



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 29, 2020 – 06:17 am BST

PDB ID : 4UWQ  
Title : Crystal structure of the disulfide-linked complex of the thiosulfodyrolase SoxB with the carrier-protein SoxYZ from *Thermus thermophilus*  
Authors : Grabarczyk, D.B.; Chappell, P.E.; Johnson, S.; Stelzl, L.S.; Lea, S.M.; Berks, B.C.  
Deposited on : 2014-08-14  
Resolution : 3.28 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](mailto: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 ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

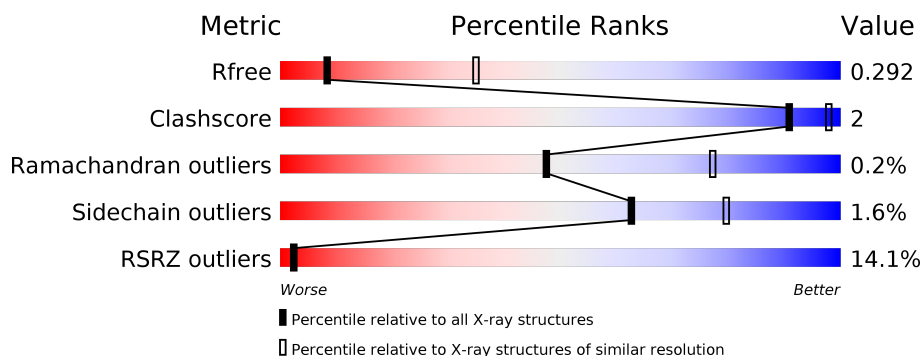
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.28 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))
$R_{free}$	130704	1177 (3.32-3.24)
Clashscore	141614	1044 (3.30-3.26)
Ramachandran outliers	138981	1026 (3.30-3.26)
Sidechain outliers	138945	1025 (3.30-3.26)
RSRZ outliers	127900	1141 (3.32-3.24)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	562	<div> <div>4%</div> <div>92%</div> <div>6%</div> <div>.</div> </div>
1	D	562	<div> <div>7%</div> <div>93%</div> <div>.</div> <div>.</div> </div>
1	G	562	<div> <div>8%</div> <div>93%</div> <div>5%</div> <div>.</div> </div>
1	J	562	<div> <div>4%</div> <div>92%</div> <div>5%</div> <div>.</div> </div>
2	B	136	<div> <div>13%</div> <div>71%</div> <div>10%</div> <div>18%</div> </div>
2	E	136	<div> <div>45%</div> <div>73%</div> <div>10%</div> <div>17%</div> </div>

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Mol	Chain	Length	Quality of chain
2	H	136	
2	K	136	
3	C	108	
3	F	108	
3	I	108	
3	L	108	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23081 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 SULFUR OXIDATION PROTEIN SOXB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	548	Total	C	N	O	S	0	0	0
			4323	2783	752	781	7			
1	D	545	Total	C	N	O	S	0	0	0
			4299	2769	749	774	7			
1	G	548	Total	C	N	O	S	0	0	0
			4323	2783	752	781	7			
1	J	547	Total	C	N	O	S	0	0	0
			4314	2778	751	778	7			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	expression tag	UNP Q72IT0
A	13	ALA	-	expression tag	UNP Q72IT0
A	14	SER	-	expression tag	UNP Q72IT0
A	15	TRP	-	expression tag	UNP Q72IT0
A	16	SER	-	expression tag	UNP Q72IT0
A	17	HIS	-	expression tag	UNP Q72IT0
A	18	PRO	-	expression tag	UNP Q72IT0
A	19	GLN	-	expression tag	UNP Q72IT0
A	20	PHE	-	expression tag	UNP Q72IT0
A	21	GLU	-	expression tag	UNP Q72IT0
A	22	LYS	-	expression tag	UNP Q72IT0
A	175	CYS	TRP	engineered mutation	UNP Q72IT0
D	12	MET	-	expression tag	UNP Q72IT0
D	13	ALA	-	expression tag	UNP Q72IT0
D	14	SER	-	expression tag	UNP Q72IT0
D	15	TRP	-	expression tag	UNP Q72IT0
D	16	SER	-	expression tag	UNP Q72IT0
D	17	HIS	-	expression tag	UNP Q72IT0
D	18	PRO	-	expression tag	UNP Q72IT0
D	19	GLN	-	expression tag	UNP Q72IT0
D	20	PHE	-	expression tag	UNP Q72IT0

