wwPDB X-ray Structure Validation Summary Report (i)

Feb 15, 2017 – 12:43 am GMT

PDB ID	:	5CK3
Title	:	Signal recognition particle receptor SRb-GTP/SRX complex from Chaetomium thermophilum
Authors	:	Jadhav, B.R.; Wild, K.; Sinning, I.
Deposited on	:	2015-07-15
Resolution	:	3.20 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 (i)) were used in the production of this report:

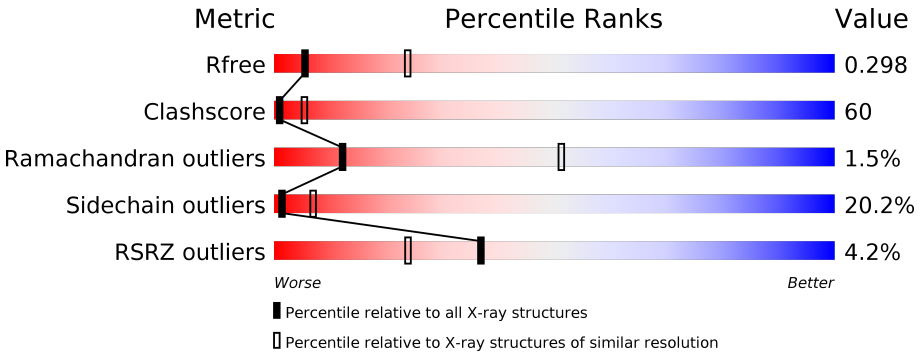
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

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 3.20 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}	100719	1015 (3.22-3.18)
Clashscore	112137	1009 (3.20-3.20)
Ramachandran outliers	110173	1118 (3.22-3.18)
Sidechain outliers	110143	1117 (3.22-3.18)
RSRZ outliers	101464	1020 (3.22-3.18)

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	181	2% 14% 49% 10% • 25%
1	C	181	14% 31% 12% • 42%
1	E	181	3% 13% 33% 12% 43%
2	B	307	3% 30% 47% 11% 12%
2	D	307	2% 22% 43% 9% • 25%
2	F	307	7% 9% 32% 6% 52%

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
4	GTP	B	402	-	-	X	-
4	GTP	F	401	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7908 atoms, of which 8 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 SRX domain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	135	Total	C	N	O	S	0	0	0
			1090	707	178	203	2			
1	C	105	Total	C	N	O	S	0	0	0
			873	576	136	160	1			
1	E	104	Total	C	N	O	S	0	0	0
			843	555	131	155	2			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP G0S1R8
A	-6	LYS	-	expression tag	UNP G0S1R8
A	-5	HIS	-	expression tag	UNP G0S1R8
A	-4	HIS	-	expression tag	UNP G0S1R8
A	-3	HIS	-	expression tag	UNP G0S1R8
A	-2	HIS	-	expression tag	UNP G0S1R8
A	-1	HIS	-	expression tag	UNP G0S1R8
A	0	HIS	-	expression tag	UNP G0S1R8
A	1	MET	-	expression tag	UNP G0S1R8
A	2	SER	-	expression tag	UNP G0S1R8
C	-7	MET	-	initiating methionine	UNP G0S1R8
C	-6	LYS	-	expression tag	UNP G0S1R8
C	-5	HIS	-	expression tag	UNP G0S1R8
C	-4	HIS	-	expression tag	UNP G0S1R8
C	-3	HIS	-	expression tag	UNP G0S1R8
C	-2	HIS	-	expression tag	UNP G0S1R8
C	-1	HIS	-	expression tag	UNP G0S1R8
C	0	HIS	-	expression tag	UNP G0S1R8
C	1	MET	-	expression tag	UNP G0S1R8
C	2	SER	-	expression tag	UNP G0S1R8
E	-7	MET	-	initiating methionine	UNP G0S1R8
E	-6	LYS	-	expression tag	UNP G0S1R8
E	-5	HIS	-	expression tag	UNP G0S1R8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
E	-4	HIS	-	expression tag	UNP G0S1R8
E	-3	HIS	-	expression tag	UNP G0S1R8
E	-2	HIS	-	expression tag	UNP G0S1R8
E	-1	HIS	-	expression tag	UNP G0S1R8
E	0	HIS	-	expression tag	UNP G0S1R8
E	1	MET	-	expression tag	UNP G0S1R8
E	2	SER	-	expression tag	UNP G0S1R8

