Full wwPDB EM Validation Report ⓘ

Nov 12, 2022 – 12:29 PM EST

PDB ID	:	6PPH
EMDB ID	:	EMD-20436
Title	:	Kaposi's sarcoma-associated herpesvirus (KSHV), C1 penton vertex register, CATC-binding structure
Authors	:	Gong, D.; Dai, X.; Jih, J.; Liu, Y.T.; Bi, G.Q.; Sun, R.; Zhou, Z.H.
Deposited on	:	2019-07-06
Resolution	:	3.80 Å(reported)

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

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

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

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

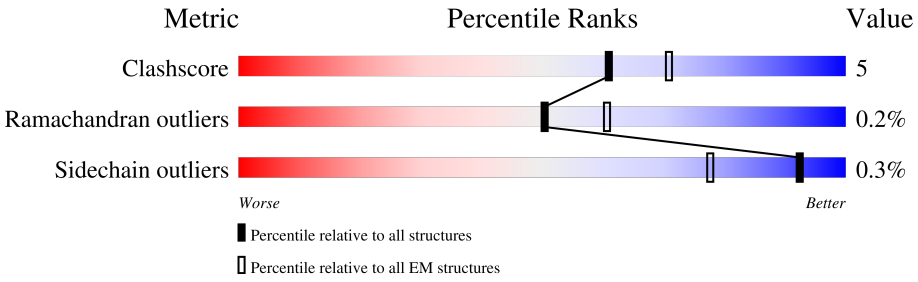
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.80 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	k	454	10% 75% 24%
2	l	549	15% 85%
2	m	549	5% 15% 85%
3	n	2635	98%
3	o	2635	98%
4	5	331	15% 83% 12% 5%
4	b	331	16% 96%
5	6	305	28% 84% 15%

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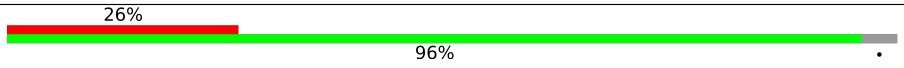
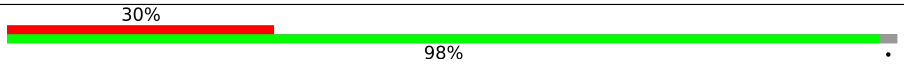
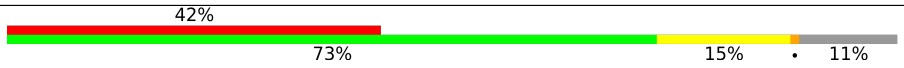
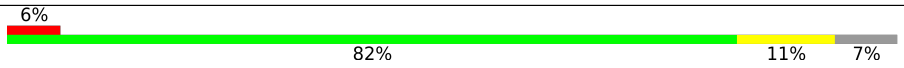
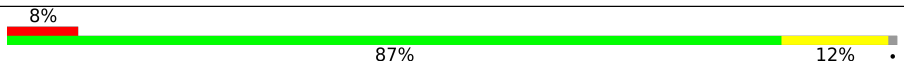
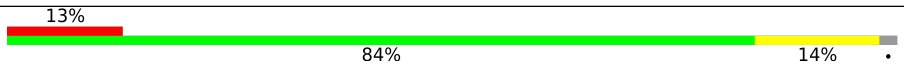
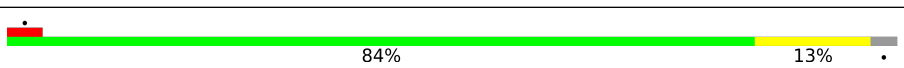
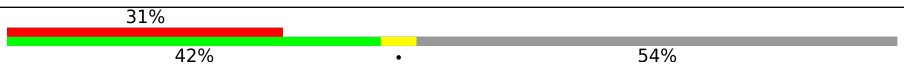
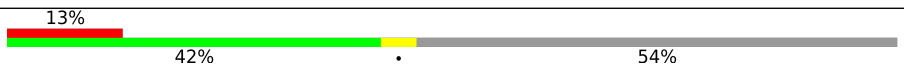
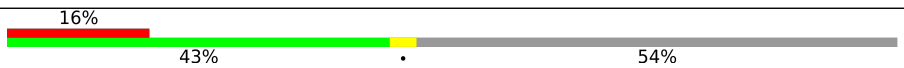
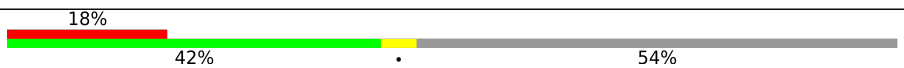
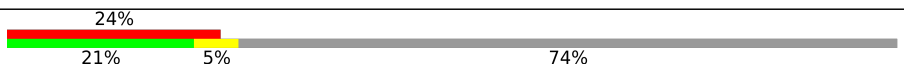
Mol	Chain	Length	Quality of chain
5	7	305	
5	c	305	
5	d	305	
6	4	1376	
6	S	1376	
6	T	1376	
6	W	1376	
6	X	1376	
7	0	170	
7	1	170	
7	2	170	
7	3	170	
7	A	170	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 73502 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 Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	k	344	Total	C	N	O	S	0	0
			2680	1722	467	477	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	165	PRO	LEU	conflict	UNP Q76RH8
k	281	SER	GLY	conflict	UNP Q76RH8

- Molecule 2 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	l	83	Total	C	N	O	S	0	0
			686	429	135	119	3		
2	m	80	Total	C	N	O	S	0	0
			645	406	121	115	3		

- Molecule 3 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	n	40	Total	C	N	O	0	0
			323	209	56	58		
3	o	40	Total	C	N	O	0	0
			323	209	56	58		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	2220	THR	PRO	conflict	UNP Q2HR64
o	2220	THR	PRO	conflict	UNP Q2HR64

- Molecule 4 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	314	Total	C	N	O	S	0	0
			2428	1557	416	442	13		
4	b	321	Total	C	N	O	S	0	0
			2478	1586	424	453	15		

- Molecule 5 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	302	Total	C	N	O	S	0	0
			2382	1514	406	447	15		
5	7	294	Total	C	N	O	S	0	0
			2315	1478	391	431	15		
5	c	294	Total	C	N	O	S	0	0
			2330	1485	397	434	14		
5	d	300	Total	C	N	O	S	0	0
			2365	1505	401	444	15		

- Molecule 6 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	1222	Total	C	N	O	S	0	0
			9634	6133	1673	1757	71		
6	S	1281	Total	C	N	O	S	0	0
			10061	6401	1739	1852	69		
6	T	1360	Total	C	N	O	S	0	0
			10667	6776	1851	1967	73		
6	X	1341	Total	C	N	O	S	0	0
			10519	6685	1824	1939	71		
6	W	1354	Total	C	N	O	S	0	0
			10622	6748	1842	1960	72		

- Molecule 7 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	44	Total	C	N	O	S	0	0
			380	244	72	62	2		
7	2	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	3	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	1	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

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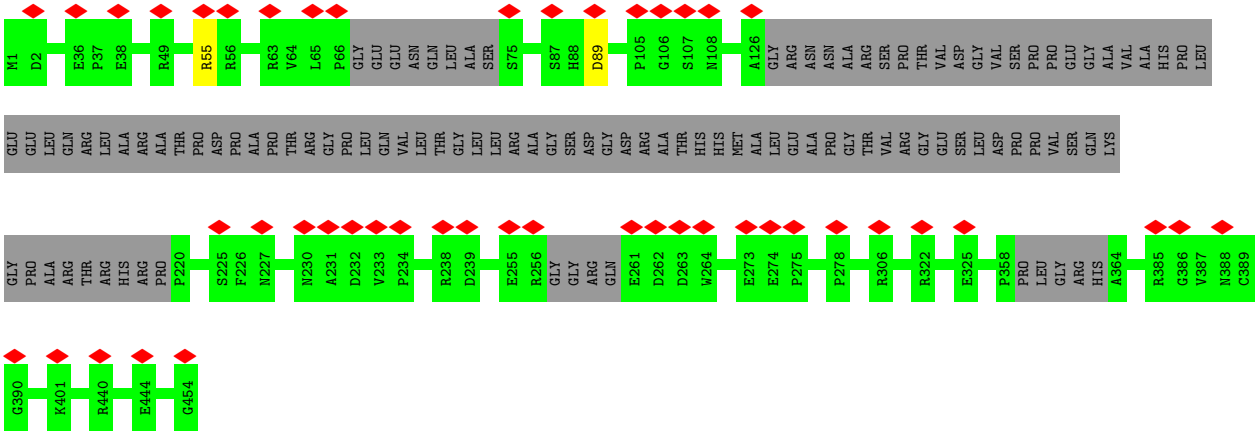
Mol	Chain	Residues	Atoms					AltConf	Trace
7	0	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

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.

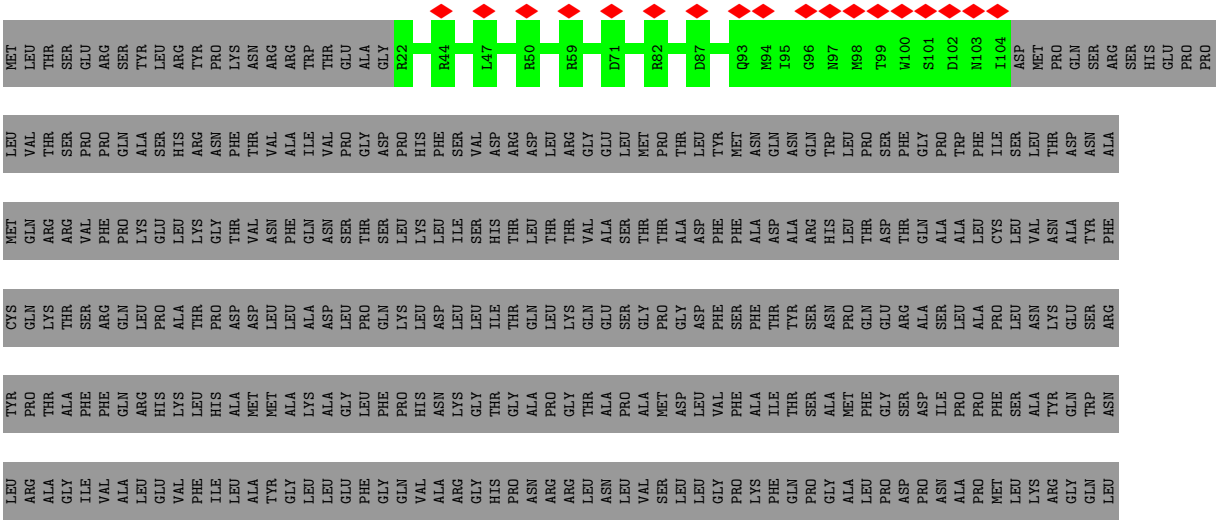
• Molecule 1: Capsid vertex component 1

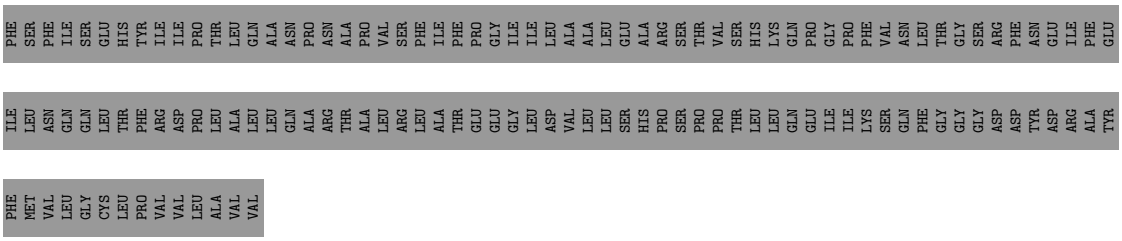
Chain k:



• Molecule 2: Capsid vertex component 2

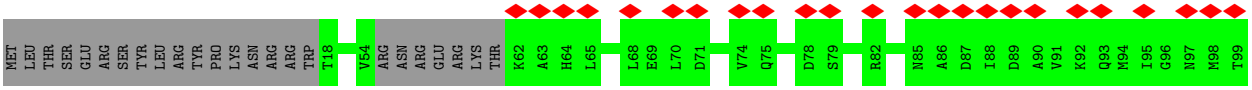
Chain l:

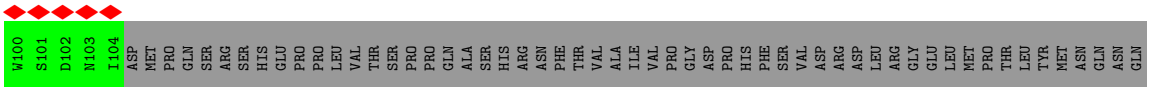




• Molecule 2: Capsid vertex component 2

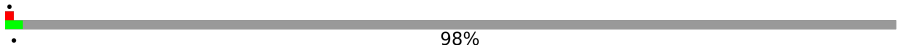
Chain m:

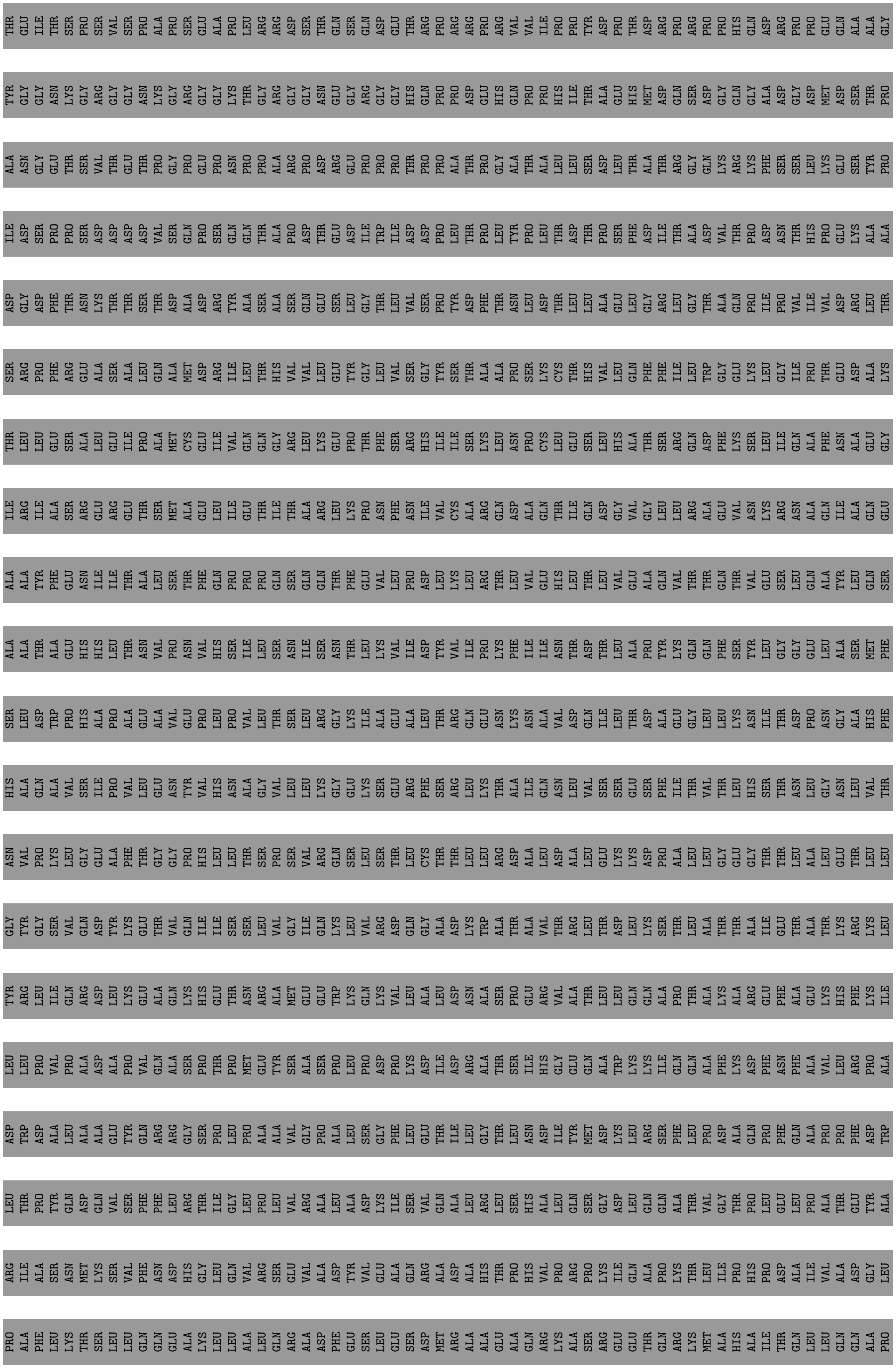




• Molecule 3: Large tegument protein deneddylase

Chain n:

