



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2016 – 11:36 PM EDT

PDB ID : 5D4Z
Title : Crystal structure of Repressor from Salmonella-temperate phage
Authors : Kim, H.J.; Yoon, H.J.; Ryu, S.; Lee, H.H.
Deposited on : 2015-08-10
Resolution : 2.98 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 ⓘ 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-20027457
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-20027457

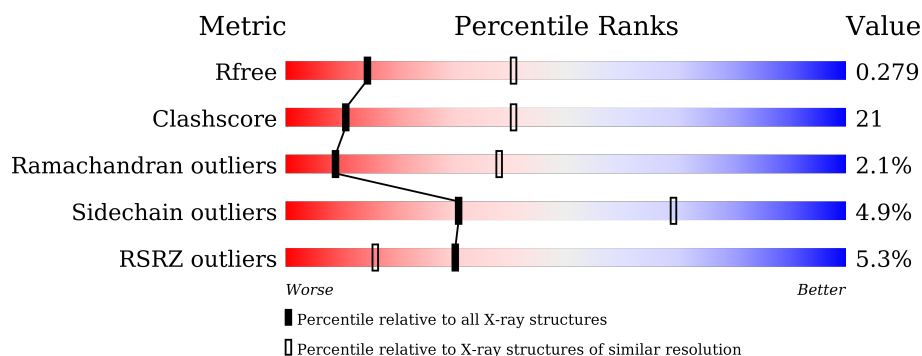
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	1992 (3.00-2.96)
Clashscore	102246	2349 (3.00-2.96)
Ramachandran outliers	100387	2274 (3.00-2.96)
Sidechain outliers	100360	2277 (3.00-2.96)
RSRZ outliers	91569	2007 (3.00-2.96)

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	1	107	<div> <div>3%</div> <div> <div></div> <div>50%</div> <div>48%</div> <div>..</div> </div> </div>
1	2	107	<div> <div>9%</div> <div> <div></div> <div>57%</div> <div>34%</div> <div>.. 6%</div> </div> </div>
1	3	107	<div> <div>2%</div> <div> <div></div> <div>50%</div> <div>38%</div> <div>5% 7%</div> </div> </div>
1	4	107	<div> <div>17%</div> <div> <div></div> <div>48%</div> <div>45%</div> <div>. 7%</div> </div> </div>
1	5	107	<div> <div>7%</div> <div> <div></div> <div>48%</div> <div>41%</div> <div>. . 7%</div> </div> </div>
1	6	107	<div> <div>17%</div> <div> <div></div> <div>50%</div> <div>33%</div> <div>11% . 6%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	7	107	
1	A	107	
1	B	107	
1	C	107	
1	D	107	
1	E	107	
1	F	107	
1	G	107	
1	H	107	
1	I	107	
1	J	107	
1	K	107	
1	L	107	
1	M	107	
1	N	107	
1	O	107	
1	P	107	
1	Q	107	
1	R	107	
1	T	107	
1	U	107	
1	V	107	
1	W	107	
1	X	107	
1	Y	107	

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Mol	Chain	Length	Quality of chain
1	Z	107	<div><div></div><div>13%</div><div>47%</div><div>38%</div><div>8%</div><div>7%</div></div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25962 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 Repressor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	B	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	C	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	D	101	Total	C	N	O	S	0	0	0
			773	493	131	144	5			
1	E	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	F	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	G	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	H	102	Total	C	N	O	S	0	0	0
			782	498	132	147	5			
1	I	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	J	103	Total	C	N	O	S	0	0	0
			791	503	134	149	5			
1	K	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	L	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	M	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	N	102	Total	C	N	O	S	0	0	0
			782	498	132	147	5			
1	O	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	P	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	R	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	T	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	U	103	Total	C	N	O	S	0	0	0
			791	503	134	149	5			
1	V	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	W	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	X	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	Y	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	Z	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			
1	1	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			
1	2	101	Total	C	N	O	S	0	0	0
			773	493	131	144	5			
1	3	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			
1	4	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			
1	5	100	Total	C	N	O	S	0	0	0
			762	484	130	143	5			
1	6	101	Total	C	N	O	S	0	0	0
			773	493	131	144	5			
1	7	105	Total	C	N	O	S	0	0	0
			808	513	138	152	5			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	21	Total	O	0	0
			21	21		
2	B	24	Total	O	0	0
			24	24		
2	C	25	Total	O	0	0
			25	25		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	D	39	Total O 39 39	0	0
2	E	21	Total O 21 21	0	0
2	F	30	Total O 30 30	0	0
2	G	19	Total O 19 19	0	0
2	H	26	Total O 26 26	0	0
2	I	3	Total O 3 3	0	0
2	J	10	Total O 10 10	0	0
2	K	5	Total O 5 5	0	0
2	L	17	Total O 17 17	0	0
2	M	5	Total O 5 5	0	0
2	N	13	Total O 13 13	0	0
2	O	3	Total O 3 3	0	0
2	P	8	Total O 8 8	0	0
2	Q	18	Total O 18 18	0	0
2	R	33	Total O 33 33	0	0
2	T	32	Total O 32 32	0	0
2	U	27	Total O 27 27	0	0
2	V	16	Total O 16 16	0	0
2	W	27	Total O 27 27	0	0
2	X	19	Total O 19 19	0	0
2	Y	17	Total O 17 17	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	Z	4	Total 4	O 4	0	0
2	1	8	Total 8	O 8	0	0
2	2	7	Total 7	O 7	0	0
2	3	18	Total 18	O 18	0	0
2	4	6	Total 6	O 6	0	0
2	5	14	Total 14	O 14	0	0
2	6	3	Total 3	O 3	0	0
2	7	9	Total 9	O 9	0	0

