



wwPDB X-ray Structure Validation Summary Report

Feb 27, 2014 – 08:05 AM GMT

PDB ID : 3R1F
Title : Crystal structure of a key regulator of virulence in Mycobacterium tuberculosis
Authors : Rosenberg, O.S.; Dovey, C.; Finer-Moore, J.; Stroud, R.M.; Cox, J.S.
Deposited on : 2011-03-10
Resolution : 2.50 Å(reported)

This is a wwPDB 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/ValidationPDFNotes.html>

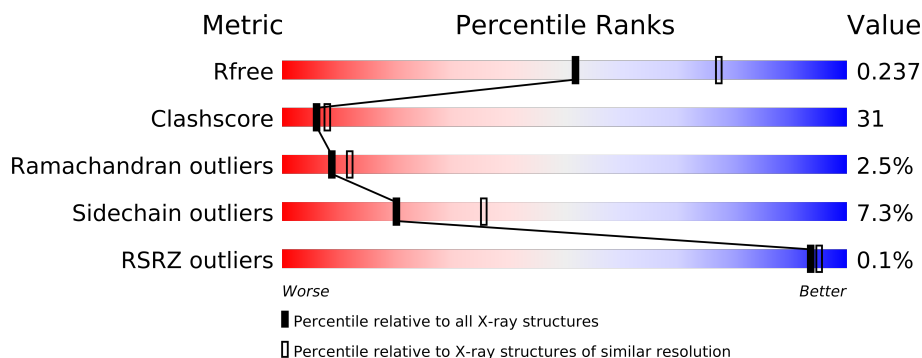
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 2.50 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))
R_{free}	66092	2784 (2.50-2.50)
Clashscore	79885	3562 (2.50-2.50)
Ramachandran outliers	78287	3480 (2.50-2.50)
Sidechain outliers	78261	3482 (2.50-2.50)
RSRZ outliers	66119	2785 (2.50-2.50)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	135	
1	B	135	
1	C	135	
1	D	135	
1	E	135	
1	F	135	
1	G	135	
1	H	135	
1	I	135	
1	J	135	
1	K	135	
1	L	135	
1	M	135	
1	N	135	

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Mol	Chain	Length	Quality of chain
1	O	135	
1	P	135	
1	Q	135	
1	R	135	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 17208 atoms, of which 0 are hydrogen and 0 are deuterium.

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 ESX-1 secretion-associated regulator EspR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	123	Total	C	N	O	S	Se	0	0	0
			967	606	178	179	1	3			
1	B	130	Total	C	N	O	S	Se	0	0	0
			1019	636	188	191	1	3			
1	C	123	Total	C	N	O	S	Se	0	0	0
			960	603	175	178	1	3			
1	D	130	Total	C	N	O	S	Se	0	0	0
			1019	636	188	191	1	3			
1	E	125	Total	C	N	O	S	Se	0	0	0
			986	617	183	182	1	3			
1	F	130	Total	C	N	O	S	Se	0	0	0
			1019	636	188	191	1	3			
1	G	123	Total	C	N	O	S	Se	0	0	0
			966	606	178	178	1	3			
1	H	130	Total	C	N	O	S	Se	0	0	0
			1016	633	188	191	1	3			
1	I	124	Total	C	N	O	S	Se	0	0	0
			974	610	179	181	1	3			
1	J	130	Total	C	N	O	S	Se	0	0	0
			1019	636	188	191	1	3			
1	K	124	Total	C	N	O	S	Se	0	0	0
			973	609	179	181	1	3			
1	L	129	Total	C	N	O	S	Se	0	0	0
			1013	633	187	189	1	3			
1	M	119	Total	C	N	O	S	Se	0	0	0
			932	587	170	171	1	3			
1	N	130	Total	C	N	O	S	Se	0	0	0
			1019	636	188	191	1	3			
1	O	90	Total	C	N	O	S	Se	0	0	0
			706	450	121	132	1	2			
1	P	92	Total	C	N	O	S	Se	0	0	0
			721	459	123	135	1	3			