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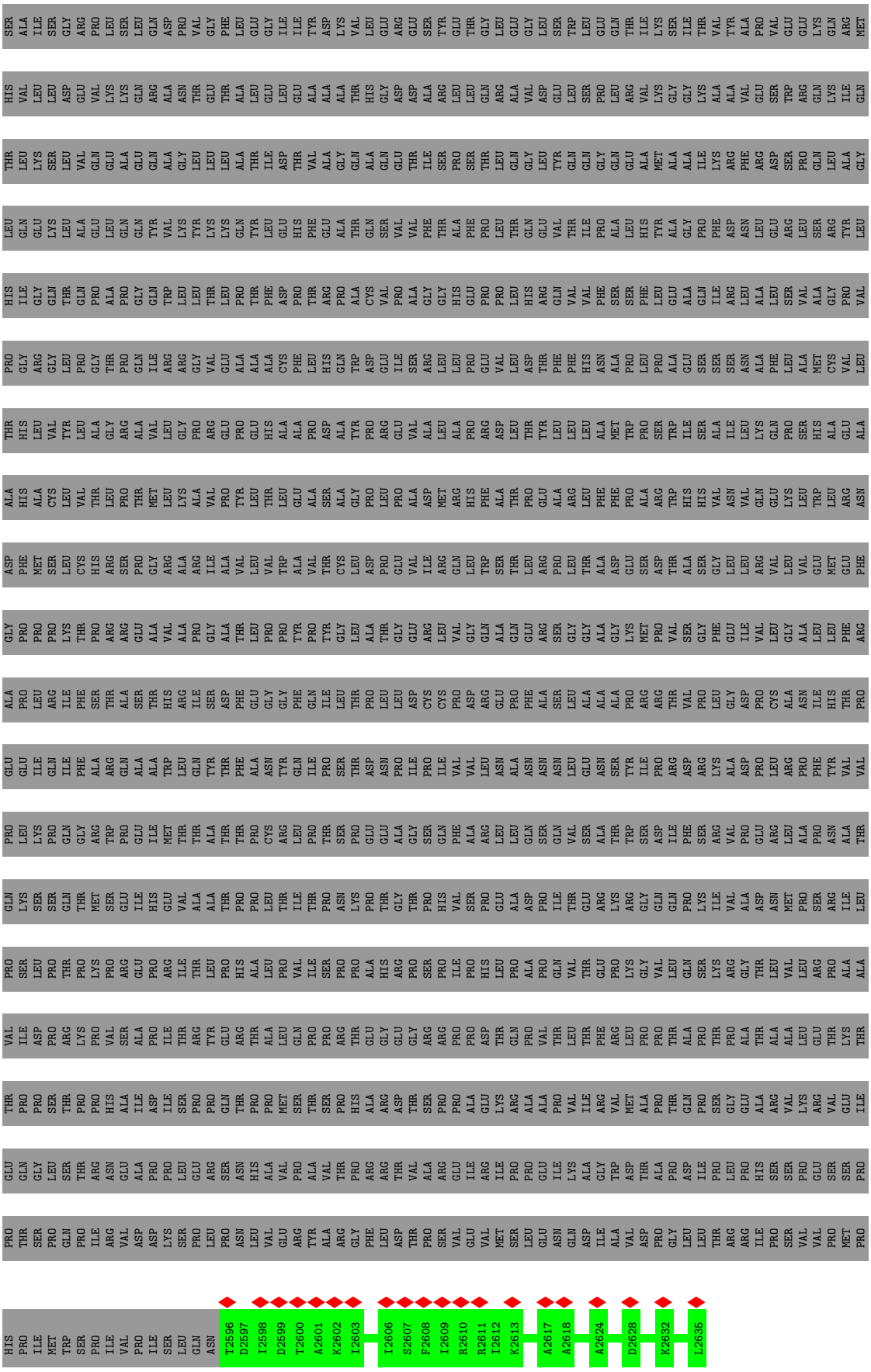
TYR GLY GLY ASN LYS GLY ARG GLY GLY ASN LYS GLY ARG GLY GLY LYS THR GLY ARG GLY GLY ASN GLU GLY ARG GLY GLY HIS GLN PRO PRO ASP GLU HIS GLN PRO PRO HIS ILE THR ALA GLU HIS MET ASP GLN SER ASP GLY GLN GLY ALA ASP GLY ASP MET ASP SER THR PRO
ALA ASN GLY GLU THR SER VAL THR GLU THR PRO GLY PRO GLU PRO ASN PRO PRO ALA ARG PRO ASP ARG GLU PRO PRO PRO THR PRO PRO ALA THR PRO GLY ALA THR ALA LEU LEU SER ASP LEU THR ALA THR ARG GLY GLN LYS ARG LYS PHE SER SER LEU LYS GLU SER TYR PRO
ILE ASP SER PRO PRO SER ASP ASP ASP ASP VAL SER GLN PRO SER GLN GLN THR ALA PRO ASP THR GLU ASP ILE TRP ILE ASP ASP PRO LEU THR PRO LEU TYR PRO LEU THR ASP THR PRO SER PHE ASP ILE THR ALA ASP VAL THR PRO ASP ASN THR HIS PRO GLU LYS ALA ALA
ASP GLY ASP PHE THR ASN LYS THR THR SER THR ASP ALA ASP ARG TYR ALA SER ALA SER GLN GLU SER LEU GLY THR LEU VAL SER PRO TYR ASP PHE THR ASN LEU ASP THR LEU LEU ALA GLU LEU GLY ARG LEU GLY THR ALA GLN PRO ILE PRO VAL ILE VAL ASP ARG LEU THR
SER ARG PRO PHE ARG GLU ALA SER ALA LEU GLN ALA MET ASP ARG ILE LEU THR HIS VAL VAL LEU GLU TYR GLY LEU VAL SER GLY TYR SER THR ALA ALA PRO SER LYS CYS THR HIS VAL LEU GLN PHE PHE ILE LEU TRP GLY GLU LYS LEU GLY ILE PRO THR GLU ASP ALA LYS
THR LEU LEU GLU SER ALA LEU GLU ILE PRO ALA MET CYS GLU ILE VAL GLN GLN GLY ARG LEU LYS GLU PRO THR PHE SER ARG HIS ILE ILE SER LYS LEU ASN PRO CYS LEU GLU SER LEU HIS ALA THR SER ARG GLN ASP PHE LYS SER LEU ILE GLN ALA PHE ASN ALA GLU GLY
ILE ARG ILE ALA SER ARG GLU ARG GLU THR SER MET ALA GLU LEU ILE GLU THR ILE THR ALA ARG LEU LYS PRO ASN PHE ASN ILE VAL CYS ALA ARG GLN ASP ALA GLN THR ILE GLN ASP GLY VAL GLY LEU LEU ARG ALA GLU VAL ASN LYS ARG ASN ALA GLN ILE ALA GLN GLU
ALA ALA TYR PHE GLU ASN ILE ILE THR ALA LEU SER THR PHE GLN PRO PRO PRO GLN SER GLN GLN THR PHE GLU VAL LEU PRO ASP LEU LYS LEU ARG THR LEU VAL GLU HIS LEU THR LEU VAL GLU ALA GLN VAL THR THR GLN THR VAL GLU SER LEU GLN ALA TYR LEU GLN SER
ALA ALA THR ALA GLU HIS HIS LEU THR ASN VAL PRO ASN VAL HIS SER ILE LEU SER ASN ILE SER ASN THR LEU LYS VAL ILE ASP TYR VAL ILE PRO LYS PHE ILE ILE ASN THR ASP THR LEU ALA PRO TYR LYS GLN GLN PHE SER TYR LEU GLY GLY GLU LEU ALA SER MET PHE
SER LEU ASP TRP PRO HIS ALA PRO ALA GLU ALA VAL GLU PRO LEU PRO VAL LEU THR SER LEU ARG GLY LYS ILE ALA GLU ALA LEU THR ARG GLN GLU ASN LYS ASN ALA VAL ASP GLN ILE LEU THR ASP ALA GLU GLY LEU LEU LYS ASN ILE THR ASP PRO ASN GLY ALA HIS PHE
HIS ALA GLN ALA VAL SER ILE PRO VAL LEU GLU ASN TYR VAL HIS ASN ALA GLY VAL LEU LEU LYS GLY GLU LYS SER GLU ARG PHE SER ARG LEU LYS THR ALA ILE GLN ASN LEU VAL SER SER GLU SER PHE ILE THR VAL THR LEU HIS SER THR ASN LEU GLY ASN LEU VAL THR
ASN VAL PRO LYS LEU GLY GLU ALA PHE THR GLY GLY PRO HIS LEU LEU THR SER PRO SER VAL ARG GLN SER LEU SER THR LEU CYS THR THR LEU LEU ARG ASP ALA LEU ASP ALA LEU GLU LYS LYS ASP PRO ALA LEU LEU GLY GLU GLY THR THR LEU ALA LEU GLU THR LEU LEU
GLY TYR GLY SER VAL GLN ASP TYR LYS GLU THR VAL GLN ILE ILE SER SER LEU VAL GLY ILE GLN LYS LEU VAL ARG ASP GLN GLY ALA ASP LYS TRP ALA THR ALA VAL THR ARG LEU THR ASP LEU LYS SER THR LEU ALA THR THR ALA ILE GLU THR ALA THR LYS ARG LYS LEU
TYR ARG LEU ILE GLN ARG ASP LEU LYS GLU ALA GLN LYS HIS GLU THR ASN ARG ALA MET GLU GLU TRP LYS GLN LYS VAL LEU ALA LEU ASP ASN ALA SER PRO GLU ARG VAL ALA THR LEU LEU GLN GLN ALA PRO THR ALA LYS ALA ARG GLU PHE ALA GLU LYS HIS PHE LYS ILE
LEU LEU PRO VAL PRO ALA ASP ALA PRO VAL GLN ALA SER PRO THR PRO MET GLU TYR SER ALA SER PRO LEU PRO ASP PRO LYS ASP ILE ASP ARG ALA THR SER ILE HIS GLY GLU GLN ALA TRP LYS LYS ILE GLN GLN ALA PHE LYS ASP PHE ASN PHE ALA VAL LEU ARG PRO ALA
ASP TRP ASP ALA LEU ALA ALA GLU TYR GLN ARG ARG GLY SER PRO LEU PRO ALA ALA VAL GLY PRO ALA LEU SER GLY PHE LEU GLU THR ILE LEU GLY THR LEU ASN ASP ILE TYR MET ASP LYS LEU ARG SER PHE LEU PRO ASP ALA GLN PRO PHE GLN ALA PRO PRO PHE ASP TRP
LEU THR PRO TYR GLN ASP GLN VAL SER PHE PHE LEU ARG THR ILE GLY LEU PRO LEU VAL ARG ALA LEU ALA ASP LYS ILE SER VAL GLN ALA LEU ARG LEU SER HIS ALA LEU GLN SER GLY ASP LEU GLN GLN ALA THR VAL GLY THR PRO LEU GLU LEU PRO ALA THR GLU TYR ALA
ARG ILE ALA SER ASN MET LYS SER VAL PHE ASN ASP HIS GLY LEU GLN VAL ARG SER GLU VAL ALA ASP TYR VAL GLU ALA GLN ARG ALA ASP ALA HIS THR PRO HIS VAL PRO ARG PRO LYS ILE GLN ALA PRO LYS THR LEU ILE PRO HIS PRO ASP ALA ILE VAL ALA ASP GLY LEU
PRO ALA PHE LEU LYS THR SER LEU LEU GLN GLN GLU ALA LYS LEU LEU ALA LEU GLN ARG ALA ASP PHE GLU SER LEU GLU SER ASP MET ARG ALA ALA ALA GLU ALA GLN ARG LYS ALA SER ARG GLU GLN THR GLN ARG LYS MET ALA HIS ALA ILE THR GLN LEU LEU GLN GLN ALA PRO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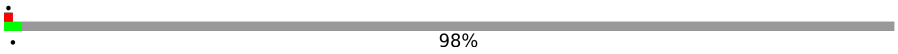
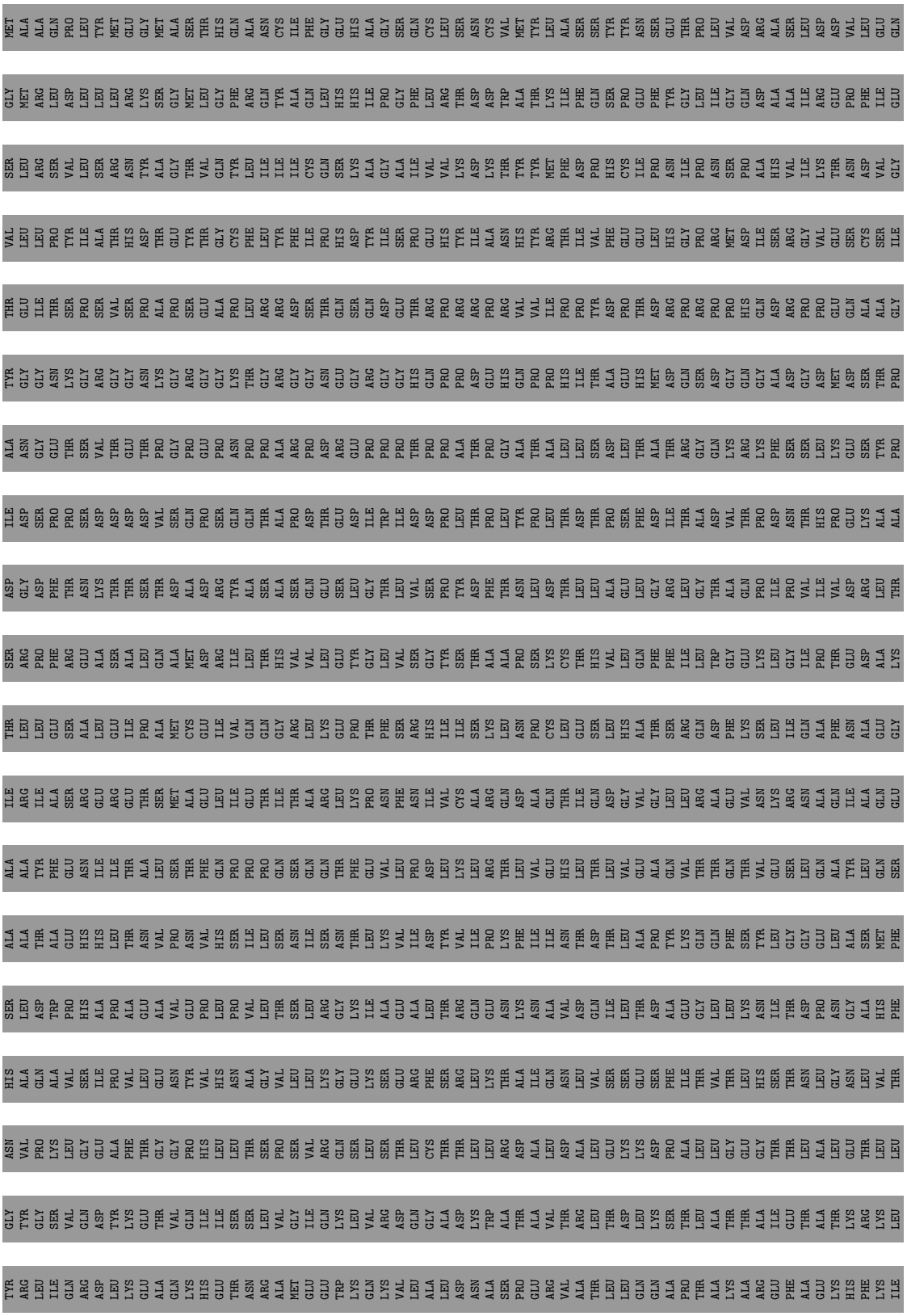
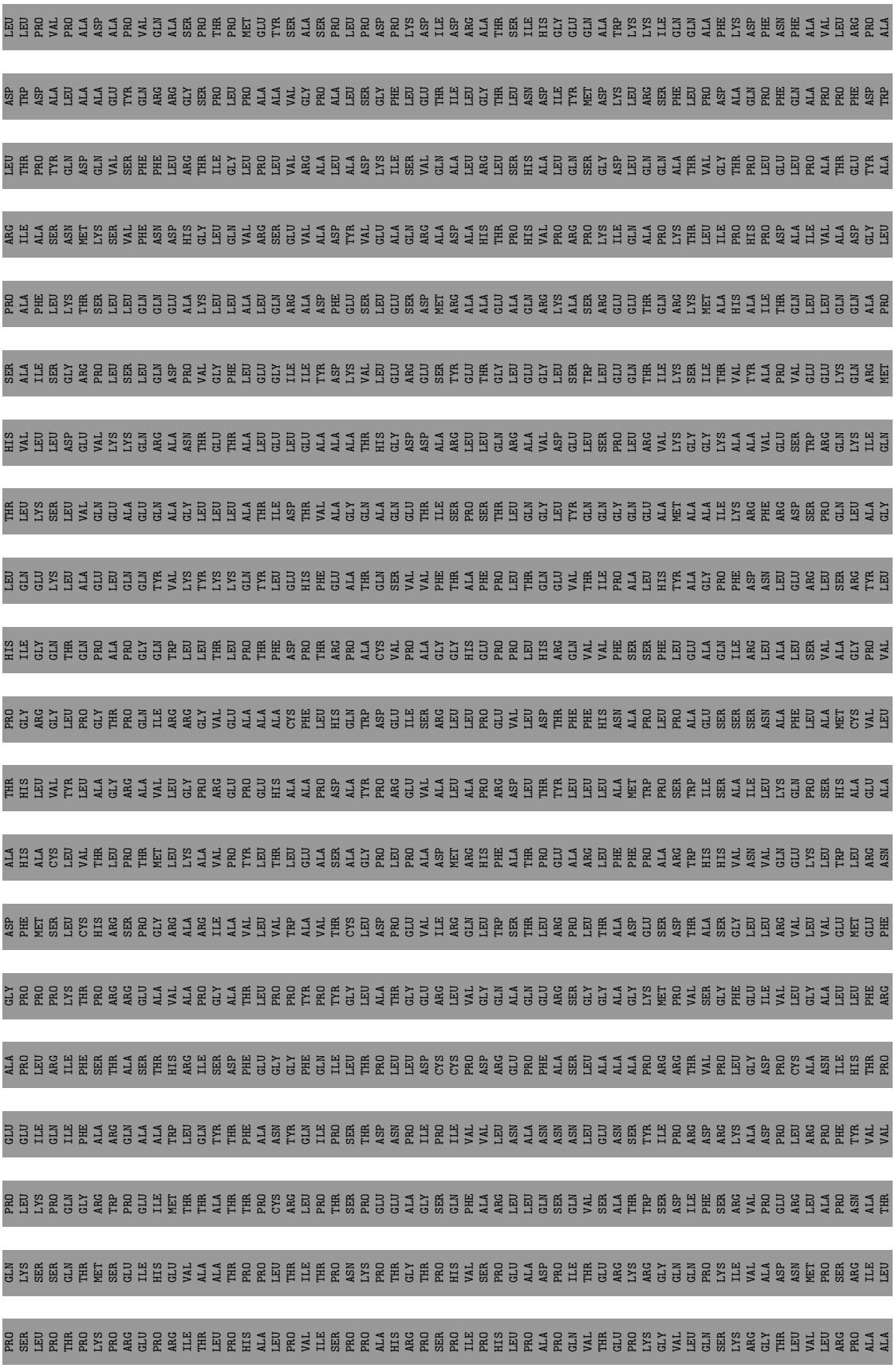
R2611
I2612
K2613
A2617
A2618
A2624
D2628
K2632
L2635

• Molecule 3: Large tegument protein deneddylase

Chain o:






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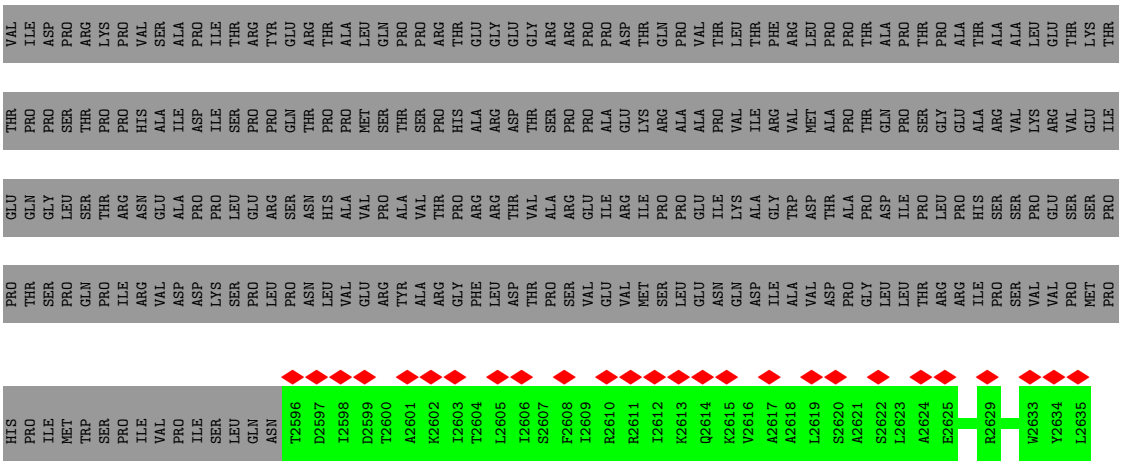
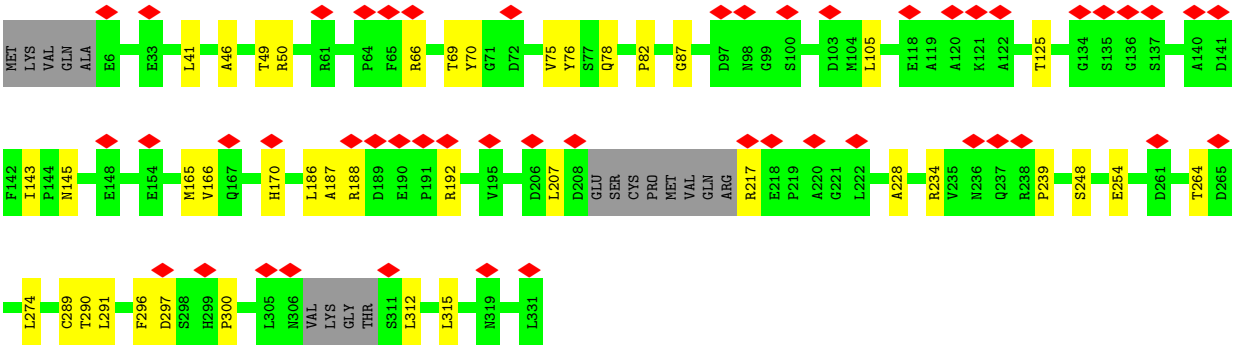
PRO LEU LYS PRO GLN GLY ARG TRP PRO GLU THR SER PRO GLU GLU ILE PRO GLN THR THR THR PRO CYS ARG LEU PRO THR SER GLN VAL SER ALA THR TRP SER ASP ILE PHE SER ARG VAL PRO GLU GLU ARG LEU ALA PRO ASN ALA THR
GLN LYS SER SER GLU ILE HIS GLU MET THR THR PRO PRO LEU THR ILE THR PRO ASN LYS PRO THR GLY THR PRO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



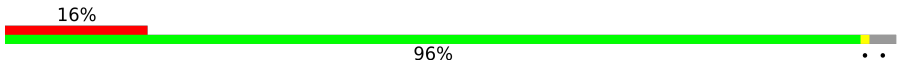
• Molecule 4: Triplex capsid protein 1

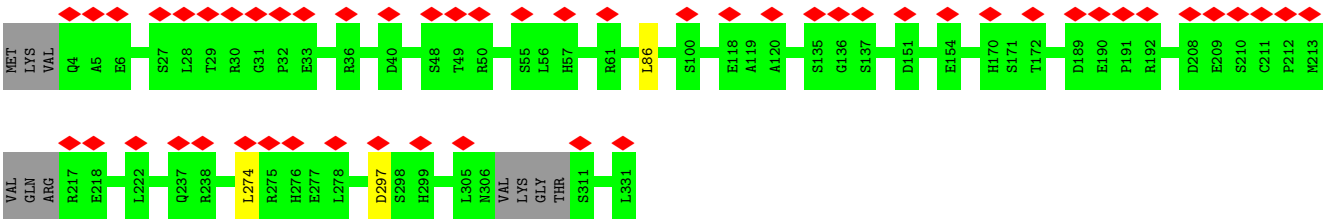
Chain 5:



• Molecule 4: Triplex capsid protein 1

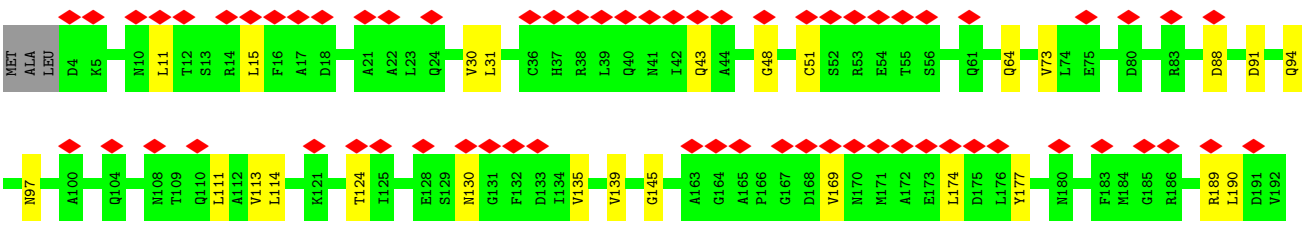
Chain b:

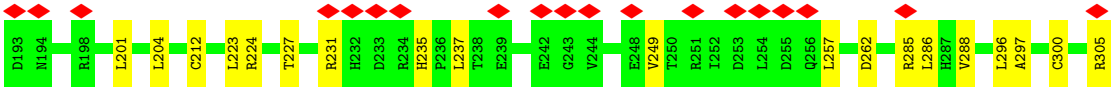




• Molecule 5: Triplex capsid protein 2

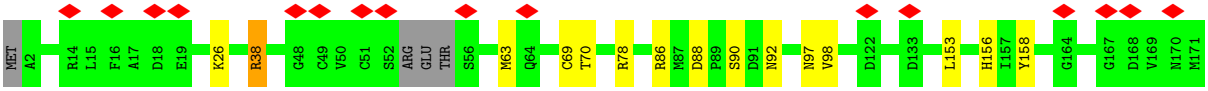
Chain 6:

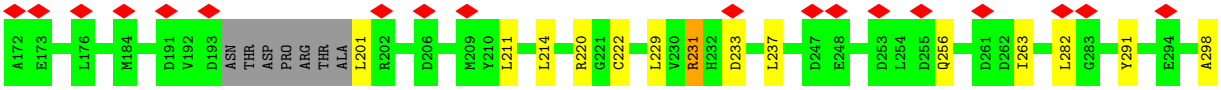




• Molecule 5: Triplex capsid protein 2

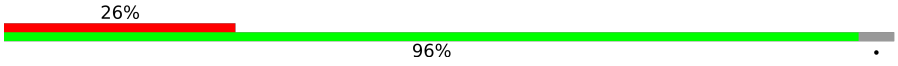
Chain 7:

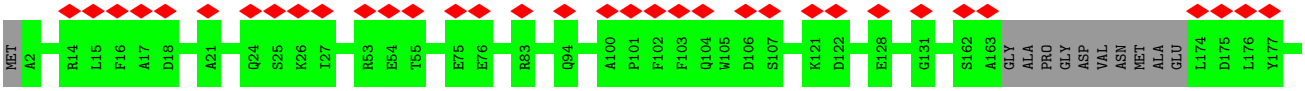


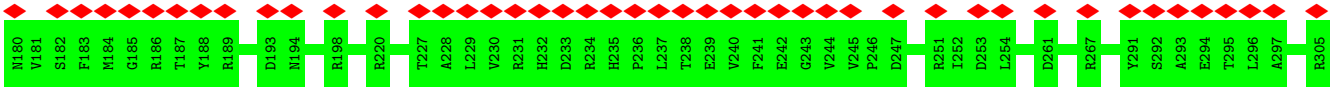


• Molecule 5: Triplex capsid protein 2

Chain c:

