



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 8, 2016 – 02:05 PM EST

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 Full wwPDB X-ray Structure Validation 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 ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
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)	:	rb-20028442

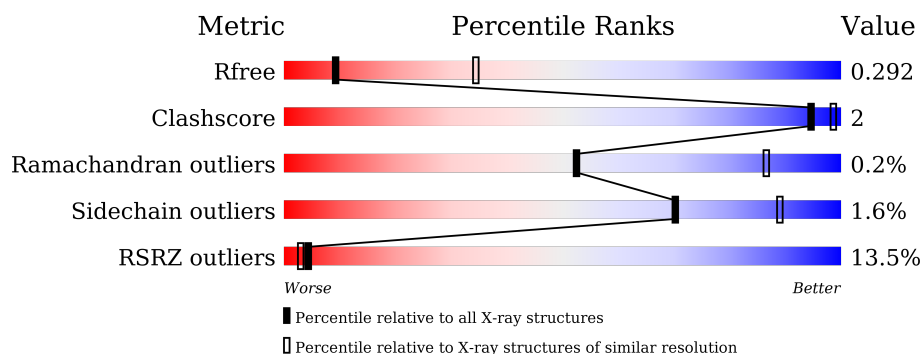
1 Overall quality at a glance

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}	91344	1756 (3.36-3.20)
Clashscore	102246	1941 (3.36-3.20)
Ramachandran outliers	100387	1905 (3.36-3.20)
Sidechain outliers	100360	1903 (3.36-3.20)
RSRZ outliers	91569	1764 (3.36-3.20)

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 $\leq 5\%$. 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>3%</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>9%</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>11%</div> <div>71%</div> <div>10%</div> <div>18%</div> </div>
2	E	136	<div> <div>41%</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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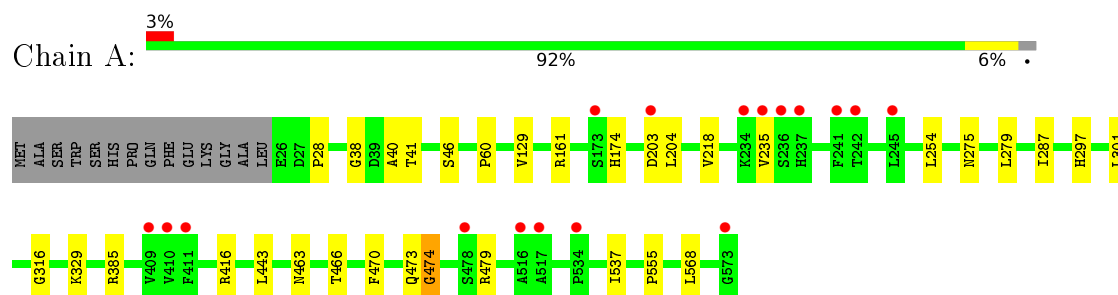
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	J	2	Total	O	0	0
			2	2		
5	K	1	Total	O	0	0
			1	1		

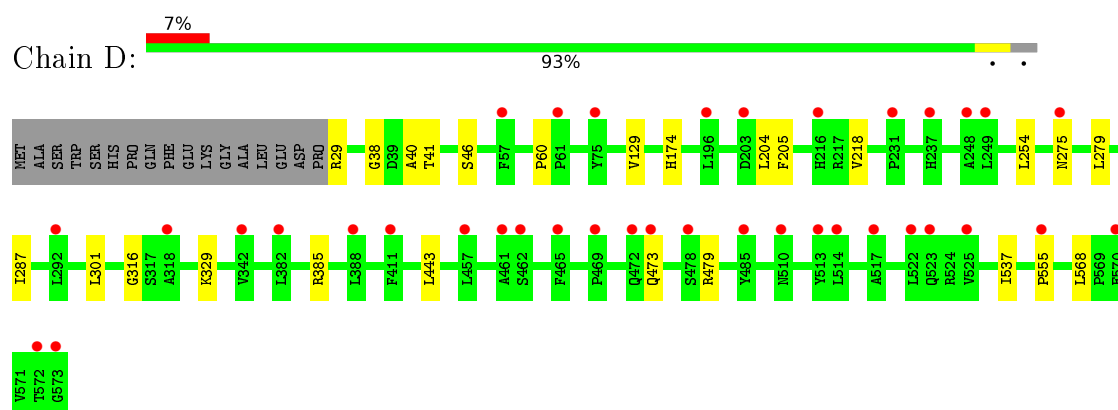
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