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Chain	Residue	Modelled	Actual	Comment	Reference
D	21	GLU	-	expression tag	UNP Q72IT0
D	22	LYS	-	expression tag	UNP Q72IT0
D	175	CYS	TRP	engineered mutation	UNP Q72IT0
G	12	MET	-	expression tag	UNP Q72IT0
G	13	ALA	-	expression tag	UNP Q72IT0
G	14	SER	-	expression tag	UNP Q72IT0
G	15	TRP	-	expression tag	UNP Q72IT0
G	16	SER	-	expression tag	UNP Q72IT0
G	17	HIS	-	expression tag	UNP Q72IT0
G	18	PRO	-	expression tag	UNP Q72IT0
G	19	GLN	-	expression tag	UNP Q72IT0
G	20	PHE	-	expression tag	UNP Q72IT0
G	21	GLU	-	expression tag	UNP Q72IT0
G	22	LYS	-	expression tag	UNP Q72IT0
G	175	CYS	TRP	engineered mutation	UNP Q72IT0
J	12	MET	-	expression tag	UNP Q72IT0
J	13	ALA	-	expression tag	UNP Q72IT0
J	14	SER	-	expression tag	UNP Q72IT0
J	15	TRP	-	expression tag	UNP Q72IT0
J	16	SER	-	expression tag	UNP Q72IT0
J	17	HIS	-	expression tag	UNP Q72IT0
J	18	PRO	-	expression tag	UNP Q72IT0
J	19	GLN	-	expression tag	UNP Q72IT0
J	20	PHE	-	expression tag	UNP Q72IT0
J	21	GLU	-	expression tag	UNP Q72IT0
J	22	LYS	-	expression tag	UNP Q72IT0
J	175	CYS	TRP	engineered mutation	UNP Q72IT0

- Molecule 2 is a protein called SOXY PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	111	Total	C	N	O	S	0	0	0
			832	526	141	161	4			
2	E	113	Total	C	N	O	S	0	0	0
			844	530	147	164	3			
2	H	103	Total	C	N	O	S	0	0	0
			771	484	132	153	2			
2	K	121	Total	C	N	O	S	0	0	0
			909	575	156	174	4			

