



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 10:58 am BST

PDB ID : 6DQL  
Title : Crystal structure of Regulator of Proteinase B RopB complexed with SIP  
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Deposited on : 2018-06-11  
Resolution : 3.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

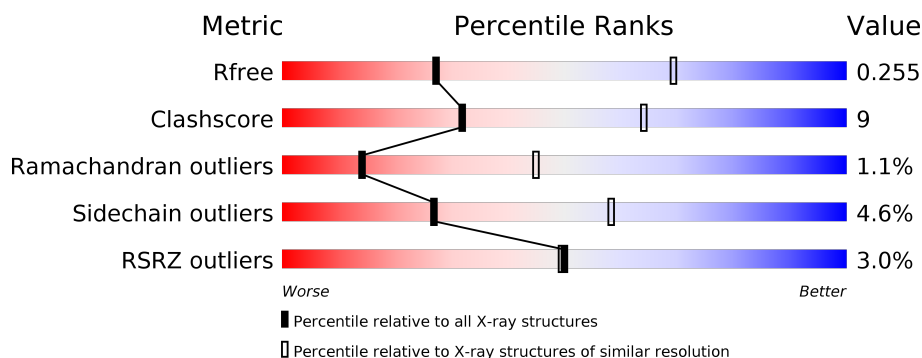
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	233	<div> <div>4%</div> <div> <div></div> <div>83%</div> <div>13%</div> <div>••</div> </div> </div>
1	B	233	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>18%</div> <div>•</div> </div> </div>
2	C	8	<div> <div>25%</div> <div>50%</div> <div>25%</div> </div>

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3868 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 Regulator of Proteinase B RopB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1895	1224	300	356	15			
1	B	226	Total	C	N	O	S	0	0	0
			1886	1219	299	353	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	281	LEU	-	expression tag	UNP D3KVD8
A	282	GLU	-	expression tag	UNP D3KVD8
A	283	HIS	-	expression tag	UNP D3KVD8
A	284	HIS	-	expression tag	UNP D3KVD8
A	285	HIS	-	expression tag	UNP D3KVD8
A	286	HIS	-	expression tag	UNP D3KVD8
A	287	HIS	-	expression tag	UNP D3KVD8
A	288	HIS	-	expression tag	UNP D3KVD8
B	281	LEU	-	expression tag	UNP D3KVD8
B	282	GLU	-	expression tag	UNP D3KVD8
B	283	HIS	-	expression tag	UNP D3KVD8
B	284	HIS	-	expression tag	UNP D3KVD8
B	285	HIS	-	expression tag	UNP D3KVD8
B	286	HIS	-	expression tag	UNP D3KVD8
B	287	HIS	-	expression tag	UNP D3KVD8
B	288	HIS	-	expression tag	UNP D3KVD8

- Molecule 2 is a protein called SpeB-inducing peptide (SIP).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	8	Total	C	N	O	S	0	0	0
			74	55	9	9	1			

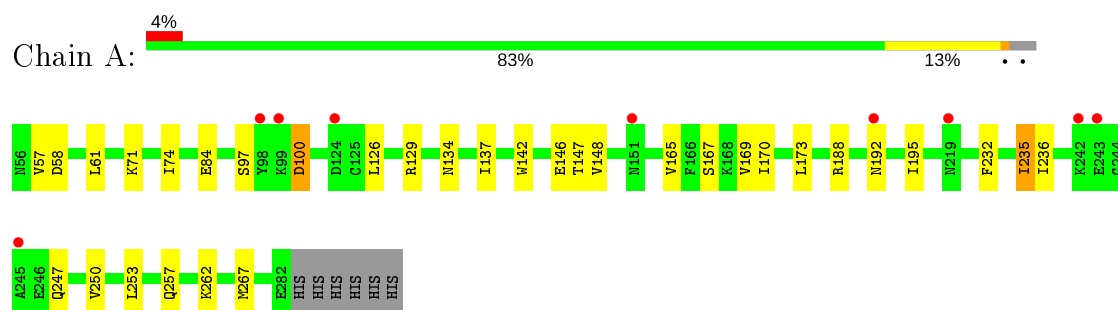
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	6	Total 6	O 6	0	0
3	B	6	Total 6	O 6	0	0
3	C	1	Total 1	O 1	0	0

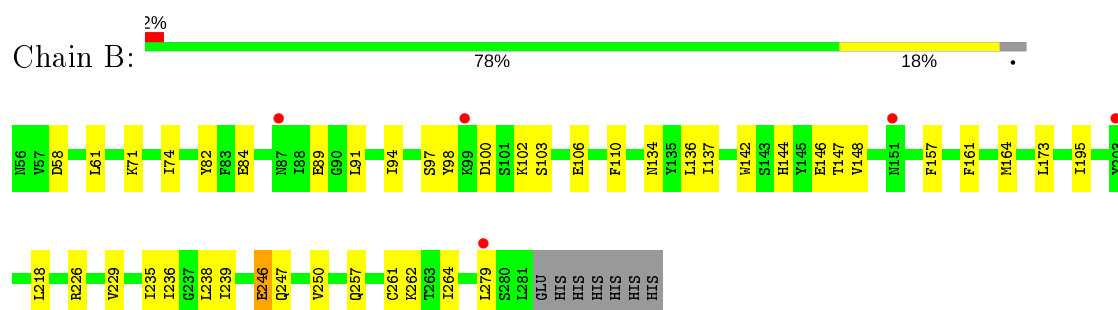
### 3 Residue-property plots [i](#)