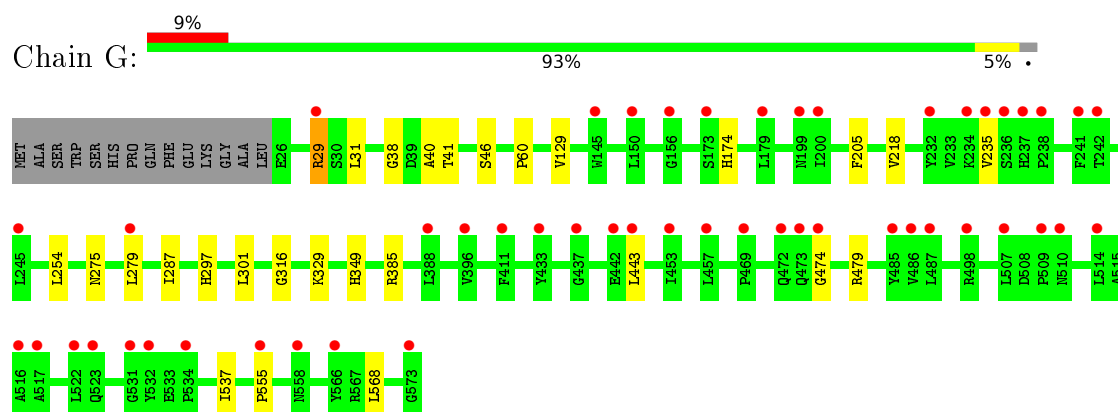
- Molecule 1: SULFUR OXIDATION PROTEIN SOXB



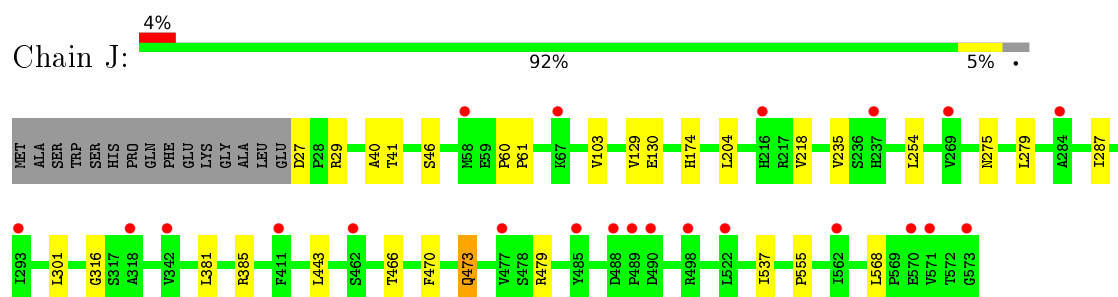
- Molecule 1: SULFUR OXIDATION PROTEIN SOXB



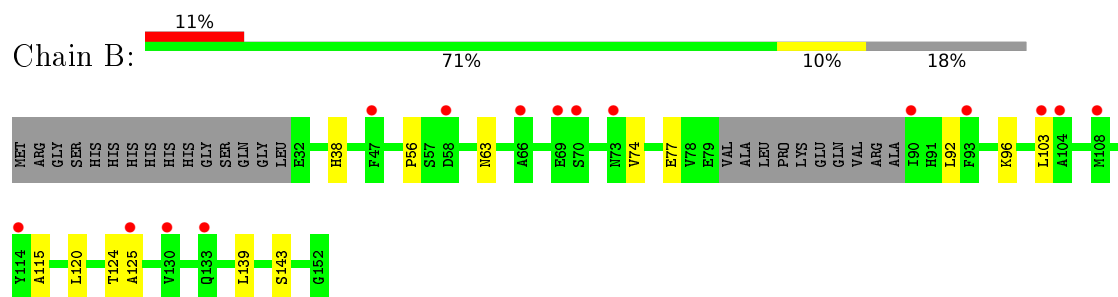
- Molecule 1: SULFUR OXIDATION PROTEIN SOXB



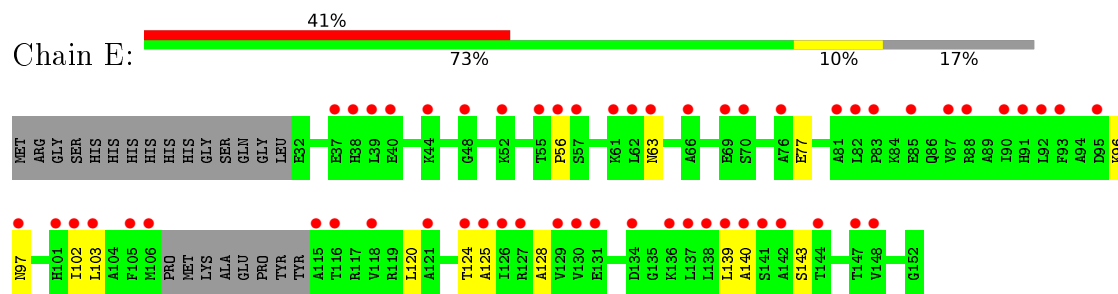
- Molecule 1: SULFUR OXIDATION PROTEIN SOXB