3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

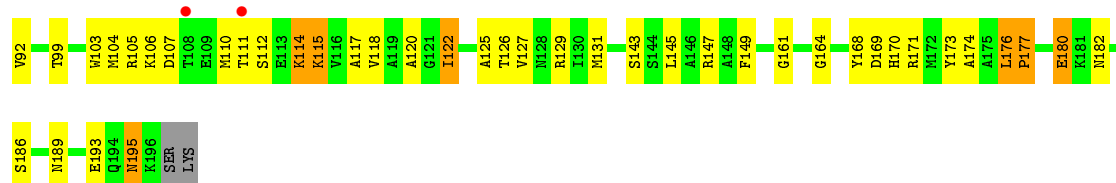
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• Molecule 1: Repressor



• Molecule 1: Repressor



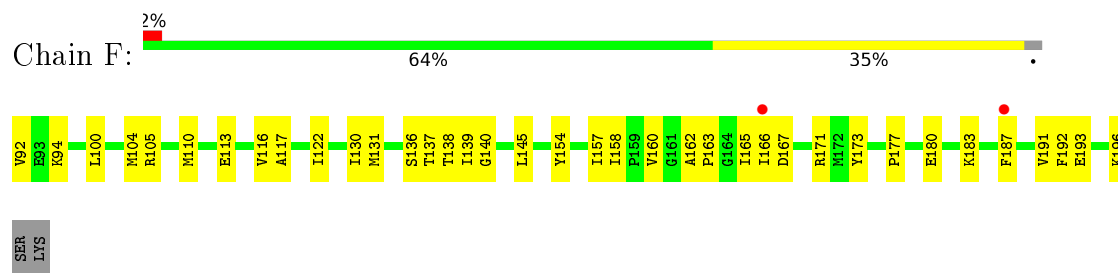
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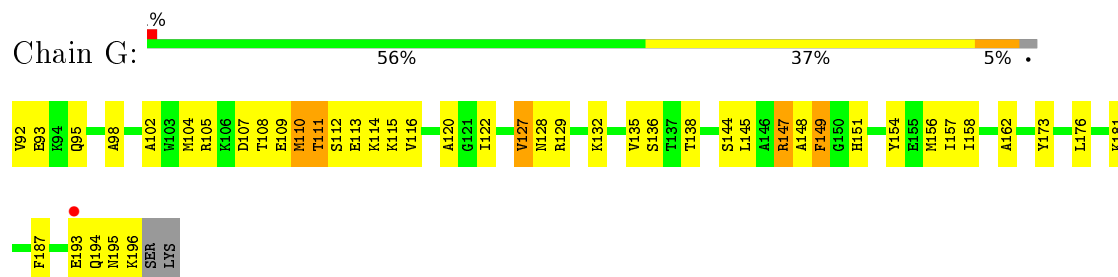
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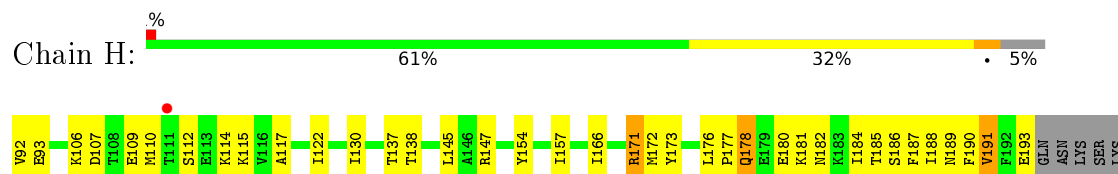
