wwPDB X-ray Structure Validation Summary Report (i)

May 22, 2020 – 02:04 am BST

PDB ID	:	4B2T
Title	:	The crystal structures of the eukaryotic chaperonin CCT reveal its functional partitioning
Authors	:	Kalisman, N.; Schroeder, G.F.; Levitt, M.
Deposited on	:	2012-07-17
Resolution	:	5.50 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 following versions of software and data (see references (1)) were used in the production of this report:

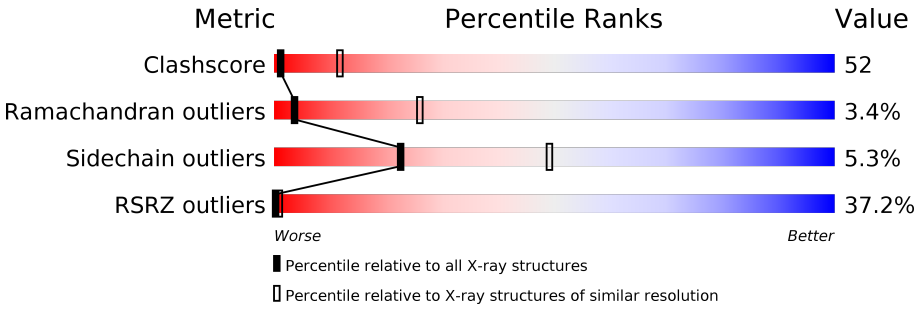
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.50 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)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1010 (7.10-3.90)
Ramachandran outliers	138981	1014 (7.12-3.82)
Sidechain outliers	138945	1191 (7.20-3.80)
RSRZ outliers	127900	1023 (7.08-3.76)

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 on 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	556	26% 29% 51% 6% 13%
1	a	556	27% 57% 6% 35%
2	B	535	43% 35% 52% 10%
2	b	535	30% 62% 5% 33%
3	D	542	29% 28% 55% 5% 11%
3	d	542	25% 61% 5% 34%
4	E	541	20% 32% 50% 7% 11%

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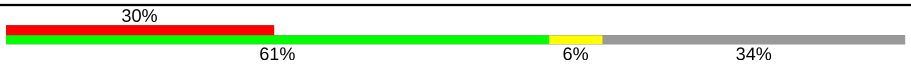
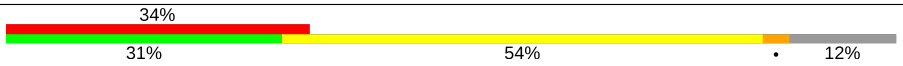
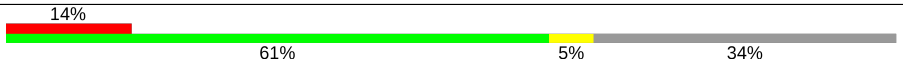
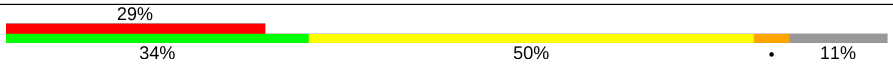
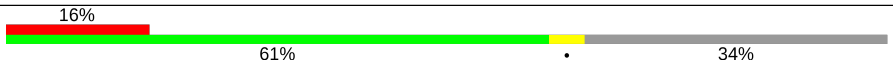
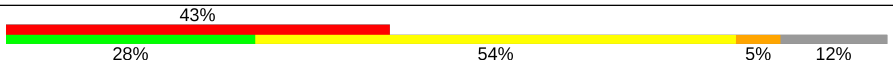
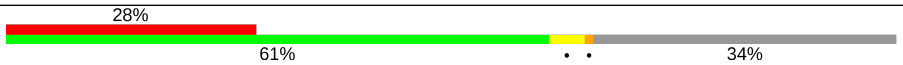
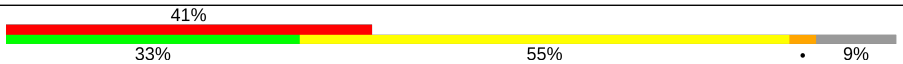
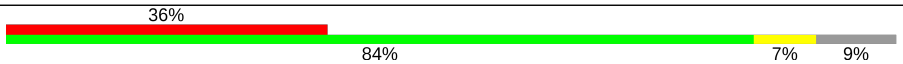
Mol	Chain	Length	Quality of chain
4	e	541	
5	G	545	
5	g	545	
6	H	543	
6	h	543	
7	Q	548	
7	q	548	
8	Z	531	
8	z	531	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 51877 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 T-COMPLEX PROTEIN 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3625	2280	633	692	20			
1	a	359	Total	C	N	O	S	0	0	0
			2705	1703	469	520	13			

- Molecule 2 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	481	Total	C	N	O	S	0	0	0
			3602	2258	629	696	19			
2	b	359	Total	C	N	O	S	0	0	0
			2658	1652	469	524	13			

- Molecule 3 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT DELTA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	481	Total	C	N	O	S	0	0	0
			3610	2259	627	703	21			
3	d	359	Total	C	N	O	S	0	0	0
			2690	1671	473	532	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	158	VAL	GLU	conflict	UNP Q2T9X2
D	510	LEU	GLN	conflict	UNP Q2T9X2
d	1158	VAL	GLU	conflict	UNP Q2T9X2
d	1510	LEU	GLN	conflict	UNP Q2T9X2

- Molecule 4 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT EPSILON.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	481	Total	C	N	O	S	0	0	0
			3674	2299	644	703	28			
4	e	359	Total	C	N	O	S	0	0	0
			2724	1688	486	528	22			

- Molecule 5 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT GAMMA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	G	481	Total	C	N	O	S	0	0	0
			3719	2326	661	705	27			
5	g	359	Total	C	N	O	S	0	0	0
			2735	1711	480	523	21			

- Molecule 6 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	H	481	Total	C	N	O	S	0	0	0
			3671	2320	633	693	25			
6	h	359	Total	C	N	O	S	0	0	0
			2724	1719	472	517	16			

- Molecule 7 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT THETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	Q	481	Total	C	N	O	S	0	0	0
			3673	2317	628	703	25			
7	q	359	Total	C	N	O	S	0	0	0
			2739	1729	467	526	17			

- Molecule 8 is a protein called T-COMPLEX PROTEIN 1 SUBUNIT ZETA.

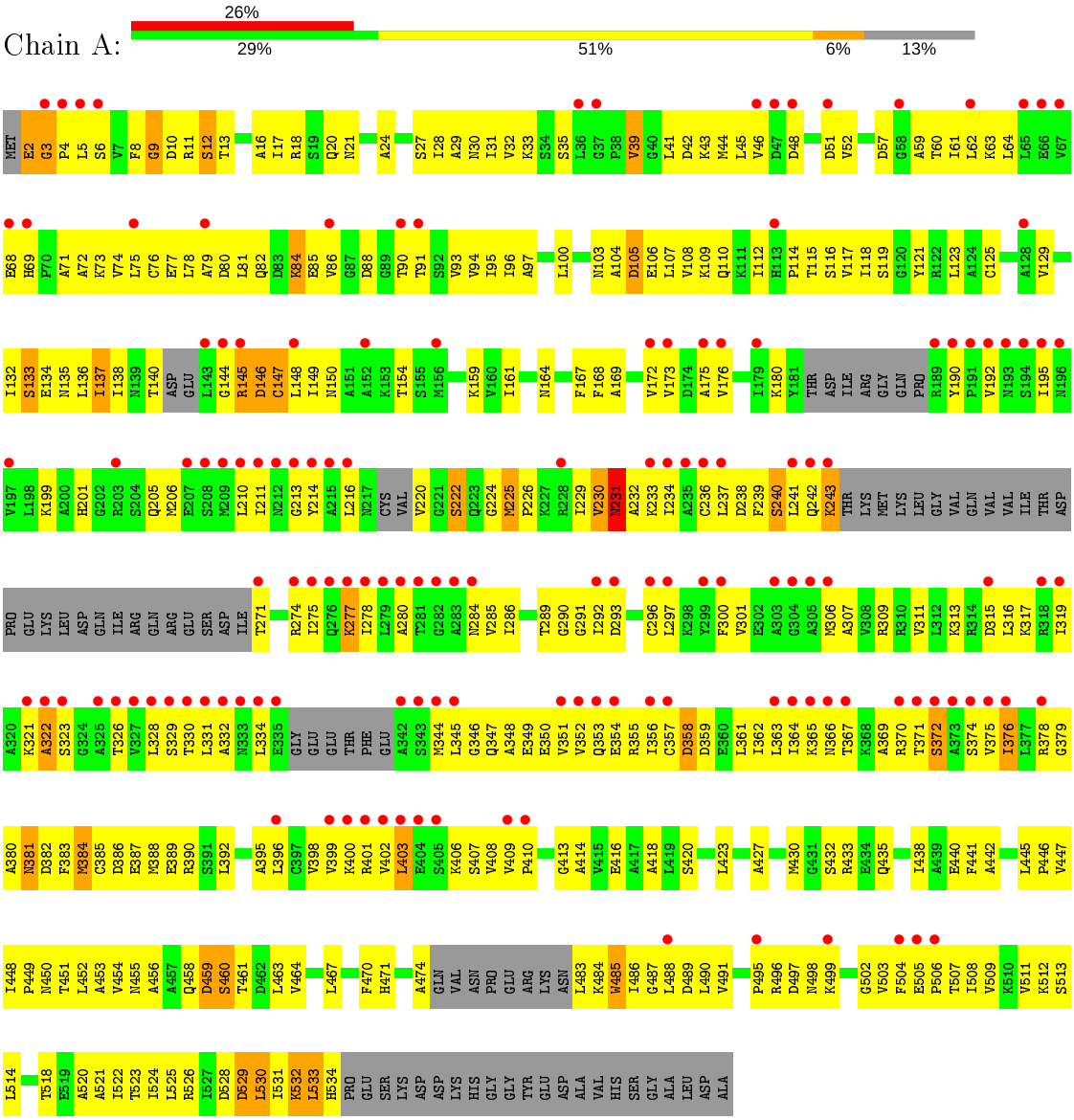
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	Z	481	Total	C	N	O	S	0	0	0
			3664	2310	638	697	19			
8	z	481	Total	C	N	O	S	0	0	0
			3664	2310	638	697	19			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