- Molecule 2 is a protein called Putative signal recognition particle protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	270	Total	C	N	O	S	0	0	0
			2067	1313	362	388	4			
2	D	230	Total	C	N	O	S	0	0	0
			1789	1148	307	330	4			
2	F	147	Total	C	N	O	S	0	0	0
			1128	725	200	202	1			

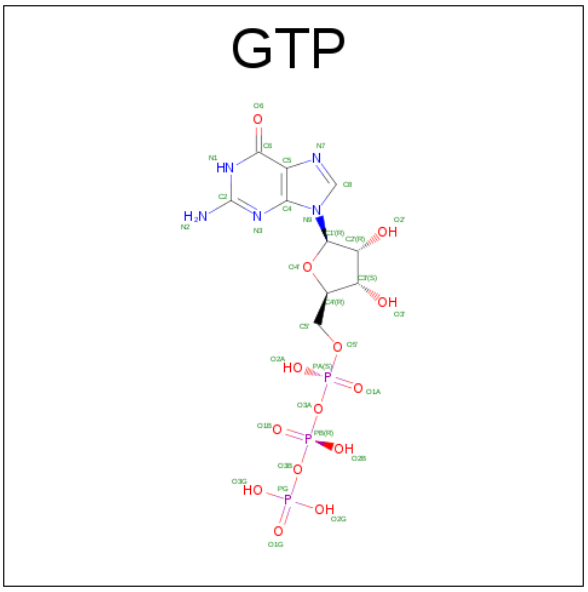
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	41	MET	-	initiating methionine	UNP G0S401
B	42	GLY	-	expression tag	UNP G0S401
D	41	MET	-	initiating methionine	UNP G0S401
D	42	GLY	-	expression tag	UNP G0S401
F	41	MET	-	initiating methionine	UNP G0S401
F	42	GLY	-	expression tag	UNP G0S401

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

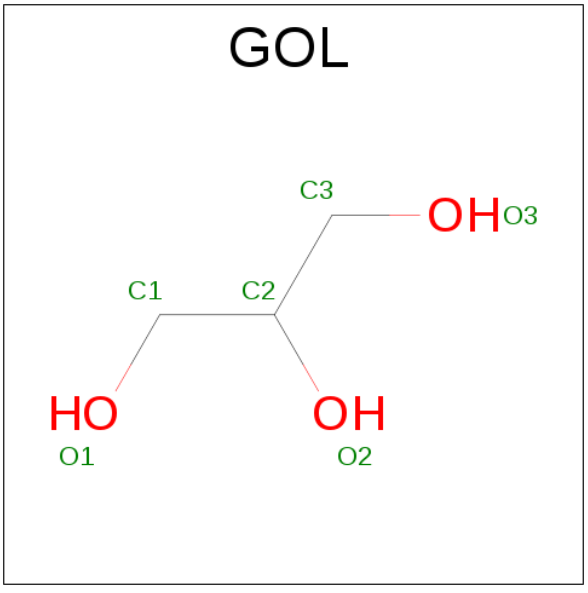
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



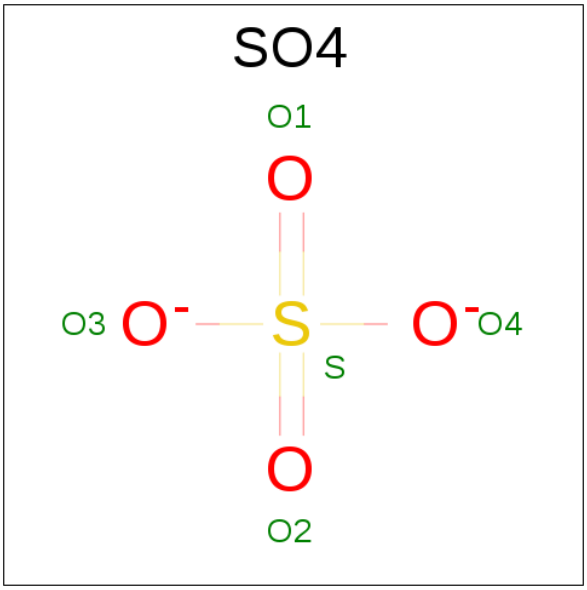
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	D	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	F	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



