W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Oct 7, 2024 – 04:46 AM EDT

PDB ID	:	4KK1
Title	:	Crystal Structure of TSC1 core domain from S. pombe
Authors	:	Sun, W.; Zhu, Y.; Wang, Z.Z.; Zhong, Q.; Gao, F.; Lou, J.Z.; Gong, W.M.; Xu, W.Q.
Deposited on	:	2013-05-05
Resolution	:	3.30 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp
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:

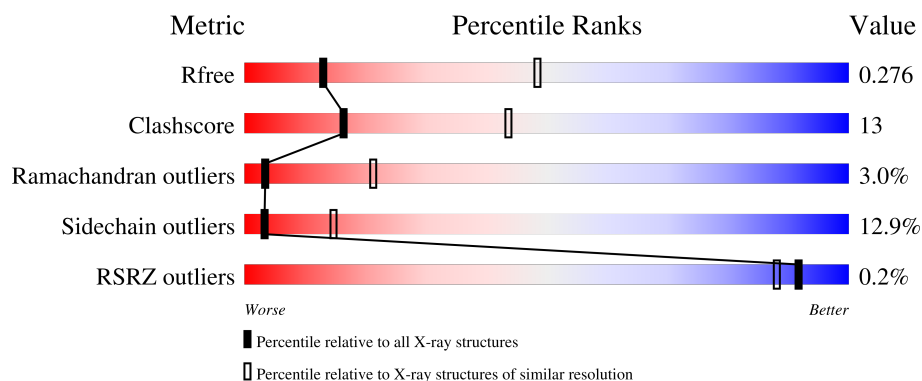|		
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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	Percentile Ranks	Value
Rfree		0.276
Clashscore		13
Ramachandran outliers		3.0%
Sidechain outliers		12.9%
RSRZ outliers		0.2%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	164625	1085 (3.32-3.28)
Clashscore	180529	1128 (3.32-3.28)
Ramachandran outliers	177936	1125 (3.32-3.28)
Sidechain outliers	177891	1124 (3.32-3.28)
RSRZ outliers	164620	1085 (3.32-3.28)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	434	53% 33% 7% 7%
1	B	434	58% 27% • • 10%
1	C	434	59% 26% 5% 10%
1	D	434	60% 26% • 10%
1	E	434	% 54% 30% 6% 10%

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Mol	Chain	Length	Quality of chain
1	F	434	57% 29% · 10%
1	G	434	56% 30% · 10%
1	H	434	49% 35% 6% 10%
1	I	434	56% 26% 8% 10%
1	J	434	52% 32% 6% 10%
1	K	434	57% 31% · 7%
1	L	434	58% 28% · 10%
1	M	434	57% 27% 6% 10%
1	N	434	54% 30% 6% 10%
1	O	434	54% 29% 6% 10%
1	P	434	59% 25% 7% 10%
1	Q	434	55% 31% · 10%
1	R	434	60% 26% · 10%
1	S	434	59% 26% 5% 10%
1	T	434	59% 27% · 10%

2   Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 63794 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 Tuberous sclerosis 1 protein homolog.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	403	Total 3268	C 2116	N 548	O 591	S 8	Se 5	0	0	0
1	B	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	C	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	D	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	E	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	F	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	G	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	H	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	I	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	J	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	K	403	Total 3268	C 2116	N 548	O 591	S 8	Se 5	0	0	0
1	L	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	M	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	N	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	O	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	P	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	R	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	S	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0
1	T	391	Total 3181	C 2066	N 532	O 570	S 8	Se 5	0	0	0

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q09778
A	-1	HIS	-	expression tag	UNP Q09778
A	0	MSE	-	expression tag	UNP Q09778
B	-2	SER	-	expression tag	UNP Q09778
B	-1	HIS	-	expression tag	UNP Q09778
B	0	MSE	-	expression tag	UNP Q09778
C	-2	SER	-	expression tag	UNP Q09778
C	-1	HIS	-	expression tag	UNP Q09778
C	0	MSE	-	expression tag	UNP Q09778
D	-2	SER	-	expression tag	UNP Q09778
D	-1	HIS	-	expression tag	UNP Q09778
D	0	MSE	-	expression tag	UNP Q09778
E	-2	SER	-	expression tag	UNP Q09778
E	-1	HIS	-	expression tag	UNP Q09778
E	0	MSE	-	expression tag	UNP Q09778
F	-2	SER	-	expression tag	UNP Q09778
F	-1	HIS	-	expression tag	UNP Q09778
F	0	MSE	-	expression tag	UNP Q09778
G	-2	SER	-	expression tag	UNP Q09778
G	-1	HIS	-	expression tag	UNP Q09778
G	0	MSE	-	expression tag	UNP Q09778
H	-2	SER	-	expression tag	UNP Q09778
H	-1	HIS	-	expression tag	UNP Q09778
H	0	MSE	-	expression tag	UNP Q09778
I	-2	SER	-	expression tag	UNP Q09778
I	-1	HIS	-	expression tag	UNP Q09778
I	0	MSE	-	expression tag	UNP Q09778
J	-2	SER	-	expression tag	UNP Q09778
J	-1	HIS	-	expression tag	UNP Q09778
J	0	MSE	-	expression tag	UNP Q09778
K	-2	SER	-	expression tag	UNP Q09778

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| Chain	Residue	Modelled	Actual	Comment	Reference
K	-1	HIS	-	expression tag	UNP Q09778
K	0	MSE	-	expression tag	UNP Q09778
L	-2	SER	-	expression tag	UNP Q09778
L	-1	HIS	-	expression tag	UNP Q09778
L	0	MSE	-	expression tag	UNP Q09778
M	-2	SER	-	expression tag	UNP Q09778
M	-1	HIS	-	expression tag	UNP Q09778
M	0	MSE	-	expression tag	UNP Q09778
N	-2	SER	-	expression tag	UNP Q09778
N	-1	HIS	-	expression tag	UNP Q09778
N	0	MSE	-	expression tag	UNP Q09778
O	-2	SER	-	expression tag	UNP Q09778
O	-1	HIS	-	expression tag	UNP Q09778
O	0	MSE	-	expression tag	UNP Q09778
P	-2	SER	-	expression tag	UNP Q09778
P	-1	HIS	-	expression tag	UNP Q09778
P	0	MSE	-	expression tag	UNP Q09778
Q	-2	SER	-	expression tag	UNP Q09778
Q	-1	HIS	-	expression tag	UNP Q09778
Q	0	MSE	-	expression tag	UNP Q09778
R	-2	SER	-	expression tag	UNP Q09778
R	-1	HIS	-	expression tag	UNP Q09778
R	0	MSE	-	expression tag	UNP Q09778
S	-2	SER	-	expression tag	UNP Q09778
S	-1	HIS	-	expression tag	UNP Q09778
S	0	MSE	-	expression tag	UNP Q09778
T	-2	SER	-	expression tag	UNP Q09778
T	-1	HIS	-	expression tag	UNP Q09778
T	0	MSE	-	expression tag	UNP Q09778