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



#### • Molecule 1: Regulator of Proteinase B RopB



#### • Molecule 2: SpeB-inducing peptide (SIP)



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 1 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.21Å 94.21Å 179.96Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.17 – 3.30 29.17 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.4 (29.17-3.30) 99.6 (29.17-3.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	14.12 (at 3.31Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.234 , 0.266 0.232 , 0.255	Depositor DCC
$R_{free}$ test set	690 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	158.7	Xtriage
Anisotropy	0.067	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 155.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.057 for -h,-k,l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	3868	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	176.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.35% 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	0.51	0/1932	0.55	0/2601
1	B	0.52	0/1923	0.56	0/2589
2	C	0.59	0/76	0.96	0/101
All	All	0.52	0/3931	0.56	0/5291

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 ⓘ

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	1895	0	1864	21	0
1	B	1886	0	1858	22	0
2	C	74	0	85	30	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
3	C	1	0	0	0	0
All	All	3868	0	3807	68	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 9.

All (68) 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)
2:C:5:LEU:O	2:C:6:LEU:HD23	1.61	1.01
2:C:5:LEU:O	2:C:6:LEU:CD2	2.10	1.00
2:C:5:LEU:O	2:C:6:LEU:CG	2.17	0.91
2:C:5:LEU:O	2:C:6:LEU:HG	1.69	0.91
2:C:5:LEU:HD13	2:C:6:LEU:N	1.89	0.87
2:C:4:LEU:O	2:C:5:LEU:HB2	1.77	0.84
2:C:5:LEU:C	2:C:6:LEU:HD23	2.00	0.80
1:B:142:TRP:HE1	1:B:147:THR:HG22	1.48	0.77
2:C:4:LEU:HD12	2:C:5:LEU:H	1.51	0.76
2:C:6:LEU:HG	2:C:7:PHE:H	1.50	0.75
1:A:142:TRP:HE1	1:A:147:THR:HG22	1.52	0.75
2:C:2:TRP:NE1	2:C:4:LEU:HB2	2.03	0.73
1:B:82:TYR:HE2	1:B:89:GLU:HB2	1.54	0.72
2:C:2:TRP:CD1	2:C:4:LEU:HB2	2.27	0.70
2:C:7:PHE:CG	2:C:8:LEU:HD12	2.29	0.67
1:A:188:ARG:NH1	2:C:8:LEU:O	2.28	0.66
1:B:238:LEU:HD12	1:B:246:GLU:HA	1.77	0.66
1:B:94:ILE:O	1:B:98:TYR:N	2.32	0.61
1:A:232:PHE:HA	1:A:235:ILE:HG22	1.83	0.60
1:A:257:GLN:OE1	1:A:262:LYS:NZ	2.34	0.59
1:B:97:SER:HA	1:B:100:ASP:HB3	1.84	0.59
2:C:7:PHE:CD1	2:C:8:LEU:HD12	2.40	0.57
1:B:257:GLN:OE1	1:B:262:LYS:NZ	2.35	0.56
2:C:6:LEU:CG	2:C:7:PHE:H	2.19	0.55
1:A:165:VAL:O	1:A:169:VAL:HG23	2.08	0.54
2:C:5:LEU:HD13	2:C:5:LEU:C	2.28	0.54
1:B:102:LYS:O	1:B:106:GLU:HB2	2.10	0.52
2:C:5:LEU:HD12	2:C:6:LEU:CD2	2.39	0.52
2:C:2:TRP:CD1	2:C:3:LEU:N	2.78	0.51
1:B:142:TRP:CE2	1:B:146:GLU:HB3	2.46	0.51
2:C:2:TRP:HE1	2:C:4:LEU:HB2	1.74	0.51
2:C:5:LEU:HD12	2:C:6:LEU:HD23	1.92	0.50
1:A:142:TRP:CE2	1:A:146:GLU:HB3	2.47	0.50
1:B:142:TRP:NE1	1:B:147:THR:HG22	2.22	0.49
1:A:142:TRP:NE1	1:A:147:THR:HG22	2.24	0.49
1:A:134:ASN:HA	1:A:137:ILE:HD12	1.94	0.49
1:B:71:LYS:HA	1:B:74:ILE:HD12	1.96	0.47
1:A:71:LYS:HA	1:A:74:ILE:HD12	1.96	0.46
2:C:4:LEU:O	2:C:5:LEU:CB	2.57	0.46
2:C:7:PHE:CD2	2:C:8:LEU:HD12	2.50	0.46
1:A:57:VAL:HG22	1:B:144:HIS:HB2	1.98	0.46
2:C:6:LEU:HG	2:C:7:PHE:N	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ASN:HA	1:B:137:ILE:HD12	1.98	0.45
1:A:267:MET:HG2	2:C:7:PHE:HE1	1.80	0.45
2:C:2:TRP:HE1	2:C:4:LEU:CD2	2.30	0.44
1:A:147:THR:OG1	1:A:148:VAL:N	2.51	0.44
1:B:147:THR:OG1	1:B:148:VAL:N	2.51	0.44
2:C:5:LEU:CD1	2:C:5:LEU:C	2.86	0.43
1:A:247:GLN:O	1:A:250:VAL:HG22	2.19	0.43
1:A:97:SER:HA	1:A:100:ASP:HB3	2.00	0.43
2:C:2:TRP:CD1	2:C:2:TRP:C	2.92	0.43
1:B:261:CYS:HB3	1:B:264:ILE:HG12	2.01	0.43
1:B:161:PHE:O	1:B:164:MET:HG2	2.19	0.43
1:A:167:SER:O	1:A:170:ILE:HG22	2.20	0.42
1:A:267:MET:CG	2:C:7:PHE:HE1	2.32	0.42
1:B:94:ILE:HG23	1:B:110:PHE:CE2	2.54	0.42
1:A:250:VAL:HA	1:A:253:LEU:HB2	2.03	0.41
1:B:247:GLN:O	1:B:250:VAL:HG12	2.19	0.41
1:B:226:ARG:HA	1:B:229:VAL:HG22	2.02	0.41
1:A:126:LEU:HA	1:A:129:ARG:HB3	2.03	0.41
2:C:4:LEU:CD1	2:C:5:LEU:H	2.26	0.41
1:B:239:ILE:HG13	1:B:279:LEU:HD13	2.03	0.41
1:A:58:ASP:N	1:A:58:ASP:OD1	2.54	0.41
1:B:58:ASP:OD1	1:B:58:ASP:N	2.54	0.40
1:A:192:ASN:ND2	2:C:6:LEU:O	2.51	0.40
1:B:136:LEU:HD12	1:B:157:PHE:CE2	2.56	0.40
1:A:192:ASN:HA	1:A:192:ASN:HD22	1.73	0.40
1:B:91:LEU:O	1:B:94:ILE:HB	2.21	0.40

