wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 02:50 AM GMT

PDB ID	:	2IUS
Title	:	E. COLI FTSK MOTOR DOMAIN
Authors	:	Massey, T.H.; Mercogliano, C.P.; Yates, J.; Sherratt, D.J.; Lowe, J.
Deposited on	:	2006-06-07
Resolution	:	2.70 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
http://wwpdb.org/validation/2016/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:

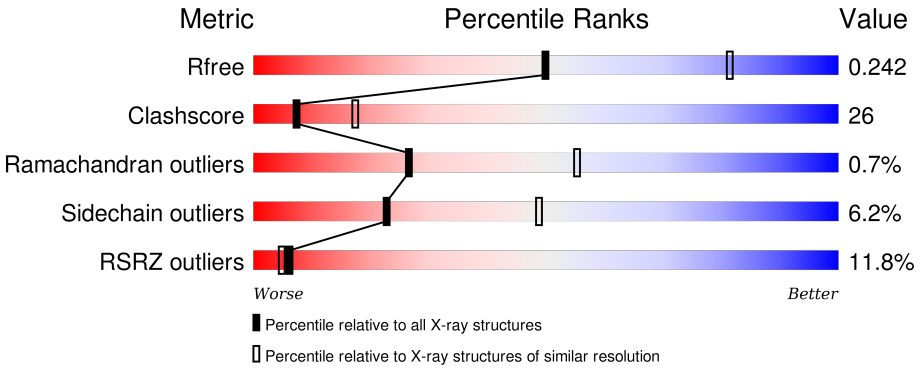
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.70 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))
R_{free}	91344	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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. 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	512	7% 43% 31% • 23%
1	B	512	6% 46% 27% • 23%
1	C	512	11% 44% 30% • 23%
1	D	512	7% 45% 30% • 23%
1	E	512	10% 43% 28% • 26%

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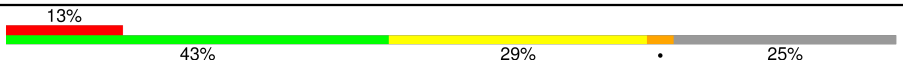
Mol	Chain	Length	Quality of chain
1	F	512	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 18569 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 DNA TRANSLOCASE FTSK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	0	1
			3029	1930	532	551	16			
1	B	393	Total	C	N	O	S	0	0	1
			3029	1930	532	551	16			
1	C	393	Total	C	N	O	S	0	0	1
			3029	1930	532	551	16			
1	D	394	Total	C	N	O	S	0	0	1
			3036	1935	533	552	16			
1	E	381	Total	C	N	O	S	0	0	1
			2941	1877	512	536	16			
1	F	382	Total	C	N	O	S	0	0	1
			2952	1883	516	537	16			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	997	ALA	LYS	ENGINEERED MUTATION	UNP P46889
B	997	ALA	LYS	ENGINEERED MUTATION	UNP P46889
C	997	ALA	LYS	ENGINEERED MUTATION	UNP P46889
D	997	ALA	LYS	ENGINEERED MUTATION	UNP P46889
E	997	ALA	LYS	ENGINEERED MUTATION	UNP P46889
F	997	ALA	LYS	ENGINEERED MUTATION	UNP P46889

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		
2	B	94	Total	O	0	0
			94	94		
2	C	80	Total	O	0	0
			80	80		

