wwPDB EM Validation Summary Report

Sep 10, 2026 – 05:56 am BST

PDB ID	:	2VDC / pdb_00002vdc
EMDB ID	:	EMD-1440
Title	:	THE 9.5 A RESOLUTION STRUCTURE OF GLUTAMATE SYNTHASE FROM CRYO-ELECTRON MICROSCOPY AND ITS OLIGOMERIZATION BEHAVIOR IN SOLUTION: FUNCTIONAL IMPLICATIONS.
Authors	:	Cottevieille, M.; Larquet, E.; Jonic, S.; Petoukhov, M.V.; Caprini, G.; Paravisi, S.; Svergun, D.I.; Vanoni, M.A.; Boisset, N.
Deposited on	:	2007-10-04
Resolution	:	9.50 Å(reported)
Based on initial model	:	2VDC

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 (i) symbol.

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

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

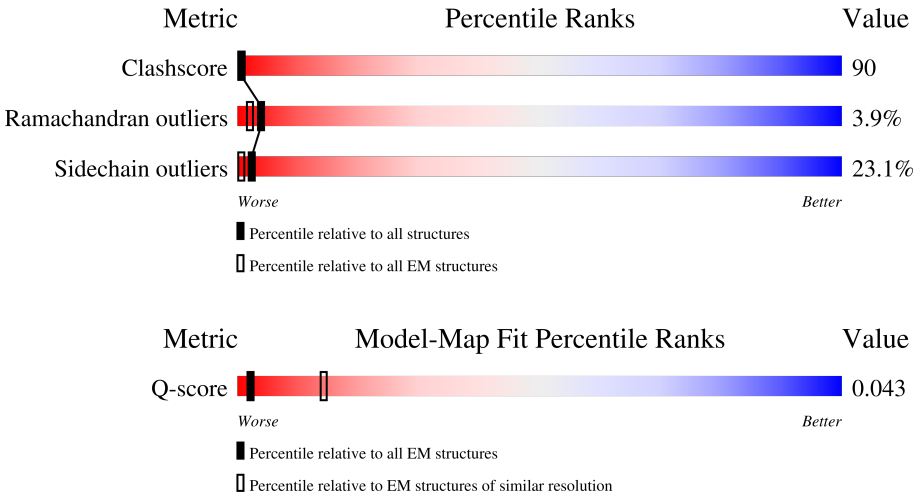
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

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 9.50 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	234 (9.00 - 10.00)

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	1472	29% 20% 48% 26% 6%
1	B	1472	29% 23% 47% 24% 6%
1	C	1472	31% 20% 49% 25% 6%

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Mol	Chain	Length	Quality of chain
1	D	1472	30% 22% 47% 24% 6%
1	E	1472	30% 20% 49% 25% 6%
1	F	1472	31% 23% 47% 24% 6%
2	G	456	21% 15% 43% 28% 14%
2	H	456	22% 15% 43% 28% 14%
2	I	456	24% 15% 43% 28% 14%
2	J	456	21% 15% 43% 28% 14%
2	K	456	24% 15% 43% 28% 14%
2	L	456	22% 15% 43% 28% 14%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OMT	A	2473	-	X	-	-
3	OMT	B	2473	-	X	-	-
3	OMT	C	2473	-	X	-	-
3	OMT	D	2473	-	X	-	-
3	OMT	E	2473	-	X	-	-
3	OMT	F	2473	-	X	-	-
6	F3S	B	2476	-	-	X	-
6	F3S	D	2476	-	-	X	-
6	F3S	E	2476	-	-	X	-
6	F3S	F	2476	-	-	X	-
7	SF4	G	483	-	-	X	-
7	SF4	H	483	-	-	X	-
7	SF4	I	483	-	-	X	-
7	SF4	J	483	-	-	X	-
7	SF4	K	483	-	-	X	-
7	SF4	L	483	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 89598 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.

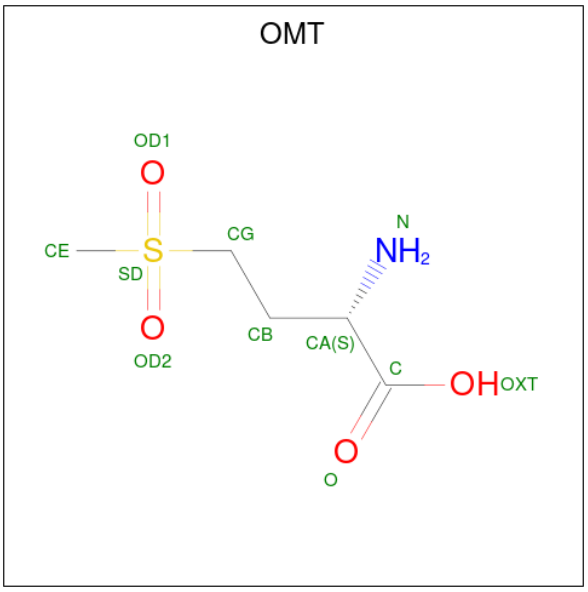
- Molecule 1 is a protein called GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	B	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	C	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	D	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	E	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		
1	F	1472	Total	C	N	O	S	0	0
			11337	7109	2036	2132	60		

- Molecule 2 is a protein called GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN.

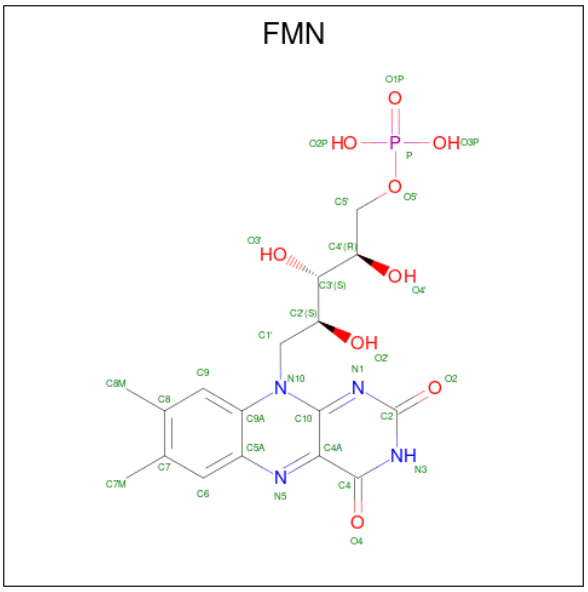
Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	H	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	I	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	J	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	K	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		
2	L	456	Total	C	N	O	S	0	0
			3468	2163	624	666	15		

- Molecule 3 is S-DIOXYMETHIONINE (CCD ID: OMT) (formula: $C_5H_{11}NO_4S$).



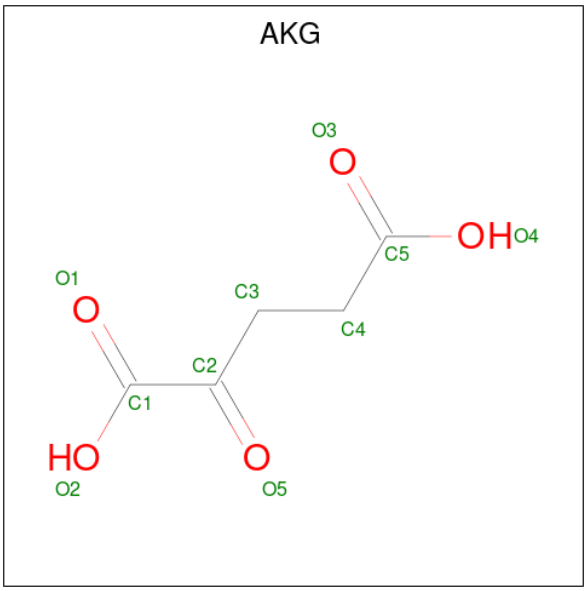
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	B	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	C	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	D	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	E	1	Total	C	N	O	S	0
			11	5	1	4	1	
3	F	1	Total	C	N	O	S	0
			11	5	1	4	1	

- Molecule 4 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$).



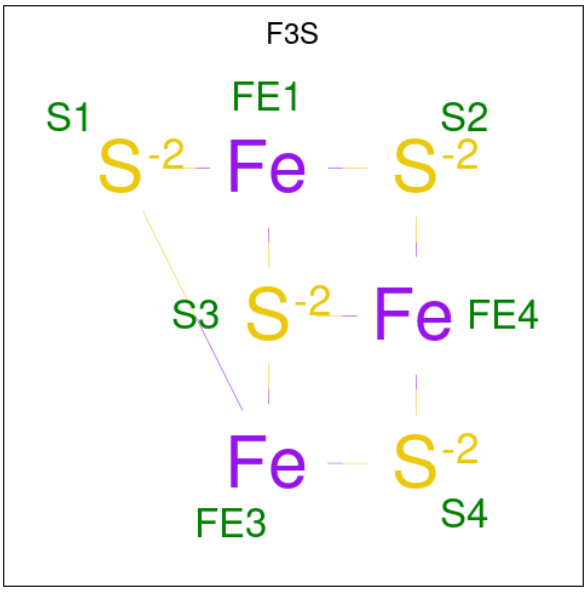
Mol	Chain	Residues	Atoms					AltConf
4	A	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	B	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	C	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	D	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	E	1	Total	C	N	O	P	0
			31	17	4	9	1	
4	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 5 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: $C_5H_6O_5$).



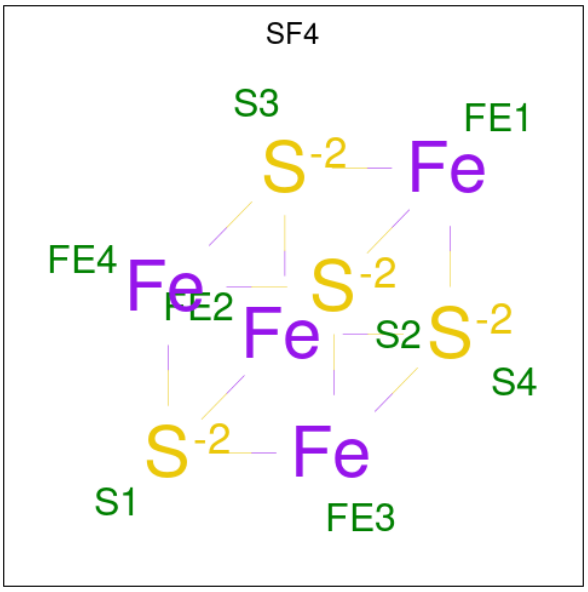
Mol	Chain	Residues	Atoms	AltConf
5	A	1	Total C O 10 5 5	0
5	B	1	Total C O 10 5 5	0
5	C	1	Total C O 10 5 5	0
5	D	1	Total C O 10 5 5	0
5	E	1	Total C O 10 5 5	0
5	F	1	Total C O 10 5 5	0

- Molecule 6 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe_3S_4).



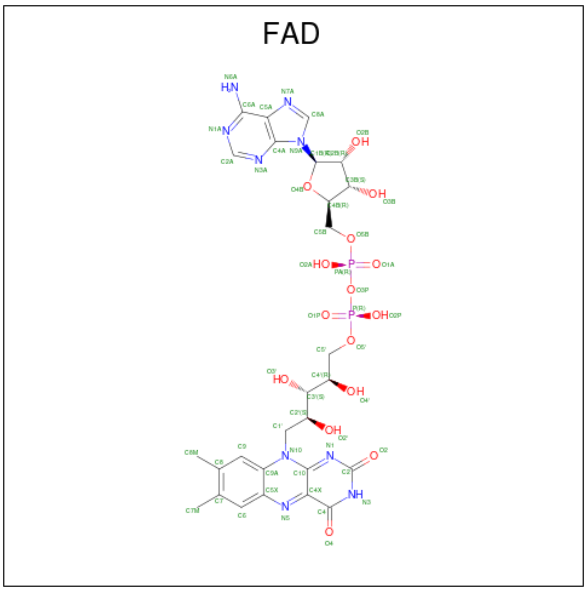
Mol	Chain	Residues	Atoms	AltConf
6	A	1	Total Fe S 7 3 4	0
6	B	1	Total Fe S 7 3 4	0
6	C	1	Total Fe S 7 3 4	0
6	D	1	Total Fe S 7 3 4	0
6	E	1	Total Fe S 7 3 4	0
6	F	1	Total Fe S 7 3 4	0

- Molecule 7 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms	AltConf
7	G	1	Total Fe S 8 4 4	0
7	G	1	Total Fe S 8 4 4	0
7	H	1	Total Fe S 8 4 4	0
7	H	1	Total Fe S 8 4 4	0
7	I	1	Total Fe S 8 4 4	0
7	I	1	Total Fe S 8 4 4	0
7	J	1	Total Fe S 8 4 4	0
7	J	1	Total Fe S 8 4 4	0
7	K	1	Total Fe S 8 4 4	0
7	K	1	Total Fe S 8 4 4	0
7	L	1	Total Fe S 8 4 4	0
7	L	1	Total Fe S 8 4 4	0

- Molecule 8 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $C_{27}H_{33}N_9O_{15}P_2$).



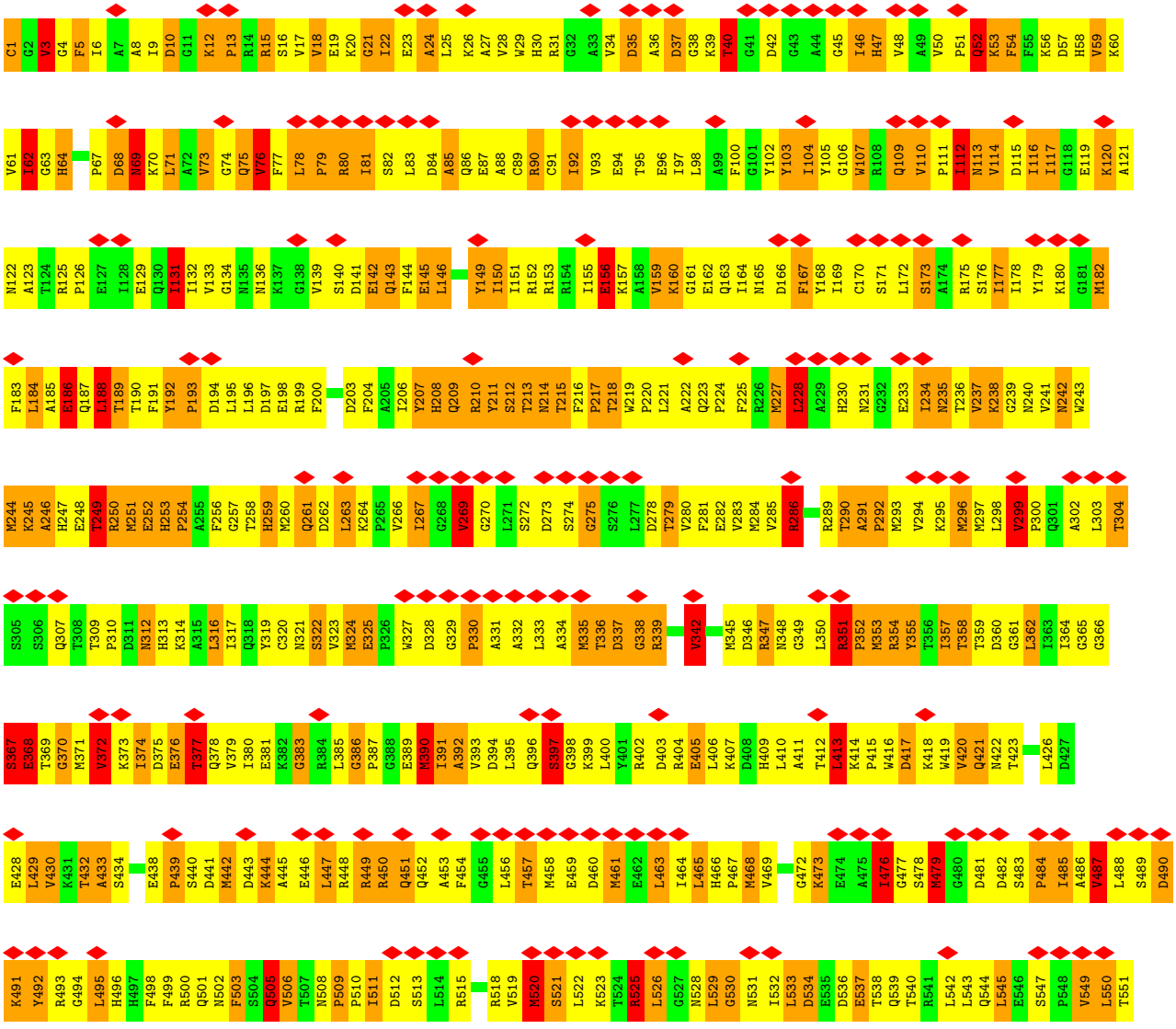
Mol	Chain	Residues	Atoms					AltConf
8	G	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	H	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	I	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	J	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	K	1	Total	C	N	O	P	0
			53	27	9	15	2	
8	L	1	Total	C	N	O	P	0
			53	27	9	15	2	

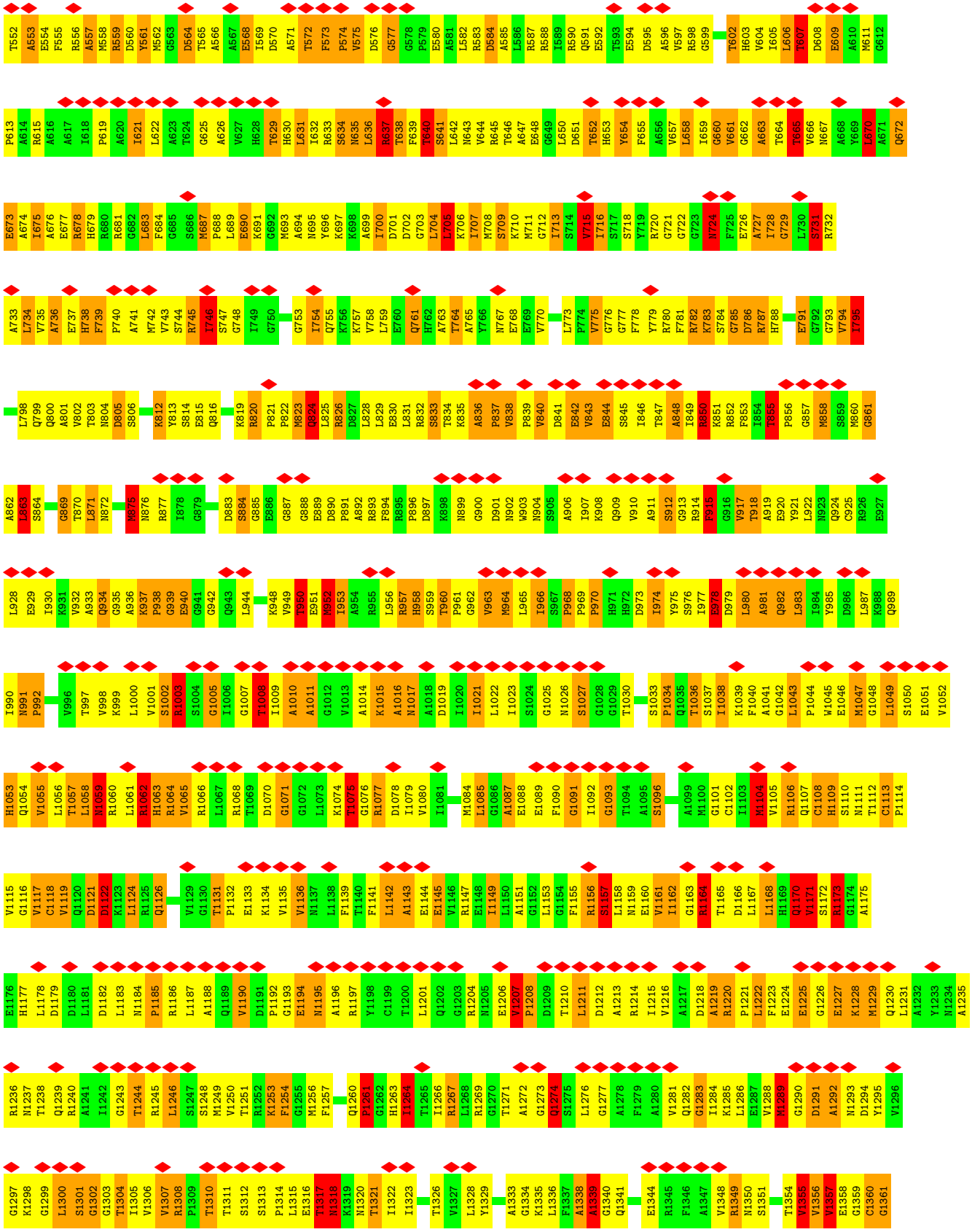
3 Residue-property plots (i)

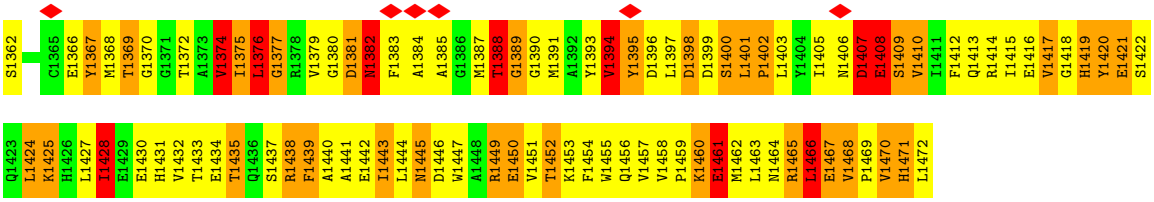
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain A: 