There are no symmetry-related clashes.

## 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	A	225/233 (97%)	211 (94%)	13 (6%)	1 (0%)	34	66
1	B	224/233 (96%)	207 (92%)	15 (7%)	2 (1%)	17	48
2	C	6/8 (75%)	3 (50%)	1 (17%)	2 (33%)	0	0
All	All	455/474 (96%)	421 (92%)	29 (6%)	5 (1%)	14	45

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	5	LEU
1	A	100	ASP
2	C	6	LEU
1	B	103	SER
1	B	218	LEU

### 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	214/220 (97%)	208 (97%)	6 (3%)	43	70
1	B	213/220 (97%)	206 (97%)	7 (3%)	38	66
2	C	8/8 (100%)	1 (12%)	7 (88%)	0	0
All	All	435/448 (97%)	415 (95%)	20 (5%)	27	58

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	LEU
1	A	84	GLU
1	A	173	LEU
1	A	195	ILE
1	A	235	ILE
1	A	236	ILE
1	B	61	LEU
1	B	84	GLU

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Mol	Chain	Res	Type
1	B	173	LEU
1	B	195	ILE
1	B	235	ILE
1	B	236	ILE
1	B	246	GLU
2	C	1	MET
2	C	2	TRP
2	C	3	LEU
2	C	4	LEU
2	C	5	LEU
2	C	6	LEU
2	C	7	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	192	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

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, 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	227/233 (97%)	-0.04	9 (3%)	38 36	103, 174, 244, 290	0
1	B	226/233 (96%)	-0.03	5 (2%)	62 60	108, 168, 236, 290	0
2	C	8/8 (100%)	0.53	0	100 100	192, 239, 252, 257	0
All	All	461/474 (97%)	-0.03	14 (3%)	50 49	103, 172, 242, 290	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	124	ASP	4.3
1	A	245	ALA	3.3
1	A	99	LYS	2.9
1	B	203	TYR	2.7
1	A	98	TYR	2.7
1	A	242	LYS	2.6
1	B	99	LYS	2.5
1	A	243	GLU	2.4
1	A	192	ASN	2.4
1	A	219	ASN	2.3
1	B	151	ASN	2.3
1	B	87	ASN	2.2
1	B	279	LEU	2.1
1	A	151	ASN	2.0

### 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 [i](#)

There are no carbohydrates 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.