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	Q	116	Total	C	N	O	S	Se	0	0	0
			906	570	165	167	1	3			
1	R	123	Total	C	N	O	S	Se	0	0	0
			974	608	179	183	1	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	EXPRESSION TAG	UNP P96228
A	-1	ASN	-	EXPRESSION TAG	UNP P96228
A	0	ALA	-	EXPRESSION TAG	UNP P96228
B	-2	SER	-	EXPRESSION TAG	UNP P96228
B	-1	ASN	-	EXPRESSION TAG	UNP P96228
B	0	ALA	-	EXPRESSION TAG	UNP P96228
C	-2	SER	-	EXPRESSION TAG	UNP P96228
C	-1	ASN	-	EXPRESSION TAG	UNP P96228
C	0	ALA	-	EXPRESSION TAG	UNP P96228
D	-2	SER	-	EXPRESSION TAG	UNP P96228
D	-1	ASN	-	EXPRESSION TAG	UNP P96228
D	0	ALA	-	EXPRESSION TAG	UNP P96228
E	-2	SER	-	EXPRESSION TAG	UNP P96228
E	-1	ASN	-	EXPRESSION TAG	UNP P96228
E	0	ALA	-	EXPRESSION TAG	UNP P96228
F	-2	SER	-	EXPRESSION TAG	UNP P96228
F	-1	ASN	-	EXPRESSION TAG	UNP P96228
F	0	ALA	-	EXPRESSION TAG	UNP P96228
G	-2	SER	-	EXPRESSION TAG	UNP P96228
G	-1	ASN	-	EXPRESSION TAG	UNP P96228
G	0	ALA	-	EXPRESSION TAG	UNP P96228
H	-2	SER	-	EXPRESSION TAG	UNP P96228
H	-1	ASN	-	EXPRESSION TAG	UNP P96228
H	0	ALA	-	EXPRESSION TAG	UNP P96228
I	-2	SER	-	EXPRESSION TAG	UNP P96228
I	-1	ASN	-	EXPRESSION TAG	UNP P96228
I	0	ALA	-	EXPRESSION TAG	UNP P96228
J	-2	SER	-	EXPRESSION TAG	UNP P96228
J	-1	ASN	-	EXPRESSION TAG	UNP P96228
J	0	ALA	-	EXPRESSION TAG	UNP P96228
K	-2	SER	-	EXPRESSION TAG	UNP P96228
K	-1	ASN	-	EXPRESSION TAG	UNP P96228
K	0	ALA	-	EXPRESSION TAG	UNP P96228
L	-2	SER	-	EXPRESSION TAG	UNP P96228

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Chain	Residue	Modelled	Actual	Comment	Reference
L	-1	ASN	-	EXPRESSION TAG	UNP P96228
L	0	ALA	-	EXPRESSION TAG	UNP P96228
M	-2	SER	-	EXPRESSION TAG	UNP P96228
M	-1	ASN	-	EXPRESSION TAG	UNP P96228
M	0	ALA	-	EXPRESSION TAG	UNP P96228
N	-2	SER	-	EXPRESSION TAG	UNP P96228
N	-1	ASN	-	EXPRESSION TAG	UNP P96228
N	0	ALA	-	EXPRESSION TAG	UNP P96228
O	-2	SER	-	EXPRESSION TAG	UNP P96228
O	-1	ASN	-	EXPRESSION TAG	UNP P96228
O	0	ALA	-	EXPRESSION TAG	UNP P96228
P	-2	SER	-	EXPRESSION TAG	UNP P96228
P	-1	ASN	-	EXPRESSION TAG	UNP P96228
P	0	ALA	-	EXPRESSION TAG	UNP P96228
Q	-2	SER	-	EXPRESSION TAG	UNP P96228
Q	-1	ASN	-	EXPRESSION TAG	UNP P96228
Q	0	ALA	-	EXPRESSION TAG	UNP P96228
R	-2	SER	-	EXPRESSION TAG	UNP P96228
R	-1	ASN	-	EXPRESSION TAG	UNP P96228
R	0	ALA	-	EXPRESSION TAG	UNP P96228

