



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 9, 2020 – 02:51 AM BST

PDB ID : 6KZ0  
Title : HRV14 3C in complex with single chain antibody GGVV  
Authors : Meng, B.; Yang, B.; Wilson, I.A.  
Deposited on : 2019-09-21  
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 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	:	2.13.1
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

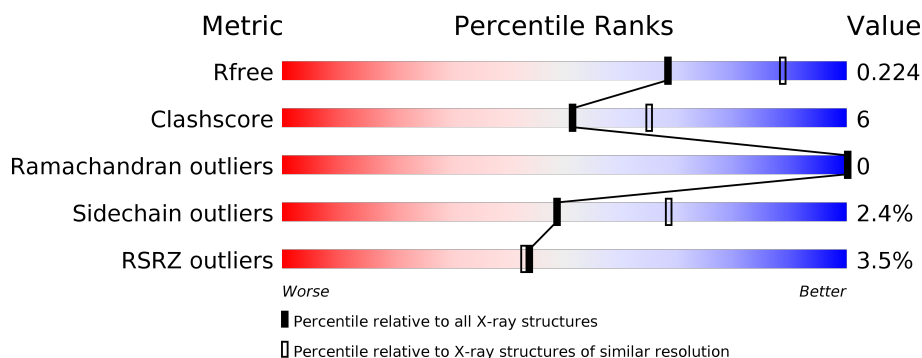
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (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 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	184	<div> <div>6%</div> <div> <div></div> <div>76%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	D	184	<div> <div>6%</div> <div> <div></div> <div>75%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	G	184	<div> <div>9%</div> <div> <div></div> <div>73%</div> <div>14%</div> <div>•</div> <div>11%</div> </div> </div>
1	J	184	<div> <div>4%</div> <div> <div></div> <div>72%</div> <div>17%</div> <div>•</div> <div>10%</div> </div> </div>
2	B	142	<div> <div>%</div> <div> <div></div> <div>77%</div> <div>7%</div> <div>•</div> <div>15%</div> </div> </div>
2	E	142	<div> <div>%</div> <div> <div></div> <div>80%</div> <div>6%</div> <div></div> <div>14%</div> </div> </div>

*Continued on next page...*

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	142	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>73%</div><div>13%</div><div>14%</div></div></div>
2	K	142	<div><div><div></div><div></div><div></div></div><div><div>2%</div><div>78%</div><div>7%</div><div>14%</div></div></div>
3	C	108	<div><div><div></div><div></div><div></div></div><div><div>%</div><div>92%</div><div>7%</div><div></div></div></div>
3	F	108	<div><div><div></div><div></div><div></div></div><div><div></div><div>94%</div><div>5%</div><div></div></div></div>
3	I	108	<div><div><div></div><div></div><div></div></div><div><div></div><div>88%</div><div>11%</div><div></div></div></div>
3	L	108	<div><div><div></div><div></div><div></div></div><div><div></div><div>91%</div><div>8%</div><div></div></div></div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12416 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	164	Total	C	N	O	S	0	0	0
			1262	797	224	235	6			
1	D	164	Total	C	N	O	S	0	0	0
			1262	797	224	235	6			
1	G	163	Total	C	N	O	S	0	0	0
			1257	794	223	234	6			
1	J	165	Total	C	N	O	S	0	0	0
			1270	801	225	238	6			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP P03303
A	0	SER	-	expression tag	UNP P03303
D	-1	GLY	-	expression tag	UNP P03303
D	0	SER	-	expression tag	UNP P03303
G	-1	GLY	-	expression tag	UNP P03303
G	0	SER	-	expression tag	UNP P03303
J	-1	GLY	-	expression tag	UNP P03303
J	0	SER	-	expression tag	UNP P03303

- Molecule 2 is a protein called GGVV H chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	121	Total	C	N	O	S	0	0	0
			917	579	154	180	4			
2	E	122	Total	C	N	O	S	0	0	0
			926	584	156	182	4			
2	H	122	Total	C	N	O	S	0	0	0
			926	584	156	182	4			
2	K	122	Total	C	N	O	S	0	0	0
			926	584	156	182	4			

- Molecule 3 is a protein called GGVV L chain.

