



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 9DT4 / pdb\_00009dt4  
Title : Crystal structure of the engineered sulfonylurea repressor CsR (L4.2-20), apo form  
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Deposited on : 2024-09-30  
Resolution : 2.40 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0  
Xtriage (Phenix) : 2.0  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.010 (Gargrove)  
Density-Fitness : 1.0.12  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.46

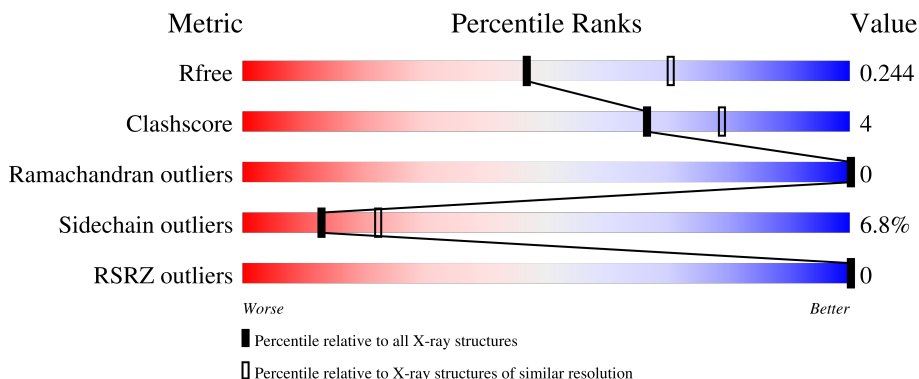
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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))
$R_{free}$	164625	4642 (2.40-2.40)
Clashscore	180529	5218 (2.40-2.40)
Ramachandran outliers	177936	5158 (2.40-2.40)
Sidechain outliers	177891	5159 (2.40-2.40)
RSRZ outliers	164620	4642 (2.40-2.40)

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 of 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	207	
1	B	207	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 3218 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 Sulfonylurea repressor CsR (L4.2-20).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1596	1016	279	297	4			
1	B	200	Total	C	N	O	S	0	0	0
			1605	1022	281	298	4			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	ALA	SER	conflict	UNP P04483
A	60	HIS	LEU	conflict	UNP P04483
A	64	GLN	HIS	conflict	UNP P04483
A	67	TYR	PHE	conflict	UNP P04483
A	68	LEU	CYS	conflict	UNP P04483
A	82	PHE	ASN	conflict	UNP P04483
A	86	MET	PHE	conflict	UNP P04483
A	88	LEU	CYS	conflict	UNP P04483
A	100	SER	HIS	conflict	UNP P04483
A	105	TRP	PRO	conflict	UNP P04483
A	108	GLN	LYS	conflict	UNP P04483
A	113	ALA	LEU	conflict	UNP P04483
A	116	MET	GLN	conflict	UNP P04483
A	121	THR	CYS	conflict	UNP P04483
A	134	THR	LEU	conflict	UNP P04483
A	135	ASP	SER	conflict	UNP P04483
A	138	ARG	GLY	conflict	UNP P04483
A	139	VAL	HIS	conflict	UNP P04483
A	144	ALA	CYS	conflict	UNP P04483
A	147	LEU	GLU	conflict	UNP P04483
A	151	GLN	HIS	conflict	UNP P04483
A	163	PRO	THR	conflict	UNP P04483
A	174	TRP	ILE	conflict	UNP P04483
A	177	LYS	PHE	conflict	UNP P04483
A	178	VAL	ASP	conflict	UNP P04483

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Chain	Residue	Modelled	Actual	Comment	Reference
A	195	ALA	CYS	conflict	UNP P04483
A	203	ARG	CYS	conflict	UNP P04483
B	2	ALA	SER	conflict	UNP P04483
B	60	HIS	LEU	conflict	UNP P04483
B	64	GLN	HIS	conflict	UNP P04483
B	67	TYR	PHE	conflict	UNP P04483
B	68	LEU	CYS	conflict	UNP P04483
B	82	PHE	ASN	conflict	UNP P04483
B	86	MET	PHE	conflict	UNP P04483
B	88	LEU	CYS	conflict	UNP P04483
B	100	SER	HIS	conflict	UNP P04483
B	105	TRP	PRO	conflict	UNP P04483
B	108	GLN	LYS	conflict	UNP P04483
B	113	ALA	LEU	conflict	UNP P04483
B	116	MET	GLN	conflict	UNP P04483
B	121	THR	CYS	conflict	UNP P04483
B	134	THR	LEU	conflict	UNP P04483
B	135	ASP	SER	conflict	UNP P04483
B	138	ARG	GLY	conflict	UNP P04483
B	139	VAL	HIS	conflict	UNP P04483
B	144	ALA	CYS	conflict	UNP P04483
B	147	LEU	GLU	conflict	UNP P04483
B	151	GLN	HIS	conflict	UNP P04483
B	163	PRO	THR	conflict	UNP P04483
B	174	TRP	ILE	conflict	UNP P04483
B	177	LYS	PHE	conflict	UNP P04483
B	178	VAL	ASP	conflict	UNP P04483
B	195	ALA	CYS	conflict	UNP P04483
B	203	ARG	CYS	conflict	UNP P04483

