



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 20, 2020 – 02:15 PM BST

PDB ID : 5KNG  
Title : CRYSTAL STRUCTURE OF ANTI-IL-13 DARPIN 6G9  
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Deposited on : 2016-06-28  
Resolution : 1.35 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 : 2.13.1  
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

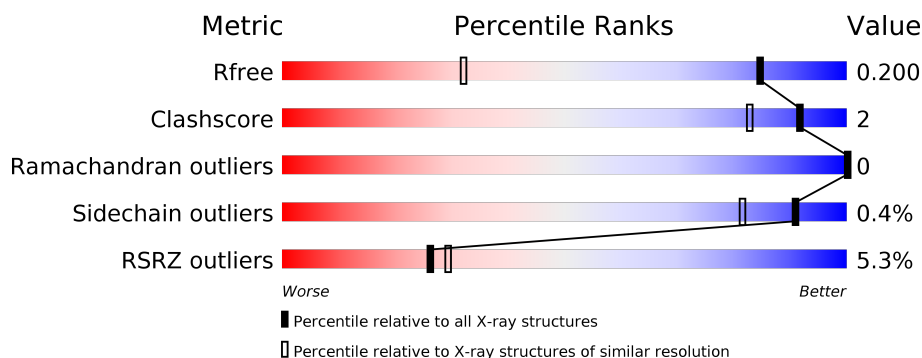
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.35 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	1509 (1.38-1.34)
Clashscore	141614	1551 (1.38-1.34)
Ramachandran outliers	138981	1530 (1.38-1.34)
Sidechain outliers	138945	1530 (1.38-1.34)
RSRZ outliers	127900	1487 (1.38-1.34)

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	169	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 91%; height: 10px; background-color: green;"></div> <div style="width: 7%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="position: absolute; left: 91%; top: -10px;">91%</div> <div style="position: absolute; left: 97%; top: -10px;">7%</div> </div>
1	B	169	<div> <div style="width: 100%; height: 10px; background-color: red;"></div> <div style="width: 92%; height: 10px; background-color: green;"></div> <div style="width: 6%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="position: absolute; left: 92%; top: -10px;">92%</div> <div style="position: absolute; left: 98%; top: -10px;">6%</div> </div>
1	C	169	<div> <div style="width: 3%; height: 10px; background-color: red;"></div> <div style="width: 88%; height: 10px; background-color: green;"></div> <div style="width: 5%; height: 10px; background-color: yellow;"></div> <div style="width: 7%; height: 10px; background-color: grey;"></div> <div style="position: absolute; left: 3%; top: -10px;">3%</div> <div style="position: absolute; left: 88%; top: -10px;">88%</div> <div style="position: absolute; left: 95%; top: -10px;">5%</div> <div style="position: absolute; left: 98%; top: -10px;">7%</div> </div>
1	D	169	<div> <div style="width: 15%; height: 10px; background-color: red;"></div> <div style="width: 87%; height: 10px; background-color: green;"></div> <div style="width: 11%; height: 10px; background-color: yellow;"></div> <div style="width: 2%; height: 10px; background-color: grey;"></div> <div style="position: absolute; left: 15%; top: -10px;">15%</div> <div style="position: absolute; left: 87%; top: -10px;">87%</div> <div style="position: absolute; left: 98%; top: -10px;">11%</div> </div>

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 5386 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 DARPIN 6G9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	158	Total	C	N	O	S	16	0	0
			1192	744	208	239	1			
1	B	159	Total	C	N	O	S	13	0	0
			1196	746	209	240	1			
1	C	158	Total	C	N	O	S	0	0	0
			1176	736	205	234	1			
1	D	151	Total	C	N	O	S	9	0	0
			1101	692	190	218	1			

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



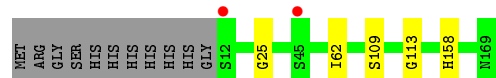
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			6	3	3		
3	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	198	Total	O	0	0
			198	198		
4	B	199	Total	O	0	0
			199	199		
4	C	184	Total	O	0	0
			184	184		
4	D	118	Total	O	0	0
			118	118		



- Molecule 1: DARPIN 6G9



MET ARG GLY SER HIS HIS HIS HIS HIS HIS G11 T112 E130 H158 N169

Amino Acid	Count (approx.)	Color	Red Dot
ARG	10	Yellow	No
GLY	10	Yellow	No
SER	10	Yellow	No
HIS	10	Yellow	No
HIS	10	Yellow	No
HIS	10	Yellow	No
HIS	10	Yellow	No
HIS	10	Yellow	No
HIS	10	Yellow	No
HIS	10	Yellow	No
GLY	10	Yellow	No
S12	10	Green	Yes
D13	10	Green	Yes
G25	10	Yellow	No
I62	10	Yellow	No
F78	10	Yellow	No
I79	10	Yellow	No
L93	10	Yellow	No
D110	10	Yellow	No
Q122	10	Yellow	No
V131	10	Yellow	No
F145	10	Green	Yes
H158	10	Yellow	No
Q166	10	Green	Yes
H169	10	Green	Yes

