100%)	412 (91%)	40 (9%)	2 (0%)	30	63
17	X	378/422 (90%)	342 (90%)	33 (9%)	3 (1%)	16	49
18	Y	376/389 (97%)	337 (90%)	39 (10%)	0	100	100
19	Z	284/324 (88%)	260 (92%)	24 (8%)	0	100	100
20	d	255/350 (73%)	208 (82%)	46 (18%)	1 (0%)	30	63
21	e	45/70 (64%)	32 (71%)	13 (29%)	0	100	100
22	f	876/908 (96%)	727 (83%)	141 (16%)	8 (1%)	14	45
23	a	371/376 (99%)	343 (92%)	27 (7%)	1 (0%)	37	69
24	b	189/377 (50%)	164 (87%)	24 (13%)	1 (0%)	25	58
25	c	285/310 (92%)	256 (90%)	29 (10%)	0	100	100
26	u	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
26	v	74/81 (91%)	73 (99%)	1 (1%)	0	100	100
26	w	74/81 (91%)	70 (95%)	4 (5%)	0	100	100
26	x	74/81 (91%)	71 (96%)	3 (4%)	0	100	100
All	All	9045/10066 (90%)	8105 (90%)	906 (10%)	34 (0%)	32	63

All (34) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
11	K	128	ALA
15	V	344	ASP
20	d	33	LEU
22	f	344	VAL
22	f	353	LEU
22	f	356	ASN
22	f	787	LEU
22	f	838	ARG
22	f	842	VAL
24	b	24	THR
2	B	181	GLN
6	F	280	PRO
4	D	367	PRO
4	D	368	ASP
11	K	133	MET

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Mol	Chain	Res	Type
17	X	188	ALA
17	X	199	ALA
22	f	335	ARG
22	f	841	PRO
23	a	16	PRO
1	A	309	PHE
1	A	399	ALA
10	J	27	LYS
16	W	312	MET
17	X	202	CYS
2	B	370	SER
2	B	169	PRO
3	C	91	PRO
1	A	378	PRO
11	K	129	ASP
6	F	87	PRO
16	W	418	PRO
1	A	157	ILE
6	F	205	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	337/372 (91%)	330 (98%)	7 (2%)	48 66
2	B	334/385 (87%)	323 (97%)	11 (3%)	33 56
3	C	311/352 (88%)	296 (95%)	15 (5%)	21 46
4	D	333/366 (91%)	318 (96%)	15 (4%)	23 47
5	E	329/341 (96%)	321 (98%)	8 (2%)	44 62
6	F	339/379 (89%)	331 (98%)	8 (2%)	44 62
7	G	193/210 (92%)	193 (100%)	0	100 100
8	H	164/191 (86%)	162 (99%)	2 (1%)	67 77
9	I	193/221 (87%)	192 (100%)	1 (0%)	86 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
10	J	154/211 (73%)	148 (96%)	6 (4%)	27 51
11	K	189/203 (93%)	185 (98%)	4 (2%)	48 66
12	L	198/224 (88%)	195 (98%)	3 (2%)	60 74
13	M	192/212 (91%)	191 (100%)	1 (0%)	86 90
14	U	695/816 (85%)	677 (97%)	18 (3%)	41 61
15	V	236/460 (51%)	231 (98%)	5 (2%)	48 66
16	W	291/416 (70%)	280 (96%)	11 (4%)	28 52
17	X	262/362 (72%)	244 (93%)	18 (7%)	13 37
18	Y	334/344 (97%)	326 (98%)	8 (2%)	44 62
19	Z	257/295 (87%)	253 (98%)	4 (2%)	58 73
20	d	212/294 (72%)	198 (93%)	14 (7%)	14 38
21	e	12/63 (19%)	11 (92%)	1 (8%)	9 32
23	a	333/336 (99%)	323 (97%)	10 (3%)	36 58
24	b	167/312 (54%)	164 (98%)	3 (2%)	54 71
25	c	252/268 (94%)	244 (97%)	8 (3%)	34 56
26	u	68/70 (97%)	67 (98%)	1 (2%)	60 74
26	v	68/70 (97%)	68 (100%)	0	100 100
26	w	68/70 (97%)	66 (97%)	2 (3%)	37 58
26	x	68/70 (97%)	67 (98%)	1 (2%)	60 74
All	All	6589/7913 (83%)	6404 (97%)	185 (3%)	40 59

All (185) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	110	LYS
1	A	150	HIS
1	A	157	ILE
1	A	160	THR
1	A	297	ARG
1	A	312	ARG
1	A	426	THR
2	B	177	GLU
2	B	178	LYS
2	B	181	GLN
2	B	186	ASP

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Mol	Chain	Res	Type
2	B	187	ILE
2	B	192	ASN
2	B	193	GLN
2	B	314	ASN
2	B	315	GLN
2	B	317	ASP
2	B	371	ARG
3	C	33	LEU
3	C	39	SER
3	C	92	GLU
3	C	125	LYS
3	C	126	ILE
3	C	134	LEU
3	C	136	SER
3	C	180	ILE
3	C	229	ARG
3	C	239	ARG
3	C	250	GLU
3	C	251	ILE
3	C	293	MET
3	C	372	ARG
3	C	383	PHE
4	D	46	LYS
4	D	47	LEU
4	D	54	LEU
4	D	56	VAL
4	D	60	TYR
4	D	96	VAL
4	D	98	GLN
4	D	99	ASN
4	D	100	THR
4	D	352	MET
4	D	353	ASN
4	D	354	LEU
4	D	358	VAL
4	D	360	LEU
4	D	368	ASP
5	E	35	GLU
5	E	134	GLU
5	E	190	GLN
5	E	223	ARG
5	E	242	ARG

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Mol	Chain	Res	Type
5	E	262	ASN
5	E	275	MET
5	E	310	LEU
6	F	69	MET
6	F	215	LEU
6	F	277	GLU
6	F	278	LYS
6	F	281	SER
6	F	282	ILE
6	F	320	PHE
6	F	435	LEU
8	H	39	LYS
8	H	70	LYS
9	I	67	LYS
10	J	52	LYS
10	J	96	LEU
10	J	98	VAL
10	J	100	ASP
10	J	118	TYR
10	J	147	THR
11	K	10	ARG
11	K	21	LEU
11	K	129	ASP
11	K	133	MET
12	L	207	THR
12	L	226	ASP
12	L	227	ASP
13	M	41	CYS
14	U	69	TYR
14	U	118	LEU
14	U	179	TYR
14	U	194	ARG
14	U	203	LYS
14	U	259	GLN
14	U	333	MET
14	U	345	ASN
14	U	387	ARG
14	U	388	ASP
14	U	415	HIS
14	U	423	MET
14	U	527	GLN
14	U	603	LEU

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Mol	Chain	Res	Type
14	U	609	ASP
14	U	612	ASP
14	U	666	LYS
14	U	755	THR
15	V	210	CYS
15	V	220	PHE
15	V	223	LYS
15	V	283	ASN
15	V	497	PRO
16	W	251	TYR
16	W	262	LYS
16	W	273	TYR
16	W	313	GLU
16	W	314	LEU
16	W	315	MET
16	W	316	ARG
16	W	341	PHE
16	W	351	TRP
16	W	412	ILE
16	W	419	LYS
17	X	155	ARG
17	X	182	ASN
17	X	190	LEU
17	X	191	THR
17	X	192	SER
17	X	194	ARG
17	X	196	THR
17	X	200	ILE
17	X	205	LYS
17	X	374	PHE
17	X	390	GLU
17	X	394	ASP
17	X	395	LYS
17	X	396	THR
17	X	397	TYR
17	X	398	GLU
17	X	408	SER
17	X	409	LYS
18	Y	50	MET
18	Y	232	GLU
18	Y	233	ARG
18	Y	242	LYS

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Mol	Chain	Res	Type
18	Y	246	ILE
18	Y	247	LEU
18	Y	248	GLU
18	Y	267	ARG
19	Z	43	TRP
19	Z	237	LEU
19	Z	257	MET
19	Z	288	LYS
20	d	11	ARG
20	d	12	LYS
20	d	33	LEU
20	d	34	ASN
20	d	36	LEU
20	d	66	LYS
20	d	67	ASP
20	d	70	SER
20	d	73	ARG
20	d	84	ASP
20	d	89	LEU
20	d	92	SER
20	d	96	HIS
20	d	97	GLN
21	e	3	GLU
23	a	9	GLN
23	a	61	GLU
23	a	63	PHE
23	a	64	ILE
23	a	89	ASP
23	a	96	PHE
23	a	106	SER
23	a	108	ASP
23	a	113	LEU
23	a	341	LEU
24	b	107	MET
24	b	133	LYS
24	b	181	ASP
25	c	26	ASP
25	c	43	LYS
25	c	196	LEU
25	c	198	ARG
25	c	204	THR
25	c	254	ASN