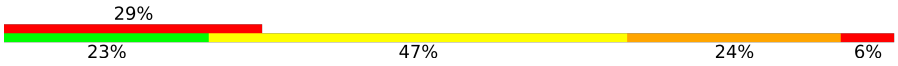


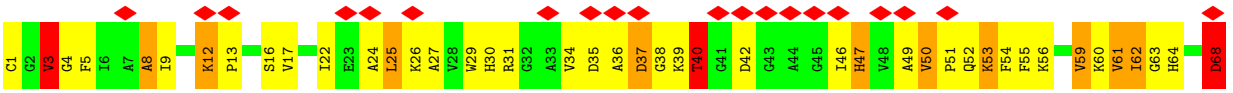


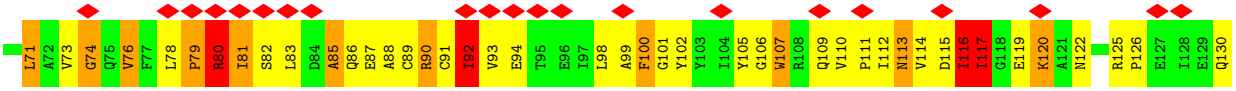


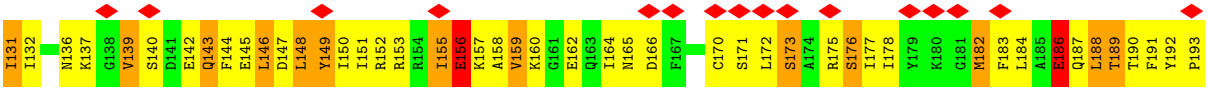
• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

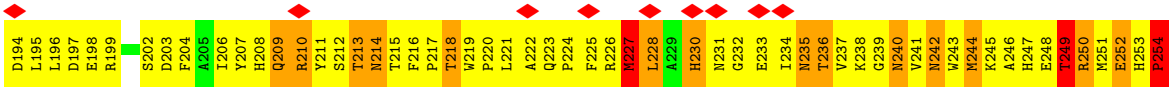
Chain B:

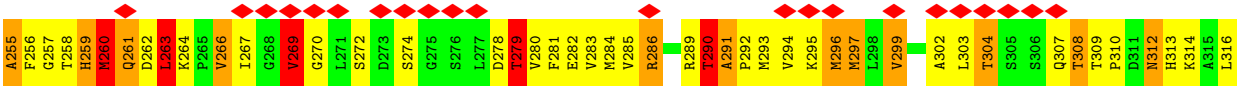


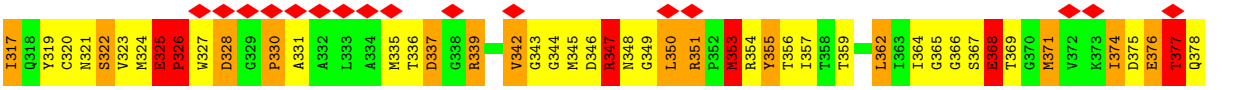


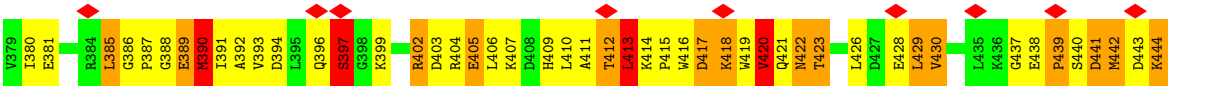




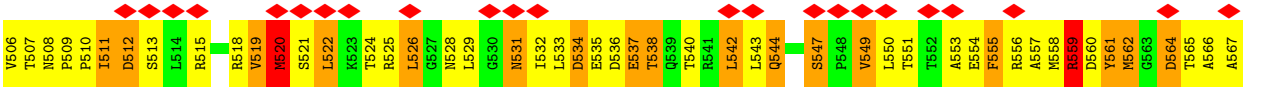




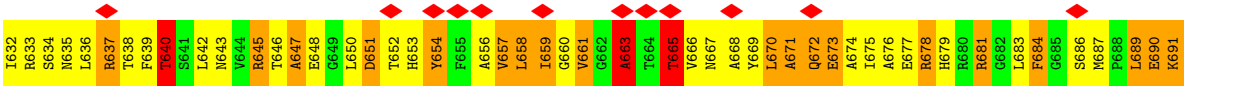


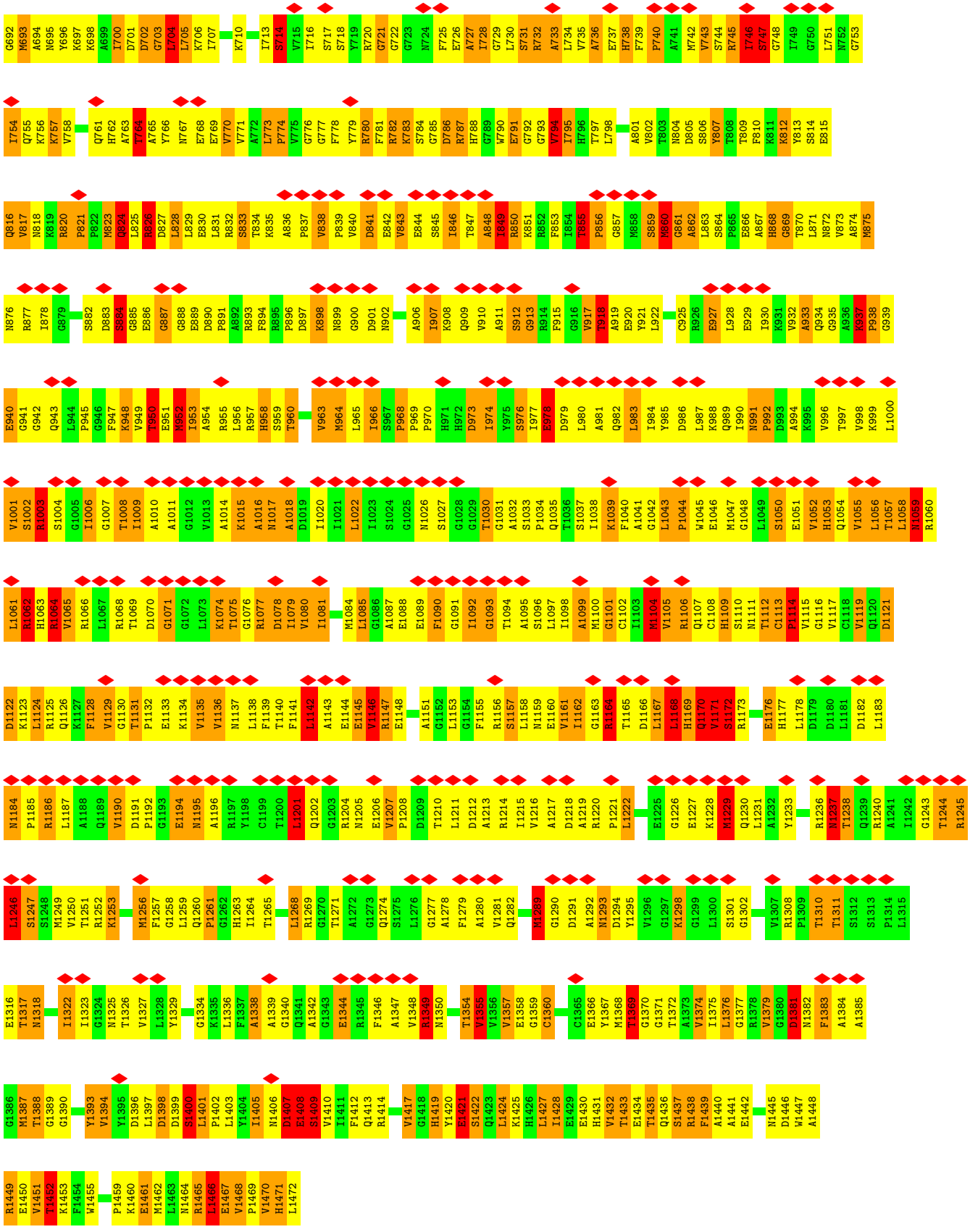






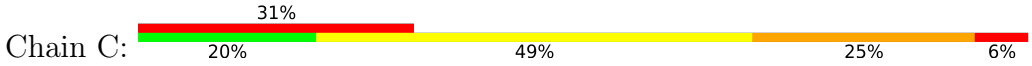


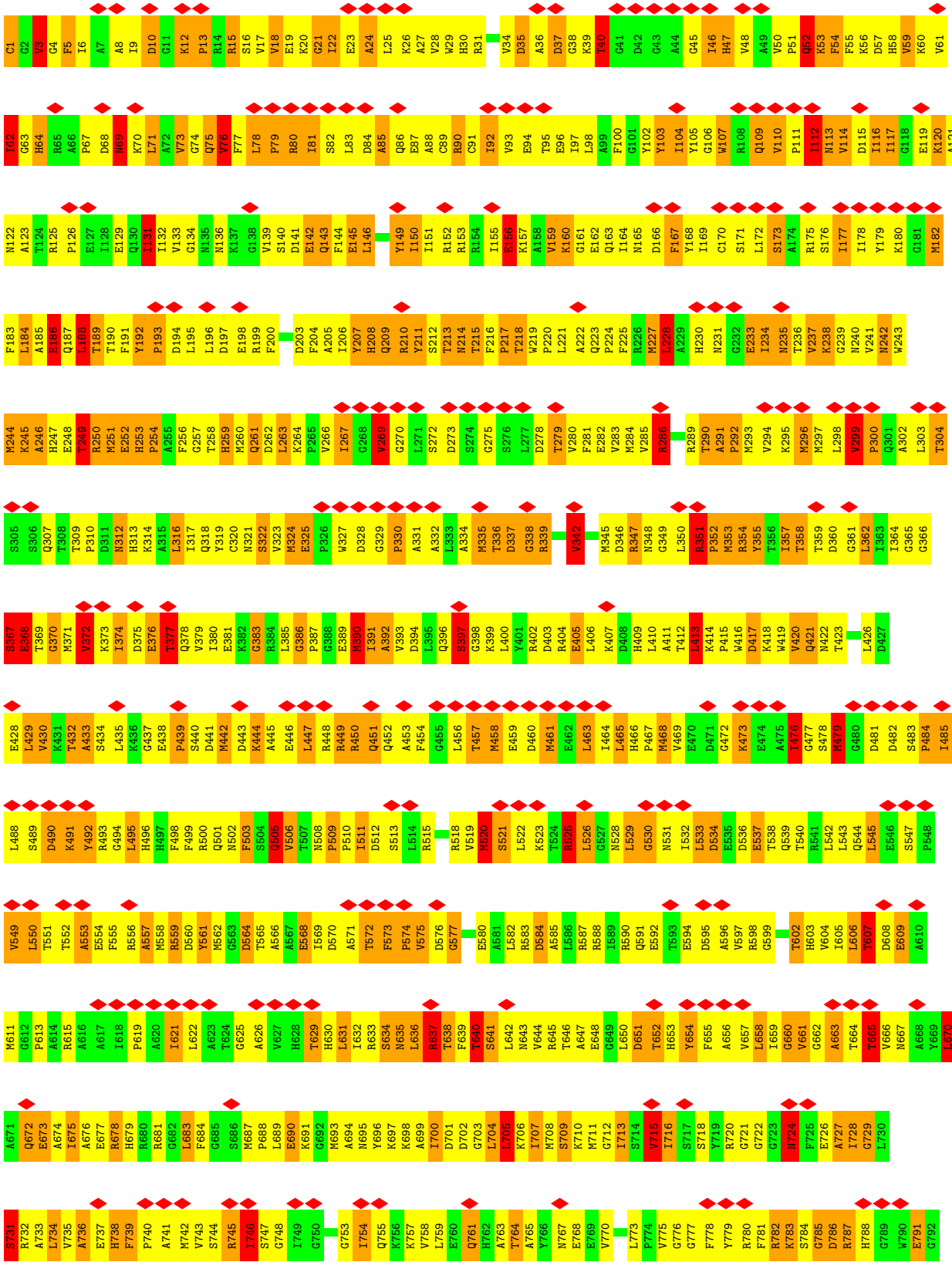


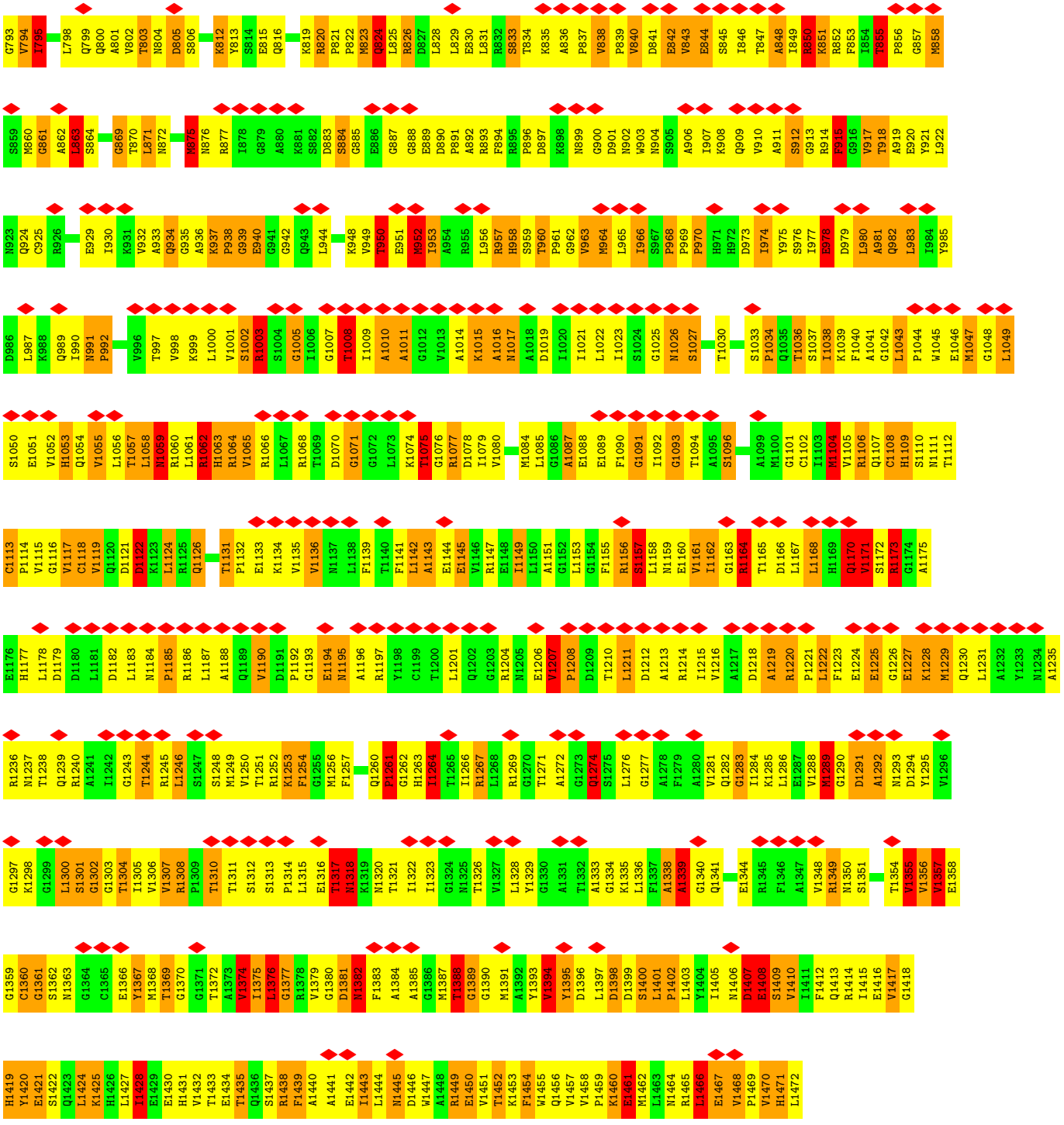


• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

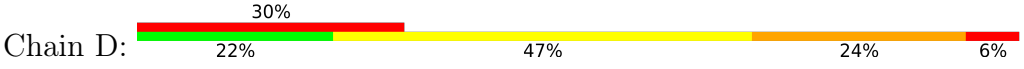
Chain C:

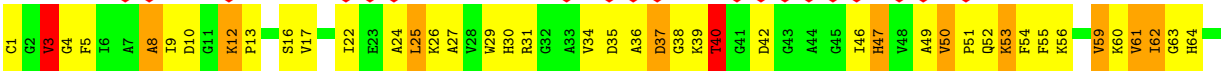

31%
20%
49%
25%
6%

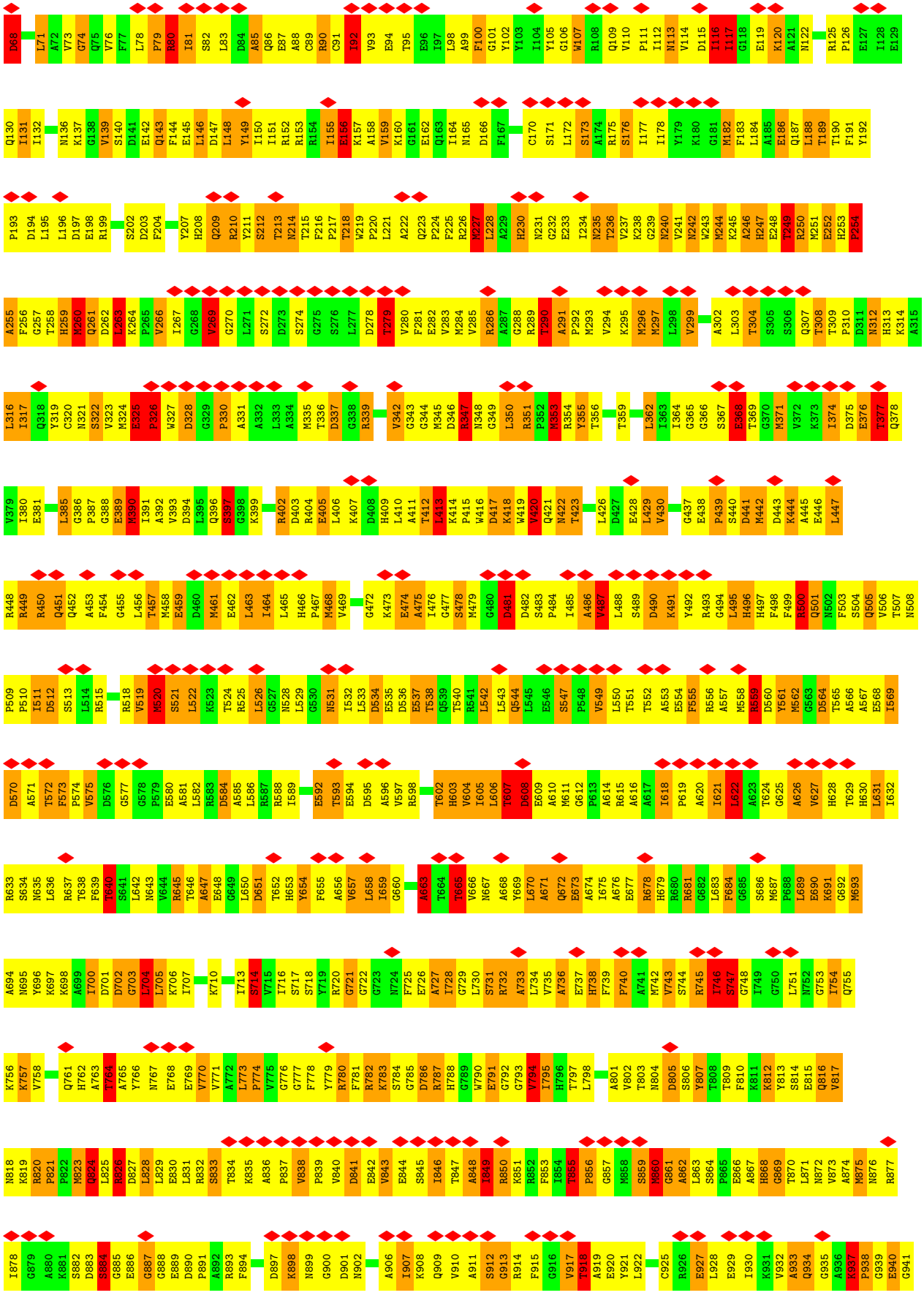

C1 G2 V3 G4 F5 I6 A7 A8 I9 D10 G11 K12 P13 R14 R15 S16 V17 V18 E19 K20 G21 I22 E23 A24 L25 K26 A27 V28 W29 H30 R31 V34 D35 A36 D37 G38 K39 T40 G41 D42 G43 A44 G45 I46 H47 V48 A49 V50 P51 Q52 K53 F54 F55 K56 D57 H58 V59 K60 V61
I62 G63 H64 R65 A66 P67 D68 N69 K70 L71 A72 V73 G74 Q75 V76 F77 L78 P79 R80 I81 S82 L83 D84 A85 Q86 E87 A88 C89 R90 C91 I92 V93 E94 T95 E96 I97 L98 A99 F100 G101 Y102 Y103 I104 Y105 G106 W107 R108 Q109 V110 P111 I112 N113 V114 D115 I116 I117 G118 E119 K120 A121
N122 A123 T124 R125 P126 E127 I128 E129 Q130 I131 I132 V133 G134 N135 N136 K137 G138 V139 S140 D141 E142 Q143 F144 E145 L146 Y149 I150 I151 R152 R153 R154 I155 E156 K157 A158 V159 K160 G161 E162 Q163 I164 N165 D166 F167 Y168 I169 C170 S171 L172 S173 A174 R175 S176 I177 I178 Y179 K180 G181 M182
F183 L184 A185 E186 Q187 L188 T189 T190 F191 Y192 P193 D194 L195 L196 D197 E198 R199 F200 D203 F204 A205 I206 Y207 H208 Q209 R210 Y211 S212 T213 N214 T215 F216 P217 T218 W219 P220 L221 A222 Q223 P224 F225 R226 M227 L228 A229 H230 N231 G232 E233 I234 N235 T236 V237 K238 G239 N240 V241 N242 W243
M244 K245 A246 H247 E248 T249 R250 M251 E252 H253 P254 A255 F256 G257 T258 H259 M260 Q261 D262 L263 K264 P265 V266 I267 G268 V269 G270 L271 S272 D273 S274 G275 S276 L277 D278 T279 V280 F281 E282 V283 M284 V285 R286 R289 T290 A291 P292 M293 V294 K295 M296 M297 L298 V299 P300 Q301 A302 L303 T304
S305 S306 Q307 T308 T309 P310 D311 N312 H313 K314 A315 L316 I317 Q318 Y319 C320 N321 S322 V323 M324 E325 P326 W327 D328 G329 P330 A331 A332 L333 A334 M335 T336 D337 G338 R339 V342 M345 D346 R347 N348 G349 L350 R351 P352 M353 R354 Y355 T356 I357 T358 T359 D360 G361 L362 I363 I364 G365 G366
S367 E368 T369 G370 M371 V372 K373 I374 D375 E376 T377 Q378 V379 I380 E381 K382 G383 R384 L385 G386 P387 G388 E389 M390 I391 A392 V393 D394 L395 Q396 S397 G398 K399 L400 Y401 R402 D403 R404 E405 L406 K407 D408 H409 L410 A411 T412 L413 K414 P415 W416 D417 K418 W419 V420 Q421 N422 T423 L426 D427
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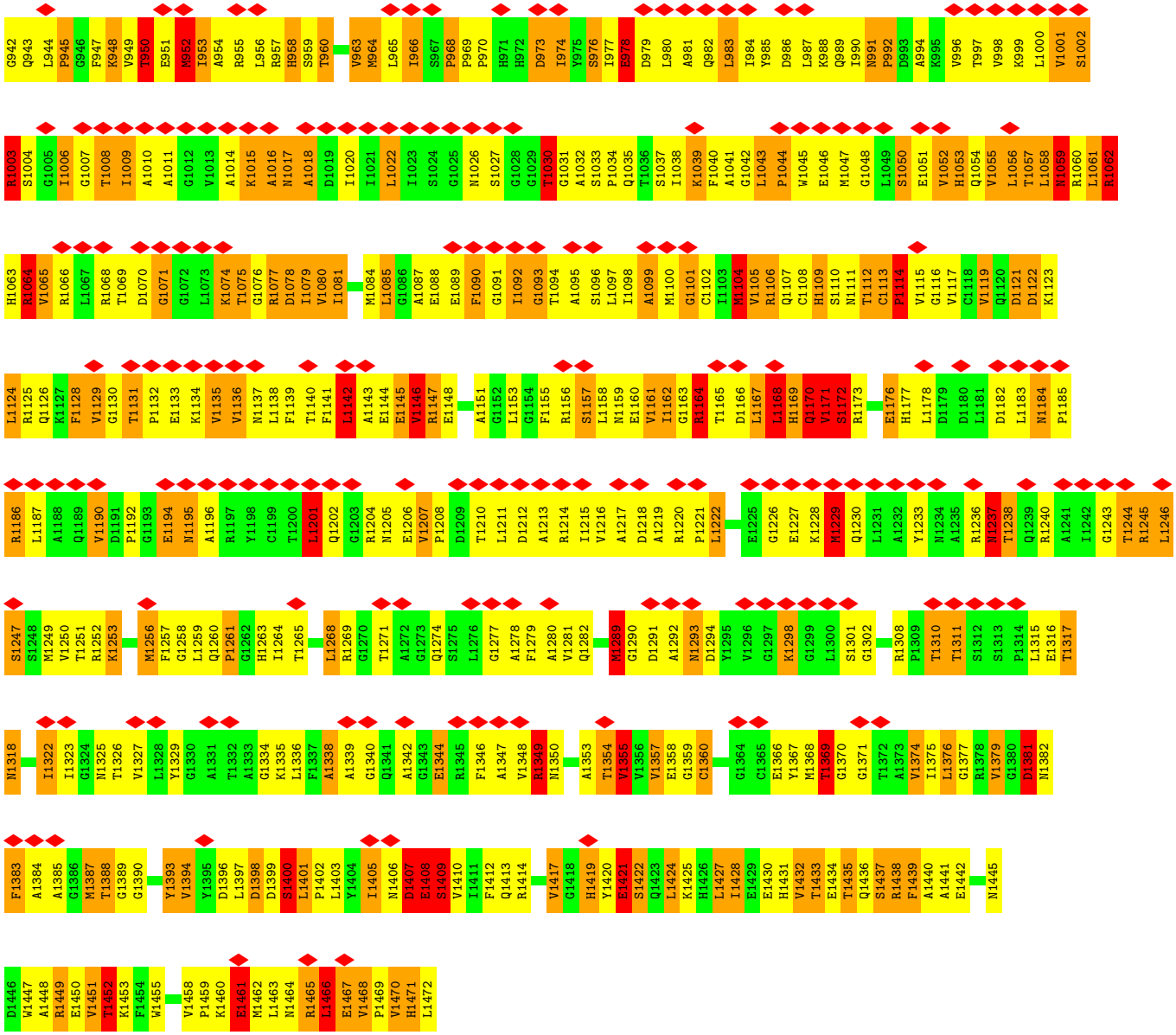


• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN



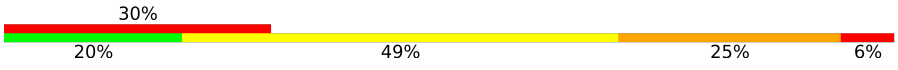


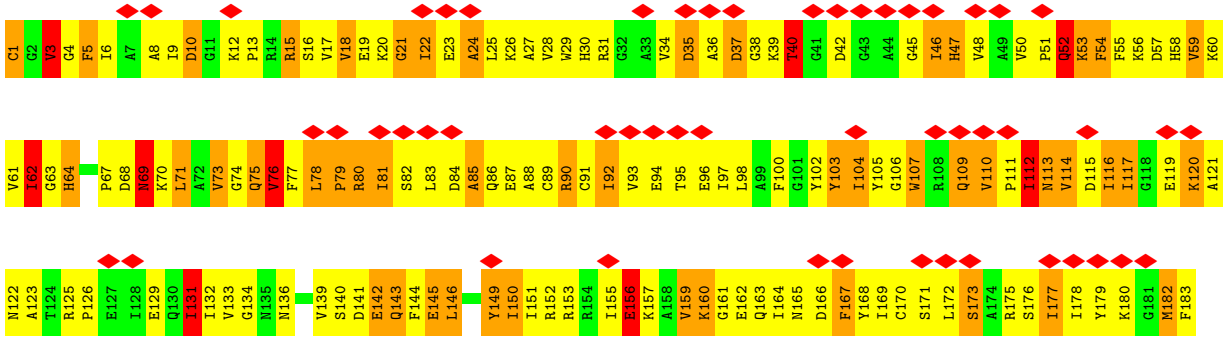

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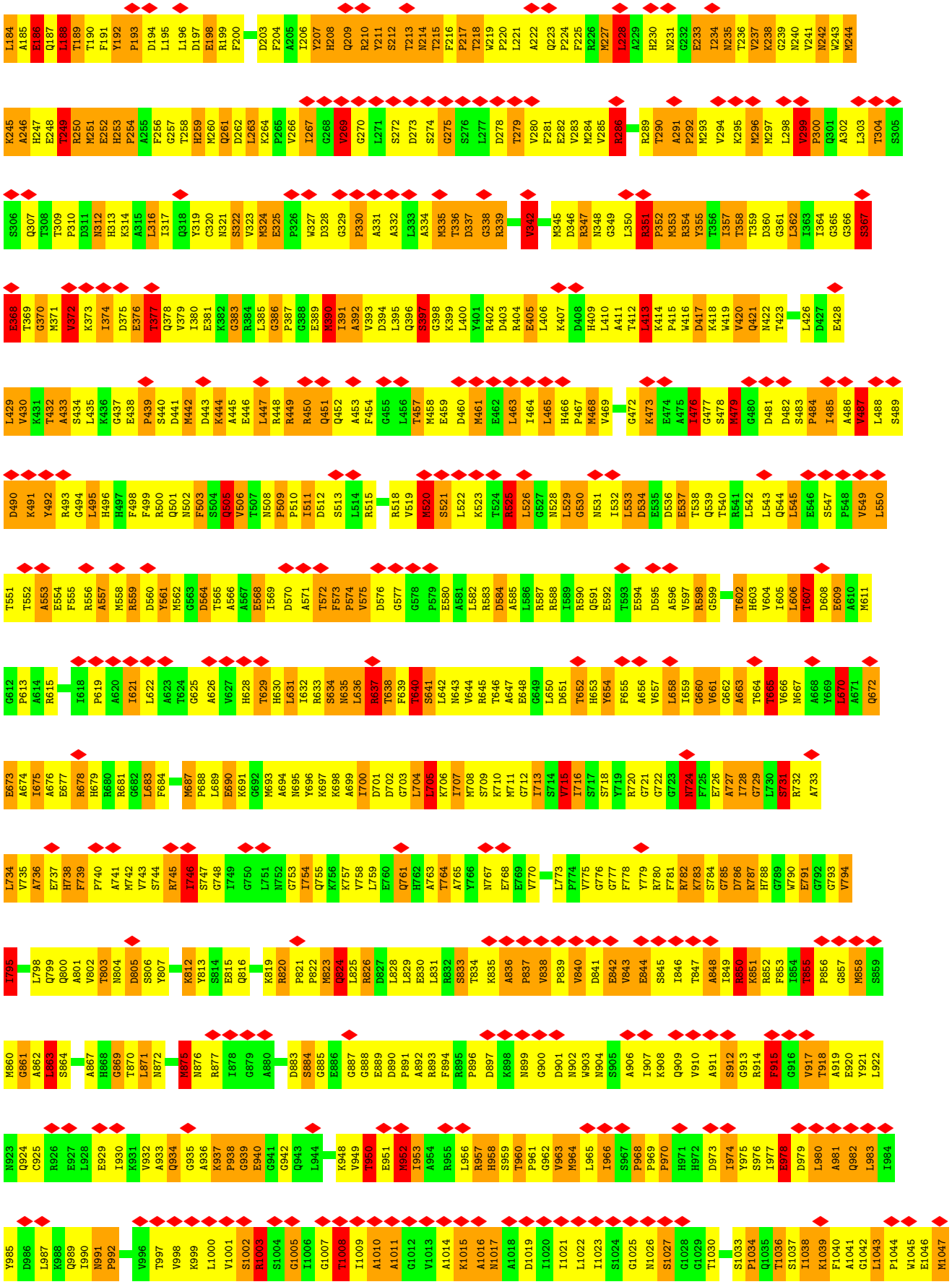


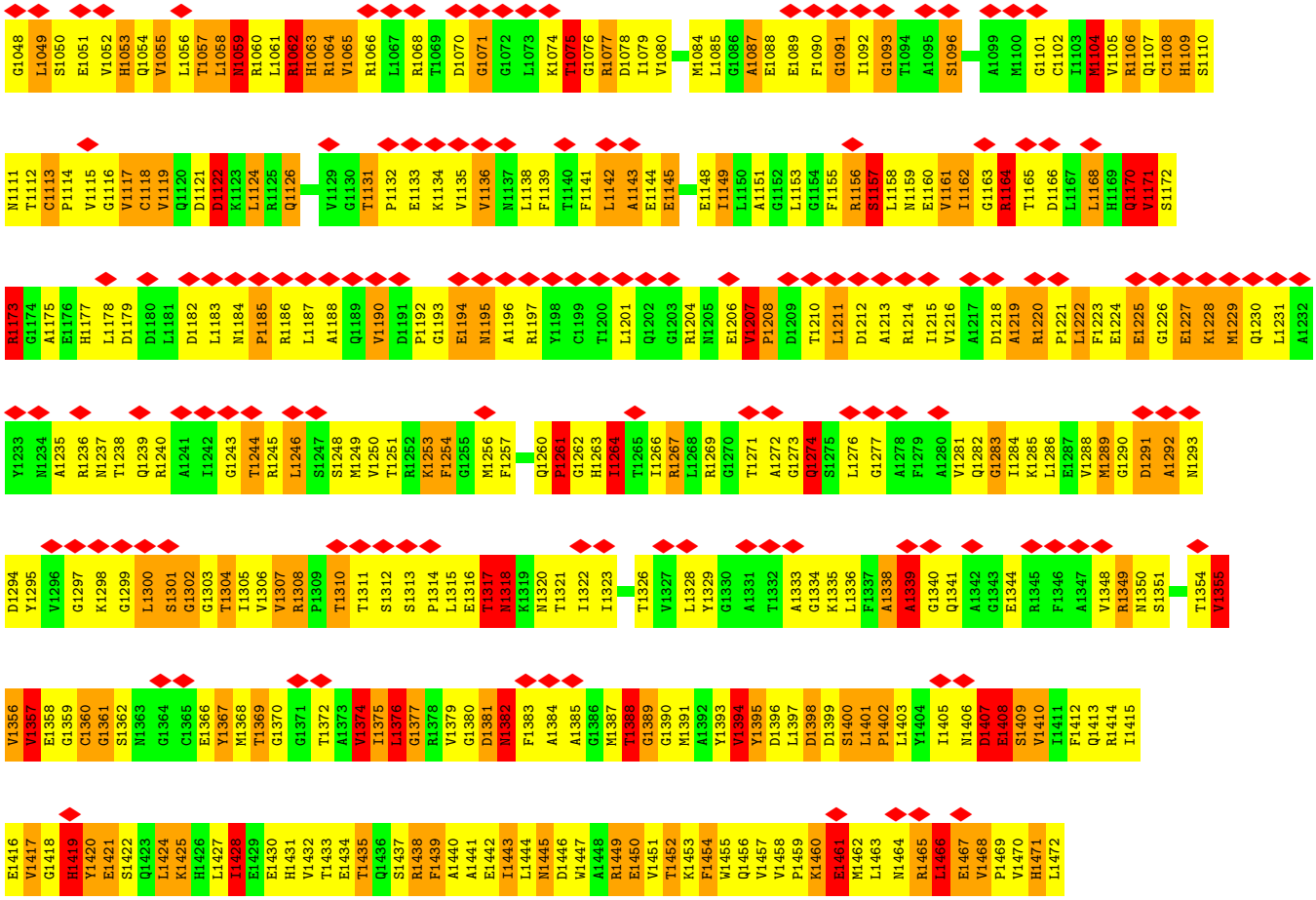
• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain E:



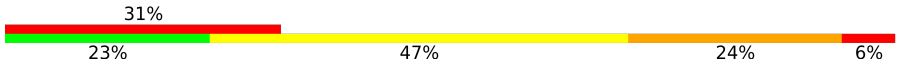


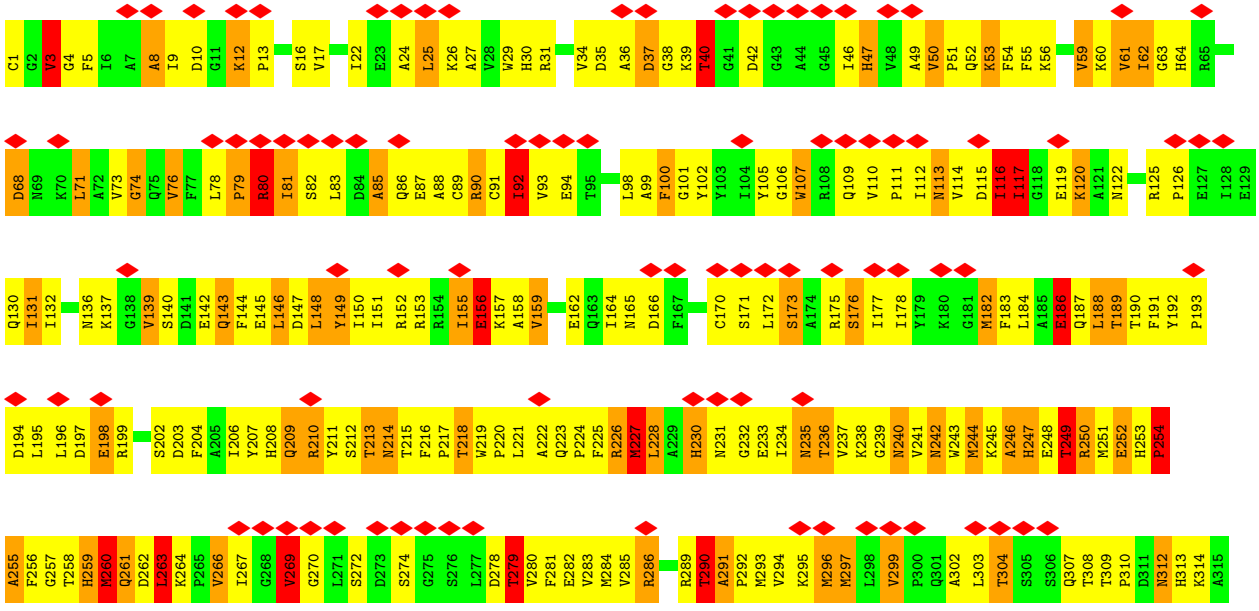


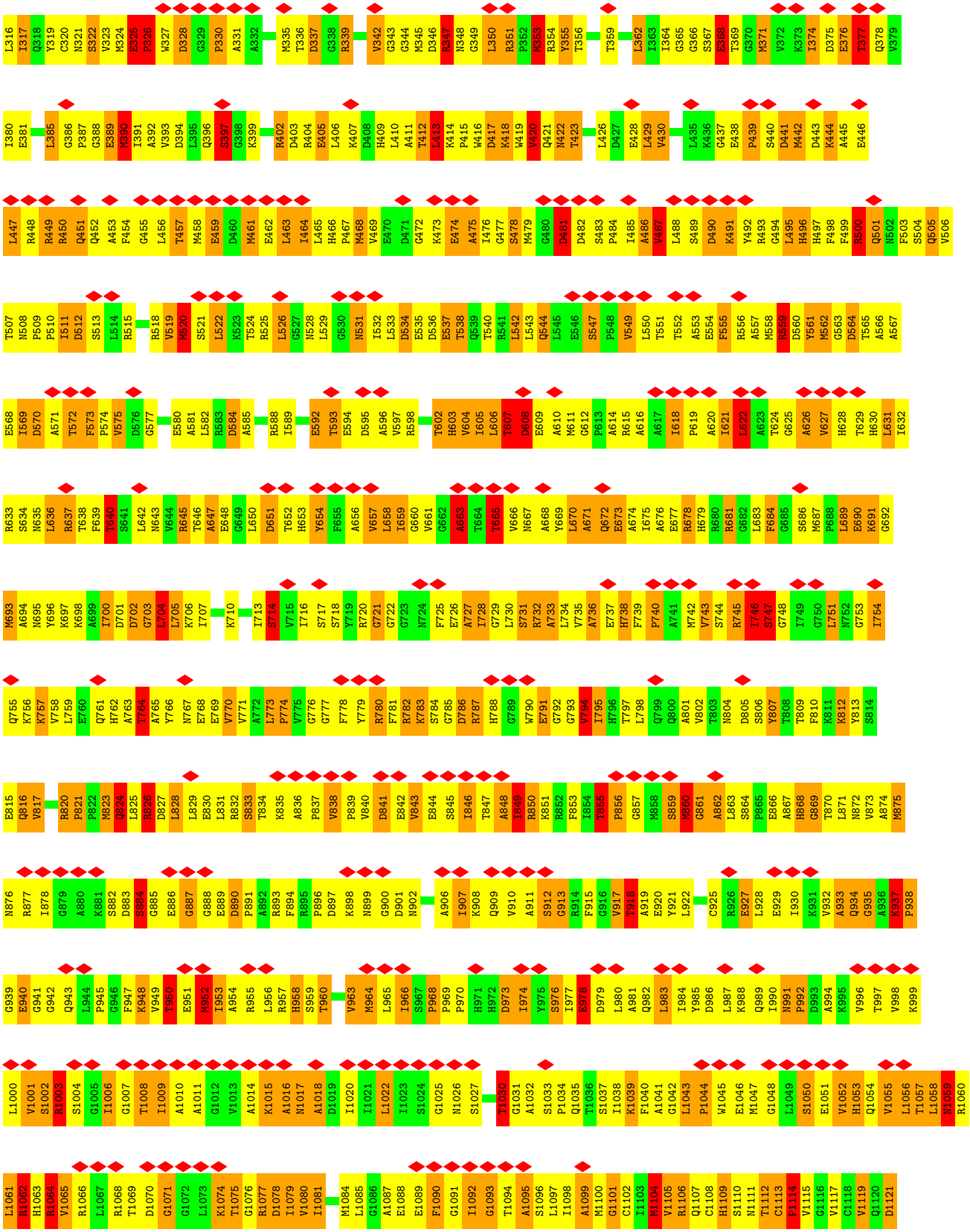


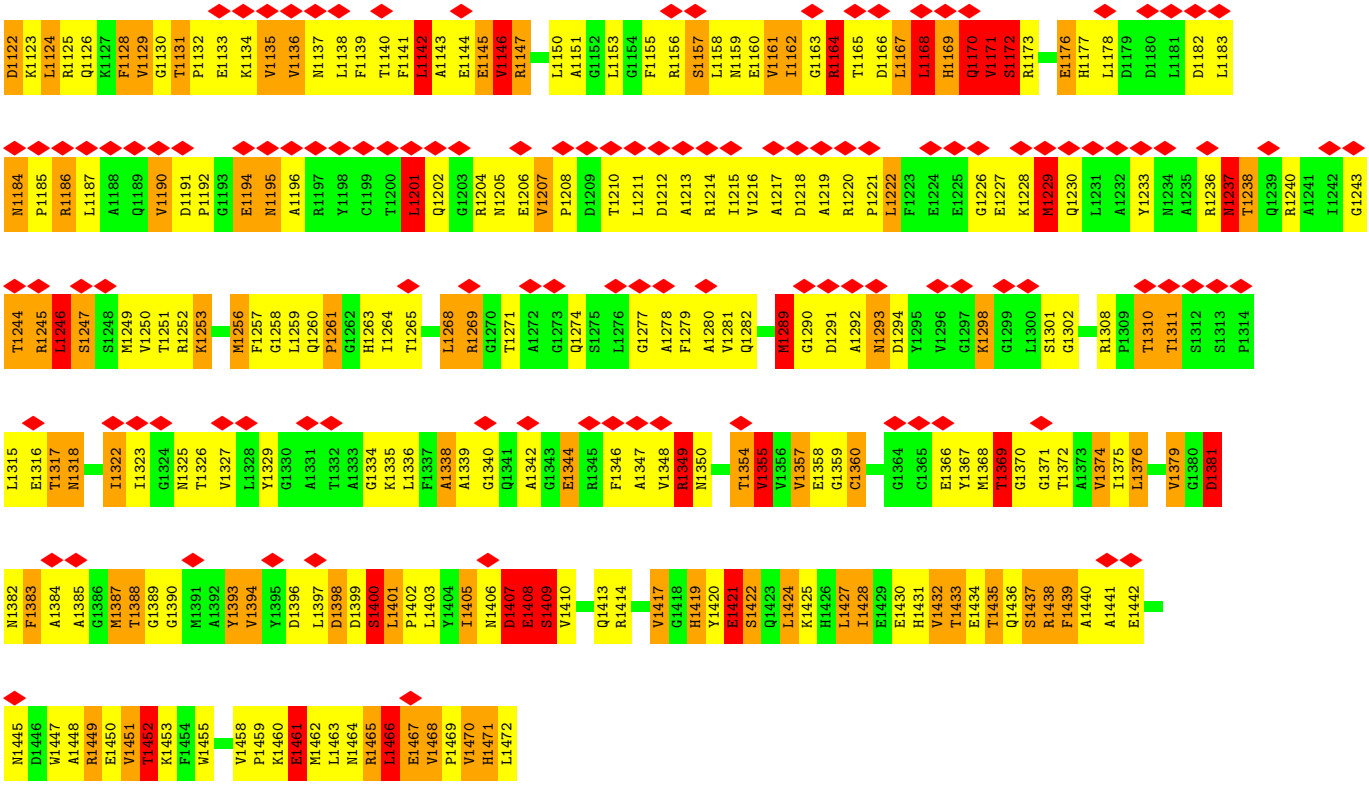
• Molecule 1: GLUTAMATE SYNTHASE [NADPH] LARGE CHAIN

