wwPDB EM Validation Summary Report

Jan 7, 2023 – 09:30 AM EST

PDB ID	:	8F5P
EMDB ID	:	EMD-28867
Title	:	Structure of Leishmania tarentolae IFT-A (state 2)
Authors	:	Zhou, H.; Brown, A.
Deposited on	:	2022-11-14
Resolution	:	3.40 Å(reported)

This is a wwPDB EM Validation Summary 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:

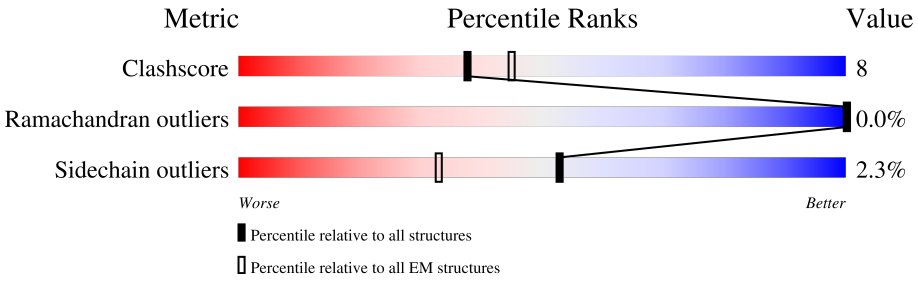
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 3.40 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	A	368	6% 14% 6% 80%
2	B	1247	6% 69% 21% 10%
3	C	1292	12% 70% 20% 9%
4	D	1642	28% 9% 63%
5	E	1654	17% 51% 13% 36%
6	F	1376	46% 59% 11% 30%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 39437 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 NET domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	75	585	361	97	120	7	0	0

- Molecule 2 is a protein called Intraflagellar transport protein 122B, putative.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1128	8917	5645	1557	1652	63	0	0

- Molecule 3 is a protein called Intraflagellar transport protein 122 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	1176	9337	5918	1619	1732	68	0	0

- Molecule 4 is a protein called TPR_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	612	4826	3026	862	912	26	0	0

- Molecule 5 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	1057	8269	5228	1430	1561	50	0	0

- Molecule 6 is a protein called WD_REPEATS_REGION domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	970	7499	4713	1315	1436	35	0	0

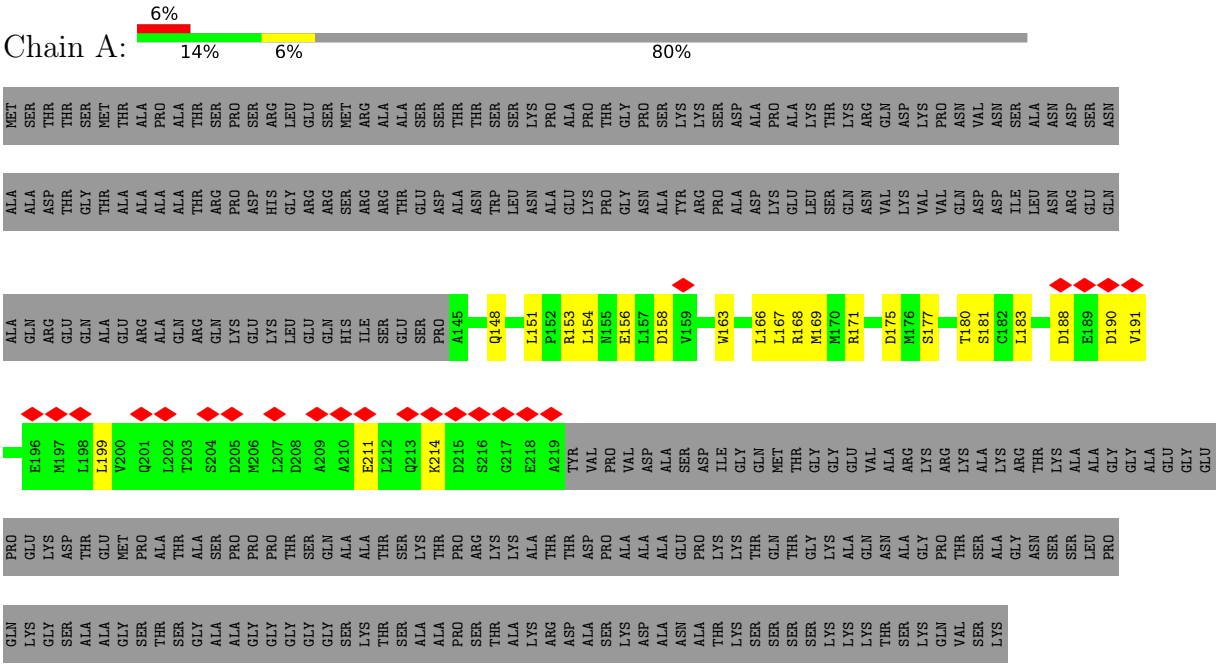
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
7	B	2	Total Zn 2 2	0
7	C	2	Total Zn 2 2	0

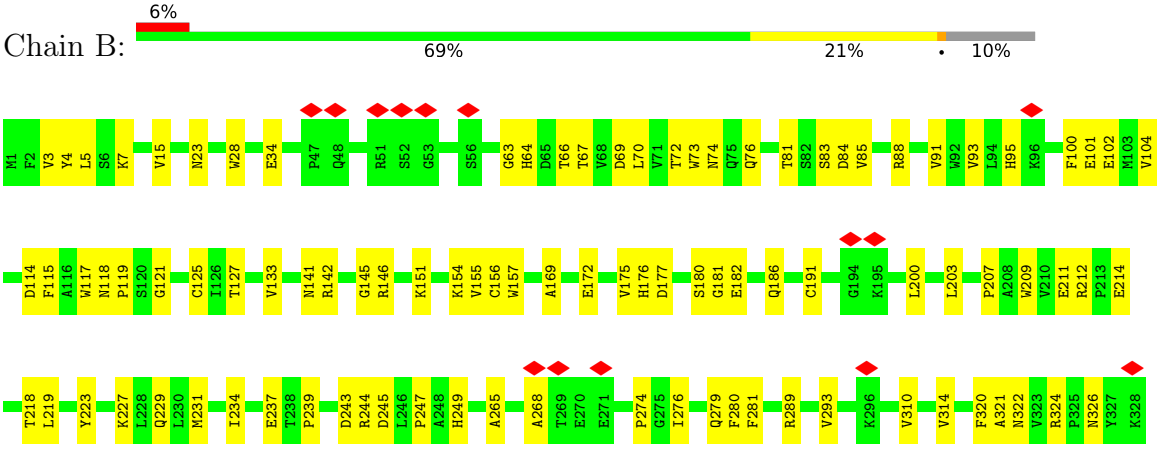
3 Residue-property plots (i)