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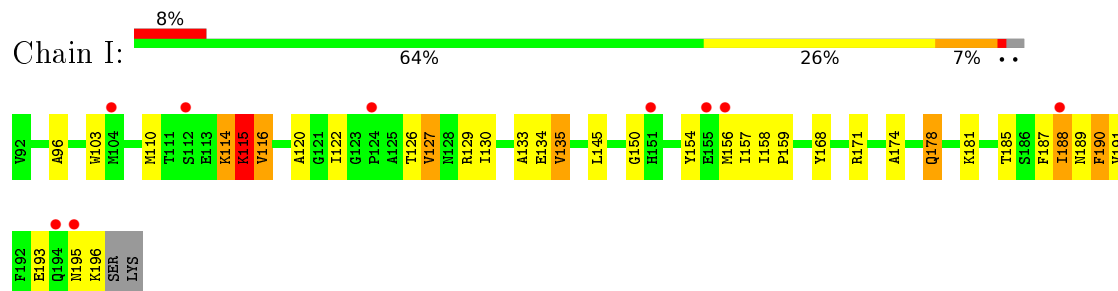
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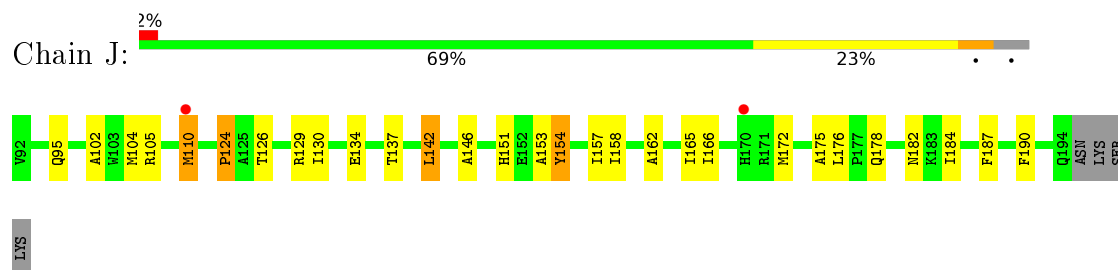
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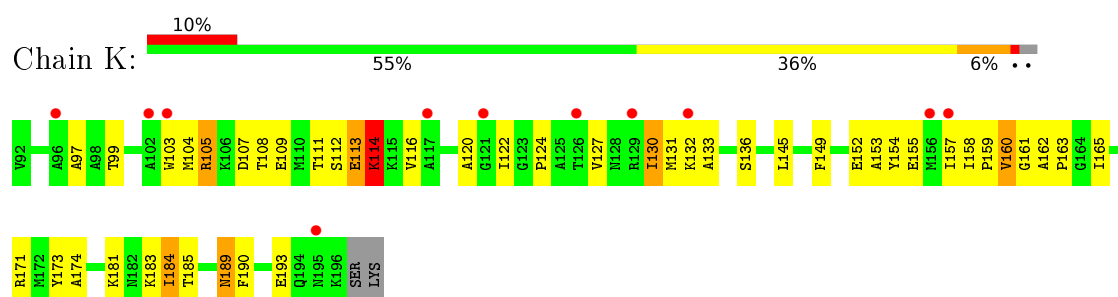
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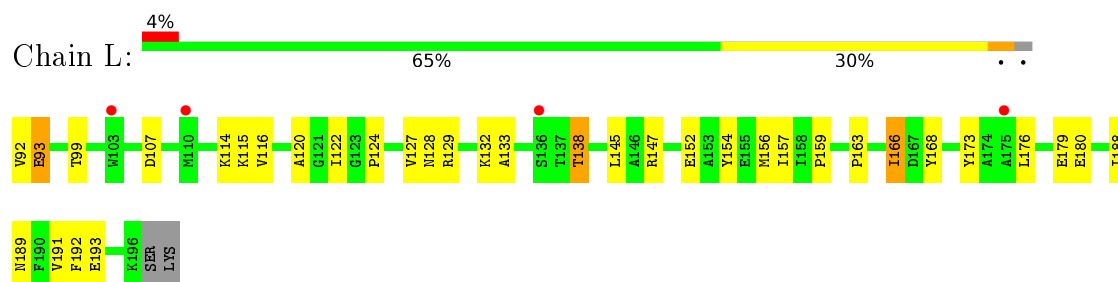
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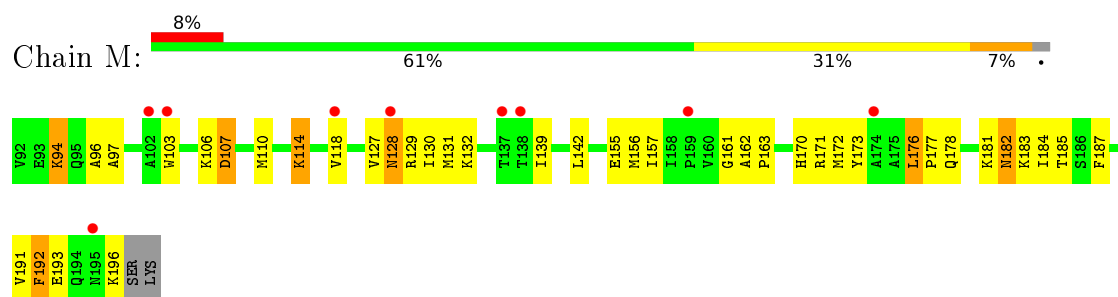
- Molecule 1: Repressor