Chain F:





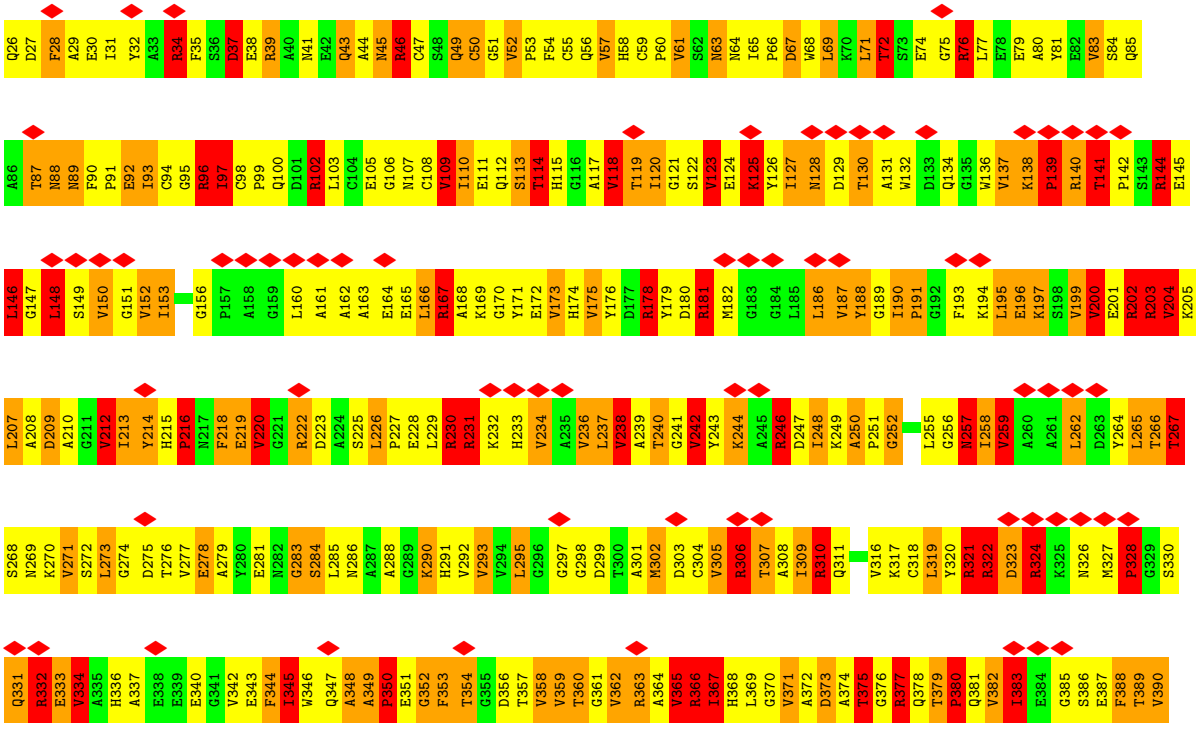

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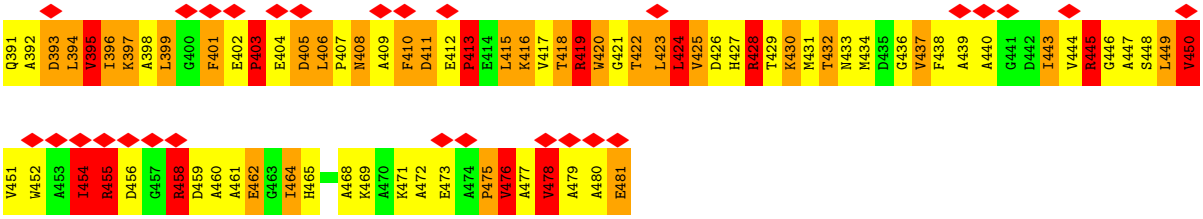


• Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN

Chain G:



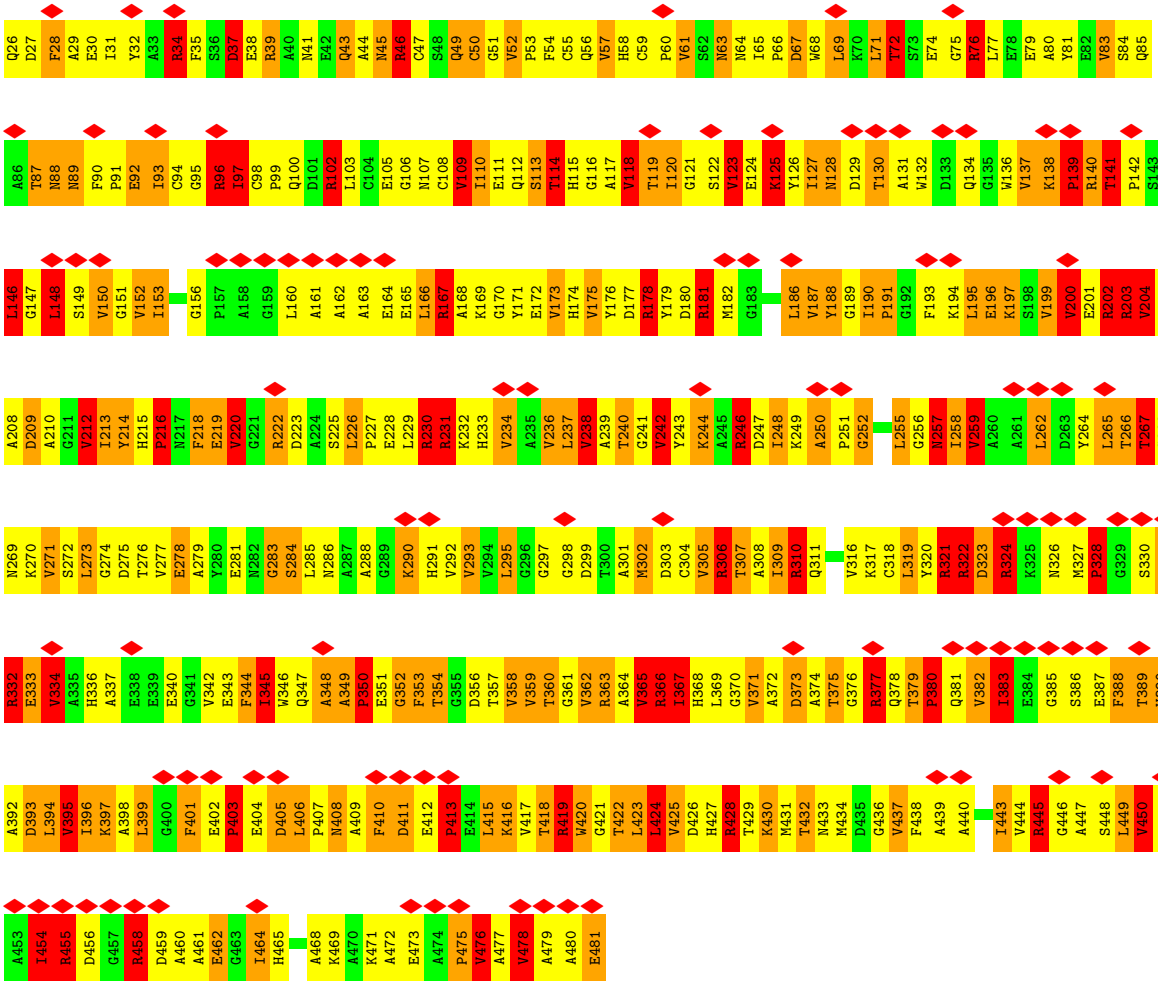




• Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN

Chain H:

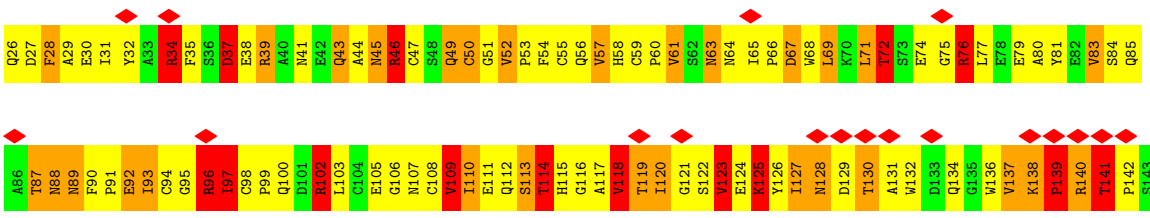


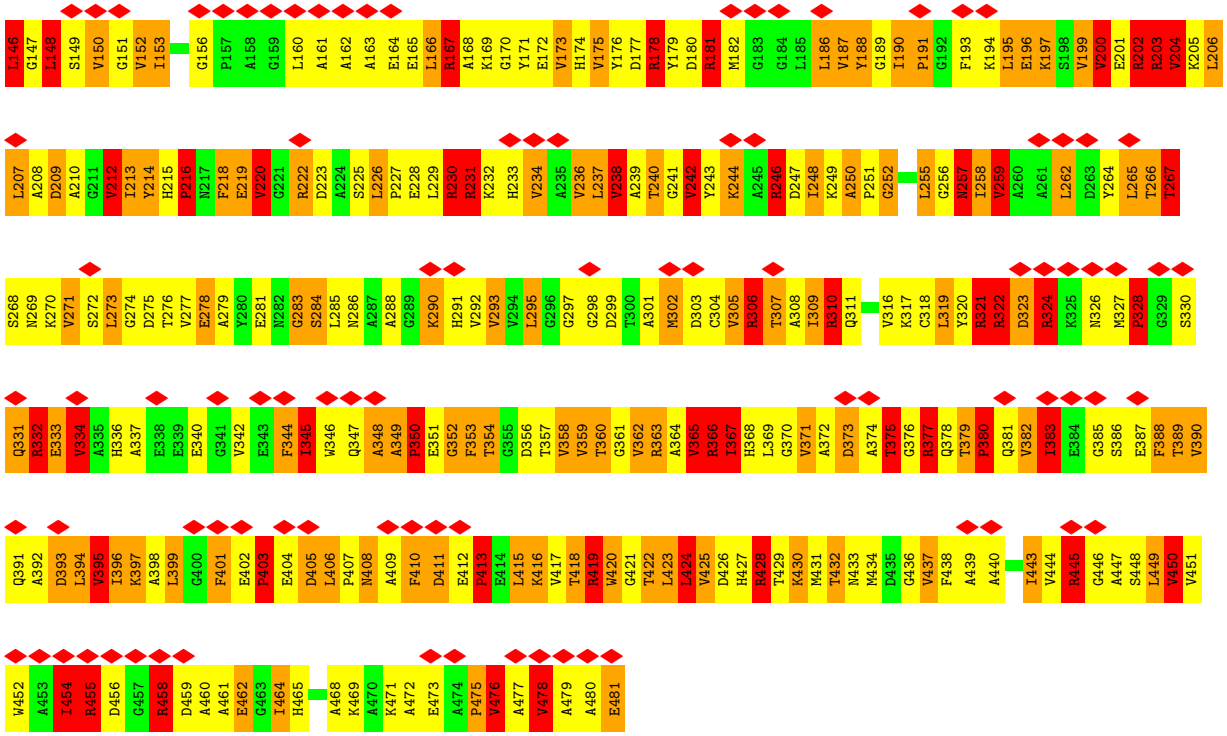


• Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN

Chain I:



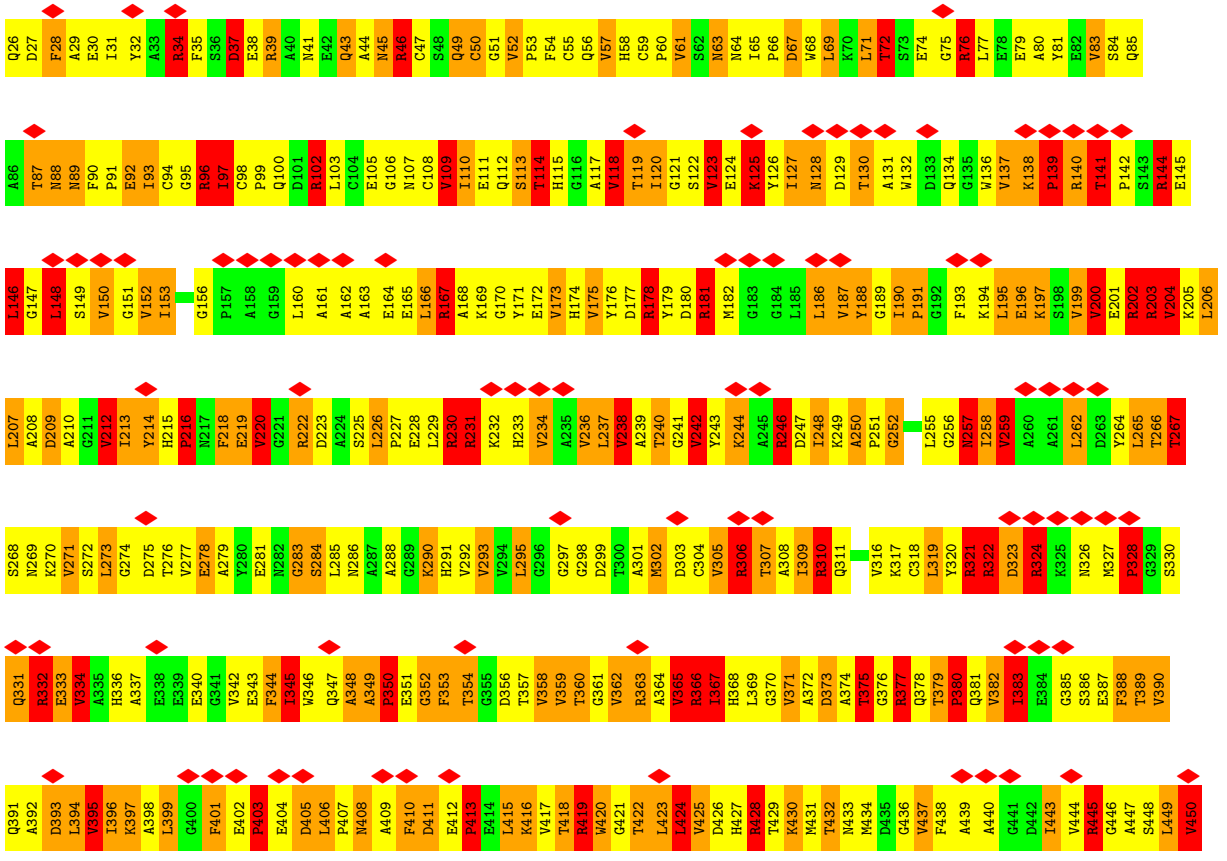


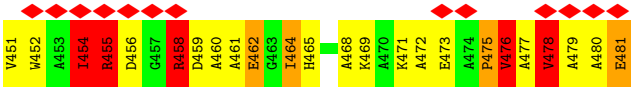


• Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN

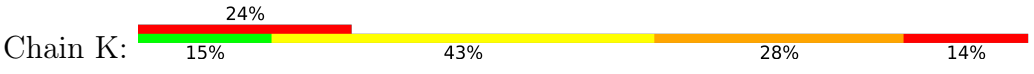
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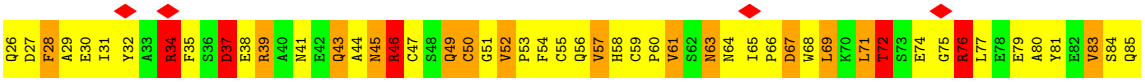


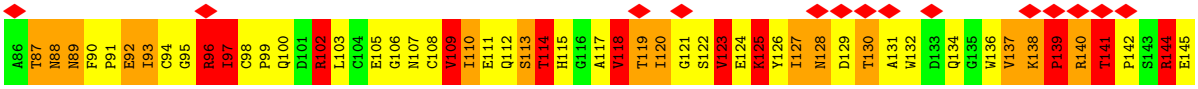




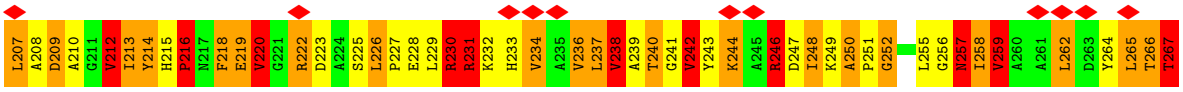
• Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN

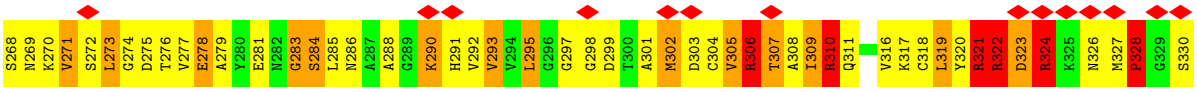


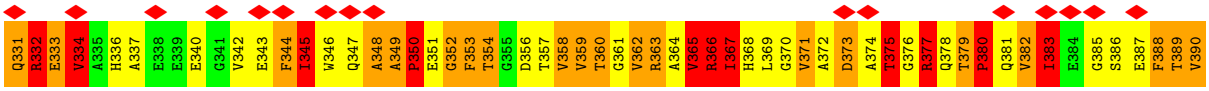




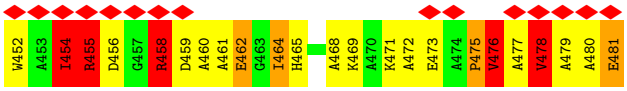








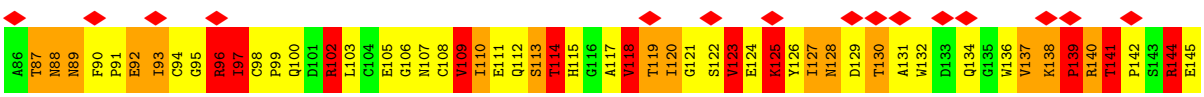


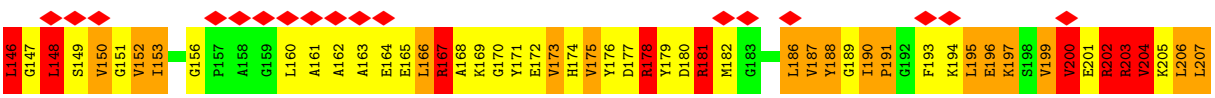


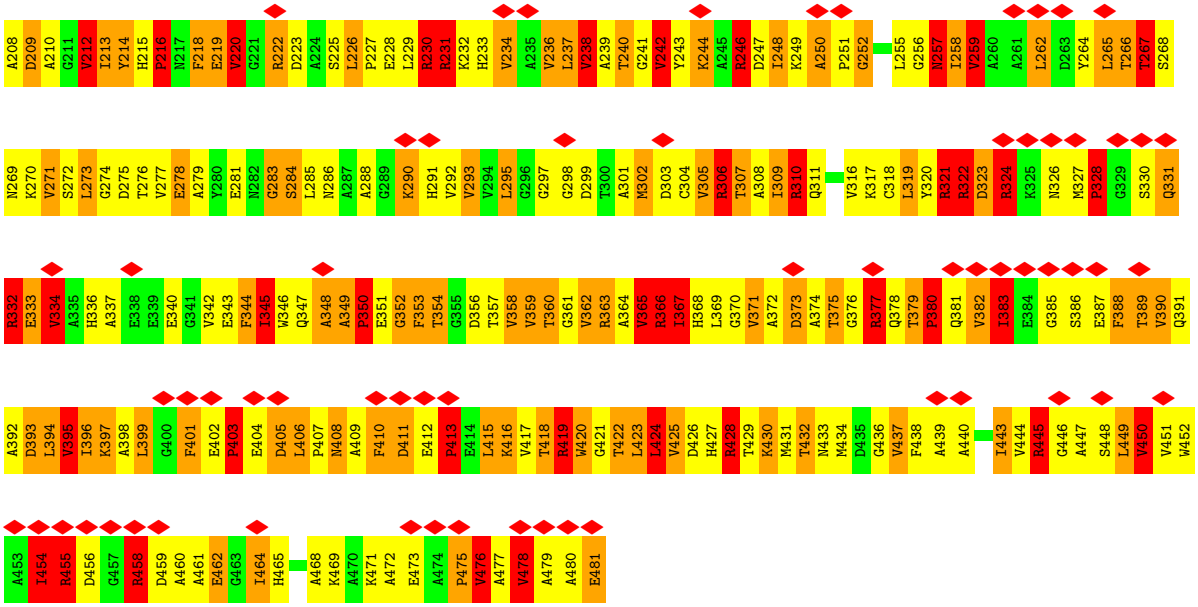
• Molecule 2: GLUTAMATE SYNTHASE [NADPH] SMALL CHAIN