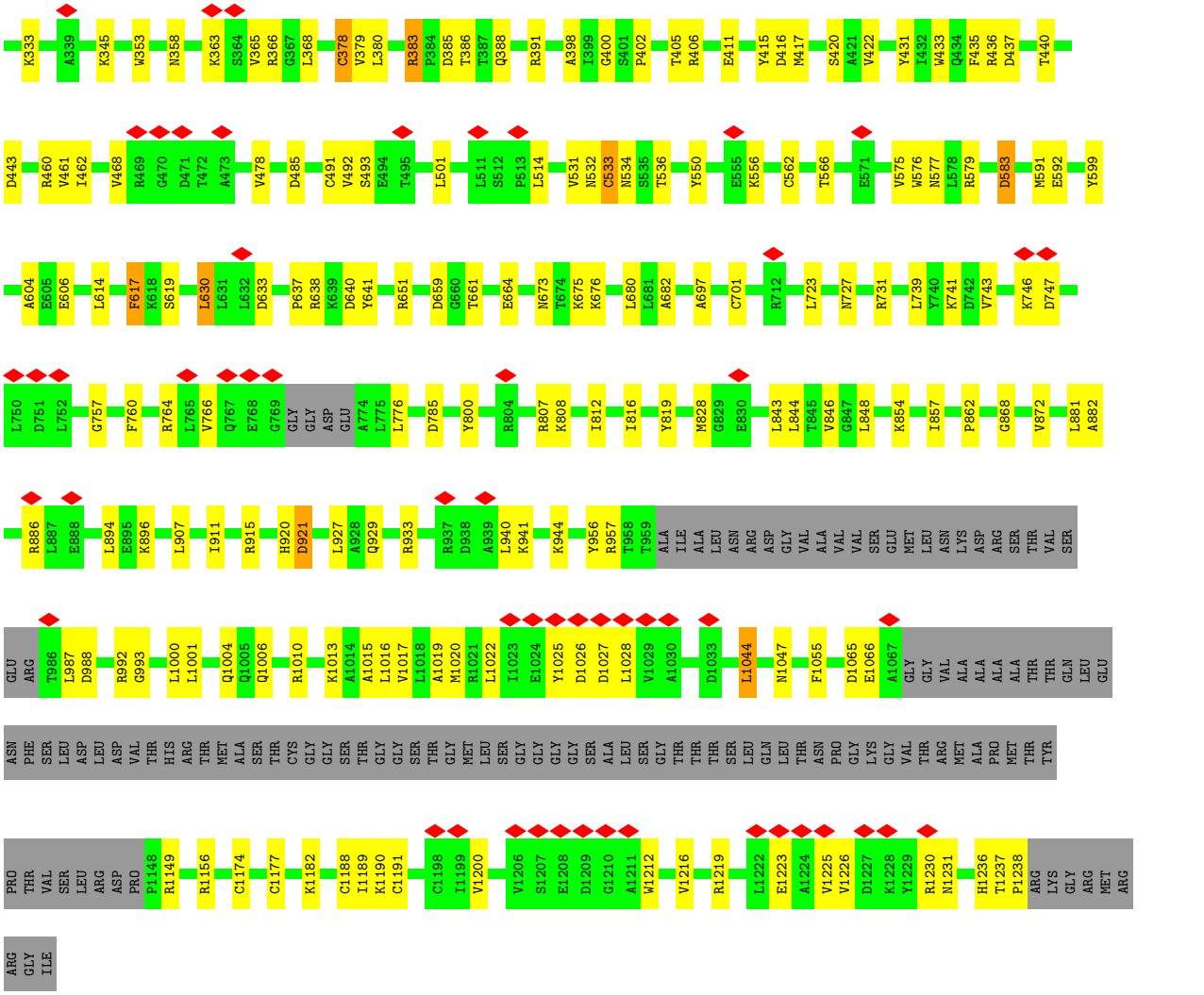
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: NET domain-containing protein



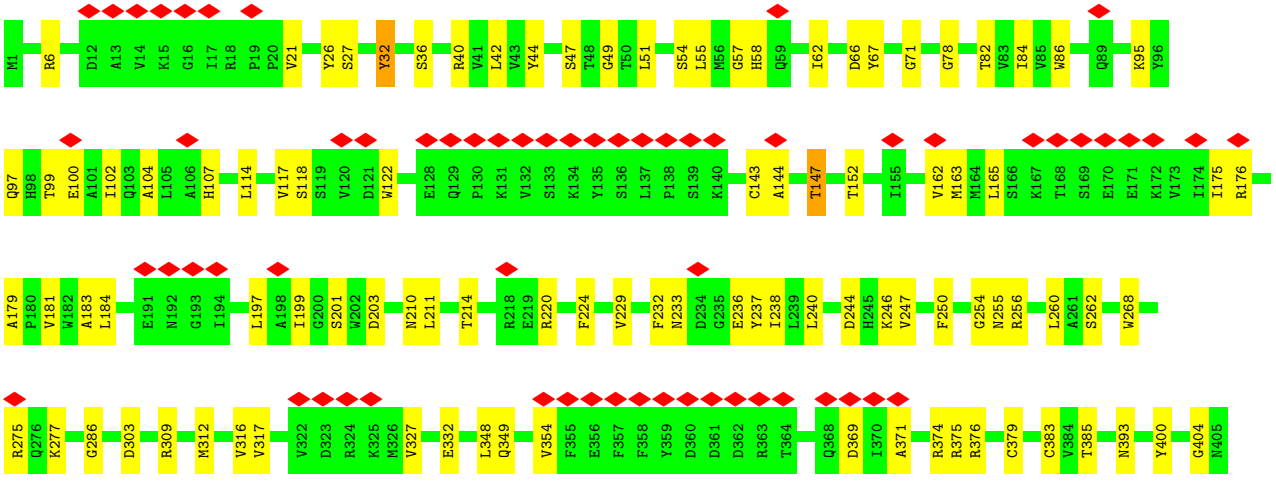
• Molecule 2: Intraflagellar transport protein 122B, putative