3   Residue-property plots ⓘ

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 electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: Tuberous sclerosis 1 protein homolog
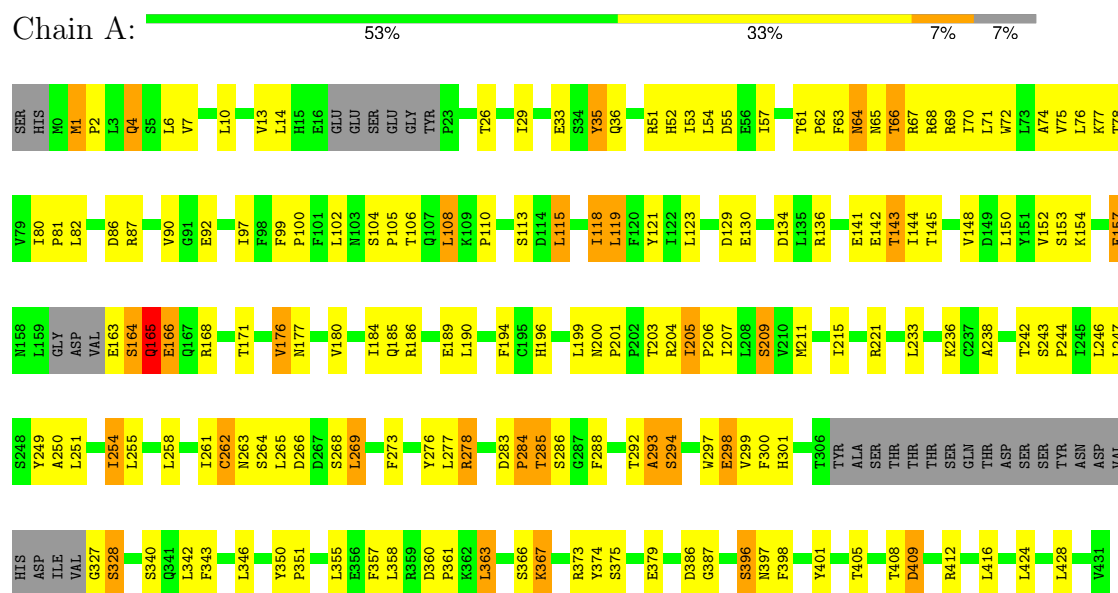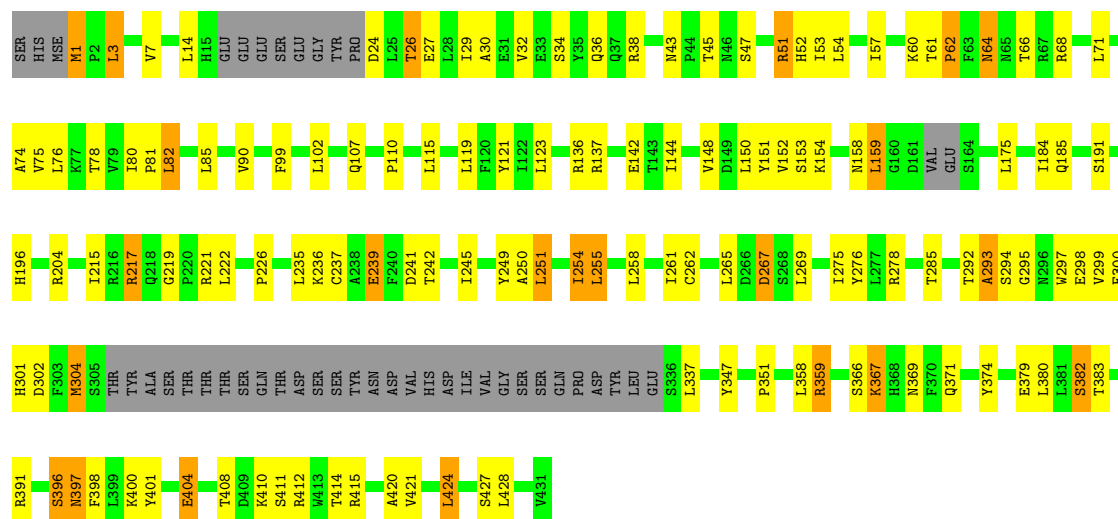
Chain A:

• Molecule 1: Tuberous sclerosis 1 protein homolog
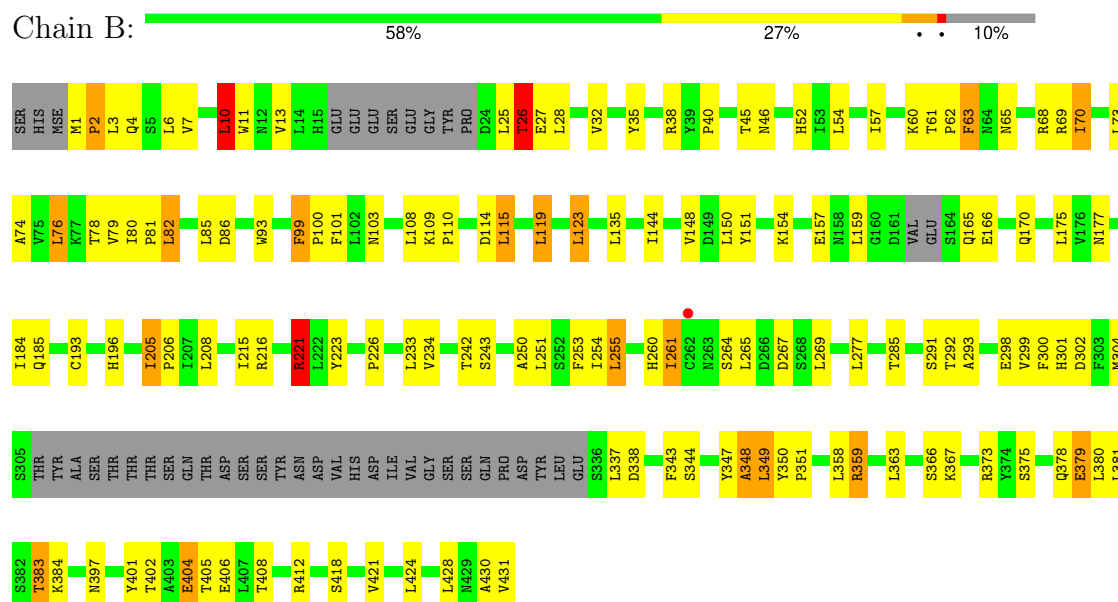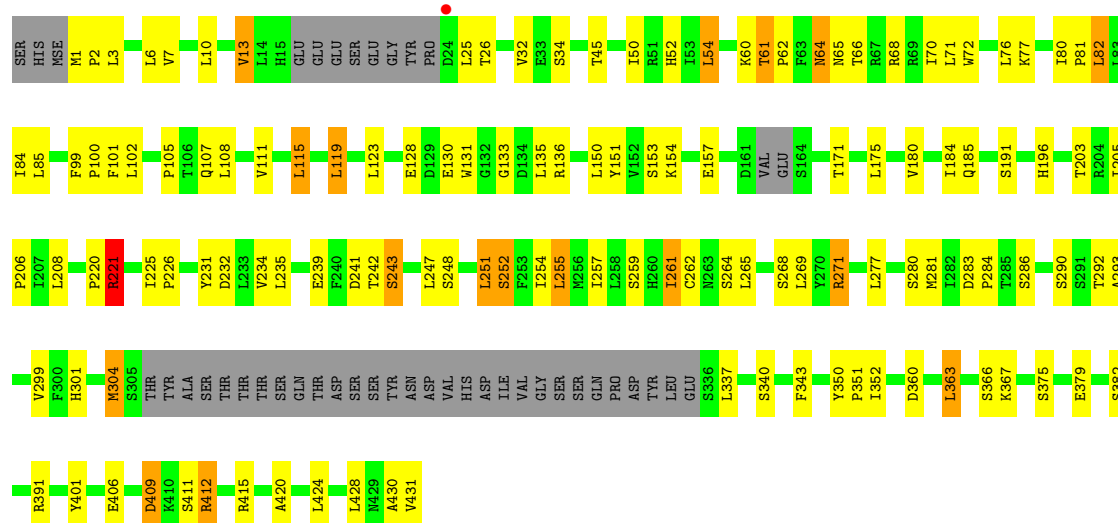
Chain B:

• Molecule 1: Tuberous sclerosis 1 protein homolog
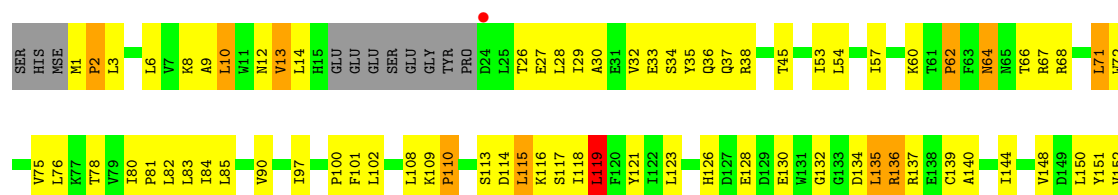
Chain C:

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain D:

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain E:

S153 K154 A155 I156 D161 VAL GLU S164 Q165 T171 L175 V180 I184 Q185 R186 P187 S191 F194 C195 H196 H197 F198 L199 N200 P201 P202 T203 R204 I205 P206 I207 I215 P220 R221 L222 Y223 E224 I225 P226 Q227 T228 Y231 D232 L233 V234 L235 K236 C237 A238 E239

F240 D241 T242 S243 L246 L251 S252 F253 I254 L255 M256 I261 C262 N263 S264 L265 D266 D267 S268 L269 Y270 R271 L272 F273 C274 I275 Y276 L277 R278 T292 A293 S294 G295 D302 F303 M304 S305 THR TYR ALA SER THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS

ASP ILE VAL GLY SER SER GLN PRO ASP TYR LEU GLU S336 Q341 I345 L363 S366 K367 R373 Y374 S375 S396 Y401 T402 A403 E404 T408 D409 K410 S411 R412 D417 S418 L424 L428 N429 A430 V431

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain F:

57%	29%	•	10%

SER HIS MSE M1 P2 L3 Q4 L10 H15 GLU GLU SER GLU GLY TYR PRO D24 L25 T26 E27 A30 E31 V32 Y35 Q36 Q42 N43 P44 T45 N46 S47 R51 H52 I53 L54 K60 T61 P62 F63 N64 N65 T66 R67 R68 R69 L76 K77 T78 V79 I80 P81

L82 L83 I84 A89 E92 F98 F99 P100 N103 Q107 L108 L115 K116 L119 F120 Y121 I122 L123 H126 E130 W131 L135 R136 I144 V148 Y151 V152 D161 VAL GLU S164 L175 L179 I184 Q185 S192 F198 P201 P202 T203

R204 I205 P206 V210 V214 I215 R221 L222 I225 P226 F230 Y231 D232 L233 V234 L235 E239 F240 D241 T242 S243 P244 I245 L246 A250 L251 S252 F253 I254 L255 M256 I257 L258 H260 I261 C262 N263 S264 L265 D266 D267 S268 L269 Y270 R271 L272 F273 L277 R278 D283

P284 T285 S291 S294 G295 N296 W297 E298 V299 D302 F303 M304 S305 THR TYR ALA SER THR THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY SER SER GLN PRO ASP TYR LEU GLU S336 L337 Q341 L342 F343 S344 I345 Y350 F354 L358

S366 K367 H368 N369 F370 Y374 S375 F376 D386 G387 L388 L399 K400 Y401 E404 T408 R412 W413 T414 R415 L416 D417 S418 I419 A420 V421 V431

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain G:

56%	30%	•	10%

SER HIS MSE M1 P2 L3 Q4 S5 L6 V7 K8 A9 L10 L14 H15 GLU GLU SER GLU GLY TYR PRO D24 L25 T26 V32 E33 S34 Y35 Y39 T45 N46 I50 L54 D55 E56 I57 P62 F63 R69 I70 L71 W72 V75 L76 V79 I80 P81 L82

D86 V90 W93 W94 D95 F99 Q107 L108 K109 P110 L115 K116 S117 I118 L119 F120 Y121 I122 L123 H126 D134 L135 R136 E142 T143 I144 T145 R146 L147 V148 D149 L150 Y151 V152 S153 K154 A155 I156 E157 D161 VAL GLU S164 R168 N169 Q170 V176 N177

V180 H181 I184 Q185 E189 L190 S191 F198 R204 I215 R216 P220 R221 L222 Y223 T228 G229 D232 L233 A238 S243 L246 L247 A250 L251 S252 F253 I254 L255 L258 S259 H260 I261 C262 N263 S264 L265 D266 L269 Y276 L277 R278 M281

T285 S290 G295 N296 W297 E298 V299 F300 H301 D302 F303 M304 S305 THR TYR ALA SER THR THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY SER SER GLN PRO ASP TYR LEU GLU S336 L337 I345 A348 L349 F354 L355 E356 F357 L358 R359

L363 Y364 A365 S366 K367 H368 Y374 S375 F376 E379 L380 L381 S382 T383 L389 G390 R391 S396 N397 Y401 E406 L407 T408 R412 W413 T414 R415 L416 D417 L424 L428 V431
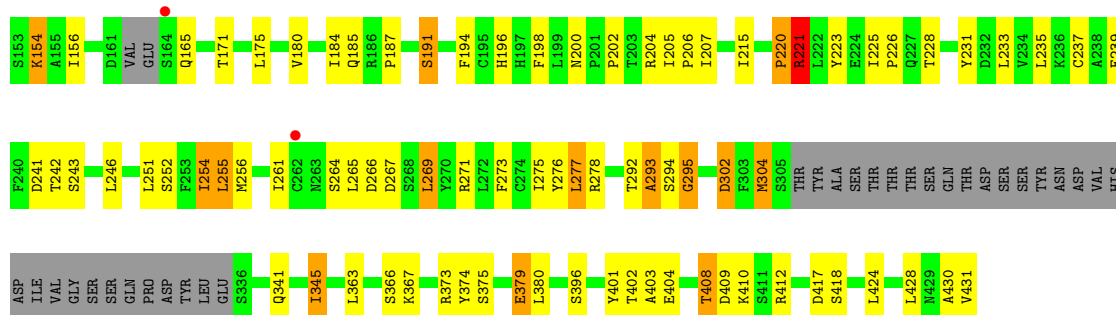
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain H:

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain I:

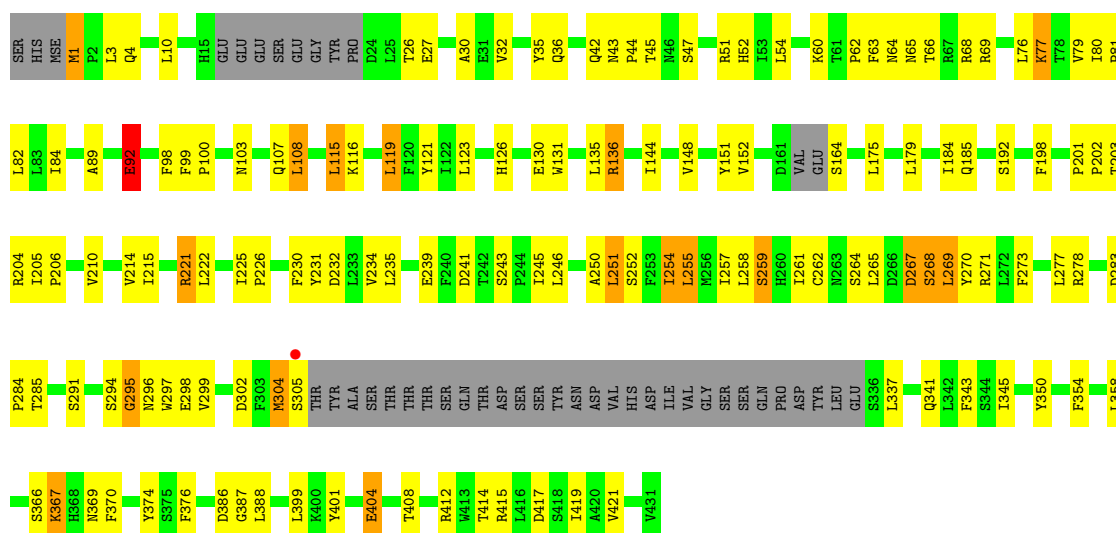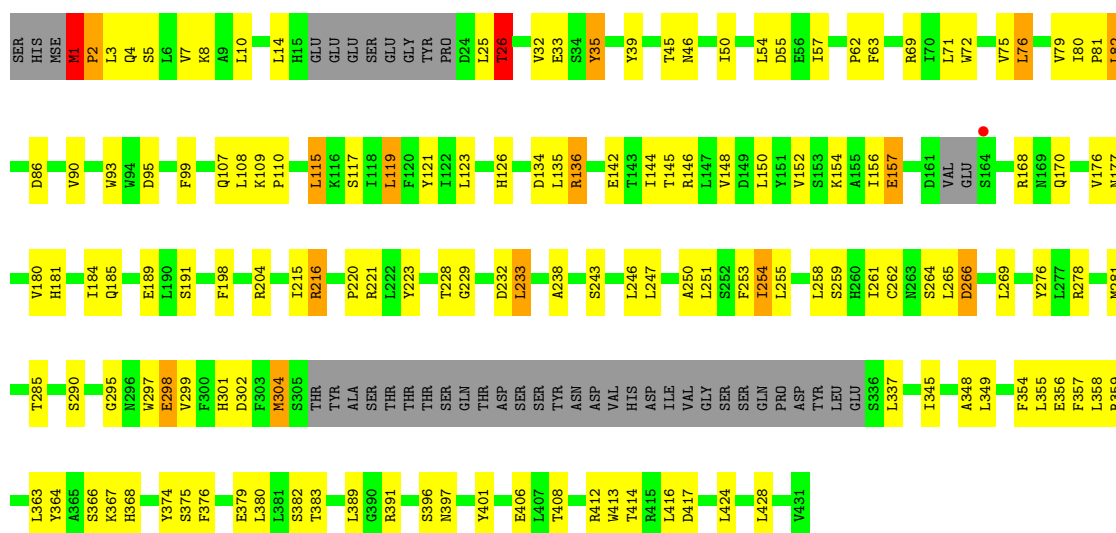• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain J:
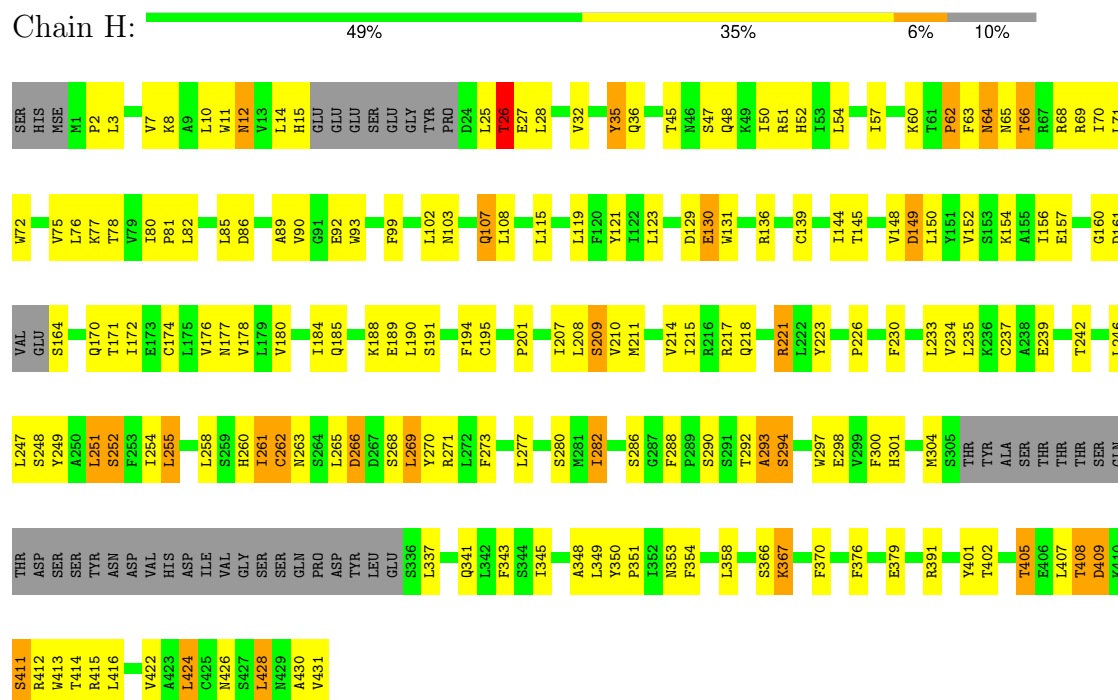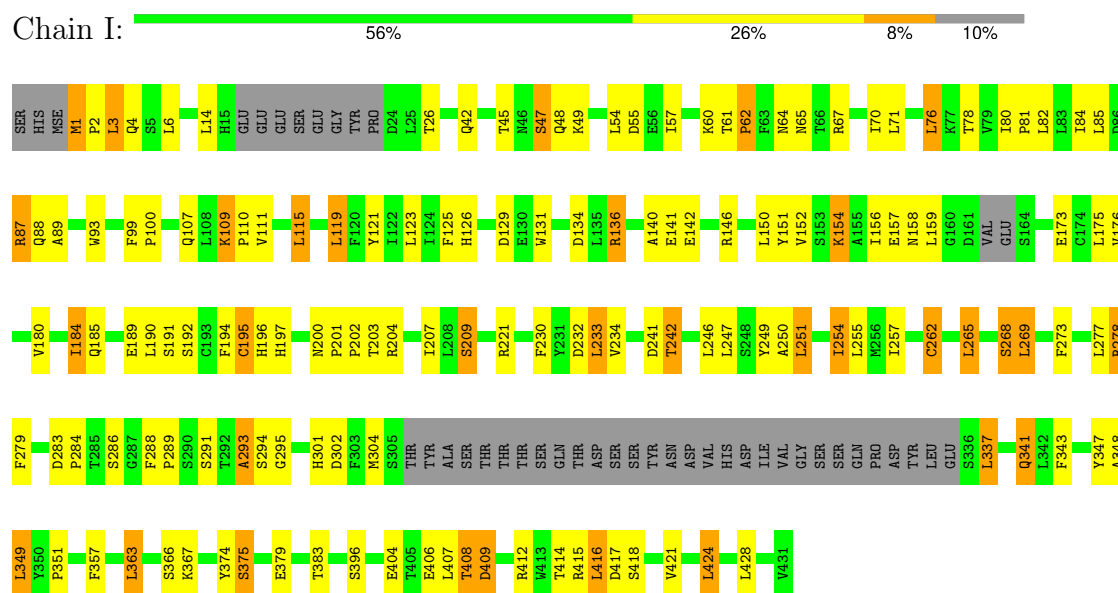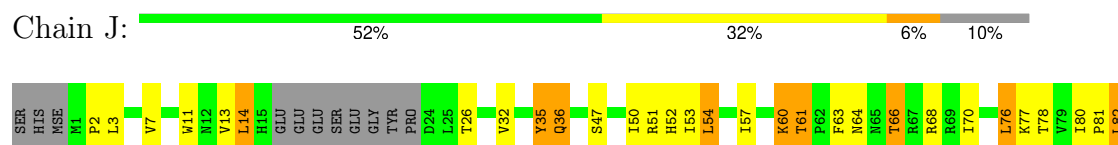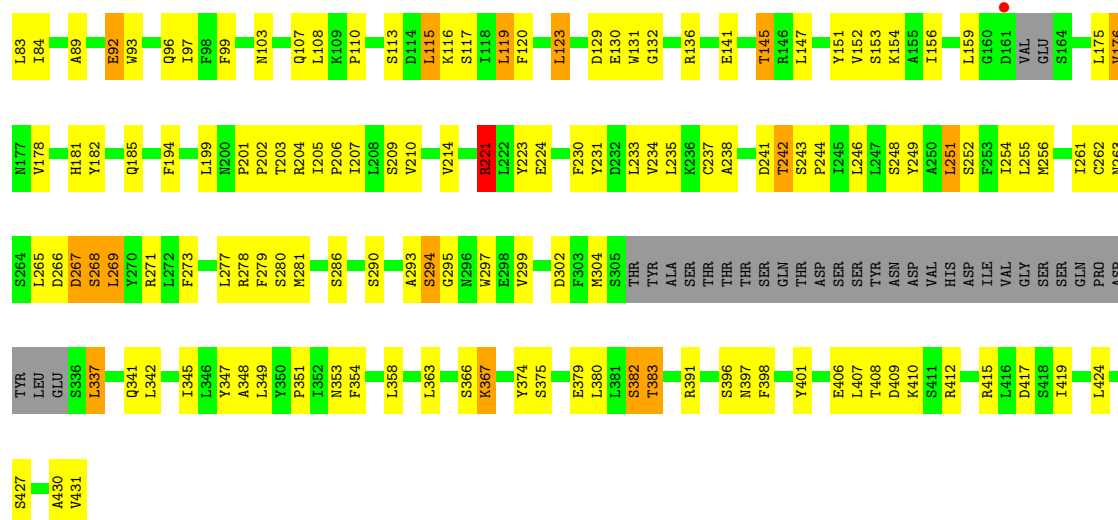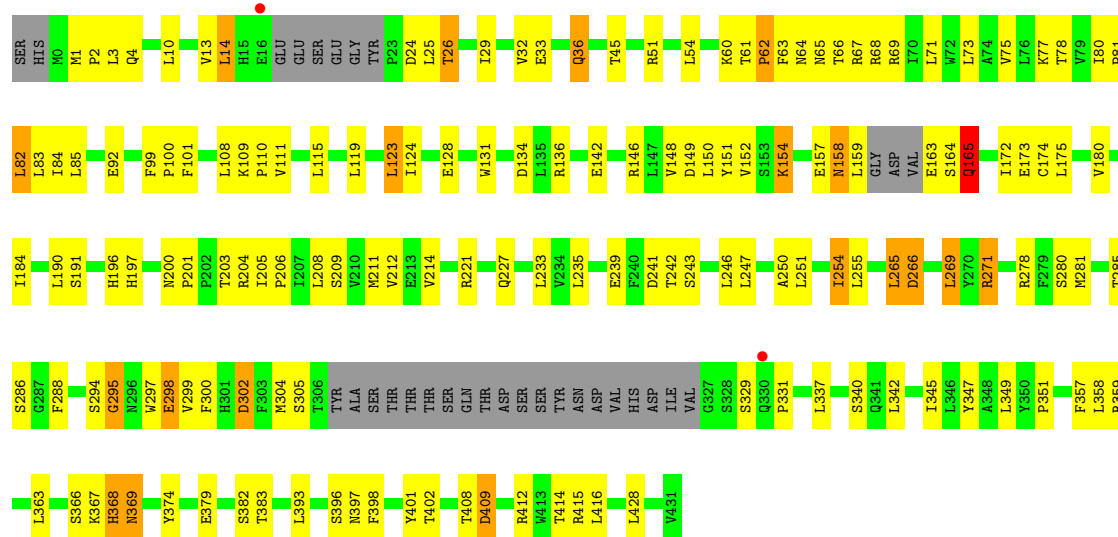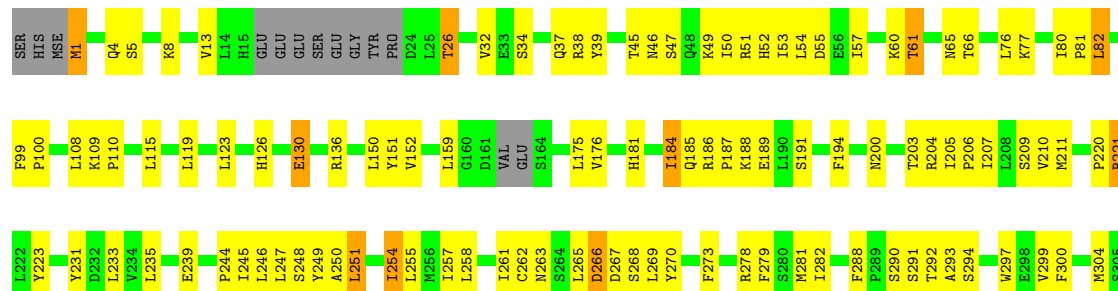