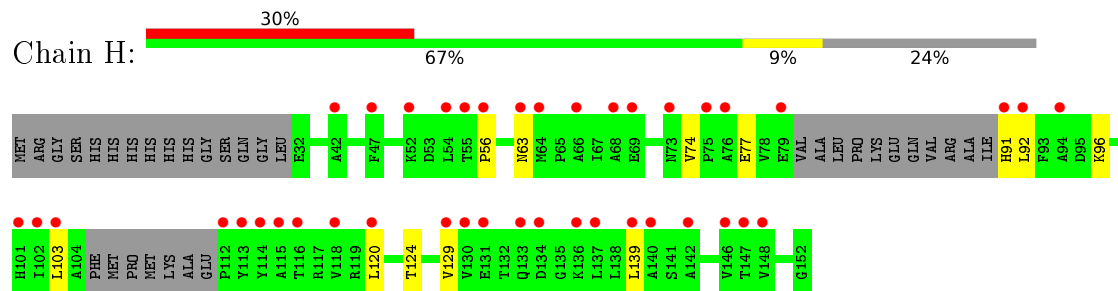
- Molecule 2: SOXY PROTEIN



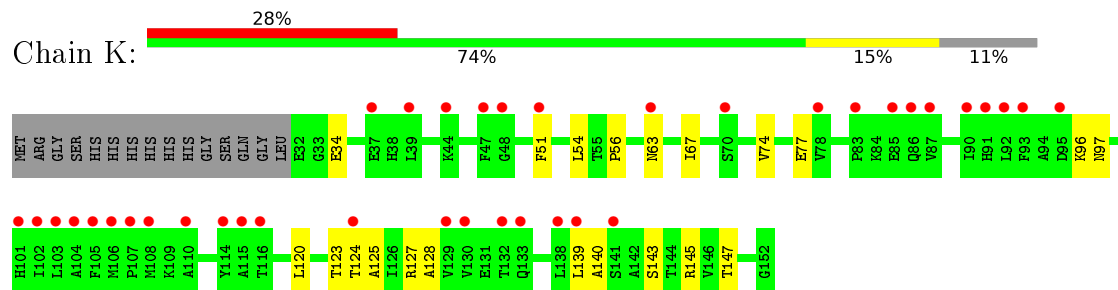
- Molecule 2: SOXY PROTEIN



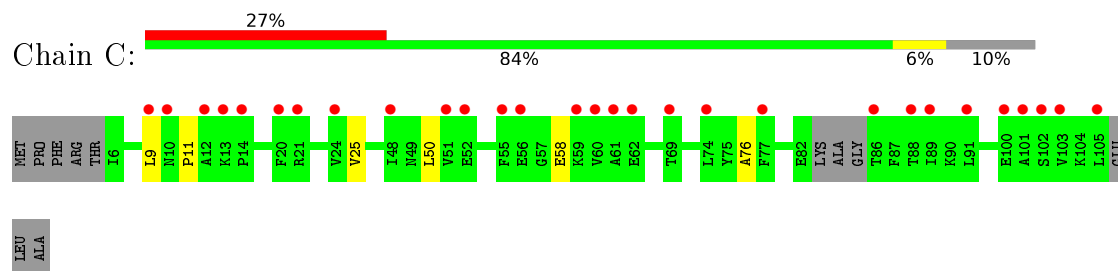
- Molecule 2: SOXY PROTEIN



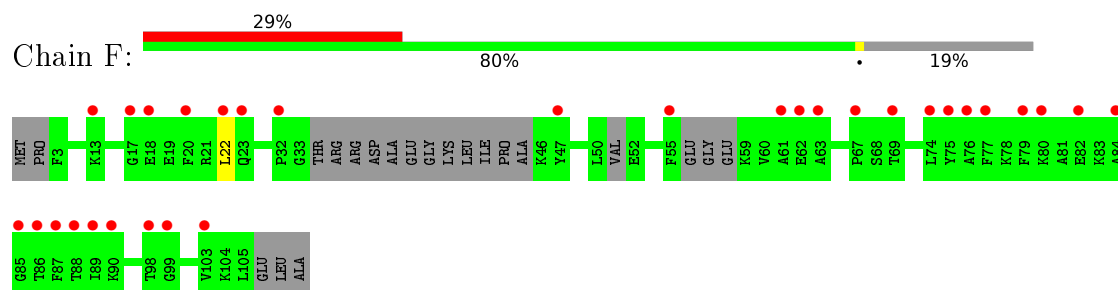
- Molecule 2: SOXY PROTEIN



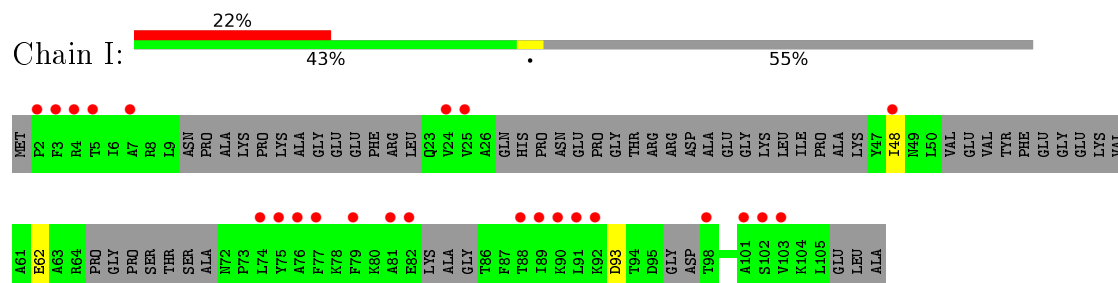
- Molecule 3: SOXZ



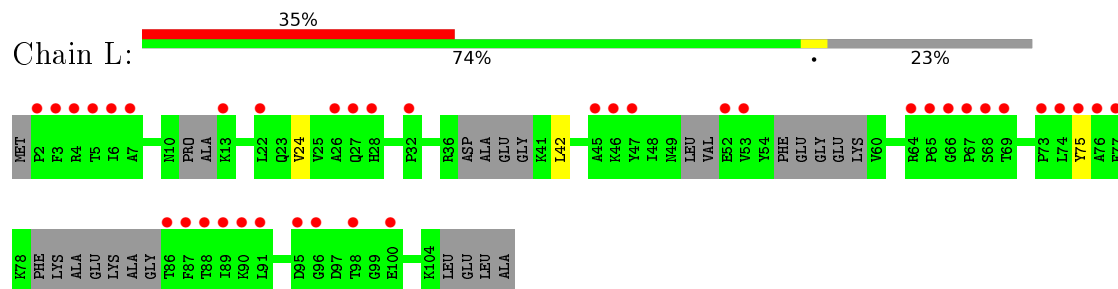
- Molecule 3: SOXZ



- Molecule 3: SOXZ



- Molecule 3: SOXZ



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	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) 96.9 (59.81-3.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.34%)	DCC
Wilson B-factor (Å ²)	79.4	Xtriage
Anisotropy	0.553	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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.

All (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
1:D:275:ASN:HB3	1:D:279:LEU:HD23	1.89	0.55
1:J:275:ASN:HB3	1:J:279:LEU:HD23	1.89	0.55
1:G:29:ARG:HE	1:G:349:HIS:CE1	2.25	0.55
1:A:297:HIS:HE2	1:A:474:GLY:HA3	1.71	0.54
1:A:275:ASN:HB3	1:A:279:LEU:HD23	1.89	0.54
2:B:63:ASN:HB3	2:B:77:GLU:HB3	1.89	0.53
1:G:275:ASN:HB3	1:G:279:LEU:HD23	1.89	0.53
2:K:63:ASN:HB3	2:K:77:GLU:HB3	1.91	0.53
2:E:56:PRO:HA	2:E:139:LEU:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:97:ASN:HD21	2:K:120:LEU:HA	1.74	0.52
2:E:128:ALA:HB3	2:E:140:ALA:HB3	1.91	0.52
2:K:96:LYS:H	2:K:124:THR:HG23	1.74	0.52
2:H:56:PRO:HA	2:H:139:LEU:HB2	1.93	0.50
2:B:115:ALA:HB3	3:C:76:ALA:HB3	1.94	0.50
2:K:128:ALA:HB3	2:K:140:ALA:HB3	1.94	0.49
2:B:96:LYS:H	2:B:124:THR:HG23	1.77	0.49
1:G:29:ARG:HH21	1:G:349:HIS:CE1	2.31	0.48
1:A:463:ASN:HD21	1:A:473:GLN:HB2	1.79	0.48
1:A:416:ARG:HH22	1:A:474:GLY:HA2	1.79	0.48
2:K:56:PRO:HA	2:K:139:LEU:HB2	1.95	0.48
1:J:443:LEU:HD13	1:J:537:ILE:HD13	1.96	0.47
1:D:40:ALA:HB2	1:D:218:VAL:HG11	1.95	0.47
1:J:254:LEU:HD23	1:J:287:ILE:HG13	1.96	0.47
1:A:161:ARG:HD3	1:J:130:GLU:O	2.13	0.47
1:A:254:LEU:HD23	1:A:287:ILE:HG13	1.96	0.47
2:E:97:ASN:HD21	2:E:120:LEU:HA	1.78	0.47