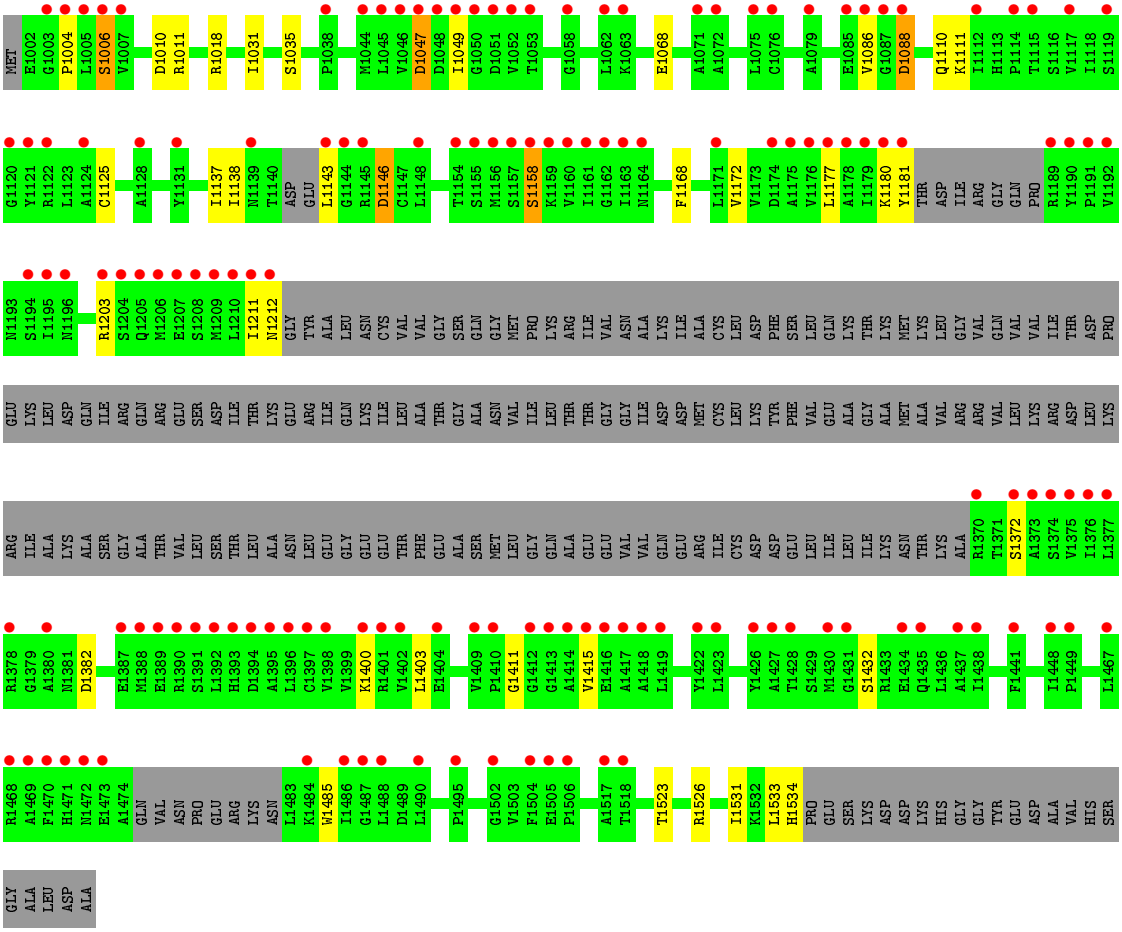
- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT ALPHA

Chain A:



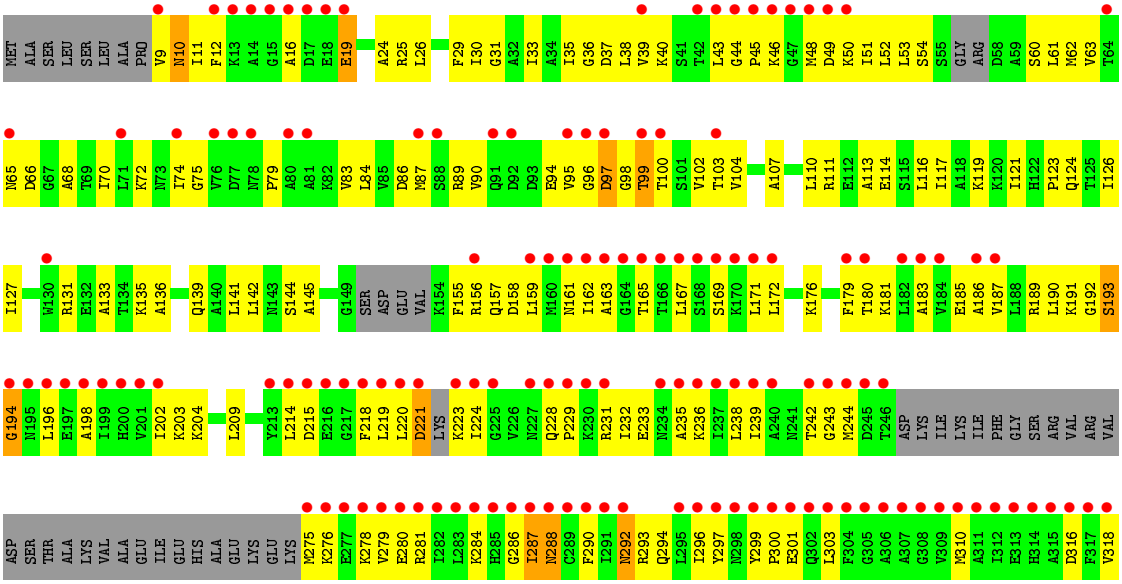
- Molecule 1: T-COMPLEX PROTEIN 1 SUBUNIT ALPHA

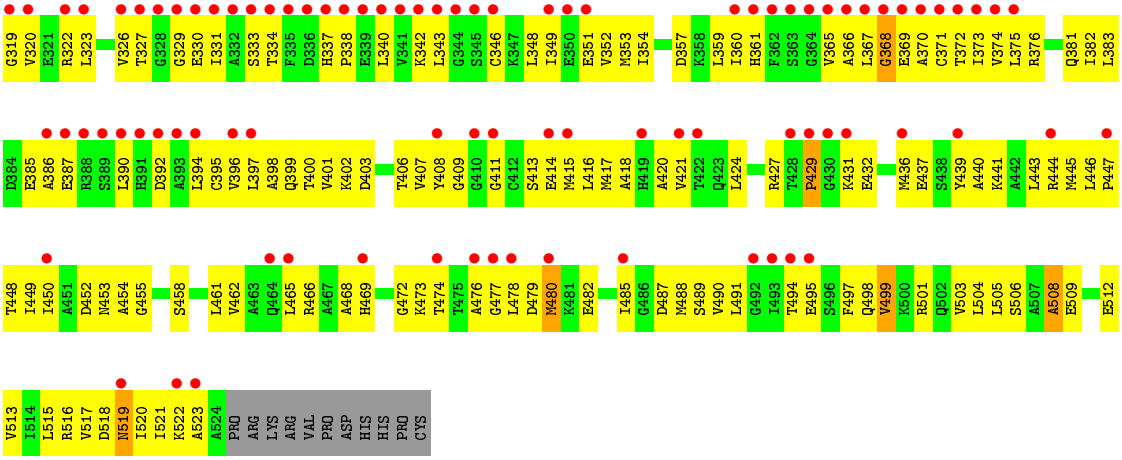
Chain a:



• Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA

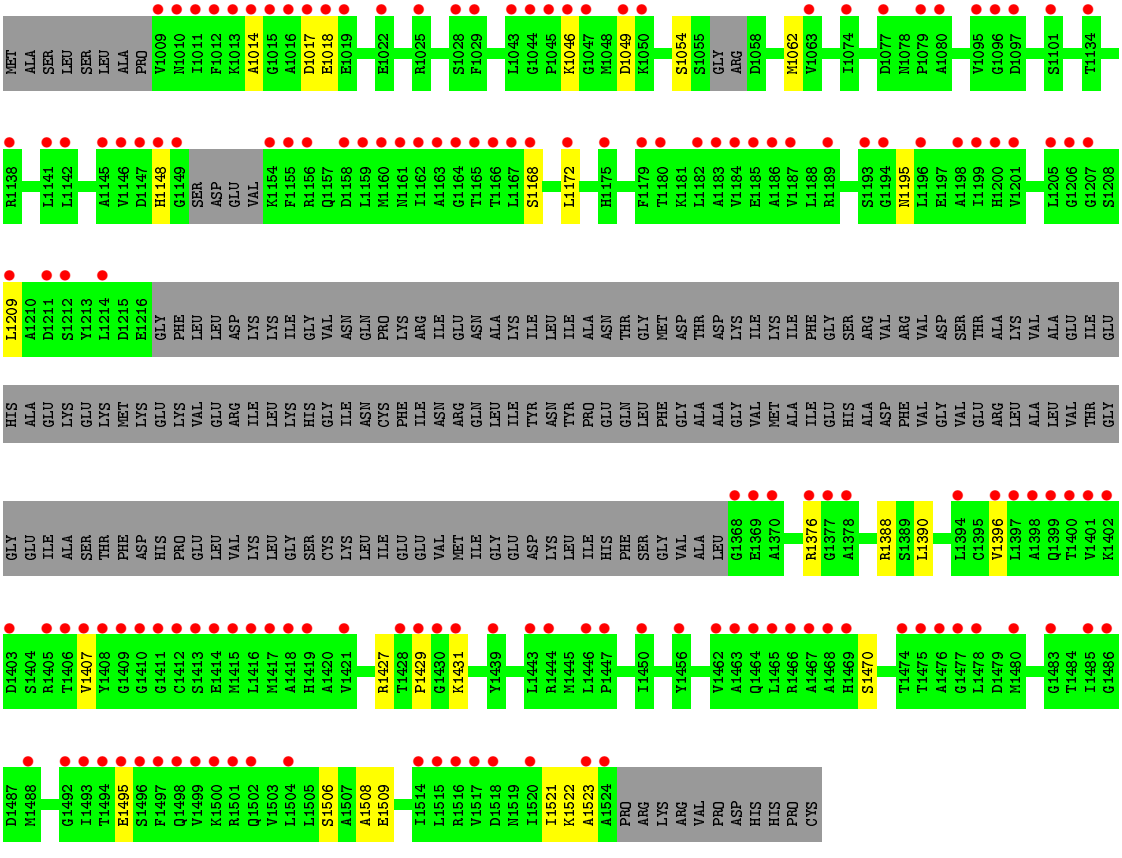
Chain B:





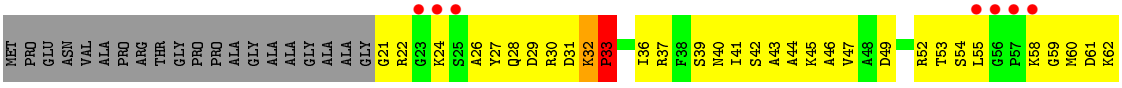
• Molecule 2: T-COMPLEX PROTEIN 1 SUBUNIT BETA

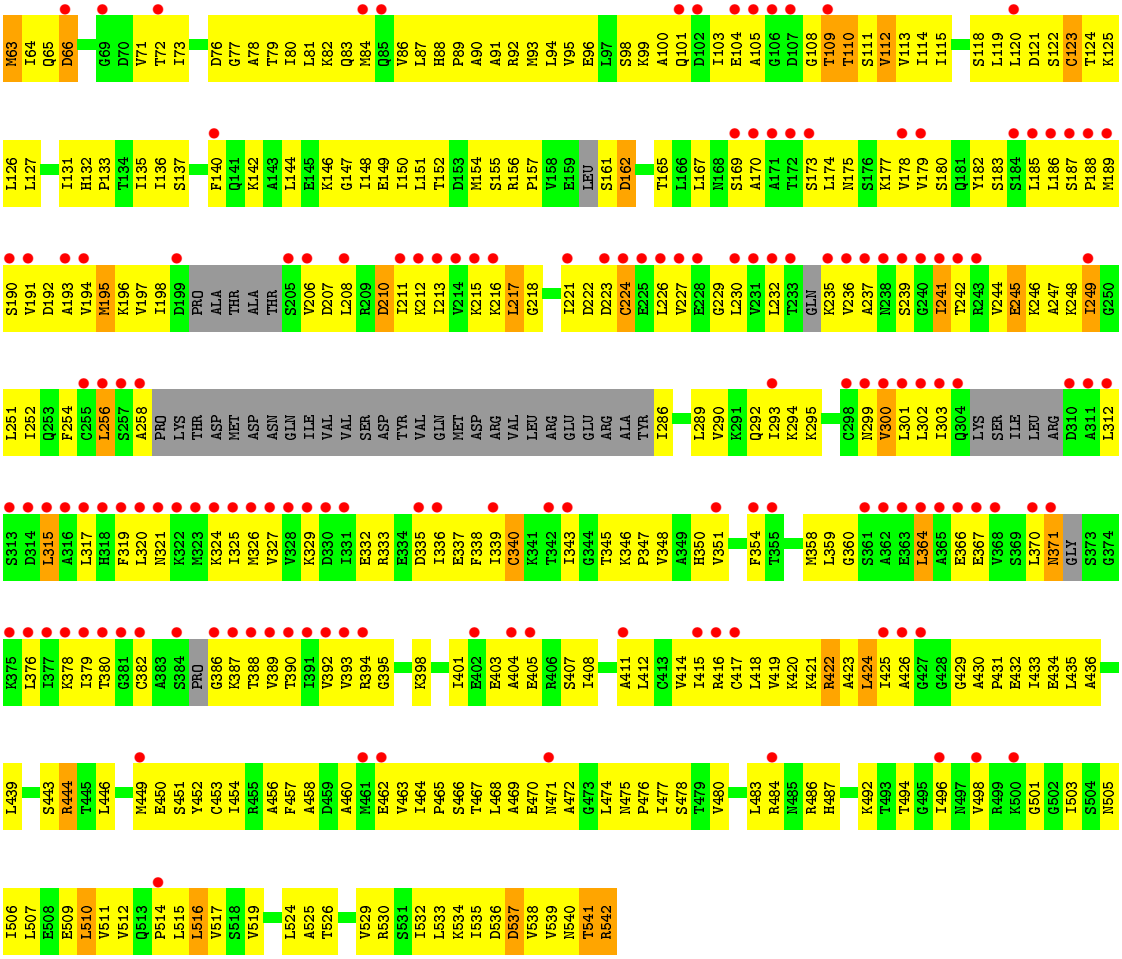
Chain b:



• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

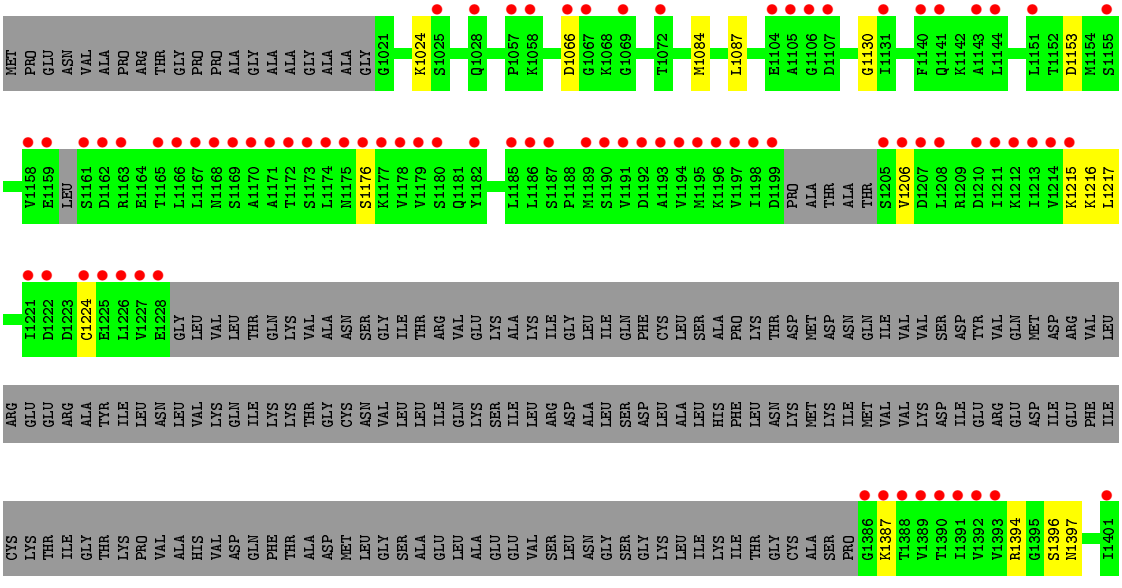
Chain D:

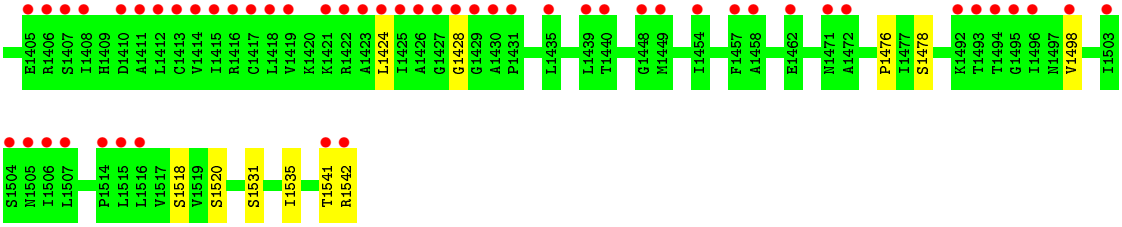




• Molecule 3: T-COMPLEX PROTEIN 1 SUBUNIT DELTA

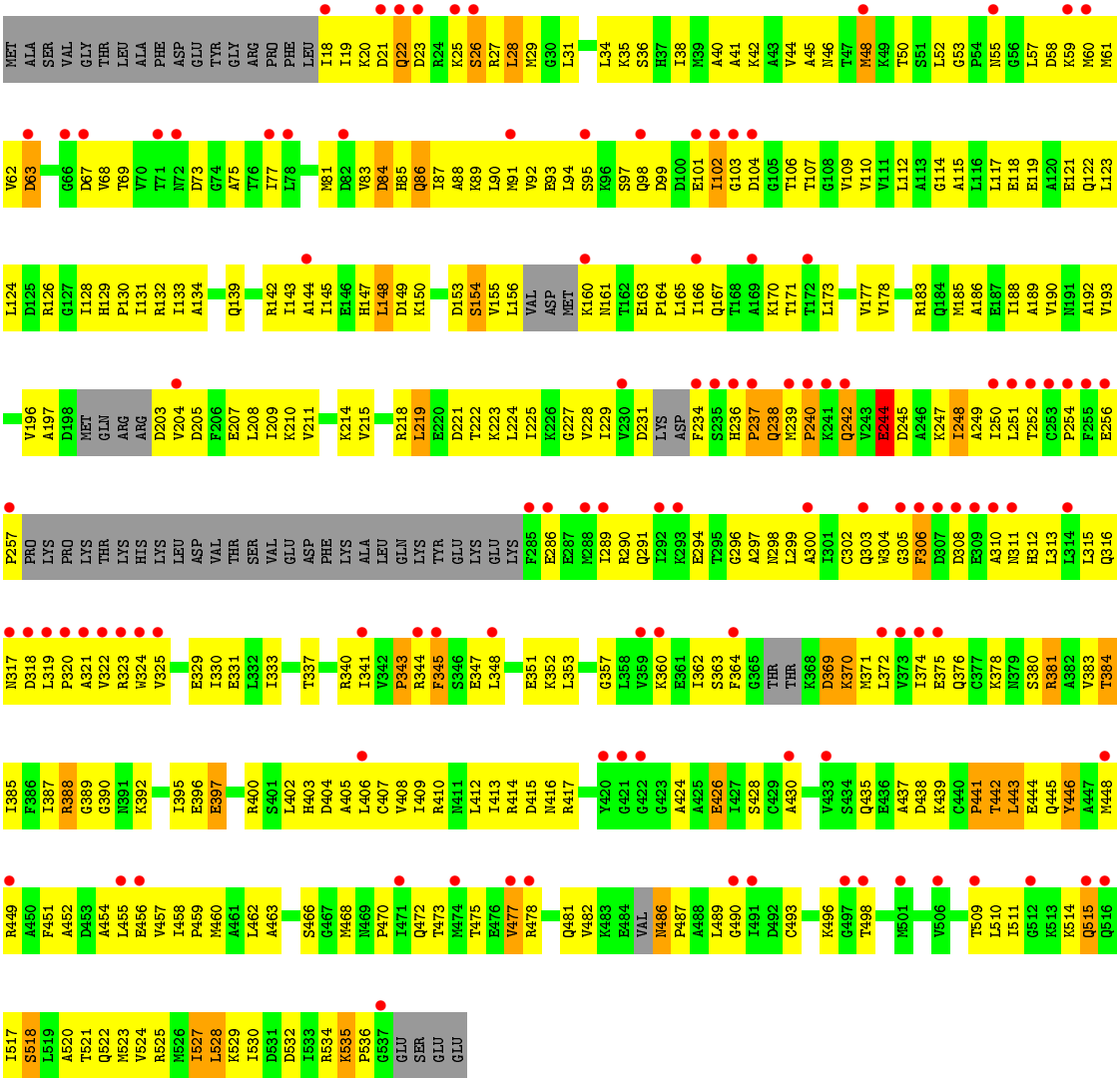
Chain d:





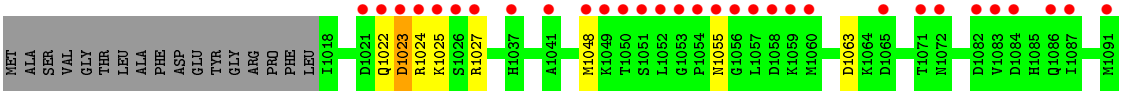
• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

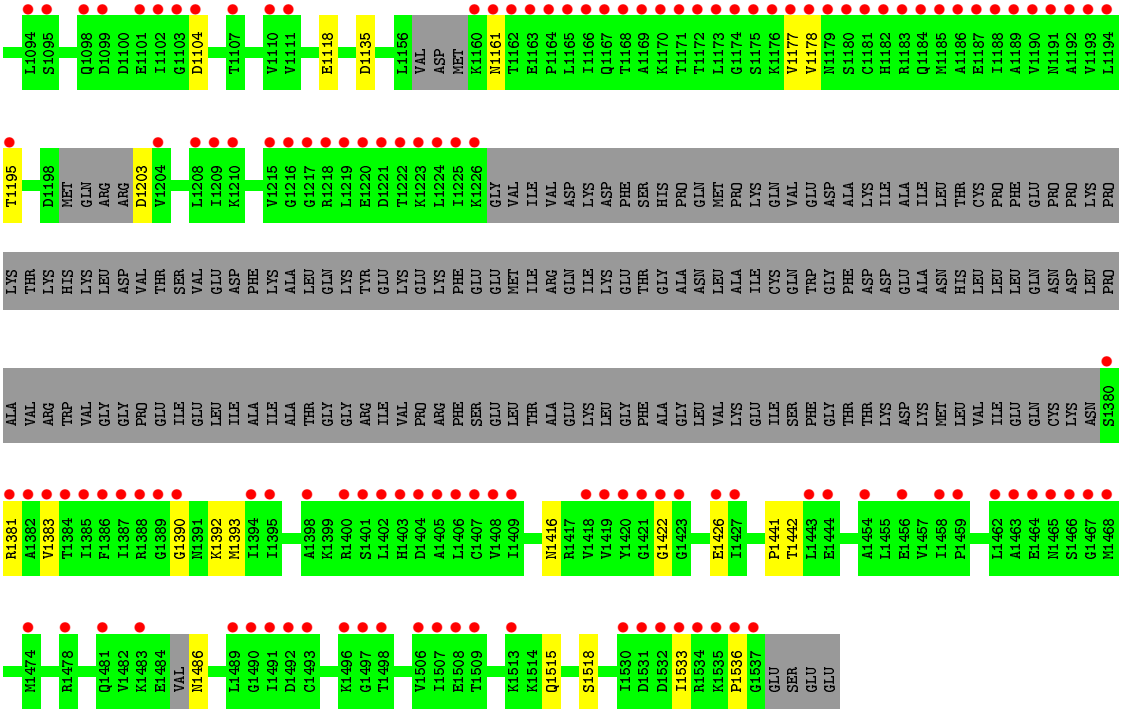
Chain E:



• Molecule 4: T-COMPLEX PROTEIN 1 SUBUNIT EPSILON

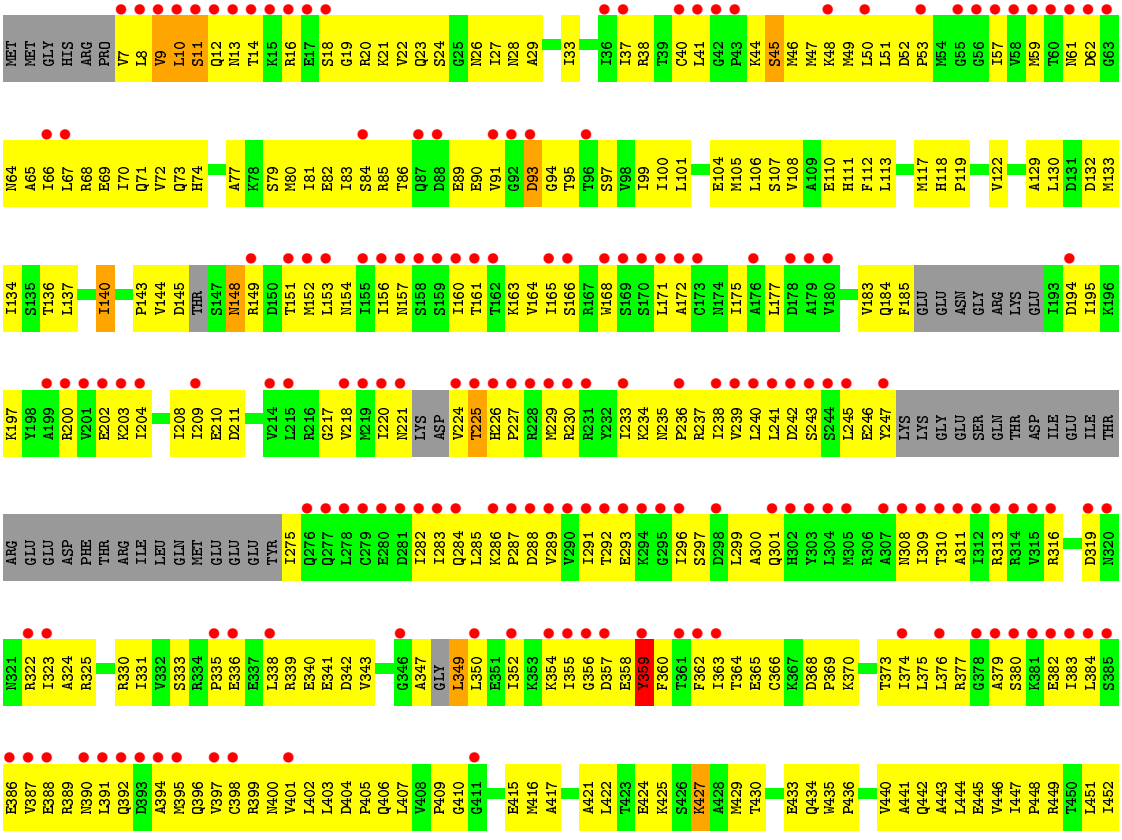
Chain e:

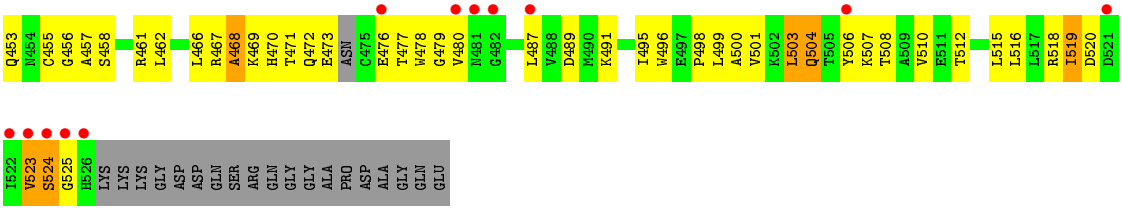




• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

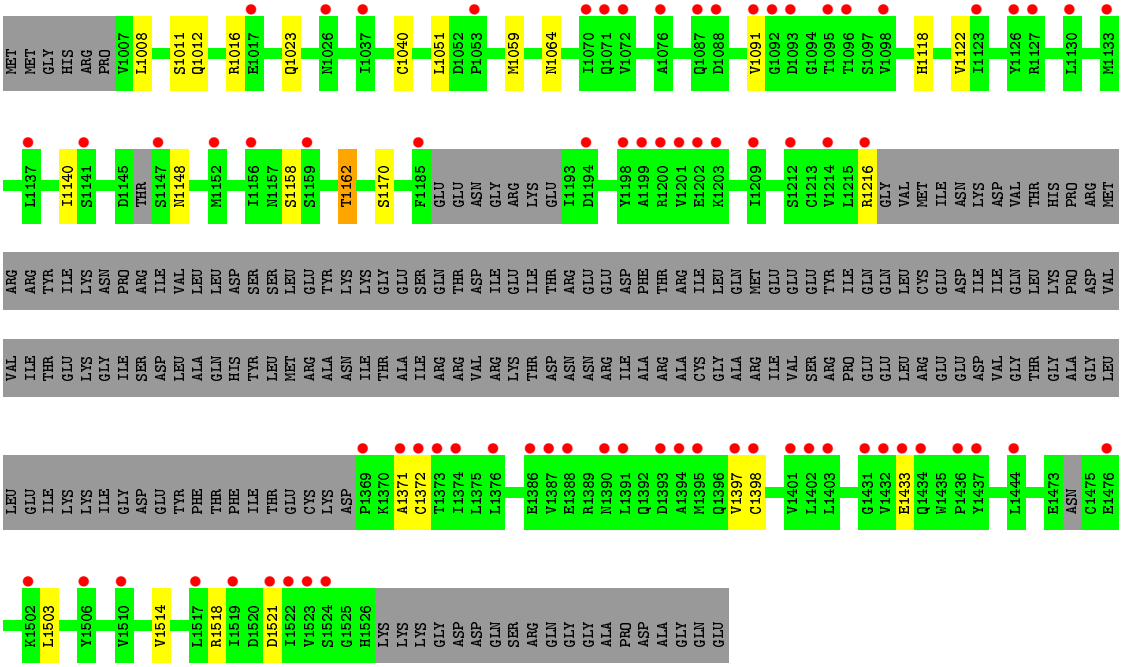
Chain G:





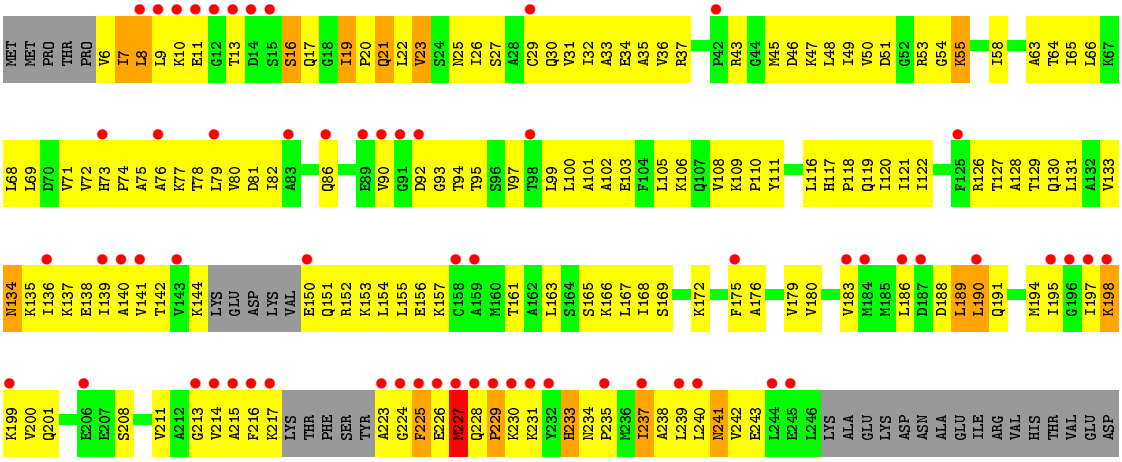
• Molecule 5: T-COMPLEX PROTEIN 1 SUBUNIT GAMMA

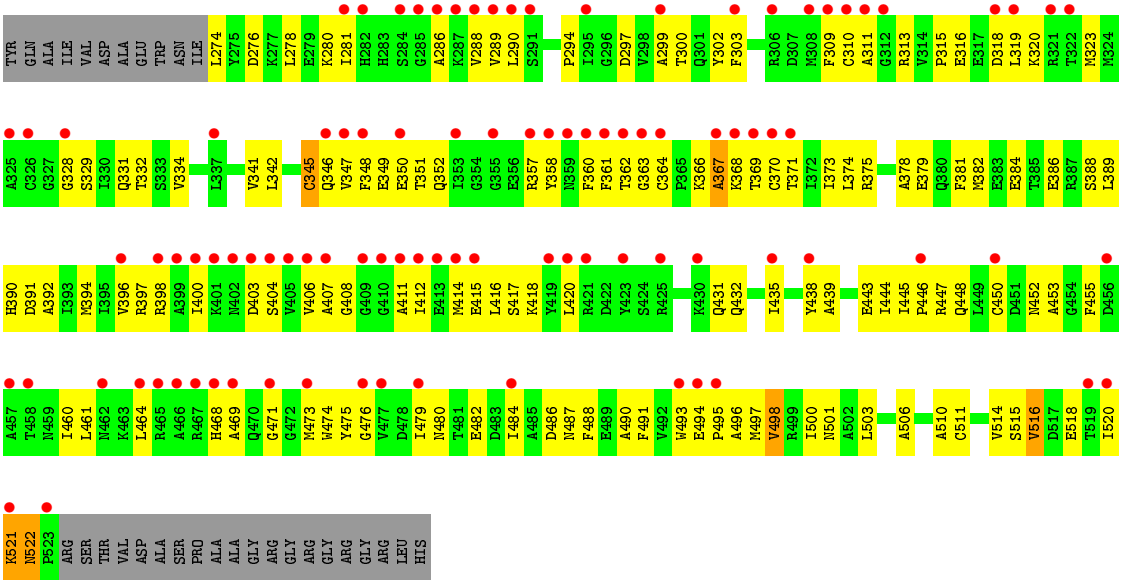
Chain g:



• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

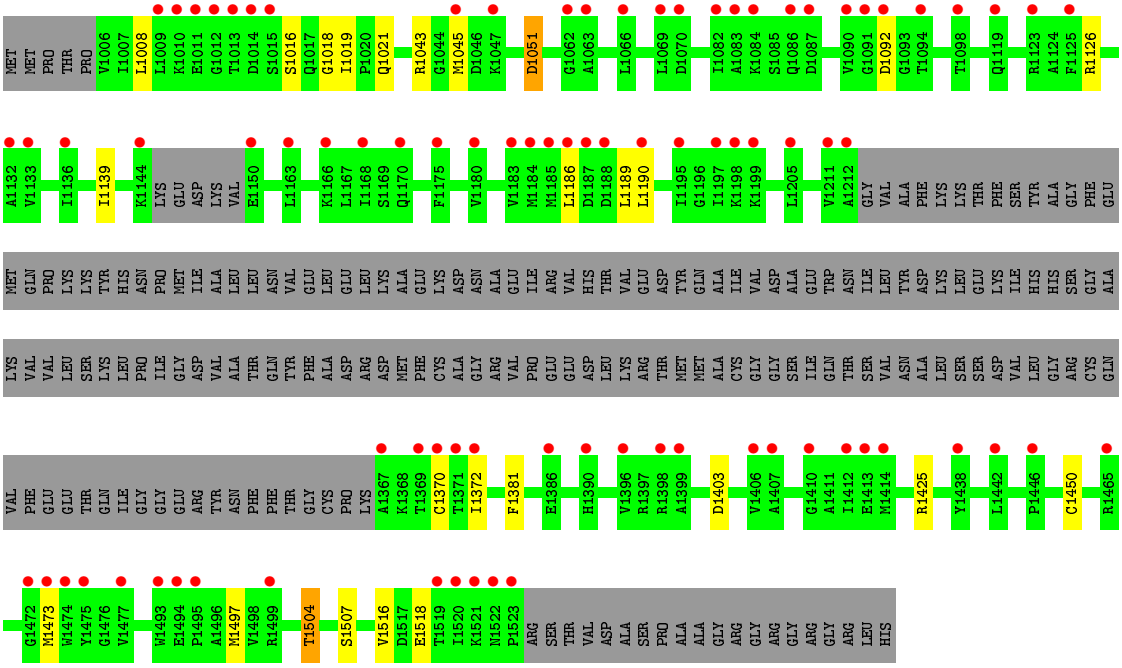
Chain H:





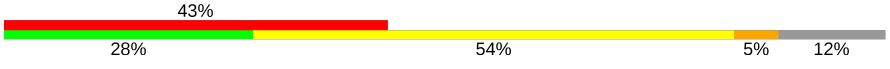
• Molecule 6: T-COMPLEX PROTEIN 1 SUBUNIT ETA

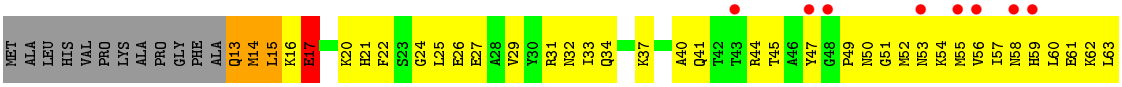
Chain h:

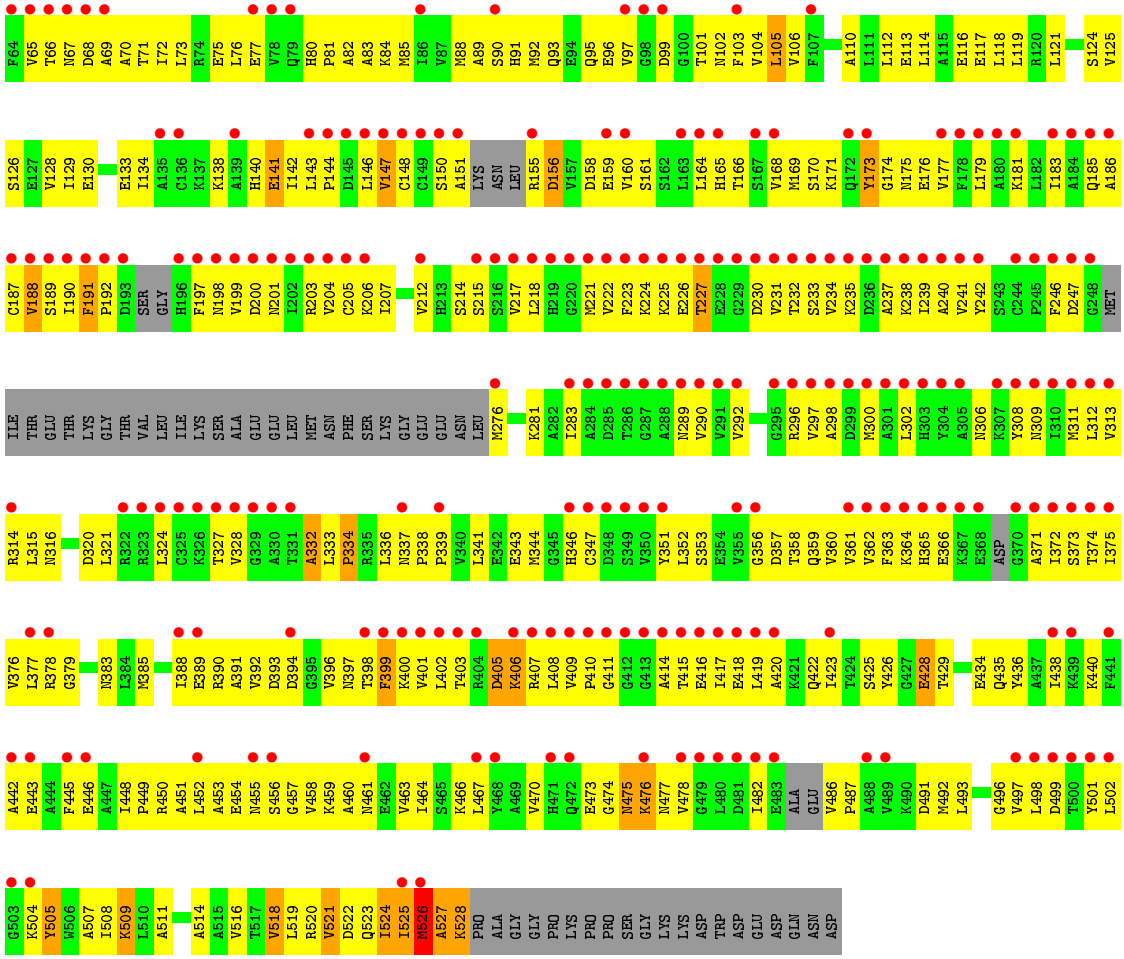


• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

Chain Q:

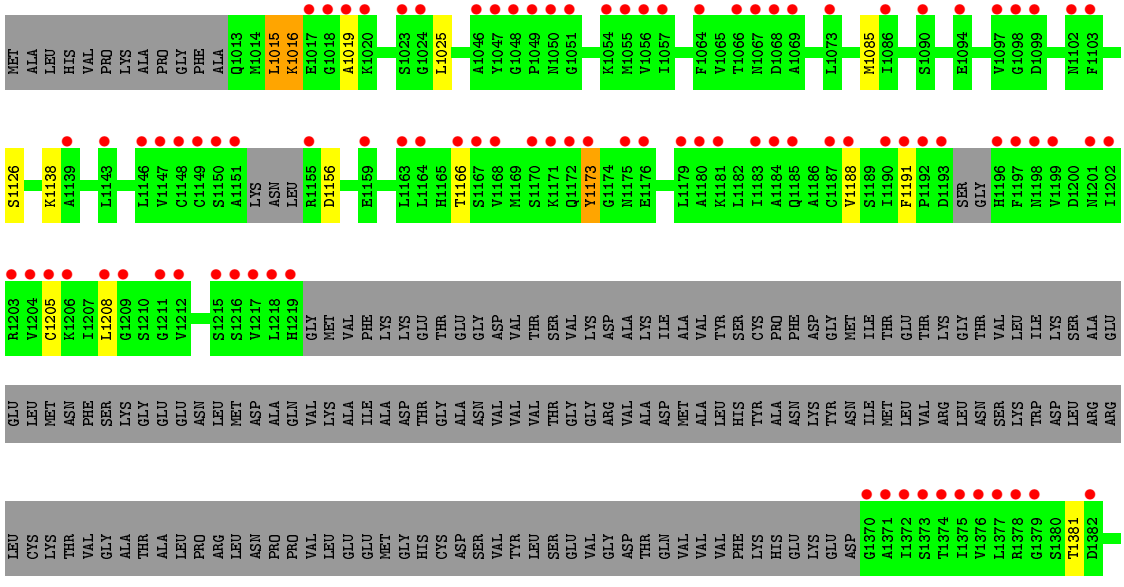


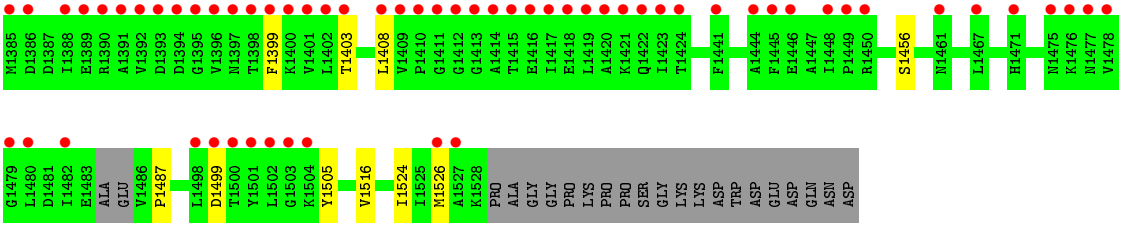




• Molecule 7: T-COMPLEX PROTEIN 1 SUBUNIT THETA

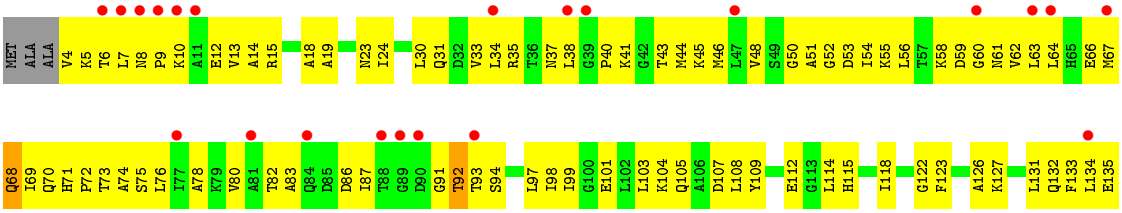
Chain q:

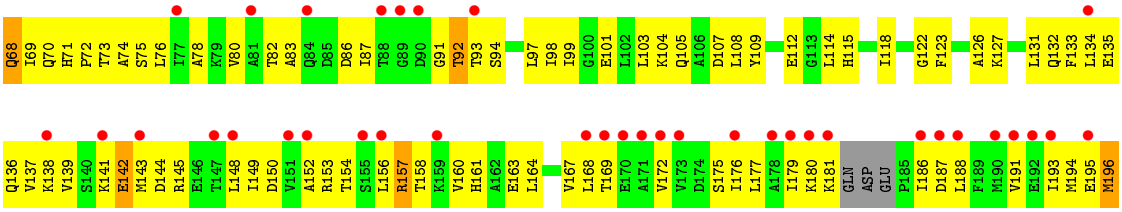


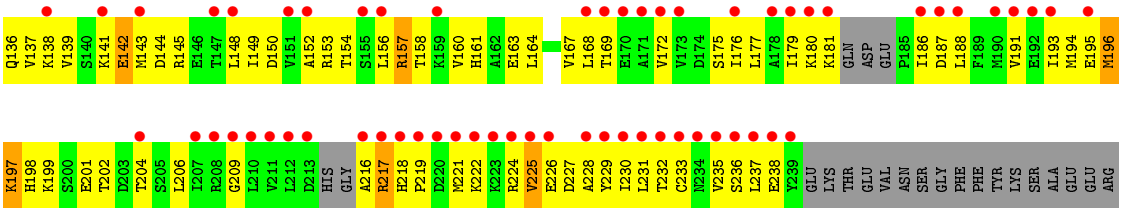


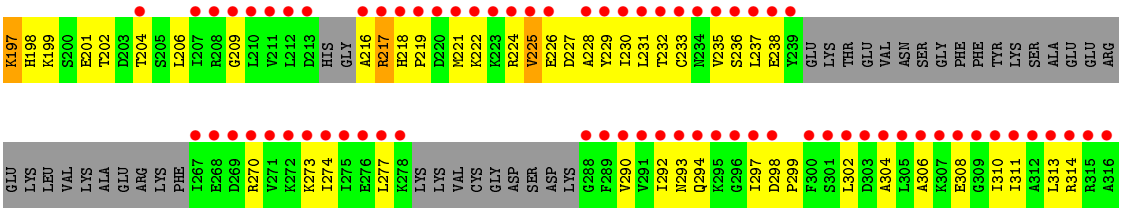
• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA

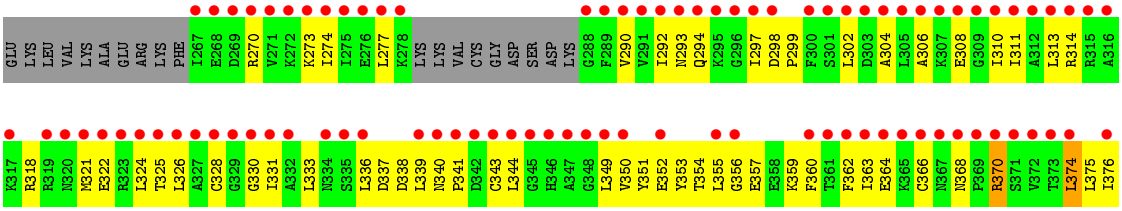
Chain Z:

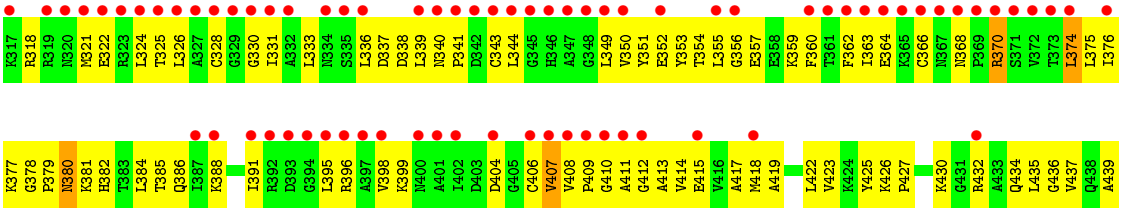


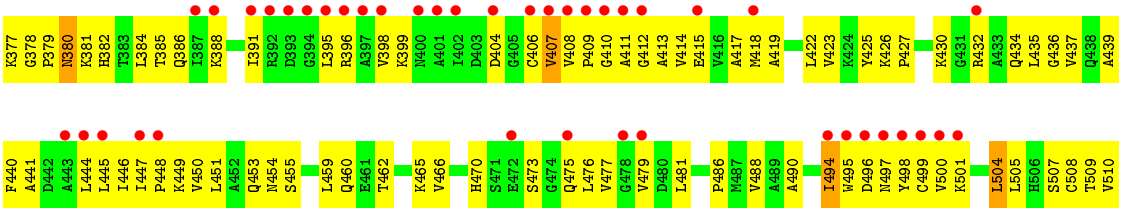


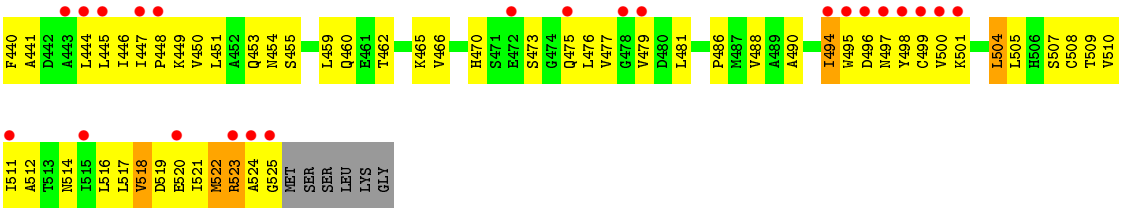


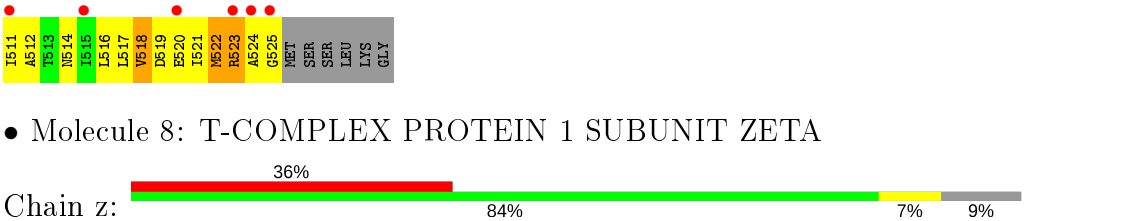


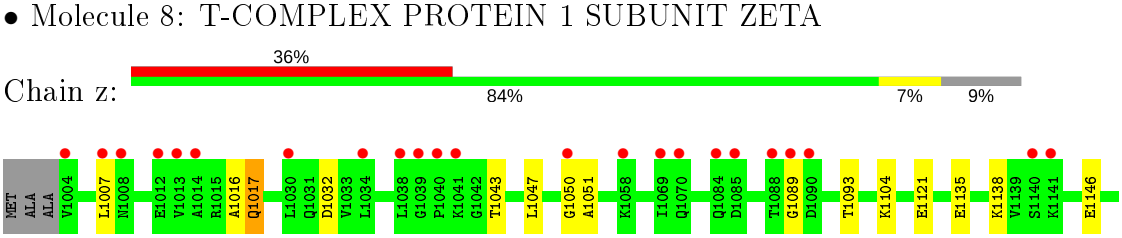


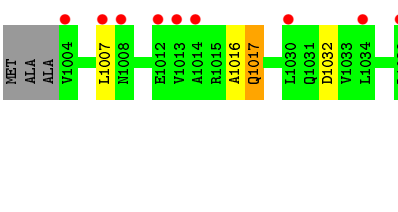






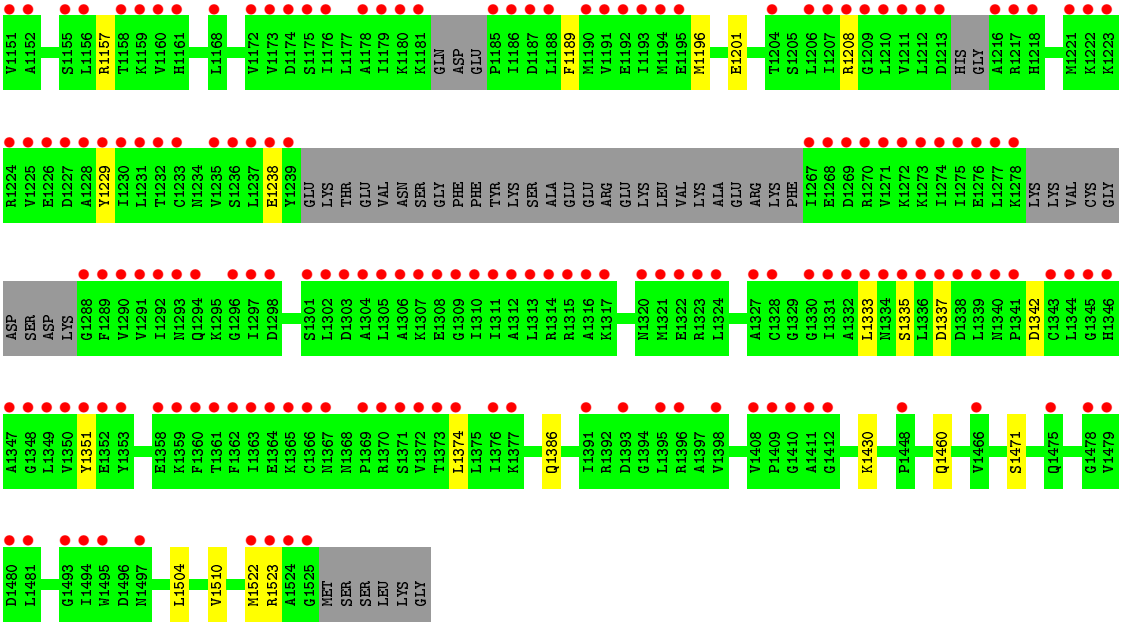






• Molecule 8: T-COMPLEX PROTEIN 1 SUBUNIT ZETA

Chain z:


V1151 A1152 S1155 L1156 R1157 T1158 K1159 V1160 H1161 L1168 V1172 V1173 D1174 S1175 I1176 L1177 A1178 I1179 K1180 K1181 GLN ASP GLU P1185 I1186 D1187 L1188 F1189 M1190 V1191 E1192 I1193 M1194 E1195 M1196 E1201 T1204 S1205 L1206 I1207 R1208 G1209 L1210 V1211 L1212 D1213 HIS GLY A1216 R1217 H1218 M1221 K1222 K1223
R1224 V1225 E1226 D1227 A1228 Y1229 I1230 L1231 T1232 C1233 N1234 V1235 S1236 L1237 E1238 Y1239 GLU LYS THR GLU VAL ASN SER GLY PHE PHE TYR LYS SER ALA GLU GLU ARG GLU LYS LEU VAL LYS ALA GLU ARG LYS PHE I1267 E1268 D1269 R1270 V1271 K1272 K1273 I1274 I1275 E1276 L1277 K1278 LYS LYS VAL CYS GLY
ASP SER ASP LYS G1288 F1289 V1290 V1291 I1292 N1293 Q1294 K1295 G1296 I1297 D1298 S1301 L1302 D1303 A1304 L1305 A1306 K1307 E1308 G1309 I1310 I1311 A1312 L1313 R1314 R1315 A1316 K1317 N1320 M1321 E1322 R1323 L1324 A1327 C1328 G1329 G1330 I1331 A1332 L1333 M1334 S1335 L1336 D1337 D1338 L1339 M1340 P1341 D1342 C1343 L1344 G1345 H1346
A1347 G1348 L1349 V1350 Y1351 E1352 Y1353 E1358 K1359 F1360 T1361 F1362 I1363 E1364 K1365 C1366 N1367 N1368 P1369 R1370 S1371 V1372 T1373 L1374 L1375 I1376 K1377 Q1386 I1391 R1392 D1393 G1394 L1395 R1396 A1397 V1398 V1408 P1409 G1410 A1411 G1412 K1430 P1448 Q1460 V1466 S1471 Q1475 G1478 V1479
D1480 L1481 G1493 I1494 W1495 D1496 N1497 L1504 V1510 M1522 R1523 A1524 G1525 MET SER SER LEU LYS GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	272.70Å 313.50Å 158.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	200.00 – 5.50 97.58 – 5.44	Depositor EDS
% Data completeness (in resolution range)	99.1 (200.00-5.50) 98.4 (97.58-5.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.37 (at 5.41Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.340 , 0.399 0.345 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	257.8	Xtriage
Anisotropy	0.400	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 427.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.32$, $< L^2 > = 0.16$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.75	EDS
Total number of atoms	51877	wwPDB-VP
Average B, all atoms (Å^2)	277.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[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

5.1 Standard geometry

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	0.22	0/3657	0.44	0/4934
1	a	0.22	0/2733	0.46	0/3695
2	B	0.22	0/3638	0.43	0/4903
2	b	0.21	0/2680	0.44	0/3615
3	D	0.21	0/3632	0.46	0/4891
3	d	0.21	0/2707	0.45	0/3650
4	E	0.22	0/3712	0.44	0/4997
4	e	0.21	0/2743	0.44	0/3687
5	G	0.21	0/3758	0.45	0/5073
5	g	0.21	0/2763	0.46	0/3733
6	H	0.23	0/3716	0.43	0/5008
6	h	0.22	0/2751	0.45	0/3711
7	Q	0.23	0/3724	0.44	0/5032
7	q	0.23	0/2774	0.43	0/3746
8	Z	0.22	0/3702	0.44	0/4995
8	z	0.21	0/3702	0.45	0/4995
All	All	0.22	0/52392	0.44	0/70665

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3625	0	3783	380	0
1	a	2705	0	2799	0	0
2	B	3602	0	3705	353	0
2	b	2658	0	2733	0	0
3	D	3610	0	3810	456	0
3	d	2690	0	2818	0	0
4	E	3674	0	3781	382	0
4	e	2724	0	2822	0	0
5	G	3719	0	3870	398	0
5	g	2735	0	2851	0	0
6	H	3671	0	3783	366	0
6	h	2724	0	2842	0	0
7	Q	3673	0	3719	383	0
7	q	2739	0	2777	0	0
8	Z	3664	0	3820	413	0
8	z	3664	0	3820	0	0
All	All	51877	0	53733	2912	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 52.

The worst 5 of 2912 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:G:456:GLY:HA3	8:Z:118:ILE:HD11	1.37	1.06
1:A:211:ILE:HG22	1:A:213:GLY:H	1.21	1.04
3:D:540:ASN:HB3	3:D:542:ARG:HD3	1.36	1.03
4:E:94:LEU:HD21	4:E:523:MET:HB2	1.39	1.03
3:D:31:ASP:HB3	3:D:36:ILE:HB	1.39	1.03

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 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	471/556 (85%)	390 (83%)	63 (13%)	18 (4%)	3	24
1	a	351/556 (63%)	283 (81%)	50 (14%)	18 (5%)	2	19
2	B	473/535 (88%)	398 (84%)	62 (13%)	13 (3%)	5	31
2	b	353/535 (66%)	301 (85%)	42 (12%)	10 (3%)	5	30
3	D	469/542 (86%)	385 (82%)	70 (15%)	14 (3%)	4	28
3	d	351/542 (65%)	300 (86%)	42 (12%)	9 (3%)	5	31
4	E	471/541 (87%)	392 (83%)	60 (13%)	19 (4%)	3	23
4	e	351/541 (65%)	295 (84%)	39 (11%)	17 (5%)	2	21
5	G	471/545 (86%)	396 (84%)	62 (13%)	13 (3%)	5	30
5	g	351/545 (64%)	291 (83%)	51 (14%)	9 (3%)	5	31
6	H	473/543 (87%)	384 (81%)	73 (15%)	16 (3%)	3	26
6	h	353/543 (65%)	289 (82%)	54 (15%)	10 (3%)	5	30
7	Q	473/548 (86%)	406 (86%)	45 (10%)	22 (5%)	2	21
7	q	351/548 (64%)	292 (83%)	48 (14%)	11 (3%)	4	27
8	Z	473/531 (89%)	400 (85%)	57 (12%)	16 (3%)	3	26
8	z	473/531 (89%)	403 (85%)	57 (12%)	13 (3%)	5	31
All	All	6708/8682 (77%)	5605 (84%)	875 (13%)	228 (3%)	3	26

5 of 228 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3	GLY
1	A	145	ARG
1	A	146	ASP
1	A	230	VAL
2	B	54	SER

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 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	395/461 (86%)	368 (93%)	27 (7%)	16 42
1	a	297/461 (64%)	269 (91%)	28 (9%)	8 29
2	B	382/429 (89%)	372 (97%)	10 (3%)	46 67
2	b	281/429 (66%)	263 (94%)	18 (6%)	17 44
3	D	407/454 (90%)	388 (95%)	19 (5%)	26 52
3	d	303/454 (67%)	285 (94%)	18 (6%)	19 46
4	E	400/455 (88%)	371 (93%)	29 (7%)	14 40
4	e	298/455 (66%)	283 (95%)	15 (5%)	24 50
5	G	416/470 (88%)	402 (97%)	14 (3%)	37 60
5	g	307/470 (65%)	288 (94%)	19 (6%)	18 45
6	H	394/445 (88%)	381 (97%)	13 (3%)	38 61
6	h	292/445 (66%)	274 (94%)	18 (6%)	18 45
7	Q	398/452 (88%)	380 (96%)	18 (4%)	27 53
7	q	296/452 (66%)	279 (94%)	17 (6%)	20 47
8	Z	398/440 (90%)	386 (97%)	12 (3%)	41 63
8	z	398/440 (90%)	374 (94%)	24 (6%)	19 46
All	All	5662/7212 (78%)	5363 (95%)	299 (5%)	22 49

5 of 299 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	Z	370	ARG
1	a	1523	THR
8	z	1017	GLN
8	Z	508	CYS
1	a	1125	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 144 such sidechains are listed below:

Mol	Chain	Res	Type
7	Q	435	GLN
1	a	1393	HIS
8	z	1070	GLN
8	Z	23	ASN
8	Z	453	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 carbohydrates 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, 95^{th} 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	481/556 (86%)	1.61	142 (29%) 0 1	260, 260, 260, 260	0
1	a	359/556 (64%)	2.09	149 (41%) 0 0	282, 282, 282, 282	0
2	B	481/535 (89%)	2.59	229 (47%) 0 0	281, 281, 281, 281	0
2	b	359/535 (67%)	2.17	159 (44%) 0 0	272, 272, 272, 272	0
3	D	481/542 (88%)	1.80	158 (32%) 0 1	289, 289, 289, 289	0
3	d	359/542 (66%)	1.80	133 (37%) 0 1	266, 266, 266, 266	0
4	E	481/541 (88%)	1.25	109 (22%) 0 2	262, 262, 262, 262	0
4	e	359/541 (66%)	2.40	164 (45%) 0 0	283, 283, 283, 283	0
5	G	481/545 (88%)	1.96	185 (38%) 0 1	283, 283, 283, 283	0
5	g	359/545 (65%)	1.17	75 (20%) 1 2	275, 275, 275, 275	0
6	H	481/543 (88%)	1.70	159 (33%) 0 1	272, 272, 272, 272	0
6	h	359/543 (66%)	1.19	86 (23%) 0 2	258, 258, 258, 258	0
7	Q	481/548 (87%)	2.59	233 (48%) 0 0	308, 308, 308, 308	0
7	q	359/548 (65%)	2.02	154 (42%) 0 0	261, 261, 261, 261	0
8	Z	481/531 (90%)	2.52	218 (45%) 0 0	297, 297, 297, 297	0
8	z	481/531 (90%)	2.37	193 (40%) 0 1	276, 276, 276, 276	0
All	All	6842/8682 (78%)	1.97	2546 (37%) 0 1	258, 276, 308, 308	0

The worst 5 of 2546 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	Z	288	GLY	25.1
8	z	1209	GLY	21.7
6	H	224	GLY	18.4
8	z	1288	GLY	16.3
4	e	1226	LYS	15.8

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 carbohydrates 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.