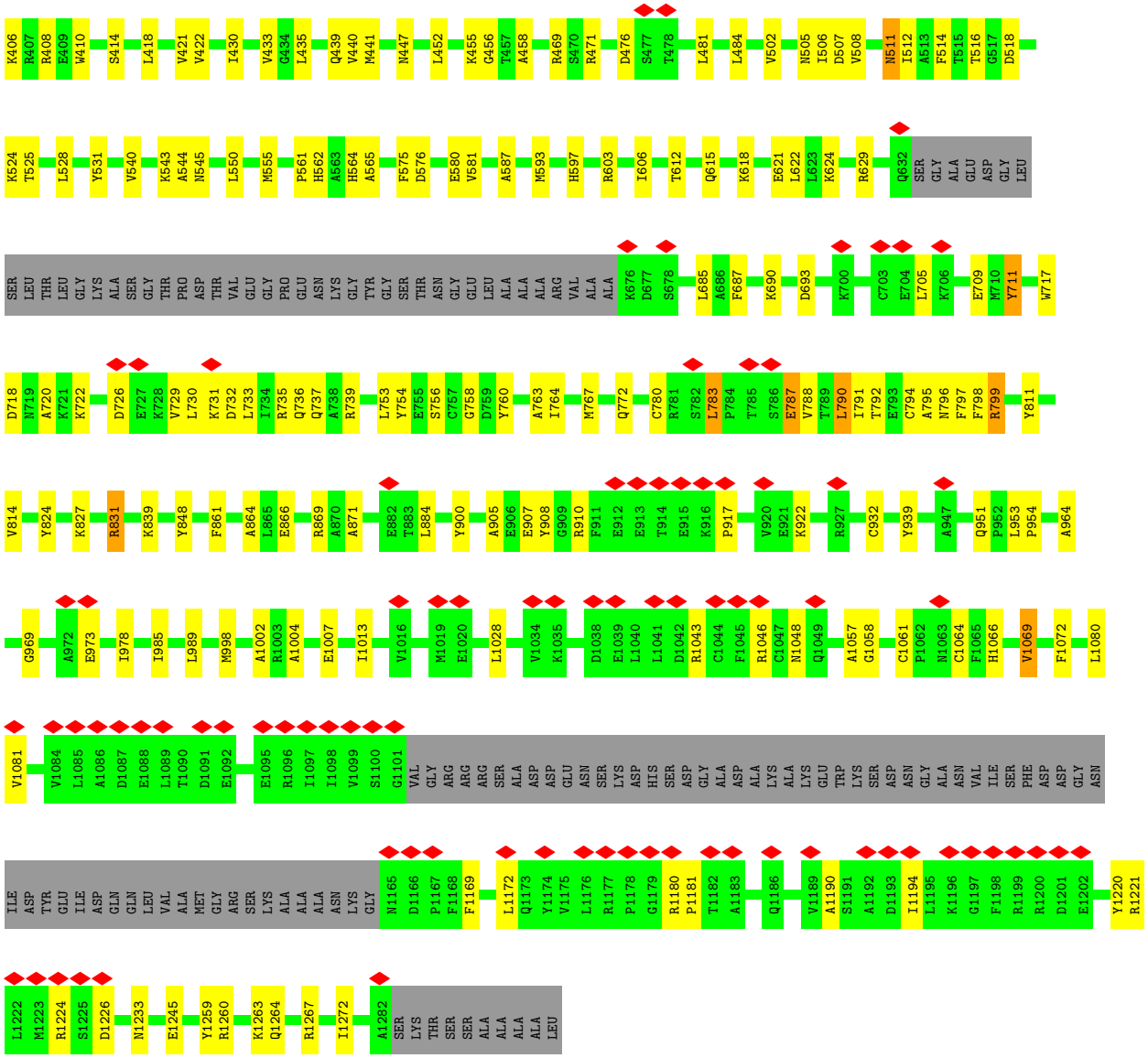




• Molecule 3: Intraflagellar transport protein 122 homolog

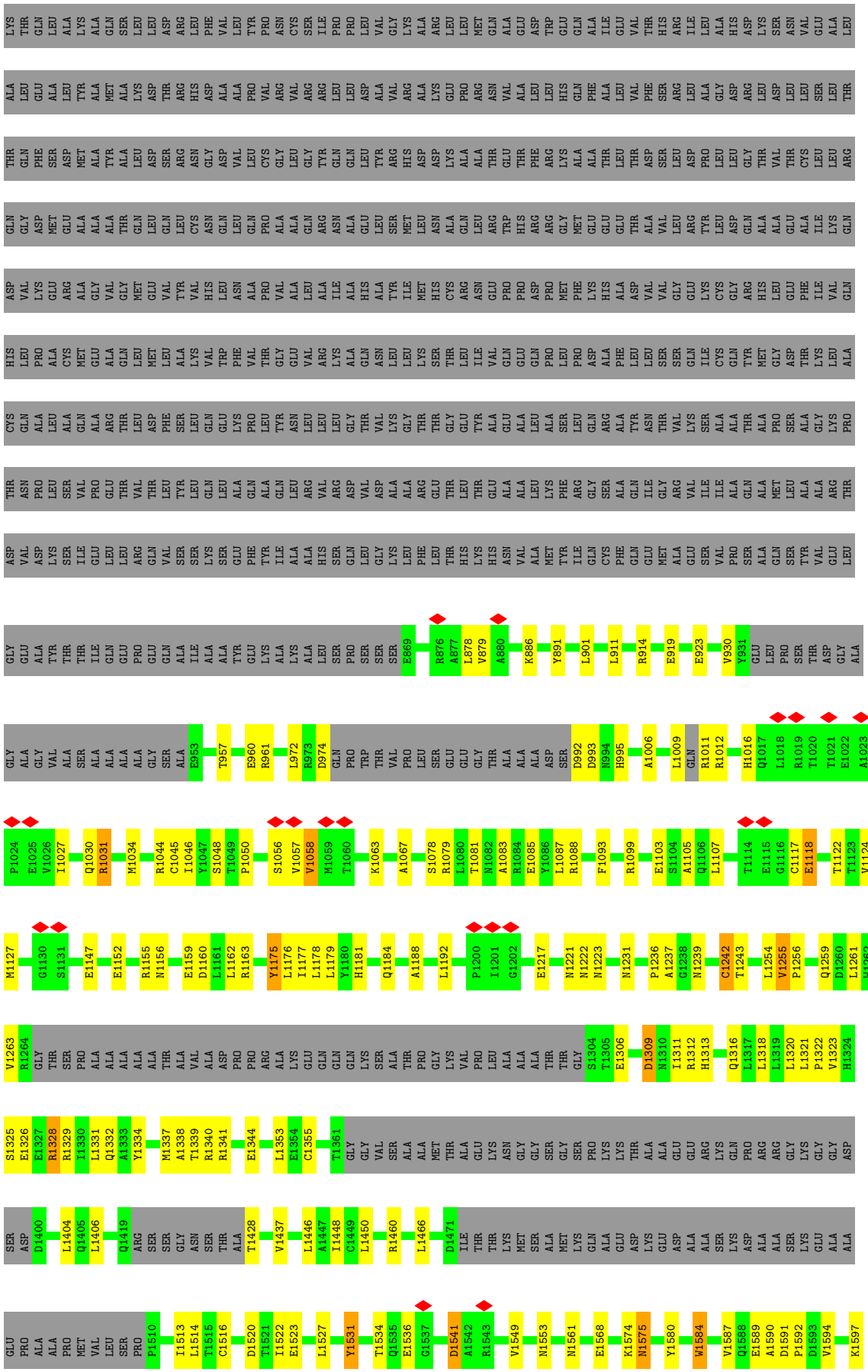
Chain C:

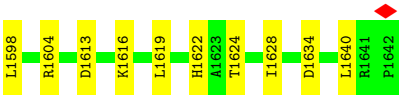




• Molecule 4: TPR_REGION domain-containing protein

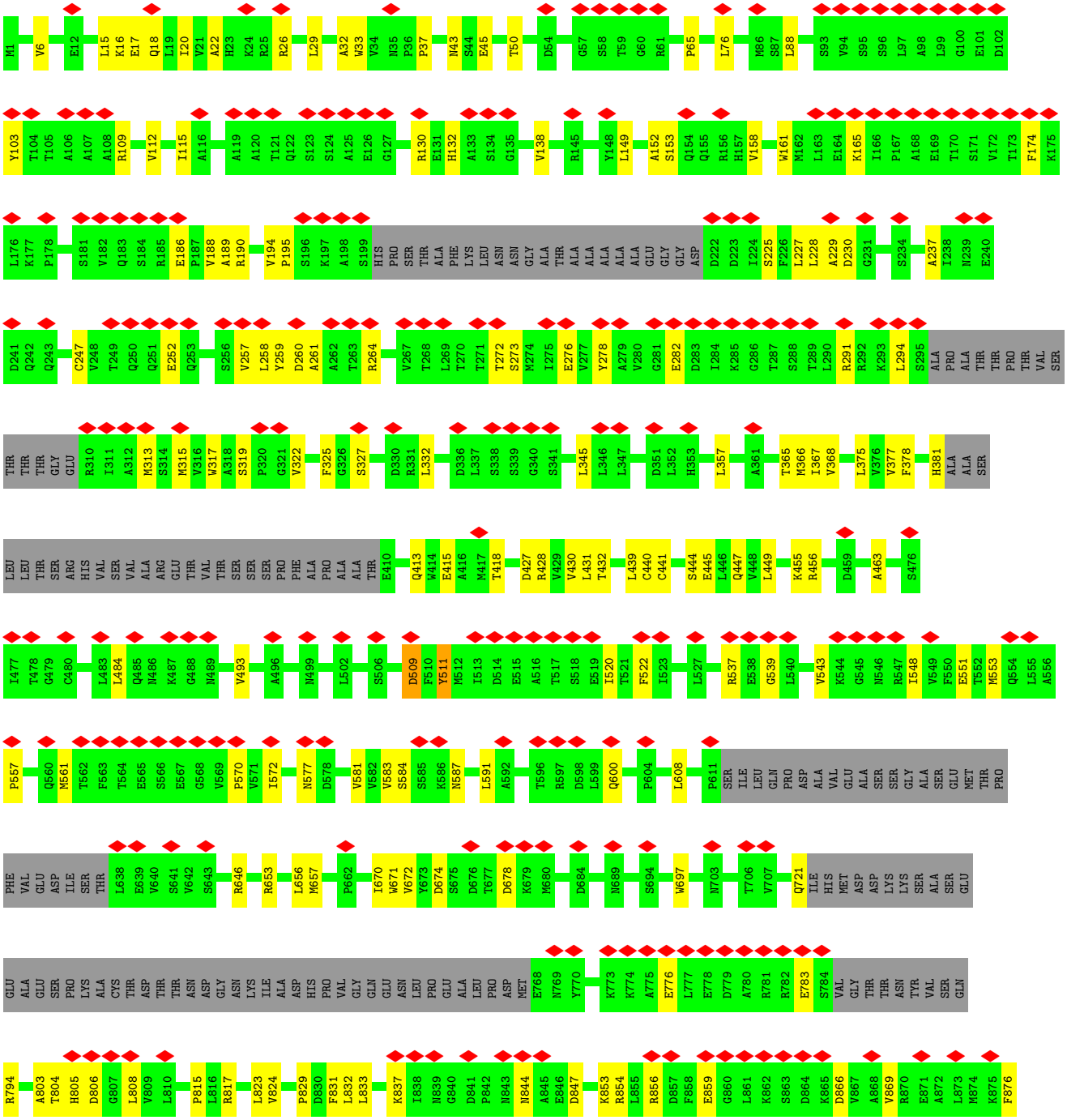
Chain D:

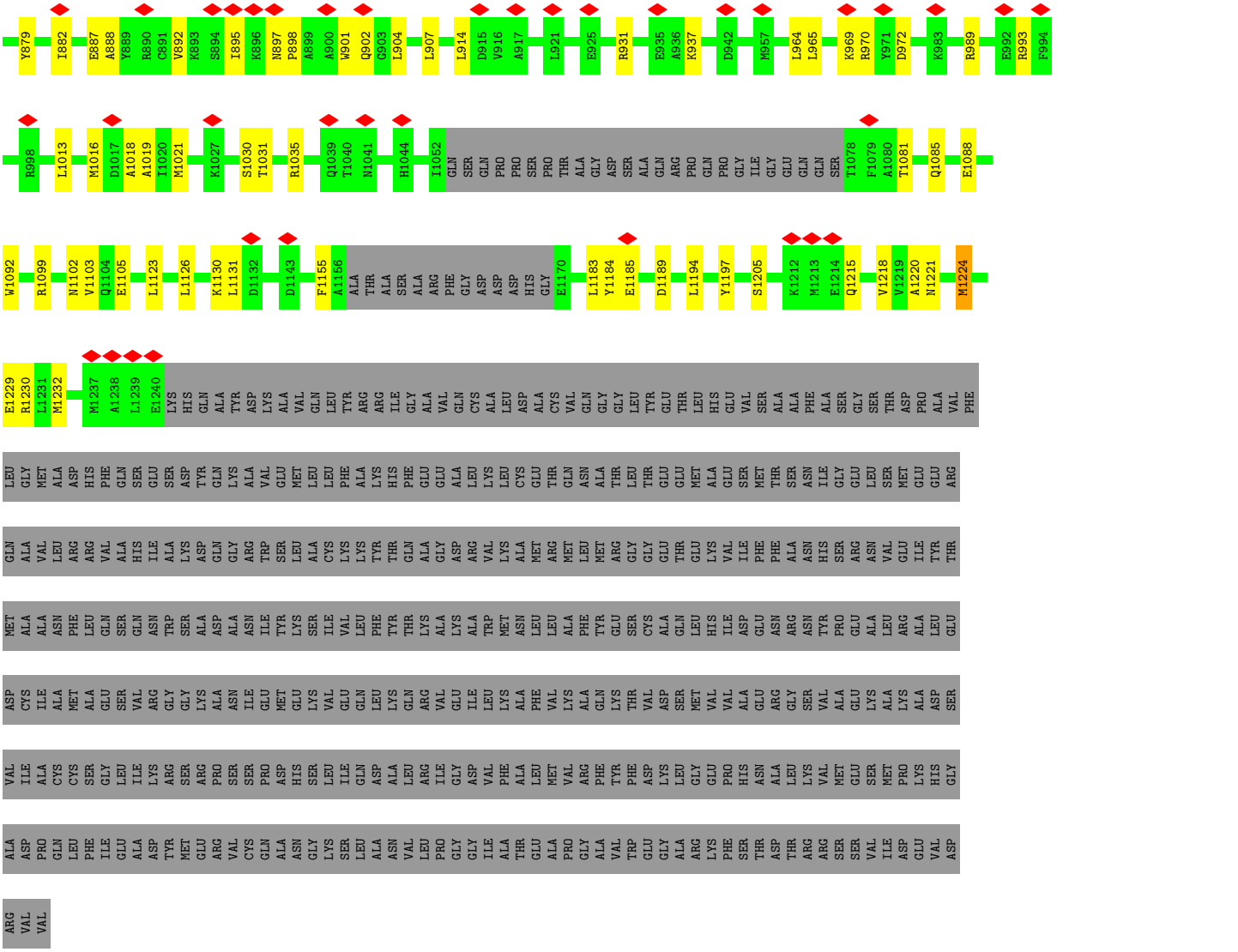




• Molecule 5: WD_REPEATS_REGION domain-containing protein

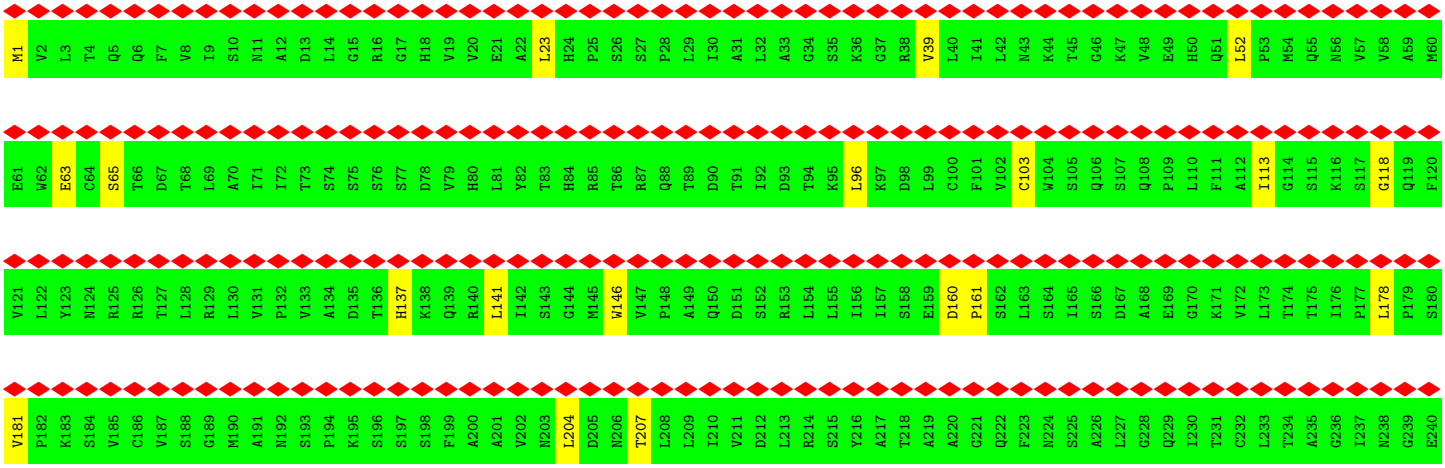
Chain E:

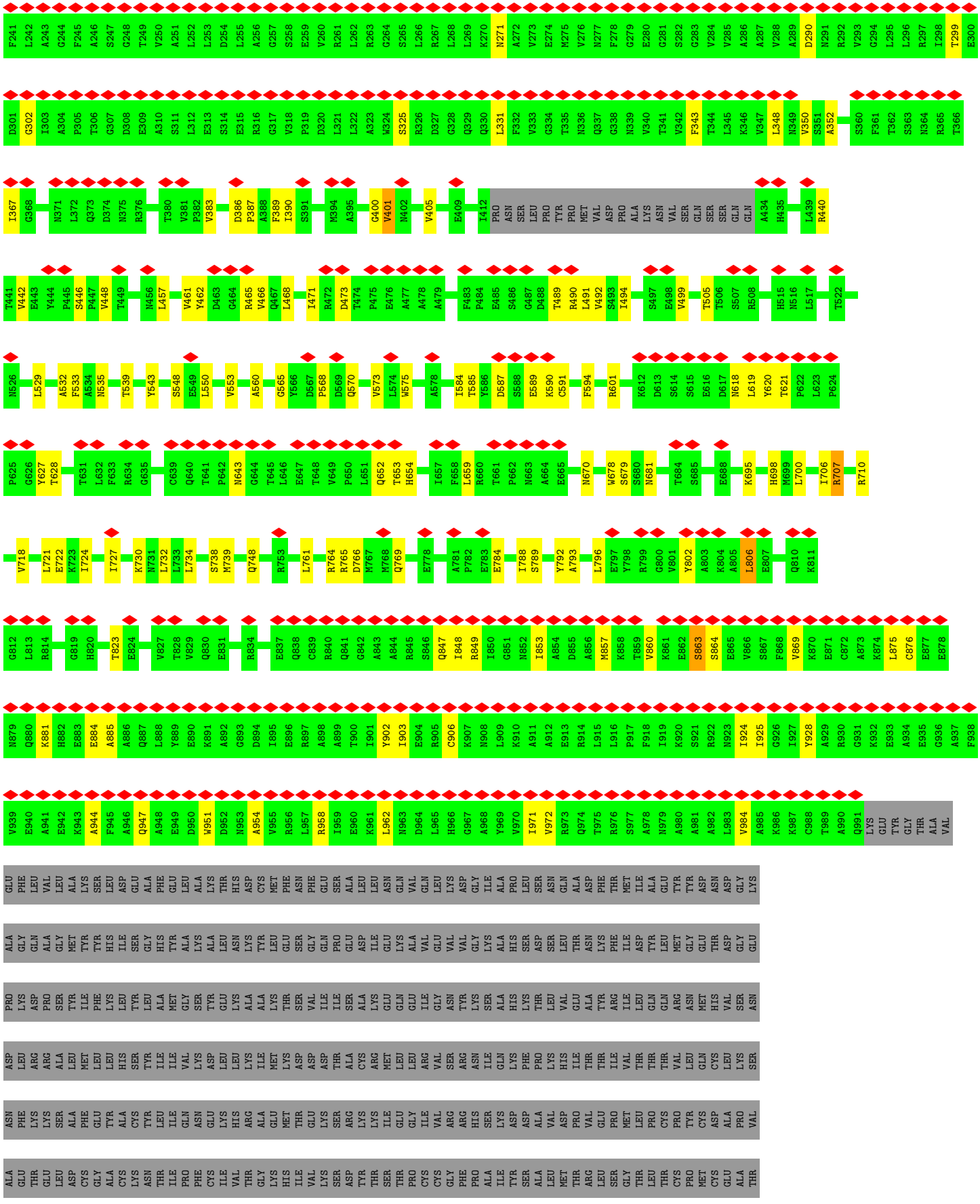




• Molecule 6: WD_REPEATS_REGION domain-containing protein

Chain F:




F241 L242 A243 G244 F245 A246 S247 G248 T249 V250 A251 L252 L253 D254 L255 A256 G257 S258 E259 V260 R261 L262 R263 G264 S265 L266 R267 L268 L269 K270 N271 A272 V273 E274 M275 V276 N277 F278 G279 E280 G281 S282 G283 V284 V285 A286 A287 V288 A289 D290 N291 R292 V293 G294 L295 L296 R297 I298 T299 E300
D301 G302 I303 A304 P305 T306 G307 D308 E309 A310 S311 L312 E313 S314 E315 R316 G317 V318 P319 D320 L321 L322 A323 W324 S325 R326 D327 G328 Q329 Q330 L331 F332 V333 G334 T335 N336 Q337 G338 N339 V340 T341 V342 F343 T344 L345 K346 V347 L348 N349 V350 S351 A352 S360 F361 T362 S363 N364 R365 T366
I367 G368 N371 L372 Q373 D374 N375 R376 T380 V381 P382 V383 D386 P387 A388 F389 I390 S391 M394 A395 G400 V401 N402 V405 E409 I412 PRO ASN SER LEU PRO TYR PRO MET VAL ASP PRO ALA LYS ASN VAL SER GLN SER GLN GLN A434 H435 L439 R440
T441 V442 E443 Y444 P445 S446 P447 V448 T449 N456 L457 V461 Y462 D463 G464 R465 V466 Q467 L468 I471 R472 D473 T474 P475 E476 A477 A478 A479 F483 P484 E485 S486 G487 D488 T489 R490 L491 V492 S493 I494 S497 E498 V499 T505 T506 S507 R508 H515 N516 L517 T522
N526 L529 A532 F533 A534 N535 T539 Y543 S548 E549 L550 V553 A560 G565 Y566 D567 P568 D569 Q570 V573 L574 W575 A578 I584 T585 Y586 D587 S588 E589 K590 C591 F594 R601 K612 D613 S614 S615 E616 D617 N618 L619 Y620 T621 P622 L623 P624
P625 G626 Y627 T628 T631 L632 F633 R634 G635 C639 Q640 T641 P642 N643 G644 T645 L646 E647 T648 V649 P650 L651 Q652 T653 H654 I657 F658 L659 R660 T661 P662 N663 A664 E665 N670 W678 S679 S680 N681 T684 S685 E688 K695 H698 M699 L700 I706 R707 R710
V718 L721 E722 K723 I724 I727 K730 N731 L732 L733 L734 S738 M739 Q748 R753 L761 R764 R765 D766 M767 M768 Q769 E778 A781 P782 E783 E784 I788 S789 Y792 A793 L796 E797 Y798 R799 G800 V801 Y802 A803 K804 A805 L806 E807 Q810 K811
G812 L813 R814 G819 H820 T823 E824 V827 T828 V829 Q830 E831 R834 E837 Q838 C839 R840 Q841 G842 A843 A844 R845 S846 Q847 I848 R849 I850 G851 N852 I853 A854 D855 A856 M857 K858 T859 V860 K861 E862 S863 S864 E865 V866 S867 F868 V869 K870 E871 C872 A873 K874 L875 C876 E877 E878
N879 Q880 K881 H882 E883 E884 A885 A886 Q887 L888 Y889 E890 K891 A892 G893 D894 I895 E896 R897 A898 A899 T900 I901 Y902 I903 E904 R905 C906 K907 N908 L909 K910 A911 A912 E913 R914 L915 L916 P917 F918 I919 K920 S921 R922 N923 I924 I925 G926 I927 Y928 A929 R930 G931 K932 E933 A934 E935 G936 A937 F938
V939 E940 A941 E942 K943 A944 F945 A946 Q947 A948 E949 D950 W951 D952 N953 A954 V955 R956 L957 R958 I959 E960 K961 L962 N963 D964 L965 H966 G967 A968 Y969 V970 I971 V972 R973 Q974 T975 R976 S977 A978 N979 A980 A981 A982 L983 V984 A985 K986 K987 C988 T989 A990 Q991 LYS GLU TYR GLY THR ALA VAL
GLU PHE LEU VAL LEU ALA LYS SER LEU ASP GLU ALA PHE GLU LEU ALA LYS THR HIS ASP CYS MET PHE ASN PHE GLU SER ALA LEU LEU ASN GLN VAL GLN LEU LYS ASP GLY ILE ALA PRO LEU SER ASN GLN ALA ASP PHE THR MET MET ILE ALA GLU TYR LEU MET GLY GLU GLY THR ASP ASN ASP GLY LYS
ALA GLY GLN ALA GLY MET TYR TYR HIS ILE SER GLY HIS TYR ALA LYS ALA LEU ASN LYS TYR LEU GLU SER GLY GLN PRO GLU ASP ILE GLU LYS ALA VAL GLU VAL VAL GLY LYS ALA HIS SER ASP SER LEU THR ASN LYS PHE ILE ASP TYR LEU MET GLY GLU GLY THR ASP GLU GLU
PRO LYS ASP PRO SER TYR ILE PHE LYS LEU TYR LEU ALA MET GLY SER TYR GLU LYS ALA ALA LYS THR SER VAL ILE ILE SER ALA LYS GLU GLN GLU ILE GLY ASN TYR LYS SER ALA HIS LYS THR LEU VAL GLU ALA TYR ARG ILE LEU LEU GLN GLN GLN ARG ASN MET HIS VAL SER ASN
ASP LEU ARG ARG ALA LEU MET LEU LEU HIS SER TYR ILE ILE VAL LYS ASP LEU LEU LYS ILE MET LYS ASP ASP THR ALA CYS ARG MET LEU LEU ARG VAL SER ARG ASN ILE GLN LYS PHE PRO LYS HIS ILE THR THR ILE VAL THR THR THR VAL LEU GLN CYS LEU LYS SER
ASN PHE LYS LYS SER ALA PHE GLU TYR ALA CYS TYR LEU ILE GLN ASN GLU LYS HIS ARG ALA GLU MET THR GLU LYS SER ARG LYS LYS ILE GLU VAL ARG ARG HIS SER LYS ASP ASP ALA VAL ASP PRO VAL GLU PRO MET LEU PRO CYS PRO TYR CYS ASP ALA PRO VAL
ALA GLU THR GLU LEU ASP CYS GLY ALA CYS LYS ASN THR ILE VAL LYS SER ASP TYR THR SER THR PRO CYS CYS GLY PHE PRO ALA ILE TYR SER ALA LEU MET THR ARG LEU SER GLY THR LEU THR CYS PRO MET CYS GLU ALA LEU PRO VAL

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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	563466	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 ($e^-/Å^2$)	57.8	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	74.154	Depositor
Minimum map value	-32.225	Depositor
Average map value	0.007	Depositor
Map value standard deviation	0.778	Depositor
Recommended contour level	7.0	Depositor
Map size (Å)	514.6, 514.6, 514.6	wwPDB
Map dimensions	620, 620, 620	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83, 0.83, 0.83	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN

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	0.25	0/592	0.47	0/800
2	B	0.28	0/9108	0.50	0/12341
3	C	0.26	0/9531	0.50	0/12900
4	D	0.26	0/4905	0.51	0/6650
5	E	0.25	0/8429	0.50	0/11438
6	F	0.24	0/7633	0.49	0/10368
All	All	0.26	0/40198	0.50	0/54497

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	585	0	565	22	0
2	B	8917	0	8815	162	0
3	C	9337	0	9275	168	0
4	D	4826	0	4799	105	0
5	E	8269	0	8212	125	0
6	F	7499	0	7503	91	0
7	B	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	2	0	0	0	0
All	All	39437	0	39169	636	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 8.