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Mol	Chain	Res	Type
25	c	303	MET
25	c	308	VAL
26	u	7	THR
26	x	52	ASP
26	w	4	PHE
26	w	31	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	GLN
1	A	85	GLN
1	A	88	GLN
2	B	84	GLN
4	D	65	GLN
4	D	222	HIS
6	F	307	GLN
15	V	266	GLN
15	V	299	GLN
15	V	387	GLN
17	X	198	ASN
20	d	252	GLN
24	b	12	ASN
26	w	41	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
27	ATP	D	501	28	26,33,33	0.80	0	31,52,52	0.92	2 (6%)
27	ATP	A	501	28	26,33,33	0.80	0	31,52,52	0.93	2 (6%)
29	ADP	C	501	-	24,29,29	0.96	1 (4%)	29,45,45	1.63	4 (13%)
29	ADP	F	501	28	24,29,29	1.09	1 (4%)	29,45,45	1.63	5 (17%)
27	ATP	B	501	28	26,33,33	0.74	0	31,52,52	0.90	2 (6%)
27	ATP	E	401	28	26,33,33	0.82	1 (3%)	31,52,52	0.94	2 (6%)

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
27	ATP	D	501	28	-	3/18/38/38	0/3/3/3
27	ATP	A	501	28	-	5/18/38/38	0/3/3/3
29	ADP	C	501	-	-	2/12/32/32	0/3/3/3
29	ADP	F	501	28	-	4/12/32/32	0/3/3/3
27	ATP	B	501	28	-	3/18/38/38	0/3/3/3
27	ATP	E	401	28	-	7/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	F	501	ADP	C2'-C1'	-2.45	1.50	1.53
29	C	501	ADP	C5-C4	2.24	1.46	1.40
27	E	401	ATP	C8-N7	-2.04	1.31	1.34

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	F	501	ADP	PA-O3A-PB	-4.77	116.44	132.83
29	C	501	ADP	PA-O3A-PB	-4.57	117.16	132.83
29	C	501	ADP	C3'-C2'-C1'	3.97	106.95	100.98
29	F	501	ADP	N3-C2-N1	-3.20	123.67	128.68
29	C	501	ADP	C4-C5-N7	-3.04	106.23	109.40
29	C	501	ADP	N3-C2-N1	-2.79	124.32	128.68
29	F	501	ADP	O3B-PB-O2B	2.72	118.03	107.64
29	F	501	ADP	O3'-C3'-C2'	-2.42	103.98	111.82
27	A	501	ATP	C3'-C2'-C1'	2.40	104.58	100.98
27	B	501	ATP	C5-C6-N6	2.36	123.94	120.35
27	A	501	ATP	C5-C6-N6	2.34	123.92	120.35
29	F	501	ADP	O4'-C1'-C2'	-2.34	103.50	106.93
27	D	501	ATP	C5-C6-N6	2.27	123.80	120.35
27	E	401	ATP	C5-C6-N6	2.14	123.60	120.35
27	B	501	ATP	C3'-C2'-C1'	2.08	104.11	100.98
27	E	401	ATP	PB-O3B-PG	2.01	139.72	132.83
27	D	501	ATP	C3'-C2'-C1'	2.01	104.00	100.98

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	A	501	ATP	C5'-O5'-PA-O1A
27	E	401	ATP	PB-O3B-PG-O2G
27	E	401	ATP	C5'-O5'-PA-O1A
27	E	401	ATP	C5'-O5'-PA-O2A
27	E	401	ATP	O4'-C4'-C5'-O5'
27	E	401	ATP	C3'-C4'-C5'-O5'
29	F	501	ADP	C5'-O5'-PA-O1A
29	F	501	ADP	C3'-C4'-C5'-O5'
27	A	501	ATP	O4'-C4'-C5'-O5'
29	F	501	ADP	O4'-C4'-C5'-O5'
27	D	501	ATP	C5'-O5'-PA-O3A
27	B	501	ATP	PB-O3A-PA-O1A
29	C	501	ADP	PB-O3A-PA-O1A
27	A	501	ATP	C5'-O5'-PA-O2A
27	B	501	ATP	O4'-C4'-C5'-O5'
27	A	501	ATP	C3'-C4'-C5'-O5'
27	B	501	ATP	C3'-C4'-C5'-O5'
27	D	501	ATP	PG-O3B-PB-O1B
27	E	401	ATP	PB-O3B-PG-O3G
27	A	501	ATP	C5'-O5'-PA-O3A
27	E	401	ATP	C5'-O5'-PA-O3A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
29	F	501	ADP	C5'-O5'-PA-O3A
29	C	501	ADP	C5'-O5'-PA-O1A
27	D	501	ATP	O4'-C4'-C5'-O5'

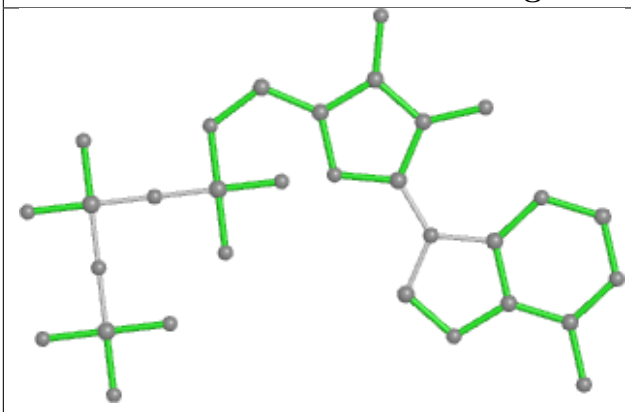
There are no ring outliers.

4 monomers are involved in 7 short contacts:

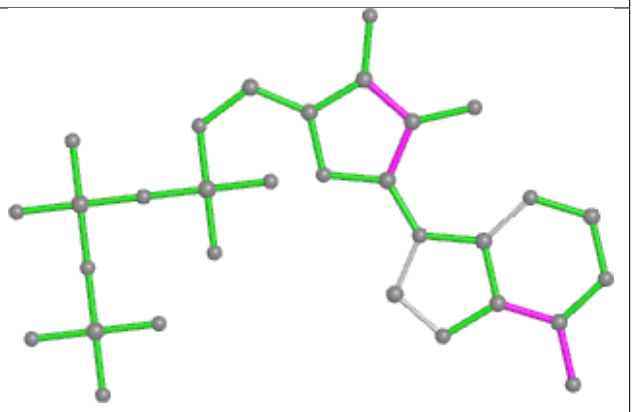
Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	D	501	ATP	1	0
29	C	501	ADP	3	0
29	F	501	ADP	1	0
27	E	401	ATP	2	0

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.