A208 D209 A210 G211 V212 I213 Y214 H215 P216 N217 F218 E219 V220 G221 R222 D223 A224 S225 L226 P227 E228 L229 R230 R231 K232 H233 V234 A235 V236 L237 V238 A239 T240 G241 V242 Y243 K244 A245 R246 D247 I248 K249 A250 P251 G252 L255 G256 N257 I258 V259 A260 A261 L262 D263 Y264 L265 T266 I267 S268
N269 K270 V271 S272 L273 G274 D275 T276 V277 E278 A279 Y280 E281 N282 G283 S284 L285 N286 A287 A288 G289 K290 H291 V292 V293 V294 L295 G296 G297 G298 D299 T300 A301 M302 D303 C304 V305 R306 T307 A308 I309 R310 Q311 V316 K317 C318 L319 Y320 R321 R322 D323 R324 K325 N326 M327 P328 G329 S330 Q331
R332 E333 V334 A335 H336 A337 E338 E339 E340 G341 V342 E343 F344 I345 W346 Q347 A348 A349 P350 E351 G352 F353 T354 G355 D356 T357 V358 V359 T360 G361 V362 R363 A364 V365 R366 I367 H368 L369 G370 V371 A372 D373 A374 T375 G376 R377 Q378 T379 P380 Q381 V382 I383 E384 G385 S386 E387 F388 T389 V390 Q391
A392 D393 L394 V395 I396 K397 A398 L399 G400 F401 E402 P403 E404 D405 L406 P407 N408 A409 F410 D411 E412 P413 E414 L415 K416 V417 T418 R419 W420 G421 T422 L423 L424 V425 D426 H427 R428 T429 K430 M431 T432 N433 M434 D435 G436 V437 F438 A439 A440 I443 V444 R445 G446 A447 S448 L449 V450 V451 W452
A453 I454 R455 D456 G457 R458 D459 A460 A461 E462 G463 I464 H465 A468 K469 A470 K471 A472 E473 A474 P475 V476 A477 V478 A479 A480 E481

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, I	Depositor
Number of particles used	12800	Depositor
Resolution determination method	Not provided	
CTF correction method	WIENER FILTERING OF VOLUMES FROM FOCAL SERIES	Depositor
Microscope	JEOL 2010UHR	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	10	Depositor
Minimum defocus (nm)	1700	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	1332.420	Depositor
Minimum map value	-799.538	Depositor
Average map value	5.063	Depositor
Map value standard deviation	98.686	Depositor
Recommended contour level	125	Depositor
Map size (Å)	304.8, 304.8, 304.8	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90, 90, 90	wwPDB
Pixel spacing (Å)	1.5875, 1.5875, 1.5875	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, AKG, OMT, FAD, F3S, FMN

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	1.45	82/11545 (0.7%)	2.02	427/15613 (2.7%)
1	B	1.49	96/11545 (0.8%)	2.00	415/15613 (2.7%)
1	C	1.45	81/11545 (0.7%)	2.02	427/15613 (2.7%)
1	D	1.49	96/11545 (0.8%)	2.00	416/15613 (2.7%)
1	E	1.45	82/11545 (0.7%)	2.02	427/15613 (2.7%)
1	F	1.49	94/11545 (0.8%)	2.00	415/15613 (2.7%)
2	G	1.39	1/3533 (0.0%)	2.29	190/4793 (4.0%)
2	H	1.39	1/3533 (0.0%)	2.29	188/4793 (3.9%)
2	I	1.39	1/3533 (0.0%)	2.29	190/4793 (4.0%)
2	J	1.39	1/3533 (0.0%)	2.29	190/4793 (4.0%)
2	K	1.39	1/3533 (0.0%)	2.29	190/4793 (4.0%)
2	L	1.39	1/3533 (0.0%)	2.29	188/4793 (3.9%)
All	All	1.45	537/90468 (0.6%)	2.08	3663/122436 (3.0%)

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
1	A	1	3
1	B	0	2
1	C	1	3
1	D	0	2
1	E	1	3
1	F	0	2
2	G	0	31
2	H	0	31
2	I	0	31
2	J	0	31
2	K	0	31

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Mol	Chain	#Chirality outliers	#Planarity outliers
2	L	0	31
All	All	3	201

The worst 5 of 537 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	838	VAL	CA-CB	-18.99	1.38	1.55
1	A	838	VAL	CA-CB	-18.92	1.38	1.55
1	E	838	VAL	CA-CB	-18.88	1.38	1.55
1	E	746	ILE	CA-CB	-13.00	1.37	1.54
1	A	746	ILE	CA-CB	-12.94	1.37	1.54

The worst 5 of 3663 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	45	ASN	CB-CG-OD1	-39.59	41.63	120.80
2	L	45	ASN	CB-CG-OD1	-39.59	41.63	120.80
2	G	45	ASN	CB-CG-OD1	-39.58	41.65	120.80
2	J	45	ASN	CB-CG-OD1	-39.58	41.65	120.80
2	I	45	ASN	CB-CG-OD1	-39.55	41.70	120.80

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	915	PHE	CA
1	C	915	PHE	CA
1	E	915	PHE	CA

5 of 201 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1002	SER	Mainchain
1	A	1171	VAL	Peptide
1	A	325	GLU	Mainchain
1	B	1168	LEU	Mainchain
1	B	725	PHE	Mainchain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11337	0	11347	1843	0
1	B	11337	0	11350	1645	0
1	C	11337	0	11347	1848	0
1	D	11337	0	11350	1640	0
1	E	11337	0	11347	1862	0
1	F	11337	0	11350	1631	0
2	G	3468	0	3397	1119	0
2	H	3468	0	3397	1113	0
2	I	3468	0	3397	1118	0
2	J	3468	0	3399	1104	0
2	K	3468	0	3399	1101	0
2	L	3468	0	3399	1110	0
3	A	11	0	10	3	0
3	B	11	0	10	2	0
3	C	11	0	10	3	0
3	D	11	0	10	2	0
3	E	11	0	10	3	0
3	F	11	0	10	2	0
4	A	31	0	19	5	0
4	B	31	0	19	8	0
4	C	31	0	19	4	0
4	D	31	0	19	8	0
4	E	31	0	19	5	0
4	F	31	0	19	7	0
5	A	10	0	4	0	0
5	B	10	0	4	2	0
5	C	10	0	4	0	0
5	D	10	0	4	3	0
5	E	10	0	4	0	0
5	F	10	0	4	2	0
6	A	7	0	0	1	0
6	B	7	0	0	3	0
6	C	7	0	0	1	0
6	D	7	0	0	3	0
6	E	7	0	0	2	0
6	F	7	0	0	3	0
7	G	16	0	0	3	0
7	H	16	0	0	3	0
7	I	16	0	0	3	0
7	J	16	0	0	3	0
7	K	16	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	L	16	0	0	3	0
8	G	53	0	31	17	0
8	H	53	0	31	17	0
8	I	53	0	31	17	0
8	J	53	0	31	17	0
8	K	53	0	31	17	0
8	L	53	0	31	17	0
All	All	89598	0	88863	16126	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 90.

The worst 5 of 16126 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1263:HIS:CE1	1:D:900:GLY:CA	1.77	1.66
1:A:782:ARG:CG	2:J:53:PRO:HD2	1.19	1.65
1:E:782:ARG:CG	2:L:53:PRO:HD2	1.19	1.64
1:C:875:MET:HE1	1:C:1139:PHE:CE2	1.35	1.62
1:F:182:MET:CE	1:F:217:PRO:HB2	1.30	1.61

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	1470/1472 (100%)	1174 (80%)	231 (16%)	65 (4%)	2	17
1	B	1470/1472 (100%)	1191 (81%)	215 (15%)	64 (4%)	2	17
1	C	1470/1472 (100%)	1175 (80%)	230 (16%)	65 (4%)	2	17
1	D	1470/1472 (100%)	1191 (81%)	215 (15%)	64 (4%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	1470/1472 (100%)	1174 (80%)	231 (16%)	65 (4%)	2	17
1	F	1470/1472 (100%)	1192 (81%)	214 (15%)	64 (4%)	2	17
2	G	454/456 (100%)	419 (92%)	25 (6%)	10 (2%)	5	29
2	H	454/456 (100%)	420 (92%)	24 (5%)	10 (2%)	5	29
2	I	454/456 (100%)	420 (92%)	24 (5%)	10 (2%)	5	29
2	J	454/456 (100%)	419 (92%)	25 (6%)	10 (2%)	5	29
2	K	454/456 (100%)	420 (92%)	24 (5%)	10 (2%)	5	29
2	L	454/456 (100%)	420 (92%)	24 (5%)	10 (2%)	5	29
All	All	11544/11568 (100%)	9615 (83%)	1482 (13%)	447 (4%)	4	19

5 of 447 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	LEU
1	A	444	LYS
1	A	451	GLN
1	A	705	LEU
1	A	712	GLY

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	1201/1201 (100%)	948 (79%)	253 (21%)	1	6
1	B	1201/1201 (100%)	953 (79%)	248 (21%)	1	6
1	C	1201/1201 (100%)	949 (79%)	252 (21%)	1	6
1	D	1201/1201 (100%)	953 (79%)	248 (21%)	1	6
1	E	1201/1201 (100%)	949 (79%)	252 (21%)	1	6
1	F	1201/1201 (100%)	953 (79%)	248 (21%)	1	6
2	G	358/358 (100%)	248 (69%)	110 (31%)	0	2
2	H	358/358 (100%)	248 (69%)	110 (31%)	0	2

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	I	358/358 (100%)	248 (69%)	110 (31%)	0 2
2	J	358/358 (100%)	248 (69%)	110 (31%)	0 2
2	K	358/358 (100%)	248 (69%)	110 (31%)	0 2
2	L	358/358 (100%)	248 (69%)	110 (31%)	0 2
All	All	9354/9354 (100%)	7193 (77%)	2161 (23%)	2 5

5 of 2161 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	152	VAL
2	J	375	THR
2	J	148	LEU
2	L	197	LYS
1	D	189	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 319 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	242	ASN
2	I	134	GLN
1	F	452	GLN
1	F	1318	ASN
2	K	45	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

42 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	AKG	B	2475	-	9,9,9	3.48	4 (44%)	11,11,11	2.80	4 (36%)
3	OMT	A	2473	-	9,10,10	4.28	5 (55%)	11,14,14	4.47	6 (54%)
4	FMN	A	2474	-	33,33,33	1.48	5 (15%)	48,50,50	2.72	20 (41%)
8	FAD	L	484	-	56,58,58	1.78	18 (32%)	81,89,89	1.17	8 (9%)
5	AKG	C	2475	-	9,9,9	3.08	4 (44%)	11,11,11	2.92	4 (36%)
4	FMN	F	2474	-	33,33,33	1.37	4 (12%)	48,50,50	2.59	20 (41%)
7	SF4	K	483	2	0,12,12	-	-	-		
7	SF4	J	482	2	0,12,12	-	-	-		
6	F3S	D	2476	1	0,9,9	-	-	-		
3	OMT	F	2473	-	9,10,10	4.15	5 (55%)	11,14,14	5.79	5 (45%)
6	F3S	E	2476	1	0,9,9	-	-	-		
6	F3S	F	2476	1	0,9,9	-	-	-		
7	SF4	I	483	2	0,12,12	-	-	-		
7	SF4	I	482	2	0,12,12	-	-	-		
6	F3S	B	2476	1	0,9,9	-	-	-		
5	AKG	A	2475	-	9,9,9	3.09	4 (44%)	11,11,11	2.92	4 (36%)
8	FAD	G	484	-	56,58,58	1.78	18 (32%)	81,89,89	1.17	7 (8%)
7	SF4	K	482	2	0,12,12	-	-	-		
4	FMN	E	2474	-	33,33,33	1.48	5 (15%)	48,50,50	2.73	20 (41%)
4	FMN	C	2474	-	33,33,33	1.48	5 (15%)	48,50,50	2.73	20 (41%)
8	FAD	J	484	-	56,58,58	1.78	18 (32%)	81,89,89	1.17	7 (8%)
5	AKG	F	2475	-	9,9,9	3.48	4 (44%)	11,11,11	2.80	4 (36%)
7	SF4	J	483	2	0,12,12	-	-	-		
3	OMT	B	2473	-	9,10,10	4.15	5 (55%)	11,14,14	5.78	5 (45%)
4	FMN	B	2474	-	33,33,33	1.37	4 (12%)	48,50,50	2.59	20 (41%)
3	OMT	D	2473	-	9,10,10	4.14	5 (55%)	11,14,14	5.79	5 (45%)
3	OMT	E	2473	-	9,10,10	4.27	5 (55%)	11,14,14	4.46	6 (54%)
6	F3S	C	2476	1	0,9,9	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	F3S	A	2476	1	0,9,9	-	-	-		
3	OMT	C	2473	-	9,10,10	4.28	5 (55%)	11,14,14	4.47	6 (54%)
5	AKG	D	2475	-	9,9,9	3.49	4 (44%)	11,11,11	2.80	4 (36%)
5	AKG	E	2475	-	9,9,9	3.08	4 (44%)	11,11,11	2.91	4 (36%)
7	SF4	H	483	2	0,12,12	-	-	-		
7	SF4	G	483	2	0,12,12	-	-	-		
8	FAD	I	484	-	56,58,58	1.78	18 (32%)	81,89,89	1.17	7 (8%)
8	FAD	K	484	-	56,58,58	1.78	18 (32%)	81,89,89	1.17	7 (8%)
7	SF4	H	482	2	0,12,12	-	-	-		
7	SF4	G	482	2	0,12,12	-	-	-		
7	SF4	L	483	2	0,12,12	-	-	-		
4	FMN	D	2474	-	33,33,33	1.37	4 (12%)	48,50,50	2.59	20 (41%)
7	SF4	L	482	2	0,12,12	-	-	-		
8	FAD	H	484	-	56,58,58	1.78	18 (32%)	81,89,89	1.17	8 (9%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	AKG	B	2475	-	-	1/9/9/9	-
3	OMT	A	2473	-	-	5/10/10/10	-
4	FMN	A	2474	-	-	7/18/18/18	0/3/3/3
8	FAD	L	484	-	-	4/34/50/50	0/6/6/6
5	AKG	C	2475	-	-	2/9/9/9	-
4	FMN	F	2474	-	-	4/18/18/18	0/3/3/3
7	SF4	K	483	2	-	-	0/6/5/5
7	SF4	J	482	2	-	-	0/6/5/5
6	F3S	D	2476	1	-	-	0/3/3/3
3	OMT	F	2473	-	-	5/10/10/10	-
6	F3S	E	2476	1	-	-	0/3/3/3
6	F3S	F	2476	1	-	-	0/3/3/3
7	SF4	I	483	2	-	-	0/6/5/5
7	SF4	I	482	2	-	-	0/6/5/5
6	F3S	B	2476	1	-	-	0/3/3/3
5	AKG	A	2475	-	-	2/9/9/9	-
8	FAD	G	484	-	-	4/34/50/50	0/6/6/6
7	SF4	K	482	2	-	-	0/6/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	FMN	E	2474	-	-	7/18/18/18	0/3/3/3
4	FMN	C	2474	-	-	7/18/18/18	0/3/3/3
8	FAD	J	484	-	-	4/34/50/50	0/6/6/6
5	AKG	F	2475	-	-	1/9/9/9	-
7	SF4	J	483	2	-	-	0/6/5/5
3	OMT	B	2473	-	-	5/10/10/10	-
4	FMN	B	2474	-	-	4/18/18/18	0/3/3/3
3	OMT	D	2473	-	-	5/10/10/10	-
3	OMT	E	2473	-	-	5/10/10/10	-
6	F3S	C	2476	1	-	-	0/3/3/3
6	F3S	A	2476	1	-	-	0/3/3/3
3	OMT	C	2473	-	-	5/10/10/10	-
5	AKG	D	2475	-	-	1/9/9/9	-
5	AKG	E	2475	-	-	2/9/9/9	-
8	FAD	K	484	-	-	4/34/50/50	0/6/6/6
8	FAD	I	484	-	-	4/34/50/50	0/6/6/6
7	SF4	G	483	2	-	-	0/6/5/5
7	SF4	H	483	2	-	-	0/6/5/5
7	SF4	H	482	2	-	-	0/6/5/5
7	SF4	G	482	2	-	-	0/6/5/5
7	SF4	L	483	2	-	-	0/6/5/5
4	FMN	D	2474	-	-	4/18/18/18	0/3/3/3
7	SF4	L	482	2	-	-	0/6/5/5
8	FAD	H	484	-	-	4/34/50/50	0/6/6/6

The worst 5 of 189 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2473	OMT	CB-CG	-7.01	1.45	1.52
3	A	2473	OMT	CB-CG	-6.97	1.45	1.52
3	E	2473	OMT	CB-CG	-6.93	1.45	1.52
3	B	2473	OMT	CG-SD	-6.88	1.69	1.78
3	F	2473	OMT	CG-SD	-6.86	1.69	1.78

The worst 5 of 221 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	2473	OMT	OD2-SD-CG	-16.66	96.68	108.34
3	F	2473	OMT	OD2-SD-CG	-16.64	96.69	108.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	2473	OMT	OD2-SD-CG	-16.63	96.70	108.34
3	C	2473	OMT	OD2-SD-CE	-11.63	97.22	108.91
3	A	2473	OMT	OD2-SD-CE	-11.61	97.24	108.91

There are no chirality outliers.

5 of 96 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2473	OMT	C-CA-CB-CG
3	A	2473	OMT	CB-CG-SD-OD1
3	A	2473	OMT	CB-CG-SD-OD2
3	B	2473	OMT	N-CA-CB-CG
3	B	2473	OMT	C-CA-CB-CG

There are no ring outliers.