The worst 5 of 636 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:539:GLY:HA3	5:E:551:GLU:O	1.71	0.91
3:C:1061:CYS:HB3	3:C:1064:CYS:SG	2.19	0.82
3:C:62:ILE:HA	3:C:78:GLY:HA2	1.66	0.76
5:E:656:LEU:HB2	5:E:671:TRP:HB2	1.68	0.76
2:B:1174:CYS:HB3	2:B:1177:CYS:SG	2.26	0.75

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	73/368 (20%)	69 (94%)	4 (6%)	0	100	100
2	B	1120/1247 (90%)	1070 (96%)	50 (4%)	0	100	100
3	C	1170/1292 (91%)	1133 (97%)	37 (3%)	0	100	100
4	D	596/1642 (36%)	567 (95%)	27 (4%)	2 (0%)	41	72
5	E	1039/1654 (63%)	1001 (96%)	38 (4%)	0	100	100
6	F	966/1376 (70%)	946 (98%)	20 (2%)	0	100	100
All	All	4964/7579 (66%)	4786 (96%)	176 (4%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	1058	VAL
4	D	1057	VAL

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	64/288 (22%)	64 (100%)	0	100	100
2	B	956/1046 (91%)	927 (97%)	29 (3%)	41	68
3	C	1012/1094 (92%)	987 (98%)	25 (2%)	47	72
4	D	505/1320 (38%)	487 (96%)	18 (4%)	35	63
5	E	892/1373 (65%)	879 (98%)	13 (2%)	65	82
6	F	822/1177 (70%)	809 (98%)	13 (2%)	62	81
All	All	4251/6298 (68%)	4153 (98%)	98 (2%)	53	74

5 of 98 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	D	1031	ARG
4	D	1624	THR
4	D	1118	GLU
4	D	1404	LEU
5	E	325	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	417	GLN
4	D	1221	ASN
4	D	1223	ASN
4	D	1622	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

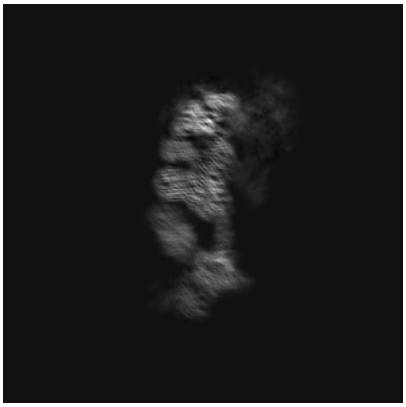
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-28867. These allow visual inspection of the internal detail of the map and identification of artifacts.

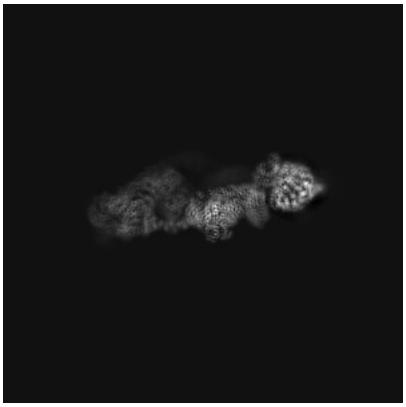
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

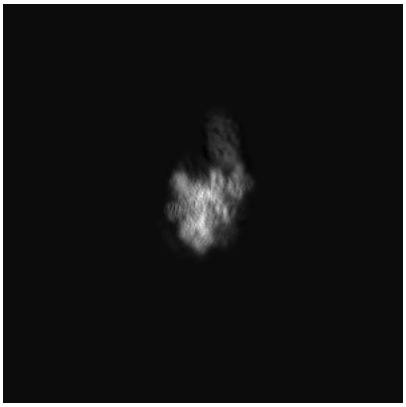
6.1.1 Primary map



X



Y



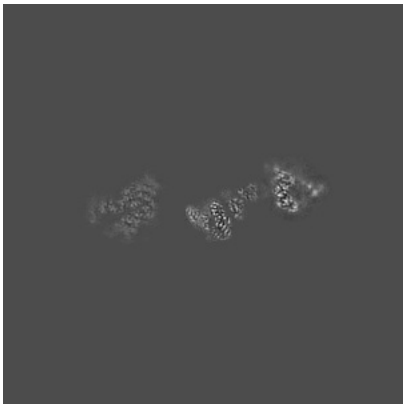
Z

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

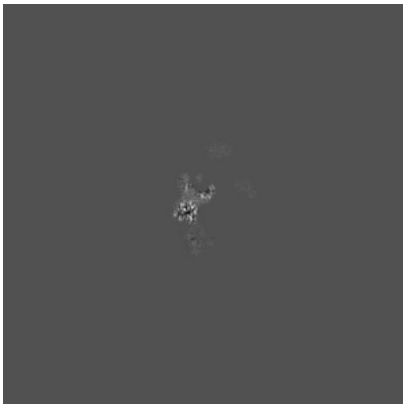
6.2 Central slices

6.2.1 Primary map

X Index: 310



Y Index: 310

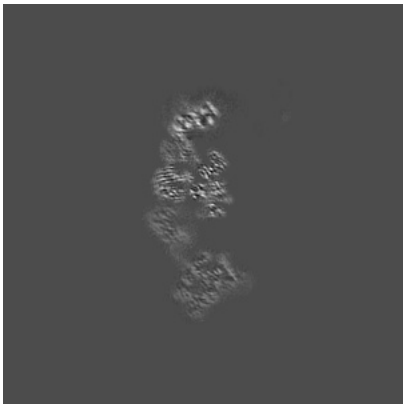


Z Index: 310

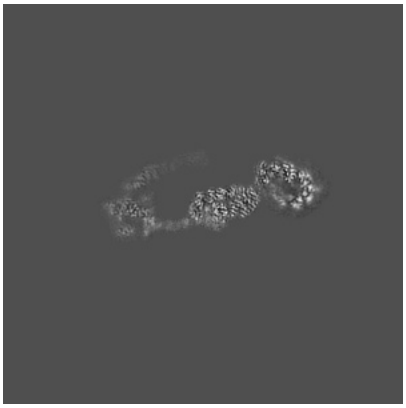
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 306



Y Index: 328

Z Index: 330

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

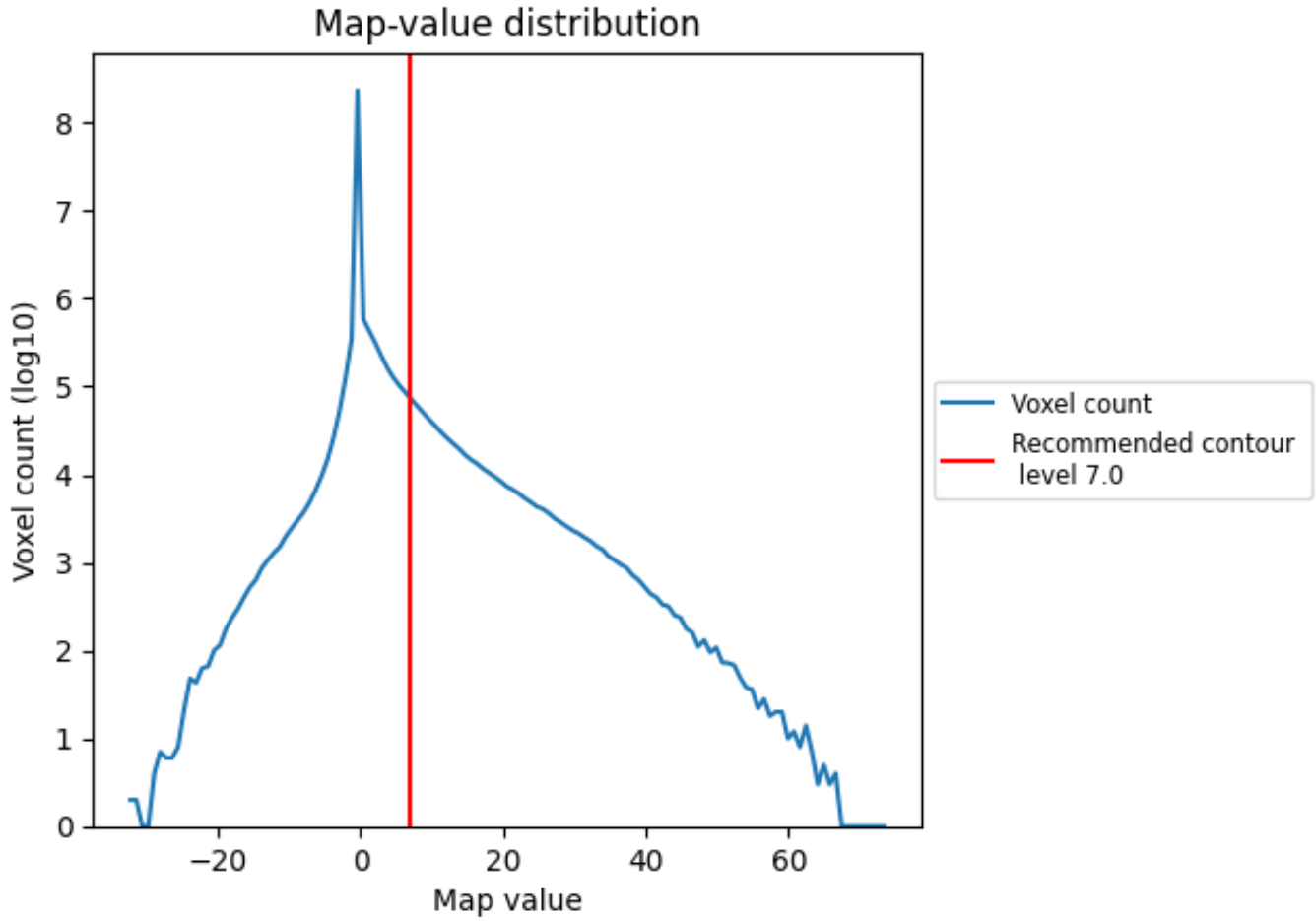
6.5 Mask visualisation (i)