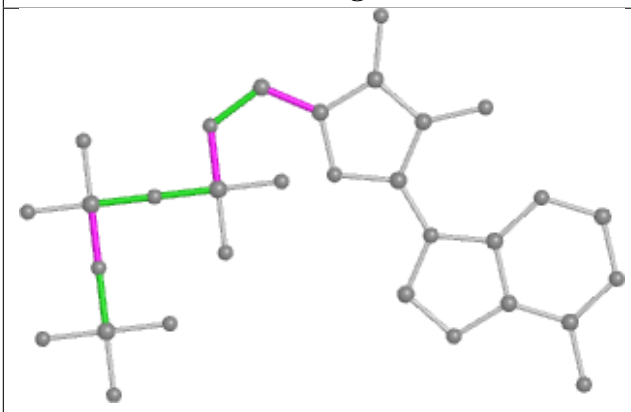
Ligand ATP D 501



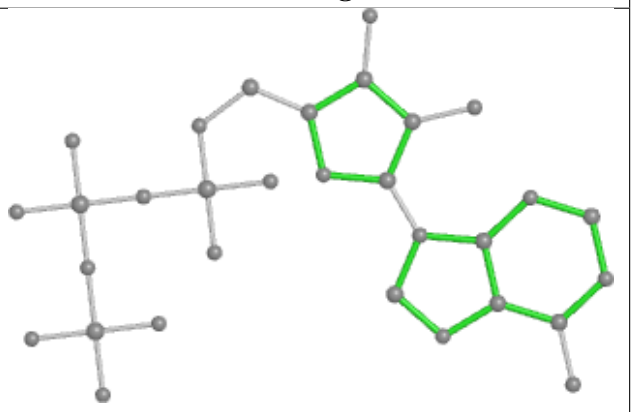
Bond lengths



Bond angles

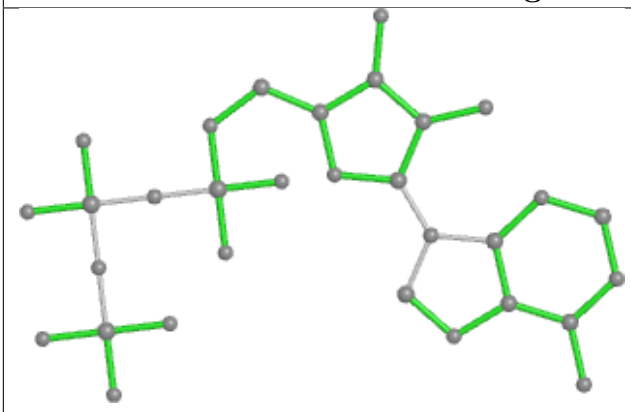


Torsions

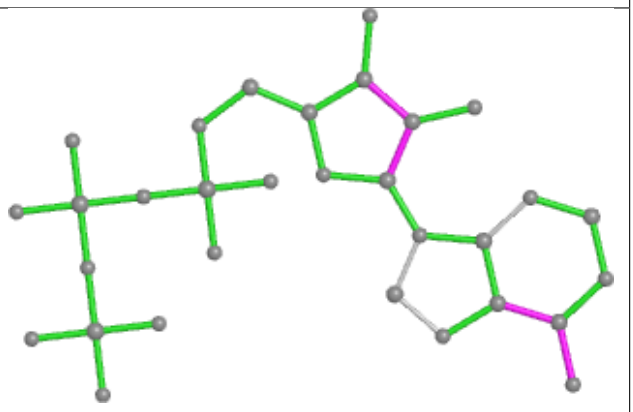


Rings

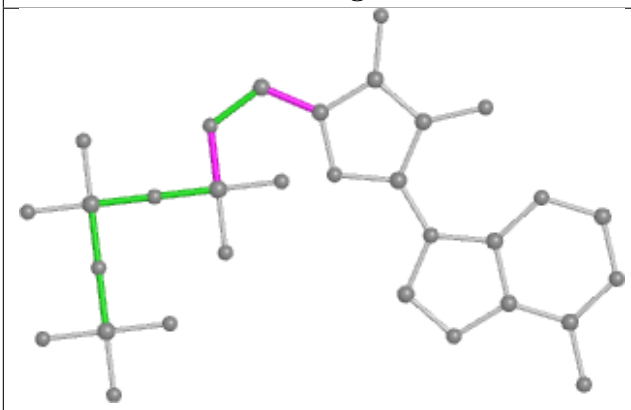
Ligand ATP A 501



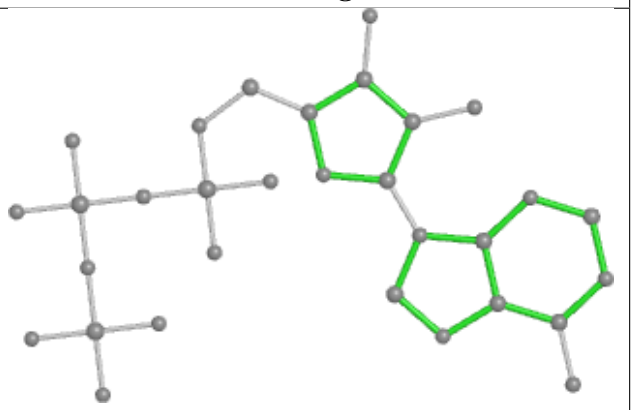
Bond lengths



Bond angles

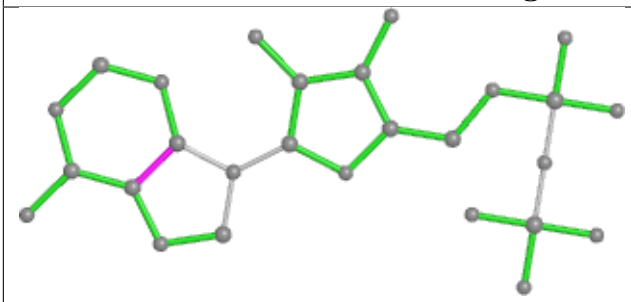


Torsions

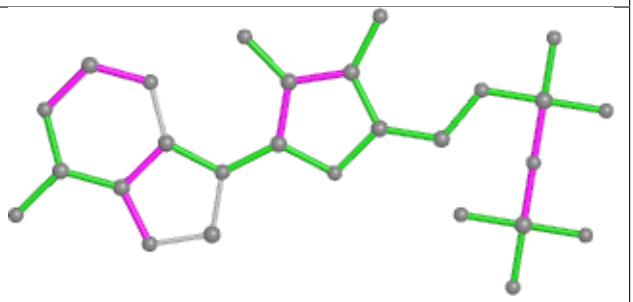


Rings

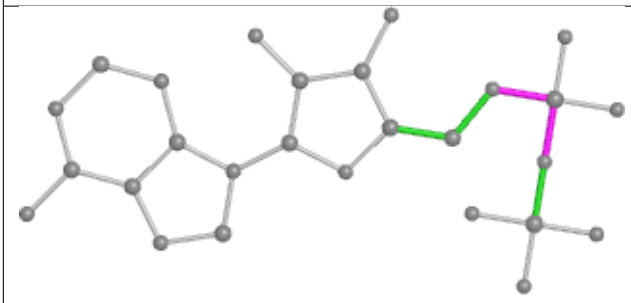
Ligand ADP C 501



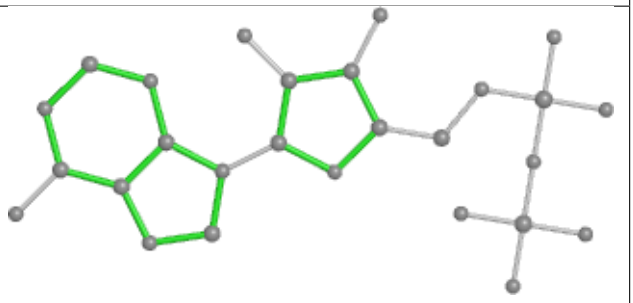
Bond lengths



Bond angles

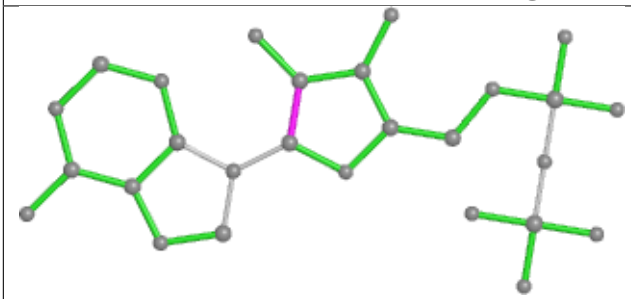


Torsions

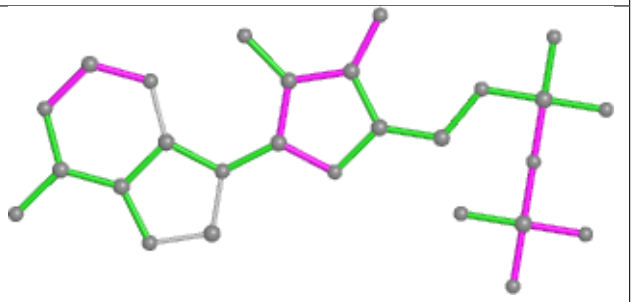


Rings