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	17	MET	-	expression tag	UNP Q72IS6
B	18	ARG	-	expression tag	UNP Q72IS6
B	19	GLY	-	expression tag	UNP Q72IS6
B	20	SER	-	expression tag	UNP Q72IS6
B	21	HIS	-	expression tag	UNP Q72IS6
B	22	HIS	-	expression tag	UNP Q72IS6
B	23	HIS	-	expression tag	UNP Q72IS6
B	24	HIS	-	expression tag	UNP Q72IS6
B	25	HIS	-	expression tag	UNP Q72IS6
B	26	HIS	-	expression tag	UNP Q72IS6
B	27	GLY	-	expression tag	UNP Q72IS6
B	28	SER	-	expression tag	UNP Q72IS6
B	88	ARG	LYS	conflict	UNP Q72IS6
E	17	MET	-	expression tag	UNP Q72IS6
E	18	ARG	-	expression tag	UNP Q72IS6
E	19	GLY	-	expression tag	UNP Q72IS6
E	20	SER	-	expression tag	UNP Q72IS6
E	21	HIS	-	expression tag	UNP Q72IS6
E	22	HIS	-	expression tag	UNP Q72IS6
E	23	HIS	-	expression tag	UNP Q72IS6
E	24	HIS	-	expression tag	UNP Q72IS6
E	25	HIS	-	expression tag	UNP Q72IS6
E	26	HIS	-	expression tag	UNP Q72IS6
E	27	GLY	-	expression tag	UNP Q72IS6
E	28	SER	-	expression tag	UNP Q72IS6
E	88	ARG	LYS	conflict	UNP Q72IS6
H	17	MET	-	expression tag	UNP Q72IS6
H	18	ARG	-	expression tag	UNP Q72IS6
H	19	GLY	-	expression tag	UNP Q72IS6
H	20	SER	-	expression tag	UNP Q72IS6
H	21	HIS	-	expression tag	UNP Q72IS6
H	22	HIS	-	expression tag	UNP Q72IS6
H	23	HIS	-	expression tag	UNP Q72IS6
H	24	HIS	-	expression tag	UNP Q72IS6
H	25	HIS	-	expression tag	UNP Q72IS6
H	26	HIS	-	expression tag	UNP Q72IS6
H	27	GLY	-	expression tag	UNP Q72IS6
H	28	SER	-	expression tag	UNP Q72IS6
H	88	ARG	LYS	conflict	UNP Q72IS6
K	17	MET	-	expression tag	UNP Q72IS6
K	18	ARG	-	expression tag	UNP Q72IS6
K	19	GLY	-	expression tag	UNP Q72IS6
K	20	SER	-	expression tag	UNP Q72IS6

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Chain	Residue	Modelled	Actual	Comment	Reference
K	21	HIS	-	expression tag	UNP Q72IS6
K	22	HIS	-	expression tag	UNP Q72IS6
K	23	HIS	-	expression tag	UNP Q72IS6
K	24	HIS	-	expression tag	UNP Q72IS6
K	25	HIS	-	expression tag	UNP Q72IS6
K	26	HIS	-	expression tag	UNP Q72IS6
K	27	GLY	-	expression tag	UNP Q72IS6
K	28	SER	-	expression tag	UNP Q72IS6
K	88	ARG	LYS	conflict	UNP Q72IS6

- Molecule 3 is a protein called SOXZ.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	97	Total	C	N	O	0	0	0
			743	471	130	142			
3	F	87	Total	C	N	O	0	0	0
			669	428	117	124			
3	I	49	Total	C	N	O	0	0	0
			393	257	66	70			
3	L	83	Total	C	N	O	0	0	0
			642	406	117	119			

- Molecule 4 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	2	Total	Mn	0	0
			2	2		
4	J	2	Total	Mn	0	0
			2	2		
4	A	2	Total	Mn	0	0
			2	2		
4	D	2	Total	Mn	0	0
			2	2		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		
5	G	3	Total	O	0	0
			3	3		

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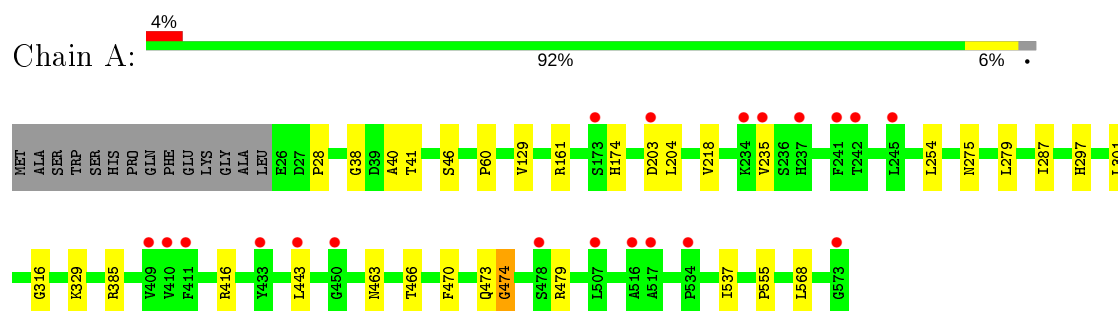
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	2	Total	O	0	0
			2	2		
5	K	1	Total	O	0	0
			1	1		