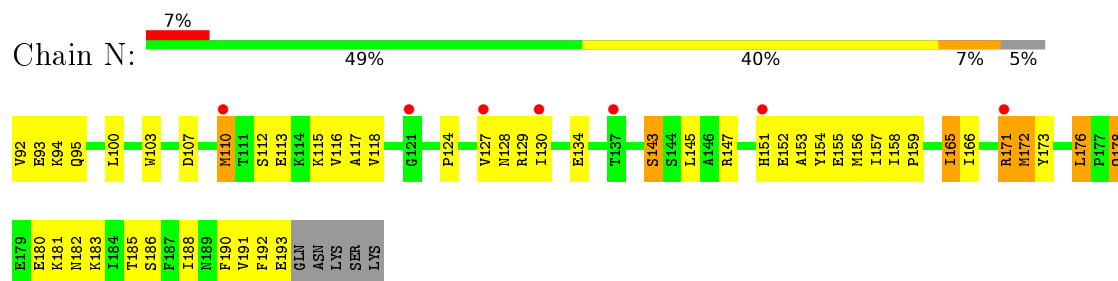
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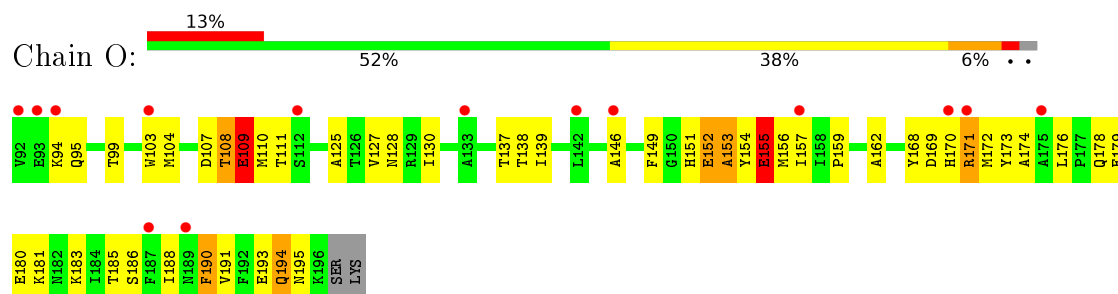
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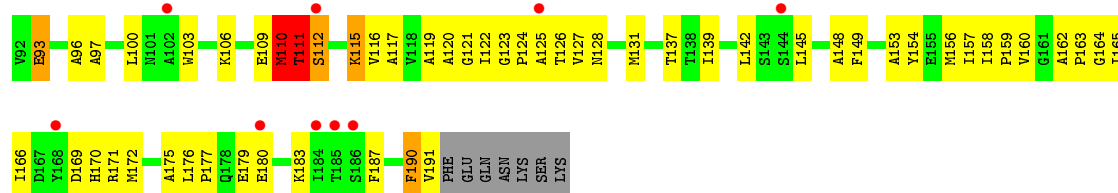
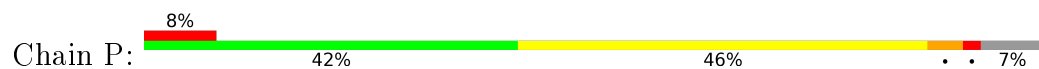
• Molecule 1: Repressor



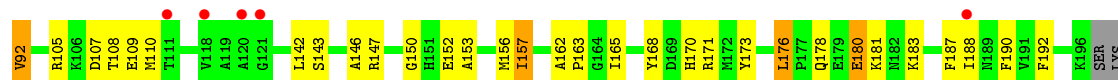
• Molecule 1: Repressor



• Molecule 1: Repressor



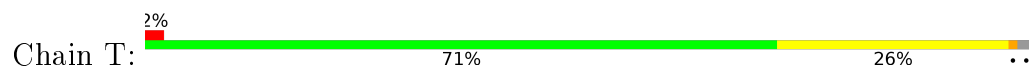
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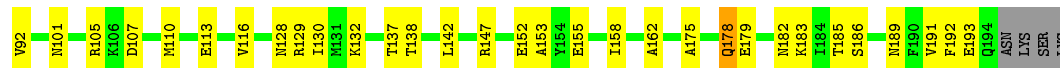
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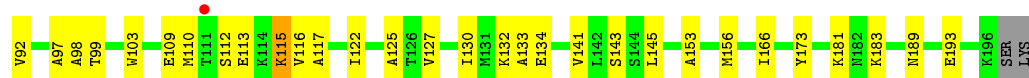
• Molecule 1: Repressor



• Molecule 1: Repressor



• Molecule 1: Repressor

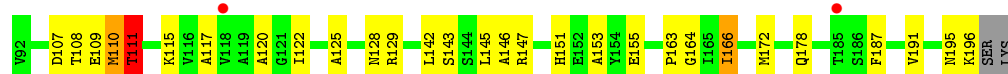


• Molecule 1: Repressor





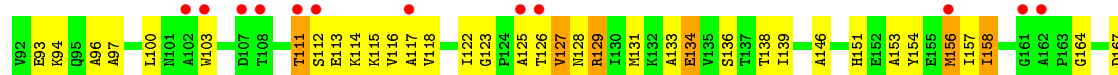
• Molecule 1: Repressor



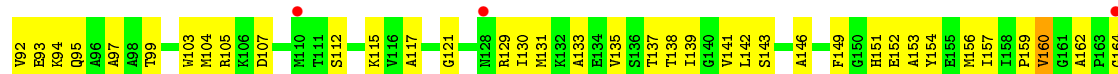
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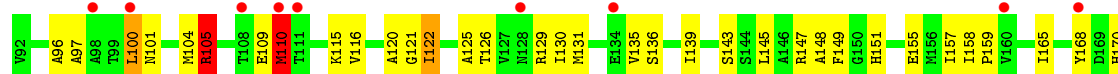
• Molecule 1: Repressor



