

# wwPDB X-ray Structure Validation Summary Report (i)

#### Nov 7, 2023 – 02:31 PM JST

PDB ID	:	6A89
Title	:	Crystal structure of the ternary complex of peptidoglycan recognition protein
		(PGRP-S) with Tartaric acid, Ribose and 2,6-DIAMINOPIMELIC ACID at
		2.11 A resolution
Authors	:	Bairagya, H.R.; Shokeen, A.; Sharma, P.; Singh, P.K.; Sharma, S.; Singh, T.P.
Deposited on	:	2018-07-06
Resolution	:	2.11  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 (i) symbol.

The types of validation reports are described at http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (1)) were used in the production of this report:

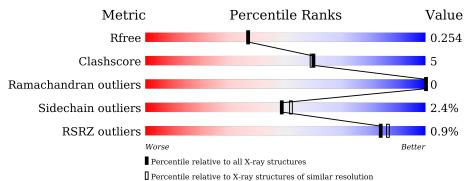
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
$\mathrm{EDS}$	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

# 1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:  $X\text{-}RAY \, DIFFRACTION$ 

The reported resolution of this entry is 2.11 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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f Similar\ resolution}\ (\#{ m Entries,\ resolution\ range}({ m \AA}))$
R <sub>free</sub>	130704	6241 (2.14-2.10)
Clashscore	141614	6778 (2.14-2.10)
Ramachandran outliers	138981	6705 (2.14-2.10)
Sidechain outliers	138945	6706 (2.14-2.10)
RSRZ outliers	127900	6112 (2.14-2.10)

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 >=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 <=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	А	167	% 94%	6%	,-
1	В	167	% <b>89</b> %	10%	
1	С	167	87%	13%	•
1	D	167	% 85%	14%	•



# 2 Entry composition (i)

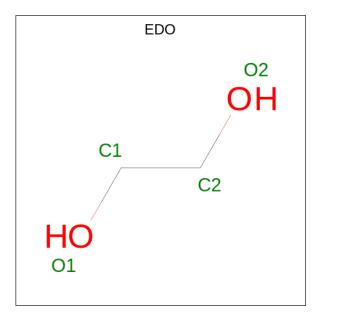
There are 7 unique types of molecules in this entry. The entry contains 5559 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues		At	oms			ZeroOcc	AltConf	Trace
1	А	167	Total	С	Ν	0	$\mathbf{S}$	0	0	0
	Л	107	1306	815	250	233	8	0	0	0
1	В	167	Total	С	Ν	0	S	0	0	0
	D	107	1306	815	250	233	8	0	0	0
1	С	167	Total	С	Ν	0	S	0	0	0
	U	107	1305	815	250	232	8	0	0	0
1	Л	167	Total	С	Ν	0	S	0	0	0
		107	1306	815	250	233	8		0	0

• Molecule 1 is a protein called Peptidoglycan recognition protein 1.

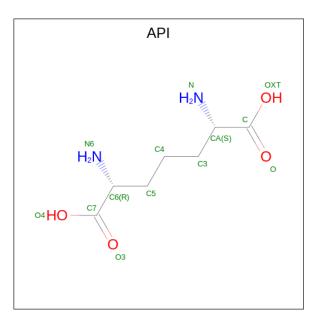
• Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



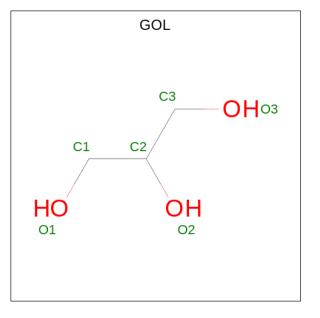
N	Aol	Chain	Residues	Atoms			ZeroOcc	AltConf
	2	А	1	Total 4	${ m C} { m 2}$	O 2	0	0

• Molecule 3 is 2,6-DIAMINOPIMELIC ACID (three-letter code: API) (formula:  $C_7H_{14}N_2O_4$ ).





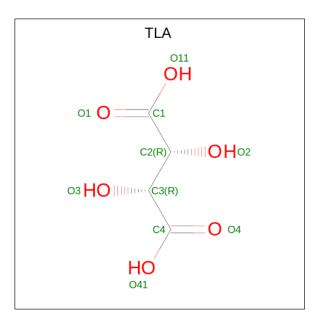
N	Aol	Chain	Residues	Atoms		ZeroOcc	AltConf
	3	В	1	Total         C         N           13         7         2	O 4	0	0



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total C 6 3	O 3	0	0

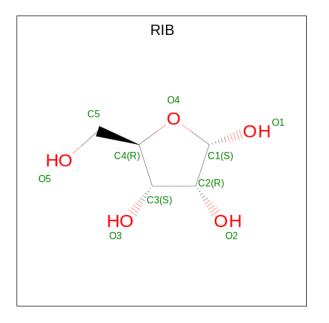
• Molecule 5 is L(+)-TARTARIC ACID (three-letter code: TLA) (formula:  $C_4H_6O_6$ ).





Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total 10	$\begin{array}{c} \mathrm{C} \\ 4 \end{array}$	O 6	0	0

• Molecule 6 is alpha-D-ribo furanose (three-letter code: RIB) (formula:  $C_5H_{10}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	D	1	Total 10	С 5	O 5	0	0

• Molecule 7 is water.



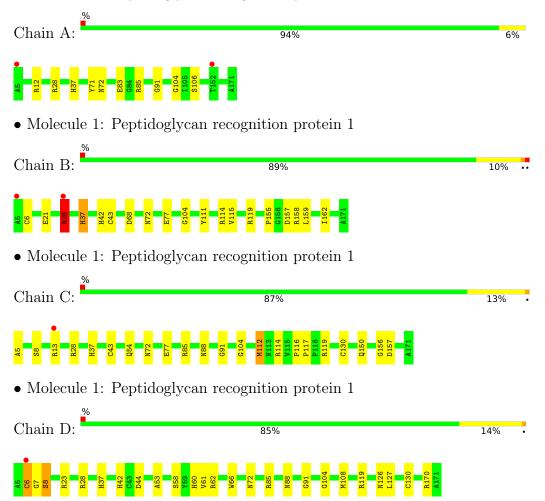
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	А	83	Total O 83 83	0	0
7	В	64	Total         O           64         64	0	0
7	С	85	Total         O           85         85	0	0
7	D	61	Total         O           61         61	0	0



# 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: Peptidoglycan recognition protein 1





## 4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants	89.50Å 101.37Å 163.04Å	Depositor
a, b, c, $\alpha$ , $\beta$ , $\gamma$	$90.00^{\circ}$ $90.00^{\circ}$ $90.00^{\circ}$	Depositor
Resolution (Å)	86.09 - 2.11	Depositor
Resolution (A)	86.09 - 2.12	EDS
% Data completeness	100.0 (86.09-2.11)	Depositor
(in resolution range)	$100.0 \ (86.09-2.12)$	EDS
R <sub>merge</sub>	0.09	Depositor
R <sub>sym</sub>	(Not available)	Depositor
$< I/\sigma(I) > 1$	2.42 (at $2.12$ Å)	Xtriage
Refinement program	REFMAC 5.8.0158	Depositor
B B.	0.191 , $0.249$	Depositor
$R, R_{free}$	0.200 , $0.254$	DCC
$R_{free}$ test set	2161 reflections $(5.07\%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	38.0	Xtriage
Anisotropy	0.851	Xtriage
Bulk solvent $k_{sol}(e/Å^3)$ , $B_{sol}(Å^2)$	0.33 , $40.3$	EDS
L-test for twinning <sup>2</sup>	$ \langle L  \rangle = 0.50, \langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5559	wwPDB-VP
Average B, all atoms $(Å^2)$	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: The largest off-origin peak in the Patterson function is 5.29% of the height of the origin peak. No significant pseudotranslation is detected.

<sup>&</sup>lt;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.



<sup>&</sup>lt;sup>1</sup>Intensities estimated from amplitudes.

# 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: EDO, TLA, RIB, GOL, API

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		
	Chain	RMSZ	# Z  > 5	RMSZ	# Z  > 5	
1	А	0.71	0/1341	0.86	0/1824	
1	В	0.73	0/1341	0.94	4/1824~(0.2%)	
1	С	0.76	0/1340	0.91	1/1824~(0.1%)	
1	D	0.80	0/1341	0.94	4/1824~(0.2%)	
All	All	0.75	0/5363	0.91	9/7296~(0.1%)	

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
1	С	112	MET	CG-SD-CE	7.47	112.16	100.20
1	D	119	ARG	NE-CZ-NH2	-6.92	116.84	120.30
1	D	6	CYS	N-CA-C	6.70	129.09	111.00
1	В	68	ASP	CB-CG-OD1	6.50	124.15	118.30
1	D	44	ASP	CB-CG-OD2	-6.22	112.70	118.30

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	А	1306	0	1261	6	0
1	В	1306	0	1261	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	С	1305	0	1261	15	0
1	D	1306	0	1261	16	1
2	А	4	0	6	0	0
3	В	13	0	7	1	0
4	D	6	0	8	0	0
5	D	10	0	4	0	0
6	D	10	0	0	0	0
7	А	83	0	0	1	0
7	В	64	0	0	1	0
7	С	85	0	0	7	1
7	D	61	0	0	5	1
All	All	5559	0	5069	48	3

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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 5.

