



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 12:53 pm BST

PDB ID : 3ZQL
Title : DNA-bound form of TetR-like repressor SimR
Authors : Le, T.B.K.; Schumacher, M.A.; Lawson, D.M.; Brennan, R.G.; Buttner, M.J.
Deposited on : 2011-06-10
Resolution : 2.99 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

<https://www.wwpdb.org/validation/2017/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
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

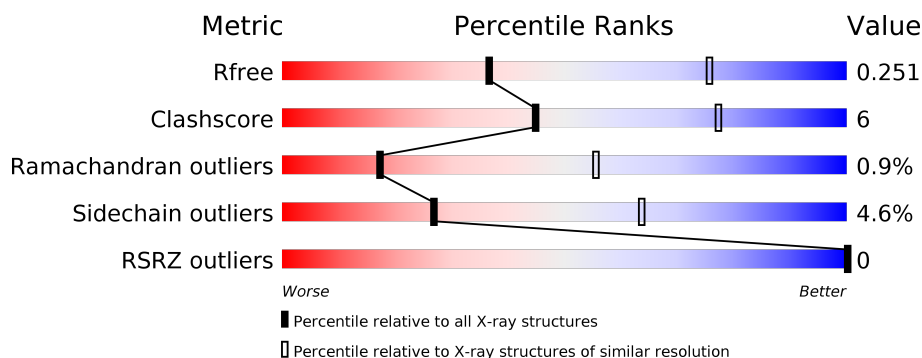
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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 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	267	<div> <div style="width: 72%;"></div> <div style="width: 15%;"></div> <div style="width: 12%;"></div> </div>
1	B	267	<div> <div style="width: 72%;"></div> <div style="width: 12%;"></div> <div style="width: 15%;"></div> </div>
1	C	267	<div> <div style="width: 73%;"></div> <div style="width: 13%;"></div> <div style="width: 12%;"></div> </div>
1	D	267	<div> <div style="width: 71%;"></div> <div style="width: 11%;"></div> <div style="width: 15%;"></div> </div>
2	E	17	<div> <div style="width: 71%;"></div> <div style="width: 29%;"></div> </div>
2	G	17	<div> <div style="width: 59%;"></div> <div style="width: 41%;"></div> </div>

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Mol	Chain	Length	Quality of chain
3	F	17	 71% 29%
3	H	17	 65% 35%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 8543 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 PUTATIVE REPRESSOR SIMREG2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	236	Total	C	N	O	S	0	0	0
			1823	1156	321	338	8			
1	B	226	Total	C	N	O	S	0	0	0
			1765	1124	304	329	8			
1	C	236	Total	C	N	O	S	0	0	0
			1825	1157	323	337	8			
1	D	226	Total	C	N	O	S	0	0	0
			1748	1117	297	326	8			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	260	LEU	-	expression tag	UNP Q9AMH9
A	261	GLU	-	expression tag	UNP Q9AMH9
A	262	HIS	-	expression tag	UNP Q9AMH9
A	263	HIS	-	expression tag	UNP Q9AMH9
A	264	HIS	-	expression tag	UNP Q9AMH9
A	265	HIS	-	expression tag	UNP Q9AMH9
A	266	HIS	-	expression tag	UNP Q9AMH9
A	267	HIS	-	expression tag	UNP Q9AMH9
B	260	LEU	-	expression tag	UNP Q9AMH9
B	261	GLU	-	expression tag	UNP Q9AMH9
B	262	HIS	-	expression tag	UNP Q9AMH9
B	263	HIS	-	expression tag	UNP Q9AMH9
B	264	HIS	-	expression tag	UNP Q9AMH9
B	265	HIS	-	expression tag	UNP Q9AMH9
B	266	HIS	-	expression tag	UNP Q9AMH9
B	267	HIS	-	expression tag	UNP Q9AMH9
C	260	LEU	-	expression tag	UNP Q9AMH9
C	261	GLU	-	expression tag	UNP Q9AMH9
C	262	HIS	-	expression tag	UNP Q9AMH9
C	263	HIS	-	expression tag	UNP Q9AMH9
C	264	HIS	-	expression tag	UNP Q9AMH9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	265	HIS	-	expression tag	UNP Q9AMH9
C	266	HIS	-	expression tag	UNP Q9AMH9
C	267	HIS	-	expression tag	UNP Q9AMH9
D	260	LEU	-	expression tag	UNP Q9AMH9
D	261	GLU	-	expression tag	UNP Q9AMH9
D	262	HIS	-	expression tag	UNP Q9AMH9
D	263	HIS	-	expression tag	UNP Q9AMH9
D	264	HIS	-	expression tag	UNP Q9AMH9
D	265	HIS	-	expression tag	UNP Q9AMH9
D	266	HIS	-	expression tag	UNP Q9AMH9
D	267	HIS	-	expression tag	UNP Q9AMH9