- Molecule 2 is water.

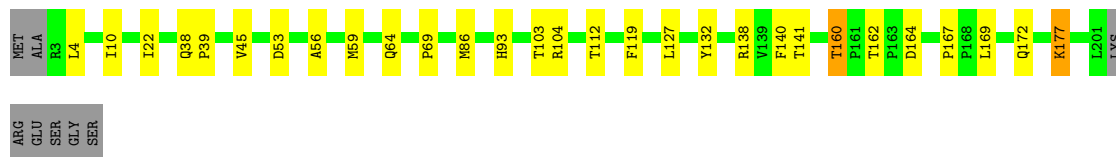
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	8	Total O 8 8	0	0
2	B	9	Total O 9 9	0	0

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

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: Sulfonylurea repressor CsR (L4.2-20)

Chain A:  82% 13% . .



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	37.12Å 56.84Å 106.01Å 90.00° 90.32° 90.00°	Depositor
Resolution (Å)	19.87 – 2.40 19.87 – 2.40	Depositor EDS
% Data completeness (in resolution range)	94.4 (19.87-2.40) 94.4 (19.87-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, $R_{free}$	0.178 , 0.241 0.185 , 0.244	Depositor DCC
$R_{free}$ test set	840 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.7	Xtriage
Anisotropy	0.191	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 29.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.044 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	3218	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.74% 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

### 5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.65	0/1627	1.20	6/2202 (0.3%)
1	B	0.65	0/1636	1.27	5/2213 (0.2%)
All	All	0.65	0/3263	1.24	11/4415 (0.2%)

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	B	0	2

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	134	THR	CA-CB-OG1	-6.98	99.13	109.60
1	A	112	THR	CA-CB-OG1	-5.91	100.73	109.60
1	B	172	GLN	CB-CA-C	-5.49	100.47	110.63
1	A	140	PHE	CA-CB-CG	-5.48	108.32	113.80
1	A	177	LYS	CB-CA-C	5.44	119.50	110.90

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	138	ARG	Sidechain
1	B	158	ARG	Sidechain

## 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	1596	0	1605	15	0
1	B	1605	0	1618	16	0
2	A	8	0	0	0	0
2	B	9	0	0	0	0
All	All	3218	0	3223	23	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 4.

The worst 5 of 23 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:132:TYR:OH	1:B:180:GLN:NE2	1.88	1.05
1:A:86:MET:HE1	1:A:138:ARG:HA	1.67	0.76
1:B:23:GLU:H	1:B:23:GLU:CD	2.00	0.69
1:A:132:TYR:HH	1:B:180:GLN:HE22	1.33	0.66
1:A:167:PRO:CG	1:B:114:GLU:HG3	2.34	0.58

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	197/207 (95%)	196 (100%)	1 (0%)	0	100	100
1	B	198/207 (96%)	196 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	395/414 (95%)	392 (99%)	3 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	169/175 (97%)	160 (95%)	9 (5%)	19	33
1	B	170/175 (97%)	156 (92%)	14 (8%)	9	15
All	All	339/350 (97%)	316 (93%)	23 (7%)	13	22

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	38	GLN
1	B	104	ARG
1	B	100	SER
1	B	107	GLU
1	A	160	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	63	HIS
1	A	93	HIS
1	A	122	GLN
1	A	172	GLN
1	B	180	GLN

### 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 oligosaccharides 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, 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	199/207 (96%)	-0.53	0 100 100	20, 36, 60, 79	0
1	B	200/207 (96%)	-0.59	0 100 100	18, 32, 62, 79	0
All	All	399/414 (96%)	-0.56	0 100 100	18, 34, 61, 79	0

There are no RSRZ outliers to report.

### 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 oligosaccharides in this entry.

### 6.4 Ligands [i](#)

There are no ligands in this entry.

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

There are no such residues in this entry.