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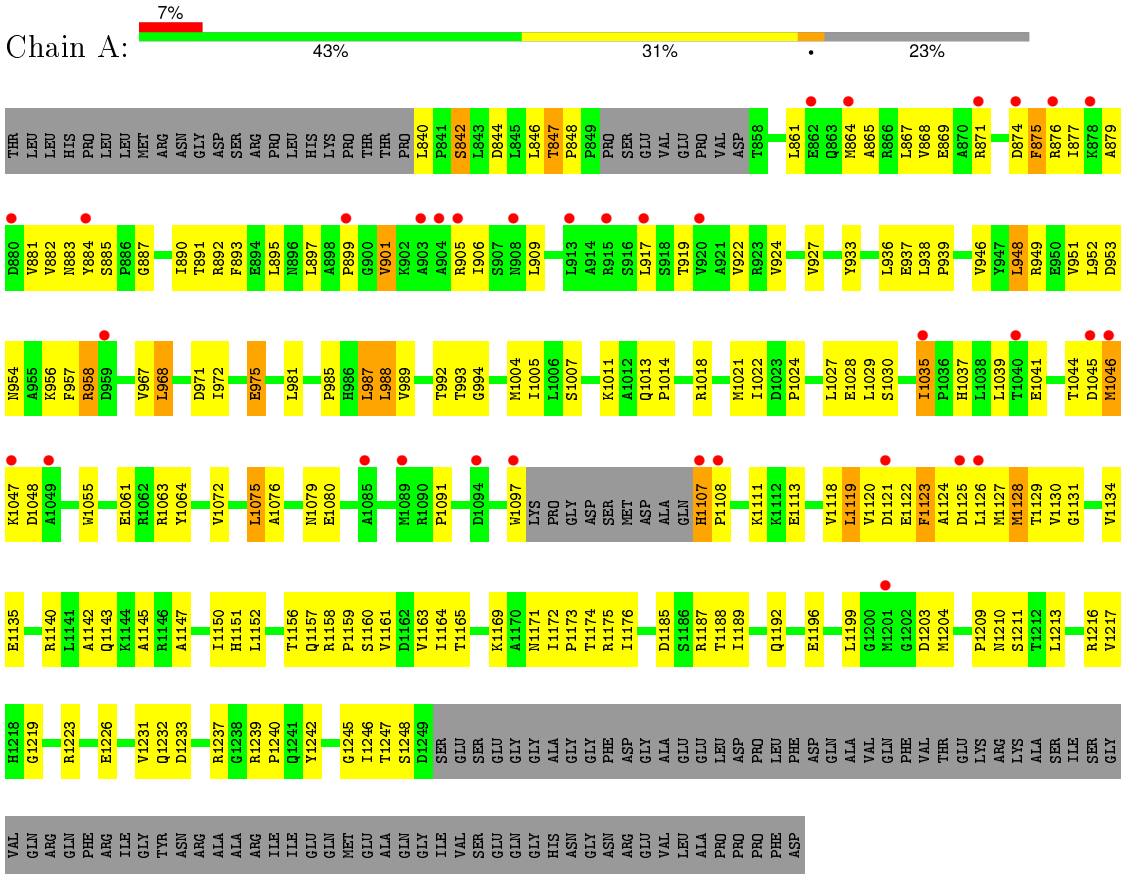
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	116	Total O 116 116	0	0
2	E	99	Total O 99 99	0	0
2	F	73	Total O 73 73	0	0

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 errors 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.