1:D:443:LEU:HD13	1:D:537:ILE:HD13	1.96	0.47
1:J:40:ALA:HB2	1:J:218:VAL:HG11	1.95	0.47
1:A:443:LEU:HD13	1:A:537:ILE:HD13	1.96	0.46
1:D:254:LEU:HD23	1:D:287:ILE:HG13	1.96	0.46
1:A:40:ALA:HB2	1:A:218:VAL:HG11	1.96	0.46
1:G:254:LEU:HD23	1:G:287:ILE:HG13	1.96	0.46
1:G:443:LEU:HD13	1:G:537:ILE:HD13	1.96	0.46
2:H:74:VAL:HG21	2:H:120:LEU:HD12	1.96	0.46
1:G:40:ALA:HB2	1:G:218:VAL:HG11	1.96	0.46
2:E:96:LYS:H	2:E:124:THR:HG23	1.81	0.46
3:L:24:VAL:HB	3:L:75:TYR:HB2	1.98	0.45
1:G:297:HIS:HE2	1:G:474:GLY:HA3	1.82	0.45
2:K:51:PHE:HA	2:K:54:LEU:HD12	1.98	0.45
2:B:74:VAL:HG21	2:B:120:LEU:HD12	1.99	0.44
2:H:96:LYS:H	2:H:124:THR:HG23	1.82	0.44
2:K:34:GLU:HG2	2:K:127:ARG:HH22	1.83	0.44
2:K:125:ALA:HA	2:K:143:SER:HA	2.00	0.44
2:B:92:LEU:HD12	2:B:103:LEU:HD11	2.00	0.43
1:J:41:THR:HG21	1:J:129:VAL:HG21	2.00	0.43
1:G:555:PRO:HB2	1:G:568:LEU:HD11	2.00	0.43
1:D:46:SER:HB3	1:D:316:GLY:HA3	2.00	0.43
1:A:555:PRO:HB2	1:A:568:LEU:HD11	2.00	0.43
1:D:41:THR:HG21	1:D:129:VAL:HG21	2.01	0.43
1:D:60:PRO:HD3	1:D:385:ARG:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:46:SER:HB3	1:G:316:GLY:HA3	2.00	0.43
1:G:60:PRO:HD3	1:G:385:ARG:HD3	2.00	0.43
2:K:74:VAL:HG21	2:K:120:LEU:HD12	2.00	0.42
1:D:555:PRO:HB2	1:D:568:LEU:HD11	2.00	0.42
1:J:60:PRO:HD3	1:J:385:ARG:HD3	2.00	0.42
2:E:125:ALA:HA	2:E:143:SER:HA	2.02	0.42
2:H:91:HIS:HB2	2:H:129:VAL:HG23	2.01	0.42
1:A:46:SER:HB3	1:A:316:GLY:HA3	2.00	0.42
1:J:555:PRO:HB2	1:J:568:LEU:HD11	2.00	0.42
1:J:46:SER:HB3	1:J:316:GLY:HA3	2.00	0.42
1:J:473:GLN:HB2	2:K:67:ILE:HD13	2.01	0.42
1:G:41:THR:HG21	1:G:129:VAL:HG21	2.01	0.42
1:A:60:PRO:HD3	1:A:385:ARG:HD3	2.00	0.42
2:E:102:ILE:HG22	2:E:103:LEU:HD23	2.01	0.41
2:K:145:ARG:HG2	2:K:147:THR:HG23	2.02	0.41
1:A:41:THR:HG21	1:A:129:VAL:HG21	2.01	0.41
2:H:92:LEU:HD12	2:H:103:LEU:HD11	2.03	0.41
3:I:48:ILE:HA	3:I:93:ASP:HA	2.03	0.41
1:J:60:PRO:HA	1:J:61:PRO:HD3	2.00	0.41
2:B:125:ALA:HA	2:B:143:SER:HA	2.03	0.40
1:A:416:ARG:HH22	1:A:474:GLY:CA	2.34	0.40
2:B:56:PRO:HA	2:B:139:LEU:HB3	2.03	0.40
1:J:103:VAL:HG22	1:J:381:LEU:HD13	2.03	0.40