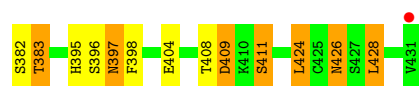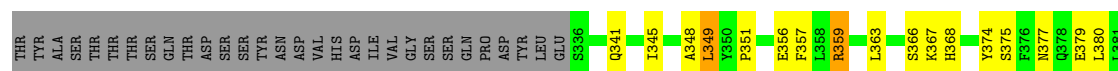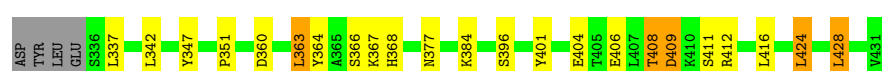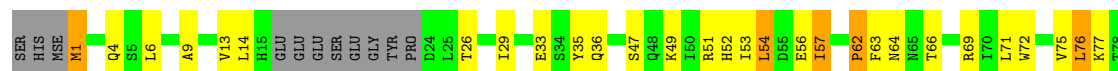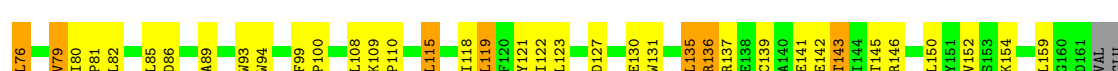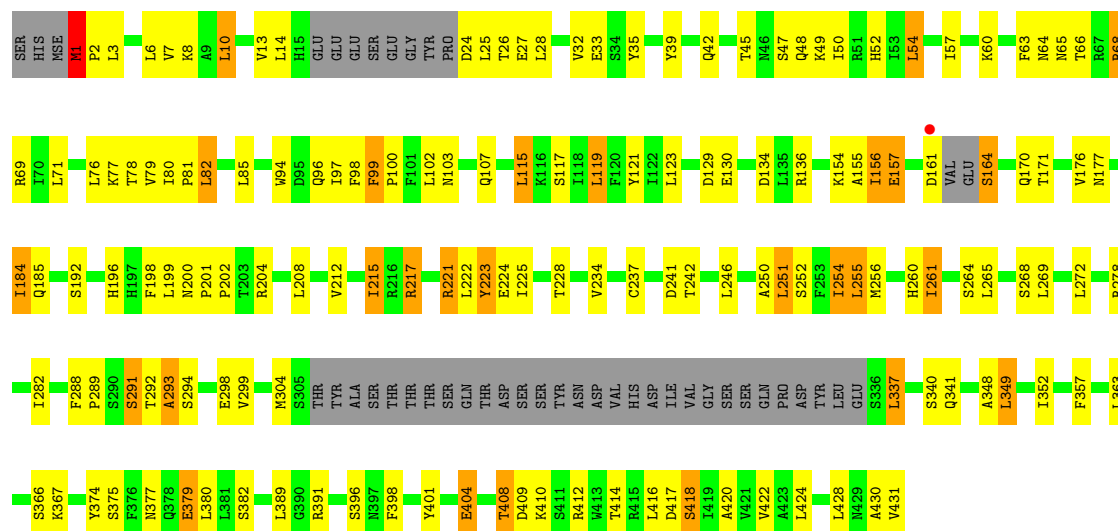
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain K:
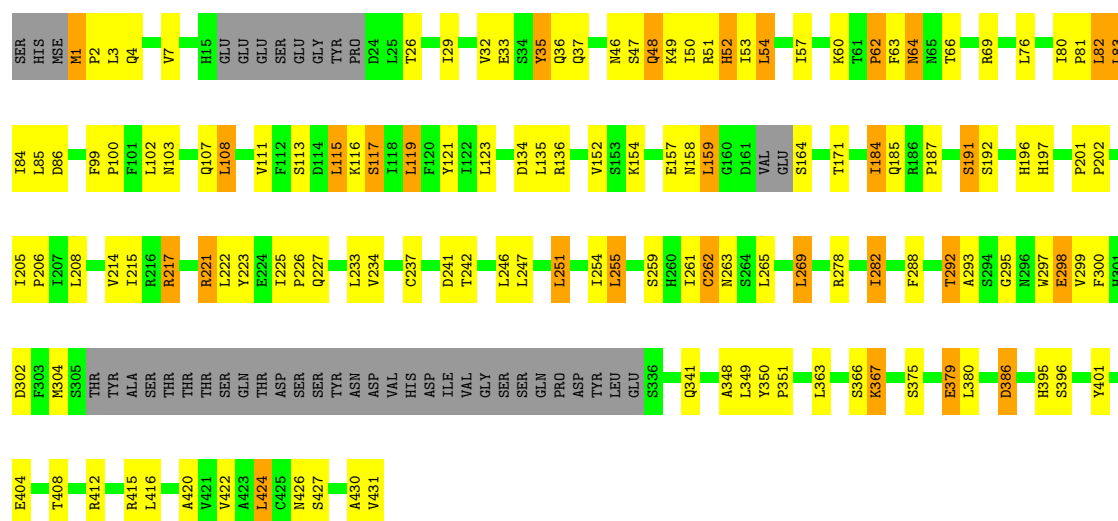