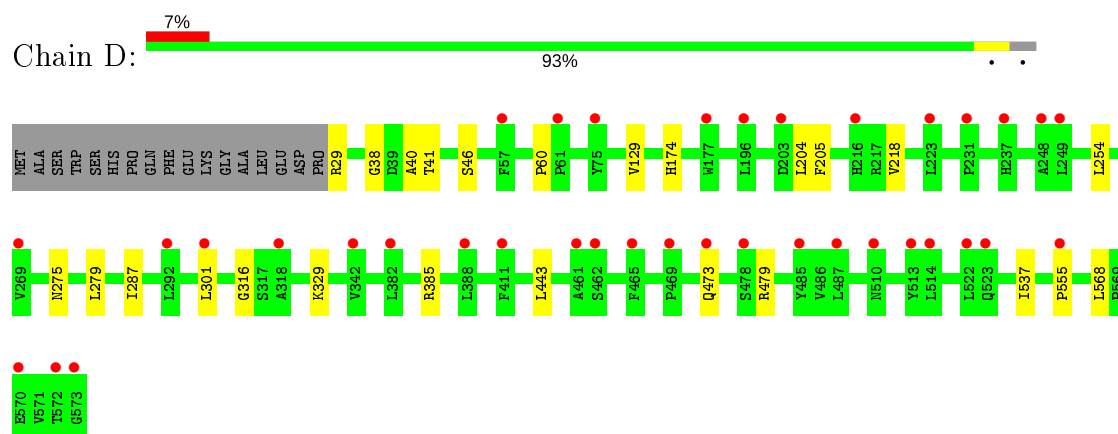
### 3 Residue-property plots [i](#)

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.

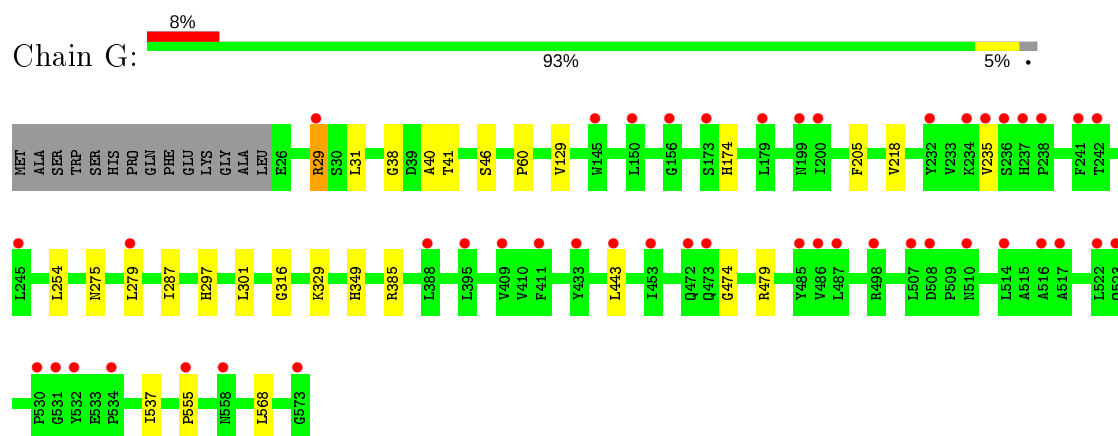
#### • Molecule 1: SULFUR OXIDATION PROTEIN SOXB



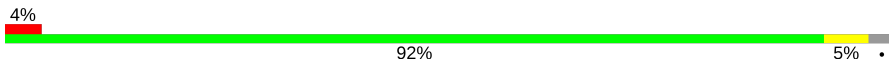
#### • Molecule 1: SULFUR OXIDATION PROTEIN SOXB