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%)	34 74
1	D	543/562 (97%)	517 (95%)	25 (5%)	1 (0%)	52 86

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	546/562 (97%)	518 (95%)	27 (5%)	1 (0%)	52	86
1	J	545/562 (97%)	517 (95%)	27 (5%)	1 (0%)	52	86
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%)	21	63
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%)	52	86

All (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
2	K	123	THR
1	A	474	GLY

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	446/457 (98%)	439 (98%)	7 (2%)	70	89
1	D	443/457 (97%)	437 (99%)	6 (1%)	74	90
1	G	446/457 (98%)	440 (99%)	6 (1%)	76	91
1	J	445/457 (97%)	436 (98%)	9 (2%)	63	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	87/108 (81%)	86 (99%)	1 (1%)	80	92
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%)	21	60
3	F	68/86 (79%)	67 (98%)	1 (2%)	72	90
3	I	41/86 (48%)	40 (98%)	1 (2%)	57	84
3	L	67/86 (78%)	66 (98%)	1 (2%)	72	90
All	All	2384/2604 (92%)	2347 (98%)	37 (2%)	70	89

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	203	ASP
1	A	204	LEU
1	A	235	VAL
1	A	301	LEU
1	A	466	THR
1	A	470	PHE
1	A	479	ARG
2	B	38	HIS
3	C	9	LEU
3	C	11	PRO
3	C	25	VAL
3	C	50	LEU
3	C	58	GLU
1	D	29	ARG
1	D	204	LEU
1	D	205	PHE
1	D	301	LEU
1	D	473	GLN
1	D	479	ARG
3	F	22	LEU
1	G	29	ARG
1	G	31	LEU
1	G	205	PHE
1	G	235	VAL
1	G	301	LEU
1	G	479	ARG

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Mol	Chain	Res	Type
3	I	62	GLU
1	J	27	ASP
1	J	29	ARG
1	J	204	LEU
1	J	235	VAL
1	J	301	LEU
1	J	466	THR
1	J	470	PHE
1	J	473	GLN
1	J	479	ARG
3	L	42	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	147	ASN
3	C	30	ASN
1	D	147	ASN
3	F	30	ASN
1	G	147	ASN
1	J	147	ASN
2	K	97	ASN
3	L	30	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 ⓘ

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](#)