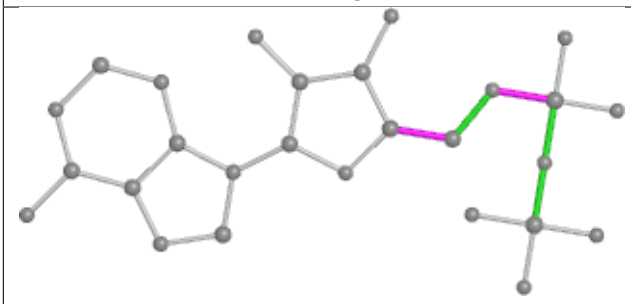
Ligand ADP F 501



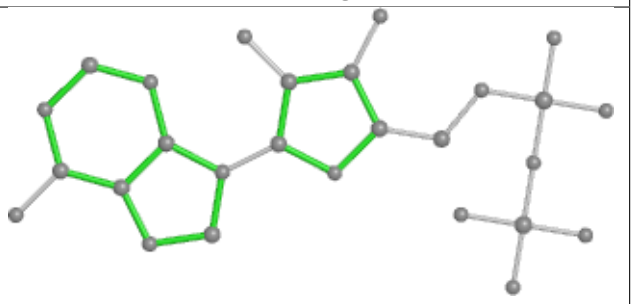
Bond lengths



Bond angles

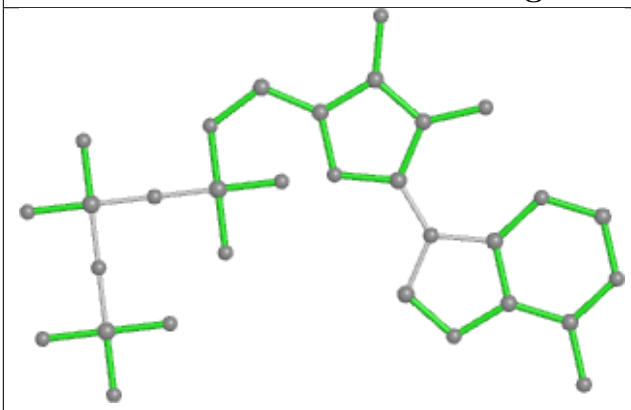


Torsions

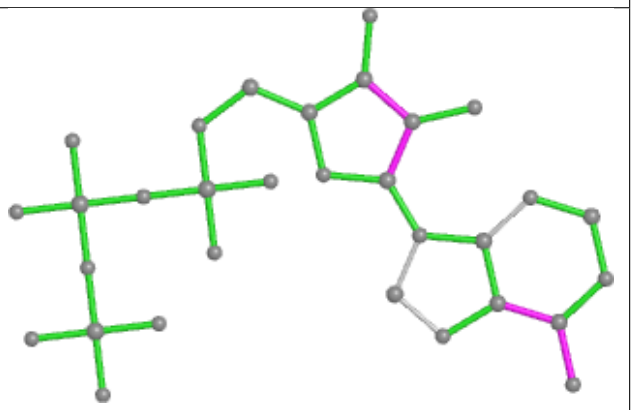


Rings

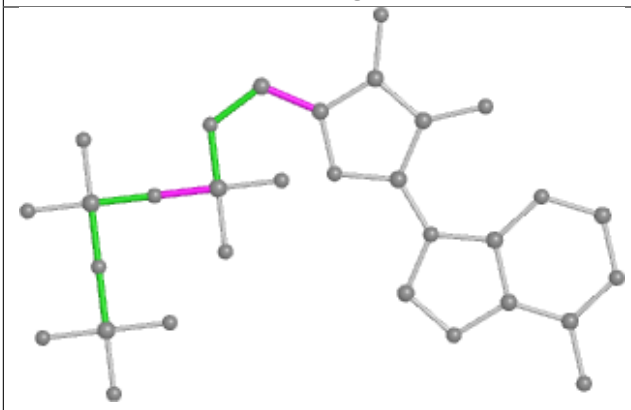
Ligand ATP B 501



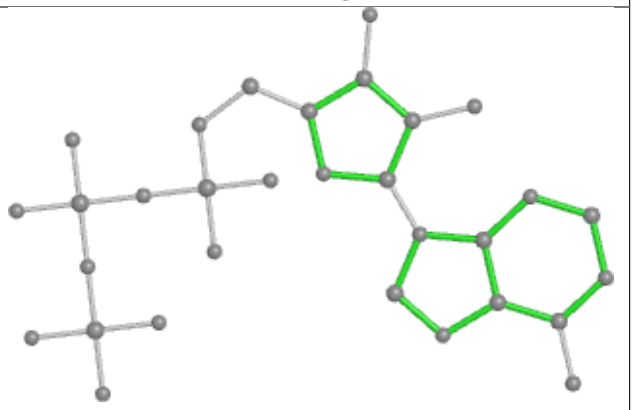
Bond lengths



Bond angles

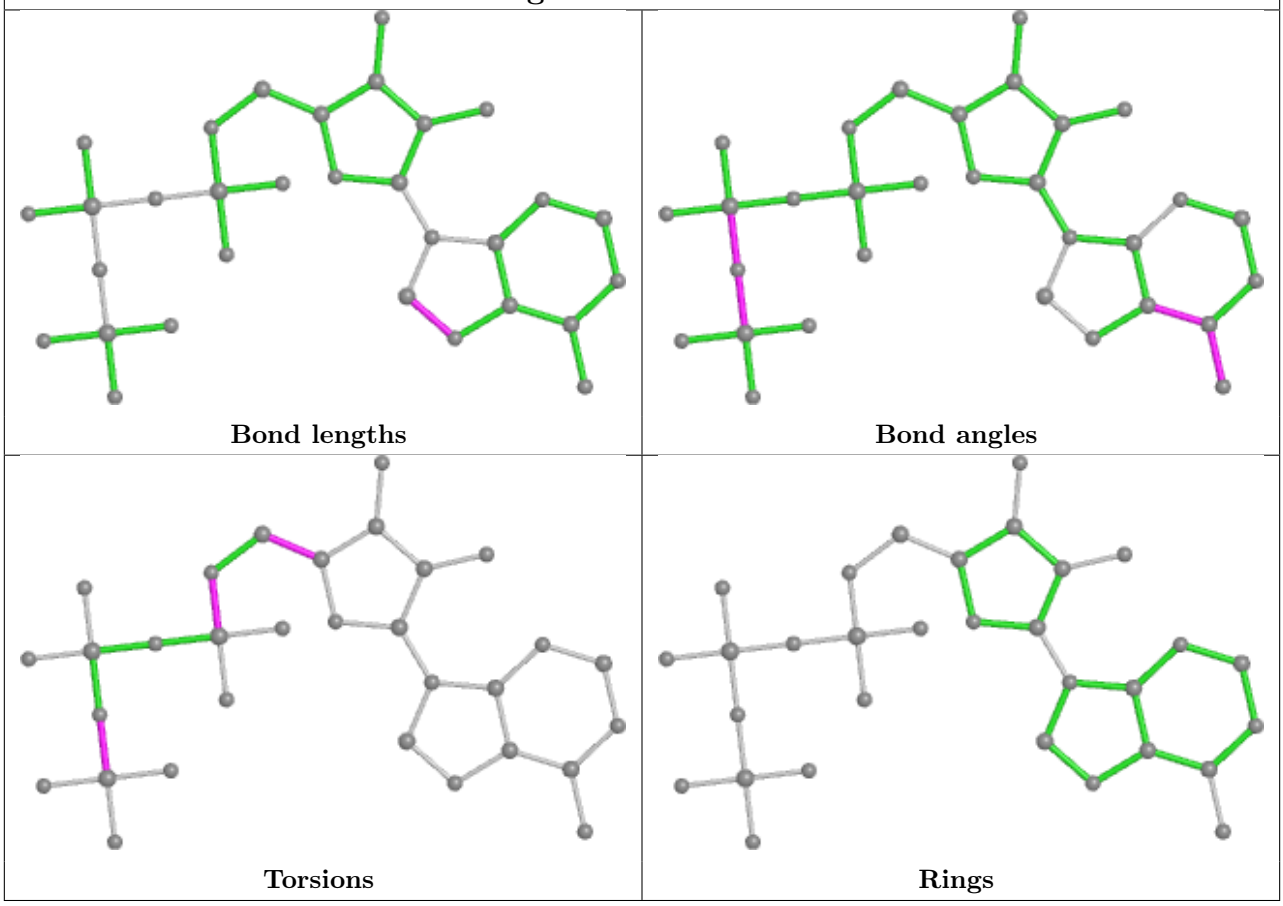


Torsions



Rings

Ligand ATP E 401



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

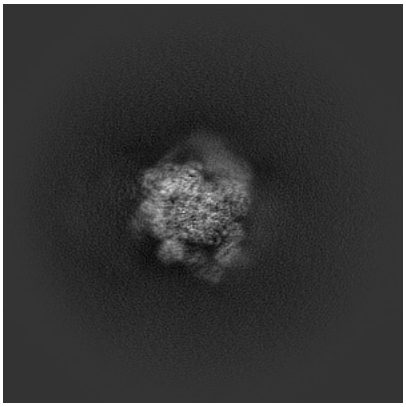
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-36645. These allow visual inspection of the internal detail of the map and identification of artifacts.