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	2	Total O 2 2	0	0
2	B	1	Total O 1 1	0	0
2	C	1	Total O 1 1	0	0
2	D	2	Total O 2 2	0	0
2	F	1	Total O 1 1	0	0
2	H	1	Total O 1 1	0	0
2	I	1	Total O 1 1	0	0
2	L	3	Total O 3 3	0	0
2	M	1	Total O 1 1	0	0

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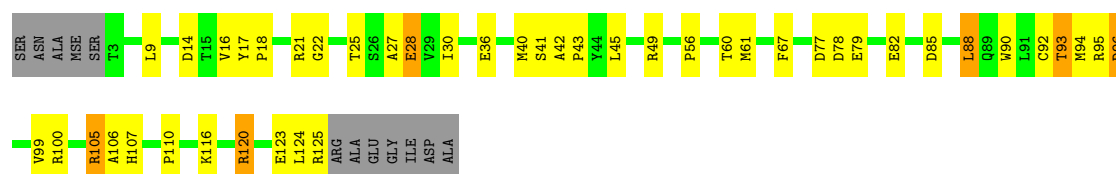
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	N	4	Total	O	0	0
			4	4		
2	P	2	Total	O	0	0
			2	2		

3 Residue-property plots

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.

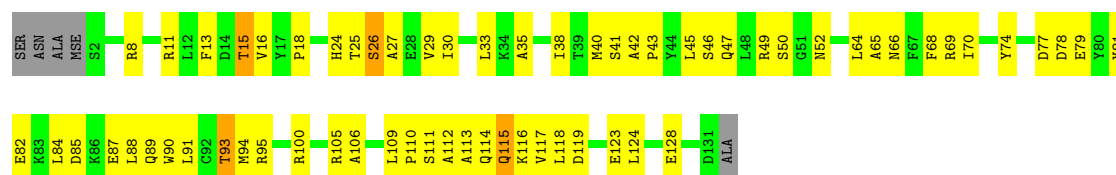
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain A: 



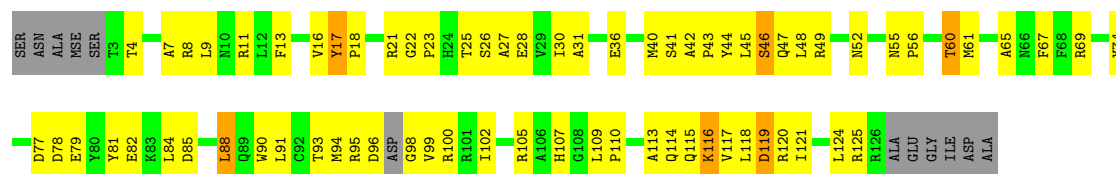
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain B: 



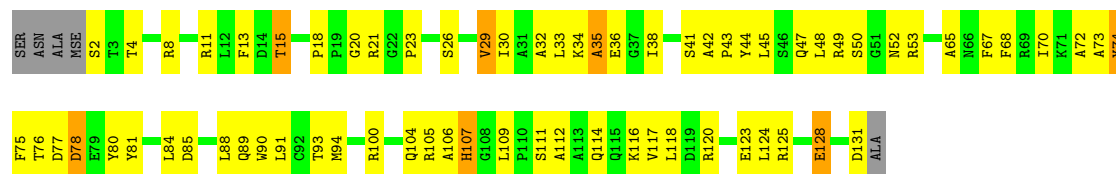
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain C: 



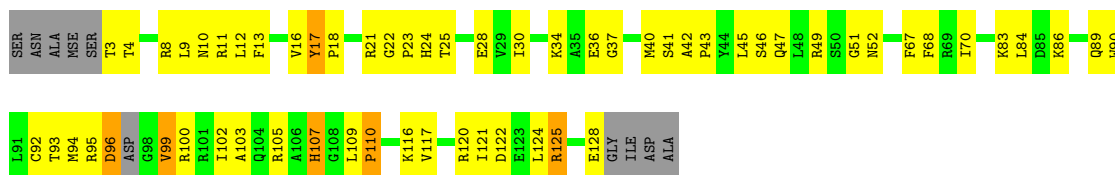
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain D: 