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	548/562 (97%)	0.48	17 (3%) 52 44	37, 63, 89, 101	0
1	D	545/562 (96%)	0.71	37 (6%) 20 15	62, 93, 115, 125	0
1	G	548/562 (97%)	0.73	50 (9%) 11 8	45, 80, 122, 137	0
1	J	547/562 (97%)	0.60	22 (4%) 42 32	47, 72, 94, 110	0
2	B	111/136 (81%)	1.08	15 (13%) 4 3	67, 110, 126, 133	0
2	E	113/136 (83%)	2.11	56 (49%) 0 0	87, 141, 154, 174	0
2	H	103/136 (75%)	1.91	41 (39%) 0 0	83, 141, 156, 182	0
2	K	121/136 (88%)	1.64	38 (31%) 1 1	69, 134, 152, 177	0
3	C	97/108 (89%)	1.37	29 (29%) 1 1	112, 127, 140, 156	0
3	F	87/108 (80%)	1.85	31 (35%) 0 1	129, 148, 163, 174	0
3	I	49/108 (45%)	2.77	24 (48%) 0 0	100, 141, 164, 188	0
3	L	83/108 (76%)	1.90	38 (45%) 0 0	123, 140, 166, 192	0
All	All	2952/3224 (91%)	0.92	398 (13%) 4 3	37, 85, 149, 192	0

All (398) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	I	5	THR	14.5
3	I	89	ILE	9.7
3	I	102	SER	8.5
3	I	88	THR	7.6
2	K	115	ALA	7.6
2	H	55	THR	6.5
3	C	89	ILE	6.4
2	H	56	PRO	6.4
2	H	115	ALA	6.3
1	G	236	SER	6.2
1	D	573	GLY	6.2