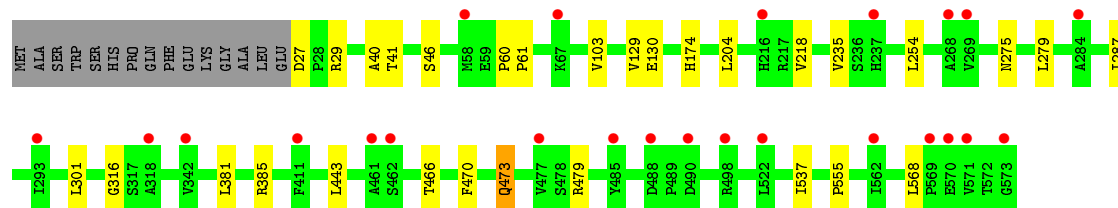


#### • Molecule 1: SULFUR OXIDATION PROTEIN SOXB



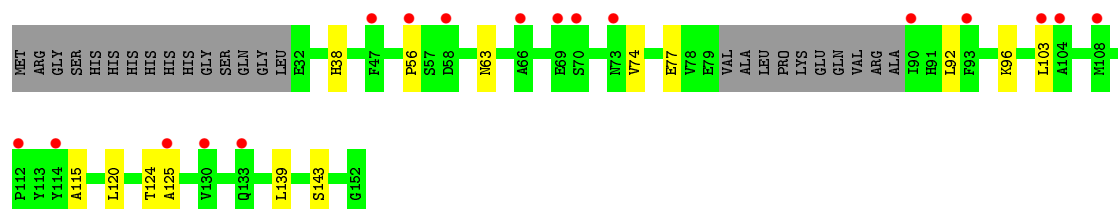
• Molecule 1: SULFUR OXIDATION PROTEIN SOXB

Chain J: 




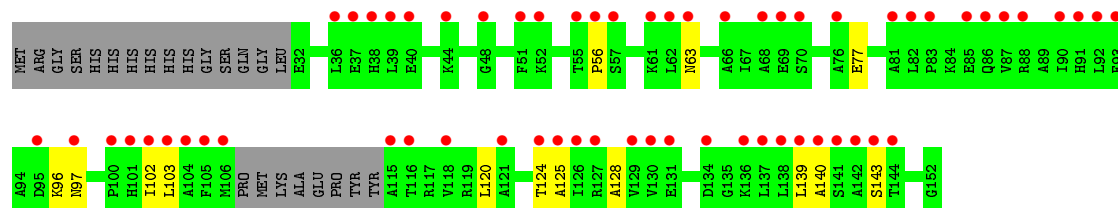
• Molecule 2: SOXY PROTEIN

Chain B: 



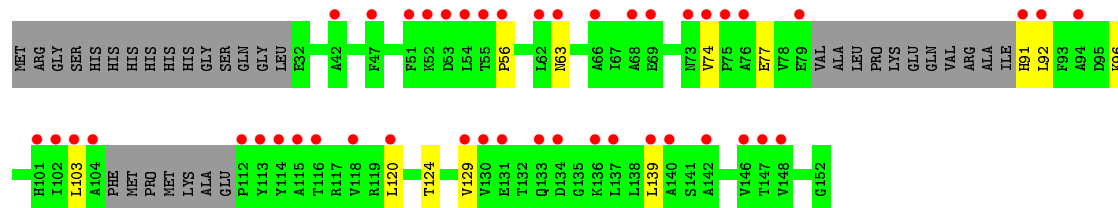
• Molecule 2: SOXY PROTEIN

Chain E: 




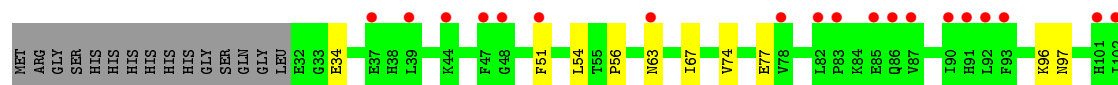
• Molecule 2: SOXY PROTEIN

Chain H: 