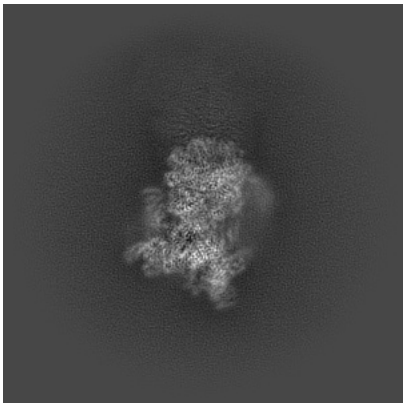
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

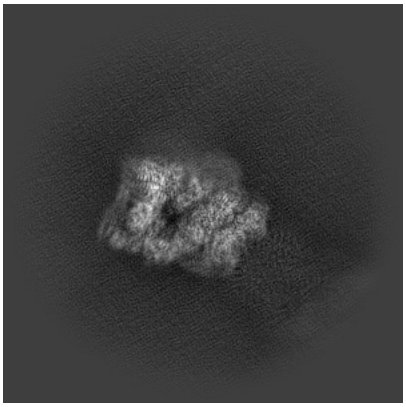
6.1.1 Primary map



X



Y

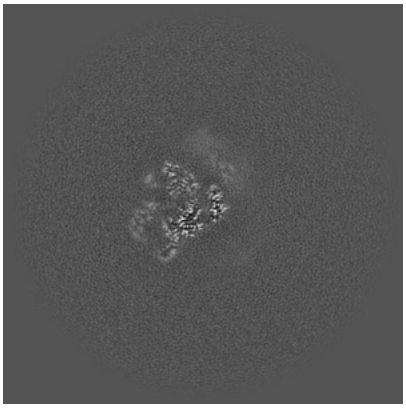


Z

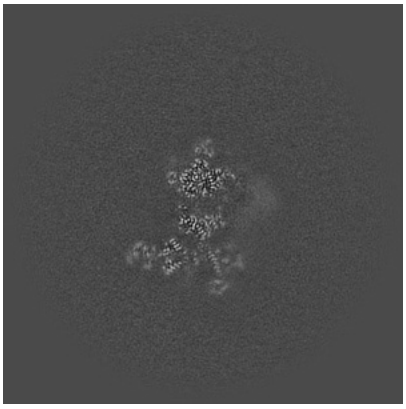
The images above show the map projected in three orthogonal directions.

6.2 Central slices

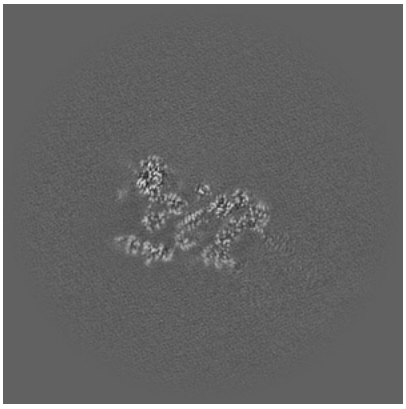
6.2.1 Primary map



X Index: 200



Y Index: 200

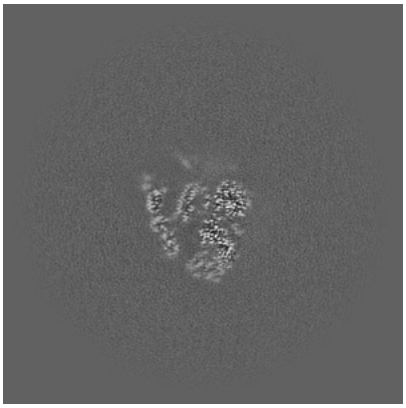


Z Index: 200

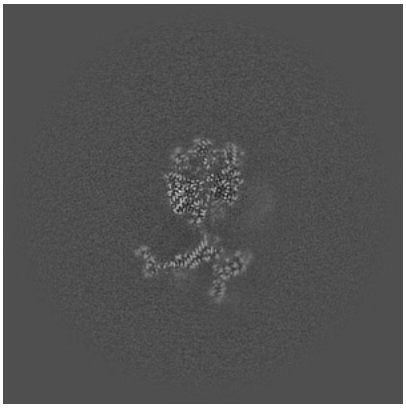
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

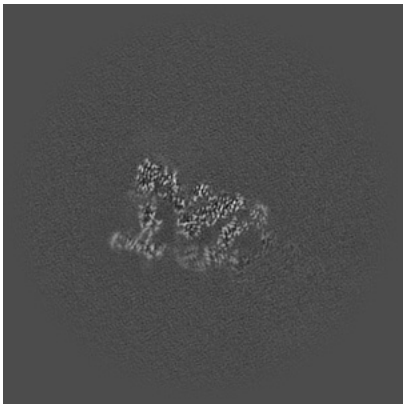
6.3.1 Primary map



X Index: 153



Y Index: 188

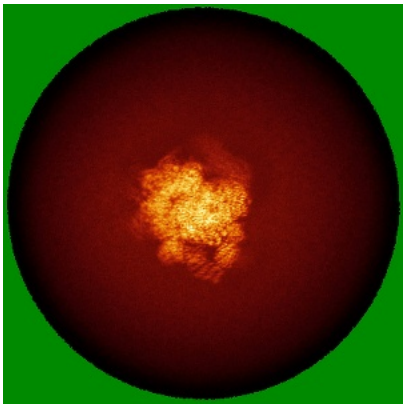


Z Index: 191

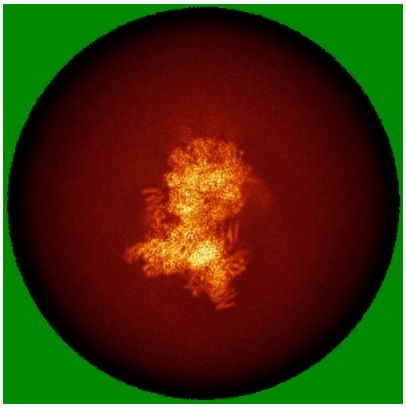
The images above show the largest variance slices of the map in three orthogonal directions.

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

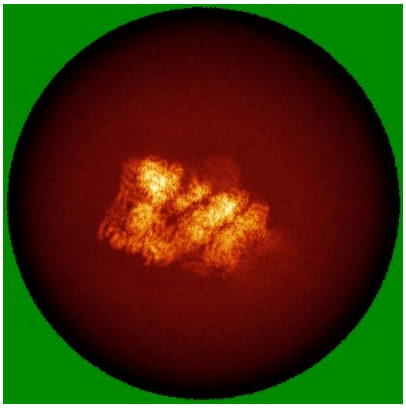
6.4.1 Primary map



X



Y

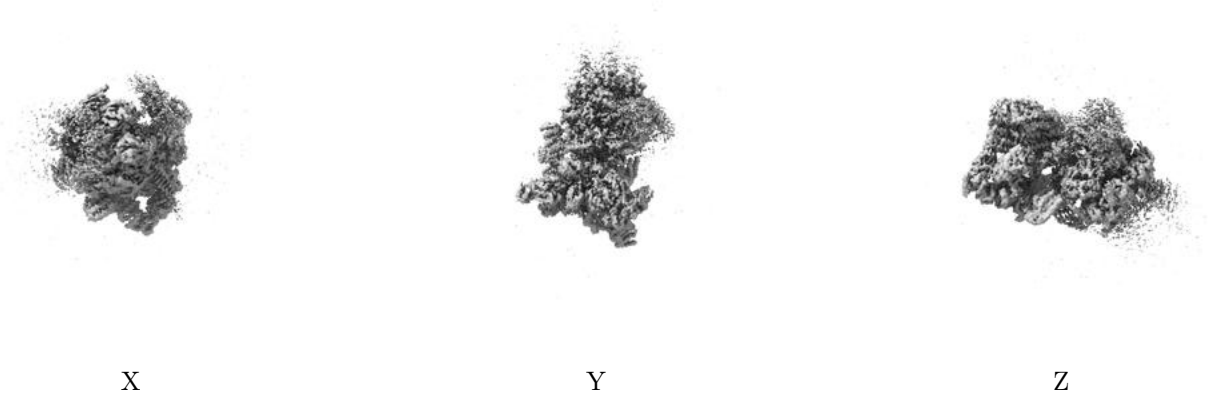


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 5.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