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

7 Map analysis

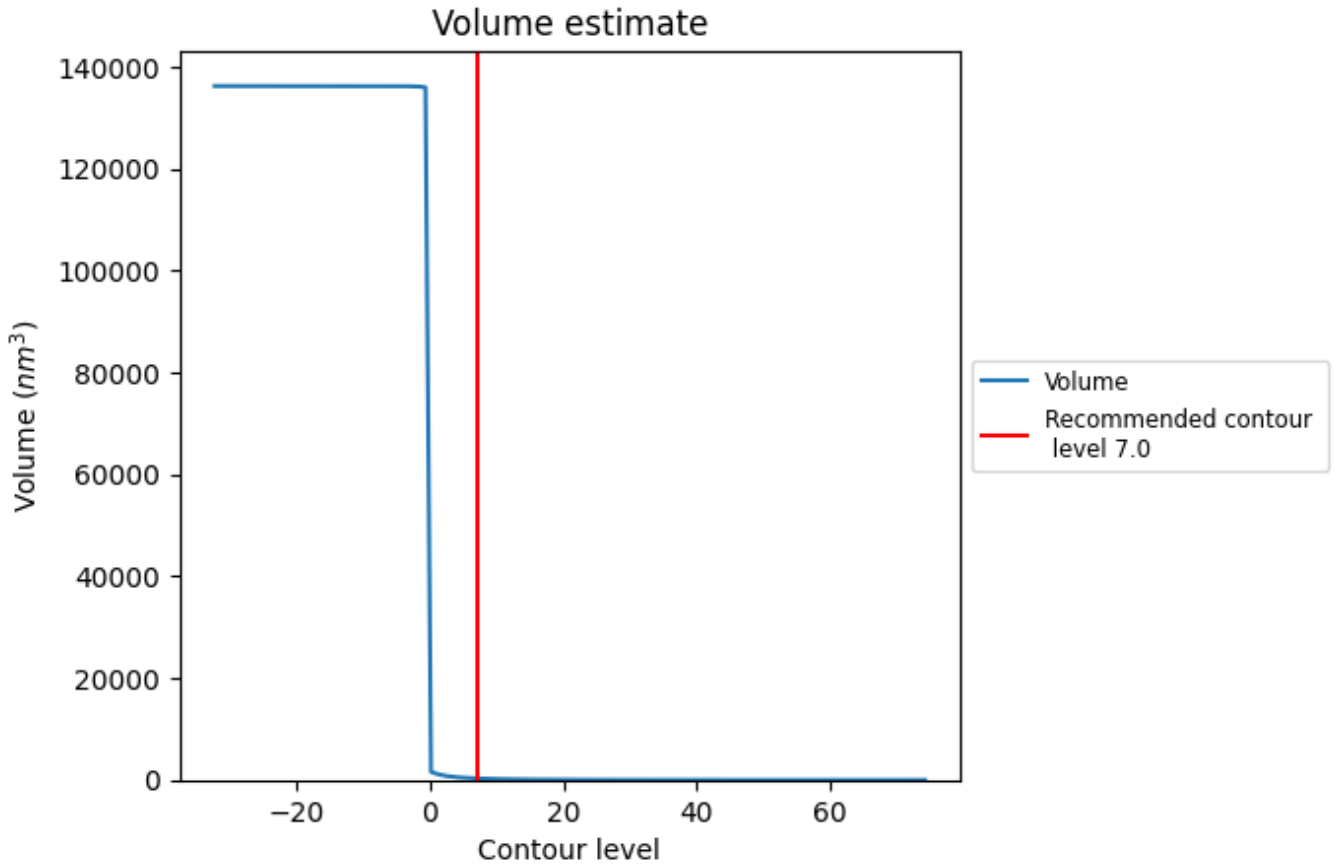
This section contains the results of statistical analysis of the map.

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.

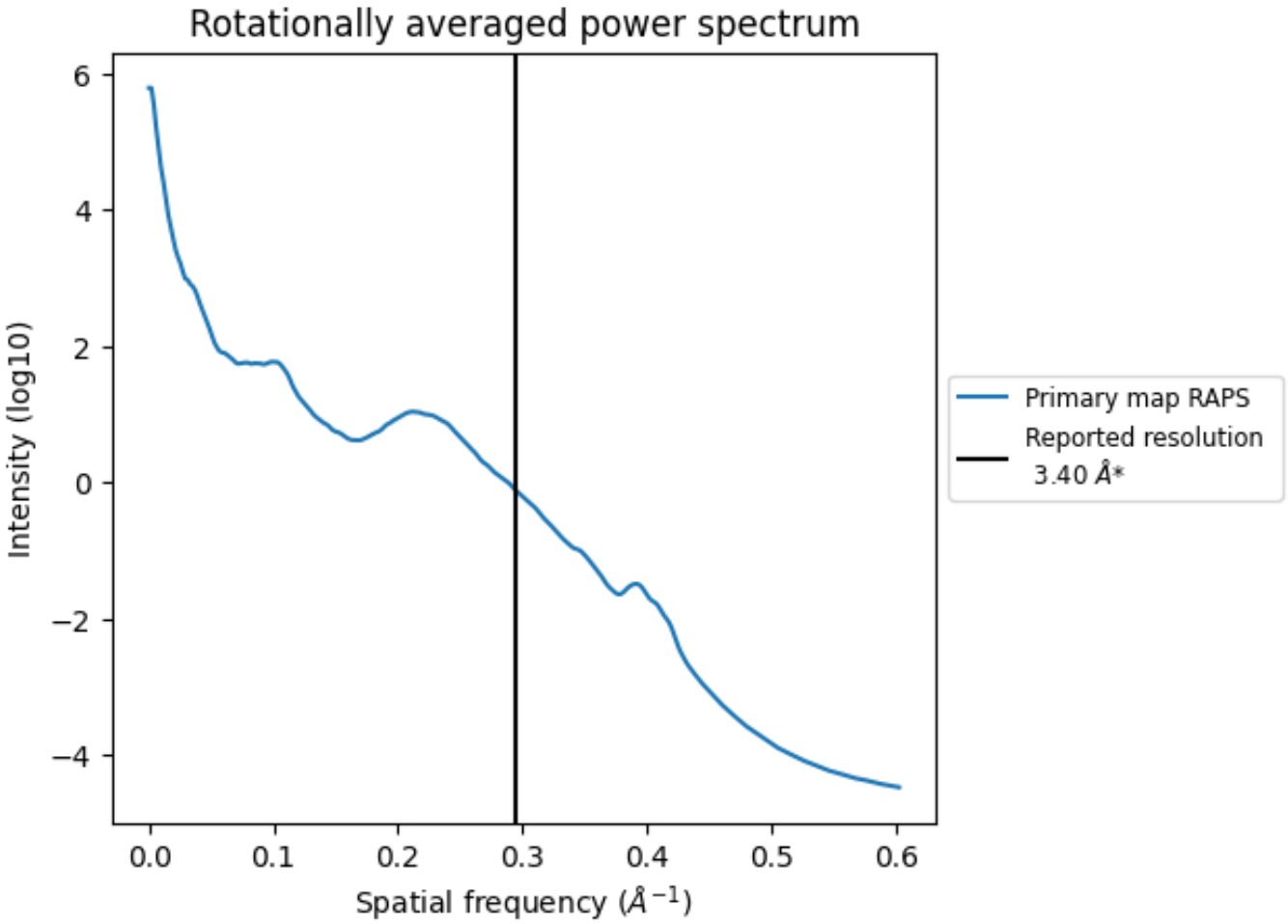
7.2 Volume estimate (i)



The volume at the recommended contour level is 303 nm^3; this corresponds to an approximate mass of 273 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 0.294 Å^{-1}

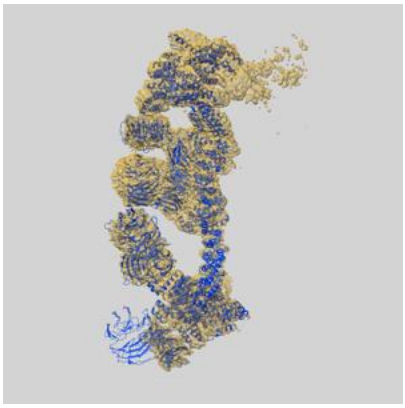
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

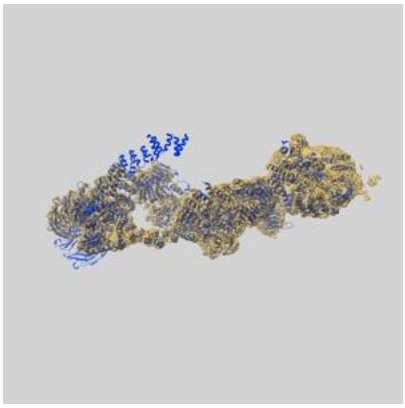
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-28867 and PDB model 8F5P. Per-residue inclusion information can be found in section 3 on page 5.