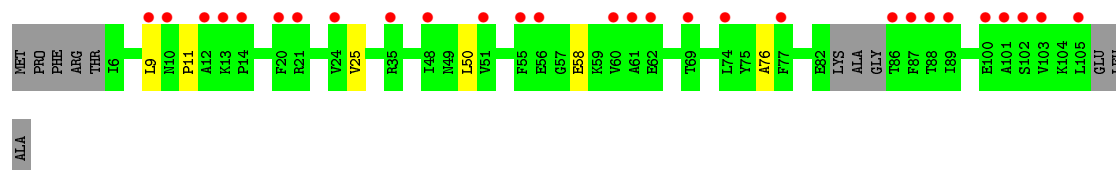
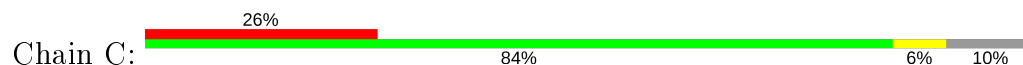
• Molecule 2: SOXY PROTEIN

Chain K: 

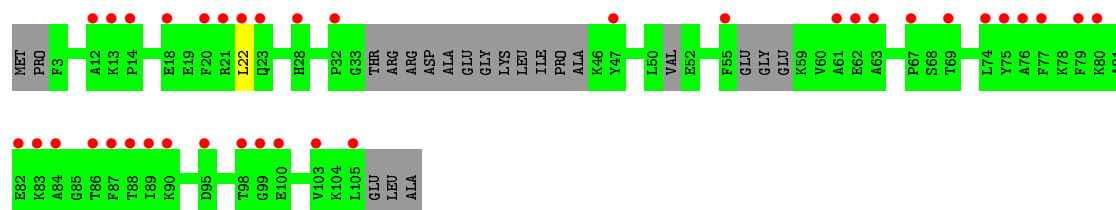
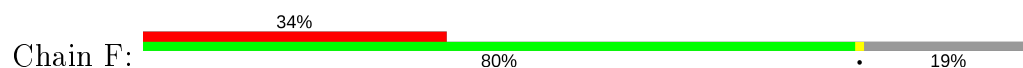




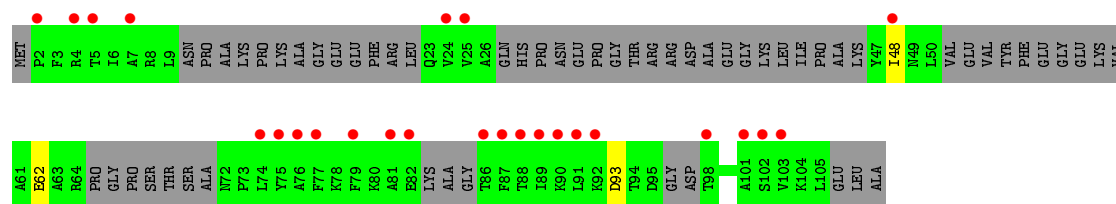
• Molecule 3: SOXZ



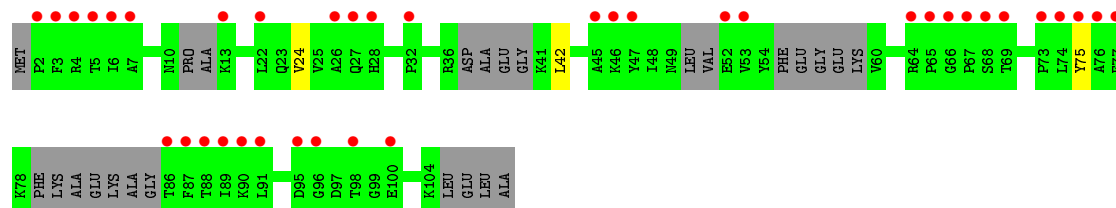
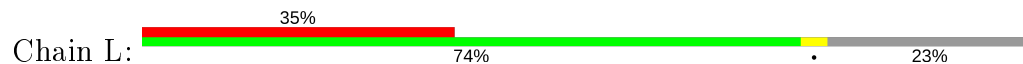
• Molecule 3: SOXZ