39 monomers are involved in 192 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	2475	AKG	2	0
3	A	2473	OMT	3	0
4	A	2474	FMN	5	0
8	L	484	FAD	17	0
4	F	2474	FMN	7	0
7	K	483	SF4	2	0
7	J	482	SF4	1	0
6	D	2476	F3S	3	0
3	F	2473	OMT	2	0
6	E	2476	F3S	2	0
6	F	2476	F3S	3	0
7	I	483	SF4	2	0
7	I	482	SF4	1	0
6	B	2476	F3S	3	0
8	G	484	FAD	17	0
7	K	482	SF4	1	0
4	E	2474	FMN	5	0
4	C	2474	FMN	4	0
8	J	484	FAD	17	0
5	F	2475	AKG	2	0
7	J	483	SF4	2	0
3	B	2473	OMT	2	0
4	B	2474	FMN	8	0

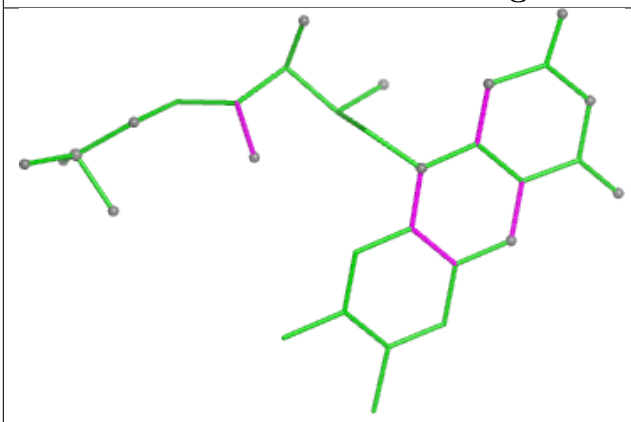
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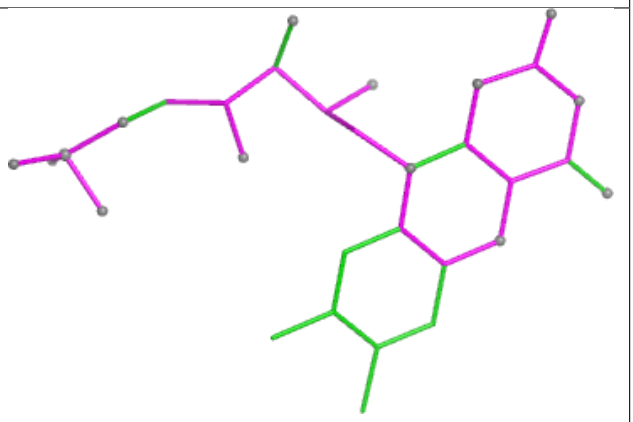
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2473	OMT	2	0
3	E	2473	OMT	3	0
6	C	2476	F3S	1	0
6	A	2476	F3S	1	0
3	C	2473	OMT	3	0
5	D	2475	AKG	3	0
7	H	483	SF4	2	0
7	G	483	SF4	2	0
8	I	484	FAD	17	0
8	K	484	FAD	17	0
7	H	482	SF4	1	0
7	G	482	SF4	1	0
7	L	483	SF4	2	0
4	D	2474	FMN	8	0
7	L	482	SF4	1	0
8	H	484	FAD	17	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

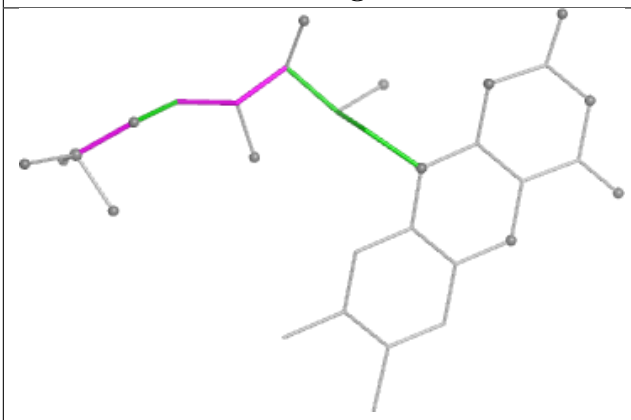
Ligand FMN A 2474



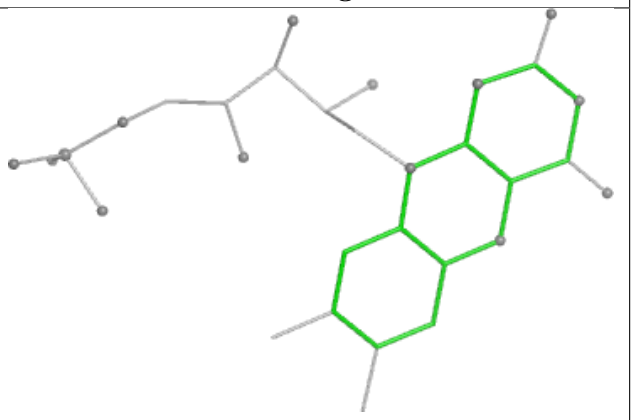
Bond lengths



Bond angles

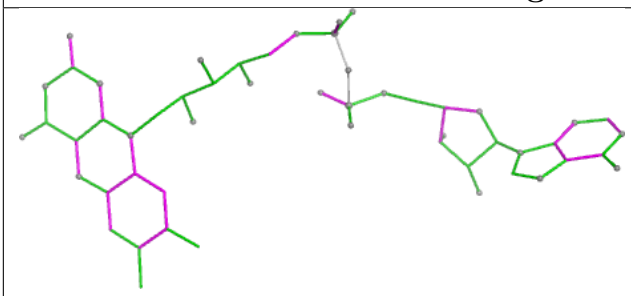


Torsions

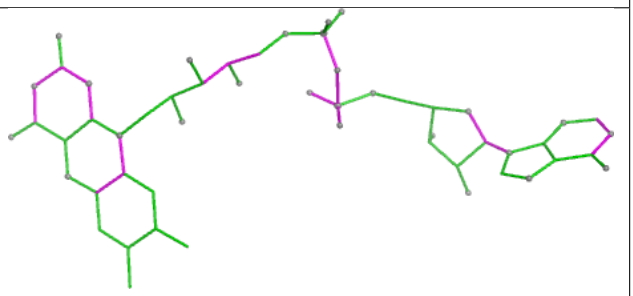


Rings

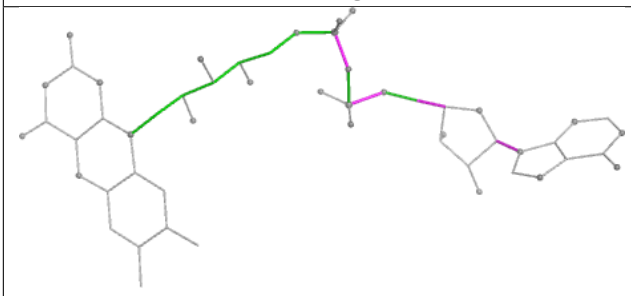
Ligand FAD L 484



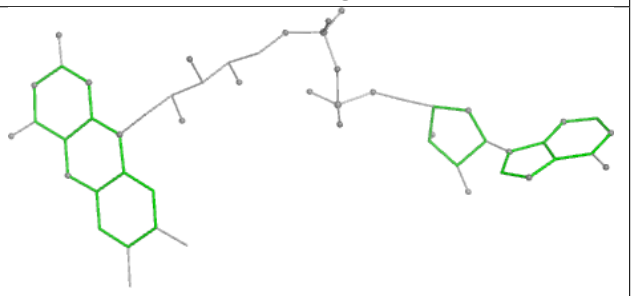
Bond lengths



Bond angles

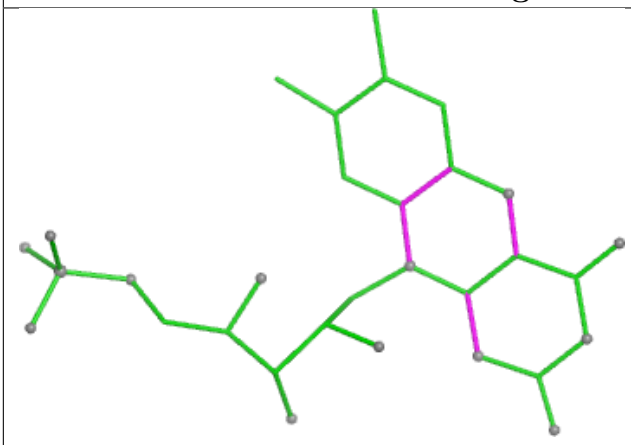


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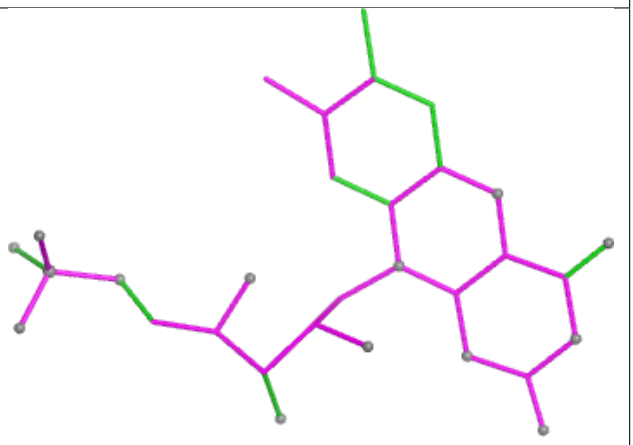


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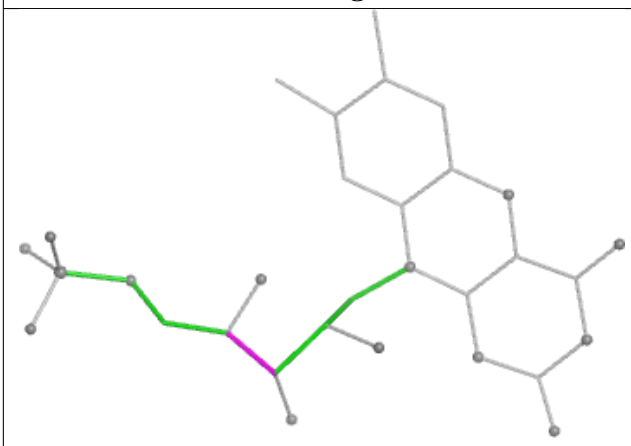
Ligand FMN F 2474



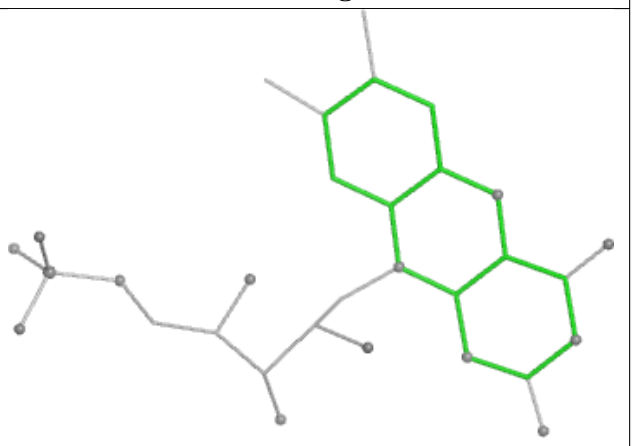
Bond lengths



Bond angles

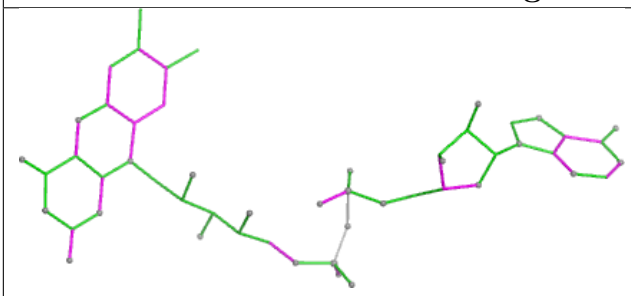


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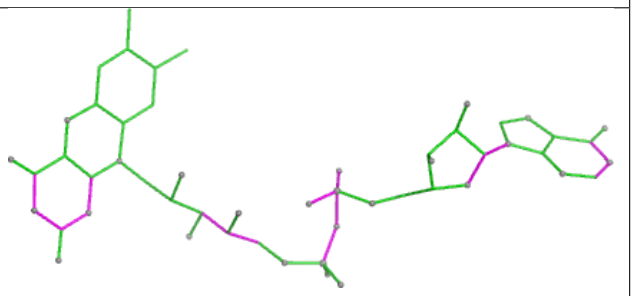


Rings

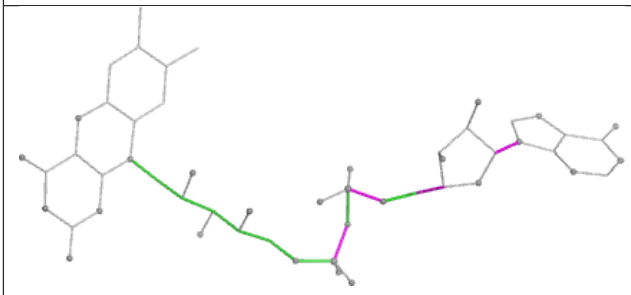
Ligand FAD G 484



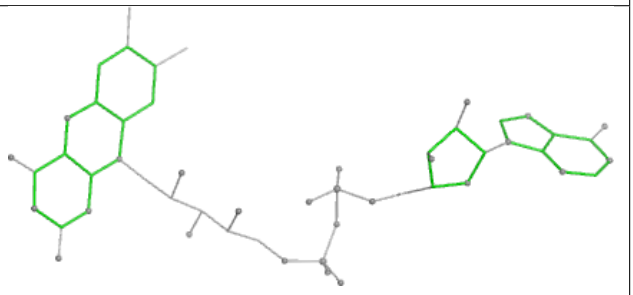
Bond lengths



Bond angles

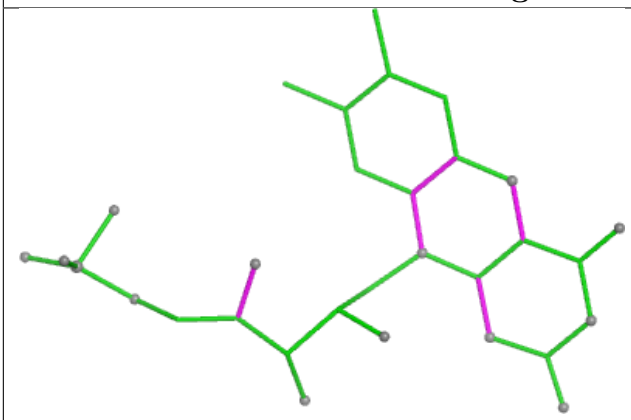


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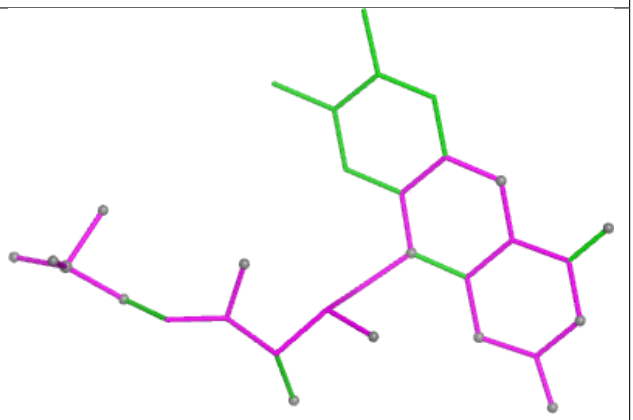


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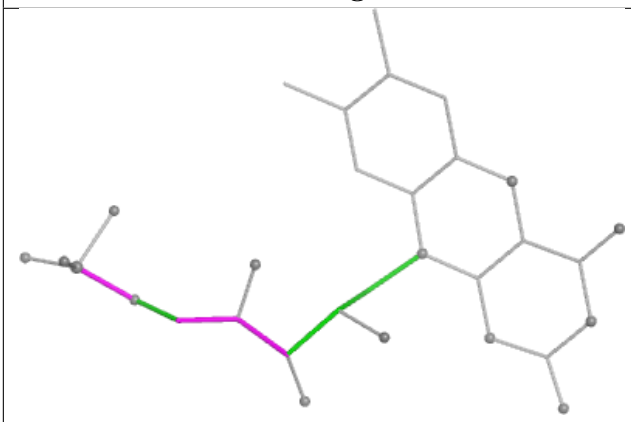
Ligand FMN E 2474



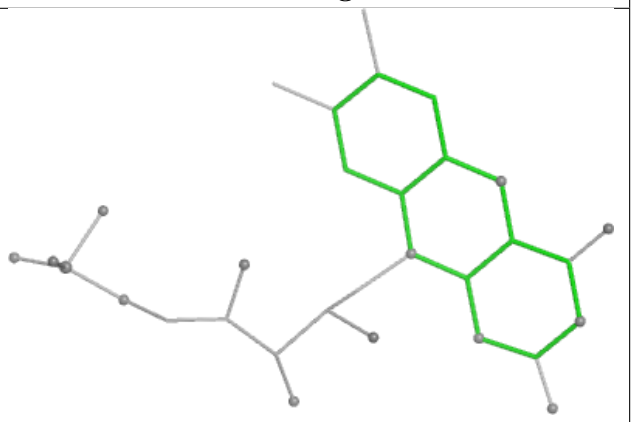
Bond lengths



Bond angles

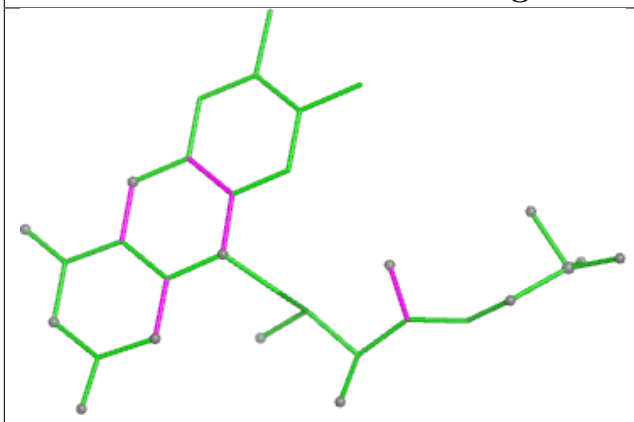


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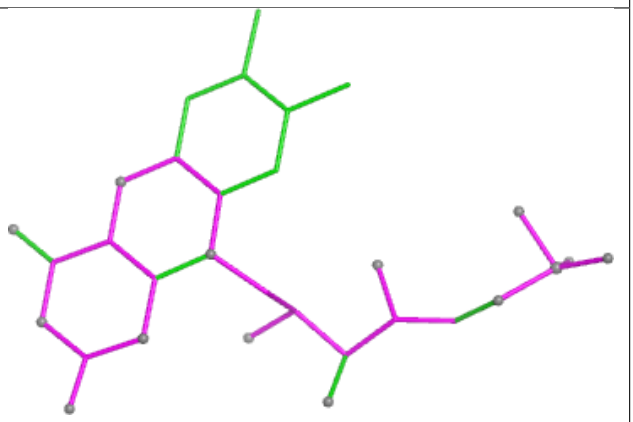


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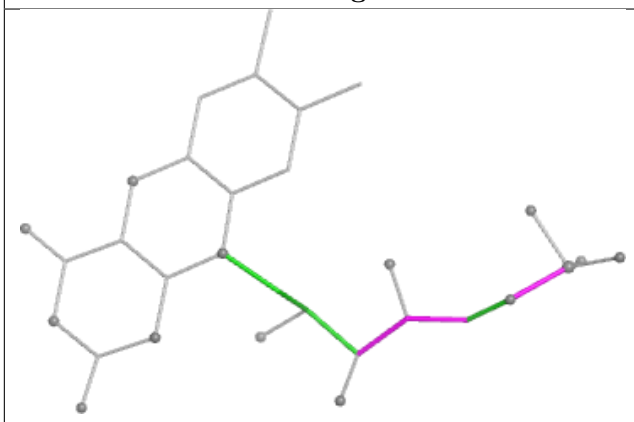
Ligand FMN C 2474



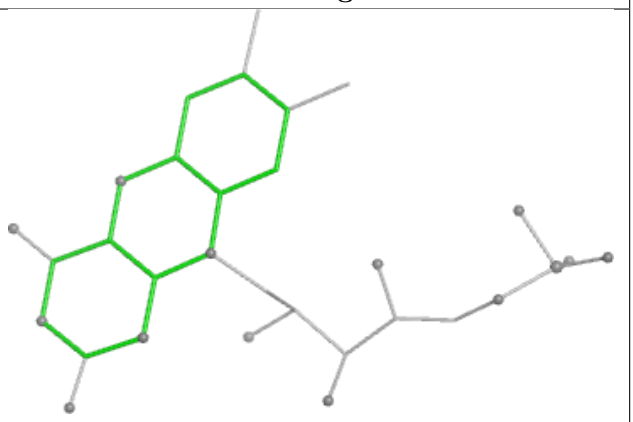
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Bond angles

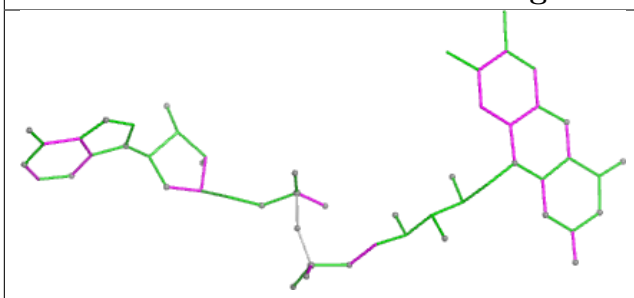


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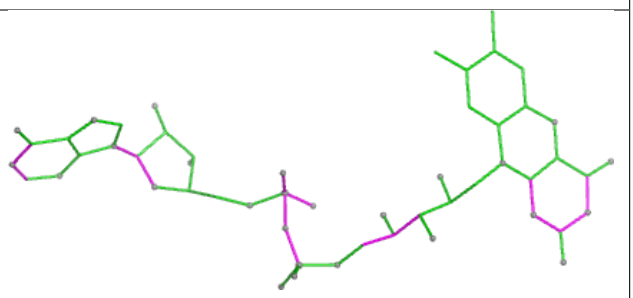


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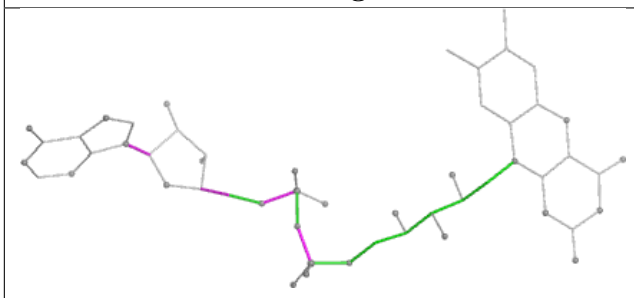
Ligand FAD J 484



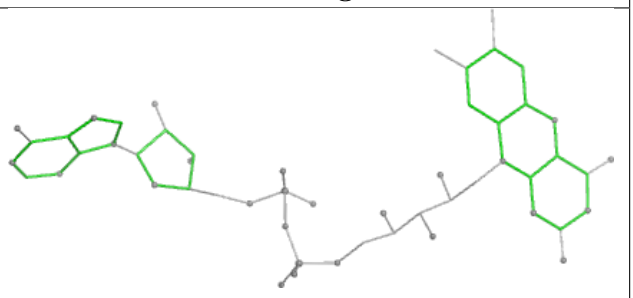
Bond lengths



Bond angles

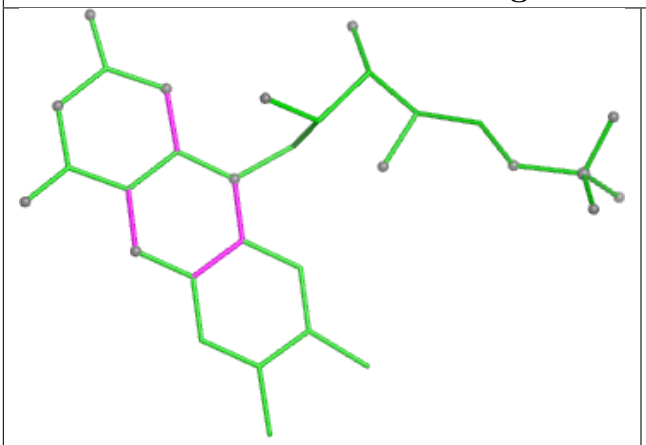


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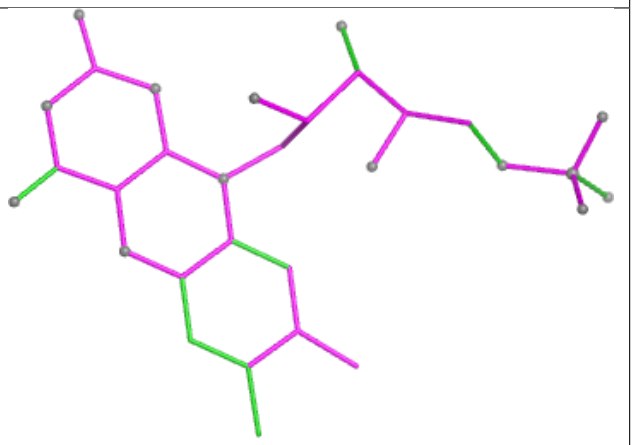