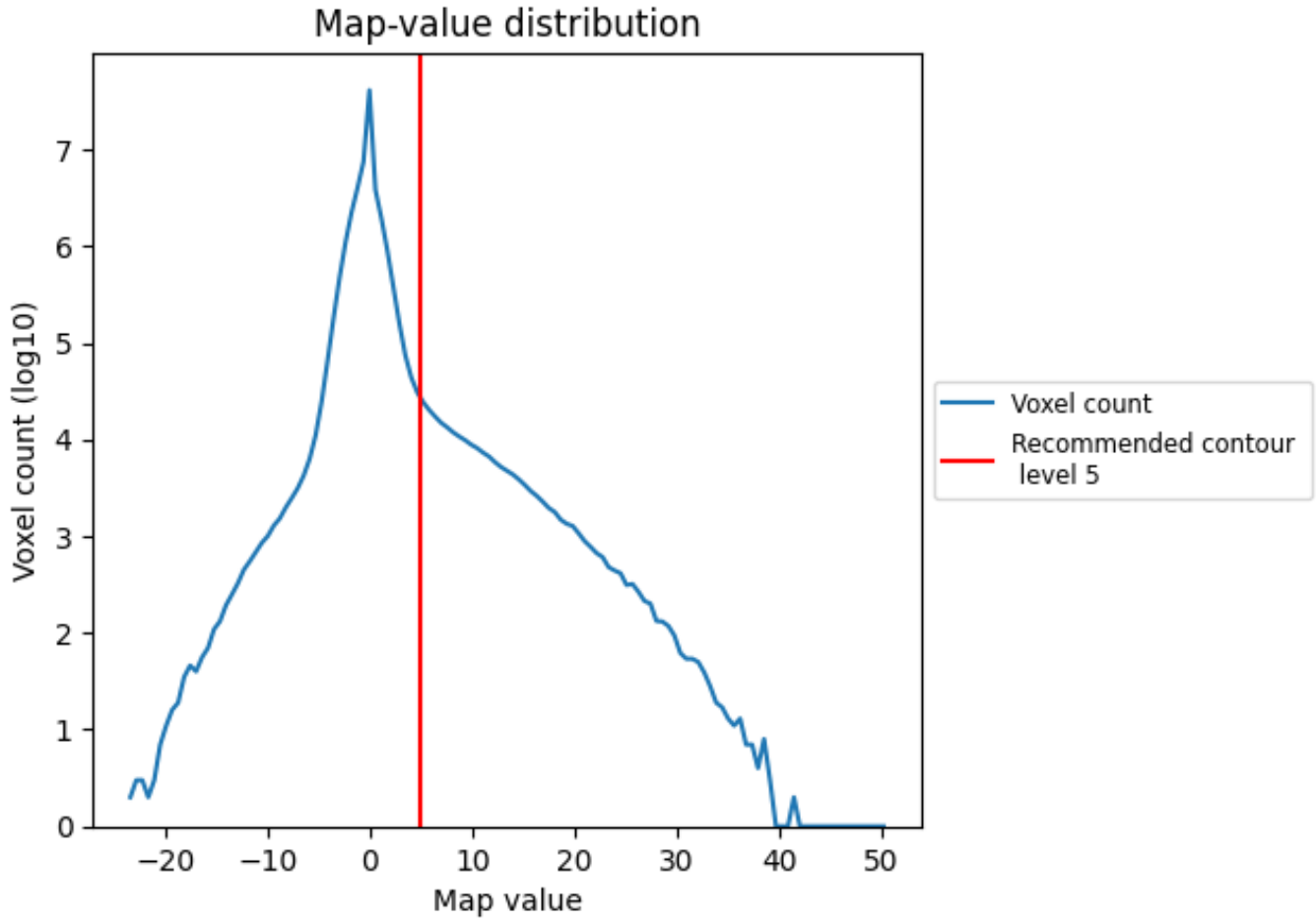
6.6 Mask visualisation (i)

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

7 Map analysis

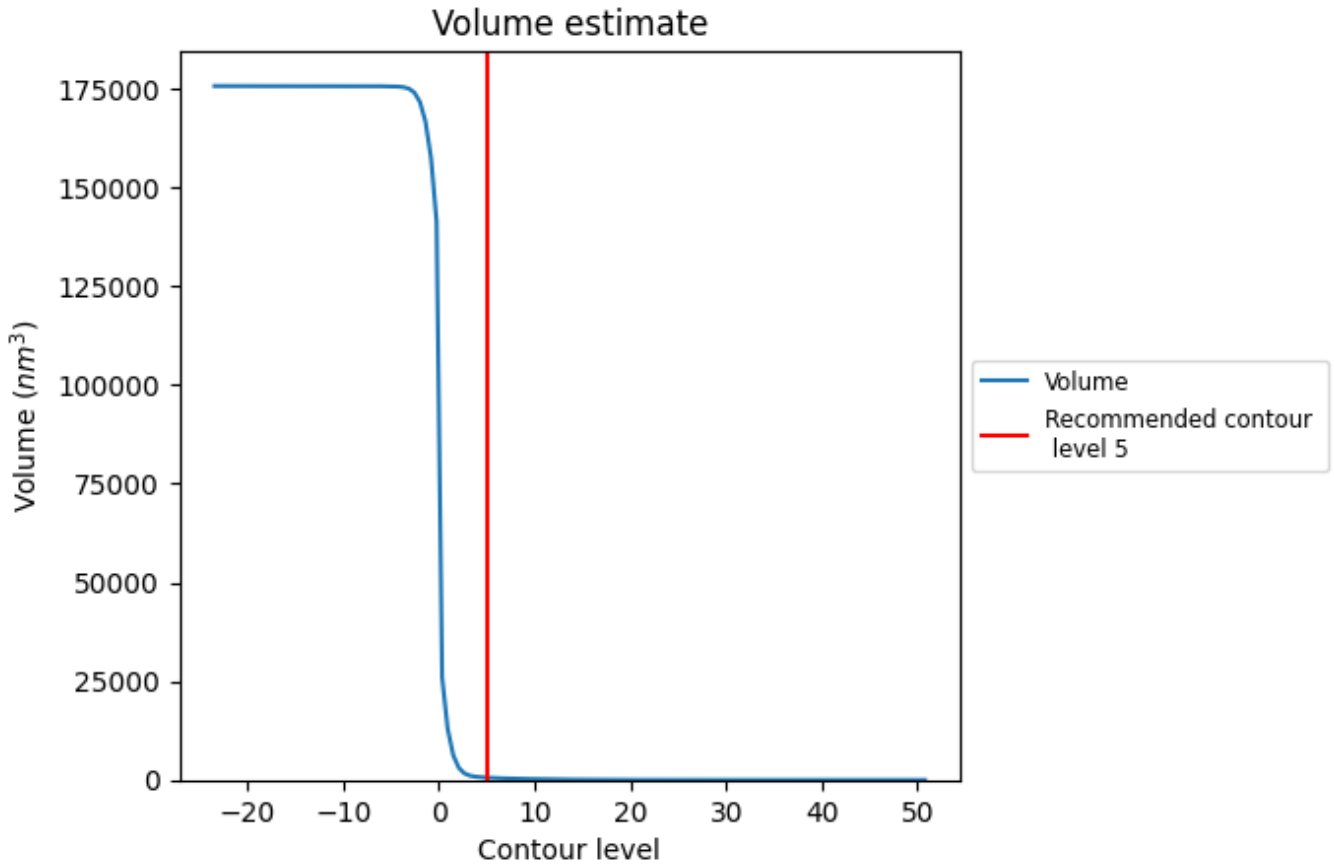
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

