



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2020 – 12:38 PM BST

PDB ID : 6WM1  
Title : Crystal structure of the Grb2 SH2 domain in complex with a tripeptide: Ac-pY-Ac6c-N-phenylpropyl  
Authors : Martin, S.F.; Clements, J.H.  
Deposited on : 2020-04-20  
Resolution : 1.80 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.

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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
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13
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)	:	2.13

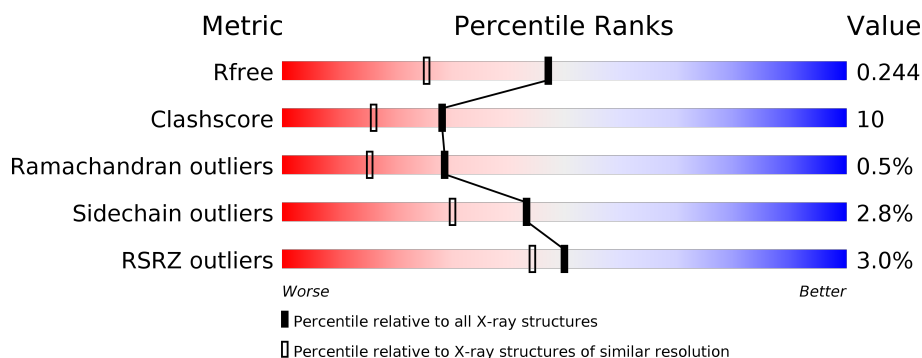
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	117	<div> <div>3%</div> <div> <div></div> <div>74%</div> <div>9%</div> <div>•</div> <div>15%</div> </div> </div>
1	C	117	<div> <div>3%</div> <div> <div></div> <div>71%</div> <div>14%</div> <div>•</div> <div>15%</div> </div> </div>
2	B	5	<div> <div></div> <div> <div>60%</div> <div>40%</div> </div> </div>
2	D	5	<div> <div></div> <div> <div>80%</div> <div>20%</div> </div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 1956 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 Growth factor receptor-bound protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	100	Total	C	N	O	S	6	3	0
			848	543	152	150	3			
1	C	100	Total	C	N	O	S	0	3	0
			855	547	155	150	3			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	164	HIS	-	expression tag	UNP P62993
A	165	HIS	-	expression tag	UNP P62993
A	166	HIS	-	expression tag	UNP P62993
A	167	HIS	-	expression tag	UNP P62993
A	168	HIS	-	expression tag	UNP P62993
A	169	HIS	-	expression tag	UNP P62993
C	164	HIS	-	expression tag	UNP P62993
C	165	HIS	-	expression tag	UNP P62993
C	166	HIS	-	expression tag	UNP P62993
C	167	HIS	-	expression tag	UNP P62993
C	168	HIS	-	expression tag	UNP P62993
C	169	HIS	-	expression tag	UNP P62993

- Molecule 2 is a protein called ACE-PTR-02K-ASN-PRA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	5	Total	C	N	O	P	0	0	0
			46	31	5	9	1			
2	D	5	Total	C	N	O	P	0	0	0
			46	31	5	9	1			

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	1	Total	Ca	0	0
			1	1		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Cl	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	81	Total	O	0	0
			81	81		
6	C	60	Total	O	0	0
			60	60		
6	B	5	Total	O	0	0
			5	5		

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



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	36.01Å 62.98Å 90.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	51.76 – 1.80 33.48 – 1.80	Depositor EDS
% Data completeness (in resolution range)	84.4 (51.76-1.80) 84.4 (33.48-1.80)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	16.91 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.177 , 0.245 0.176 , 0.244	Depositor DCC
$R_{free}$ test set	850 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	23.0	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 47.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	1956	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.00% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PRA, ACE, CL, CA, 02K, PTR

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	1.21	1/870 (0.1%)	1.00	2/1168 (0.2%)
1	C	1.10	2/877 (0.2%)	0.98	2/1175 (0.2%)
2	B	1.18	0/7	1.16	0/8
2	D	1.15	0/7	1.65	0/8
All	All	1.15	3/1761 (0.2%)	0.99	4/2359 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	78	ARG	CB-CG	-8.14	1.30	1.52
1	C	118	TYR	CD1-CE1	6.21	1.48	1.39
1	C	83	PHE	CG-CD1	5.18	1.46	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	113	ASP	CB-CG-OD1	6.68	124.32	118.30
1	A	144	GLN	CB-CA-C	-6.09	98.21	110.40
1	C	100	LYS	CD-CE-NZ	-5.91	98.11	111.70
1	A	67	ARG	NE-CZ-NH1	-5.01	117.80	120.30

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	848	0	829	19	1
1	C	855	0	839	30	1
2	B	46	0	39	0	0
2	D	46	0	39	1	0
3	C	6	0	8	0	0
3	D	6	0	8	0	0
4	C	1	0	0	0	0
5	C	1	0	0	0	0
6	A	81	0	0	2	0
6	B	5	0	0	0	0
6	C	60	0	0	1	0
6	D	1	0	0	0	0
All	All	1956	0	1762	35	1

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 10.