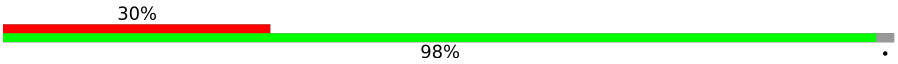


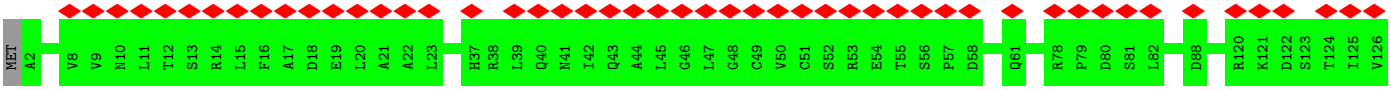


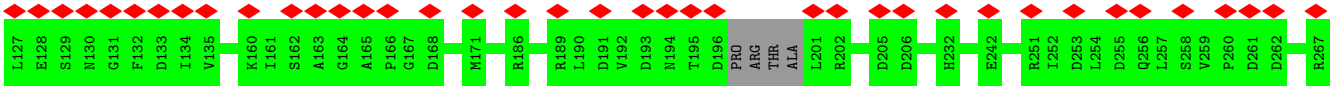


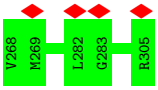
• Molecule 5: Triplex capsid protein 2

Chain d:



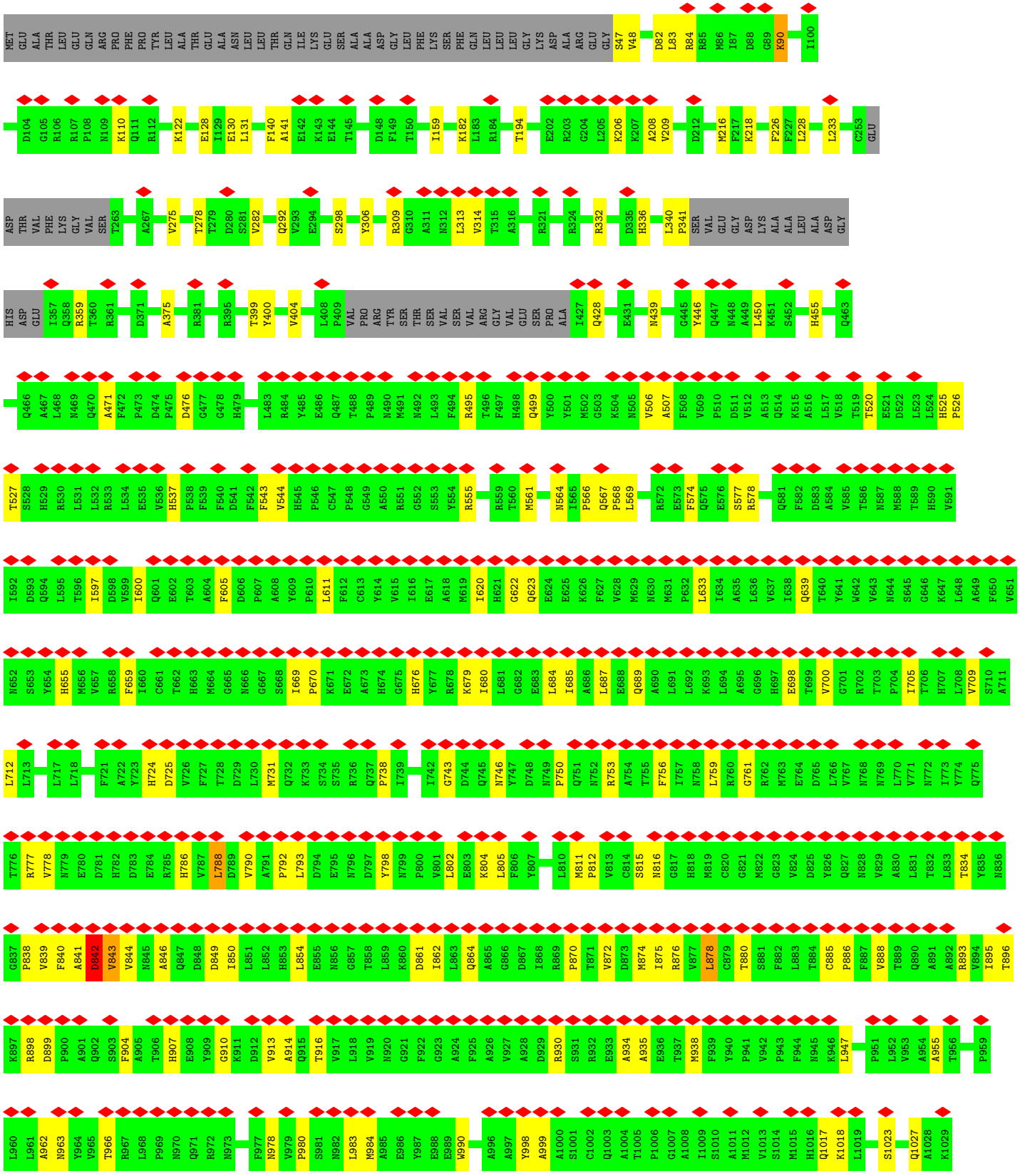






• Molecule 6: Major capsid protein

Chain 4: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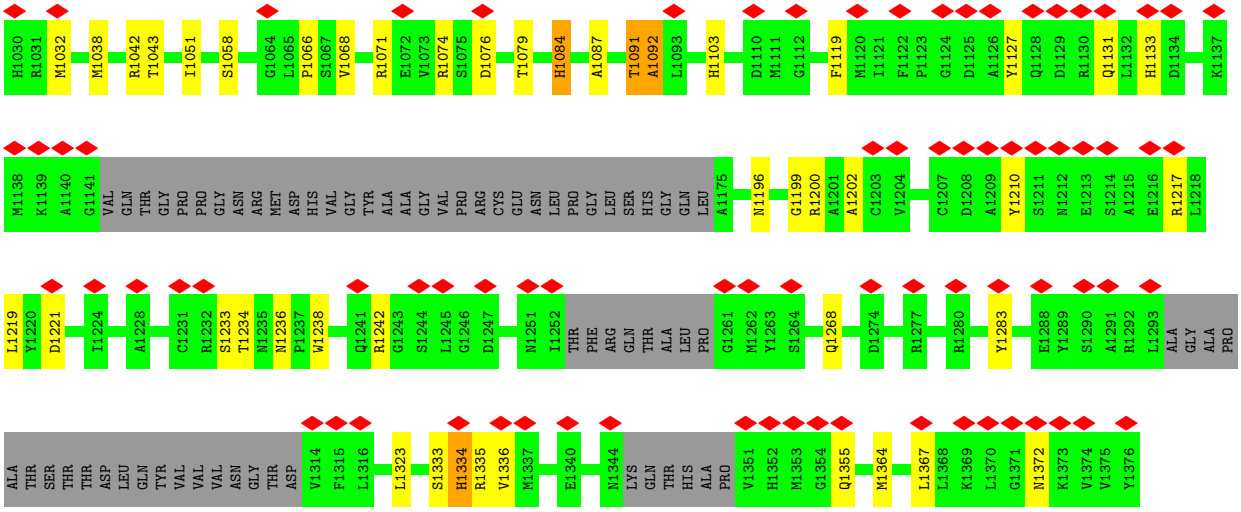
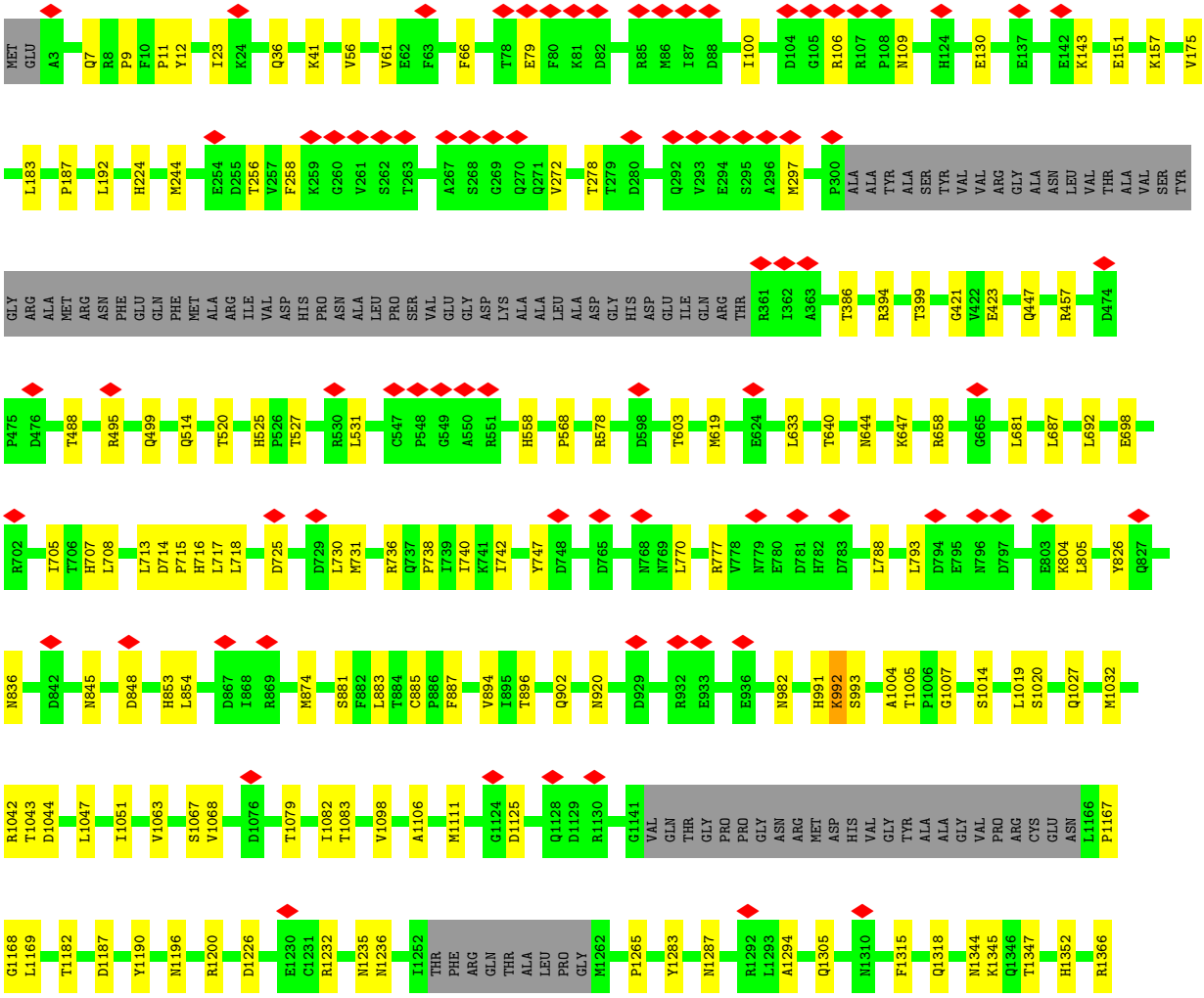
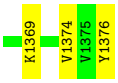
D104 G105 R106 R107 P108 N109 K110 Q111 R112 K122 E128 I129 E130 L131 F140 A141 E142 K143 E144 T145 D148 F149 T150 I159 K182 L183 R184 T194 E202 R203 G204 L205 K206 K207 A208 V209 D212 M216 F217 K218 F226 F227 L228 L233 C253 GLU
ASP THR VAL PHE LYS GLY VAL SER T263 A267 V275 T278 T279 D280 S281 V282 Q292 V293 E294 S298 Y306 R309 G310 A311 N312 L313 V314 T315 A316 R321 R324 R332 D335 H336 L340 P341 SER VAL GLU GLY ASP LYS ALA ALA LEU ALA ASP GLY
HIS ASP GLU I357 Q358 R359 T360 R361 D371 A375 R381 R395 T399 Y400 V404 L408 P409 VAL PRO ARG TYR SER THR SER VAL SER VAL ARG GLY VAL GLU SER PRO ALA I427 Q428 E431 N439 G445 Y446 Q447 N448 A449 L450 K451 S452 H455 Q463
Q466 A467 L468 N469 Q470 A471 F472 P473 D474 P475 D476 G477 G478 H479 L483 R484 Y485 E486 Q487 T488 P489 N490 M491 N492 L493 F494 R495 T496 F497 H498 Q499 Y500 Y501 M502 G503 K504 N505 V506 A507 F508 V509 P510 D511 V512 A513 Q514 K515 A516 L517 V518 T519 T520 E521 D522 L523 L524 H525 P526
T527 S528 H529 R530 L531 L532 R533 L534 E535 V536 H537 P538 F539 F540 D541 F542 F543 V544 H545 P546 C547 P548 G549 A550 R551 G552 S553 Y554 R555 R559 T560 M561 N564 I565 P566 Q567 P568 L569 R572 E573 F574 Q575 E576 S577 R578 Q581 F582 D583 A584 V585 T586 N587 M588 T589 H590 V591
I592 D593 Q594 L595 T596 I597 D598 V599 I600 Q601 E602 T603 A604 F605 D606 P607 A608 Y609 P610 L611 F612 C613 Y614 V615 I616 E617 A618 M619 I620 H621 G622 Q623 E624 E625 K626 F627 V628 M629 N630 M631 P632 L633 I634 A635 L636 V637 I638 Q639 T640 Y641 W642 V643 N644 S645 G646 K647 L648 A649 F650 V651
N652 S653 Y654 H655 M656 V657 R658 F659 I660 C661 T662 H663 M664 G665 N666 G667 S668 I669 P670 K671 E672 A673 H674 G675 H676 Y677 R678 K679 I680 L681 G682 E683 L684 I685 A686 L687 E688 Q689 A690 L691 L692 K693 L694 A695 G696 H697 E698 T699 V700 G701 R702 T703 P704 I705 T706 H707 L708 V709 S710 A711
L712 L713 L717 L718 F721 A722 Y723 H724 D725 V726 F727 T728 D729 L730 M731 Q732 K733 S734 S735 R736 Q737 P738 I739 I742 G743 D744 Q745 N746 Y747 D748 N749 P750 Q751 N752 R753 A754 T755 F756 I757 N758 L759 R760 G761 R762 M763 E764 D765 L766 V767 N768 N769 L770 V771 N772 I773 Y774 Q775
T776 R777 V778 N779 E780 D781 H782 D783 E784 R785 H786 V787 L788 D789 V790 A791 P792 L793 D794 E795 N796 D797 Y798 N799 P800 V801 L802 E803 K804 L805 F806 Y807 L810 M811 P812 V813 C814 S815 N816 G817 H818 M819 C820 G821 M822 G823 V824 D825 Y826 Q827 N828 V829 A830 L831 T832 L833 T834 Y835 N836
G837 P838 V839 F840 A841 D842 V843 V844 N845 A846 Q847 D848 D849 I850 L851 L852 H853 L854 E855 N856 G857 T858 L859 K860 D861 I862 L863 Q864 A865 G866 D867 I868 R869 P870 T871 V872 D873 M874 I875 R876 V877 L878 C879 T880 S881 F882 L883 T884 C885 P886 F887 V888 T889 Q890 A891 A892 R893 V894 I895 T896
K897 R898 D899 P900 A901 Q902 S903 F904 A905 T906 H907 E908 Y909 G910 K911 D912 V913 A914 Q915 T916 V917 L918 V919 N920 G921 F922 G923 A924 F925 A926 V927 A928 D929 R930 S931 R932 E933 A934 A935 E936 T937 M938 F939 Y940 P941 V942 P943 F944 N945 K946 L947 P951 L952 V953 A954 A955 T956 P959
L960 L961 A962 N963 Y964 V965 T966 R967 L968 P969 N970 Q971 R972 N973 F977 N978 V979 P980 S981 N982 L983 M984 A985 E986 Y987 E988 E989 W990 A996 A997 Y998 A999 A1000 S1001 C1002 Q1003 A1004 T1005 P1006 G1007 A1008 I1009 S1010 A1011 M1012 V1013 S1014 M1015 H1016 Q1017 K1018 L1019 S1023 Q1027 A1028 K1029



• Molecule 6: Major capsid protein

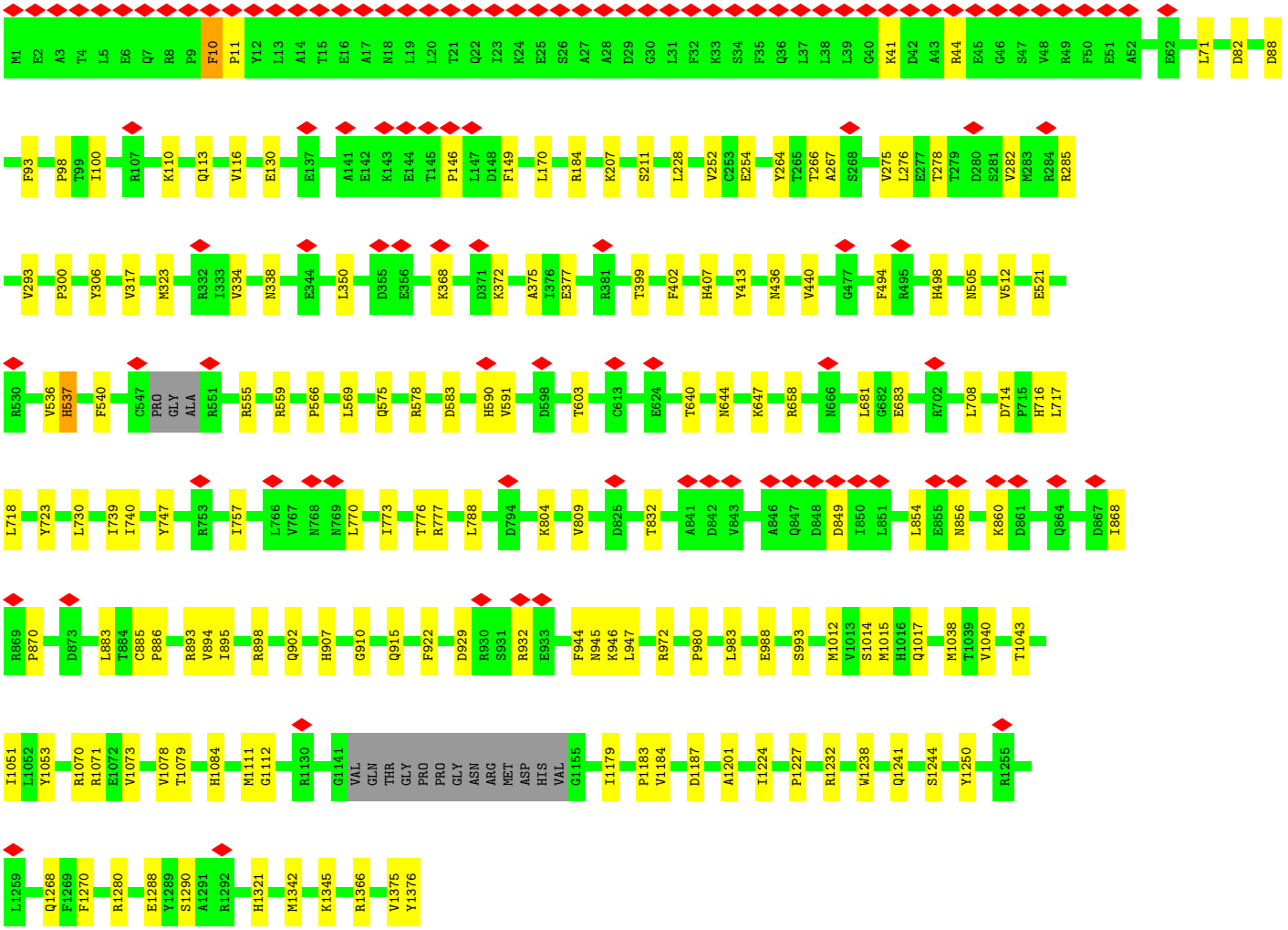
Chain S:





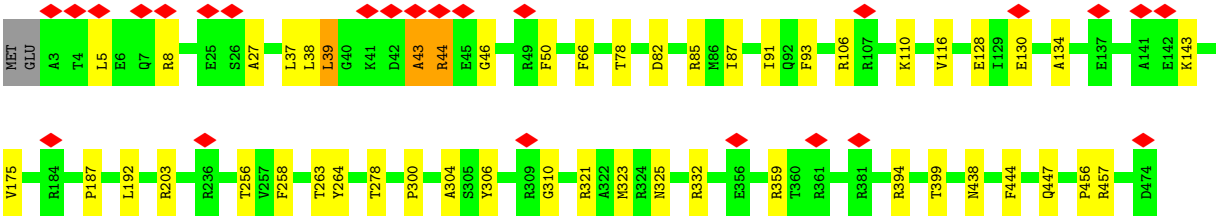
• Molecule 6: Major capsid protein

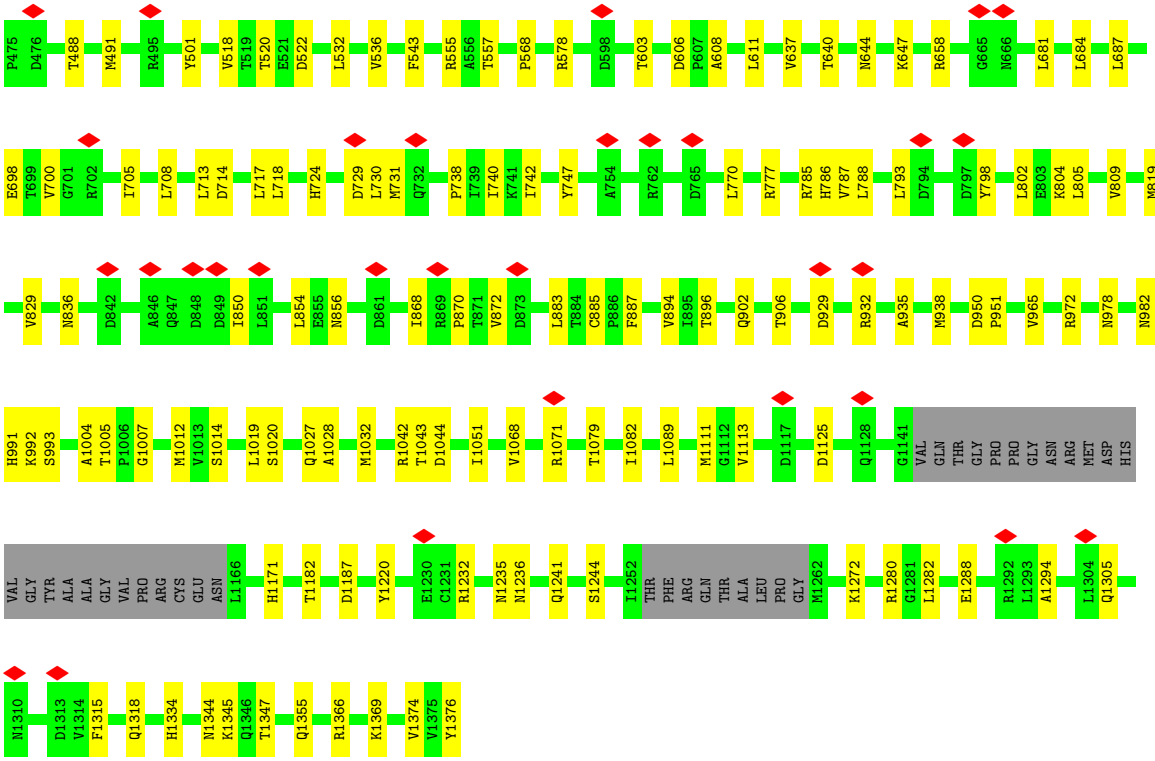
Chain T:



• Molecule 6: Major capsid protein

Chain X:





• Molecule 6: Major capsid protein

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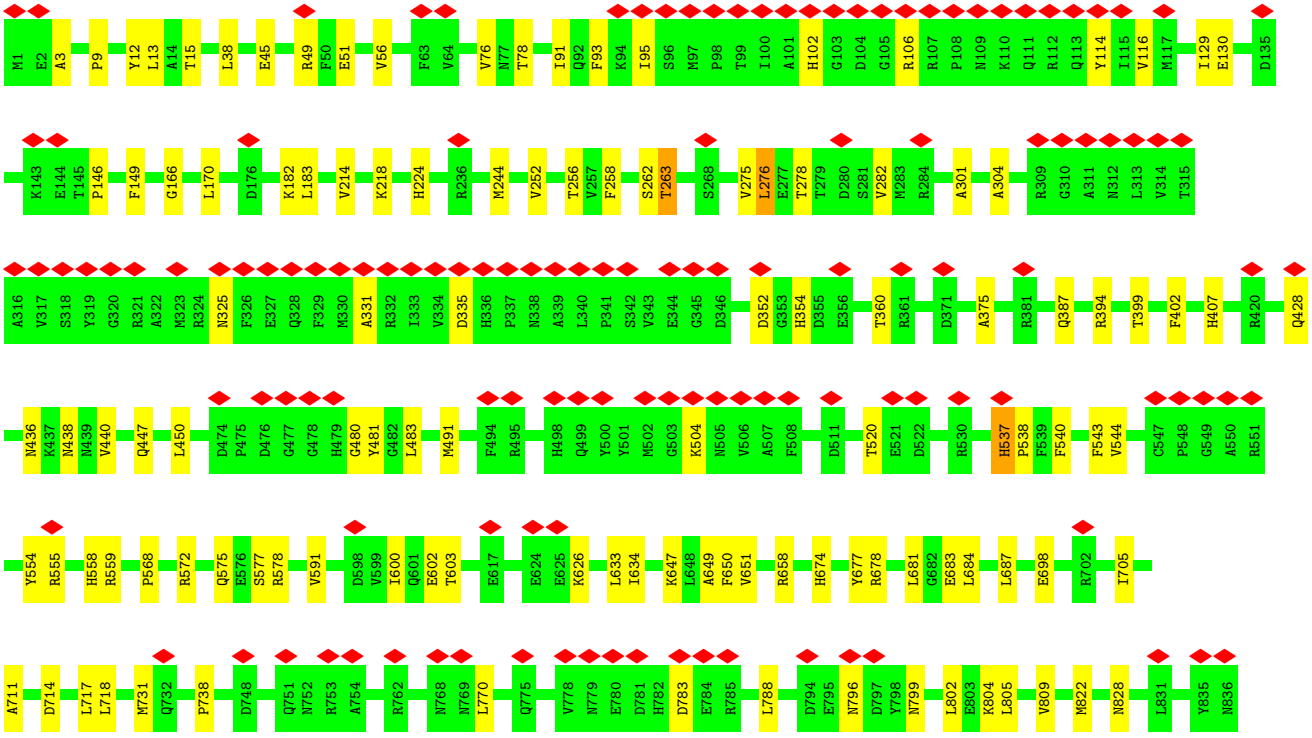
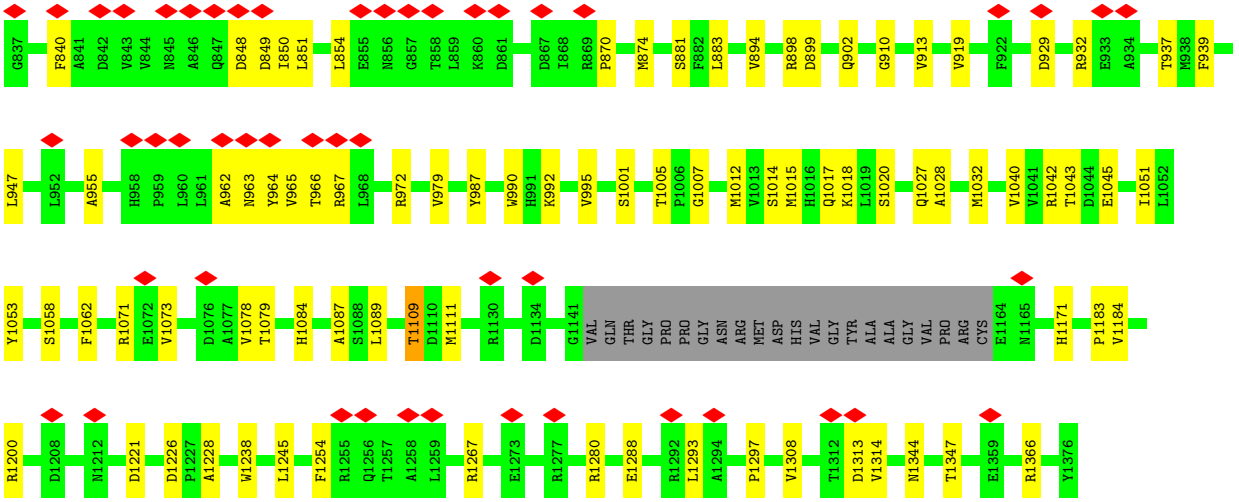
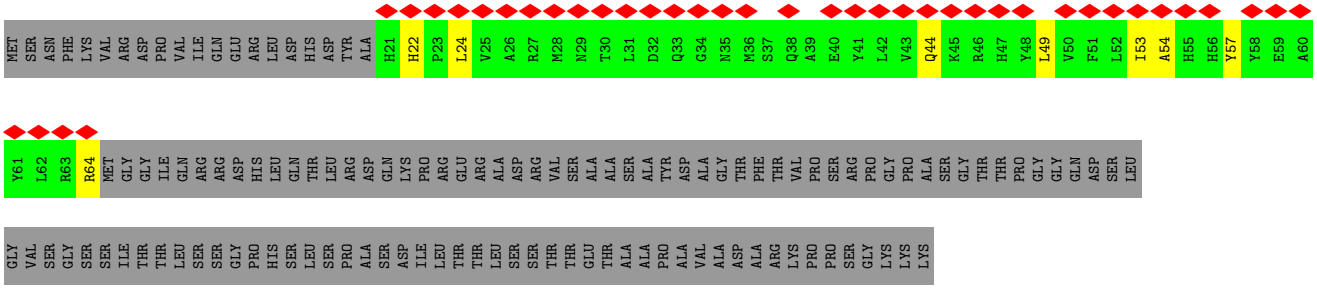




• Molecule 7: Small capsomere-interacting protein

Chain A:



• Molecule 7: Small capsomere-interacting protein

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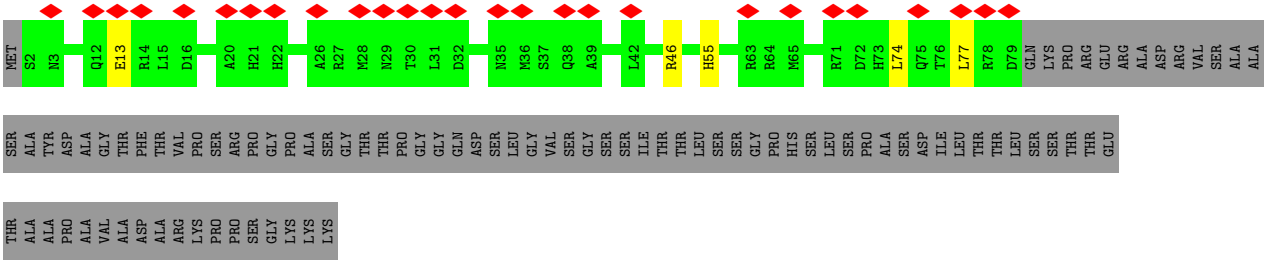

• Molecule 7: Small capsomere-interacting protein

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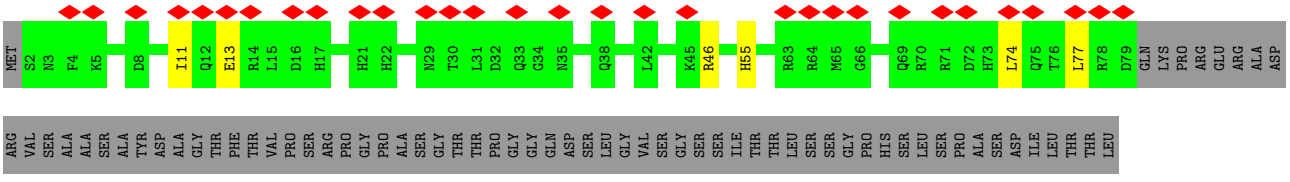
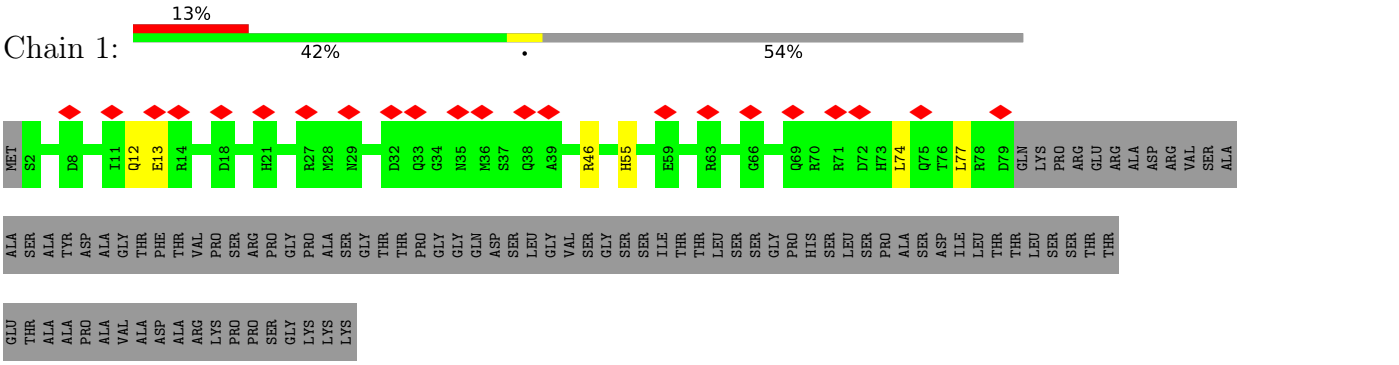
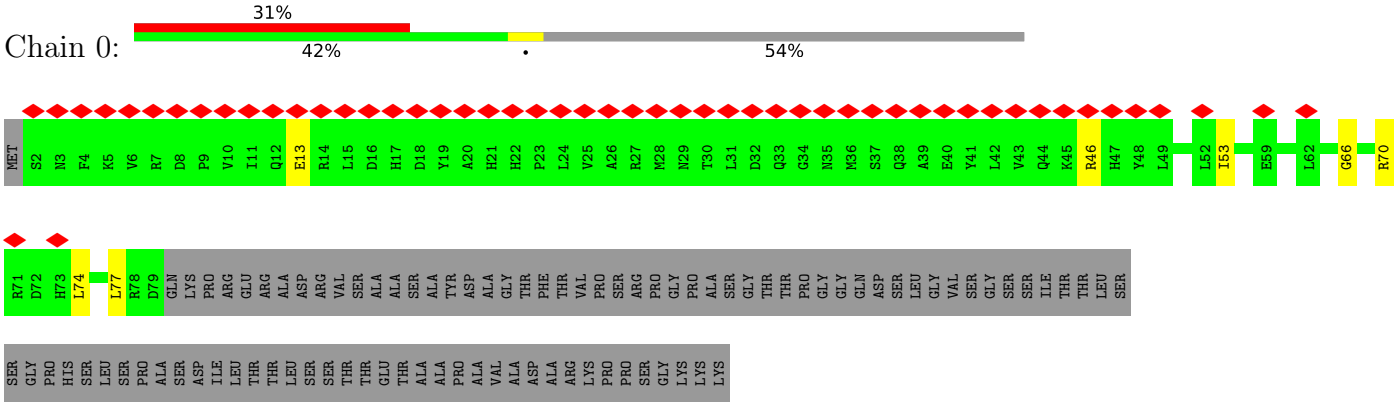


• Molecule 7: Small capsomere-interacting protein



• Molecule 7: Small capsomere-interacting protein



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	928740	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 ($e^-/Å^2$)	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.135	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	k	0.33	0/2753	0.54	1/3755 (0.0%)
2	l	0.26	0/698	0.47	0/942
2	m	0.25	0/656	0.47	0/887
3	n	0.28	0/326	0.50	0/437
3	o	0.28	0/326	0.50	0/437
4	5	0.31	0/2489	0.59	2/3383 (0.1%)
4	b	0.35	0/2540	0.63	3/3452 (0.1%)
5	6	0.31	0/2430	0.61	1/3309 (0.0%)
5	7	0.31	0/2360	0.60	1/3210 (0.0%)
5	c	0.32	0/2376	0.60	0/3234
5	d	0.31	0/2411	0.58	0/3281
6	4	0.32	0/9861	0.61	4/13391 (0.0%)
6	S	0.35	0/10300	0.60	3/13998 (0.0%)
6	T	0.38	0/10919	0.63	1/14839 (0.0%)
6	W	0.37	0/10874	0.61	1/14780 (0.0%)
6	X	0.37	0/10768	0.60	5/14635 (0.0%)
7	0	0.27	0/682	0.48	0/919
7	1	0.28	0/682	0.48	0/919
7	2	0.27	0/682	0.48	0/919
7	3	0.27	0/682	0.48	0/919
7	A	0.24	0/391	0.46	0/528
All	All	0.35	0/75206	0.60	22/102174 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
6	4	0	13
6	S	0	1
6	T	0	6
6	W	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	X	0	2
All	All	0	28

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	T	708	LEU	CA-CB-CG	7.85	133.36	115.30
6	S	1004	ALA	C-N-CA	7.79	141.18	121.70
6	X	708	LEU	CA-CB-CG	7.60	132.78	115.30
6	S	1019	LEU	CA-CB-CG	7.57	132.72	115.30
4	b	297	ASP	CB-CG-OD1	7.57	125.11	118.30
6	S	708	LEU	CA-CB-CG	7.26	132.00	115.30
6	X	39	LEU	CA-CB-CG	7.04	131.50	115.30
4	b	274	LEU	CA-CB-CG	7.04	131.48	115.30
4	5	297	ASP	CB-CG-OD1	6.97	124.57	118.30
6	X	1019	LEU	CA-CB-CG	6.75	130.84	115.30
6	X	1004	ALA	C-N-CA	6.50	137.95	121.70
6	4	878	LEU	CA-CB-CG	5.88	128.81	115.30
4	5	296	PHE	C-N-CA	5.51	135.47	121.70
6	4	888	VAL	CG1-CB-CG2	-5.47	102.14	110.90
6	4	788	LEU	CB-CG-CD2	5.37	120.13	111.00
4	b	86	LEU	CA-CB-CG	5.29	127.47	115.30
6	4	798	TYR	C-N-CA	5.21	134.74	121.70
5	7	214	LEU	CA-CB-CG	5.21	127.27	115.30
5	6	31	LEU	CA-CB-CG	5.17	127.19	115.30
6	X	1282	LEU	CA-CB-CG	5.15	127.14	115.30
1	k	89	ASP	CB-CG-OD1	5.10	122.89	118.30
6	W	276	LEU	CA-CB-CG	5.02	126.85	115.30

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	4	1084	HIS	Peptide
6	4	1091	THR	Peptide
6	4	1092	ALA	Peptide
6	4	110	LYS	Peptide
6	4	1334	HIS	Peptide
6	4	292	GLN	Peptide
6	4	313	LEU	Peptide

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Mol	Chain	Res	Type	Group
6	4	506	VAL	Peptide
6	4	842	ASP	Peptide
6	4	843	VAL	Peptide
6	4	886	PRO	Peptide
6	4	899	ASP	Peptide
6	4	90	LYS	Peptide
6	S	991	HIS	Peptide
6	T	10	PHE	Peptide
6	T	1112	GLY	Peptide
6	T	505	ASN	Peptide
6	T	537	HIS	Peptide
6	T	886	PRO	Peptide
6	T	944	PHE	Peptide
6	W	262	SER	Peptide
6	W	263	THR	Mainchain
6	W	354	HIS	Peptide
6	W	537	HIS	Peptide
6	W	848	ASP	Peptide
6	W	849	ASP	Peptide
6	X	43	ALA	Peptide
6	X	991	HIS	Peptide

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	k	2680	0	2675	0	0
2	l	686	0	704	0	0
2	m	645	0	653	0	0
3	n	323	0	353	0	0
3	o	323	0	353	0	0
4	5	2428	0	2421	25	0
4	b	2478	0	2466	0	0
5	6	2382	0	2396	26	0
5	7	2315	0	2335	20	0
5	c	2330	0	2354	0	0
5	d	2365	0	2379	0	0
6	4	9634	0	9527	128	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	S	10061	0	9955	88	0
6	T	10667	0	10543	95	0
6	W	10622	0	10500	118	0
6	X	10519	0	10398	99	0
7	0	666	0	647	5	0
7	1	666	0	647	4	0
7	2	666	0	647	3	0
7	3	666	0	647	4	0
7	A	380	0	369	7	0
All	All	73502	0	72969	560	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 5.