• Molecule 1: Repressor

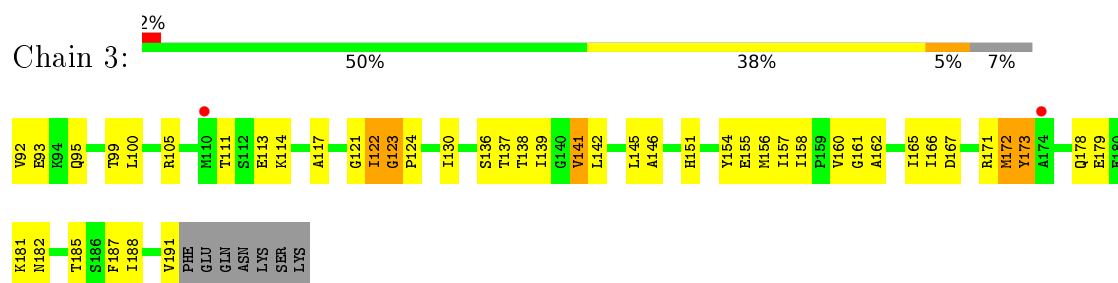


• Molecule 1: Repressor

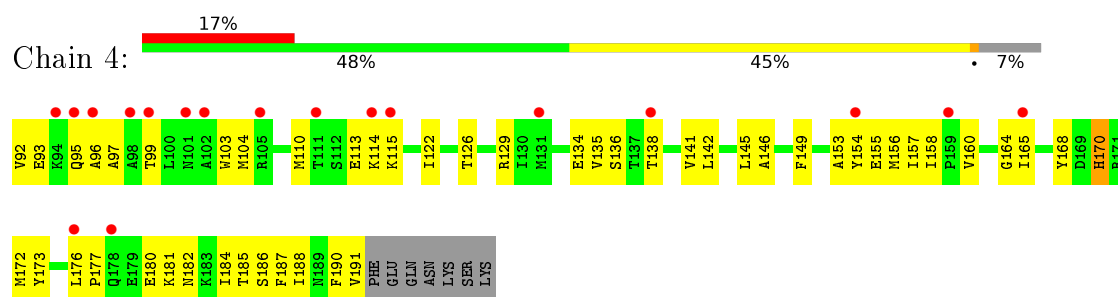


• Molecule 1: Repressor

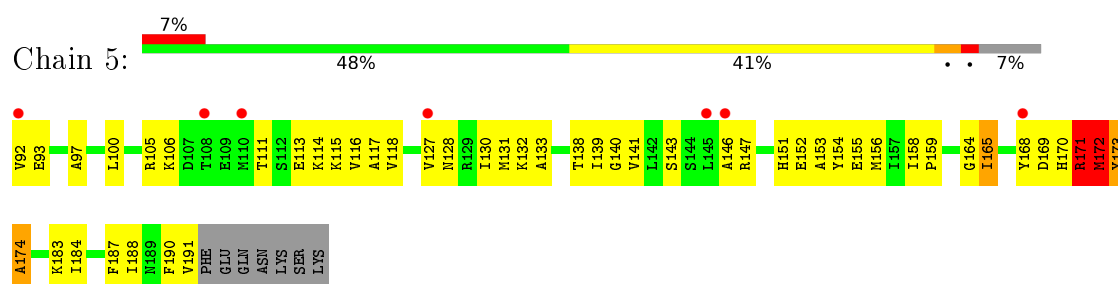




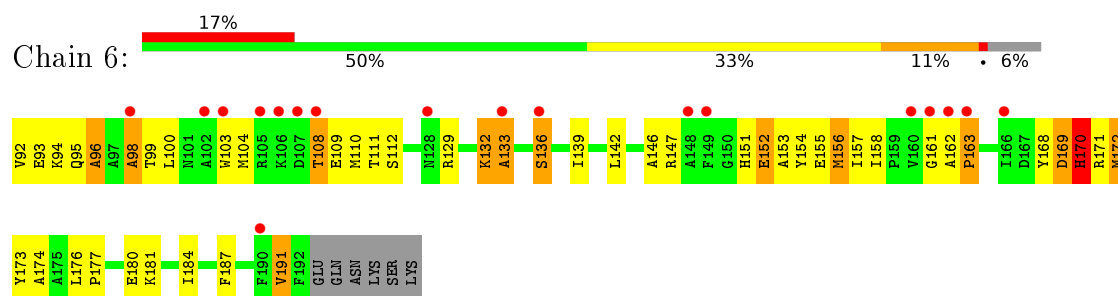
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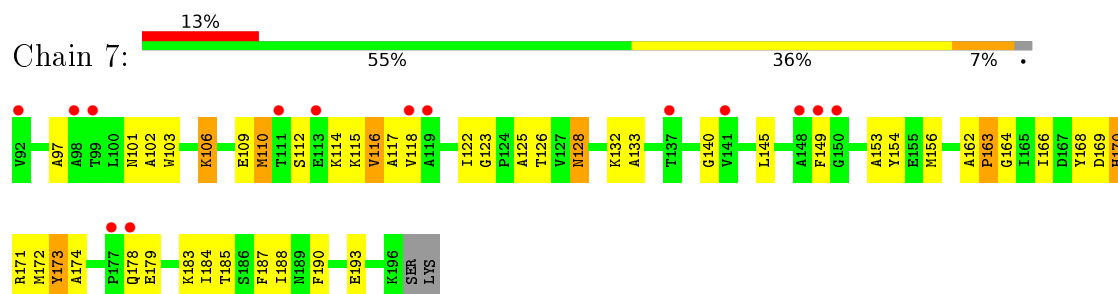
• Molecule 1: Repressor