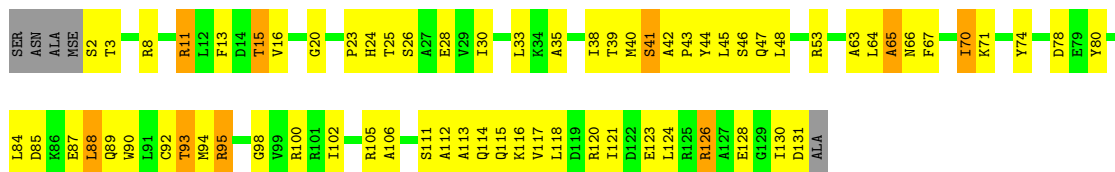
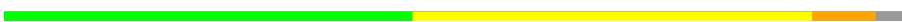
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain E: 



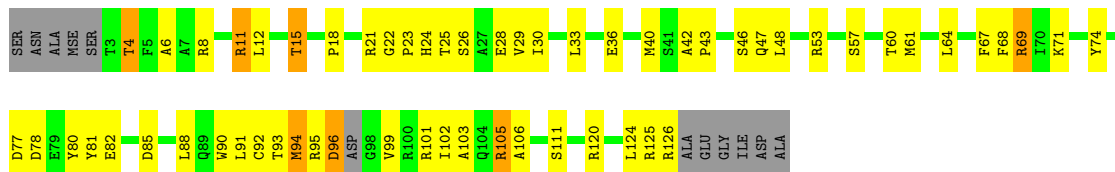
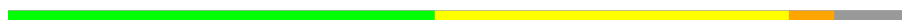
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain F:



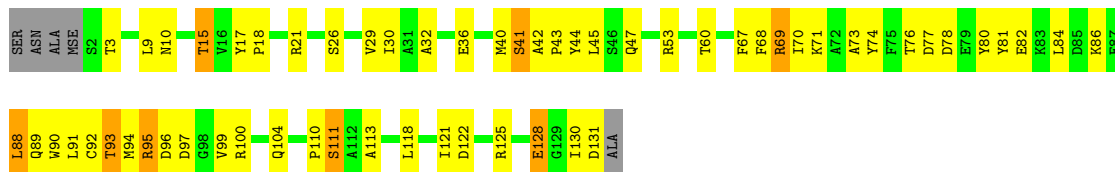
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain G:



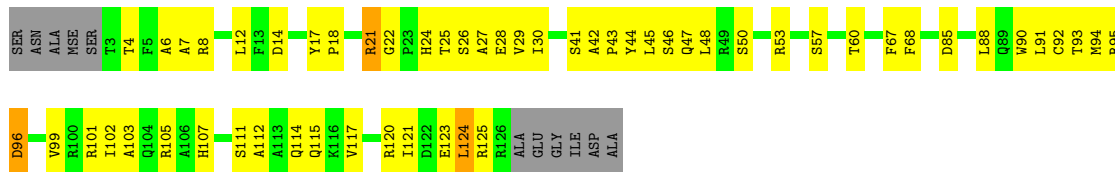
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain H:



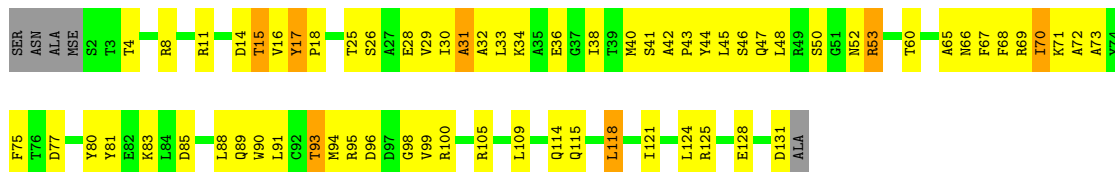
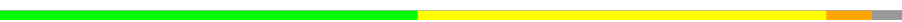
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain I:

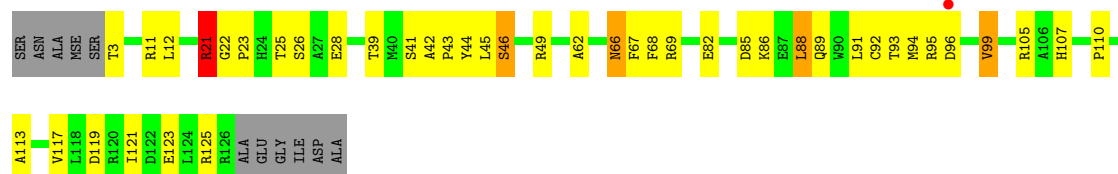


- Molecule 1: ESX-1 secretion-associated regulator EspR

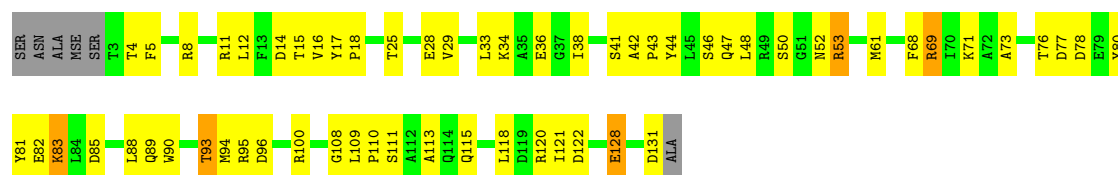
Chain J:



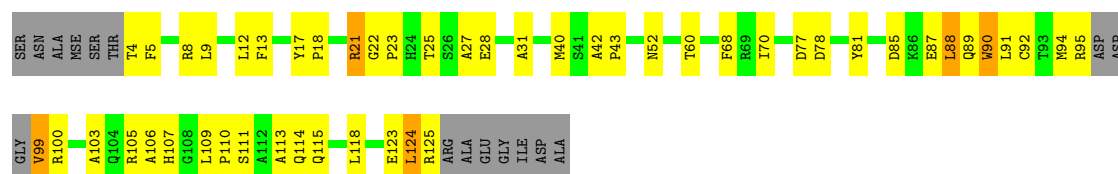
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain K: 

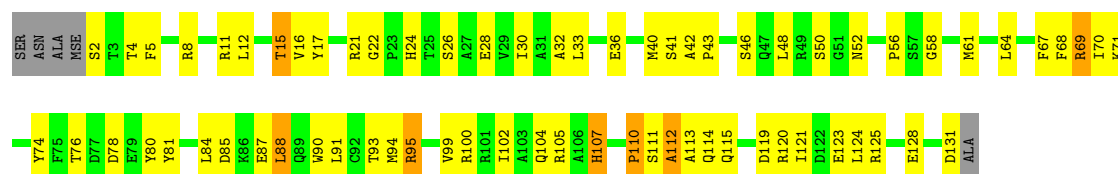
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain L: 

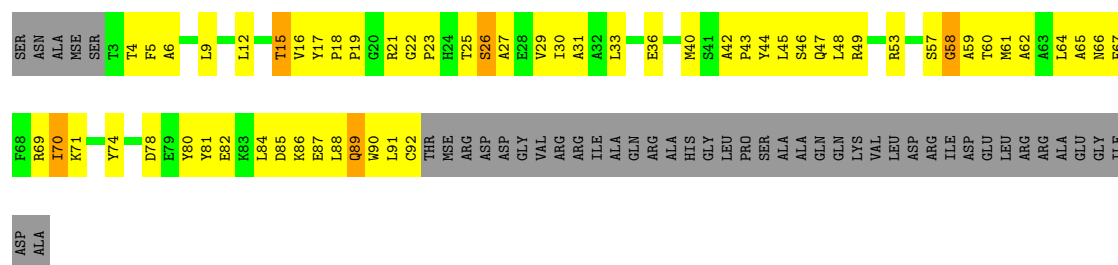
- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain M: 

- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain N: 

- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain O: 

- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain P:

SER ASN ALA MSE SER T3 T4 F5 R8 L9 F13 D14 V16 T15 Y17 P18 R21 G22 P23 H24 T25 S26 T30 K34 A35 E36 M40 S41 A42 P43 S46 Q47 L48 R49 S50 G51 N52 R53 T60 M61 A62 M66 F67 F68 R69 I70 A72 A73 Y74 F75

T76 D77 E78 E79 Y81 L84 E87 L88 Q89 W90 L91 G92 T93 M94 ARG ASP ASP GLY VAL ARG ARG ILE ALA GLN ARG ALA HIS GLY LEU PRO SER ALA ALA GLN GLN LYS VAL LEU ASP ASP ILE ARG ASP GLU LEU ARG ARG ALA GLU GLY ILE ASP ALA

- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain Q:

SER ASN ALA MSE SER T3 T4 F5 L9 N10 R11 L12 F13 D14 Y17 P18 R21 G22 P23 H24 T25 S26 A27 E28 V29 K34 A35 E36 G37 I38 A42 P43 Y44 L45 S46 Q47 L48 R49 S50 G51 N52 R53 A59 T60 M61 A62 A63 L64 A65 M66 F67 F68 R69 I70

K71 F75 T76 D77 E79 D85 K86 E87 L88 Q89 W90 L91 C92 T93 M94 R95 D96 D97 G98 V99 R100 R101 I102 R106 A107 H107 G108 L109 P110 S111 A112 A113 L113 ASP ARG ILE LEU LEU ARG ARG ALA GLY ILE ASP ALA

- Molecule 1: ESX-1 secretion-associated regulator EspR

Chain R:

SER ASN ALA MSE SER T3 T4 R8 R11 L12 F13 D14 V16 T15 Y17 P18 R21 G22 P23 H24 T25 S26 A27 E28 V29 I30 L33 K34 A35 E36 T39 A42 P43 Y44 L45 S46 Q47 L48 R49 S50 G51 N52 S57 G58 T60 R69 I70 K71 A72 A73 Y74

F75 T76 Y80 Y81 E82 L88 Q89 L91 C92 T93 M94 R95 D96 D97 G98 V99 R100 R101 I102 A103 Q104 R105 A106 HIS GLY LEU PRO SER ALA Q114 Q115 K116 V117 L118 D119 R120 I121 D122 E123 L124 R125 R126 A127 G128 E129 I130 D131 ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	148.49Å 148.49Å 129.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.84 – 2.50 48.84 – 2.40	Depositor EDS
% Data completeness (in resolution range)	91.0 (48.84-2.50) 90.4 (48.84-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.44 (at 2.39Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.1_743)	Depositor
R, R_{free}	0.197 , 0.232 0.205 , 0.237	Depositor DCC
R_{free} test set	5682 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	32.1	Xtriage
Anisotropy	0.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 10.3	EDS
Estimated twinning fraction	0.045 for -h,-k,l 0.048 for h,-h-k,-l 0.438 for -k,-h,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 112973 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17208	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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 71.56 % 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 2.5717e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

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	0.49	0/983	0.62	0/1324
1	B	0.48	0/1035	0.64	0/1393
1	C	0.50	0/975	0.66	0/1313
1	D	0.47	0/1035	0.64	0/1393
1	E	0.49	0/1001	0.65	0/1346
1	F	0.47	0/1035	0.63	0/1393
1	G	0.47	0/981	0.63	0/1320
1	H	0.49	0/1032	0.63	0/1389
1	I	0.47	0/990	0.63	0/1334
1	J	0.51	0/1035	0.67	0/1393
1	K	0.49	0/989	0.65	0/1332
1	L	0.50	0/1029	0.66	0/1385
1	M	0.44	0/947	0.60	0/1276
1	N	0.48	0/1035	0.68	0/1393
1	O	0.49	0/721	0.66	0/975
1	P	0.45	0/735	0.62	0/992
1	Q	0.44	0/922	0.63	0/1243
1	R	0.43	0/987	0.59	0/1325
All	All	0.48	0/17467	0.64	0/23519