MET	ARG	GLY	SER	SER	HIS	HIS	HIS	HIS	HIS	HIS	GLY	SER	SER	ASP	LEU	ASP	K16	K17	K18	L18	L19	E20	A21	D27	D28	E29	V30	R31	R30	I32	I33	I33	N34	ALA	ASN	GLY	A38	D39	V40	N41	A42	S45	V65	L66	L67	K68	V69	G70	A71	Y102	I111	Q122	F145	H158	T169
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## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.08 Å 96.08 Å 206.43 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	15.00 – 1.35 29.31 – 1.35	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-1.35) 100.0 (29.31-1.35)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.15 (at 1.35 Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.174 , 0.197 0.177 , 0.200	Depositor DCC
$R_{free}$ test set	3121 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.9	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	5386	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.10% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4

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	0.36	0/1209	0.56	0/1640
1	B	0.38	0/1213	0.55	0/1645
1	C	0.35	0/1193	0.53	0/1622
1	D	0.40	1/1117 (0.1%)	0.53	0/1522
All	All	0.37	1/4732 (0.0%)	0.54	0/6429

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	29	GLU	CG-CD	-5.45	1.43	1.51

There are no bond angle outliers.

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	1192	0	1172	3	0
1	B	1196	0	1175	3	0
1	C	1176	0	1138	7	0
1	D	1101	0	1044	2	0
2	A	5	0	0	0	0
2	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	16	1	0
4	A	198	0	0	1	0
4	B	199	0	0	1	0
4	C	184	0	0	2	0
4	D	118	0	0	1	0
All	All	5386	0	4545	15	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 2.

The worst 5 of 15 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:93:LEU:HD11	1:C:131:VAL:HG21	1.55	0.89
1:B:112:THR:OG1	3:B:202:GOL:H12	1.94	0.68
1:D:158:HIS:HD2	4:D:307:HOH:O	1.91	0.52
1:B:158:HIS:HD2	4:B:479:HOH:O	1.93	0.51
1:B:130:GLU:HG2	4:C:1118:HOH:O	2.10	0.51

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	156/169 (92%)	154 (99%)	2 (1%)	0	100	100
1	B	157/169 (93%)	155 (99%)	2 (1%)	0	100	100
1	C	156/169 (92%)	154 (99%)	2 (1%)	0	100	100
1	D	147/169 (87%)	143 (97%)	4 (3%)	0	100	100
All	All	616/676 (91%)	606 (98%)	10 (2%)	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	122/131 (93%)	122 (100%)	0	100	100
1	B	122/131 (93%)	122 (100%)	0	100	100
1	C	116/131 (88%)	115 (99%)	1 (1%)	78	53
1	D	105/131 (80%)	104 (99%)	1 (1%)	76	49
All	All	465/524 (89%)	463 (100%)	2 (0%)	91	81

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	78	PHE
1	D	34	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	158	HIS
1	C	135	HIS
1	C	158	HIS
1	B	36	ASN
1	C	140	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

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

4 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	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	PO4	A	201	-	4,4,4	0.92	0	6,6,6	0.25	0
3	GOL	B	201	-	5,5,5	0.36	0	5,5,5	0.34	0
2	PO4	C	1001	-	4,4,4	0.97	0	6,6,6	0.69	0
3	GOL	B	202	-	5,5,5	0.35	0	5,5,5	0.32	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	B	201	-	-	0/4/4/4	-
3	GOL	B	202	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

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
3	B	202	GOL	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<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	158/169 (93%)	-0.00	2 (1%) 77 81	11, 15, 33, 44	5 (3%)
1	B	159/169 (94%)	0.00	1 (0%) 89 91	11, 14, 35, 57	4 (2%)
1	C	158/169 (93%)	0.24	5 (3%) 47 53	12, 18, 35, 62	0
1	D	151/169 (89%)	0.91	25 (16%) 1 1	12, 23, 66, 84	3 (1%)
All	All	626/676 (92%)	0.28	33 (5%) 26 29	11, 17, 46, 84	12 (1%)

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	38	ALA	12.6
1	D	32	ILE	8.9
1	D	30	VAL	5.9
1	C	12	SER	5.4
1	D	18	LEU	5.3

### 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<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	B	202	6/6	0.82	0.25	24,35,47,64	0
3	GOL	B	201	6/6	0.90	0.12	24,27,36,47	0
2	PO4	A	201	5/5	0.96	0.11	17,18,20,24	0
2	PO4	C	1001	5/5	0.97	0.09	17,17,20,22	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.