All (560) 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)
6:4:864:GLN:HB2	6:4:930:ARG:HH22	1.58	0.68
6:4:698:GLU:HG3	6:4:705:ILE:HD12	1.76	0.67
5:7:220:ARG:HH22	5:7:256:GLN:HE21	1.42	0.66
6:4:916:THR:HG23	6:4:984:MET:HG2	1.77	0.66
6:T:536:VAL:HG13	6:T:1244:SER:HA	1.78	0.66
6:4:777:ARG:NH2	6:4:885:CYS:O	2.30	0.65
6:4:875:ILE:HG23	6:4:878:LEU:HD12	1.79	0.64
6:S:187:PRO:HG2	6:S:192:LEU:HD12	1.78	0.64
7:1:55:HIS:HD2	6:X:770:LEU:HD22	1.61	0.64
6:4:566:PRO:HB2	6:4:568:PRO:HD2	1.79	0.64
6:S:845:ASN:HB3	6:S:848:ASP:HB2	1.78	0.64
6:W:278:THR:HG22	6:W:1051:ILE:HG12	1.80	0.64
6:T:113:GLN:HB3	6:W:38:LEU:HB2	1.80	0.64
6:4:893:ARG:NH2	6:4:984:MET:SD	2.71	0.64
6:4:611:LEU:HD22	6:4:862:ILE:HD13	1.80	0.63
7:2:55:HIS:HD2	6:S:770:LEU:HD22	1.63	0.63
6:S:1068:VAL:HG22	6:S:1082:ILE:HG12	1.78	0.63
6:W:658:ARG:HA	6:W:681:LEU:HD11	1.80	0.63
6:W:1073:VAL:HG13	6:W:1078:VAL:HG22	1.81	0.63
6:W:1200:ARG:NH1	6:W:1221:ASP:O	2.32	0.62
6:X:603:THR:HG22	6:X:647:LYS:HB3	1.81	0.62
5:6:114:LEU:HD11	5:6:145:GLY:HA2	1.80	0.62
6:T:1280:ARG:NH2	6:T:1288:GLU:OE1	2.33	0.62
6:4:861:ASP:O	6:4:930:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:254:GLU:OE2	6:T:372:LYS:NZ	2.32	0.61
6:W:929:ASP:OD1	6:W:932:ARG:NH2	2.33	0.61
4:5:41:LEU:HD21	6:4:1068:VAL:HG11	1.82	0.61
6:T:407:HIS:HB2	6:T:1184:VAL:HG12	1.83	0.61
6:T:929:ASP:OD1	6:T:932:ARG:NH2	2.34	0.61
6:T:717:LEU:HA	6:T:915:GLN:HE22	1.65	0.60
6:X:37:LEU:HB2	6:X:50:PHE:HB2	1.81	0.60
6:T:566:PRO:HG2	6:T:569:LEU:HD12	1.82	0.60
6:T:868:ILE:HG22	6:T:870:PRO:HD3	1.83	0.60
6:4:525:HIS:HD2	6:4:527:THR:HG22	1.66	0.60
7:3:11:ILE:HD11	6:T:832:THR:HG22	1.84	0.60
6:S:692:LEU:HD13	6:T:972:ARG:HG2	1.82	0.60
6:T:275:VAL:HG22	6:T:375:ALA:HB3	1.84	0.60
6:T:1241:GLN:HB3	6:T:1244:SER:HB3	1.83	0.60
6:W:130:GLU:HG2	6:W:1079:THR:HG22	1.83	0.60
6:X:608:ALA:HB3	6:W:678:ARG:HH22	1.67	0.59
6:S:1182:THR:HG23	6:S:1236:ASN:HB3	1.83	0.59
5:7:38:ARG:HH22	6:S:1083:THR:HG22	1.67	0.59
6:T:1201:ALA:HB3	6:T:1227:PRO:HG2	1.83	0.59
6:4:838:PRO:HD2	6:4:854:LEU:HA	1.83	0.59
6:X:698:GLU:HG3	6:X:705:ILE:HD12	1.84	0.59
6:T:1187:ASP:OD2	6:T:1232:ARG:NH2	2.36	0.59
5:6:113:VAL:HG22	5:6:139:VAL:HG12	1.85	0.59
6:W:1293:LEU:HD21	6:W:1297:PRO:HG3	1.84	0.59
6:4:684:LEU:HD11	6:4:805:LEU:HB2	1.85	0.59
6:X:1187:ASP:OD2	6:X:1232:ARG:NH2	2.36	0.59
6:T:578:ARG:NH2	6:T:1017:GLN:OE1	2.35	0.58
6:W:256:THR:HG22	6:W:258:PHE:H	1.67	0.58
6:T:640:THR:O	6:T:644:ASN:ND2	2.36	0.58
6:X:203:ARG:NH1	6:W:1313:ASP:OD2	2.35	0.58
6:X:39:LEU:HB3	6:X:43:ALA:HB1	1.86	0.58
6:S:1111:MET:SD	6:S:1366:ARG:NH2	2.70	0.58
6:4:399:THR:HG21	6:4:1268:GLN:HE22	1.69	0.58
6:4:439:ASN:ND2	6:4:1372:ASN:O	2.36	0.58
6:4:838:PRO:HA	6:4:841:ALA:HB3	1.84	0.58
6:W:1045:GLU:N	6:W:1109:THR:OG1	2.35	0.58
5:7:86:ARG:NH1	5:7:88:ASP:OD1	2.36	0.58
6:4:731:MET:HG2	6:4:738:PRO:HG2	1.86	0.58
6:S:578:ARG:NH1	6:S:1014:SER:O	2.37	0.58
6:W:214:VAL:HG12	6:W:218:LYS:HE2	1.86	0.58
5:6:111:LEU:HB2	5:6:286:LEU:HB2	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:1344:ASN:ND2	6:X:1347:THR:OG1	2.37	0.57
6:W:78:THR:HG22	6:W:304:ALA:HB3	1.86	0.57
6:W:543:PHE:HZ	6:W:555:ARG:HH11	1.52	0.57
6:W:537:HIS:HA	6:W:1238:TRP:CD1	2.39	0.57
6:W:850:ILE:HD12	6:W:870:PRO:HG2	1.86	0.57
6:S:7:GLN:NE2	6:S:36:GLN:OE1	2.38	0.57
6:X:606:ASP:OD1	6:W:678:ARG:NH1	2.37	0.57
6:W:538:PRO:O	6:W:559:ARG:NH1	2.37	0.57
6:4:623:GLN:NE2	6:4:761:GLY:O	2.37	0.57
6:S:698:GLU:HG3	6:S:705:ILE:HD12	1.85	0.57
6:X:128:GLU:OE2	6:X:1071:ARG:NH2	2.37	0.57
6:4:1066:PRO:HB3	6:4:1084:HIS:HA	1.86	0.57
6:X:777:ARG:NH2	6:X:885:CYS:O	2.38	0.57
6:4:1199:GLY:HA3	6:4:1236:ASN:H	1.70	0.57
6:W:578:ARG:NH2	6:W:1017:GLN:OE1	2.38	0.57
6:4:128:GLU:OE2	6:4:1071:ARG:NH2	2.37	0.57
6:4:724:HIS:HB3	6:4:793:LEU:HB2	1.87	0.57
6:S:1344:ASN:ND2	6:S:1347:THR:OG1	2.38	0.57
6:S:488:THR:OG1	6:S:982:ASN:ND2	2.39	0.56
6:4:639:GLN:HA	6:4:670:PRO:HG3	1.87	0.56
6:S:770:LEU:HD21	6:S:883:LEU:HD22	1.87	0.56
6:W:965:VAL:HG13	6:W:972:ARG:HG2	1.87	0.56
6:W:1071:ARG:O	6:W:1079:THR:OG1	2.24	0.56
6:W:799:ASN:HD21	6:W:802:LEU:HD12	1.69	0.56
6:4:507:ALA:HB1	6:4:978:ASN:HD21	1.71	0.56
6:X:1294:ALA:HB3	6:X:1318:GLN:HE21	1.69	0.56
6:W:481:TYR:OH	6:W:979:VAL:O	2.23	0.56
6:S:1294:ALA:HB3	6:S:1318:GLN:HE21	1.69	0.56
6:T:93:PHE:HB2	6:T:116:VAL:HB	1.88	0.56
7:2:13:GLU:OE1	7:2:46:ARG:NH2	2.37	0.56
6:T:1250:TYR:HB2	6:T:1270:PHE:HD2	1.70	0.56
6:W:91:ILE:HD12	6:W:1089:LEU:HD22	1.87	0.56
6:W:275:VAL:HG22	6:W:375:ALA:HB3	1.88	0.56
5:6:11:LEU:HG	5:6:15:LEU:HD23	1.87	0.56
6:S:640:THR:O	6:S:644:ASN:ND2	2.39	0.56
6:X:856:ASN:ND2	7:0:66:GLY:O	2.39	0.56
5:6:189:ARG:NH1	5:6:190:LEU:O	2.39	0.55
4:5:143:ILE:HG22	4:5:145:ASN:H	1.71	0.55
6:T:537:HIS:HA	6:T:1238:TRP:CD1	2.42	0.55
6:T:717:LEU:HD23	6:T:804:LYS:HD3	1.88	0.55
6:T:1070:ARG:HH21	6:T:1073:VAL:HG21	1.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:1111:MET:SD	6:T:1366:ARG:NH2	2.79	0.55
6:X:640:THR:O	6:X:644:ASN:ND2	2.40	0.55
6:W:182:LYS:NZ	6:W:1058:SER:OG	2.39	0.55
5:6:177:TYR:HB3	5:7:263:ILE:HG21	1.87	0.55
5:6:94:GLN:HE21	5:6:297:ALA:HB1	1.70	0.55
6:S:658:ARG:HA	6:S:681:LEU:HD11	1.87	0.55
6:T:399:THR:HG22	6:T:1043:THR:HG22	1.88	0.55
6:X:399:THR:HG22	6:X:1043:THR:HG22	1.88	0.55
6:W:1027:GLN:HB3	6:W:1032:MET:HB2	1.89	0.55
6:4:428:GLN:NE2	6:4:577:SER:OG	2.34	0.55
6:T:306:TYR:OH	6:T:323:MET:O	2.24	0.55
6:4:1333:SER:HB2	6:4:1355:GLN:HB2	1.88	0.55
6:X:777:ARG:HG2	6:X:887:PHE:HE1	1.71	0.55
6:S:902:GLN:NE2	6:S:1020:SER:OG	2.40	0.55
6:T:334:VAL:HG21	6:X:310:GLY:HA2	1.89	0.55
6:W:1280:ARG:NH2	6:W:1288:GLU:OE1	2.40	0.55
7:3:13:GLU:OE1	7:3:46:ARG:NH2	2.37	0.54
6:X:1043:THR:OG1	6:X:1305:GLN:NE2	2.39	0.54
4:5:50:ARG:NH2	6:4:140:PHE:O	2.40	0.54
4:5:254:GLU:HG2	5:6:64:GLN:HE21	1.72	0.54
6:S:603:THR:HG22	6:S:647:LYS:HB3	1.89	0.54
6:T:777:ARG:NH2	6:T:885:CYS:O	2.40	0.54
7:1:13:GLU:OE1	7:1:46:ARG:NH2	2.37	0.54
4:5:66:ARG:NH1	5:7:90:SER:O	2.41	0.54
6:S:447:GLN:NE2	6:T:521:GLU:OE1	2.41	0.54
6:T:578:ARG:NH1	6:T:1014:SER:O	2.40	0.54
4:5:289:CYS:SG	4:5:290:THR:N	2.80	0.54
6:S:1167:PRO:HD3	6:T:1224:ILE:HD13	1.89	0.54
6:T:146:PRO:HA	6:T:149:PHE:HD2	1.72	0.54
6:4:309:ARG:HD3	6:X:38:LEU:HD12	1.89	0.54
6:X:130:GLU:HG2	6:X:1079:THR:HG22	1.90	0.54
6:X:729:ASP:OD2	6:X:798:TYR:OH	2.25	0.54
6:4:846:ALA:HA	6:4:872:VAL:HB	1.88	0.54
6:S:1283:TYR:O	6:S:1287:ASN:ND2	2.41	0.54
6:4:834:THR:HG22	7:A:53:ILE:HD12	1.90	0.54
6:T:658:ARG:HA	6:T:681:LEU:HD11	1.89	0.54
6:X:1280:ARG:NH2	6:X:1288:GLU:OE1	2.40	0.53
6:4:567:GLN:HE21	6:4:998:TYR:HA	1.73	0.53
6:X:770:LEU:HD21	6:X:883:LEU:HD22	1.90	0.53
6:X:1068:VAL:HG22	6:X:1082:ILE:HG12	1.90	0.53
6:W:1308:VAL:HG21	6:W:1314:VAL:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:130:GLU:HG2	6:S:1079:THR:HG22	1.90	0.53
6:4:700:VAL:O	6:4:1131:GLN:NE2	2.41	0.53
6:S:157:LYS:HD2	6:T:338:ASN:HA	1.90	0.53
5:6:201:LEU:HD13	5:7:231:ARG:HH12	1.72	0.53
6:S:707:HIS:HD2	6:S:715:PRO:HD3	1.72	0.53
6:4:47:SER:OG	6:4:48:VAL:N	2.41	0.53
6:S:399:THR:HG22	6:S:1043:THR:HG22	1.90	0.53
7:0:13:GLU:OE1	7:0:46:ARG:NH2	2.37	0.53
5:7:291:TYR:HD1	5:7:298:ALA:HB2	1.73	0.53
6:4:1071:ARG:O	6:4:1079:THR:OG1	2.25	0.53
6:T:1071:ARG:O	6:T:1079:THR:OG1	2.24	0.53
6:X:278:THR:HG22	6:X:1051:ILE:HG12	1.90	0.53
6:4:495:ARG:O	6:4:499:GLN:N	2.41	0.53
6:T:591:VAL:HB	6:T:683:GLU:HB2	1.90	0.53
6:X:785:ARG:NH1	6:X:787:VAL:O	2.41	0.53
4:5:186:LEU:HD23	4:5:192:ARG:HB3	1.91	0.53
6:X:91:ILE:HD11	6:X:1089:LEU:HD22	1.89	0.53
4:5:264:THR:HA	5:7:237:LEU:HD21	1.91	0.52
5:6:285:ARG:HD2	5:7:305:ARG:HE	1.73	0.52
6:4:206:LYS:HG3	6:4:208:ALA:H	1.73	0.52
6:X:687:LEU:HD23	6:X:805:LEU:HD22	1.90	0.52
6:W:963:ASN:HA	6:W:966:THR:HG22	1.91	0.52
6:W:399:THR:HG22	6:W:1043:THR:HG22	1.91	0.52
6:4:684:LEU:HA	6:4:687:LEU:HB2	1.91	0.52
6:S:11:PRO:HB2	6:X:332:ARG:HD2	1.91	0.52
6:S:421:GLY:HA3	6:T:413:TYR:HA	1.91	0.52
6:T:854:LEU:HD13	6:T:860:LYS:HG2	1.91	0.52
4:5:217:ARG:NH2	5:6:43:GLN:O	2.43	0.52
6:T:946:LYS:HE2	6:T:993:SER:HA	1.91	0.52
4:5:234:ARG:HD3	4:5:274:LEU:HD11	1.91	0.52
6:4:84:ARG:HH21	6:X:134:ALA:HB2	1.74	0.52
6:X:578:ARG:NH1	6:X:1014:SER:O	2.43	0.52
6:4:913:VAL:HG12	6:4:990:TRP:HD1	1.75	0.52
6:4:963:ASN:HA	6:4:966:THR:HG22	1.92	0.52
6:W:603:THR:HG22	6:W:647:LYS:HB3	1.92	0.52
6:W:851:LEU:HD23	6:W:854:LEU:HD12	1.92	0.52
6:4:275:VAL:HG22	6:4:375:ALA:HB3	1.92	0.52
6:X:488:THR:OG1	6:X:982:ASN:ND2	2.43	0.52
6:4:130:GLU:HG2	6:4:1079:THR:HG22	1.90	0.52
6:S:731:MET:HG2	6:S:738:PRO:HG2	1.91	0.52
6:X:66:PHE:HD1	6:X:175:VAL:HG22	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:902:GLN:NE2	6:W:1020:SER:OG	2.42	0.52
6:4:399:THR:HG22	6:4:1043:THR:HG22	1.91	0.51
6:4:935:ALA:HA	6:4:938:MET:HB2	1.91	0.51
6:S:1042:ARG:NH1	6:S:1044:ASP:OD2	2.43	0.51
6:X:306:TYR:OH	6:X:323:MET:O	2.28	0.51
6:T:512:VAL:HG12	6:T:993:SER:HB3	1.92	0.51
6:X:394:ARG:HD3	6:X:1315:PHE:HB3	1.91	0.51
6:4:182:LYS:NZ	6:4:1058:SER:OG	2.44	0.51
6:W:183:LEU:HD13	6:W:394:ARG:HH21	1.74	0.51
6:4:759:LEU:HD22	6:4:792:PRO:HB3	1.93	0.51
6:S:777:ARG:NH2	6:S:885:CYS:O	2.43	0.51
6:T:350:LEU:HD12	6:W:13:LEU:HD23	1.92	0.51
6:W:602:GLU:HB3	6:W:647:LYS:HE2	1.92	0.51
6:T:1342:MET:HA	6:T:1375:VAL:HG21	1.93	0.51
6:W:1005:THR:HG22	6:W:1007:GLY:H	1.74	0.51
5:6:97:ASN:HB3	5:6:296:LEU:HB3	1.93	0.51
6:W:407:HIS:HB2	6:W:1184:VAL:HG12	1.93	0.51
4:5:207:LEU:HB2	4:5:248:SER:HB3	1.91	0.51
6:S:687:LEU:HD23	6:S:805:LEU:HD22	1.93	0.51
6:T:603:THR:HG22	6:T:647:LYS:HB3	1.92	0.51
6:4:676:HIS:HA	6:4:679:LYS:HB2	1.93	0.50
4:5:300:PRO:HB2	4:5:315:LEU:HD22	1.92	0.50
5:6:124:THR:HG22	5:6:135:VAL:HG22	1.93	0.50
6:X:87:ILE:HD11	6:W:49:ARG:HD3	1.93	0.50
6:X:1345:LYS:NZ	6:X:1376:TYR:OXT	2.37	0.50
6:W:963:ASN:O	6:W:967:ARG:N	2.43	0.50
6:4:778:VAL:HG13	7:A:44:GLN:HE22	1.76	0.50
6:S:192:LEU:HD13	6:S:1098:VAL:HG22	1.92	0.50
4:5:70:TYR:HB2	4:5:188:ARG:HH11	1.75	0.50
6:S:716:HIS:HD2	6:S:736:ARG:HH21	1.59	0.50
6:T:278:THR:HG22	6:T:1051:ILE:HG12	1.93	0.50
6:X:829:VAL:HG22	6:X:938:MET:HE3	1.94	0.50
6:W:93:PHE:HB2	6:W:116:VAL:HB	1.91	0.50
6:W:537:HIS:HB2	6:W:1245:LEU:HB2	1.94	0.50
6:T:436:ASN:HD22	6:T:440:VAL:HB	1.77	0.50
6:T:1073:VAL:HG22	6:T:1078:VAL:HG13	1.92	0.50
6:W:447:GLN:HB3	6:W:1028:ALA:HB1	1.93	0.50
6:4:1200:ARG:HG3	6:4:1234:THR:HG23	1.93	0.50
6:X:93:PHE:HB2	6:X:116:VAL:HB	1.93	0.50
6:W:633:LEU:HD12	6:W:874:MET:HB3	1.94	0.50
6:4:471:ALA:HB1	6:4:1242:ARG:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:743:GLY:O	6:4:746:ASN:ND2	2.45	0.49
4:5:234:ARG:HG2	4:5:239:PRO:HA	1.93	0.49
5:6:48:GLY:HA2	5:6:51:CYS:HB3	1.93	0.49
6:4:537:HIS:HA	6:4:1238:TRP:HD1	1.75	0.49
6:X:611:LEU:HD11	6:X:935:ALA:HB2	1.94	0.49
4:5:228:ALA:HB2	4:5:291:LEU:HD11	1.94	0.49
6:S:12:TYR:HA	6:W:56:VAL:HG12	1.93	0.49
6:W:828:ASN:ND2	6:W:937:THR:O	2.45	0.49
6:T:1268:GLN:HG2	6:T:1321:HIS:CD2	2.46	0.49
5:6:30:VAL:HG22	5:6:73:VAL:HG22	1.94	0.49
6:4:1217:ARG:HG3	6:4:1221:ASP:HB2	1.94	0.49
6:X:740:ILE:HB	6:X:747:TYR:HB3	1.95	0.49
6:4:725:ASP:HB2	6:4:790:VAL:HG11	1.95	0.49
6:4:898:ARG:NH1	6:4:904:PHE:O	2.45	0.49
5:6:169:VAL:HG11	5:6:174:LEU:HD13	1.95	0.49
6:S:66:PHE:HD1	6:S:175:VAL:HG22	1.78	0.49
6:S:495:ARG:HE	6:S:499:GLN:HE21	1.59	0.49
6:4:82:ASP:N	6:4:82:ASP:OD1	2.46	0.49
6:4:340:LEU:HD12	6:4:341:PRO:HD2	1.94	0.49
6:X:658:ARG:HA	6:X:681:LEU:HD11	1.94	0.49
6:W:1344:ASN:ND2	6:W:1347:THR:OG1	2.45	0.49
5:6:262:ASP:OD2	5:7:158:TYR:OH	2.31	0.48
6:X:1369:LYS:HG2	6:X:1374:VAL:HG22	1.95	0.48
6:W:1073:VAL:HG22	6:W:1078:VAL:HG13	1.95	0.48
6:W:578:ARG:NH1	6:W:1014:SER:O	2.42	0.48
6:W:591:VAL:HB	6:W:683:GLU:HB2	1.95	0.48
6:W:600:ILE:HG23	6:W:651:VAL:HG11	1.94	0.48
6:S:23:ILE:HB	6:W:387:GLN:HE22	1.78	0.48
6:4:633:LEU:HD11	6:4:874:MET:HA	1.94	0.48
6:S:725:ASP:HB3	6:S:793:LEU:HD22	1.94	0.48
6:T:740:ILE:HB	6:T:747:TYR:HB3	1.94	0.48
6:X:256:THR:HG22	6:X:258:PHE:H	1.79	0.48
6:X:929:ASP:HA	6:X:932:ARG:HG3	1.96	0.48
6:W:731:MET:HG2	6:W:738:PRO:HG2	1.96	0.48
4:5:87:GLY:H	4:5:165:MET:HB2	1.78	0.48
6:4:228:LEU:HD22	6:4:1103:HIS:HB2	1.95	0.48
6:S:740:ILE:HB	6:S:747:TYR:HB3	1.96	0.48
6:T:739:ILE:HB	6:T:895:ILE:HB	1.95	0.48
6:W:276:LEU:HB3	6:W:1053:TYR:HD1	1.79	0.48
6:4:206:LYS:HB3	6:4:209:VAL:HG23	1.96	0.48
6:4:756:PHE:O	6:4:788:LEU:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:1369:LYS:HG2	6:S:1374:VAL:HG22	1.95	0.48
6:X:932:ARG:HH12	6:W:796:ASN:HB3	1.79	0.48
5:7:69:CYS:SG	5:7:70:THR:N	2.86	0.48
6:4:520:THR:HG22	6:4:568:PRO:HA	1.96	0.48
6:4:578:ARG:NH2	6:4:1017:GLN:OE1	2.46	0.48
6:4:895:ILE:HG13	6:4:914:ALA:HB2	1.96	0.48
6:S:826:TYR:OH	6:S:920:ASN:O	2.31	0.48
6:X:742:ILE:HG12	6:X:788:LEU:HD22	1.94	0.48
6:W:95:ILE:HB	6:W:114:TYR:HB2	1.96	0.48
6:S:619:MET:SD	6:S:881:SER:OG	2.69	0.48
5:6:212:CYS:N	5:7:222:CYS:SG	2.87	0.47
6:X:518:VAL:HG13	6:X:522:ASP:HB3	1.94	0.47
6:X:718:LEU:HD12	6:X:894:VAL:HG21	1.96	0.47
6:4:685:ILE:O	6:4:689:GLN:N	2.46	0.47
6:W:9:PRO:HB3	6:W:45:GLU:HB3	1.97	0.47
6:S:1187:ASP:OD2	6:S:1232:ARG:NH2	2.47	0.47
6:X:532:LEU:O	6:X:1241:GLN:NE2	2.40	0.47
6:S:714:ASP:OD1	6:S:736:ARG:NH2	2.48	0.47
6:S:1047:LEU:HD12	6:S:1106:ALA:HB3	1.97	0.47
6:X:836:ASN:HD21	6:X:854:LEU:HD12	1.79	0.47
6:X:1027:GLN:HB3	6:X:1032:MET:HB2	1.96	0.47
4:5:76:TYR:HB3	4:5:78:GLN:HG2	1.97	0.47
6:S:514:GLN:HG3	6:S:531:LEU:HD21	1.97	0.47
6:S:558:HIS:O	6:S:992:LYS:NZ	2.46	0.47
6:S:1043:THR:OG1	6:S:1305:GLN:NE2	2.47	0.47
6:T:228:LEU:HD21	6:T:285:ARG:HG3	1.97	0.47
6:T:494:PHE:HB3	6:T:498:HIS:HD2	1.80	0.47
6:X:902:GLN:NE2	6:X:1020:SER:OG	2.43	0.47
6:W:276:LEU:HA	6:W:1053:TYR:HA	1.97	0.47
6:W:438:ASN:HD22	6:W:1171:HIS:CD2	2.32	0.47
6:4:218:LYS:NZ	6:4:1323:LEU:O	2.47	0.47
6:4:750:PRO:HA	6:4:753:ARG:HB3	1.96	0.47
6:S:742:ILE:HG12	6:S:788:LEU:HD22	1.96	0.47
6:X:110:LYS:HD2	6:W:130:GLU:HG3	1.96	0.47
6:X:491:MET:HE3	6:X:786:HIS:HA	1.96	0.47
6:W:278:THR:HB	6:W:282:VAL:HB	1.97	0.47
6:W:325:ASN:ND2	6:W:352:ASP:OD2	2.47	0.47
5:6:305:ARG:O	5:7:305:ARG:NH2	2.48	0.47
6:4:1210:TYR:HB3	6:4:1283:TYR:HE2	1.79	0.47
6:S:423:GLU:HG2	6:S:1352:HIS:HE1	1.80	0.47
6:T:41:LYS:O	6:T:44:ARG:NH1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:276:LEU:HB3	6:T:1053:TYR:HD1	1.80	0.47
6:T:856:ASN:OD1	6:T:860:LYS:NZ	2.43	0.47
6:W:626:LYS:NZ	6:W:881:SER:O	2.44	0.47
6:W:711:ALA:HB2	6:W:1018:LYS:HD3	1.97	0.47
6:W:718:LEU:HD12	6:W:894:VAL:HG21	1.96	0.47
6:T:770:LEU:HD21	6:T:883:LEU:HD22	1.97	0.46
6:W:955:ALA:HB1	6:W:962:ALA:HA	1.97	0.46
6:X:543:PHE:HE1	6:X:557:THR:HG23	1.80	0.46
6:W:575:GLN:NE2	6:W:1015:MET:SD	2.88	0.46
6:T:718:LEU:HD12	6:T:894:VAL:HG21	1.98	0.46
6:T:898:ARG:HD3	6:T:902:GLN:HG3	1.96	0.46
6:W:438:ASN:HB2	6:W:1171:HIS:HD2	1.80	0.46
6:4:278:THR:HG22	6:4:1051:ILE:HG12	1.98	0.46
6:X:717:LEU:HD23	6:X:804:LYS:HD3	1.98	0.46
6:W:591:VAL:N	6:W:683:GLU:OE1	2.37	0.46
5:6:204:LEU:HB3	5:7:229:LEU:HD11	1.97	0.46
6:4:1196:ASN:HD22	6:4:1202:ALA:H	1.63	0.46
6:S:718:LEU:HD12	6:S:894:VAL:HG21	1.97	0.46
4:5:125:THR:HG22	4:5:312:LEU:HD11	1.98	0.46
6:S:1169:LEU:O	6:T:211:SER:OG	2.26	0.46
6:T:350:LEU:HD21	6:W:15:THR:HG22	1.98	0.46
6:X:1005:THR:HG22	6:X:1007:GLY:H	1.80	0.46
6:T:82:ASP:OD1	6:T:82:ASP:N	2.48	0.46
6:X:444:PHE:HB2	6:X:1113:VAL:HG11	1.98	0.46
6:W:402:PHE:HD2	6:W:1040:VAL:HB	1.80	0.46
6:W:770:LEU:HD21	6:W:883:LEU:HD22	1.97	0.46
6:4:655:HIS:O	6:4:659:PHE:N	2.46	0.45
6:S:836:ASN:HD21	6:S:854:LEU:HD12	1.82	0.45
6:W:331:ALA:HA	6:W:335:ASP:HB2	1.98	0.45
6:W:913:VAL:HG21	6:W:990:TRP:HE1	1.80	0.45
6:S:718:LEU:HD21	6:S:730:LEU:HD12	1.99	0.45
6:X:78:THR:HG22	6:X:304:ALA:HB3	1.97	0.45
6:4:839:VAL:HG11	6:4:875:ILE:HB	1.98	0.45
6:X:456:PRO:HG2	6:X:1125:ASP:HB3	1.98	0.45
6:W:684:LEU:HD23	6:W:802:LEU:HD22	1.99	0.45
6:W:822:MET:SD	6:W:939:PHE:HB3	2.57	0.45
6:S:9:PRO:HG2	6:T:317:VAL:HG13	1.98	0.45
6:S:1169:LEU:H	6:S:1169:LEU:HG	1.63	0.45
6:X:714:ASP:O	6:X:804:LYS:NZ	2.48	0.45
6:W:717:LEU:HD23	6:W:804:LYS:HD3	1.97	0.45
6:4:122:LYS:HD2	6:4:1087:ALA:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:457:ARG:NE	6:S:1125:ASP:OD2	2.50	0.45
7:3:55:HIS:HD2	6:T:770:LEU:HD22	1.81	0.45
6:X:520:THR:HG22	6:X:568:PRO:HA	1.99	0.45
6:X:700:VAL:HG23	6:X:705:ILE:HG12	1.99	0.45
6:X:1220:TYR:HE2	6:X:1272:LYS:HD3	1.81	0.45
6:4:574:PHE:O	6:4:578:ARG:N	2.49	0.45
6:S:386:THR:HG21	6:T:100:ILE:HG13	1.98	0.45
6:S:717:LEU:HD23	6:S:804:LYS:HD3	1.98	0.45
6:W:987:TYR:O	6:W:992:LYS:NZ	2.50	0.45
6:S:56:VAL:HG12	6:W:12:TYR:HA	1.98	0.45
6:S:79:GLU:HG2	6:S:1063:VAL:HB	1.98	0.45
6:S:100:ILE:O	6:S:109:ASN:ND2	2.50	0.45
6:T:555:ARG:HE	6:T:907:HIS:CD2	2.35	0.45
6:T:1345:LYS:NZ	6:T:1376:TYR:OXT	2.50	0.45
5:7:156:HIS:HD2	5:7:201:LEU:HB2	1.82	0.45
6:4:90:LYS:HE2	6:X:27:ALA:HB3	1.99	0.45
6:S:151:GLU:HG2	6:X:85:ARG:HH22	1.82	0.45
6:T:293:VAL:HG21	6:T:368:LYS:HE3	1.98	0.45
6:T:757:ILE:HG12	6:T:788:LEU:HD22	1.98	0.45
6:T:907:HIS:HB2	6:T:910:GLY:N	2.31	0.45
6:T:264:TYR:HE1	6:T:300:PRO:HD2	1.82	0.45
6:W:447:GLN:HA	6:W:450:LEU:HB2	1.98	0.45
6:W:572:ARG:NH2	6:W:1001:SER:O	2.50	0.45
6:S:394:ARG:HD3	6:S:1315:PHE:HB3	1.99	0.45
6:X:1111:MET:SD	6:X:1366:ARG:NH2	2.81	0.45
6:W:1062:PHE:HB2	6:W:1087:ALA:HB3	1.99	0.45
6:4:842:ASP:O	6:4:844:VAL:N	2.49	0.44
6:W:504:LYS:HG2	6:W:964:TYR:HE1	1.82	0.44
6:4:404:VAL:HG13	6:4:1038:MET:HG3	1.98	0.44
6:S:1345:LYS:NZ	6:S:1376:TYR:OXT	2.41	0.44
6:W:491:MET:HB2	6:W:783:ASP:HA	1.99	0.44
6:W:520:THR:HG22	6:W:568:PRO:HA	1.99	0.44
6:4:278:THR:HB	6:4:282:VAL:HB	1.99	0.44
6:T:170:LEU:HD11	6:T:1084:HIS:HB2	1.98	0.44
6:T:494:PHE:O	6:T:498:HIS:N	2.35	0.44
6:4:298:SER:HB3	6:4:359:ARG:HD2	1.98	0.44
6:4:306:TYR:HE1	6:X:39:LEU:HD23	1.82	0.44
6:4:455:HIS:HD2	6:4:1119:PHE:HD1	1.65	0.44
6:X:447:GLN:HB3	6:X:1028:ALA:HB1	2.00	0.44
6:W:898:ARG:NH1	6:W:910:GLY:O	2.51	0.44
6:S:1043:THR:HG23	6:S:1265:PRO:HB3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:6:223:LEU:HD22	5:6:249:VAL:HG13	1.99	0.44
6:4:684:LEU:HD22	6:4:802:LEU:HA	1.98	0.44
6:X:724:HIS:HB3	6:X:793:LEU:HB3	1.99	0.44
6:W:102:HIS:HE1	6:W:106:ARG:HD2	1.83	0.44
6:4:476:ASP:H	6:4:544:VAL:HG11	1.82	0.44
6:T:130:GLU:HG2	6:T:1079:THR:HG22	1.99	0.44
6:W:540:PHE:HD1	6:W:558:HIS:HA	1.82	0.44
6:W:788:LEU:HD11	6:W:919:VAL:HG21	2.00	0.44
6:4:812:PRO:HB2	6:4:999:ALA:HB1	1.99	0.44
6:4:980:PRO:HD2	6:4:983:LEU:HD12	1.99	0.44
6:X:718:LEU:HD21	6:X:730:LEU:HD12	2.00	0.44
6:X:965:VAL:HG13	6:X:972:ARG:HG2	1.99	0.44
6:4:332:ARG:O	6:4:336:HIS:N	2.50	0.44
6:S:777:ARG:HG2	6:S:887:PHE:HE1	1.83	0.44
6:W:252:VAL:HG21	6:W:1053:TYR:HD2	1.83	0.44
6:4:777:ARG:HH22	6:4:885:CYS:H	1.66	0.43
6:4:1017:GLN:NE2	6:4:1023:SER:O	2.48	0.43
6:S:633:LEU:HG	6:S:874:MET:HE2	1.99	0.43
6:X:738:PRO:HB3	6:X:896:THR:HG22	1.99	0.43
5:7:231:ARG:HG2	5:7:233:ASP:H	1.83	0.43
6:4:620:ILE:HG22	6:4:622:GLY:H	1.83	0.43
6:4:1127:TYR:HB2	6:4:1133:HIS:HB2	1.99	0.43
6:S:256:THR:HG22	6:S:258:PHE:H	1.82	0.43
6:X:5:LEU:HD13	6:X:8:ARG:HH22	1.83	0.43
6:W:428:GLN:NE2	6:W:577:SER:OG	2.43	0.43
6:W:1254:PHE:HB2	6:W:1267:ARG:HH22	1.83	0.43
6:4:712:LEU:HD23	6:4:804:LYS:HD2	1.99	0.43
6:4:743:GLY:HA3	6:4:786:HIS:CE1	2.54	0.43
6:W:129:ILE:HD11	6:W:166:GLY:HA3	2.01	0.43
6:S:130:GLU:HG3	6:T:110:LYS:HD2	2.01	0.43
6:S:224:HIS:HB3	6:S:244:MET:HE3	2.00	0.43
6:S:520:THR:HG22	6:S:568:PRO:HA	1.99	0.43
6:T:402:PHE:HD2	6:T:1040:VAL:HB	1.83	0.43
6:T:714:ASP:O	6:T:804:LYS:NZ	2.51	0.43
6:X:187:PRO:HG2	6:X:192:LEU:HD12	2.00	0.43
6:X:731:MET:HG2	6:X:738:PRO:HG2	1.98	0.43
6:X:1182:THR:HG23	6:X:1236:ASN:HB3	2.00	0.43
6:4:680:ILE:O	6:4:684:LEU:HB2	2.18	0.43
6:W:301:ALA:HB2	6:W:360:THR:HB	2.00	0.43
6:W:947:LEU:HD21	6:W:995:VAL:HG12	2.00	0.43
6:X:950:ASP:HA	6:X:951:PRO:HD3	1.90	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:0:53:ILE:HD13	6:W:840:PHE:CE1	2.54	0.43
6:W:714:ASP:O	6:W:804:LYS:NZ	2.51	0.43
6:4:811:MET:O	6:4:815:SER:N	2.50	0.43
6:X:536:VAL:HG13	6:X:1244:SER:HA	2.00	0.43
6:X:809:VAL:HG13	6:X:1012:MET:HB2	2.01	0.43
6:W:674:HIS:CE1	6:W:678:ARG:HH21	2.37	0.43
5:7:63:MET:HG3	5:7:282:LEU:HD12	2.00	0.43
6:S:272:VAL:HG21	6:S:297:MET:HE1	2.00	0.43
6:T:893:ARG:NH2	6:T:988:GLU:OE1	2.51	0.43
5:7:26:LYS:HA	5:7:98:VAL:HG21	2.01	0.43
6:4:605:PHE:HZ	6:4:816:ASN:HB2	1.84	0.43
6:4:1074:ARG:HG2	6:4:1076:ASP:H	1.84	0.43
6:T:88:ASP:HB3	6:W:3:ALA:HB2	2.01	0.42
6:W:224:HIS:HB3	6:W:244:MET:HE3	2.01	0.42
6:W:809:VAL:HG13	6:W:1012:MET:HB2	2.01	0.42
6:W:1183:PRO:HB3	6:W:1238:TRP:HZ3	1.84	0.42
4:5:82:PRO:HB3	4:5:170:HIS:CD2	2.54	0.42
6:4:934:ALA:O	6:4:938:MET:N	2.40	0.42
6:4:1027:GLN:HB3	6:4:1032:MET:HB2	2.01	0.42
6:4:1334:HIS:O	6:4:1336:VAL:N	2.51	0.42
6:S:278:THR:HG22	6:S:1051:ILE:HG12	2.01	0.42
6:X:264:TYR:CE1	6:X:300:PRO:HD2	2.54	0.42
6:W:170:LEU:HD11	6:W:1084:HIS:HB2	2.02	0.42
6:4:226:PHE:HD2	6:4:1364:MET:HB3	1.84	0.42
6:S:525:HIS:HD2	6:S:527:THR:HG22	1.84	0.42
6:S:1027:GLN:HB3	6:S:1032:MET:HB2	2.01	0.42
6:4:1196:ASN:ND2	6:4:1202:ALA:H	2.17	0.42
6:S:707:HIS:CD2	6:S:715:PRO:HD3	2.54	0.42
6:T:71:LEU:N	6:T:377:GLU:OE2	2.52	0.42
6:X:777:ARG:HG2	6:X:887:PHE:CE1	2.53	0.42
7:0:74:LEU:HD23	7:0:77:LEU:HD12	2.02	0.42
6:W:698:GLU:HG3	6:W:705:ILE:HD12	2.01	0.42
6:W:1226:ASP:O	6:W:1228:ALA:N	2.47	0.42
6:4:709:VAL:O	6:4:1018:LYS:HB2	2.20	0.42
6:4:955:ALA:HB1	6:4:962:ALA:HA	2.01	0.42
6:T:893:ARG:HG3	6:T:915:GLN:O	2.20	0.42
5:6:288:VAL:HG22	5:6:300:CYS:HB3	2.01	0.42
6:4:1127:TYR:H	6:4:1133:HIS:CD2	2.37	0.42
6:X:501:TYR:OH	6:X:978:ASN:O	2.32	0.42
6:W:480:GLY:HA3	6:W:483:LEU:HD11	2.01	0.42
5:6:88:ASP:HB2	5:6:91:ASP:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:561:MET:H	6:4:564:ASN:ND2	2.18	0.42
6:4:834:THR:HB	7:A:49:LEU:HB3	2.02	0.42
6:4:1200:ARG:NE	6:4:1219:LEU:O	2.52	0.42
6:X:819:MET:N	6:X:950:ASP:OD2	2.44	0.42
6:4:446:TYR:O	6:4:450:LEU:N	2.52	0.42
6:4:898:ARG:NE	6:4:910:GLY:O	2.52	0.42
6:S:738:PRO:HB3	6:S:896:THR:HG22	2.00	0.42
6:T:723:TYR:OH	6:T:922:PHE:HB3	2.20	0.42
6:W:634:ILE:HB	6:W:650:PHE:HE2	1.85	0.42
6:4:525:HIS:CD2	6:4:527:THR:HG22	2.50	0.42
6:4:880:THR:HG22	7:A:54:ALA:HA	2.01	0.42
6:S:1190:TYR:OH	6:S:1196:ASN:O	2.31	0.42
6:4:543:PHE:CZ	6:4:555:ARG:HD3	2.55	0.41
6:4:839:VAL:HG13	6:4:872:VAL:HG13	2.02	0.41
6:W:1042:ARG:NH2	6:W:1111:MET:O	2.53	0.41
5:6:224:ARG:HD3	5:6:257:LEU:HD21	2.02	0.41
6:4:526:PRO:HB3	6:4:1233:SER:HB2	2.02	0.41
6:4:896:THR:HG1	6:4:990:TRP:HZ2	1.68	0.41
6:T:278:THR:HB	6:T:282:VAL:HB	2.01	0.41
6:T:540:PHE:O	6:T:559:ARG:NH1	2.53	0.41
6:X:321:ARG:NH1	6:W:51:GLU:OE2	2.53	0.41
6:X:1042:ARG:NH1	6:X:1044:ASP:OD2	2.52	0.41
6:W:146:PRO:HA	6:W:149:PHE:HD2	1.85	0.41
6:W:544:VAL:HG22	6:W:554:TYR:HE1	1.86	0.41
6:W:899:ASP:OD1	6:W:899:ASP:N	2.53	0.41
4:5:69:THR:HG21	5:7:92:ASN:HD21	1.85	0.41
6:4:131:LEU:HD22	6:4:159:ILE:HG13	2.02	0.41
6:4:1058:SER:O	6:4:1091:THR:OG1	2.26	0.41
6:T:809:VAL:HG13	6:T:1012:MET:HB2	2.01	0.41
6:T:980:PRO:HD2	6:T:983:LEU:HD12	2.02	0.41
7:2:74:LEU:HD23	7:2:77:LEU:HD12	2.02	0.41
4:5:75:VAL:HG21	4:5:105:LEU:HD22	2.03	0.41
6:4:566:PRO:HD2	6:4:569:LEU:HD12	2.03	0.41
6:4:876:ARG:HG2	7:A:57:TYR:CG	2.55	0.41
6:X:850:ILE:HD11	6:X:872:VAL:HA	2.01	0.41
6:T:1038:MET:HB2	6:T:1179:ILE:HG23	2.03	0.41
6:X:263:THR:O	6:X:359:ARG:NH1	2.48	0.41
6:X:438:ASN:HD22	6:X:1171:HIS:CD2	2.38	0.41
6:X:457:ARG:NE	6:X:1125:ASP:OD2	2.54	0.41
6:W:649:ALA:O	6:W:677:TYR:OH	2.29	0.41
4:5:46:ALA:O	4:5:50:ARG:NH1	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:555:ARG:HG3	6:4:907:HIS:ND1	2.36	0.41
6:T:266:THR:OG1	6:T:267:ALA:O	2.32	0.41
6:X:850:ILE:HG13	6:X:870:PRO:HG2	2.02	0.41
7:A:22:HIS:NE2	7:A:24:LEU:HB2	2.36	0.41
7:3:74:LEU:HD23	7:3:77:LEU:HD12	2.02	0.41
4:5:49:THR:HG22	6:S:1067:SER:HB2	2.02	0.41
5:6:227:THR:HB	5:6:231:ARG:HH12	1.86	0.41
5:6:235:HIS:CD2	5:6:237:LEU:HG	2.56	0.41
6:4:400:TYR:N	6:4:1042:ARG:O	2.38	0.41
6:S:61:VAL:HG11	6:T:98:PRO:HG3	2.01	0.41
6:S:633:LEU:HD12	6:S:874:MET:HB3	2.02	0.41
6:T:184:ARG:O	6:T:1290:SER:OG	2.39	0.41
7:1:74:LEU:HD23	7:1:77:LEU:HD12	2.02	0.41
6:X:1334:HIS:HB2	6:X:1355:GLN:HG2	2.03	0.41
6:4:233:LEU:HD11	6:4:1367:LEU:HD21	2.02	0.41
7:1:12:GLN:O	7:0:70:ARG:NH1	2.54	0.41
6:X:684:LEU:HB3	6:X:802:LEU:HD22	2.03	0.41
6:4:597:ILE:HA	6:4:600:ILE:HB	2.02	0.40
6:4:840:PHE:CG	7:A:53:ILE:HG12	2.56	0.40
6:S:1005:THR:HG22	6:S:1007:GLY:H	1.86	0.40
6:S:1200:ARG:HG2	6:S:1226:ASP:HB3	2.02	0.40
6:T:773:ILE:O	6:T:776:THR:OG1	2.37	0.40
6:4:194:THR:HG21	6:4:216:MET:HB3	2.03	0.40
6:S:183:LEU:HD13	6:S:394:ARG:HH21	1.86	0.40
6:S:848:ASP:OD2	6:S:853:HIS:NE2	2.43	0.40
6:X:637:VAL:HG22	6:X:868:ILE:HD13	2.02	0.40
4:5:50:ARG:HH21	6:4:141:ALA:HA	1.86	0.40
6:4:669:ILE:H	6:4:669:ILE:HG13	1.82	0.40
6:T:575:GLN:HE21	6:T:1015:MET:HG3	1.86	0.40
6:T:947:LEU:H	6:T:947:LEU:HG	1.74	0.40
6:W:687:LEU:HD23	6:W:805:LEU:HD22	2.03	0.40
4:5:166:VAL:HG13	4:5:187:ALA:HA	2.04	0.40
5:7:153:LEU:HD21	5:7:211:LEU:HD13	2.02	0.40
6:S:1168:GLY:HA2	6:T:207:LYS:HD3	2.04	0.40
6:T:252:VAL:HG21	6:T:1053:TYR:HD2	1.86	0.40
6:X:82:ASP:OD1	6:X:82:ASP:N	2.52	0.40
6:W:436:ASN:HB2	6:W:440:VAL:O	2.21	0.40
6:4:850:ILE:HD12	6:4:870:PRO:HG2	2.04	0.40
6:T:583:ASP:OD1	6:T:590:HIS:NE2	2.54	0.40
6:T:716:HIS:HA	6:T:730:LEU:HD11	2.03	0.40
6:T:1183:PRO:HD3	6:T:1238:TRP:CE3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:44:ARG:HB3	6:X:46:GLY:H	1.87	0.40
6:X:555:ARG:HA	6:X:906:THR:HG21	2.04	0.40
6:W:76:VAL:HG21	6:W:258:PHE:HD2	1.87	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	k	334/454 (74%)	321 (96%)	13 (4%)	0	100	100
2	l	81/549 (15%)	81 (100%)	0	0	100	100
2	m	76/549 (14%)	76 (100%)	0	0	100	100
3	n	38/2635 (1%)	38 (100%)	0	0	100	100
3	o	38/2635 (1%)	38 (100%)	0	0	100	100
4	5	308/331 (93%)	297 (96%)	11 (4%)	0	100	100
4	b	315/331 (95%)	309 (98%)	6 (2%)	0	100	100
5	6	300/305 (98%)	289 (96%)	11 (4%)	0	100	100
5	7	288/305 (94%)	273 (95%)	15 (5%)	0	100	100
5	c	290/305 (95%)	283 (98%)	7 (2%)	0	100	100
5	d	296/305 (97%)	290 (98%)	6 (2%)	0	100	100
6	4	1206/1376 (88%)	1120 (93%)	80 (7%)	6 (0%)	29	66
6	S	1273/1376 (92%)	1196 (94%)	75 (6%)	2 (0%)	47	79
6	T	1354/1376 (98%)	1274 (94%)	76 (6%)	4 (0%)	41	74
6	W	1350/1376 (98%)	1276 (94%)	73 (5%)	1 (0%)	51	83
6	X	1335/1376 (97%)	1261 (94%)	71 (5%)	3 (0%)	47	79
7	0	76/170 (45%)	75 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	1	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	2	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	3	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	A	42/170 (25%)	42 (100%)	0	0	100	100
All	All	9228/16434 (56%)	8764 (95%)	448 (5%)	16 (0%)	50	79