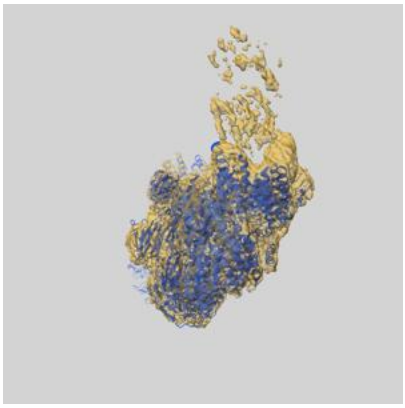
9.1 Map-model overlay



X



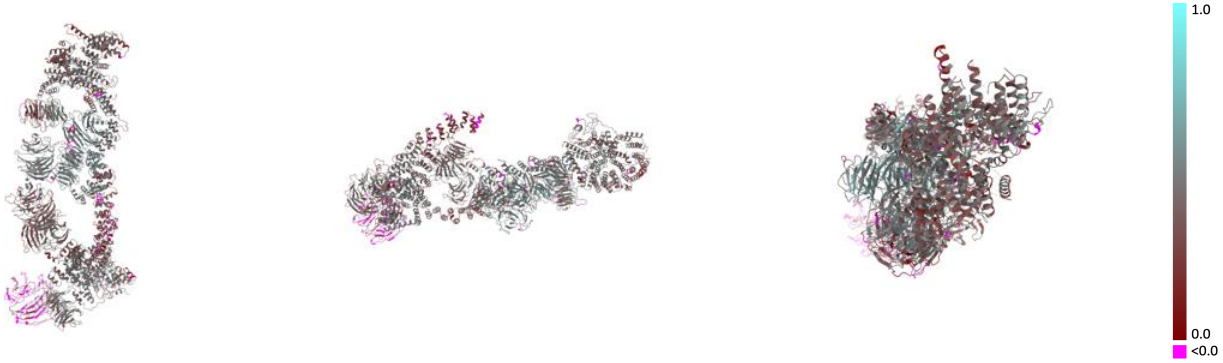
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 7.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

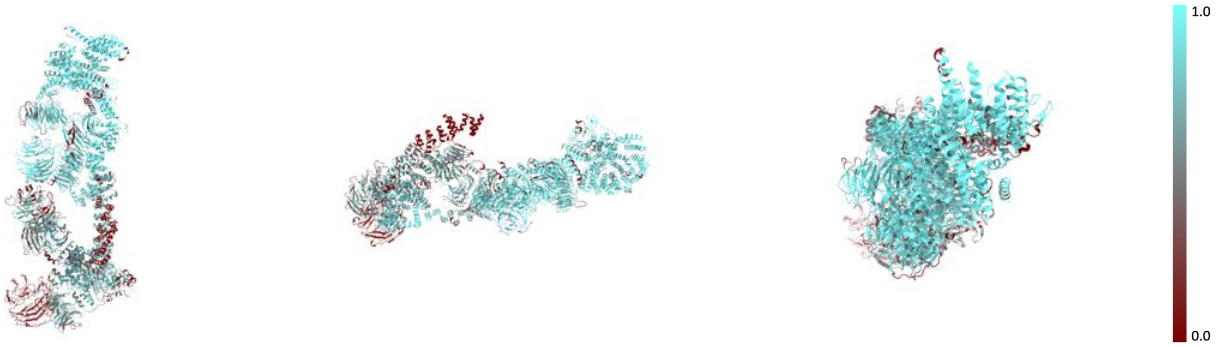
9.2 Q-score mapped to coordinate model (i)



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.

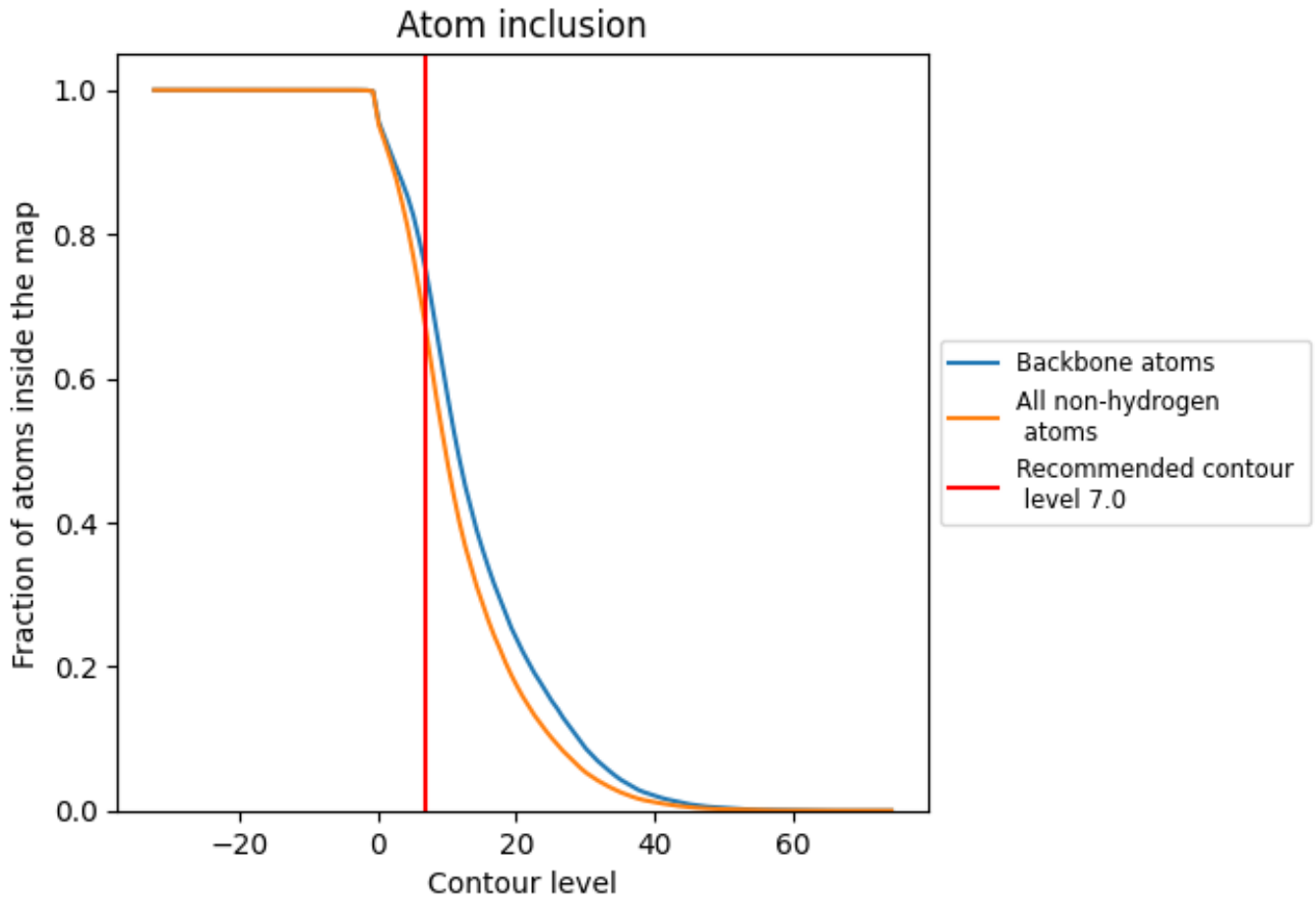
9.3 Atom inclusion mapped to coordinate model (i)



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 (7.0).

9.4 Atom inclusion (i)



At the recommended contour level, 75% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (7.0) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6664	0.3860
A	0.6463	0.3640
B	0.8720	0.4660
C	0.7463	0.4180
D	0.9017	0.3900
E	0.5746	0.3960
F	0.2758	0.2390