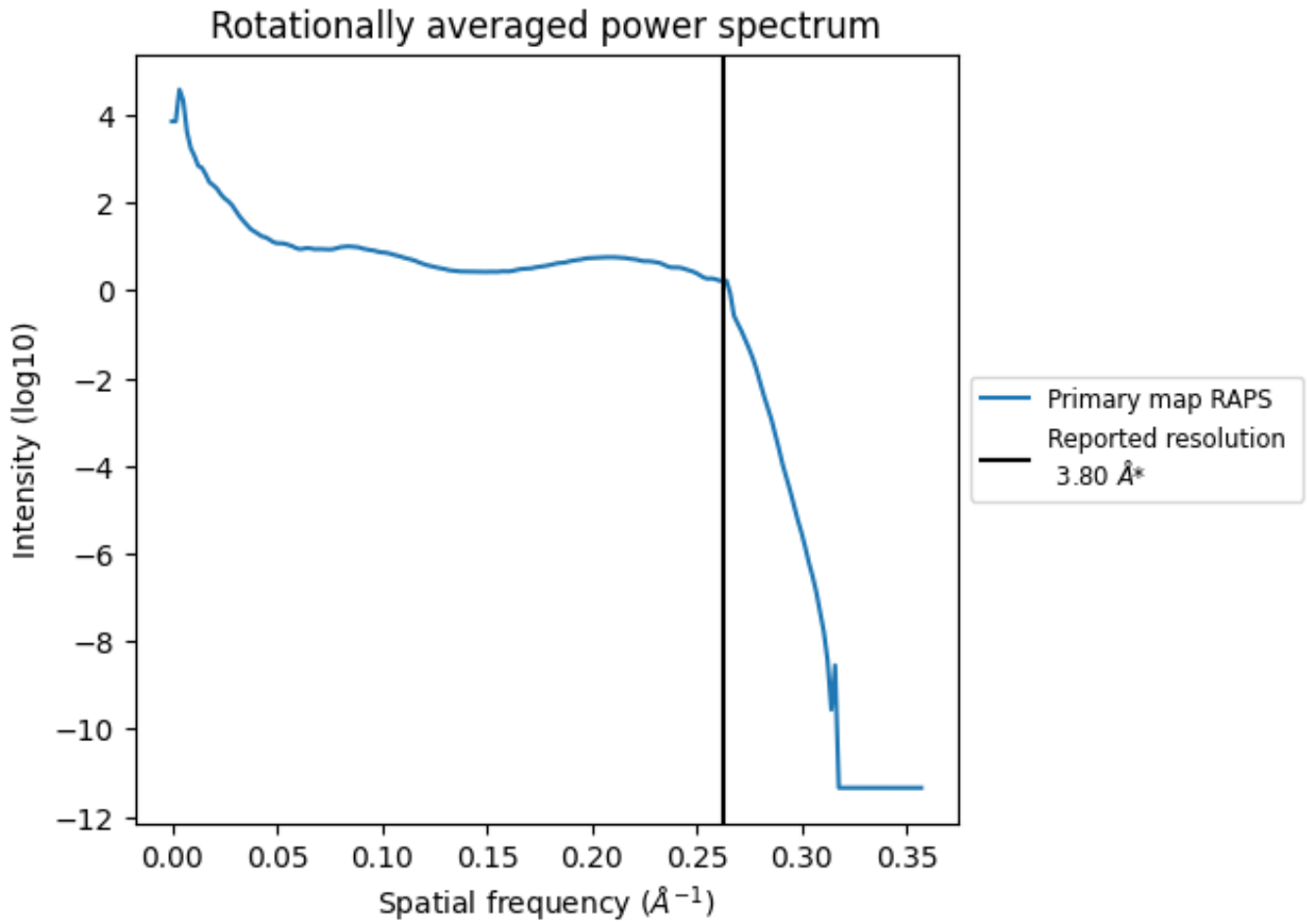
7.2 Volume estimate



The volume at the recommended contour level is 587 nm^3; this corresponds to an approximate mass of 530 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)

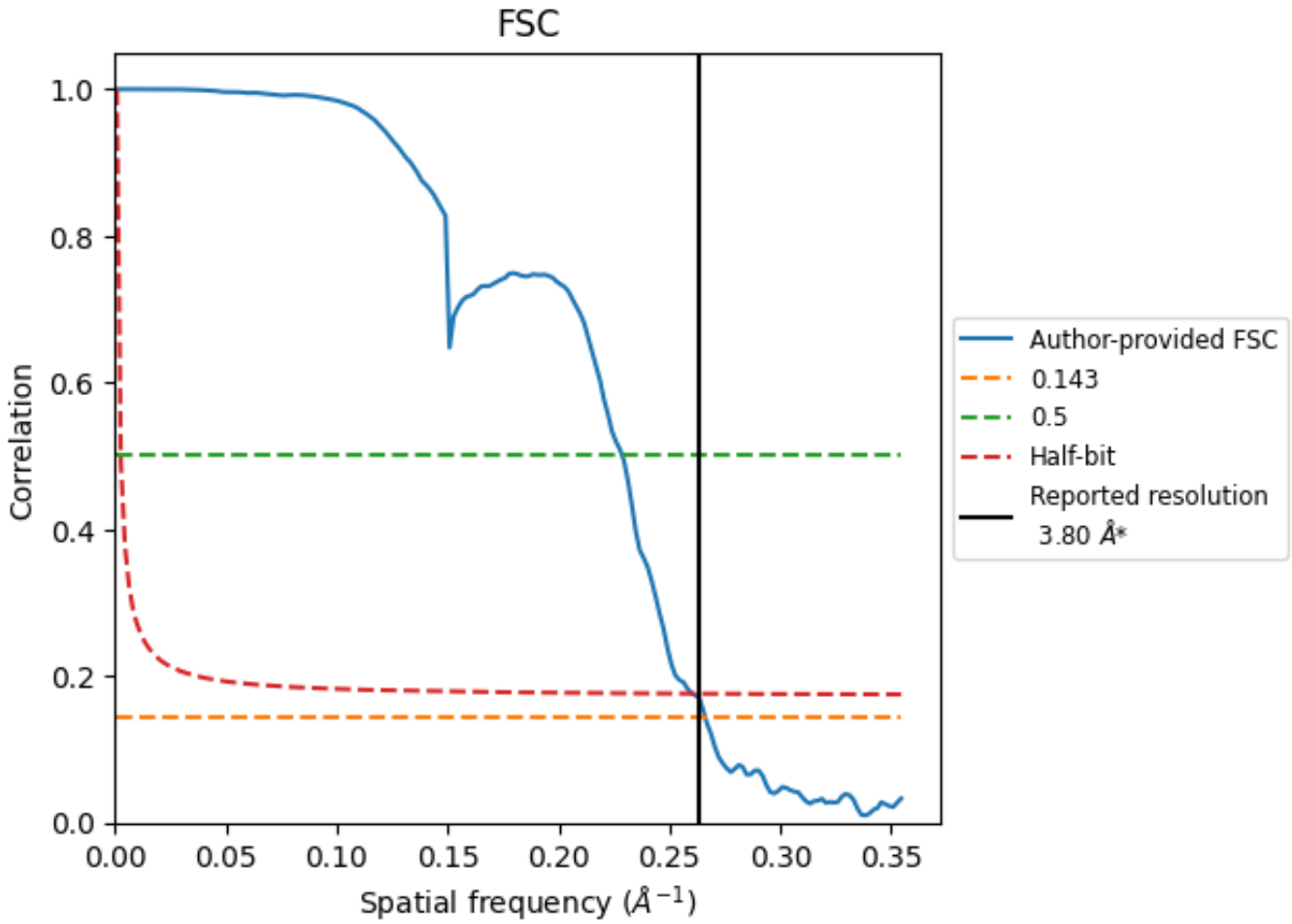


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

8.2 Resolution estimates (i)

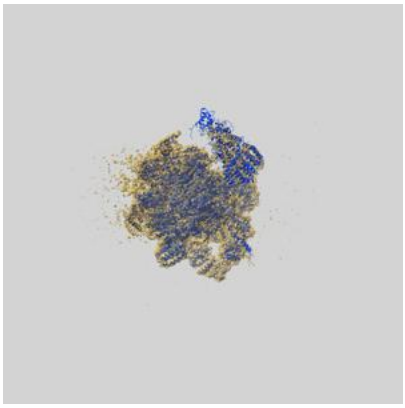
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.76	4.37	3.84
Unmasked-calculated*	-	-	-

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

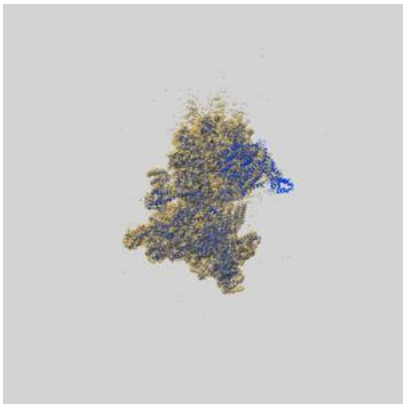
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-36645 and PDB model 8JTI. Per-residue inclusion information can be found in section 3 on page 11.