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	4	843	VAL
6	W	263	THR
6	S	992	LYS
6	T	10	PHE
6	X	992	LYS
6	4	842	ASP
6	T	945	ASN
6	X	44	ARG
6	4	849	ASP
6	4	1092	ALA
6	S	993	SER
6	X	993	SER
6	T	849	ASP
6	4	1335	ARG
6	4	314	VAL
6	T	11	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	k	293/377 (78%)	292 (100%)	1 (0%)	92	96
2	l	76/473 (16%)	76 (100%)	0	100	100
2	m	71/473 (15%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	n	35/2239 (2%)	35 (100%)	0	100 100
3	o	35/2239 (2%)	35 (100%)	0	100 100
4	5	266/281 (95%)	266 (100%)	0	100 100
4	b	272/281 (97%)	272 (100%)	0	100 100
5	6	272/274 (99%)	271 (100%)	1 (0%)	91 95
5	7	264/274 (96%)	259 (98%)	5 (2%)	57 76
5	c	267/274 (97%)	267 (100%)	0	100 100
5	d	270/274 (98%)	270 (100%)	0	100 100
6	4	1044/1166 (90%)	1042 (100%)	2 (0%)	93 97
6	S	1094/1166 (94%)	1089 (100%)	5 (0%)	88 94
6	T	1154/1166 (99%)	1154 (100%)	0	100 100
6	W	1150/1166 (99%)	1148 (100%)	2 (0%)	93 97
6	X	1139/1166 (98%)	1134 (100%)	5 (0%)	91 95
7	0	70/141 (50%)	70 (100%)	0	100 100
7	1	70/141 (50%)	70 (100%)	0	100 100
7	2	70/141 (50%)	70 (100%)	0	100 100
7	3	70/141 (50%)	70 (100%)	0	100 100
7	A	39/141 (28%)	38 (97%)	1 (3%)	46 69
All	All	8021/13994 (57%)	7999 (100%)	22 (0%)	92 96