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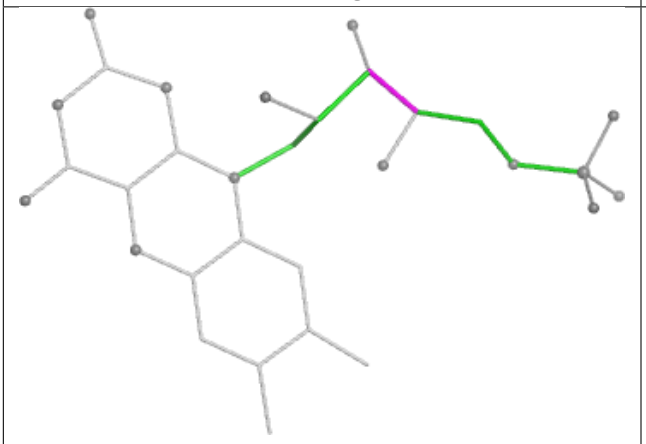
Ligand FMN B 2474



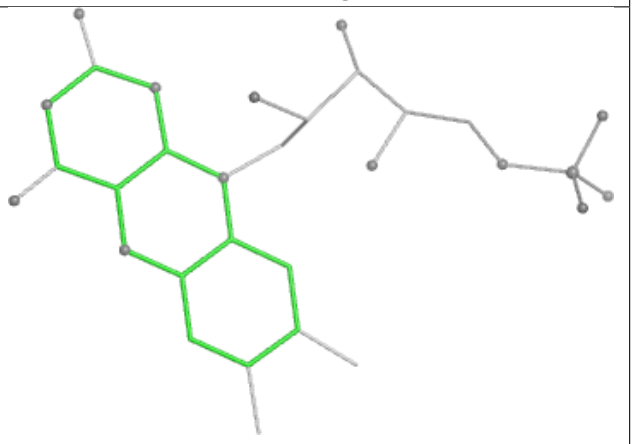
Bond lengths



Bond angles

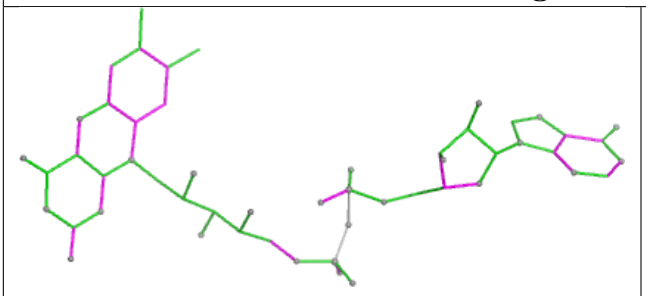


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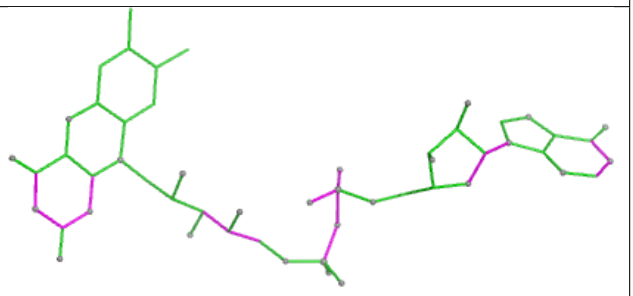


Rings

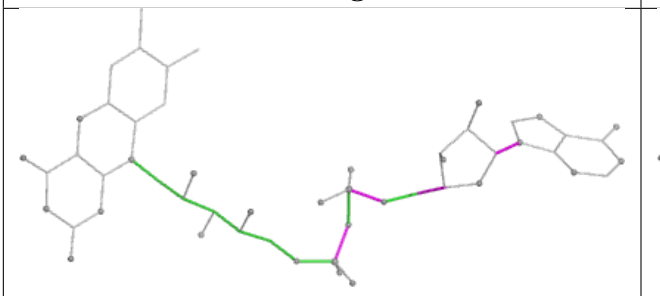
Ligand FAD I 484



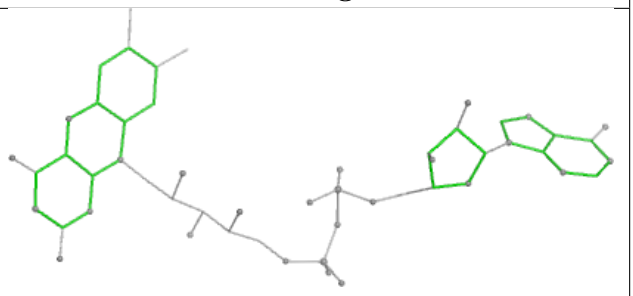
Bond lengths



Bond angles

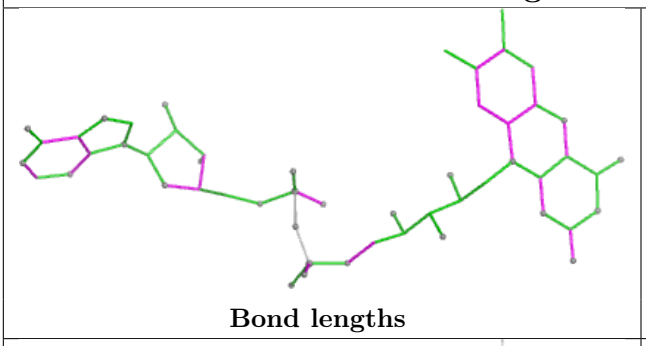


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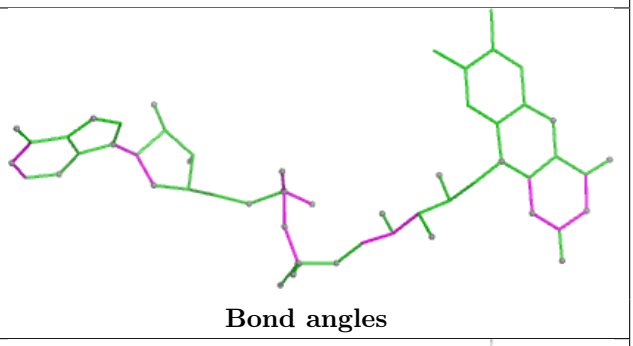


Rings

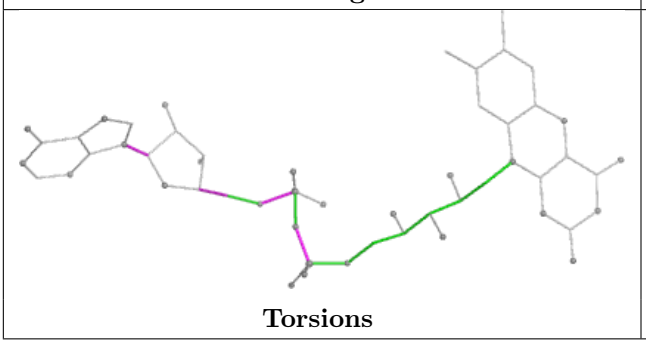
Ligand FAD K 484



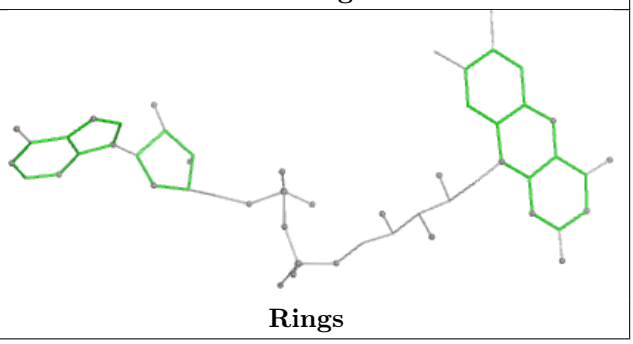
Bond lengths



Bond angles

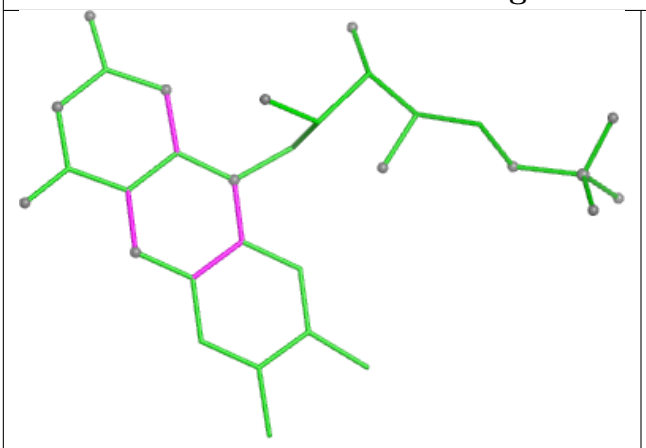


Torsions

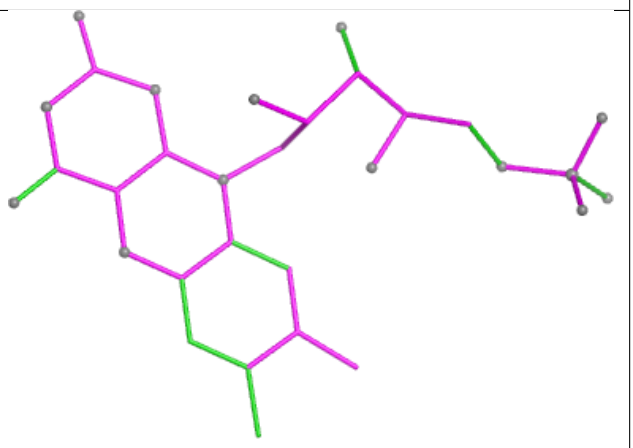


Rings

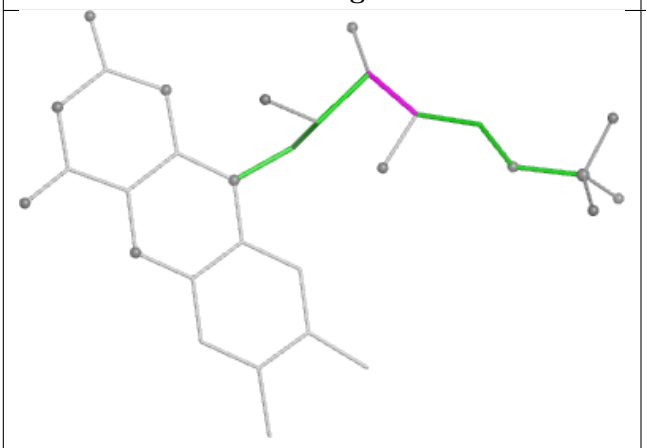
Ligand FMN D 2474



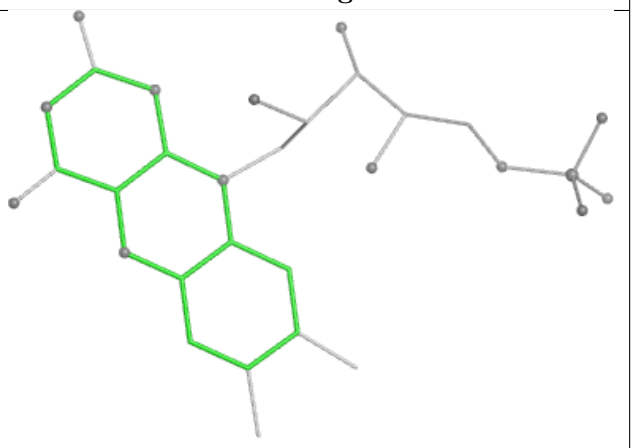
Bond lengths



Bond angles

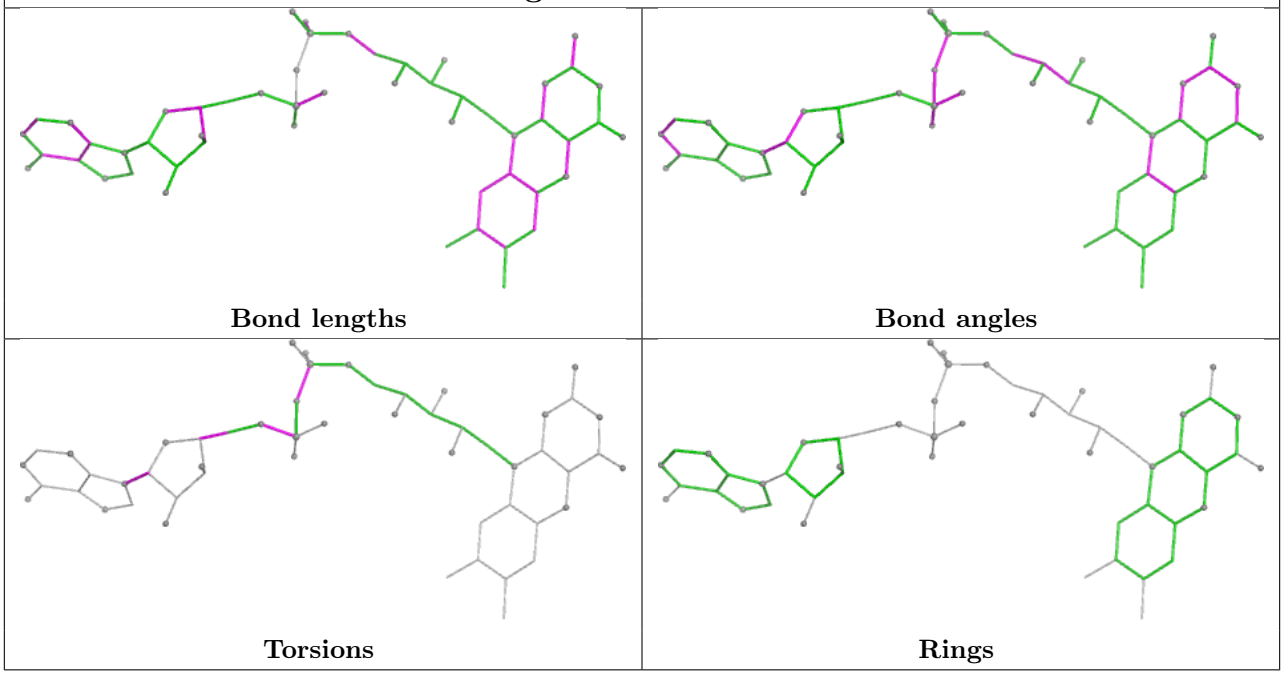


Torsions



Rings

Ligand FAD H 484



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.

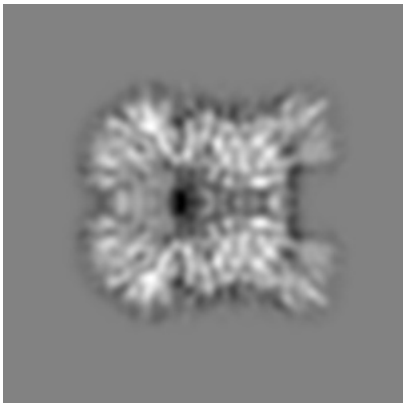
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-1440. These allow visual inspection of the internal detail of the map and identification of artifacts.

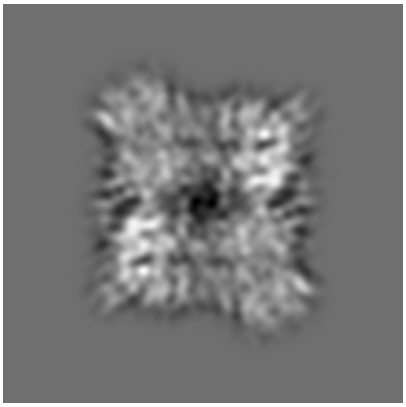
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

6.1.1 Primary map



X



Y

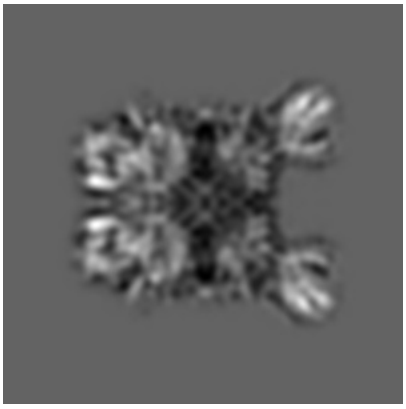


Z

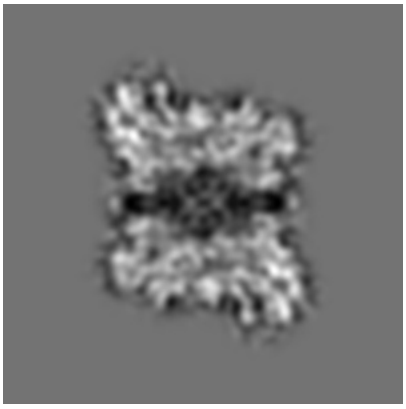
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 96



Y Index: 96

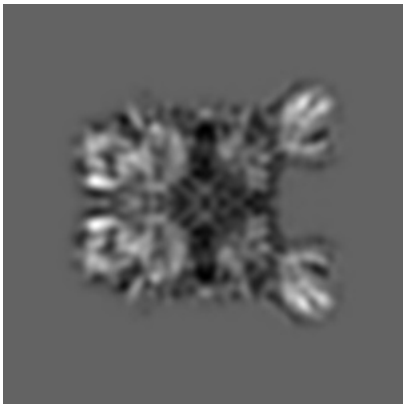


Z Index: 96

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: 96



Y Index: 98



Z Index: 59

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

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

6.4.1 Primary map



X



Y

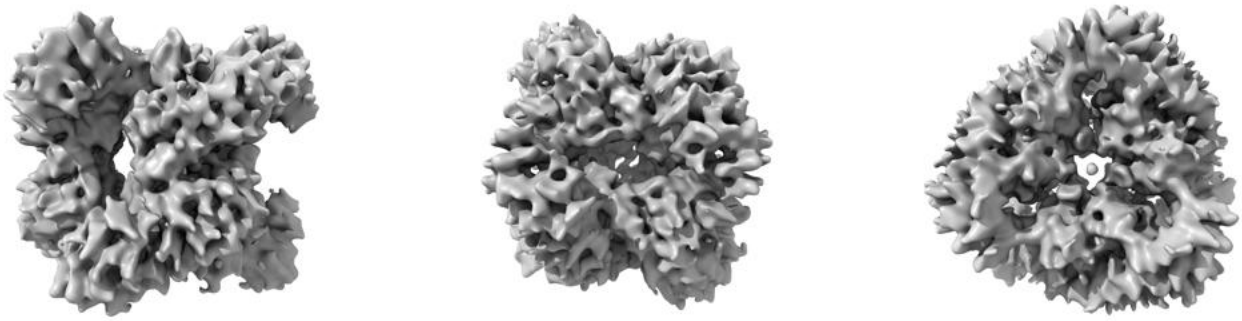


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 125.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

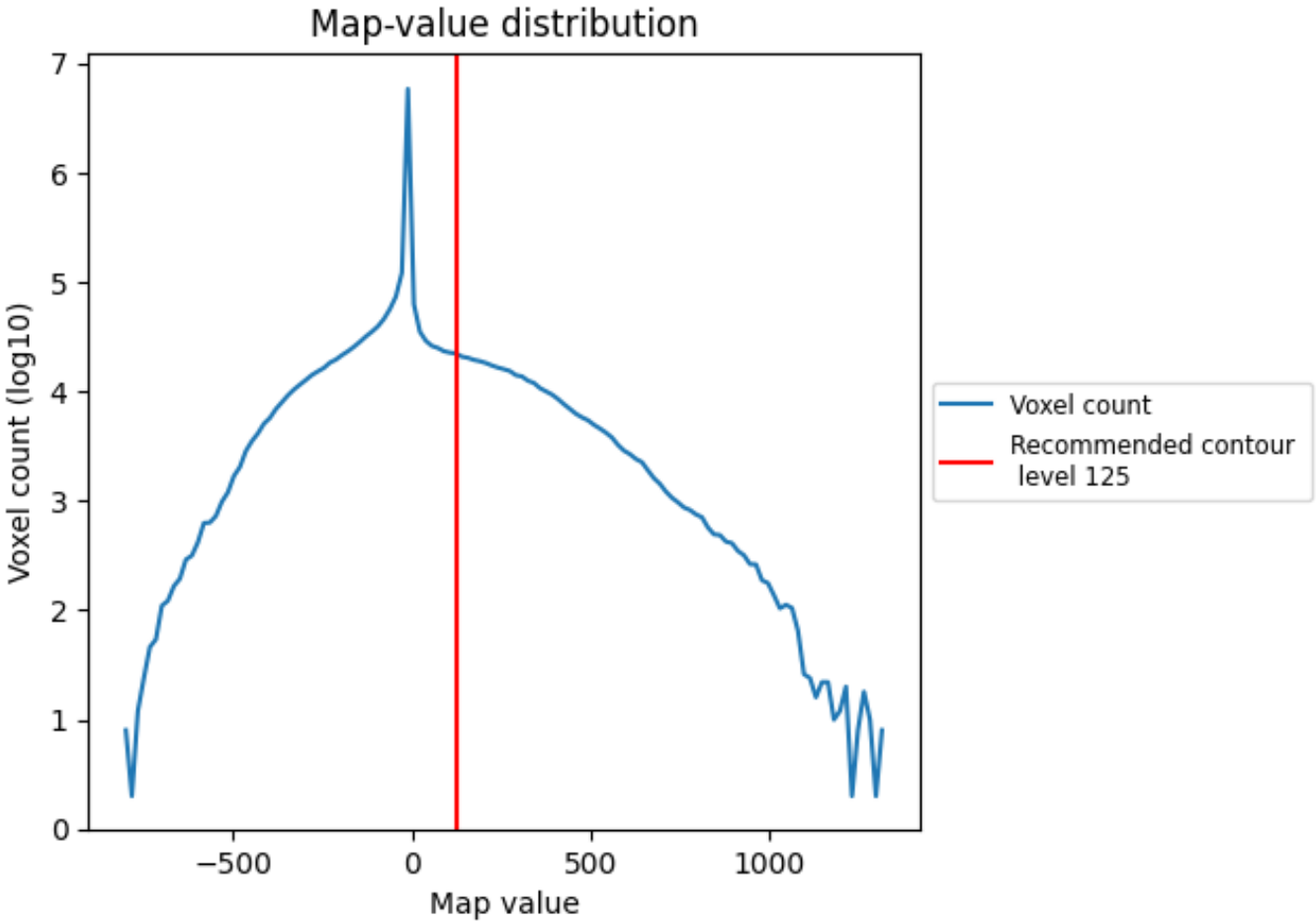
6.6 Mask visualisation (i)