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Mol	Chain	Res	Type	RSRZ
3	I	75	TYR	6.1
3	F	74	LEU	6.1
2	H	134	ASP	5.9
3	I	76	ALA	5.9
3	I	74	LEU	5.8
2	E	106	MET	5.7
1	G	237	HIS	5.6
2	B	90	ILE	5.6
3	I	98	THR	5.4
2	K	91	HIS	5.3
2	K	105	PHE	5.3
2	K	107	PRO	5.2
3	F	88	THR	5.0
2	E	76	ALA	5.0
3	L	75	TYR	5.0
2	K	103	LEU	5.0
2	E	115	ALA	5.0
3	L	5	THR	4.9
2	H	133	GLN	4.8
3	L	86	THR	4.8
2	H	130	VAL	4.8
2	H	114	TYR	4.7
2	E	139	LEU	4.6
3	F	75	TYR	4.6
3	L	3	PHE	4.6
2	K	104	ALA	4.6
3	C	14	PRO	4.5
2	E	56	PRO	4.5
2	K	85	GLU	4.5
3	F	89	ILE	4.4
3	L	28	HIS	4.4
2	E	82	LEU	4.4
2	K	87	VAL	4.4
3	L	89	ILE	4.4
2	B	70	SER	4.3
2	E	55	THR	4.3
3	F	86	THR	4.3
2	K	51	PHE	4.2
2	K	47	PHE	4.2
3	C	48	ILE	4.2
2	E	63	ASN	4.1
1	G	522	LEU	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	142	ALA	4.0
2	K	90	ILE	4.0
1	D	249	LEU	4.0
1	A	237	HIS	4.0
3	C	77	PHE	4.0
3	I	101	ALA	4.0
3	I	77	PHE	3.9
3	C	102	SER	3.9
1	G	510	ASN	3.9
3	I	48	ILE	3.9
3	L	77	PHE	3.9
2	K	93	PHE	3.9
3	C	103	VAL	3.8
3	F	55	PHE	3.8
3	L	22	LEU	3.8
2	B	69	GLU	3.8
2	B	133	GLN	3.8
3	C	86	THR	3.8
3	C	88	THR	3.8
1	J	237	HIS	3.7
2	K	132	THR	3.7
2	E	103	LEU	3.7
3	L	66	GLY	3.7
1	D	469	PRO	3.7
2	H	139	LEU	3.7
1	G	241	PHE	3.7
3	L	69	THR	3.7
2	K	138	LEU	3.7
3	C	56	GLU	3.6
2	H	136	LYS	3.6
2	E	105	PHE	3.6
1	D	462	SER	3.6
2	K	114	TYR	3.6
2	E	70	SER	3.6
3	C	100	GLU	3.6
1	J	269	VAL	3.6
2	E	129	VAL	3.6
2	K	102	ILE	3.6
3	I	4	ARG	3.6
3	L	67	PRO	3.6
1	A	203	ASP	3.6
3	F	79	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
3	L	6	ILE	3.5
1	G	573	GLY	3.5
3	L	90	LYS	3.5
2	E	125	ALA	3.5
2	E	85	GLU	3.5
1	D	237	HIS	3.5
2	K	139	LEU	3.4
1	G	242	THR	3.4
3	C	74	LEU	3.4
3	F	23	GLN	3.4
3	I	2	PRO	3.4
3	F	103	VAL	3.4
2	E	91	HIS	3.4
2	K	129	VAL	3.4
2	H	69	GLU	3.4
3	F	32	PRO	3.3
1	A	234	LYS	3.3
1	J	573	GLY	3.3
1	G	234	LYS	3.3
2	E	44	LYS	3.3
3	I	103	VAL	3.3
2	B	58	ASP	3.3
2	E	66	ALA	3.3
3	F	22	LEU	3.3
3	I	92	LYS	3.3
2	K	37	GLU	3.2
1	G	238	PRO	3.2
2	E	95	ASP	3.2
2	E	39	LEU	3.2
2	K	86	GLN	3.2
3	C	60	VAL	3.2
2	E	144	THR	3.2
3	C	9	LEU	3.2
2	E	90	ILE	3.2
2	B	108	MET	3.2
3	F	87	PHE	3.2
1	G	473	GLN	3.2
2	E	87	VAL	3.1
2	H	54	LEU	3.1
3	L	68	SER	3.1
3	F	61	ALA	3.1
2	H	118	VAL	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	411	PHE	3.1
2	H	92	LEU	3.1
2	H	137	LEU	3.1
2	E	97	ASN	3.1
2	K	78	VAL	3.1
2	H	112	PRO	3.1
3	C	10	ASN	3.1
2	K	92	LEU	3.1
3	F	13	LYS	3.1
3	L	96	GLY	3.1
2	H	131	GLU	3.0
2	E	69	GLU	3.0
2	E	124	THR	3.0
3	L	7	ALA	3.0
1	J	562	ILE	3.0
2	K	48	GLY	3.0
2	H	73	ASN	3.0
1	G	486	VAL	3.0
2	K	124	THR	3.0
3	L	100	GLU	3.0
2	E	121	ALA	3.0
2	E	127	ARG	3.0
1	G	232	TYR	3.0
1	G	517	ALA	3.0
2	H	42	ALA	3.0
2	H	68	ALA	3.0
3	F	76	ALA	3.0
2	H	146	VAL	3.0
1	G	411	PHE	3.0
2	E	83	PRO	3.0
3	I	91	LEU	3.0
1	G	433	TYR	3.0
3	L	27	GLN	3.0
3	C	51	VAL	2.9
3	I	81	ALA	2.9
2	E	81	ALA	2.9
2	E	131	GLU	2.9
1	G	179	LEU	2.9
1	A	173	SER	2.9
3	I	82	GLU	2.9
2	K	39	LEU	2.9
2	E	116	THR	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	487	LEU	2.9
2	H	94	ALA	2.9
3	L	87	PHE	2.9
2	E	62	LEU	2.9
3	I	25	VAL	2.9
2	H	147	THR	2.8
2	B	130	VAL	2.8
1	D	555	PRO	2.8
2	B	93	PHE	2.8
2	H	76	ALA	2.8
3	C	20	PHE	2.8
1	G	507	LEU	2.8
3	C	62	GLU	2.8
3	L	88	THR	2.8
2	B	104	ALA	2.8
1	G	531	GLY	2.8
1	D	216	HIS	2.8
2	H	129	VAL	2.8
2	E	40	GLU	2.8
1	G	558	ASN	2.8
1	A	242	THR	2.8
3	L	2	PRO	2.8
1	J	477	VAL	2.8
2	E	130	VAL	2.8
1	D	75	TYR	2.8
2	H	63	ASN	2.8
2	H	113	TYR	2.8
3	F	63	ALA	2.7
3	F	90	LYS	2.7
2	K	106	MET	2.7
1	D	231	PRO	2.7
1	G	472	GLN	2.7
1	D	473	GLN	2.7
1	G	156	GLY	2.7
3	I	24	VAL	2.7
3	F	80	LYS	2.7
2	E	92	LEU	2.7
3	L	76	ALA	2.7
2	H	102	ILE	2.7
2	H	91	HIS	2.7
2	E	137	LEU	2.7
2	H	120	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
3	L	47	TYR	2.7
3	F	69	THR	2.7
2	E	93	PHE	2.7
1	D	570	GLU	2.7
2	E	134	ASP	2.7
3	L	64	ARG	2.7
1	G	485	TYR	2.6
2	E	102	ILE	2.6
3	I	90	LYS	2.6
2	H	103	LEU	2.6
1	D	248	ALA	2.6
1	G	150	LEU	2.6
2	K	110	ALA	2.6
3	L	13	LYS	2.6
2	B	66	ALA	2.6
1	G	29	ARG	2.6
1	J	488	ASP	2.6
3	F	18	GLU	2.6
3	I	79	PHE	2.6
2	K	130	VAL	2.6
3	C	101	ALA	2.6
1	G	279	LEU	2.6
3	F	20	PHE	2.6
2	K	44	LYS	2.6
2	H	101	HIS	2.6
2	H	47	PHE	2.6
2	E	57	SER	2.6
1	J	570	GLU	2.6
3	L	74	LEU	2.6
1	D	485	TYR	2.6
2	E	37	GLU	2.6
2	E	141	SER	2.5
2	B	103	LEU	2.5
2	E	38	HIS	2.5
2	E	140	ALA	2.5
2	E	61	LYS	2.5
2	H	75	PRO	2.5
2	K	108	MET	2.5
1	D	478	SER	2.5
3	F	47	TYR	2.5
2	H	140	ALA	2.5
3	F	62	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	292	LEU	2.5
1	J	284	ALA	2.5
2	H	142	ALA	2.5
3	F	77	PHE	2.5
2	E	138	LEU	2.5
3	F	82	GLU	2.5
1	A	573	GLY	2.5
1	D	196	LEU	2.5
1	D	514	LEU	2.5
2	E	148	VAL	2.4
2	H	148	VAL	2.4
2	H	116	THR	2.4
1	J	522	LEU	2.4
2	E	126	ILE	2.4
1	G	555	PRO	2.4
3	C	59	LYS	2.4
3	C	55	PHE	2.4
3	F	99	GLY	2.4
3	L	53	VAL	2.4
1	D	203	ASP	2.4
1	G	516	ALA	2.4
1	A	241	PHE	2.4
2	B	114	TYR	2.4
2	H	66	ALA	2.4
3	L	98	THR	2.4
1	G	532	TYR	2.4
3	C	12	ALA	2.4
3	L	32	PRO	2.4
1	J	571	VAL	2.4
2	E	48	GLY	2.4
2	K	141	SER	2.4
2	K	63	ASN	2.4
1	J	216	HIS	2.4
1	G	145	TRP	2.3
3	C	61	ALA	2.3
3	I	7	ALA	2.3
1	J	462	SER	2.3
2	B	73	ASN	2.3
2	E	147	THR	2.3
1	G	245	LEU	2.3
3	L	65	PRO	2.3
2	K	101	HIS	2.3