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the

chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	967	0	957	54	0
1	B	1019	0	1009	62	0
1	C	960	0	948	68	0
1	D	1019	0	1009	70	0
1	E	986	0	981	65	0
1	F	1019	0	1009	82	1
1	G	966	0	959	67	2
1	H	1016	0	1000	71	0
1	I	974	0	964	55	0
1	J	1019	0	1009	74	1
1	K	973	0	960	52	0
1	L	1013	0	1004	62	0
1	M	932	0	921	66	1
1	N	1019	0	1009	74	2
1	O	706	0	691	62	0
1	P	721	0	707	59	0
1	Q	906	0	900	92	0
1	R	974	0	965	89	0
2	A	2	0	0	0	0
2	B	1	0	0	1	0
2	C	1	0	0	0	0
2	D	2	0	0	0	0
2	F	1	0	0	0	0
2	H	1	0	0	0	0
2	I	1	0	0	0	0
2	L	3	0	0	0	0
2	M	1	0	0	0	1
2	N	4	0	0	0	0
2	P	2	0	0	0	0
All	All	17208	0	17002	1052	4

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 31.

The worst 5 of 1052 close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:94:MSE:HE2	1:H:94:MSE:CG	1.54	1.36
1:G:94:MSE:HE1	1:H:94:MSE:HA	1.28	1.13
1:O:15:THR:HG21	1:O:88:LEU:HG	1.25	1.12
1:G:94:MSE:HE2	1:H:94:MSE:HG3	1.17	1.10

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:M:94:MSE:HB2	1:N:94:MSE:HE2	1.33	1.09

All (4) 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	Distance(Å)	Clash(Å)
1:F:126:ARG:NH2	1:G:126:ARG:O[3_654]	2.05	0.15
1:M:52:ASN:ND2	1:N:50:SER:O[2_544]	2.13	0.07
1:G:53:ARG:NH2	1:J:14:ASP:OD1[2_544]	2.16	0.04
1:N:4:THR:OG1	2:M:133:HOH:O[3_655]	2.17	0.03

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	121/135 (90%)	106 (88%)	11 (9%)	4 (3%)	6	7
1	B	128/135 (95%)	116 (91%)	10 (8%)	2 (2%)	14	23
1	C	119/135 (88%)	106 (89%)	12 (10%)	1 (1%)	27	46
1	D	128/135 (95%)	115 (90%)	9 (7%)	4 (3%)	7	8
1	E	121/135 (90%)	104 (86%)	14 (12%)	3 (2%)	9	12
1	F	128/135 (95%)	116 (91%)	11 (9%)	1 (1%)	27	46
1	G	119/135 (88%)	106 (89%)	9 (8%)	4 (3%)	6	7
1	H	128/135 (95%)	114 (89%)	11 (9%)	3 (2%)	10	14
1	I	122/135 (90%)	99 (81%)	21 (17%)	2 (2%)	14	23
1	J	128/135 (95%)	116 (91%)	10 (8%)	2 (2%)	14	23
1	K	122/135 (90%)	112 (92%)	9 (7%)	1 (1%)	27	46
1	L	127/135 (94%)	112 (88%)	12 (9%)	3 (2%)	9	13
1	M	115/135 (85%)	103 (90%)	11 (10%)	1 (1%)	25	42
1	N	128/135 (95%)	111 (87%)	13 (10%)	4 (3%)	7	8
1	O	88/135 (65%)	64 (73%)	21 (24%)	3 (3%)	6	7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	P	90/135 (67%)	79 (88%)	8 (9%)	3 (3%)	6	7
1	Q	114/135 (84%)	85 (75%)	24 (21%)	5 (4%)	4	4
1	R	119/135 (88%)	99 (83%)	12 (10%)	8 (7%)	2	1
All	All	2145/2430 (88%)	1863 (87%)	228 (11%)	54 (2%)	9	12