• Molecule 3: SOXZ



• Molecule 3: SOXZ



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.22Å 115.95Å 120.94Å 86.51° 83.21° 89.77°	Depositor
Resolution (Å)	59.81 – 3.28 59.81 – 3.28	Depositor EDS
% Data completeness (in resolution range)	98.5 (59.81-3.28) 98.8 (59.81-3.28)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.22 (at 3.26Å)	Xtriage
Refinement program	BUSTER 2.10.1	Depositor
R, $R_{free}$	0.269 , 0.275 0.288 , 0.292	Depositor DCC
$R_{free}$ test set	2894 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.4	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 57.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	23081	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.68% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MN

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	0.37	0/4439	0.54	0/6047
1	D	0.37	0/4414	0.54	0/6012
1	G	0.37	0/4439	0.54	0/6047
1	J	0.37	0/4430	0.54	0/6035
2	B	0.36	0/846	0.50	0/1145
2	E	0.37	0/855	0.52	0/1156
2	H	0.35	0/781	0.49	0/1054
2	K	0.36	0/924	0.51	0/1251
3	C	0.35	0/757	0.50	0/1021
3	F	0.34	0/681	0.46	0/914
3	I	0.33	0/394	0.42	0/521
3	L	0.33	0/651	0.46	0/872
All	All	0.37	0/23611	0.53	0/32075

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 [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	4323	0	4295	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4299	0	4278	9	0
1	G	4323	0	4295	12	0
1	J	4314	0	4289	12	0
2	B	832	0	833	7	0
2	E	844	0	858	7	0
2	H	771	0	767	6	0
2	K	909	0	919	11	0
3	C	743	0	743	1	0
3	F	669	0	669	0	0
3	I	393	0	405	1	0
3	L	642	0	645	1	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
4	G	2	0	0	0	0
4	J	2	0	0	0	0
5	A	5	0	0	0	0
5	G	3	0	0	0	0
5	J	2	0	0	0	0
5	K	1	0	0	0	0
All	All	23081	0	22996	78	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 2.

The worst 5 of 78 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:38:GLY:HA2	1:G:329:LYS:HD2	1.75	0.68
1:A:38:GLY:HA2	1:A:329:LYS:HD2	1.75	0.67
1:D:38:GLY:HA2	1:D:329:LYS:HD2	1.76	0.67
2:E:63:ASN:HB3	2:E:77:GLU:HB3	1.87	0.56
2:H:63:ASN:HB3	2:H:77:GLU:HB3	1.88	0.55

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	546/562 (97%)	516 (94%)	27 (5%)	3 (0%)	29	62
1	D	543/562 (97%)	517 (95%)	25 (5%)	1 (0%)	47	77
1	G	546/562 (97%)	518 (95%)	27 (5%)	1 (0%)	47	77
1	J	545/562 (97%)	517 (95%)	27 (5%)	1 (0%)	47	77
2	B	107/136 (79%)	98 (92%)	9 (8%)	0	100	100
2	E	109/136 (80%)	104 (95%)	5 (5%)	0	100	100
2	H	95/136 (70%)	91 (96%)	4 (4%)	0	100	100
2	K	117/136 (86%)	110 (94%)	6 (5%)	1 (1%)	17	50
3	C	93/108 (86%)	82 (88%)	11 (12%)	0	100	100
3	F	79/108 (73%)	70 (89%)	9 (11%)	0	100	100
3	I	35/108 (32%)	34 (97%)	1 (3%)	0	100	100
3	L	71/108 (66%)	66 (93%)	5 (7%)	0	100	100
All	All	2886/3224 (90%)	2723 (94%)	156 (5%)	7 (0%)	47	77