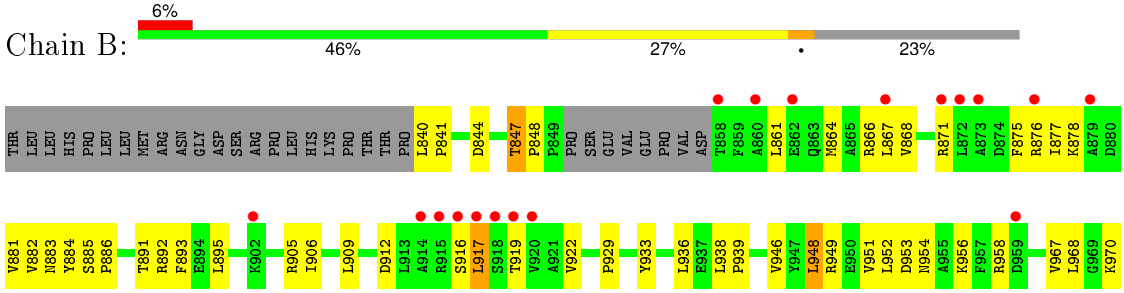
- Molecule 1: DNA TRANSLOCASE FTSK

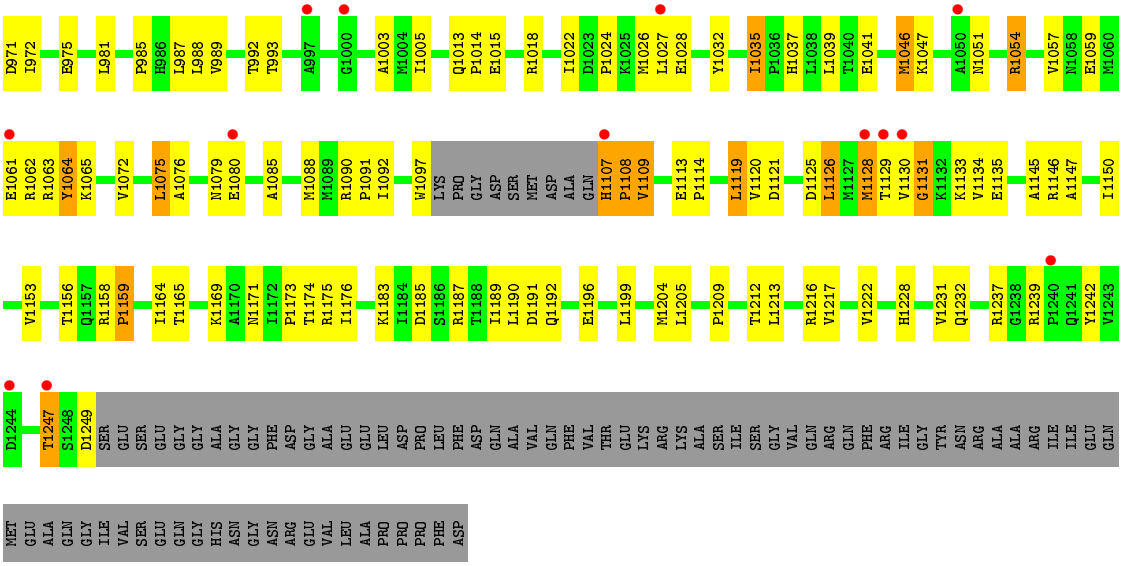
Chain A:



- Molecule 1: DNA TRANSLOCASE FTSK

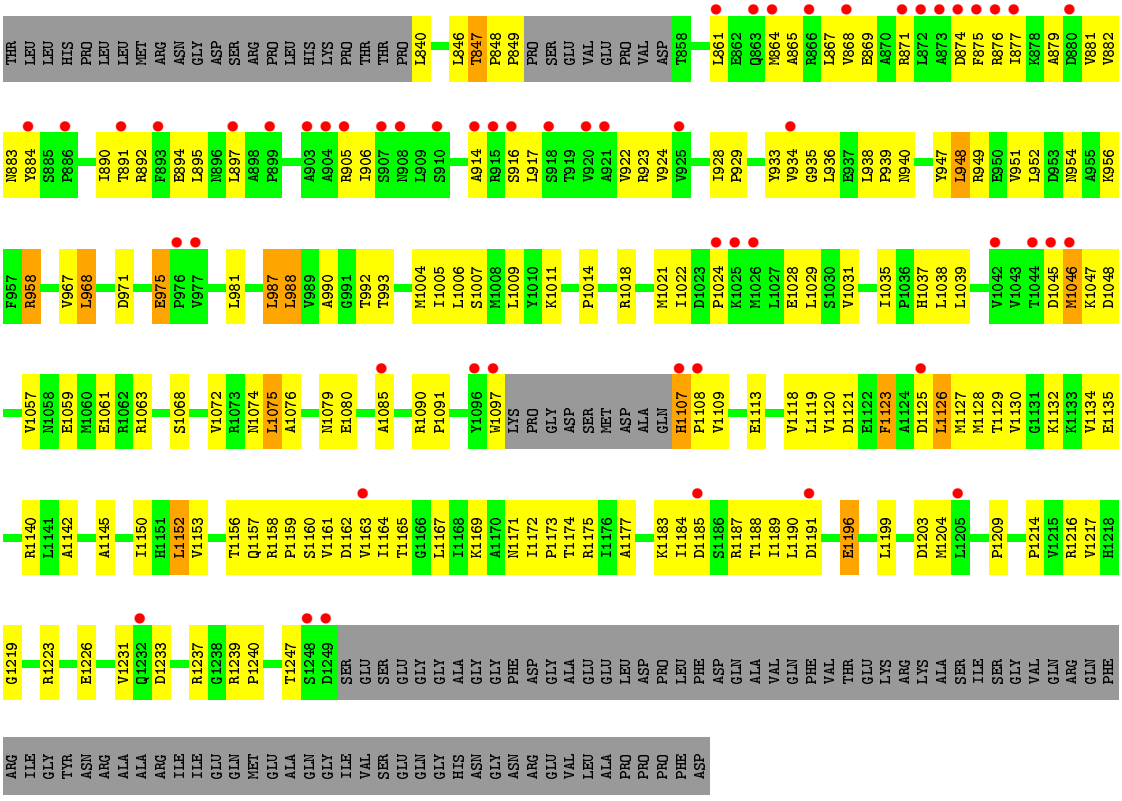
Chain B:





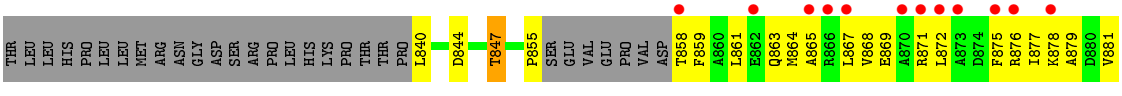
• Molecule 1: DNA TRANSLOCASE FTSK

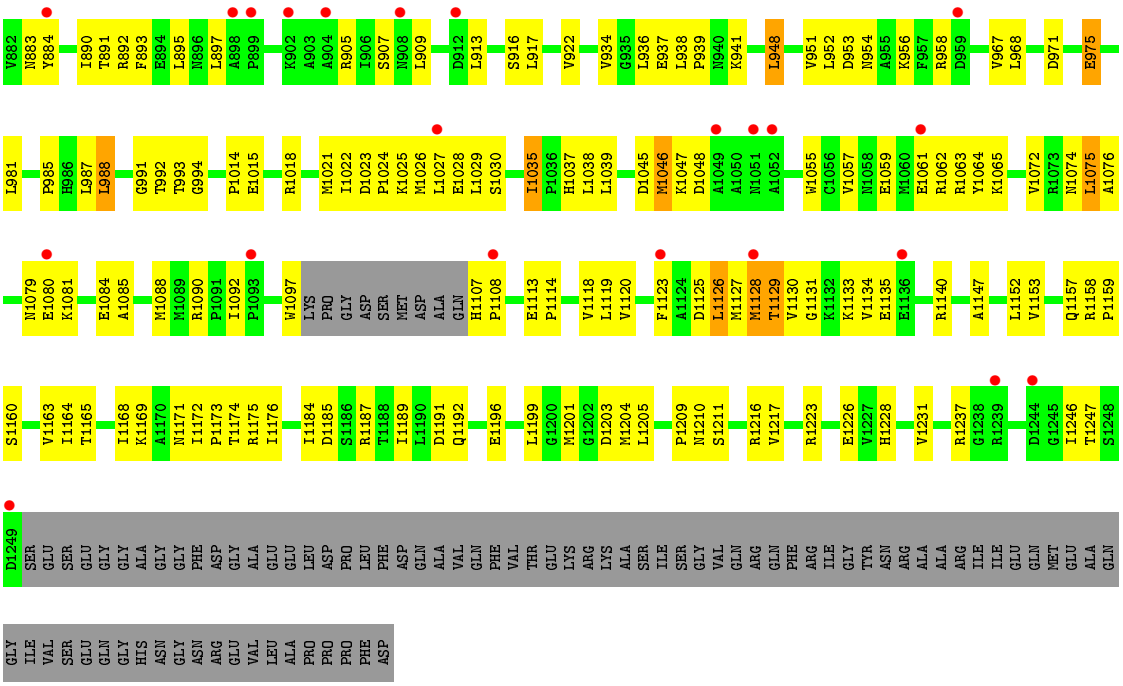
Chain C:



• Molecule 1: DNA TRANSLOCASE FTSK

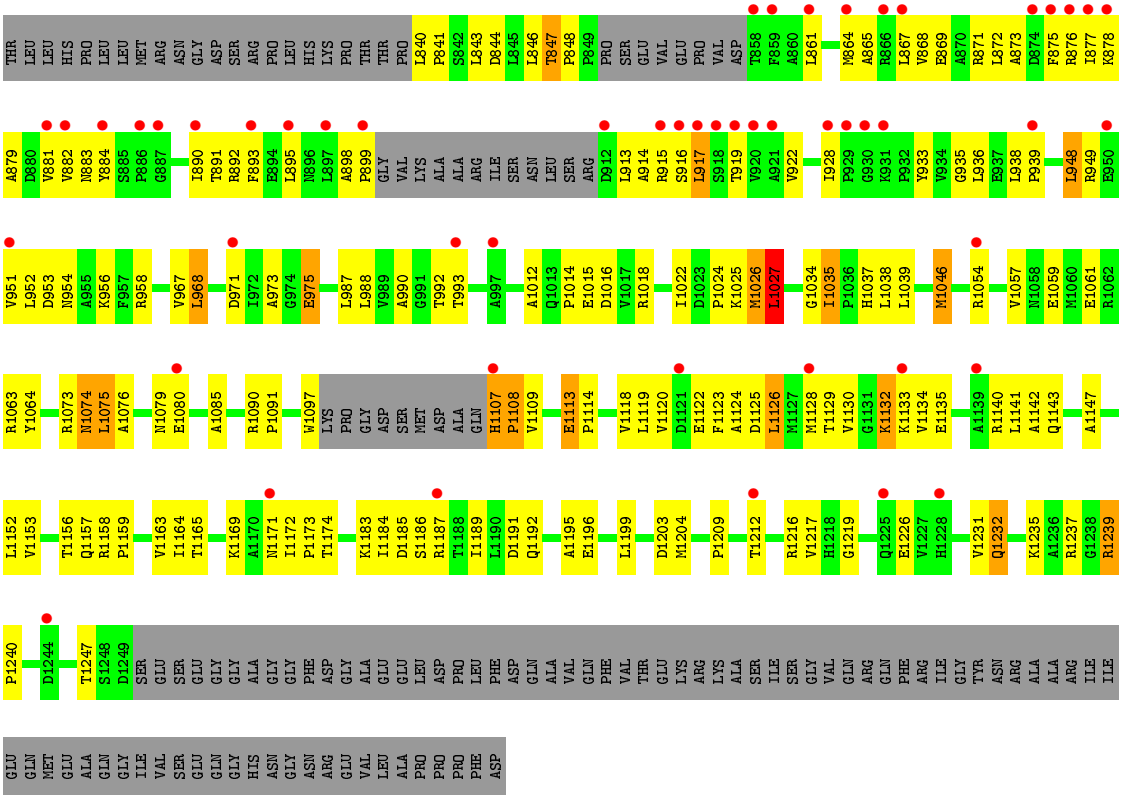
Chain D:





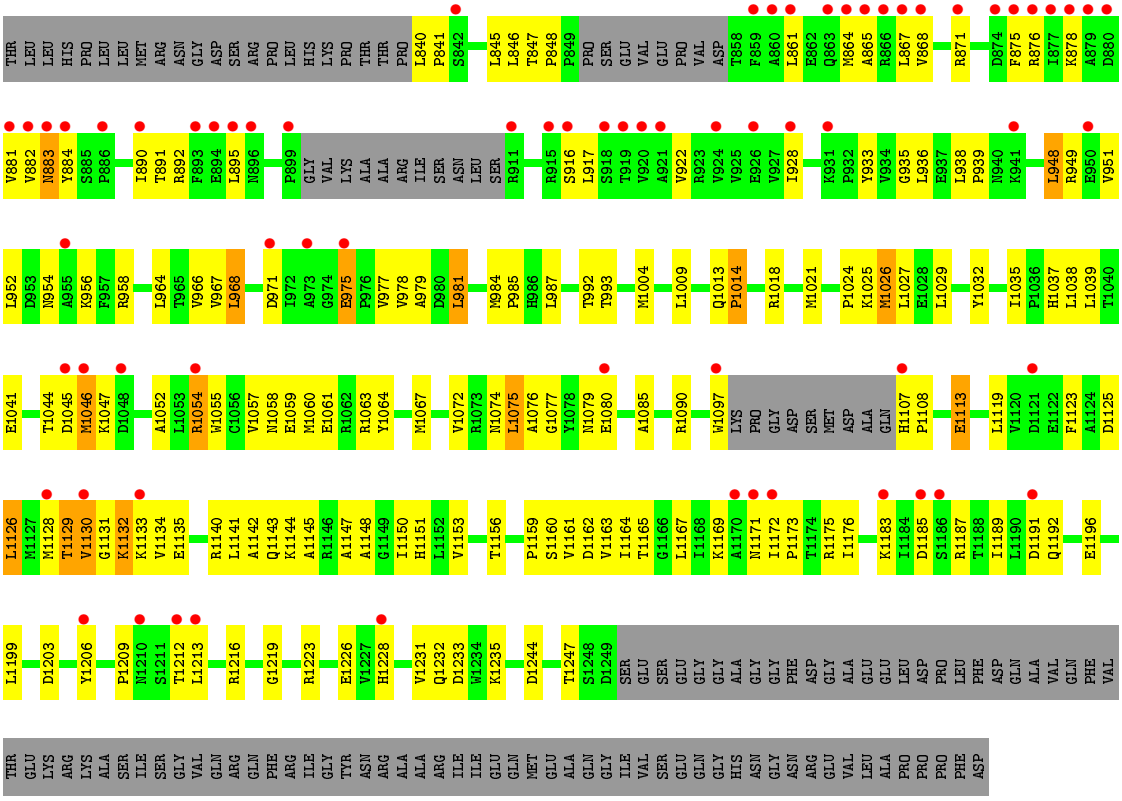
• Molecule 1: DNA TRANSLOCASE FTSK

Chain E:



• Molecule 1: DNA TRANSLOCASE FTSK

Chain F:


THR LEU LEU HIS PRO LEU LEU MET ARG ASN GLY ASP SER ARG PRO LEU HIS LYS PRO THR THR PRO L840 P841 S842 L845 L846 T847 P848 P849 PRO SER GLU VAL GLU PRO VAL ASP T858 F859 A860 L861 E862 Q863 M864 A865 R866 L867 V868 R871 D874 F875 R876 I877 K878 A879 D880
V881 V882 N883 Y884 S885 P886 I890 T891 R892 F893 E894 L895 N896 P899 GLY VAL LYS ALA ALA ARG ILE SER ASN LEU SER R911 R915 S916 L917 S918 T919 V920 A921 V922 R923 V924 V925 E926 V927 I928 K931 P932 Y933 V934 G935 L936 E937 L938 P939 N940 K941 L948 R949 E950 V951
L952 D953 N954 A955 K956 F957 R958 L964 T965 V966 V967 L968 D971 I972 A973 G974 E975 P976 V977 V978 A979 D980 L981 M984 P985 H986 L987 T992 T993 M1004 L1009 Q1013 P1014 R1018 M1021 P1024 K1025 M1026 L1027 E1028 L1029 Y1032 I1035 P1036 H1037 L1038 L1039 T1040
E1041 T1044 D1045 M1046 K1047 D1048 A1052 L1053 R1054 W1055 C1056 V1057 N1058 E1059 M1060 E1061 R1062 R1063 Y1064 M1067 V1072 R1073 N1074 L1075 A1076 G1077 Y1078 N1079 E1080 A1085 R1090 W1097 LYS PRO GLY ASP SER MET ASP ALA GLN H1107 P1108 E1113 L1119 V1120 D1121 E1122 F1123 A1124 D1125
L1126 M1127 M1128 T1129 V1130 G1131 K1132 K1133 V1134 E1135 R1140 L1141 A1142 Q1143 K1144 A1145 R1146 A1147 A1148 G1149 I1150 H1151 L1152 V1153 T1156 P1159 S1160 V1161 D1162 V1163 I1164 T1165 G1166 L1167 I1168 K1169 A1170 N1171 I1172 P1173 T1174 R1175 I1176 K1183 I1184 D1185 S1186 R1187 T1188 I1189 L1190 D1191 Q1192 E1196
L1199 D1203 Y1206 P1209 N1210 S1211 T1212 L1213 R1216 G1219 R1223 E1226 V1227 H1228 V1231 Q1232 D1233 W1234 K1235 D1244 T1247 S1248 D1249 SER GLU SER GLU GLY GLY GLY ALA GLY GLY GLY PHE ASP GLY ALA GLU GLU LEU ASP PRO LEU PHE ASP GLN ALA VAL GLN PHE VAL
THR GLU LYS ARG LYS ALA SER ILE SER GLY VAL GLN ARG GLN PHE ARG ILE GLY TYR ASN ARG ALA ALA ARG ILE ILE GLU GLN MET GLU ALA GLN GLY ILE VAL SER GLU GLN GLY HIS ASN GLY ASN ARG GLU VAL LEU ALA PRO PRO PRO PHE ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	97.60Å 117.20Å 132.80Å 90.00° 100.50° 90.00°	Depositor
Resolution (Å)	100.00 – 2.70 130.58 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (100.00-2.70) 99.7 (130.58-2.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.69Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.246 , 0.298 0.248 , 0.242	Depositor DCC
R_{free} test set	4055 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	45.5	Xtriage
Anisotropy	0.266	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 63.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Outliers	1 of 80835 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	18569	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 23.21 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.8823e-03.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.36	0/3083	0.66	0/4186
1	B	0.39	0/3083	0.66	0/4186
1	C	0.35	0/3083	0.63	0/4186
1	D	0.38	0/3090	0.65	0/4194
1	E	0.38	0/2994	0.67	0/4066
1	F	0.35	0/3005	0.63	0/4080
All	All	0.37	0/18338	0.65	0/24898