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain L:

THR TYR ALA SER THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY SER SER GLN PRO ASP TYR LEU GLU S336 Q341 I345 A348 L349 Y350 P351 E356 F357 L358 R359 L363 S366 K367 H368 Y374 S375 F376 Q378 E379 L380 L381

S382 T383 H395 S396 N397 F398 E404 T408 D409 K410 S411 L424 C425 N426 S427 L428 V431

● Molecule 1: Tuberous sclerosis 1 protein homolog

Chain M: █████████████████████████ 57% ████████ 27% ██ 6% ██ 10%

SER HIS MSE M1 Q4 S5 L6 A9 V13 L14 H15 GLU GLU GLU SER GLU GLY TYR PRO D24 L25 T26 I29 E33 S34 Y35 Q36 S47 Q48 K49 I50 R51 H52 I53 L54 D55 E56 I57 P62 F63 N64 N65 T66 R69 I70 L71 W72 V75 L76 K77 T78

V79 L82 L85 D86 A89 V90 G91 E92 Q96 F99 P100 F101 L102 N103 T106 Q107 L108 K109 P110 V111 L115 K116 S117 I118 L119 L123 E130 W131 G132 G133 D134 L135 R136 R137 L150 Y151 V152 S153 K154 L159 G160 D161 VAL GLU S164 T171 I184

Q185 S191 H196 H197 F198 P201 P202 T203 R204 L208 S209 V210 V214 R217 Q218 G219 P220 R221 L222 Y223 T228 G229 F230 Y231 D232 L233 V234 L235 K236 C237 A238 E239 T242 L246 L247 S248 Y249 A250 L251 S252 F253 I254 L255 L258 S259 H260 I261 C262 N263 S264

L265 D266 D267 S268 L269 Y270 R271 L272 F273 C274 I275 Y276 L277 R278 F279 S280 M281 I282 S286 G287 F288 S291 W297 E298 V299 F300 H301 D302 F303 M304 S305 THR TYR ALA SER THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY SER SER GLN PRO

ASP TYR LEU GLU S336 L337 L342 Y347 P351 D360 L363 Y364 A365 S366 K367 H368 N377 K384 S396 Y401 E404 T405 E406 L407 T408 D409 K410 S411 R412 L416 L424 L428 V431

● Molecule 1: Tuberous sclerosis 1 protein homolog

Chain N: ████████████████████████ 54% █████████ 30% ██ 6% ██ 10%

SER HIS MSE M1 Q4 S5 L6 A9 L10 W11 N12 V13 L14 H15 GLU GLU GLU SER GLU GLY TYR PRO D24 L25 T26 E27 L28 V32 E33 S34 Y35 Q36 P40 T45 N46 S47 Q48 K49 I50 R51 H52 I53 L54 I57 Y58 T61 P62 I70 L71 W72 V75

L76 V79 I80 P81 L82 L85 D86 A89 W93 W94 F99 P100 L108 K109 P110 L115 I118 L119 F120 Y121 I122 L123 D127 E130 W131 L135 R136 R137 E138 C139 A140 E141 E142 T143 I144 T145 R146 L150 Y151 V152 S153 K154 L159 G160 D161 VAL GLU

S164 V176 N177 H181 I184 Q185 R186 P187 K188 E189 L190 S191 S192 C193 F194 H197 F198 L199 N200 P201 P202 T203 R204 I205 P206 I207 L208 M211 I215 R216 R217 R221 L233 V234 L235 K236 C237 A238 E239 F240 D241 T242 L246 L247 S248 L251 I254 L265

L258 S259 H260 I261 S264 L265 D266 D267 S268 L269 L272 F273 R278 I282 D283 S286 G287 F288 P289 S290 S291 T292 A293 S294 W297 E298 V299 F300 H301 M304 S305 THR TYR ALA SER THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY

SER SER GLN PRO ASP TYR LEU GLU S336 L337 A348 L349 I352 L363 S366 K367 Y374 E379 L380 R391 A394 Y401 T402 A403 E404 T405 E406 L407 T408 D409 K410 S411 R412 W413 T414 D417 S418 I419 A420 L424 L428 V431

● Molecule 1: Tuberous sclerosis 1 protein homolog

Chain O: ████████████████████████ 54% █████████ 29% ██ 6% ██ 10%
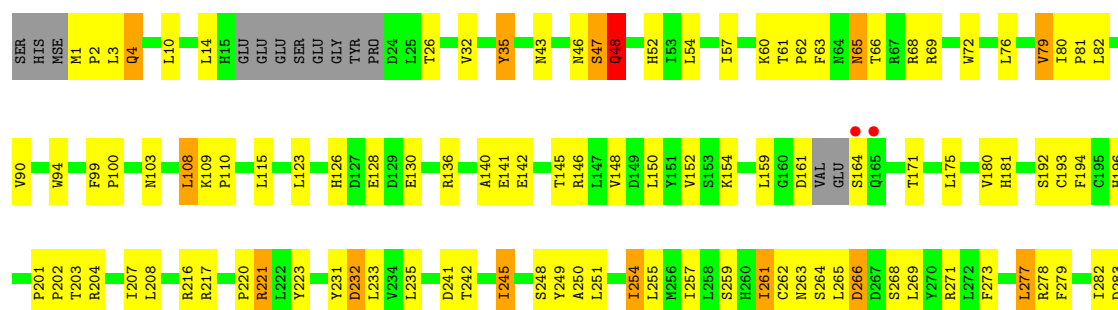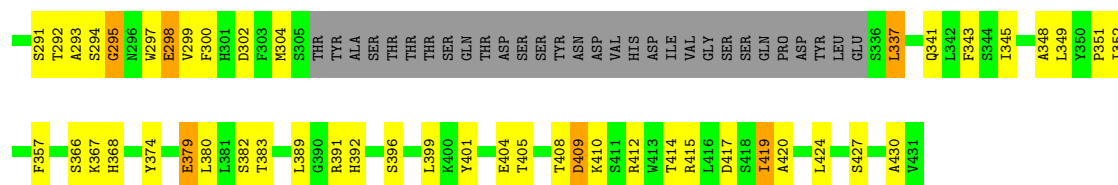
• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain P:

59%   25%   7%   10%
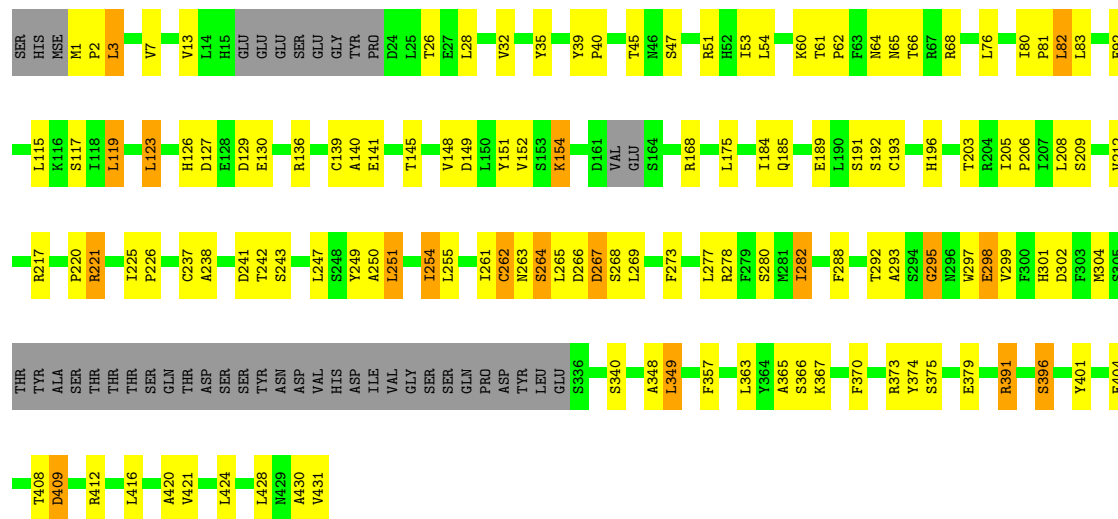
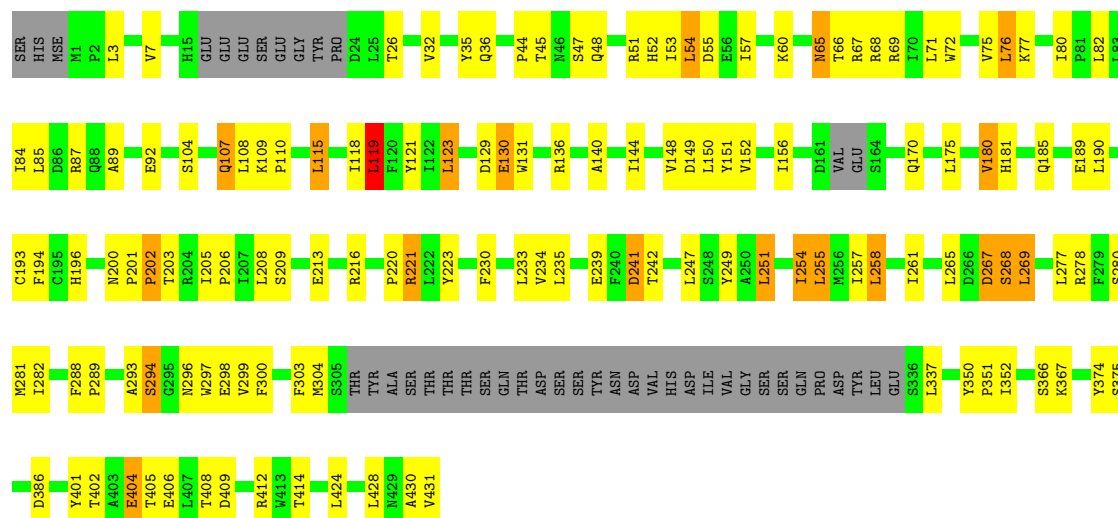• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain Q:

55%   31%   •   10%

S291 T292 A293 S294 G295 N296 W297 E298 V299 F300 H301 D302 F303 M304 S305 THR TYR ALA SER THR THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY SER SER GLN PRO ASP TYR LEU GLU S336 L337 Q341 L342 F343 S344 I345 A348 L349 Y350 P351 I352

F357 S366 K367 H368 Y374 E379 L380 L381 S382 T383 L389 G390 R391 H392 S396 L399 K400 Y401 E404 T405 T408 D409 K410 S411 R412 W413 T414 R415 L416 D417 S418 I419 A420 L424 S427 A430 V431

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain R:	60%	26%	•	10%

SER HIS MSE M1 P2 L3 V7 V13 L14 H15 GLU GLU GLU SER GLU GLY TYR PRO D24 L25 T26 E27 L28 V32 Y35 Y39 P40 T45 N46 S47 R51 H52 I53 L54 K60 T61 P62 F63 N64 N65 T66 R67 R68 L76 I80 P81 L82 L83 E92

L115 K116 S117 I118 L119 L123 H126 D127 E128 D129 E130 R136 C139 A140 E141 T145 V148 D149 L150 Y151 V152 S153 K154 D161 VAL GLU S164 R168 L175 I184 Q185 E189 L190 S191 S192 C193 H196 T203 R204 I205 P206 I207 L208 S209 V212

R217 P220 R221 I225 P226 C237 A238 D241 T242 S243 L247 S248 Y249 A250 L251 I254 L255 I261 C262 N263 S264 L265 D266 D267 S268 L269 F273 L277 R278 F279 S280 M281 I282 F288 T292 A293 S294 G295 N296 W297 E298 V299 F300 H301 D302 F303 M304 S305

THR TYR ALA SER THR THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY SER SER GLN PRO ASP TYR LEU GLU S336 S340 A348 L349 F357 L363 Y364 A365 S366 K367 F370 R373 Y374 S375 E379 R391 S396 Y401 E404

T408 D409 R412 L416 A420 V421 L424 L428 N429 A430 V431

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain S:	59%	26%	5%	10%

SER HIS MSE M1 P2 L3 V7 H15 GLU GLU GLU SER GLU GLY TYR PRO D24 L25 T26 V32 Y35 Q36 P44 T45 N46 S47 Q48 R51 H52 I53 L54 D55 E56 I57 K60 N65 T66 R67 R68 R69 I70 L71 W72 V75 L76 K77 I80 P81 L82 L83

I84 L85 D86 R87 Q88 A89 E92 S104 Q107 L108 K109 P110 L115 I118 L119 F120 Y121 I122 L123 D129 E130 W131 R136 A140 I144 V148 D149 L150 Y151 V152 I156 D161 VAL GLU S164 Q170 L175 V180 H181 Q185 E189 L190

C193 F194 C195 H196 N200 P201 P202 T203 R204 I205 P206 I207 L208 S209 E213 R216 P220 R221 L222 Y223 F230 L233 V234 L235 E239 F240 D241 T242 L247 S248 Y249 A250 L251 I254 L255 M256 I257 L258 I261 L265 D266 D267 S268 L269 L277 R278 F279 S280

M281 I282 F288 P289 A293 S294 G295 N296 W297 E298 V299 F300 F303 M304 S305 THR TYR ALA SER THR THR THR SER GLN THR ASP SER SER TYR ASN ASP VAL HIS ASP ILE VAL GLY SER SER GLN PRO ASP TYR LEU GLU S336 L337 Y350 P351 I352 S366 K367 Y374 S375

D386 Y401 T402 A403 E404 T405 E406 L407 T408 D409 R412 W413 T414 L424 L428 N429 A430 V431

• Molecule 1: Tuberous sclerosis 1 protein homolog

Chain T:	59%	27%	•	10%

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	109.32Å 254.83Å 228.47Å 90.00° 99.71° 90.00°	Depositor
Resolution (Å)	39.82 – 3.30 39.82 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.82-3.30) 99.2 (39.82-3.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.15 (at 3.18Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.186 , 0.268 0.186 , 0.276	Depositor DCC
R_{free} test set	9230 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	85.9	Xtriage
Anisotropy	0.283	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 53.9	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	63794	wwPDB-VP
Average B, all atoms (Å^2)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.70% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	A	0.63	0/3343	0.86	1/4535 (0.0%)
1	B	0.64	0/3257	0.85	1/4421 (0.0%)
1	C	0.65	0/3257	0.85	3/4421 (0.1%)
1	D	0.65	0/3257	0.85	4/4421 (0.1%)
1	E	0.62	0/3257	0.87	3/4421 (0.1%)
1	F	0.61	1/3257 (0.0%)	0.83	1/4421 (0.0%)
1	G	0.65	0/3257	0.88	5/4421 (0.1%)
1	H	0.61	0/3257	0.81	0/4421
1	I	0.66	0/3257	0.87	2/4421 (0.0%)
1	J	0.63	0/3257	0.86	2/4421 (0.0%)
1	K	0.61	0/3343	0.85	1/4535 (0.0%)
1	L	0.66	0/3257	0.86	0/4421
1	M	0.65	0/3257	0.88	1/4421 (0.0%)
1	N	0.68	0/3257	0.88	2/4421 (0.0%)
1	O	0.71	0/3257	0.91	3/4421 (0.1%)
1	P	0.64	0/3257	0.86	3/4421 (0.1%)
1	Q	0.64	0/3257	0.84	1/4421 (0.0%)
1	R	0.64	0/3257	0.86	2/4421 (0.0%)
1	S	0.58	0/3257	0.79	0/4421
1	T	0.60	0/3257	0.82	2/4421 (0.0%)
All	All	0.64	1/65312 (0.0%)	0.85	37/88648 (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
1	E	0	1
1	F	0	1
1	I	0	1
1	K	0	1
1	O	0	2

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WORLDWIDE
wwPDB
PROTEIN DATA BANK

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	P	0	1
All	All	0	7

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	92	GLU	CG-CD	5.12	1.59	1.51