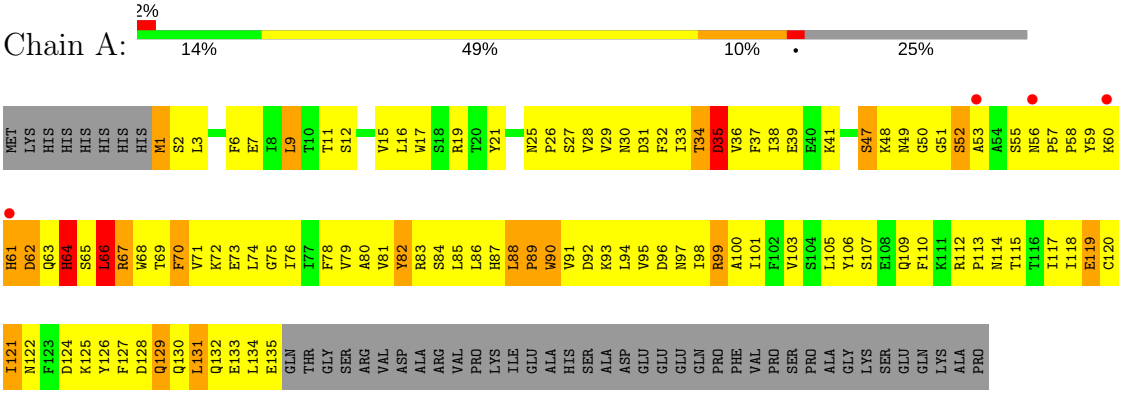
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total O S 5 4 1	0	0

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 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.

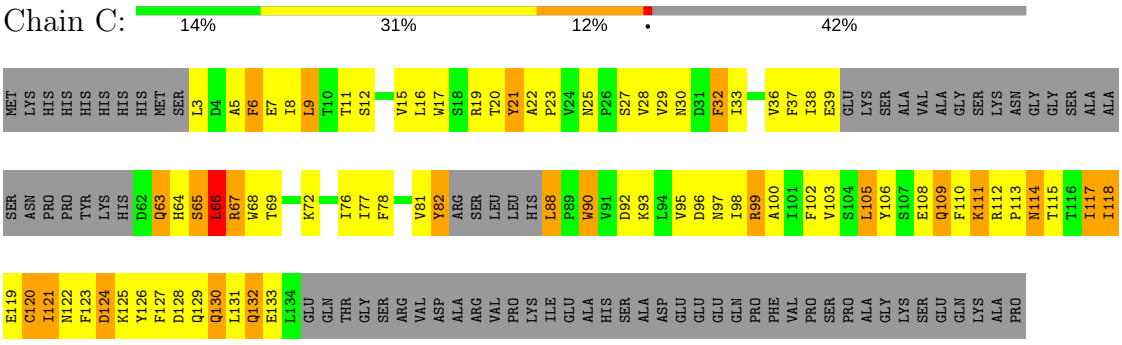
• Molecule 1: SRX domain

Chain A:



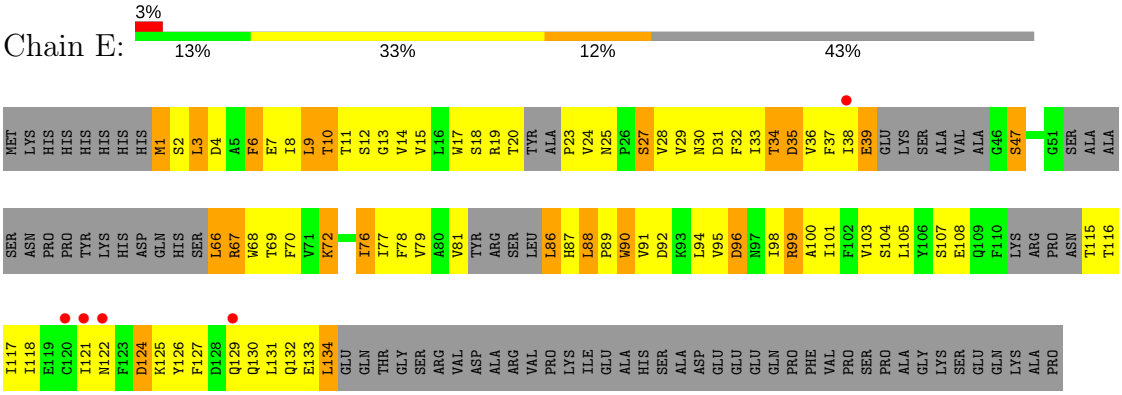
• Molecule 1: SRX domain

Chain C:



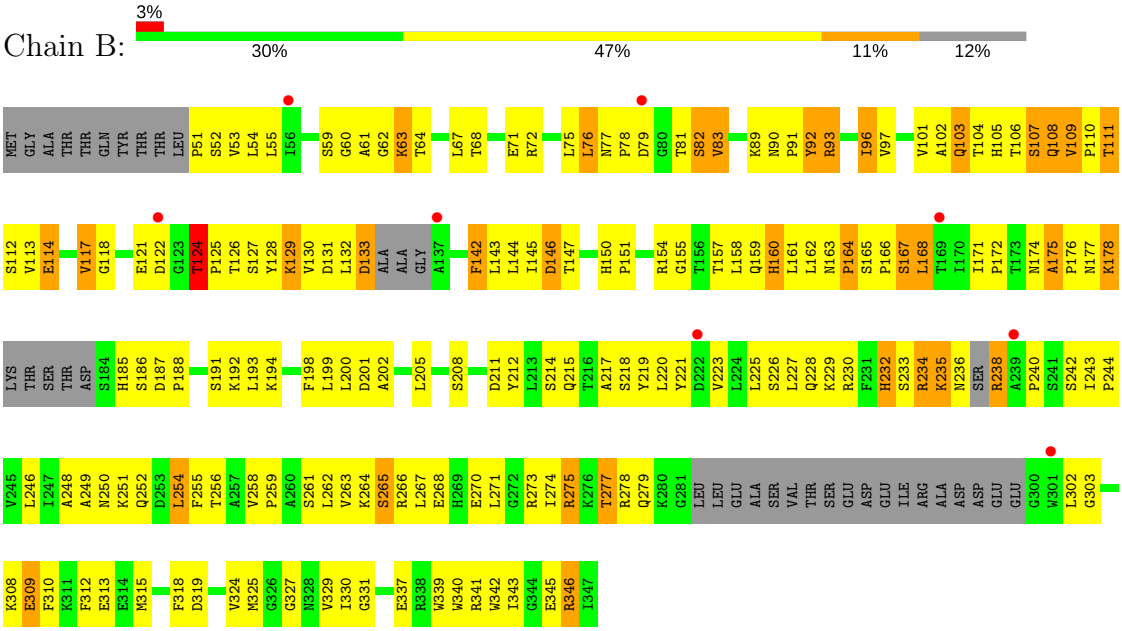
• Molecule 1: SRX domain

Chain E:



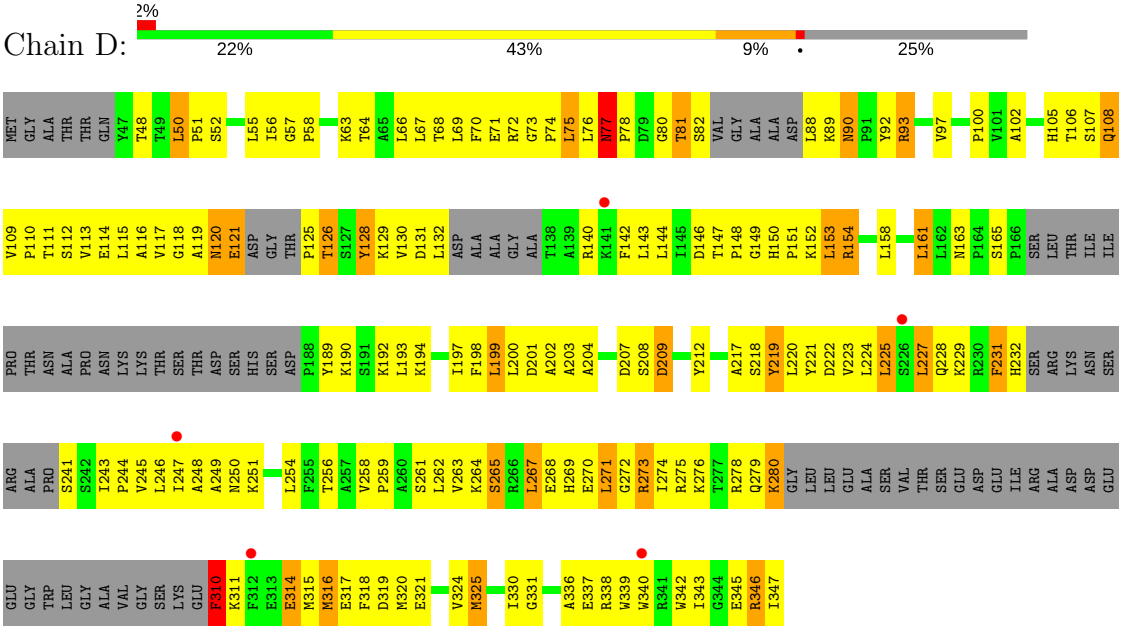
• Molecule 2: Putative signal recognition particle protein