- Molecule 2 is a DNA chain called 5'-D(*DTP*TP*CP*GP*TP*AP*CP*GP*CP*CP*GP*TP*AP*DCP *GP*AP*A)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	17	Total	C	N	O	P	0	0	0
			344	165	63	100	16			
2	G	17	Total	C	N	O	P	0	0	0
			344	165	63	100	16			

- Molecule 3 is a DNA chain called 5'-D(*DTP*TP*CP*GP*TP*AP*CP*GP*GP*CP*GP*TP*AP*DCP *GP*AP*A)-3'.

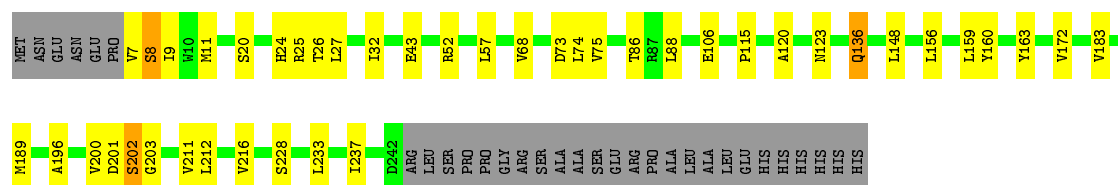
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	17	Total	C	N	O	P	0	0	0
			347	166	65	100	16			
3	H	17	Total	C	N	O	P	0	0	0
			347	166	65	100	16			

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.

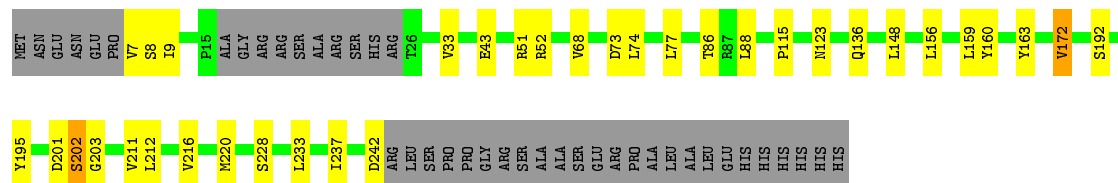
• Molecule 1: PUTATIVE REPRESSOR SIMREG2

Chain A: 



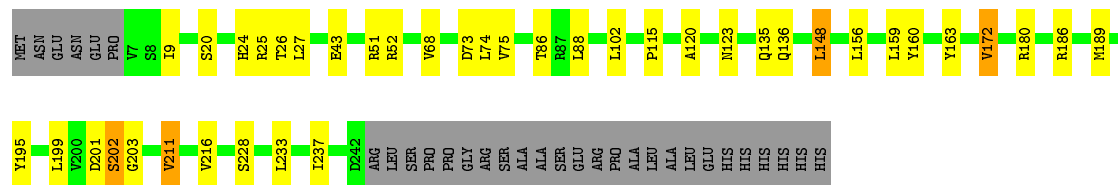
• Molecule 1: PUTATIVE REPRESSOR SIMREG2

Chain B: 



• Molecule 1: PUTATIVE REPRESSOR SIMREG2

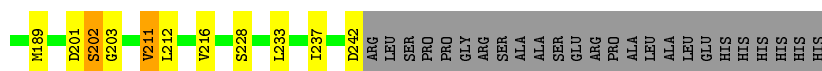
Chain C: 



• Molecule 1: PUTATIVE REPRESSOR SIMREG2

Chain D: 

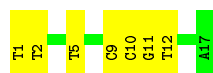




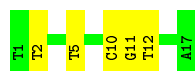
- Molecule 2: 5'-D(*DTP*TP*CP*GP*TP*AP*CP*GP*CP*CP*GP*TP*AP*DCP*GP*AP*A)-3'



- Molecule 2: 5'-D(*DTP*TP*CP*GP*TP*AP*CP*GP*CP*CP*GP*TP*AP*DCP*GP*AP*A)-3'



- Molecule 3: 5'-D(*DTP*TP*CP*GP*TP*AP*CP*GP*GP*CP*GP*TP*AP*DCP*GP*AP*A)-3'



- Molecule 3: 5'-D(*DTP*TP*CP*GP*TP*AP*CP*GP*GP*CP*GP*TP*AP*DCP*GP*AP*A)-3'