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Mol	Chain	Res	Type	RSRZ
2	K	83	PRO	2.3
1	G	523	GLN	2.3
1	A	245	LEU	2.3
2	H	52	LYS	2.3
1	A	410	VAL	2.3
3	L	4	ARG	2.3
1	G	453	ILE	2.3
1	D	411	PHE	2.3
2	E	52	LYS	2.3
1	D	388	LEU	2.3
2	K	70	SER	2.3
1	D	461	ALA	2.3
1	G	388	LEU	2.3
1	A	236	SER	2.3
2	E	101	HIS	2.3
3	C	24	VAL	2.3
3	L	91	LEU	2.3
3	L	52	GLU	2.2
3	L	46	LYS	2.2
1	A	235	VAL	2.2
1	A	478	SER	2.2
1	D	522	LEU	2.2
1	D	572	THR	2.2
3	F	67	PRO	2.2
1	G	442	GLU	2.2
2	K	133	GLN	2.2
3	L	95	ASP	2.2
1	D	342	VAL	2.2
1	G	498	ARG	2.2
1	D	513	TYR	2.2
3	F	85	GLY	2.2
1	G	443	LEU	2.2
1	A	516	ALA	2.2
1	G	514	LEU	2.2
2	K	116	THR	2.2
1	A	409	VAL	2.2
3	L	73	PRO	2.2
1	D	510	ASN	2.2
1	G	235	VAL	2.2
1	J	411	PHE	2.2
1	J	293	ILE	2.2
3	C	69	THR	2.2

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Mol	Chain	Res	Type	RSRZ
3	C	91	LEU	2.1
1	J	318	ALA	2.1
2	H	79	GLU	2.1
1	J	489	PRO	2.1
3	C	13	LYS	2.1
1	G	199	ASN	2.1
1	G	200	ILE	2.1
1	A	534	PRO	2.1
1	J	490	ASP	2.1
1	D	465	PHE	2.1
1	D	517	ALA	2.1
1	G	396	VAL	2.1
3	C	105	LEU	2.1
1	D	57	PHE	2.1
1	J	498	ARG	2.1
3	L	45	ALA	2.1
3	C	52	GLU	2.1
1	J	485	TYR	2.1
2	B	125	ALA	2.1
1	J	342	VAL	2.1
3	F	98	THR	2.1
2	E	136	LYS	2.1
1	J	67	LYS	2.1
1	G	509	PRO	2.1
1	A	517	ALA	2.1
1	G	173	SER	2.1
1	D	318	ALA	2.1
2	B	47	PHE	2.1
1	D	61	PRO	2.1
1	D	523	GLN	2.1
1	G	534	PRO	2.1
3	L	26	ALA	2.1
1	G	457	LEU	2.1
1	D	472	GLN	2.0
2	K	95	ASP	2.1
2	E	118	VAL	2.0
1	D	382	LEU	2.0
1	G	469	PRO	2.0
1	J	58	MET	2.0
2	E	88	ARG	2.0
3	C	21	ARG	2.0
3	F	17	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	H	64	MET	2.0
3	F	84	ALA	2.0
1	G	474	GLY	2.0
1	D	525	VAL	2.0
1	D	457	LEU	2.0
1	G	437	GLY	2.0
3	I	3	PHE	2.0
1	D	275	ASN	2.0
1	G	566	TYR	2.0

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. 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, 95th 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
4	MN	D	580	1/1	0.99	0.18	-0.82	60,60,60,60	0
4	MN	A	580	1/1	0.96	0.19	-0.94	50,50,50,50	0
4	MN	G	580	1/1	0.97	0.18	-1.22	63,63,63,63	0
4	MN	G	581	1/1	0.97	0.14	-1.60	59,59,59,59	0
4	MN	A	581	1/1	0.96	0.13	-1.84	51,51,51,51	0
4	MN	D	581	1/1	0.96	0.12	-1.89	63,63,63,63	0
4	MN	J	580	1/1	0.99	0.19	-1.92	46,46,46,46	0
4	MN	J	581	1/1	0.99	0.19	-3.24	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.