Chain B:



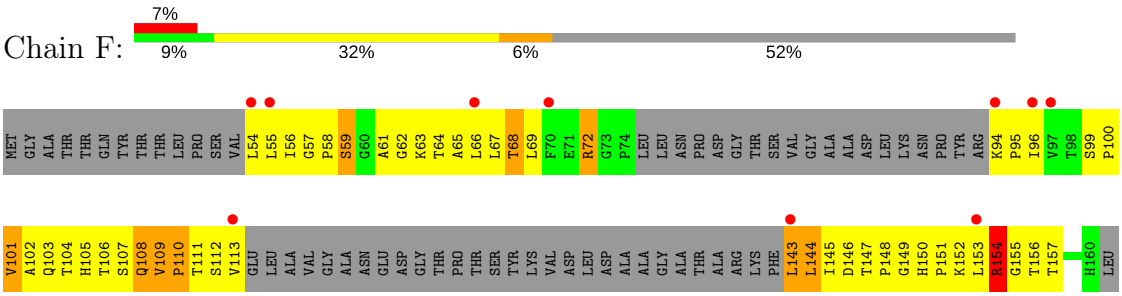
• Molecule 2: Putative signal recognition particle protein

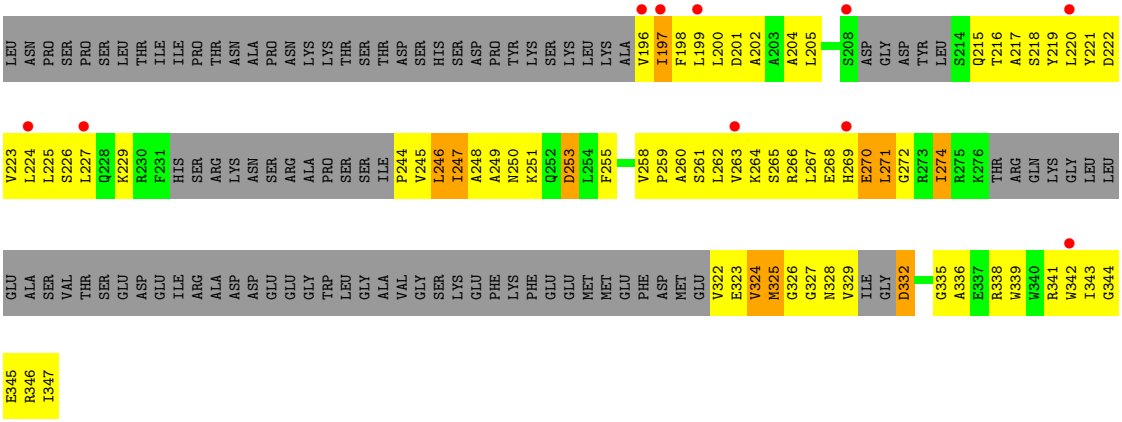
Chain D:



• Molecule 2: Putative signal recognition particle protein

Chain F:




LEU ASN PRO SER PRO SER LEU THR ILE ILE PRO THR ASN ALA PRO ASN LYS LYS THR SER THR ASP SER HIS SER ASP PRO TYR LYS SER LYS LEU LYS ALA V196 I197 F198 L199 L200 D201 A202 A203 A204 L205 S208 ASP GLY ASP TYR LEU S214 Q215 T216 A217 S218 Y219 L220 Y221 D222
V223 L224 L225 S226 L227 Q228 K229 R230 F231 HIS SER ARG LYS ASN SER ARG ALA PRO SER SER ILE P244 V245 L246 I247 A248 A249 N250 K251 Q252 D253 L254 F255 V258 P259 A260 S261 L262 V263 K264 S265 R266 L267 E268 H269 E270 L271 G272 R273 I274 R275 K276 THR ARG GLN LYS GLY LEU LEU
GLU ALA SER VAL THR SER GLU ASP GLU ILE ARG ALA ASP ASP GLU GLU GLY TRP LEU GLY ALA VAL GLY SER LYS GLU PHE LYS PHE GLU GLU MET MET GLU PHE ASP MET GLU V322 E323 V324 M325 G326 G327 N328 V329 ILE GLY D332 G335 A336 E337 R338 W339 W340 R341 W342 I343 G344
E345 R346 I347

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	88.28Å 83.61Å 90.21Å 90.00° 105.23° 90.00°	Depositor
Resolution (Å)	45.47 – 3.20 45.47 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.2 (45.47-3.20) 99.2 (45.47-3.20)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.35 (at 3.19Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.276 , 0.300 0.275 , 0.298	Depositor DCC
R_{free} test set	1076 reflections (5.14%)	DCC
Wilson B-factor (Å^2)	73.2	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 90.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Estimated twinning fraction	0.045 for l,-k,h	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	7908	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.21% 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

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GOL, MG, SO4

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	0.38	0/1118	0.73	4/1522 (0.3%)
1	C	0.35	0/894	0.63	1/1218 (0.1%)
1	E	0.25	0/858	0.47	0/1160
2	B	0.36	0/2110	0.55	1/2859 (0.0%)
2	D	0.40	2/1825 (0.1%)	0.60	2/2469 (0.1%)
2	F	0.35	1/1146 (0.1%)	0.56	1/1549 (0.1%)
All	All	0.36	3/7951 (0.0%)	0.59	9/10777 (0.1%)

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	0	2
1	C	0	2
2	D	0	2
All	All	0	6

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	310	PHE	CD2-CE2	5.28	1.49	1.39
2	F	110	PRO	N-CD	5.23	1.55	1.47
2	D	110	PRO	N-CD	5.04	1.54	1.47

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	35	ASP	CB-CG-OD2	-6.60	112.36	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	109	VAL	C-N-CD	6.09	141.19	128.40
1	C	66	LEU	CA-CB-CG	6.07	129.27	115.30
2	F	109	VAL	C-N-CD	5.87	140.73	128.40
2	D	109	VAL	C-N-CD	5.59	140.15	128.40

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	61	HIS	Peptide
1	A	64	HIS	Peptide
1	C	63	GLN	Peptide
1	C	65	SER	Peptide
2	D	88	LEU	Peptide

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	1090	0	1076	152	0
1	C	873	0	859	90	0
1	E	843	0	839	123	0
2	B	2067	0	2093	201	0
2	D	1789	0	1821	224	0
2	F	1128	0	1166	226	0
3	B	1	0	0	0	0
3	D	1	0	0	0	0
3	F	1	0	0	0	0
4	B	32	0	12	14	0
4	D	32	0	12	1	0
4	F	32	0	12	14	0
5	B	6	8	8	1	0
6	B	5	0	0	1	0
All	All	7900	8	7898	948	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 60.

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)
2:F:197:ILE:HG22	2:F:246:LEU:HB3	1.29	1.15
2:F:111:THR:O	2:F:145:ILE:HG23	1.46	1.14
2:D:55:LEU:HD21	2:D:146:ASP:HA	1.24	1.13
2:D:246:LEU:HB2	2:D:342:TRP:HZ3	1.03	1.11
2:F:259:PRO:HG2	2:F:262:LEU:HB2	1.24	1.08

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	133/181 (74%)	111 (84%)	18 (14%)	4 (3%)	5 32
1	C	99/181 (55%)	90 (91%)	7 (7%)	2 (2%)	9 44
1	E	92/181 (51%)	88 (96%)	4 (4%)	0	100 100
2	B	260/307 (85%)	237 (91%)	18 (7%)	5 (2%)	9 46
2	D	216/307 (70%)	204 (94%)	10 (5%)	2 (1%)	20 64
2	F	131/307 (43%)	116 (88%)	14 (11%)	1 (1%)	22 65
All	All	931/1464 (64%)	846 (91%)	71 (8%)	14 (2%)	12 51