• Molecule 1: Repressor



• Molecule 1: Repressor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.60 Å 62.50 Å 267.90 Å 89.99° 89.97° 72.70°	Depositor
Resolution (Å)	49.13 – 2.98 49.13 – 2.98	Depositor EDS
% Data completeness (in resolution range)	97.5 (49.13-2.98) 98.8 (49.13-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 2.96 Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.216 , 0.273 0.228 , 0.279	Depositor DCC
R_{free} test set	3856 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	70.5	Xtriage
Anisotropy	0.028	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 97.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	0.069 for -h,-k,l 0.001 for k,h,-l 0.002 for -k,-h,-l	Xtriage
Reported twinning fraction	0.509 for H, K, L 0.491 for -H, -K, L	Depositor
Outliers	0 of 76987 reflections	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	25962	wwPDB-VP
Average B, all atoms (Å ²)	77.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.46% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.38	0/822	0.61	0/1110
1	2	0.35	0/787	0.63	0/1064
1	3	0.34	0/775	0.62	0/1048
1	4	0.34	0/775	0.63	0/1048
1	5	0.37	0/775	0.62	0/1048
1	6	0.40	0/787	0.69	0/1064
1	7	0.42	0/822	0.73	0/1110
1	A	0.35	0/822	0.58	0/1110
1	B	0.38	0/822	0.59	0/1110
1	C	0.37	0/822	0.59	0/1110
1	D	0.38	0/787	0.60	0/1064
1	E	0.34	0/822	0.55	0/1110
1	F	0.38	0/822	0.58	0/1110
1	G	0.36	0/822	0.64	0/1110
1	H	0.40	0/796	0.61	0/1076
1	I	0.35	0/822	0.62	0/1110
1	J	0.35	0/805	0.56	0/1088
1	K	0.38	0/822	0.65	0/1110
1	L	0.36	0/822	0.65	0/1110
1	M	0.39	0/822	0.66	0/1110
1	N	0.38	0/796	0.64	0/1076
1	O	0.35	0/822	0.62	0/1110
1	P	0.39	0/775	0.65	0/1048
1	Q	0.37	0/822	0.57	0/1110
1	R	0.37	0/822	0.58	0/1110
1	T	0.35	0/822	0.62	0/1110
1	U	0.38	0/805	0.59	0/1088
1	V	0.37	0/822	0.59	0/1110
1	W	0.39	0/822	0.63	1/1110 (0.1%)
1	X	0.38	0/822	0.63	0/1110
1	Y	0.38	0/822	0.62	0/1110
1	Z	0.38	0/775	0.70	0/1048
All	All	0.37	0/25878	0.62	1/34960 (0.0%)

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	2	0	2
1	5	0	1
1	6	0	2
1	7	0	1
1	O	0	1
All	All	0	7

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	W	105	ARG	NE-CZ-NH1	5.57	123.08	120.30

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	2	105	ARG	Peptide
1	2	183	LYS	Peptide
1	5	171	ARG	Peptide
1	6	110	MET	Peptide
1	O	155	GLU	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	1	808	0	817	47	0
1	2	773	0	784	43	0
1	3	762	0	775	52	0
1	4	762	0	775	47	0
1	5	762	0	775	64	0
1	6	773	0	784	75	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	7	808	0	817	56	0
1	A	808	0	817	20	0
1	B	808	0	817	27	0
1	C	808	0	817	33	0
1	D	773	0	784	20	0
1	E	808	0	817	30	0
1	F	808	0	817	38	0
1	G	808	0	817	47	0
1	H	782	0	790	37	0
1	I	808	0	817	39	1
1	J	791	0	798	25	0
1	K	808	0	817	41	0
1	L	808	0	817	28	1
1	M	808	0	817	43	0
1	N	782	0	790	59	0
1	O	808	0	817	50	0
1	P	762	0	775	68	0
1	Q	808	0	817	35	0
1	R	808	0	817	24	1
1	T	808	0	817	22	0
1	U	791	0	798	24	0
1	V	808	0	817	32	0
1	W	808	0	817	37	0
1	X	808	0	817	28	0
1	Y	808	0	817	34	1
1	Z	762	0	775	53	0
2	1	8	0	0	3	0
2	2	7	0	0	0	0
2	3	18	0	0	2	0
2	4	6	0	0	0	0
2	5	14	0	0	2	0
2	6	3	0	0	0	0
2	7	9	0	0	2	0
2	A	21	0	0	4	0
2	B	24	0	0	4	0
2	C	25	0	0	4	0
2	D	39	0	0	2	0
2	E	21	0	0	2	0
2	F	30	0	0	3	0
2	G	19	0	0	4	0
2	H	26	0	0	1	0
2	I	3	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	J	10	0	0	0	0
2	K	5	0	0	0	0
2	L	17	0	0	2	0
2	M	5	0	0	1	0
2	N	13	0	0	5	0
2	O	3	0	0	1	0
2	P	8	0	0	3	0
2	Q	18	0	0	2	0
2	R	33	0	0	2	0
2	T	32	0	0	4	0
2	U	27	0	0	2	0
2	V	16	0	0	2	0
2	W	27	0	0	4	0
2	X	19	0	0	3	0
2	Y	17	0	0	5	0
2	Z	4	0	0	2	0
All	All	25962	0	25743	1083	2

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 21.