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	k	55	ARG
5	6	130	ASN
5	7	38	ARG
5	7	78	ARG
5	7	97	ASN
5	7	231	ARG
5	7	305	ARG
6	4	83	LEU
6	4	947	LEU
7	A	64	ARG
6	S	41	LYS
6	S	106	ARG
6	S	143	LYS

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Mol	Chain	Res	Type
6	S	713	LEU
6	S	1235	ASN
6	X	106	ARG
6	X	143	LYS
6	X	325	ASN
6	X	713	LEU
6	X	1235	ASN
6	W	1109	THR
6	W	1366	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (118) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	7	ASN
1	k	88	HIS
1	k	91	ASN
1	k	93	HIS
1	k	333	HIS
2	l	77	HIS
2	l	103	ASN
4	5	24	HIS
4	5	145	ASN
5	6	64	GLN
5	6	110	GLN
5	6	150	GLN
5	6	151	GLN
5	6	232	HIS
5	7	92	ASN
5	7	97	ASN
5	7	156	HIS
5	7	256	GLN
5	7	274	GLN
5	7	281	ASN
4	b	124	GLN
4	b	262	HIS
5	c	40	GLN
5	c	110	GLN
5	c	130	ASN
5	c	146	HIS
5	c	150	GLN
5	c	151	GLN
5	d	94	GLN

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Mol	Chain	Res	Type
5	d	108	ASN
5	d	150	GLN
5	d	194	ASN
5	d	274	GLN
6	4	77	ASN
6	4	397	GLN
6	4	498	HIS
6	4	525	HIS
6	4	537	HIS
6	4	545	HIS
6	4	564	ASN
6	4	567	GLN
6	4	590	HIS
6	4	652	ASN
6	4	689	GLN
6	4	978	ASN
6	4	1131	GLN
6	4	1133	HIS
6	4	1196	ASN
7	A	44	GLN
7	A	47	HIS
7	2	17	HIS
7	2	38	GLN
7	2	55	HIS
7	2	73	HIS
6	S	224	HIS
6	S	384	ASN
6	S	499	GLN
6	S	525	HIS
6	S	575	GLN
6	S	590	HIS
6	S	630	ASN
6	S	652	ASN
6	S	707	HIS
6	S	716	HIS
6	S	746	ASN
6	S	902	GLN
6	S	982	ASN
6	S	1084	HIS
6	S	1171	HIS
6	S	1235	ASN
6	S	1318	GLN

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Mol	Chain	Res	Type
6	S	1344	ASN
7	3	17	HIS
7	3	38	GLN
7	3	55	HIS
6	T	312	ASN
6	T	436	ASN
6	T	498	HIS
6	T	746	ASN
6	T	827	GLN
6	T	907	HIS
6	T	915	GLN
6	T	978	ASN
6	T	1133	HIS
6	T	1171	HIS
6	T	1305	GLN
6	T	1321	HIS
6	T	1344	ASN
7	1	17	HIS
7	1	38	GLN
7	1	55	HIS
6	X	312	ASN
6	X	325	ASN
6	X	490	ASN
6	X	663	HIS
6	X	716	HIS
6	X	746	ASN
6	X	982	ASN
6	X	1084	HIS
6	X	1171	HIS
6	X	1235	ASN
6	X	1318	GLN
6	X	1344	ASN
7	0	17	HIS
7	0	38	GLN
7	0	73	HIS
6	W	92	GLN
6	W	102	HIS
6	W	224	HIS
6	W	537	HIS
6	W	674	HIS
6	W	746	ASN
6	W	799	ASN

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Mol	Chain	Res	Type
6	W	902	GLN
6	W	978	ASN
6	W	1171	HIS
6	W	1222	HIS
6	W	1344	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

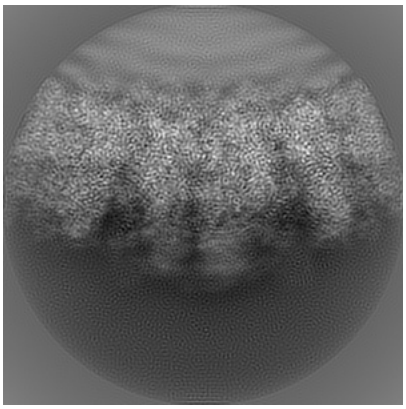
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-20436. These allow visual inspection of the internal detail of the map and identification of artifacts.

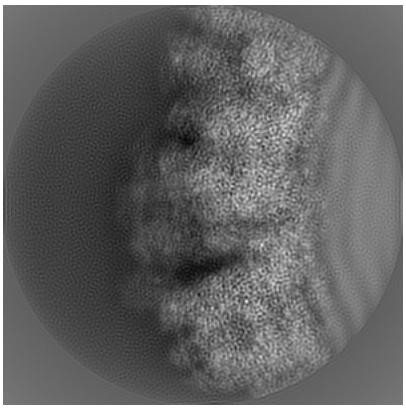
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

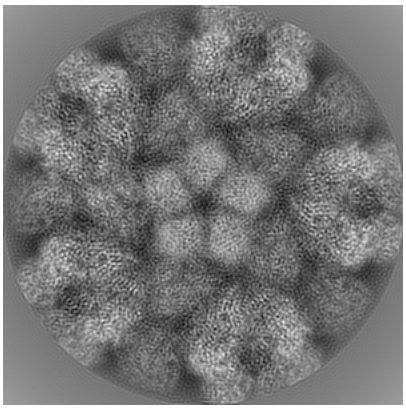
6.1.1 Primary map



X

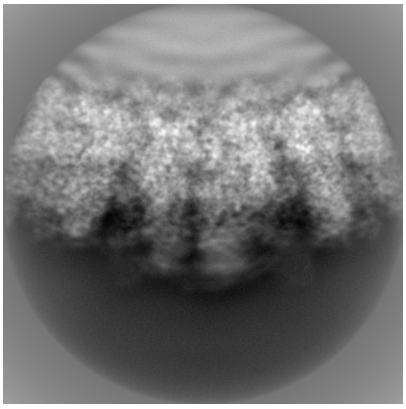


Y

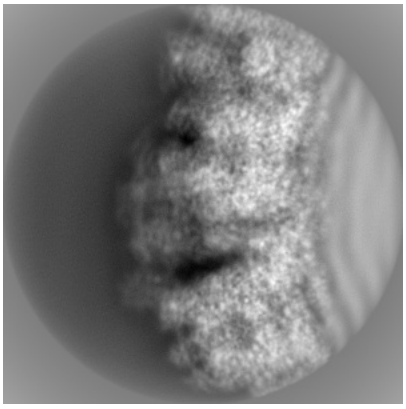


Z

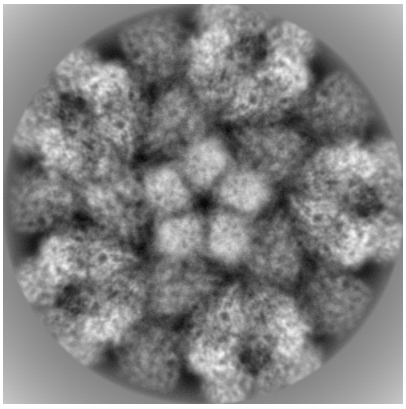
6.1.2 Raw map



X



Y

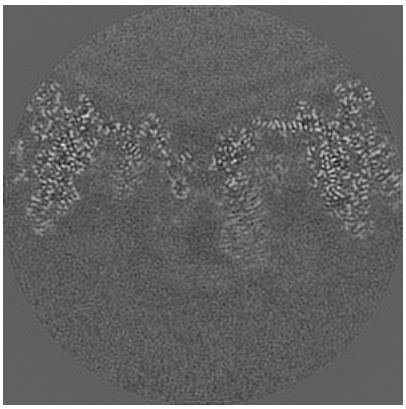


Z

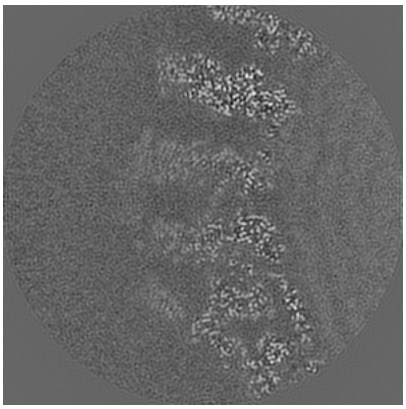
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

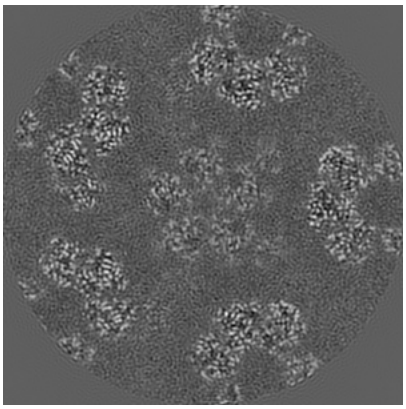
6.2.1 Primary map



X Index: 192

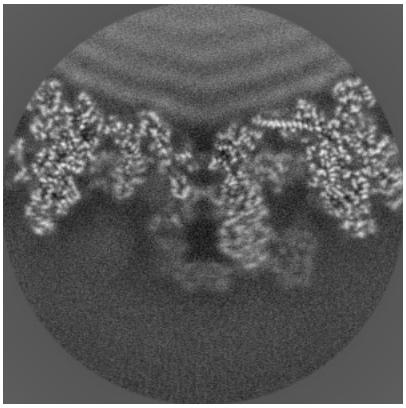


Y Index: 192

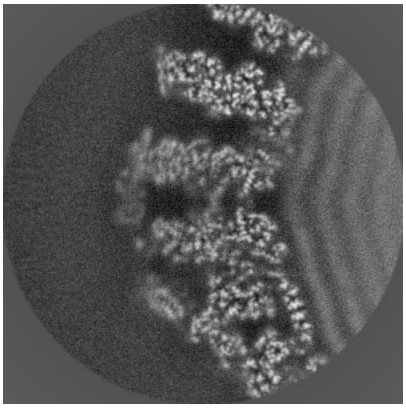


Z Index: 192

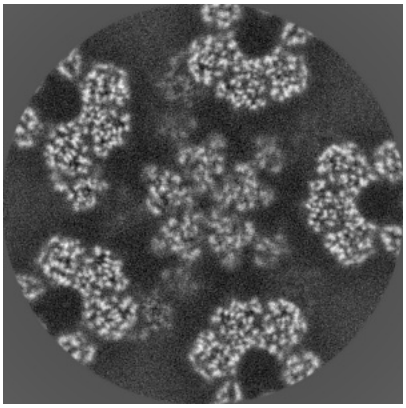
6.2.2 Raw map



X Index: 192



Y Index: 192

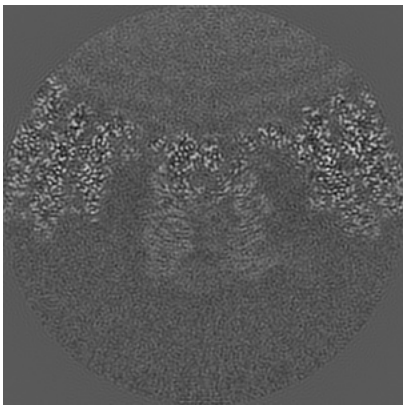


Z Index: 192

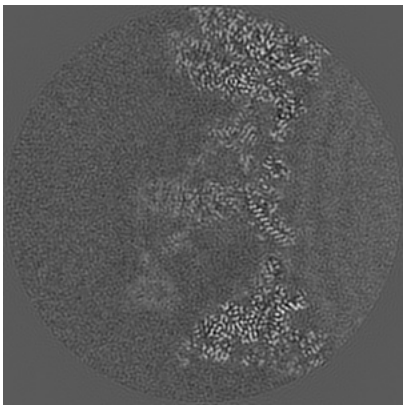
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

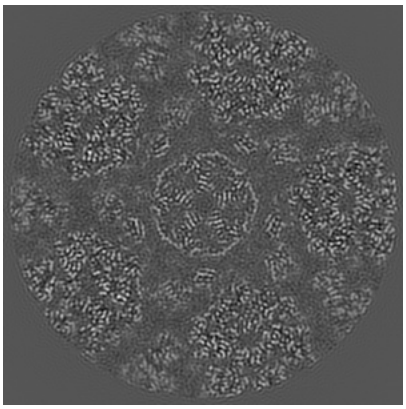
6.3.1 Primary map



X Index: 207

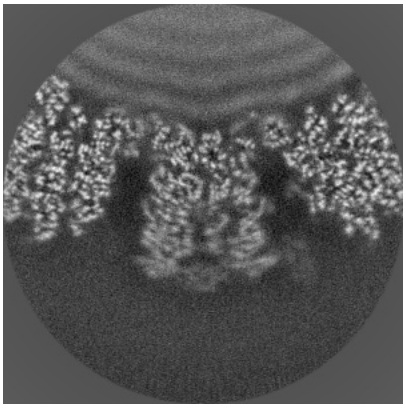


Y Index: 229

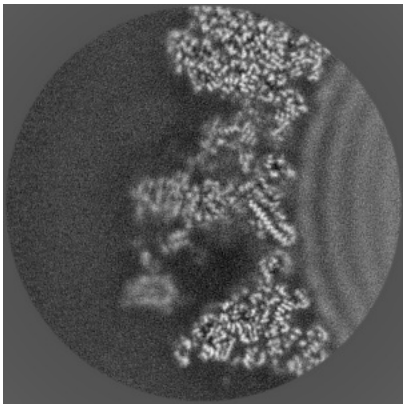


Z Index: 246

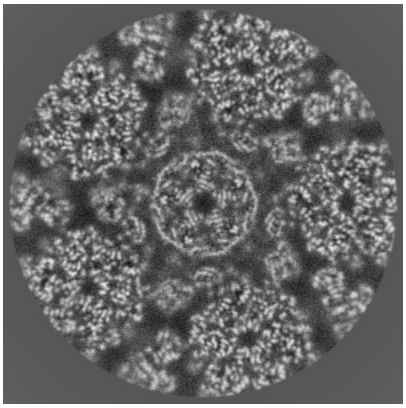
6.3.2 Raw map



X Index: 210



Y Index: 230

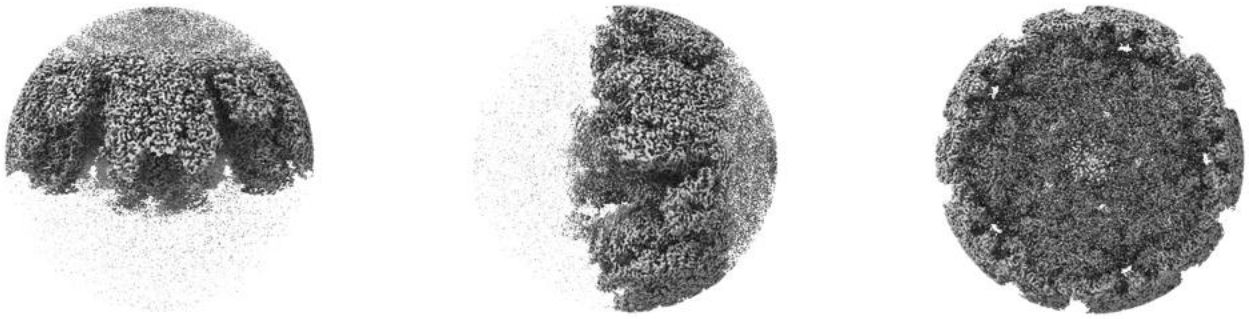


Z Index: 246

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

6.4 Orthogonal surface views (i)

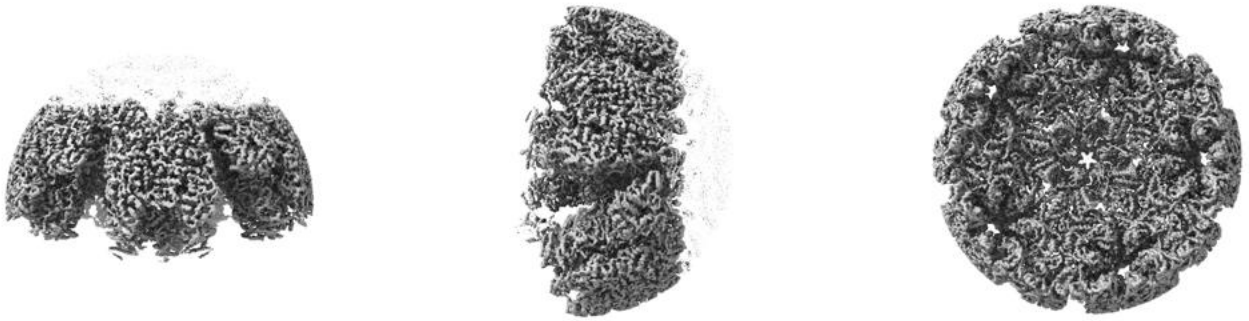
6.4.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 Raw map



X Y Z

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

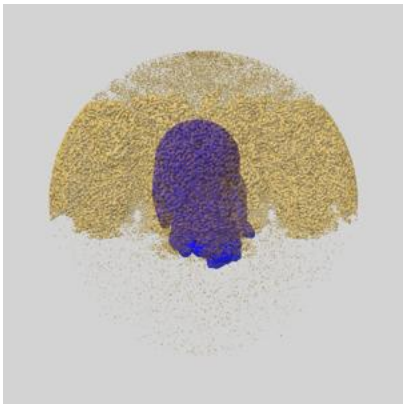
6.5 Mask visualisation (i)

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

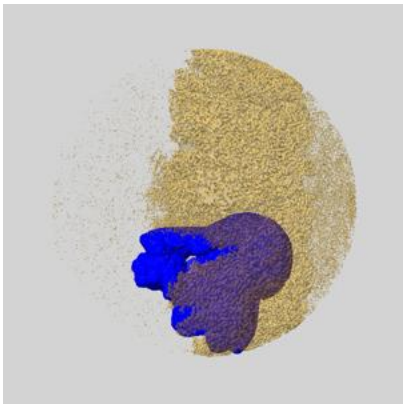
A mask typically either:

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

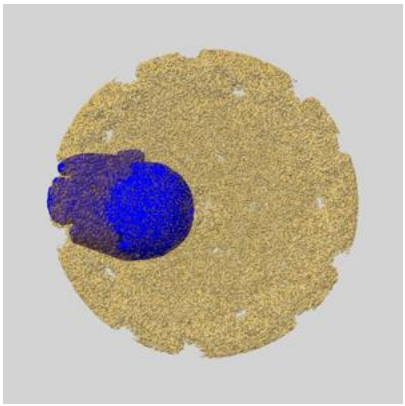
6.5.1 emd_20436_msk_1.map (i)