The worst 5 of 35 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:55:MET:HE2	1:C:73[A]:MET:HE2	1.06	1.04
1:A:55:MET:CE	1:C:73[A]:MET:HE2	1.87	1.03
1:A:55:MET:HE2	1:C:73[A]:MET:CE	1.90	1.00
1:A:129:ASN:HD22	1:C:64:LYS:H	1.08	0.91
1:C:142[B]:ARG:CG	1:C:142[B]:ARG:HH11	1.83	0.90

All (1) 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:A:152:GLU:OE2	1:C:152:GLU:OE2[4_455]	2.09	0.11

## 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	101/117 (86%)	96 (95%)	4 (4%)	1 (1%)	15	5
1	C	101/117 (86%)	99 (98%)	2 (2%)	0	100	100
2	B	1/5 (20%)	1 (100%)	0	0	100	100
2	D	1/5 (20%)	1 (100%)	0	0	100	100
All	All	204/244 (84%)	197 (97%)	6 (3%)	1 (0%)	29	15

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	56	LYS

### 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	92/105 (88%)	90 (98%)	2 (2%)	52	39
1	C	92/105 (88%)	87 (95%)	5 (5%)	22	9
2	B	1/1 (100%)	1 (100%)	0	100	100
2	D	1/1 (100%)	1 (100%)	0	100	100
All	All	186/212 (88%)	179 (96%)	7 (4%)	43	18

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	109[A]	LYS
1	C	149	ARG
1	C	109[B]	LYS
1	A	73[B]	MET
1	C	112	ARG

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	C	106	GLN
1	C	153	GLN
1	C	129	ASN
1	A	129	ASN
1	C	144	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	PTR	B	2	2	15,16,17	2.03	1 (6%)	19,22,24	1.40	3 (15%)
2	PTR	D	2	2	15,16,17	1.09	0	19,22,24	1.30	2 (10%)
2	02K	B	3	2	5,9,10	1.42	1 (20%)	5,12,14	1.55	1 (20%)
2	02K	D	3	2	5,9,10	1.14	0	5,12,14	1.30	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PTR	B	2	2	-	0/10/11/13	0/1/1/1
2	PTR	D	2	2	-	0/10/11/13	0/1/1/1
2	02K	B	3	2	-	0/2/13/16	0/1/1/1
2	02K	D	3	2	-	0/2/13/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	PTR	P-OH	6.49	1.69	1.59
2	B	3	02K	O-C	2.59	1.28	1.19

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	PTR	O2P-P-O1P	2.91	122.08	110.68
2	B	2	PTR	OH-P-O1P	-2.59	99.53	109.31
2	B	3	02K	CH-CE-CD	2.57	115.34	111.37
2	B	2	PTR	CE2-CD2-CG	-2.37	117.77	121.03
2	D	2	PTR	O2P-P-OH	2.19	112.10	105.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	PTR	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 for Mogul analysis.

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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
3	GOL	C	201	-	5,5,5	0.61	0	5,5,5	0.71	0
3	GOL	D	101	-	5,5,5	0.28	0	5,5,5	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	201	-	-	4/4/4/4	-
3	GOL	D	101	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	201	GOL	O1-C1-C2-C3
3	C	201	GOL	C1-C2-C3-O3
3	D	101	GOL	O1-C1-C2-C3
3	C	201	GOL	O1-C1-C2-O2
3	C	201	GOL	O2-C2-C3-O3

There are no ring outliers.

No monomer is involved in short contacts.

## 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	100/117 (85%)	-0.40	3 (3%) 50 44	14, 20, 31, 56	1 (1%)
1	C	100/117 (85%)	-0.46	3 (3%) 50 44	14, 22, 33, 51	0
2	B	1/5 (20%)	-0.57	0 100 100	16, 16, 16, 16	0
2	D	1/5 (20%)	-0.51	0 100 100	24, 24, 24, 24	0
All	All	202/244 (82%)	-0.43	6 (2%) 50 44	14, 21, 33, 56	1 (0%)

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	VAL	6.4
1	A	55	MET	4.4
1	C	54	GLU	4.0
1	A	153	GLN	3.8
1	C	153	GLN	3.2

### 6.2 Non-standard residues in protein, DNA, RNA chains [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<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
2	02K	B	3	9/10	0.97	0.07	15,16,18,22	0
2	02K	D	3	9/10	0.97	0.06	17,20,21,23	0
2	PTR	D	2	16/17	0.98	0.07	21,24,27,27	0
2	PTR	B	2	16/17	0.99	0.07	14,17,19,21	0

### 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<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	GOL	C	201	6/6	0.79	0.23	53,54,55,57	0
3	GOL	D	101	6/6	0.88	0.23	51,53,54,55	0
5	CL	C	203	1/1	0.94	0.07	64,64,64,64	0
4	CA	C	202	1/1	0.99	0.09	23,23,23,23	0

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

There are no such residues in this entry.