The worst 5 of 1083 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:P:111:THR:O	1:P:115:LYS:HE2	1.42	1.18
1:P:109:GLU:CD	1:P:115:LYS:HZ2	1.54	1.09
1:P:111:THR:O	1:P:115:LYS:CE	2.00	1.09
1:6:94:LYS:HD3	1:6:132:LYS:O	1.53	1.09
1:M:114:LYS:NZ	2:M:201:HOH:O	1.89	1.06

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:167:ASP:OD1	1:Y:111:THR:O[1_465]	2.04	0.16
1:I:133:ALA:O	1:L:147:ARG:NH1[1_455]	2.12	0.08

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	1	103/107 (96%)	92 (89%)	9 (9%)	2 (2%)	10	41
1	2	99/107 (92%)	85 (86%)	13 (13%)	1 (1%)	19	60
1	3	98/107 (92%)	88 (90%)	6 (6%)	4 (4%)	3	18
1	4	98/107 (92%)	81 (83%)	15 (15%)	2 (2%)	9	39
1	5	98/107 (92%)	85 (87%)	10 (10%)	3 (3%)	5	26
1	6	99/107 (92%)	73 (74%)	17 (17%)	9 (9%)	1	4
1	7	103/107 (96%)	79 (77%)	19 (18%)	5 (5%)	3	15
1	A	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
1	B	103/107 (96%)	95 (92%)	7 (7%)	1 (1%)	19	60
1	C	103/107 (96%)	95 (92%)	7 (7%)	1 (1%)	19	60
1	D	99/107 (92%)	93 (94%)	6 (6%)	0	100	100
1	E	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
1	F	103/107 (96%)	101 (98%)	2 (2%)	0	100	100
1	G	103/107 (96%)	96 (93%)	7 (7%)	0	100	100
1	H	100/107 (94%)	94 (94%)	4 (4%)	2 (2%)	9	39
1	I	103/107 (96%)	87 (84%)	11 (11%)	5 (5%)	3	15
1	J	101/107 (94%)	89 (88%)	11 (11%)	1 (1%)	19	60
1	K	103/107 (96%)	84 (82%)	13 (13%)	6 (6%)	2	11
1	L	103/107 (96%)	90 (87%)	11 (11%)	2 (2%)	10	41
1	M	103/107 (96%)	80 (78%)	21 (20%)	2 (2%)	10	41
1	N	100/107 (94%)	85 (85%)	11 (11%)	4 (4%)	4	19
1	O	103/107 (96%)	86 (84%)	13 (13%)	4 (4%)	4	20
1	P	98/107 (92%)	82 (84%)	10 (10%)	6 (6%)	2	9
1	Q	103/107 (96%)	98 (95%)	5 (5%)	0	100	100
1	R	103/107 (96%)	99 (96%)	3 (3%)	1 (1%)	19	60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	T	103/107 (96%)	97 (94%)	5 (5%)	1 (1%)	19	60
1	U	101/107 (94%)	98 (97%)	3 (3%)	0	100	100
1	V	103/107 (96%)	97 (94%)	6 (6%)	0	100	100
1	W	103/107 (96%)	100 (97%)	3 (3%)	0	100	100
1	X	103/107 (96%)	96 (93%)	6 (6%)	1 (1%)	19	60
1	Y	103/107 (96%)	90 (87%)	12 (12%)	1 (1%)	19	60
1	Z	98/107 (92%)	82 (84%)	13 (13%)	3 (3%)	5	26
All	All	3249/3424 (95%)	2893 (89%)	289 (9%)	67 (2%)	9	38

5 of 67 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	I	115	LYS
1	I	190	PHE
1	N	110	MET
1	N	165	ILE
1	P	112	SER