X



Y

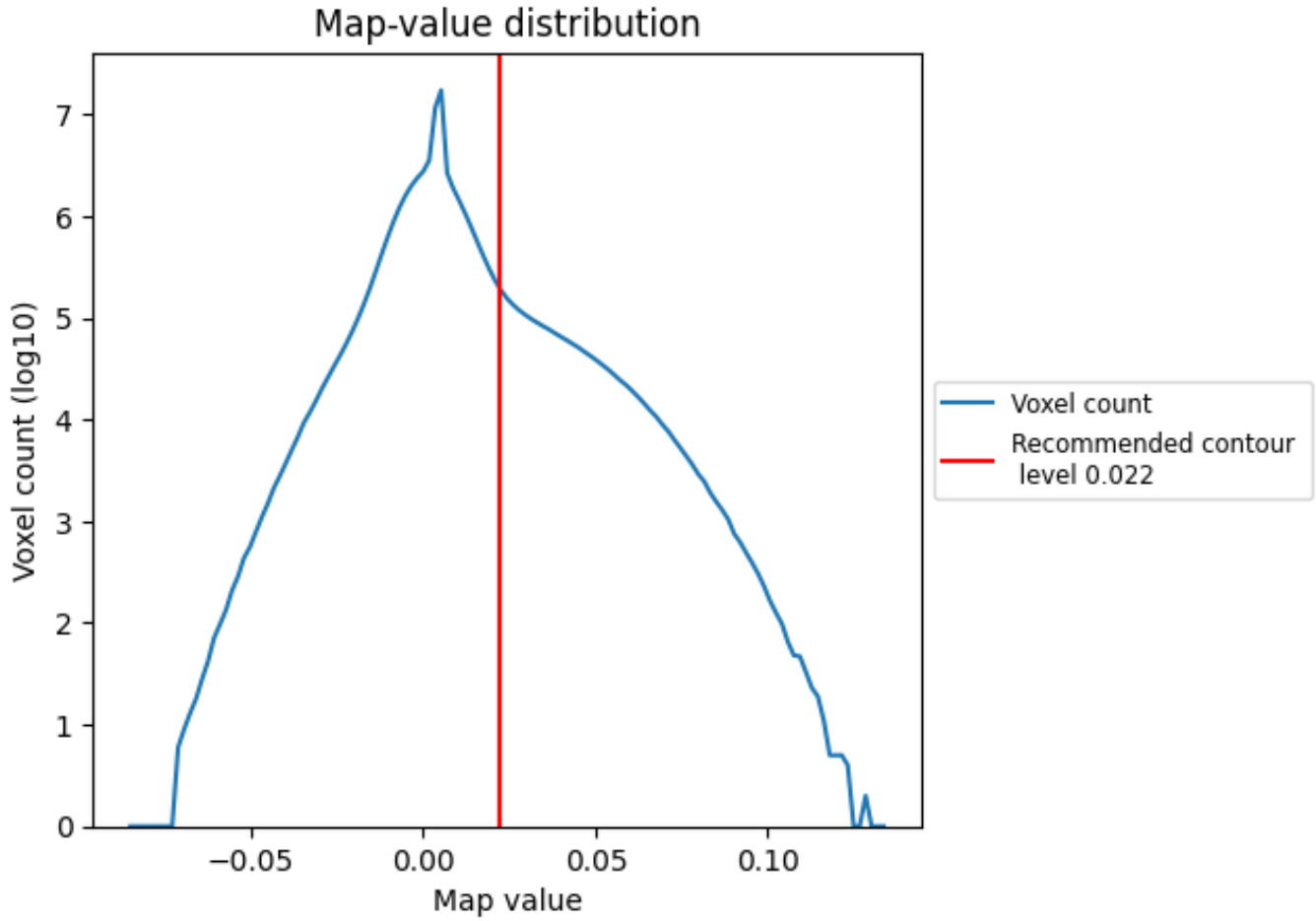


Z

7 Map analysis

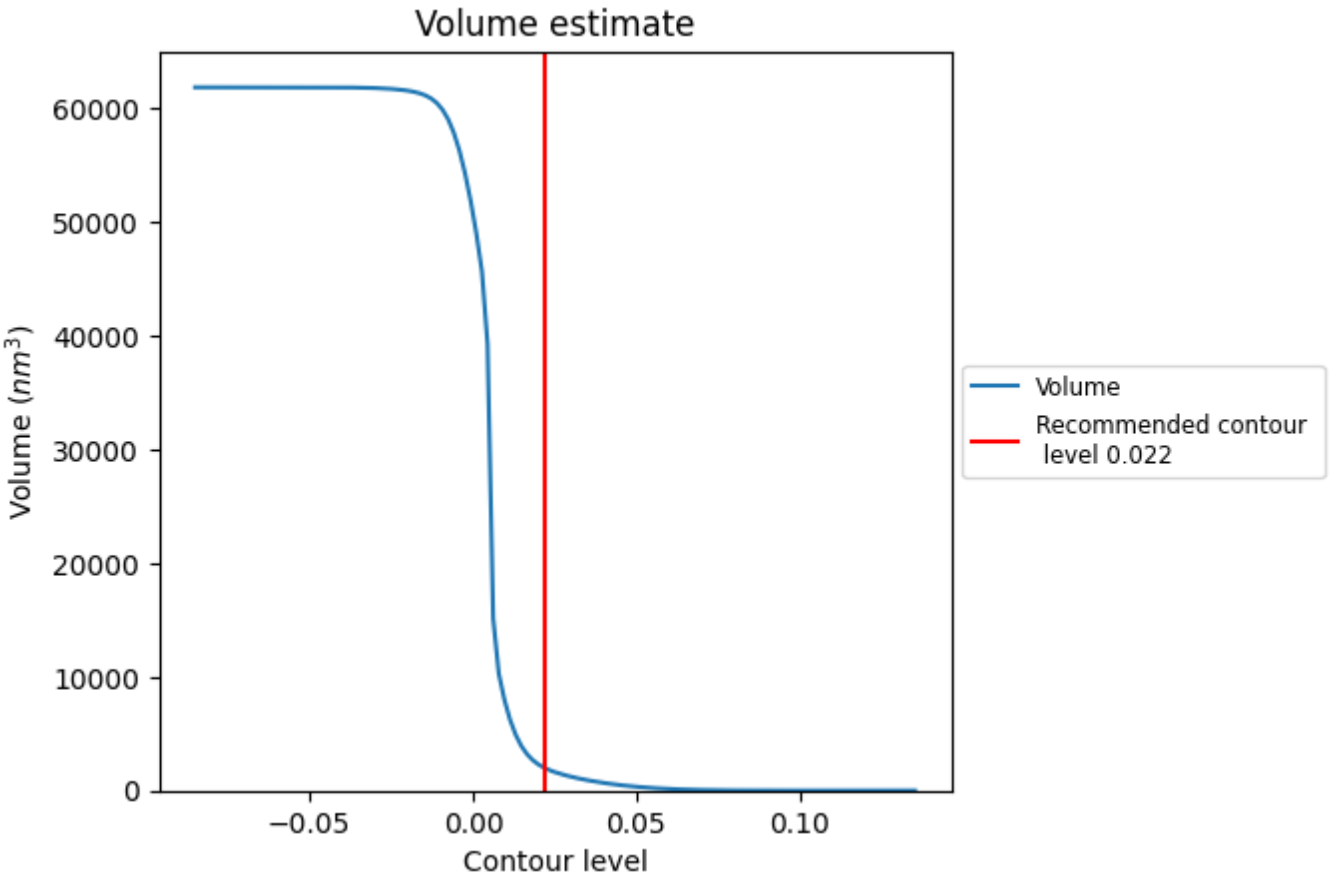
This section contains the results of statistical analysis of the map.

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.

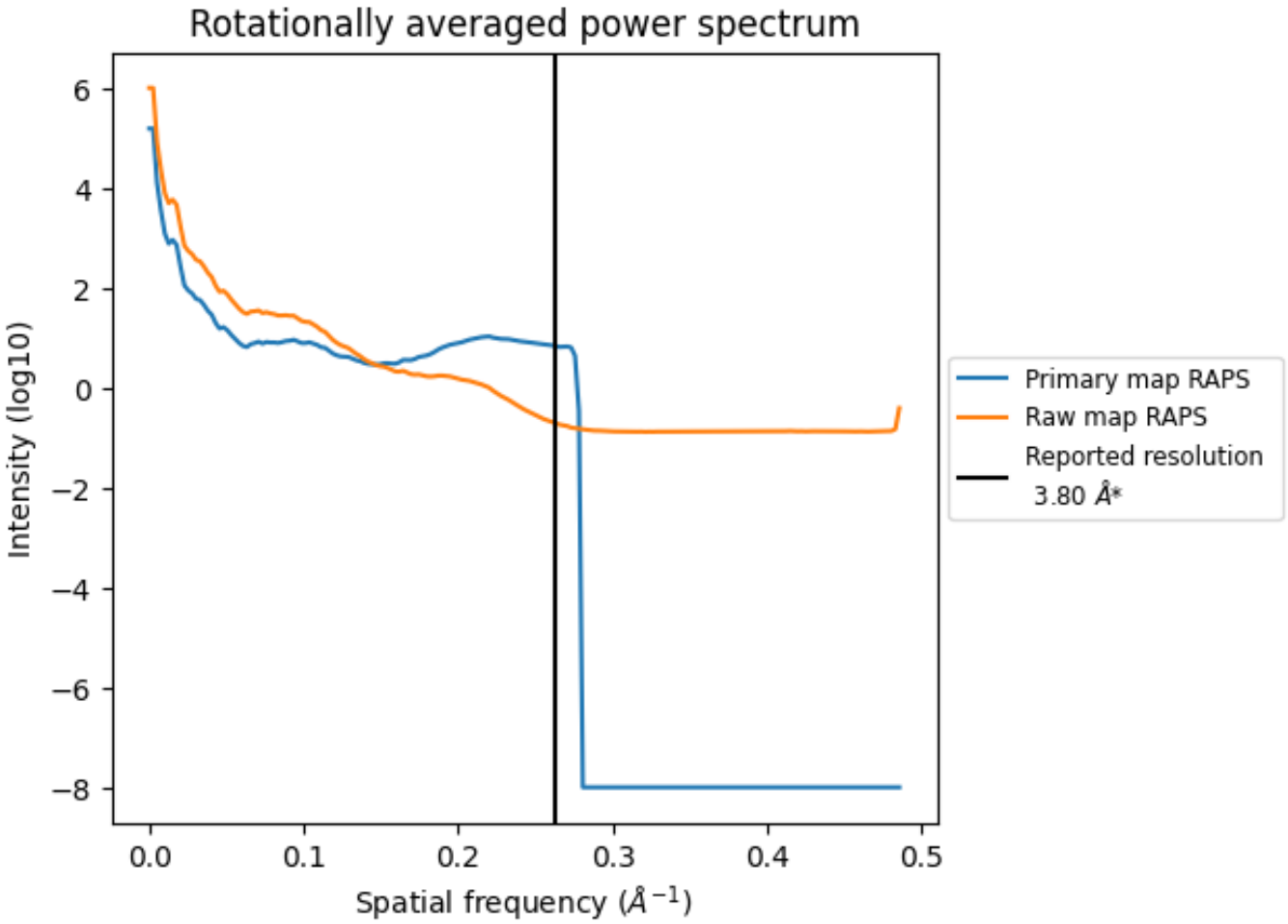
7.2 Volume estimate



The volume at the recommended contour level is 1988 nm^3; this corresponds to an approximate mass of 1796 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)

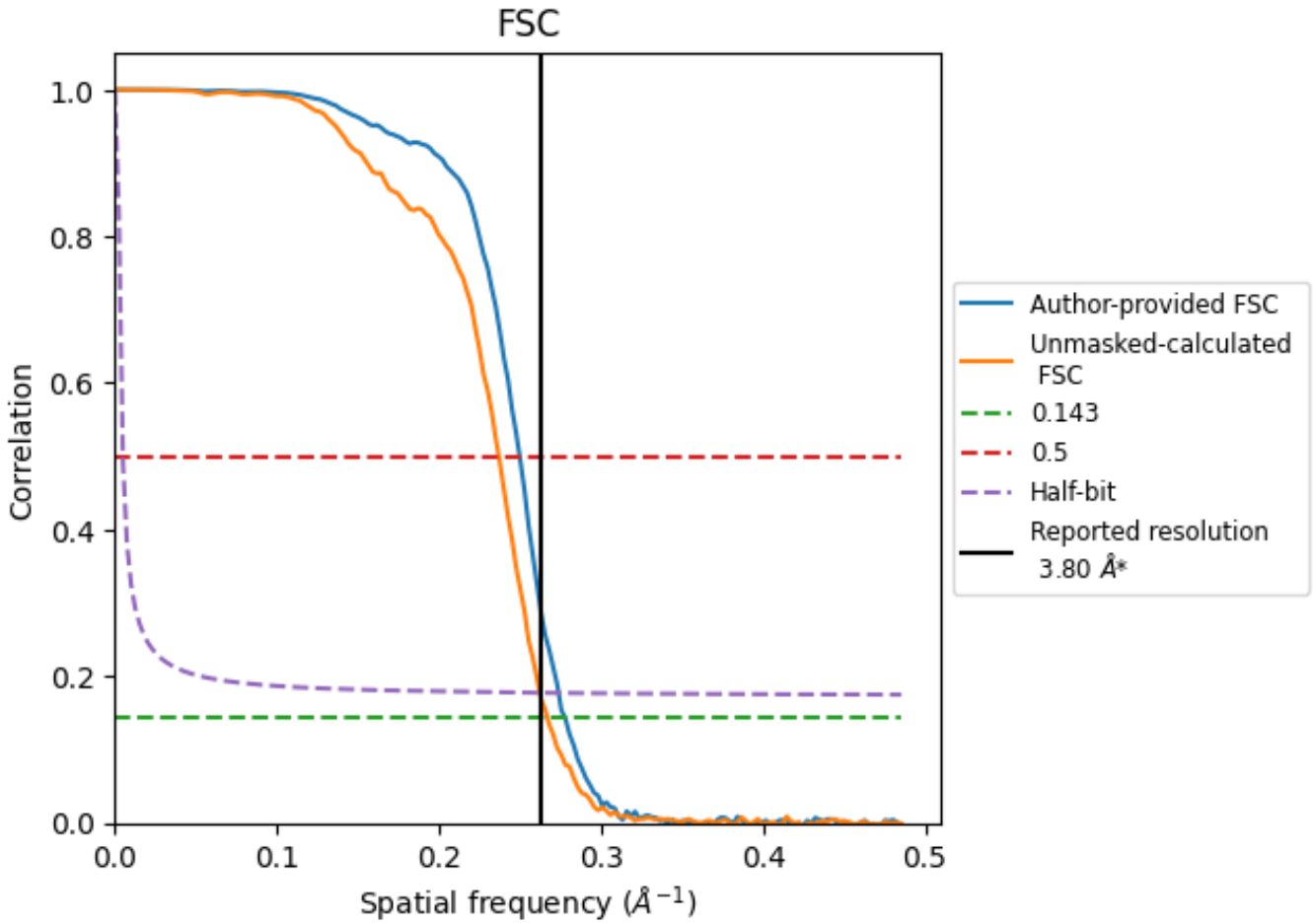


*Reported resolution corresponds to spatial frequency of 0.263 Å^{-1}

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)

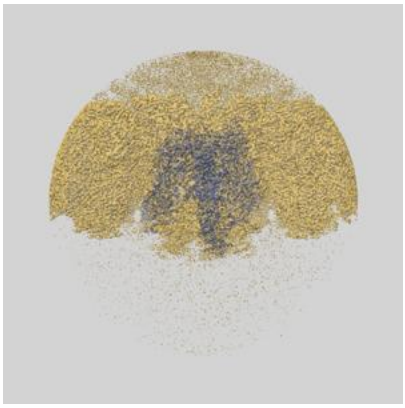
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.60	4.00	3.65
Unmasked-calculated*	3.75	4.22	3.81

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

9 Map-model fit

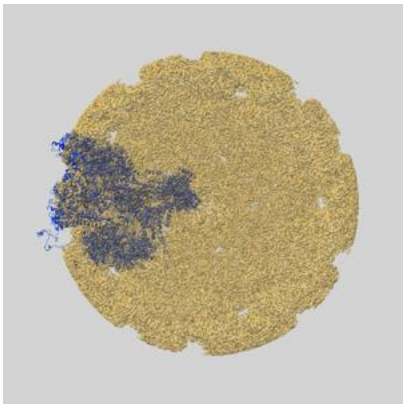
This section contains information regarding the fit between EMDB map EMD-20436 and PDB model 6PPH. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay



X

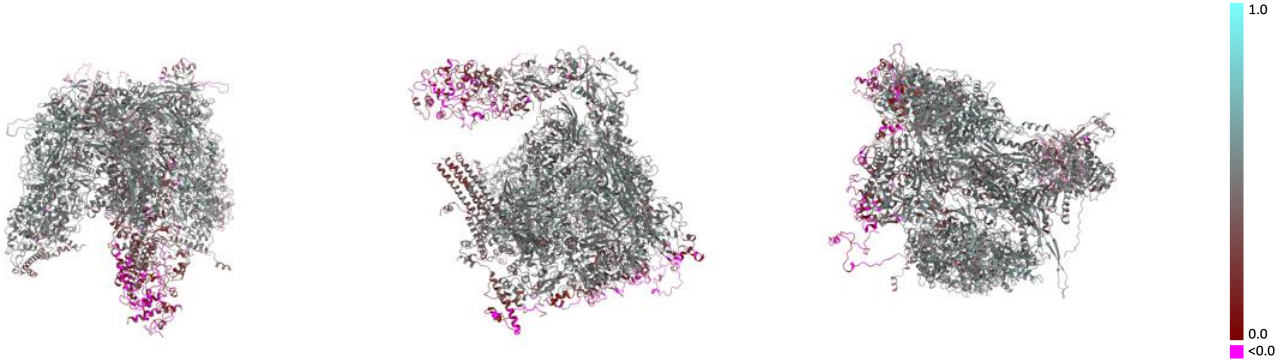
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

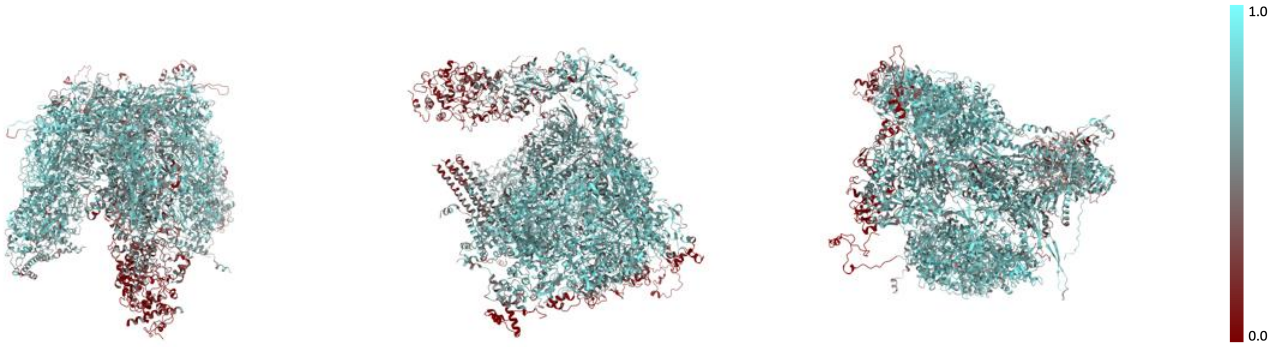
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

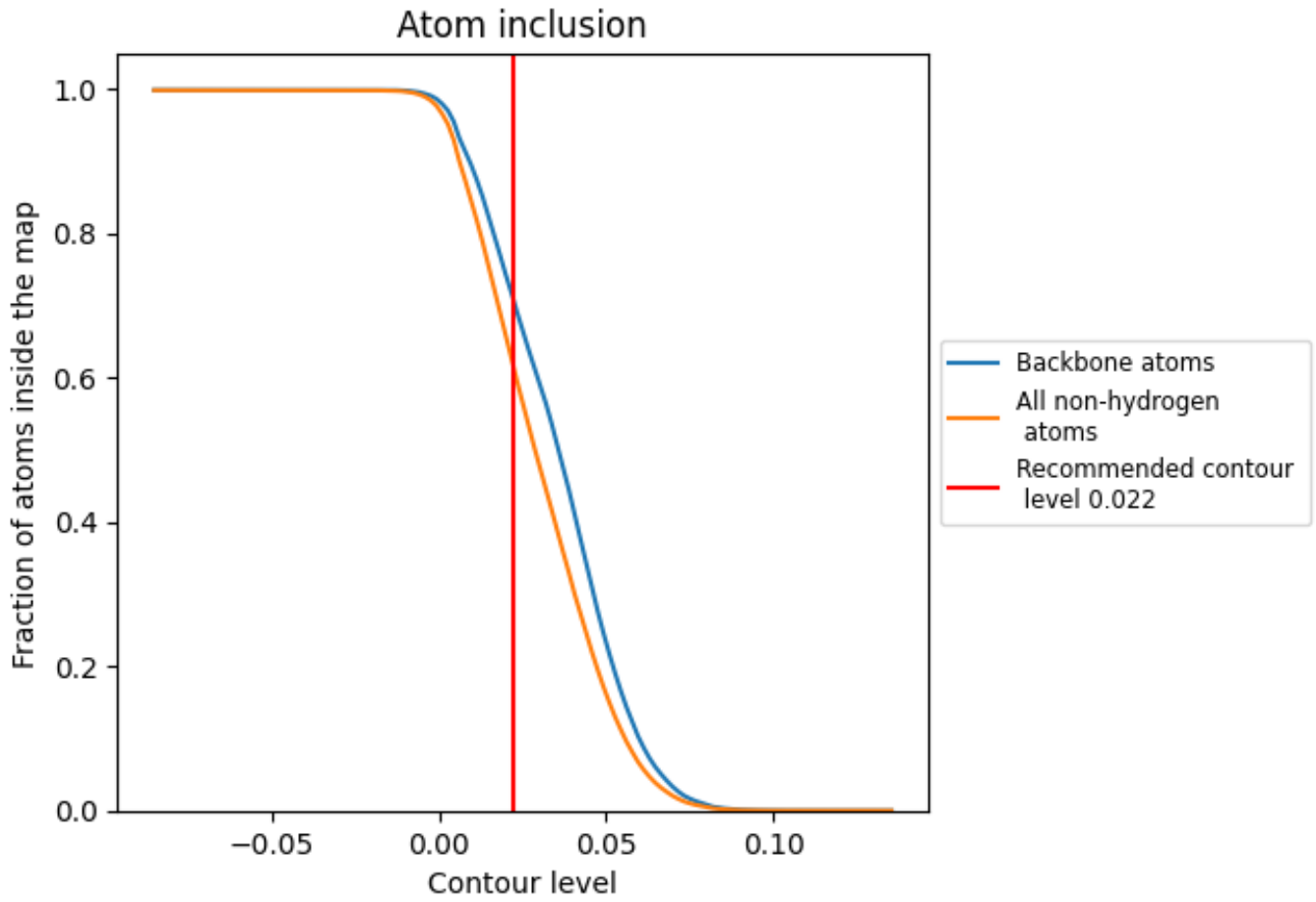
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.022).

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6223	0.4280
0	0.2196	0.1440
1	0.5763	0.3820
2	0.5140	0.3540
3	0.5062	0.3590
4	0.4214	0.2970
5	0.6057	0.4710
6	0.5430	0.4440
7	0.6389	0.4720
A	0.1553	0.1670
S	0.7179	0.4930
T	0.6938	0.4510
W	0.6551	0.4320
X	0.7425	0.5020
b	0.6442	0.4370
c	0.5409	0.3610
d	0.5179	0.3400
k	0.6557	0.4910
l	0.5271	0.4210
m	0.4881	0.4040
n	0.4222	0.3150
o	0.3460	0.3170