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.79Å 112.61Å 163.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	92.78 – 2.99 92.78 – 2.99	Depositor EDS
% Data completeness (in resolution range)	94.3 (92.78-2.99) 94.3 (92.78-2.99)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0110	Depositor
R, R_{free}	0.210 , 0.251 0.212 , 0.251	Depositor DCC
R_{free} test set	1577 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	52.7	Xtriage
Anisotropy	0.890	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 15.5	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	0.94	EDS
Total number of atoms	8543	wwPDB-VP
Average B, all atoms (Å ²)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.51% 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](#)

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	0.53	0/1867	0.61	0/2546
1	B	0.55	0/1808	0.61	0/2465
1	C	0.52	0/1868	0.62	0/2546
1	D	0.53	0/1791	0.58	0/2444
2	E	1.17	4/385 (1.0%)	1.40	7/592 (1.2%)
2	G	1.24	5/385 (1.3%)	1.42	8/592 (1.4%)
3	F	1.20	3/389 (0.8%)	1.41	8/599 (1.3%)
3	H	1.23	5/389 (1.3%)	1.35	9/599 (1.5%)
All	All	0.70	17/8882 (0.2%)	0.82	32/12383 (0.3%)

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	DT	P-OP2	8.24	1.62	1.49
2	G	5	DT	P-OP2	8.23	1.62	1.49
3	H	5	DT	P-OP2	8.06	1.62	1.49
3	F	5	DT	P-OP2	7.98	1.62	1.49
2	G	2	DT	P-OP2	7.82	1.62	1.49

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	12	DT	C5-C4-O4	-7.67	119.53	124.90
2	G	5	DT	N3-C2-O2	-7.56	117.77	122.30
2	G	2	DT	N3-C4-O4	7.21	124.22	119.90
3	F	12	DT	N3-C4-O4	7.04	124.12	119.90
2	G	12	DT	C1'-O4'-C4'	-6.97	103.13	110.10

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	1823	0	1749	33	0
1	B	1765	0	1701	25	0
1	C	1825	0	1759	24	0
1	D	1748	0	1675	27	0
2	E	344	0	193	1	0
2	G	344	0	193	3	0
3	F	347	0	193	2	0
3	H	347	0	193	2	0
All	All	8543	0	7656	105	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 6.

The worst 5 of 105 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:A:159:LEU:HG	1:A:233:LEU:HD11	1.61	0.81
1:B:159:LEU:HG	1:B:233:LEU:HD11	1.62	0.81
1:D:9:ILE:HD13	1:D:73:ASP:HB3	1.61	0.81
1:D:159:LEU:HG	1:D:233:LEU:HD11	1.60	0.81
1:C:159:LEU:HG	1:C:233:LEU:HD11	1.63	0.80

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	234/267 (88%)	225 (96%)	6 (3%)	3 (1%)	12	45
1	B	222/267 (83%)	216 (97%)	5 (2%)	1 (0%)	29	68
1	C	234/267 (88%)	223 (95%)	8 (3%)	3 (1%)	12	45
1	D	222/267 (83%)	216 (97%)	5 (2%)	1 (0%)	29	68
All	All	912/1068 (85%)	880 (96%)	24 (3%)	8 (1%)	17	55

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	THR
1	C	26	THR
1	B	202	SER
1	C	202	SER
1	D	202	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	A	182/221 (82%)	176 (97%)	6 (3%)	38	73
1	B	180/221 (81%)	172 (96%)	8 (4%)	28	65
1	C	182/221 (82%)	173 (95%)	9 (5%)	25	61
1	D	176/221 (80%)	166 (94%)	10 (6%)	20	56
All	All	720/884 (81%)	687 (95%)	33 (5%)	27	64

5 of 33 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	SER
1	C	148	LEU
1	D	211	VAL
1	C	123	ASN
1	C	135	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	224	GLN
1	D	136	GLN
1	C	136	GLN
1	B	136	GLN
1	D	123	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 ⓘ

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	236/267 (88%)	-0.00	0 100 100	41, 55, 75, 94	0
1	B	226/267 (84%)	-0.06	0 100 100	39, 54, 76, 101	0
1	C	236/267 (88%)	-0.07	0 100 100	38, 56, 73, 89	0
1	D	226/267 (84%)	0.08	0 100 100	36, 59, 89, 111	0
2	E	17/17 (100%)	-0.63	0 100 100	42, 54, 63, 63	0
2	G	17/17 (100%)	-0.60	0 100 100	46, 55, 65, 65	0
3	F	17/17 (100%)	-0.55	0 100 100	43, 52, 65, 67	0
3	H	17/17 (100%)	-0.57	0 100 100	46, 52, 65, 66	0
All	All	992/1136 (87%)	-0.05	0 100 100	36, 56, 79, 111	0

There are no RSRZ outliers to report.

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.