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	1	84/86 (98%)	82 (98%)	2 (2%)	57	86
1	2	80/86 (93%)	75 (94%)	5 (6%)	22	58
1	3	79/86 (92%)	76 (96%)	3 (4%)	40	77
1	4	79/86 (92%)	75 (95%)	4 (5%)	29	67
1	5	79/86 (92%)	75 (95%)	4 (5%)	29	67
1	6	80/86 (93%)	73 (91%)	7 (9%)	12	41
1	7	84/86 (98%)	80 (95%)	4 (5%)	31	70
1	A	84/86 (98%)	81 (96%)	3 (4%)	42	78
1	B	84/86 (98%)	80 (95%)	4 (5%)	31	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	84/86 (98%)	77 (92%)	7 (8%)	14	44
1	D	80/86 (93%)	78 (98%)	2 (2%)	55	85
1	E	84/86 (98%)	82 (98%)	2 (2%)	57	86
1	F	84/86 (98%)	84 (100%)	0	100	100
1	G	84/86 (98%)	79 (94%)	5 (6%)	24	61
1	H	81/86 (94%)	79 (98%)	2 (2%)	55	85
1	I	84/86 (98%)	80 (95%)	4 (5%)	31	70
1	J	82/86 (95%)	77 (94%)	5 (6%)	23	60
1	K	84/86 (98%)	79 (94%)	5 (6%)	24	61
1	L	84/86 (98%)	78 (93%)	6 (7%)	18	53
1	M	84/86 (98%)	75 (89%)	9 (11%)	8	29
1	N	81/86 (94%)	76 (94%)	5 (6%)	23	59
1	O	84/86 (98%)	76 (90%)	8 (10%)	11	36
1	P	79/86 (92%)	75 (95%)	4 (5%)	29	67
1	Q	84/86 (98%)	80 (95%)	4 (5%)	31	70
1	R	84/86 (98%)	82 (98%)	2 (2%)	57	86
1	T	84/86 (98%)	81 (96%)	3 (4%)	42	78
1	U	82/86 (95%)	80 (98%)	2 (2%)	57	86
1	V	84/86 (98%)	83 (99%)	1 (1%)	78	93
1	W	84/86 (98%)	82 (98%)	2 (2%)	57	86
1	X	84/86 (98%)	78 (93%)	6 (7%)	18	53
1	Y	84/86 (98%)	82 (98%)	2 (2%)	57	86
1	Z	79/86 (92%)	71 (90%)	8 (10%)	9	33
All	All	2641/2752 (96%)	2511 (95%)	130 (5%)	31	69

5 of 130 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	N	178	GLN
1	Q	157	ILE
1	6	132	LYS
1	O	109	GLU
1	O	194	GLN

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	R	194	GLN
1	U	182	ASN
1	6	170	HIS
1	T	195	ASN
1	W	101	ASN

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](#)

There are no ligands in this entry.

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 [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, 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	1	105/107 (98%)	0.13	3 (2%) 55 33	47, 87, 110, 116	0
1	2	101/107 (94%)	0.48	10 (9%) 9 5	61, 99, 133, 140	0
1	3	100/107 (93%)	0.20	2 (2%) 68 46	41, 83, 111, 139	0
1	4	100/107 (93%)	0.67	18 (18%) 2 1	64, 100, 138, 150	0
1	5	100/107 (93%)	0.41	7 (7%) 19 9	54, 94, 122, 139	0
1	6	101/107 (94%)	0.93	18 (17%) 2 1	55, 111, 136, 154	0
1	7	105/107 (98%)	0.54	14 (13%) 4 2	63, 99, 124, 129	0
1	A	105/107 (98%)	-0.06	2 (1%) 70 48	33, 64, 96, 105	0
1	B	105/107 (98%)	-0.00	1 (0%) 84 66	31, 54, 87, 99	0
1	C	105/107 (98%)	-0.08	2 (1%) 70 48	34, 60, 92, 117	0
1	D	101/107 (94%)	-0.19	0 100 100	33, 49, 69, 79	0
1	E	105/107 (98%)	-0.16	0 100 100	37, 60, 84, 102	0
1	F	105/107 (98%)	-0.26	2 (1%) 70 48	24, 46, 72, 83	0
1	G	105/107 (98%)	-0.17	1 (0%) 84 66	35, 63, 116, 127	0
1	H	102/107 (95%)	-0.19	1 (0%) 84 66	30, 52, 76, 85	0
1	I	105/107 (98%)	0.52	9 (8%) 13 6	60, 100, 126, 137	0
1	J	103/107 (96%)	0.13	2 (1%) 70 48	62, 89, 121, 134	0
1	K	105/107 (98%)	0.49	11 (10%) 8 4	69, 105, 132, 158	0
1	L	105/107 (98%)	0.31	4 (3%) 44 25	61, 85, 115, 118	0
1	M	105/107 (98%)	0.53	9 (8%) 13 6	75, 105, 142, 168	0
1	N	102/107 (95%)	0.37	7 (6%) 20 9	52, 92, 119, 125	0
1	O	105/107 (98%)	0.62	14 (13%) 4 2	66, 106, 123, 131	0
1	P	100/107 (93%)	0.38	9 (9%) 12 6	59, 91, 120, 133	0
1	Q	105/107 (98%)	0.06	5 (4%) 34 19	34, 64, 94, 104	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	R	105/107 (98%)	-0.03	1 (0%) 84 66	32, 53, 80, 106	0
1	T	105/107 (98%)	0.02	2 (1%) 70 48	41, 58, 100, 118	0
1	U	103/107 (96%)	-0.25	0 100 100	29, 42, 64, 74	0
1	V	105/107 (98%)	-0.07	1 (0%) 84 66	40, 65, 89, 110	0
1	W	105/107 (98%)	-0.19	2 (1%) 70 48	27, 45, 80, 97	0
1	X	105/107 (98%)	-0.10	2 (1%) 70 48	38, 68, 111, 117	0
1	Y	105/107 (98%)	-0.05	3 (2%) 55 33	32, 58, 95, 128	0
1	Z	100/107 (93%)	0.56	14 (14%) 4 2	64, 104, 132, 140	0
All	All	3313/3424 (96%)	0.17	176 (5%) 30 16	24, 77, 122, 168	0

The worst 5 of 176 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	4	102	ALA	7.7
1	K	117	ALA	7.1
1	O	92	VAL	6.4
1	M	195	ASN	6.0
1	6	160	VAL	5.5

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.