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	164	PRO
1	A	84	SER
2	B	124	THR
1	C	121	ILE
1	A	62	ASP

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	122/161 (76%)	96 (79%)	26 (21%)	1 6
1	C	99/161 (62%)	73 (74%)	26 (26%)	0 2
1	E	96/161 (60%)	72 (75%)	24 (25%)	1 2
2	B	225/255 (88%)	186 (83%)	39 (17%)	2 11
2	D	196/255 (77%)	157 (80%)	39 (20%)	1 7
2	F	122/255 (48%)	102 (84%)	20 (16%)	2 12
All	All	860/1248 (69%)	686 (80%)	174 (20%)	1 7

5 of 174 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	90	TRP
2	D	108	GLN
2	F	144	LEU
1	C	109	GLN
1	C	130	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	132	GLN
2	D	77	ASN
2	D	250	ASN
1	C	130	GLN
2	D	108	GLN

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 3 are monoatomic - leaving 5 for Mogul analysis.

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	$\#\|Z\| > 2$
4	GTP	B	402	3	27,34,34	0.93	1 (3%)	27,54,54	1.76	6 (22%)
5	GOL	B	403	-	5,5,5	0.38	0	5,5,5	0.28	0
6	SO4	B	404	-	4,4,4	0.18	0	6,6,6	0.06	0
4	GTP	D	401	3	27,34,34	1.00	1 (3%)	27,54,54	1.83	7 (25%)
4	GTP	F	401	3	27,34,34	0.91	1 (3%)	27,54,54	1.74	5 (18%)

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
4	GTP	B	402	3	-	0/18/38/38	0/3/3/3
5	GOL	B	403	-	-	0/4/4/4	0/0/0/0
6	SO4	B	404	-	-	0/0/0/0	0/0/0/0
4	GTP	D	401	3	-	0/18/38/38	0/3/3/3
4	GTP	F	401	3	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	401	GTP	C6-N1	2.81	1.38	1.33
4	B	402	GTP	C6-N1	3.09	1.38	1.33
4	D	401	GTP	C6-N1	3.11	1.38	1.33

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	401	GTP	N3-C2-N1	-5.40	119.58	127.46
4	B	402	GTP	N3-C2-N1	-5.10	120.01	127.46
4	F	401	GTP	N3-C2-N1	-4.92	120.27	127.46
4	F	401	GTP	C5-C6-N1	-2.60	119.78	123.48
4	D	401	GTP	C5-C6-N1	-2.55	119.85	123.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	402	GTP	14	0
5	B	403	GOL	1	0
6	B	404	SO4	1	0
4	D	401	GTP	1	0
4	F	401	GTP	14	0

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 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	135/181 (74%)	0.10	4 (2%) 51 35	36, 74, 119, 132	0
1	C	105/181 (58%)	-0.07	0 100 100	40, 68, 96, 105	0
1	E	104/181 (57%)	0.29	5 (4%) 31 19	72, 94, 112, 117	0
2	B	270/307 (87%)	0.07	8 (2%) 51 35	37, 66, 113, 131	0
2	D	230/307 (74%)	0.18	5 (2%) 62 48	47, 81, 121, 135	0
2	F	147/307 (47%)	0.81	20 (13%) 3 2	84, 121, 153, 160	0
All	All	991/1464 (67%)	0.22	42 (4%) 37 24	36, 83, 129, 160	0

The worst 5 of 42 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	4.5
2	F	197	ILE	4.5
1	A	60	LYS	4.4
1	E	38	ILE	4.4
1	E	120	CYS	3.9

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 (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	SO4	B	404	5/5	0.84	0.31	0.46	111,113,123,128	0
5	GOL	B	403	6/6	0.88	0.22	-0.07	50,68,78,81	0
4	GTP	D	401	32/32	0.95	0.19	-0.39	49,58,67,78	0
4	GTP	F	401	32/32	0.90	0.17	-0.83	86,108,117,121	0
4	GTP	B	402	32/32	0.96	0.17	-0.98	26,42,51,59	0
3	MG	D	400	1/1	0.94	0.10	-1.78	53,53,53,53	0
3	MG	F	400	1/1	0.94	0.09	-2.04	104,104,104,104	0
3	MG	B	401	1/1	0.96	0.14	-2.40	42,42,42,42	0

6.5 Other polymers (i)

There are no such residues in this entry.