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

7 Map analysis

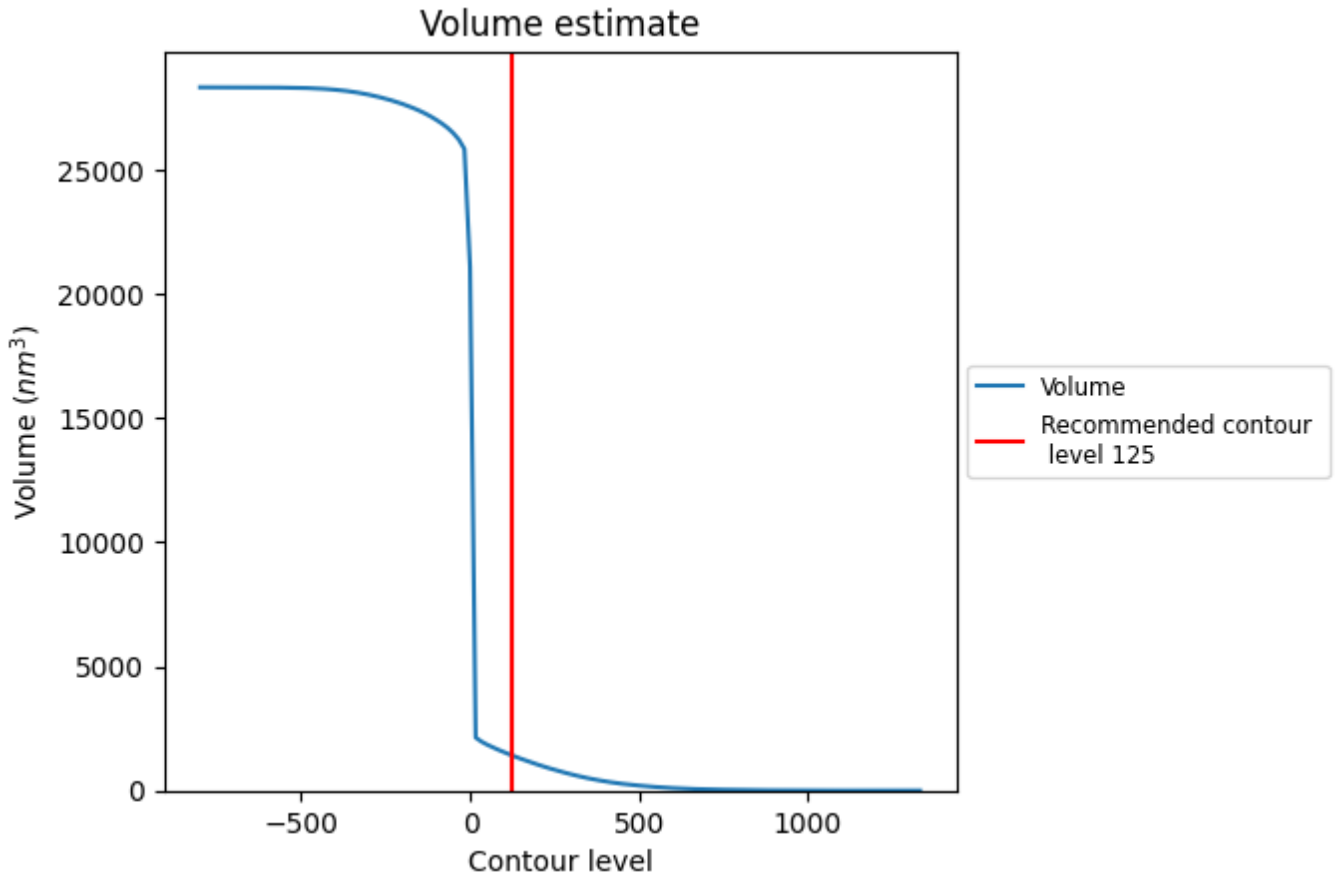
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

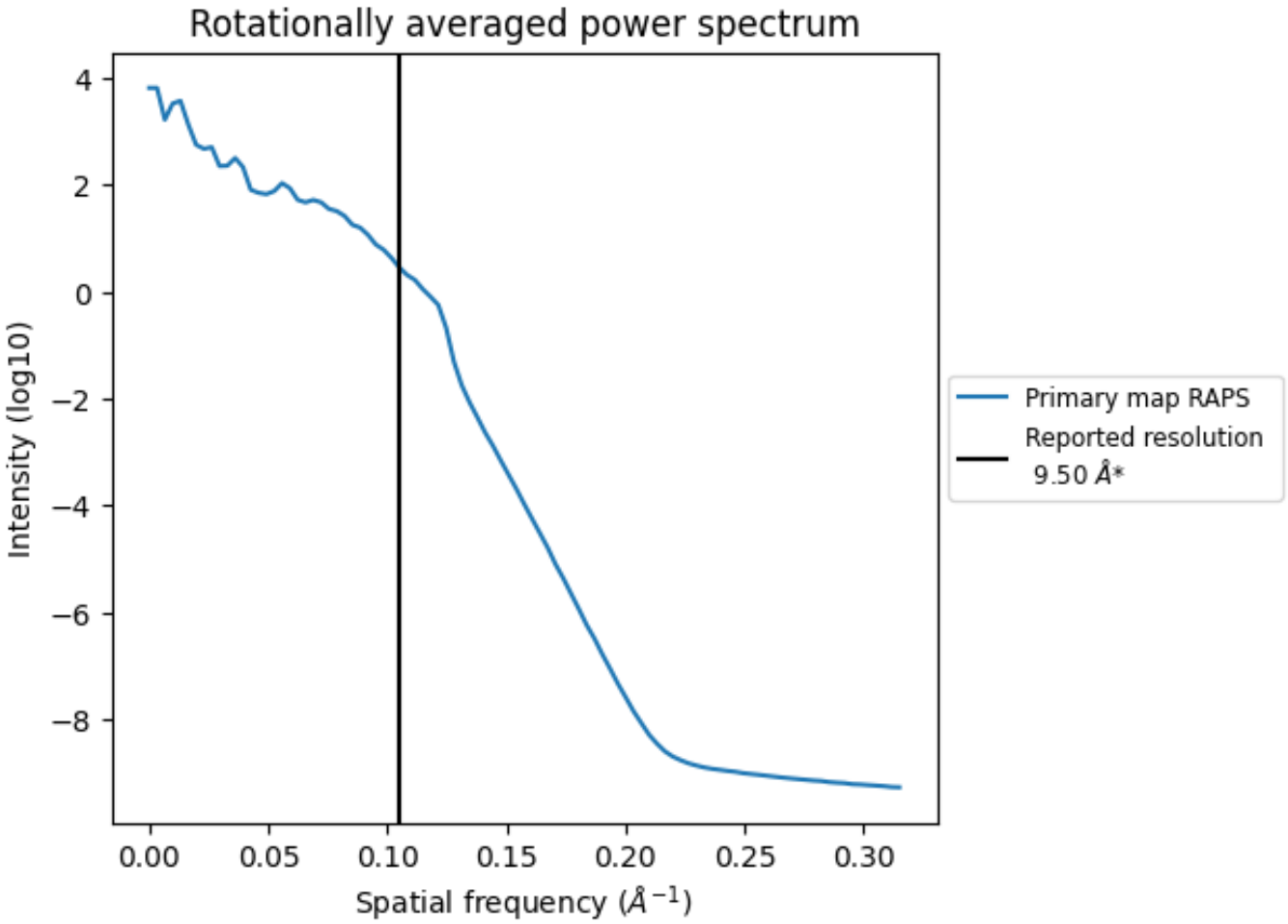
7.2 Volume estimate (i)



The volume at the recommended contour level is 1412 nm^3; this corresponds to an approximate mass of 1276 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)

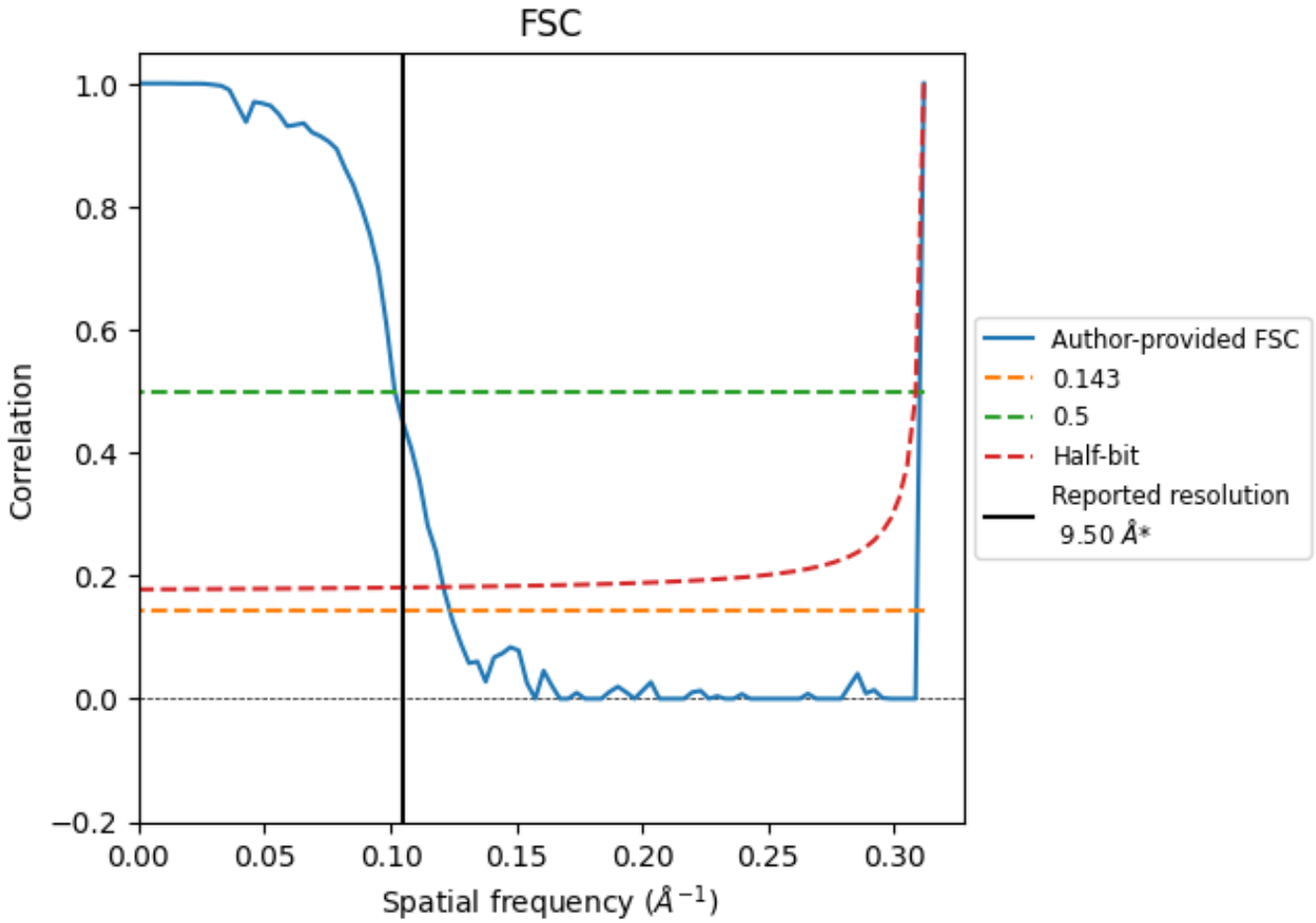


*Reported resolution corresponds to spatial frequency of 0.105 Å^{-1}

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 0.105 Å^{-1}

8.2 Resolution estimates (i)

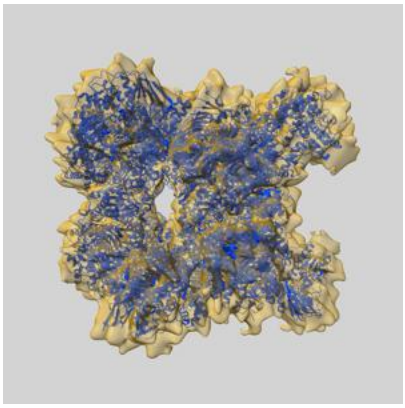
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	-	-	-
Author-provided FSC curve	8.10	9.83	8.26
Unmasked-calculated*	-	-	-

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

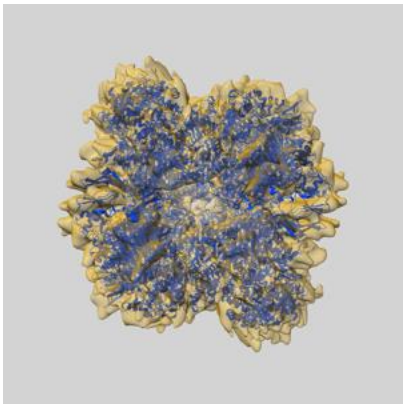
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-1440 and PDB model 2VDC. Per-residue inclusion information can be found in section 3 on page 11.

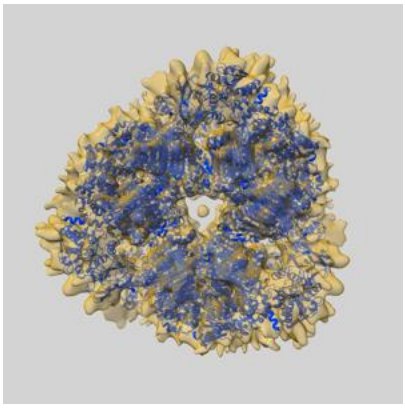
9.1 Map-model overlay



X



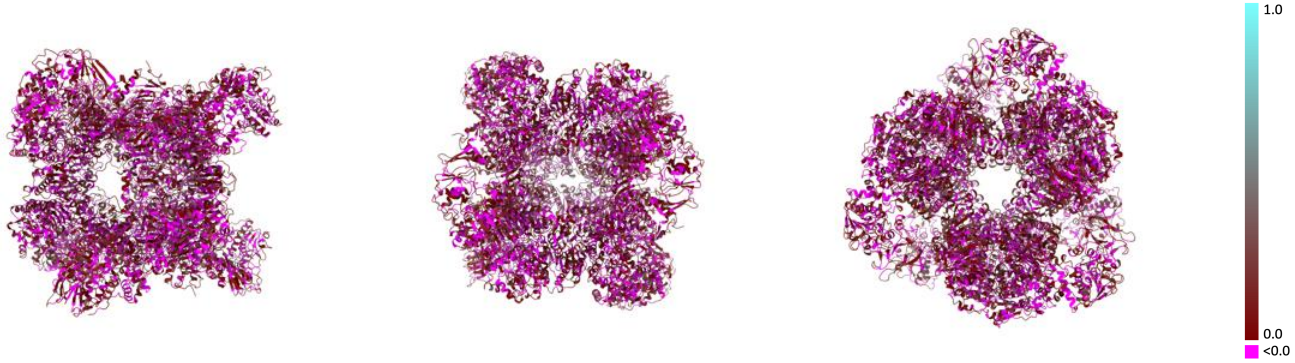
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 125.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

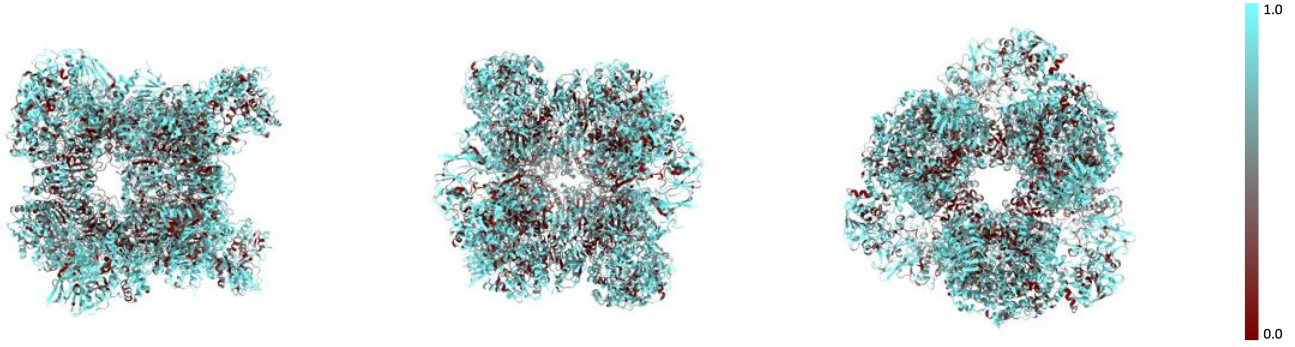
9.2 Q-score mapped to coordinate model



X Y Z

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

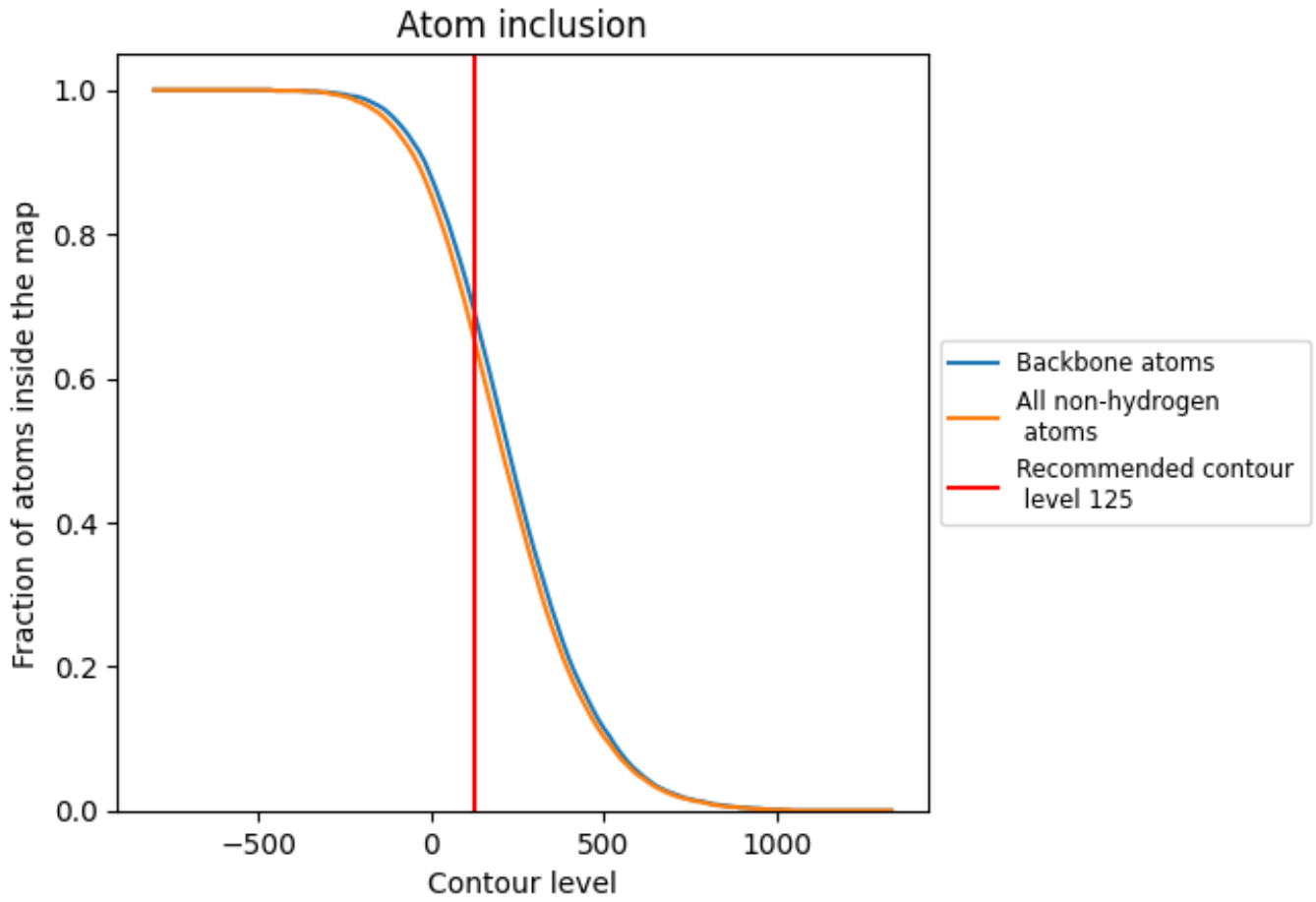
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (125).

9.4 Atom inclusion (i)



At the recommended contour level, 70% of all backbone atoms, 66% 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 (125) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6560	0.0430
A	0.6470	0.0430
B	0.6460	0.0430
C	0.6350	0.0400
D	0.6350	0.0430
E	0.6360	0.0450
F	0.6350	0.0410
G	0.7250	0.0460
H	0.7080	0.0430
I	0.7010	0.0470
J	0.7250	0.0490
K	0.7010	0.0470
L	0.7080	0.0430