The worst 5 of 48 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:C:150:GLN:HG2	7:C:214:HOH:O	1.53	1.09
1:D:8:SER:HA	7:D:315:HOH:O	1.55	1.04
1:C:117:PRO:HB2	7:C:209:HOH:O	1.62	0.98
1:C:8:SER:HA	7:C:201:HOH:O	1.73	0.87
1:D:28:ARG:HH21	1:D:88:ASN:HD21	1.26	0.83

All (3) 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)
7:C:204:HOH:O	7:C:209:HOH:O[4_556]	1.99	0.21
7:D:301:HOH:O	7:D:301:HOH:O[2_565]	2.01	0.19
1:D:6:CYS:O	$1:D:126:ASN:OD1[2_565]$	2.10	0.10

### 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	Percenti	iles
1	А	165/167~(99%)	$160 \ (97\%)$	5(3%)	0	100 1	00
1	В	165/167~(99%)	156~(94%)	9~(6%)	0	100 1	00
1	С	165/167~(99%)	158 (96%)	7 (4%)	0	100 1	00
1	D	165/167~(99%)	155~(94%)	10 (6%)	0	100 1	00
All	All	660/668~(99%)	629~(95%)	31 (5%)	0	100 1	00

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	А	135/135~(100%)	134~(99%)	1 (1%)	84 88
1	В	135/135~(100%)	131~(97%)	4 (3%)	41 43
1	С	135/135~(100%)	131~(97%)	4 (3%)	41 43
1	D	135/135~(100%)	131~(97%)	4 (3%)	41 43
All	All	540/540~(100%)	527~(98%)	13 (2%)	49 52

 $5~{\rm of}~13$  residues with a non-rotameric side chain are listed below:

Mol	Chain	Res	Type
1	С	116	PRO
1	С	130	CYS
1	D	170	ARG
1	D	23	ARG
1	D	37	HIS

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such side chains are listed below:



Mol	Chain	Res	Type
1	С	72	ASN
1	С	88	ASN
1	D	168	HIS
1	D	72	ASN
1	В	72	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 monosaccharides in this entry.

#### 5.6 Ligand geometry (i)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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| > 2 is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Turne	Chain	hain Res		Bo	ond leng	ths	В	ond ang	les
	Type	Chain	nes	Link	Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	RIB	D	203	-	$10,\!10,\!10$	0.54	0	$13,\!14,\!14$	1.25	1 (7%)
4	GOL	D	201	-	$5,\!5,\!5$	0.57	0	$5,\!5,\!5$	0.60	0
3	API	В	201	-	$10,\!12,\!12$	0.91	0	$13,\!15,\!15$	1.10	1 (7%)
2	EDO	А	201	-	3,3,3	0.51	0	2,2,2	0.12	0
5	TLA	D	202	-	$9,\!9,\!9$	1.09	0	$12,\!12,\!12$	1.40	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.



Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	RIB	D	203	-	-	1/2/18/18	0/1/1/1
4	GOL	D	201	-	-	3/4/4/4	-
3	API	В	201	-	-	8/14/14/14	-
2	EDO	А	201	-	-	0/1/1/1	-
5	TLA	D	202	-	-	0/12/12/12	-

'-' means no outliers of that kind were identified.

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Ζ	$Observed(^{o})$	$Ideal(^{o})$
5	D	202	TLA	O11-C1-C2	2.68	120.51	113.27
6	D	203	RIB	C1-C2-C3	2.50	105.42	102.30
5	D	202	TLA	O11-C1-O1	-2.37	118.72	124.09
3	В	201	API	OXT-C-CA	2.30	121.22	113.38

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	В	201	API	C4-C5-C6-C7
3	В	201	API	N6-C6-C7-O3
3	В	201	API	N6-C6-C7-O4
3	В	201	API	CA-C3-C4-C5
4	D	201	GOL	O1-C1-C2-C3

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	201	API	1	0

### 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,  $95^{th}$  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	$\langle RSRZ \rangle$	#RSRZ>2		$OWAB(Å^2)$	Q<0.9
1	А	167/167~(100%)	-0.29	2 (1%) 79	9 82	35, 45, 69, 100	0
1	В	167/167~(100%)	-0.13	2 (1%) 79	9 82	35, 48, 73, 113	0
1	С	167/167~(100%)	-0.33	1 (0%) 89	9 91	33, 42, 65, 96	0
1	D	167/167~(100%)	-0.13	1 (0%) 89	9 91	32, 44, 73, 102	0
All	All	668/668~(100%)	-0.22	6 (0%) 84	4 86	32, 45, 71, 113	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	В	5	ALA	6.0
1	А	5	ALA	4.1
1	D	6	CYS	3.3
1	В	28	ARG	2.7
1	А	152	THR	2.6

## 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 monosaccharides 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. The B-factors column lists the minimum, median,  $95^{th}$  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	$\mathbf{B} ext{-factors}(\mathrm{\AA}^2)$	Q < 0.9
2	EDO	А	201	4/4	0.69	0.19	67, 71, 73, 78	0
3	API	В	201	13/13	0.76	0.16	76,86,88,90	0
6	RIB	D	203	10/10	0.83	0.20	$55,\!61,\!66,\!68$	10
5	TLA	D	202	10/10	0.94	0.14	37,39,43,47	0
4	GOL	D	201	6/6	0.95	0.18	48,55,62,68	0

## 6.5 Other polymers (i)

There are no such residues in this entry.