5 of 54 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	93	THR
1	B	26	SER
1	H	95	ARG
1	P	35	ALA
1	Q	35	ALA

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	98/103 (95%)	93 (95%)	5 (5%)	33	57
1	B	104/103 (101%)	99 (95%)	5 (5%)	35	60
1	C	97/103 (94%)	91 (94%)	6 (6%)	26	45
1	D	104/103 (101%)	98 (94%)	6 (6%)	28	49
1	E	100/103 (97%)	94 (94%)	6 (6%)	27	47
1	F	104/103 (101%)	90 (86%)	14 (14%)	6	10
1	G	98/103 (95%)	89 (91%)	9 (9%)	13	24
1	H	103/103 (100%)	96 (93%)	7 (7%)	22	39
1	I	99/103 (96%)	93 (94%)	6 (6%)	26	46
1	J	104/103 (101%)	98 (94%)	6 (6%)	28	49
1	K	99/103 (96%)	91 (92%)	8 (8%)	17	30
1	L	103/103 (100%)	97 (94%)	6 (6%)	28	49
1	M	94/103 (91%)	89 (95%)	5 (5%)	32	54
1	N	104/103 (101%)	97 (93%)	7 (7%)	23	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	O	72/103 (70%)	65 (90%)	7 (10%)	12	21
1	P	74/103 (72%)	70 (95%)	4 (5%)	31	53
1	Q	92/103 (89%)	85 (92%)	7 (8%)	19	33
1	R	100/103 (97%)	87 (87%)	13 (13%)	6	11
All	All	1749/1854 (94%)	1622 (93%)	127 (7%)	20	36

5 of 127 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	131	ASP
1	K	21	ARG
1	R	39	THR
1	I	46	SER
1	J	15	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	114	GLN
1	J	52	ASN
1	R	47	GLN
1	I	107	HIS
1	K	107	HIS

5.3.3 RNA ⓘ

There are no RNA chains 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, 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	123/135 (91%)	-0.42	0	100	100	21, 31, 60, 77	0
1	B	130/135 (96%)	-0.36	0	100	100	21, 31, 47, 57	0
1	C	123/135 (91%)	-0.41	0	100	100	19, 32, 62, 71	0
1	D	130/135 (96%)	-0.42	0	100	100	21, 31, 50, 59	0
1	E	125/135 (92%)	-0.40	0	100	100	20, 33, 57, 67	0
1	F	130/135 (96%)	-0.40	0	100	100	18, 29, 44, 54	0
1	G	123/135 (91%)	-0.41	0	100	100	21, 31, 56, 70	0
1	H	130/135 (96%)	-0.42	0	100	100	19, 29, 48, 63	0
1	I	124/135 (91%)	-0.41	0	100	100	21, 31, 62, 74	0
1	J	130/135 (96%)	-0.42	0	100	100	19, 28, 48, 62	0
1	K	124/135 (91%)	-0.44	1 (0%)	83	84	17, 29, 56, 74	0
1	L	129/135 (95%)	-0.38	0	100	100	22, 30, 47, 61	0
1	M	119/135 (88%)	-0.34	0	100	100	26, 37, 55, 64	0
1	N	130/135 (96%)	-0.53	0	100	100	23, 33, 45, 61	0
1	O	90/135 (66%)	-0.47	0	100	100	30, 36, 51, 60	0
1	P	92/135 (68%)	-0.49	1 (1%)	77	79	23, 33, 42, 58	0
1	Q	116/135 (85%)	-0.45	0	100	100	27, 37, 57, 69	0
1	R	123/135 (91%)	-0.39	1 (0%)	83	84	26, 35, 61, 75	0
All	All	2191/2430 (90%)	-0.42	3 (0%)	93	95	17, 33, 56, 77	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	R	104	GLN	2.7
1	P	92	CYS	2.4
1	K	96	ASP	2.1

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.