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	3029	0	3146	167	0
1	B	3029	0	3146	157	3
1	C	3029	0	3146	163	0
1	D	3036	0	3153	166	0
1	E	2941	0	3046	159	3
1	F	2952	0	3059	146	0
2	A	91	0	0	18	0
2	B	94	0	0	27	0
2	C	80	0	0	20	0
2	D	116	0	0	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	99	0	0	22	0
2	F	73	0	0	25	0
All	All	18569	0	18696	948	3

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 26.

The worst 5 of 948 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:E:1046:MET:HG2	1:E:1129:THR:HG21	1.20	1.10
1:D:1159:PRO:HB3	1:D:1189:ILE:HD11	1.38	1.06
1:E:1159:PRO:HB3	1:E:1189:ILE:HD11	1.34	1.05
1:B:1159:PRO:HB3	1:B:1189:ILE:HD11	1.33	1.05
1:F:1035:ILE:HG22	1:F:1038:LEU:HG	1.45	0.99

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:919:THR:N	1:E:919:THR:N[1_465]	1.90	0.30
1:B:919:THR:O	1:E:919:THR:O[1_465]	2.09	0.11
1:B:917:LEU:O	1:E:919:THR:CG2[1_465]	2.18	0.02

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	387/512 (76%)	355 (92%)	29 (8%)	3 (1%)	24 51
1	B	387/512 (76%)	360 (93%)	23 (6%)	4 (1%)	19 45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	387/512 (76%)	354 (92%)	33 (8%)	0	100	100
1	D	387/512 (76%)	355 (92%)	30 (8%)	2 (0%)	34	63
1	E	373/512 (73%)	347 (93%)	22 (6%)	4 (1%)	17	42
1	F	374/512 (73%)	347 (93%)	24 (6%)	3 (1%)	24	51
All	All	2295/3072 (75%)	2118 (92%)	161 (7%)	16 (1%)	26	55

5 of 16 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1131	GLY
1	D	1129	THR
1	E	1026	MET
1	E	1027	LEU
1	E	1108	PRO

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	330/429 (77%)	310 (94%)	20 (6%)	23	49
1	B	330/429 (77%)	310 (94%)	20 (6%)	23	49
1	C	330/429 (77%)	309 (94%)	21 (6%)	22	47
1	D	331/429 (77%)	314 (95%)	17 (5%)	29	59
1	E	321/429 (75%)	300 (94%)	21 (6%)	21	46
1	F	322/429 (75%)	299 (93%)	23 (7%)	18	41
All	All	1964/2574 (76%)	1842 (94%)	122 (6%)	23	49

5 of 122 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	1123	PHE
1	D	1014	PRO

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Mol	Chain	Res	Type
1	F	1075	LEU
1	C	1126	LEU
1	D	847	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 83 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1171	ASN
1	D	1051	ASN
1	F	1143	GLN
1	C	1192	GLN
1	D	883	ASN

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	393/512 (76%)	0.71	34 (8%) 13 10	18, 43, 85, 100	0
1	B	393/512 (76%)	0.67	31 (7%) 15 13	14, 37, 77, 94	0
1	C	393/512 (76%)	1.05	55 (13%) 4 3	21, 49, 106, 120	0
1	D	394/512 (76%)	0.72	34 (8%) 13 10	16, 37, 76, 103	0
1	E	381/512 (74%)	1.05	52 (13%) 4 3	20, 45, 106, 128	0
1	F	382/512 (74%)	1.16	69 (18%) 2 1	19, 51, 118, 138	0
All	All	2336/3072 (76%)	0.89	275 (11%) 6 5	14, 43, 96, 138	0

The worst 5 of 275 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	918	SER	13.5
1	C	904	ALA	10.8
1	E	920	VAL	10.2
1	E	877	ILE	9.4
1	F	874	ASP	8.9

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 (i)

There are no such residues in this entry.