5 of 7 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	28	PRO
1	A	174	HIS
1	D	174	HIS
1	G	174	HIS
1	J	174	HIS

### 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	446/457 (98%)	439 (98%)	7 (2%)	62	79
1	D	443/457 (97%)	437 (99%)	6 (1%)	67	82
1	G	446/457 (98%)	440 (99%)	6 (1%)	69	82
1	J	445/457 (97%)	436 (98%)	9 (2%)	55	76
2	B	87/108 (81%)	86 (99%)	1 (1%)	73	85
2	E	89/108 (82%)	89 (100%)	0	100	100
2	H	81/108 (75%)	81 (100%)	0	100	100
2	K	95/108 (88%)	95 (100%)	0	100	100
3	C	76/86 (88%)	71 (93%)	5 (7%)	16	46
3	F	68/86 (79%)	67 (98%)	1 (2%)	65	81
3	I	41/86 (48%)	40 (98%)	1 (2%)	49	73
3	L	67/86 (78%)	66 (98%)	1 (2%)	65	81
All	All	2384/2604 (92%)	2347 (98%)	37 (2%)	62	79

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	301	LEU
1	G	29	ARG
1	J	473	GLN
1	D	473	GLN
1	D	479	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
3	F	30	ASN
3	L	30	ASN
1	J	147	ASN
1	D	147	ASN
1	G	147	ASN

### 5.3.3 RNA ⓘ

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, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	H	1
2	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	114:TYR	C	115:ALA	N	3.34
1	H	114:TYR	C	115:ALA	N	3.32

## 6 Fit of model and data [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	548/562 (97%)	0.50	20 (3%) 42 40	37, 63, 89, 101	0
1	D	545/562 (96%)	0.74	37 (6%) 17 17	62, 93, 115, 125	0
1	G	548/562 (97%)	0.74	46 (8%) 11 11	45, 80, 122, 137	0
1	J	547/562 (97%)	0.62	24 (4%) 34 33	47, 72, 94, 110	0
2	B	111/136 (81%)	1.11	17 (15%) 2 2	67, 110, 126, 133	0
2	E	113/136 (83%)	2.20	61 (53%) 0 0	87, 141, 154, 174	0
2	H	103/136 (75%)	1.97	45 (43%) 0 0	83, 141, 156, 182	0
2	K	121/136 (88%)	1.70	38 (31%) 0 0	69, 134, 152, 177	0
3	C	97/108 (89%)	1.43	28 (28%) 0 0	112, 127, 140, 156	0
3	F	87/108 (80%)	1.97	37 (42%) 0 0	129, 148, 163, 174	0
3	I	49/108 (45%)	2.80	25 (51%) 0 0	100, 141, 164, 188	0
3	L	83/108 (76%)	1.99	38 (45%) 0 0	123, 140, 166, 192	0
All	All	2952/3224 (91%)	0.95	416 (14%) 2 2	37, 85, 149, 192	0

The worst 5 of 416 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	5	THR	13.1
3	I	89	ILE	9.9
3	I	102	SER	8.6
2	K	115	ALA	8.0
3	I	88	THR	7.5

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
4	MN	A	581	1/1	0.96	0.13	51,51,51,51	0
4	MN	D	581	1/1	0.97	0.12	63,63,63,63	0
4	MN	G	581	1/1	0.97	0.14	59,59,59,59	0
4	MN	A	580	1/1	0.97	0.18	50,50,50,50	0
4	MN	G	580	1/1	0.98	0.17	63,63,63,63	0
4	MN	D	580	1/1	0.99	0.18	60,60,60,60	0
4	MN	J	581	1/1	0.99	0.19	45,45,45,45	0
4	MN	J	580	1/1	0.99	0.19	46,46,46,46	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.