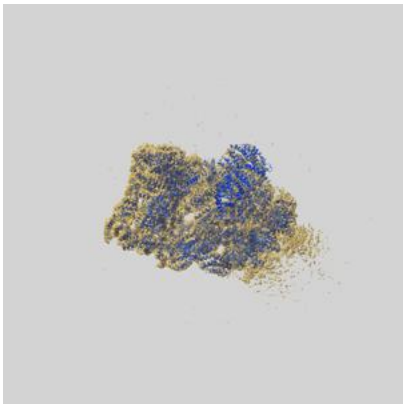
9.1 Map-model overlay



X



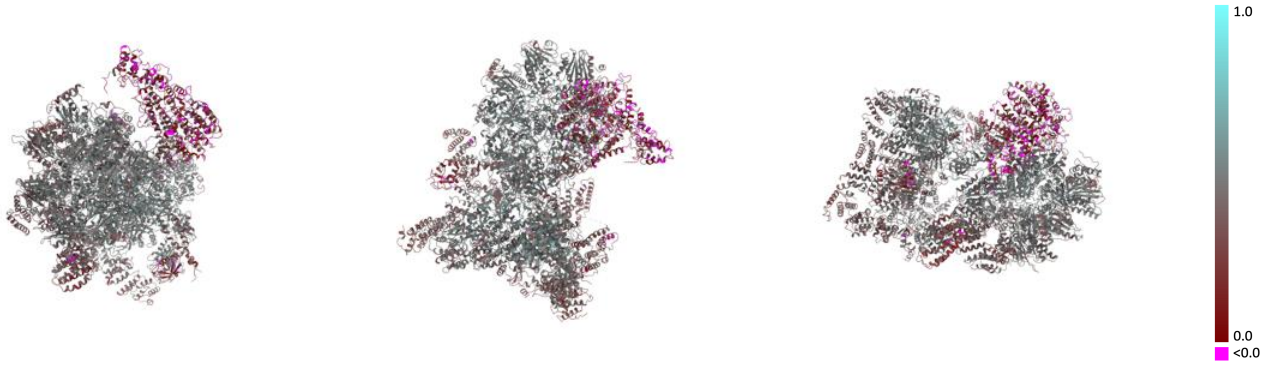
Y



Z

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

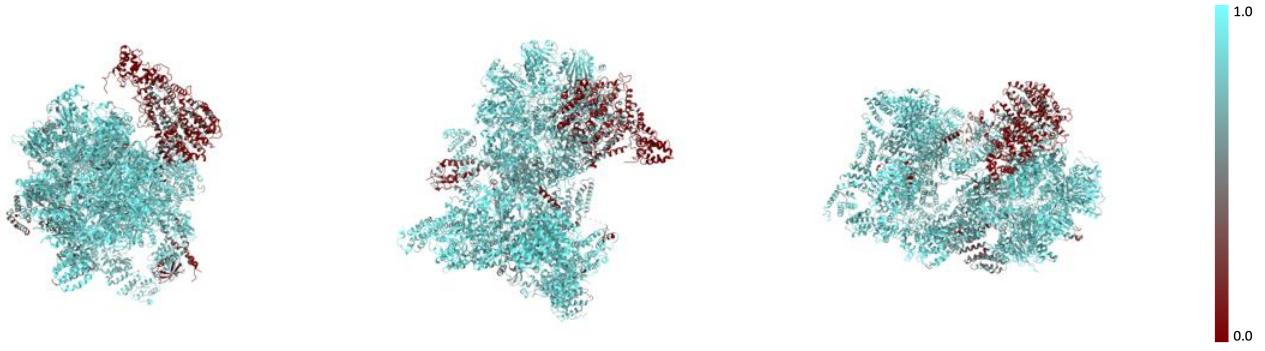
9.2 Q-score mapped to coordinate model



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.

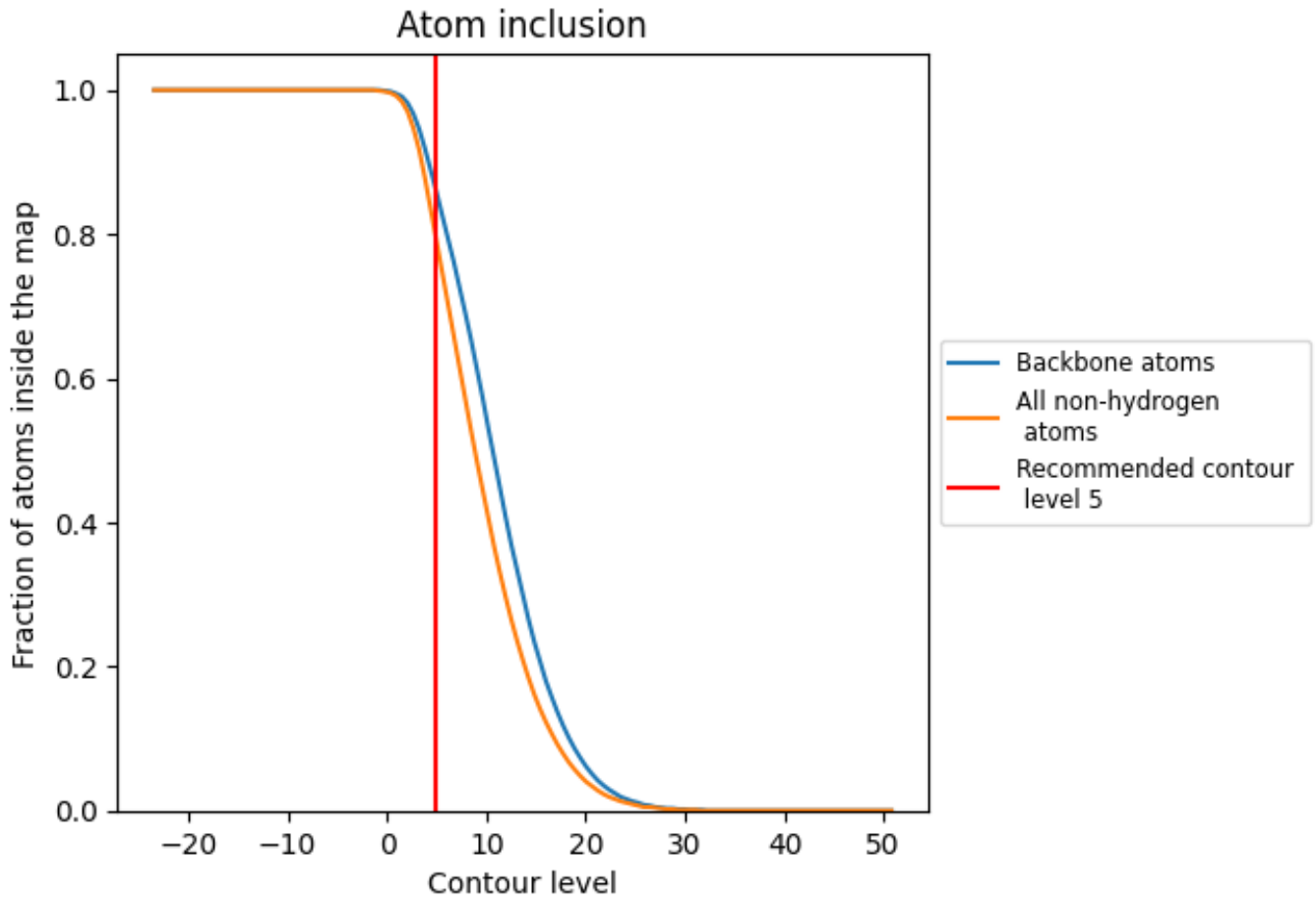
9.3 Atom inclusion mapped to coordinate model



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 (5).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

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

Chain	Atom inclusion	Q-score
All	0.7900	0.4230
A	0.8510	0.4690
B	0.7980	0.4490
C	0.7880	0.4450
D	0.8520	0.4740
E	0.8650	0.4910
F	0.8530	0.4870
G	0.8750	0.4800
H	0.8750	0.4650
I	0.8260	0.4350
J	0.8450	0.4500
K	0.8570	0.4740
L	0.8850	0.4830
M	0.8750	0.4640
U	0.8730	0.4550
V	0.8310	0.3900
W	0.8360	0.3810
X	0.6250	0.3710
Y	0.8330	0.3710
Z	0.8730	0.4800
a	0.8450	0.4070
b	0.8980	0.4580
c	0.8920	0.5020
d	0.8040	0.3550
e	0.7860	0.3390
f	0.1810	0.1890
u	0.9340	0.4690
v	0.2430	0.2040
w	0.8290	0.4200
x	0.5880	0.3900