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	304	MSE	CB-CA-C	9.11	128.63	110.40
1	C	1	MSE	CG-SE-CE	7.77	116.00	98.90
1	J	221	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	E	304	MSE	CB-CA-C	6.98	124.36	110.40
1	G	337	LEU	CA-CB-CG	6.82	130.99	115.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	220	PRO	Peptide
1	F	164	SER	Peptide
1	I	3	LEU	Peptide
1	K	368	HIS	Peptide
1	O	24	ASP	Peptide

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	3268	0	3216	108	0
1	B	3181	0	3145	81	0
1	C	3181	0	3145	73	0
1	D	3181	0	3145	74	0
1	E	3181	0	3145	80	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	3181	0	3145	80	0
1	G	3181	0	3145	81	0
1	H	3181	0	3145	114	0
1	I	3181	0	3145	78	0
1	J	3181	0	3145	99	0
1	K	3268	0	3216	81	0
1	L	3181	0	3145	83	0
1	M	3181	0	3145	95	0
1	N	3181	0	3145	99	0
1	O	3181	0	3145	89	0
1	P	3181	0	3145	79	0
1	Q	3181	0	3145	84	0
1	R	3181	0	3145	74	0
1	S	3181	0	3145	85	0
1	T	3181	0	3145	73	0
All	All	63794	0	63042	1624	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 13.

The worst 5 of 1624 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:G:115:LEU:HD22	1:G:119:LEU:HD22	1.43	0.98
1:M:401:TYR:CZ	1:M:412:ARG:HG3	1.99	0.96
1:A:121:TYR:O	1:A:136:ARG:NH2	2.05	0.90
1:I:142:GLU:OE2	1:I:146:ARG:NH1	2.08	0.86
1:Q:279:PHE:O	1:Q:282:ILE:HG22	1.76	0.85

There are no symmetry-related clashes.

5.3   Torsion angles ⓘ

5.3.1   Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	395/434 (91%)	331 (84%)	45 (11%)	19 (5%)	2	12
1	B	383/434 (88%)	333 (87%)	33 (9%)	17 (4%)	2	14
1	C	383/434 (88%)	335 (88%)	36 (9%)	12 (3%)	3	21
1	D	383/434 (88%)	333 (87%)	41 (11%)	9 (2%)	5	26
1	E	383/434 (88%)	336 (88%)	35 (9%)	12 (3%)	3	21
1	F	383/434 (88%)	347 (91%)	29 (8%)	7 (2%)	7	30
1	G	383/434 (88%)	325 (85%)	48 (12%)	10 (3%)	4	23
1	H	383/434 (88%)	320 (84%)	46 (12%)	17 (4%)	2	14
1	I	383/434 (88%)	328 (86%)	39 (10%)	16 (4%)	2	15
1	J	383/434 (88%)	314 (82%)	55 (14%)	14 (4%)	2	17
1	K	395/434 (91%)	346 (88%)	36 (9%)	13 (3%)	3	19
1	L	383/434 (88%)	327 (85%)	47 (12%)	9 (2%)	5	26
1	M	383/434 (88%)	327 (85%)	46 (12%)	10 (3%)	4	23
1	N	383/434 (88%)	323 (84%)	50 (13%)	10 (3%)	4	23
1	O	383/434 (88%)	331 (86%)	42 (11%)	10 (3%)	4	23
1	P	383/434 (88%)	342 (89%)	31 (8%)	10 (3%)	4	23
1	Q	383/434 (88%)	308 (80%)	63 (16%)	12 (3%)	3	21
1	R	383/434 (88%)	334 (87%)	41 (11%)	8 (2%)	5	27
1	S	383/434 (88%)	315 (82%)	58 (15%)	10 (3%)	4	23
1	T	383/434 (88%)	343 (90%)	35 (9%)	5 (1%)	10	36
All	All	7684/8680 (88%)	6598 (86%)	856 (11%)	230 (3%)	3	21

5 of 230 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	64	ASN
1	A	164	SER
1	A	165	GLN
1	A	262	CYS

5.3.2   Protein sidechains   ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

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	361/398 (91%)	311 (86%)	50 (14%)	3	13
1	B	352/398 (88%)	310 (88%)	42 (12%)	4	17
1	C	352/398 (88%)	306 (87%)	46 (13%)	3	14
1	D	352/398 (88%)	307 (87%)	45 (13%)	3	15
1	E	352/398 (88%)	300 (85%)	52 (15%)	2	11
1	F	352/398 (88%)	312 (89%)	40 (11%)	4	18
1	G	352/398 (88%)	310 (88%)	42 (12%)	4	17
1	H	352/398 (88%)	309 (88%)	43 (12%)	4	16
1	I	352/398 (88%)	298 (85%)	54 (15%)	2	10
1	J	352/398 (88%)	306 (87%)	46 (13%)	3	14
1	K	361/398 (91%)	313 (87%)	48 (13%)	3	14
1	L	352/398 (88%)	309 (88%)	43 (12%)	4	16
1	M	352/398 (88%)	311 (88%)	41 (12%)	4	18
1	N	352/398 (88%)	306 (87%)	46 (13%)	3	14
1	O	352/398 (88%)	300 (85%)	52 (15%)	2	11
1	P	352/398 (88%)	304 (86%)	48 (14%)	3	14
1	Q	352/398 (88%)	303 (86%)	49 (14%)	3	13
1	R	352/398 (88%)	313 (89%)	39 (11%)	5	19
1	S	352/398 (88%)	313 (89%)	39 (11%)	5	19
1	T	352/398 (88%)	309 (88%)	43 (12%)	4	16
All	All	7058/7960 (89%)	6150 (87%)	908 (13%)	3	15

5 of 908 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	13	VAL
1	T	196	HIS
1	M	248	SER
1	T	108	LEU
1	R	117	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 39 such sidechains are listed below:

Mol	Chain	Res	Type
1	P	107	GLN
1	S	197	HIS
1	P	426	ASN
1	R	368	HIS
1	T	36	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	397/434 (91%)	-0.64	0	100	100	56, 93, 146, 184	0
1	B	386/434 (88%)	-0.63	1 (0%)	90	85	55, 89, 133, 176	0
1	C	386/434 (88%)	-0.75	0	100	100	56, 80, 125, 155	0
1	D	386/434 (88%)	-0.65	1 (0%)	90	85	56, 86, 126, 166	0
1	E	386/434 (88%)	-0.68	3 (0%)	82	72	55, 86, 144, 192	0
1	F	386/434 (88%)	-0.66	1 (0%)	90	85	57, 93, 130, 164	0
1	G	386/434 (88%)	-0.68	1 (0%)	90	85	53, 84, 123, 149	0
1	H	386/434 (88%)	-0.53	0	100	100	56, 102, 155, 199	0
1	I	386/434 (88%)	-0.68	0	100	100	51, 85, 124, 171	0
1	J	386/434 (88%)	-0.65	1 (0%)	90	85	52, 93, 137, 179	0
1	K	397/434 (91%)	-0.66	2 (0%)	87	80	58, 89, 139, 212	0
1	L	386/434 (88%)	-0.70	1 (0%)	90	85	51, 84, 126, 168	0
1	M	386/434 (88%)	-0.64	0	100	100	48, 85, 144, 176	0
1	N	386/434 (88%)	-0.66	2 (0%)	87	80	50, 85, 133, 177	0
1	O	386/434 (88%)	-0.74	1 (0%)	90	85	47, 77, 117, 162	0
1	P	386/434 (88%)	-0.69	0	100	100	53, 85, 142, 188	0
1	Q	386/434 (88%)	-0.58	2 (0%)	87	80	51, 101, 154, 201	0
1	R	386/434 (88%)	-0.75	0	100	100	54, 85, 129, 164	0
1	S	386/434 (88%)	-0.56	0	100	100	69, 106, 155, 189	0
1	T	386/434 (88%)	-0.64	0	100	100	62, 94, 151, 193	0
All	All	7742/8680 (89%)	-0.66	16 (0%)	92	88	47, 89, 141, 212	0

The worst 5 of 16 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	O	161	ASP	3.2
1	E	24	ASP	2.8
1	Q	164	SER	2.7
1	K	16	GLU	2.5
1	E	164	SER	2.3

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.