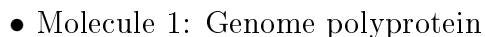
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	107	Total	C	N	O	S	0	0	0
			805	506	134	162	3			
3	F	107	Total	C	N	O	S	0	0	0
			805	506	134	162	3			
3	I	107	Total	C	N	O	S	0	0	0
			805	506	134	162	3			
3	L	107	Total	C	N	O	S	0	0	0
			805	506	134	162	3			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	19	Total	O	0	0
			19	19		
4	B	47	Total	O	0	0
			47	47		
4	C	28	Total	O	0	0
			28	28		
4	D	19	Total	O	0	0
			19	19		
4	E	56	Total	O	0	0
			56	56		
4	F	51	Total	O	0	0
			51	51		
4	G	13	Total	O	0	0
			13	13		
4	H	52	Total	O	0	0
			52	52		
4	I	26	Total	O	0	0
			26	26		
4	J	29	Total	O	0	0
			29	29		
4	K	64	Total	O	0	0
			64	64		
4	L	46	Total	O	0	0
			46	46		

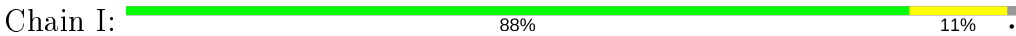


- Molecule 1: Genome polypotein





● Molecule 3: GGVV L chain



● Molecule 3: GGVV L chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	193.78 Å   133.26 Å   78.79 Å 90.00°   93.55°   90.00°	Depositor
Resolution (Å)	48.35 – 2.40 48.35 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.35-2.40) 98.7 (48.35-2.40)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.99 (at 2.39 Å)	Xtriage
Refinement program	PHENIX 1.13 _2998	Depositor
R, $R_{free}$	0.185 , 0.223 0.185 , 0.224	Depositor DCC
$R_{free}$ test set	3842 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.6	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12416	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 41.06 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.4949e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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](#)

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	0.47	0/1279	0.64	0/1721
1	D	0.62	0/1279	0.66	0/1721
1	G	0.61	0/1274	0.72	0/1714
1	J	0.72	0/1287	0.68	1/1732 (0.1%)
2	B	0.47	0/936	0.60	0/1270
2	E	0.50	0/945	0.62	0/1282
2	H	0.42	0/945	0.62	0/1282
2	K	0.55	0/945	0.64	0/1282
3	C	0.40	0/821	0.59	0/1115
3	F	0.45	0/821	0.63	0/1115
3	I	0.53	0/821	0.62	0/1115
3	L	0.49	0/821	0.66	0/1115
All	All	0.54	0/12174	0.65	1/16464 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	138	ASP	CB-CG-OD2	5.18	122.96	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	A	1262	0	1288	13	0
1	D	1262	0	1288	17	0
1	G	1257	0	1283	17	0
1	J	1270	0	1292	22	0
2	B	917	0	886	8	0
2	E	926	0	894	9	0
2	H	926	0	894	10	0
2	K	926	0	894	9	0
3	C	805	0	799	5	0
3	F	805	0	799	3	0
3	I	805	0	801	6	0
3	L	805	0	799	11	0
4	A	19	0	0	0	0
4	B	47	0	0	0	0
4	C	28	0	0	0	0
4	D	19	0	0	0	0
4	E	56	0	0	0	0
4	F	51	0	0	1	0
4	G	13	0	0	1	0
4	H	52	0	0	0	0
4	I	26	0	0	0	0
4	J	29	0	0	0	0
4	K	64	0	0	2	0
4	L	46	0	0	0	0
All	All	12416	0	11917	126	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 6.

The worst 5 of 126 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:J:138:ASP:OD2	1:J:167:GLN:HG2	1.66	0.94
3:L:39:LYS:HB2	3:L:42:LYS:HD3	1.66	0.77
2:B:24:CYS:HG	2:B:98:CYS:HG	0.91	0.73
2:E:24:CYS:HG	2:E:98:CYS:HG	0.80	0.72
1:G:70:LEU:HG	1:G:71:GLU:H	1.54	0.72

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	158/184 (86%)	153 (97%)	5 (3%)	0	100	100
1	D	158/184 (86%)	152 (96%)	6 (4%)	0	100	100
1	G	157/184 (85%)	151 (96%)	6 (4%)	0	100	100
1	J	159/184 (86%)	153 (96%)	6 (4%)	0	100	100
2	B	119/142 (84%)	114 (96%)	5 (4%)	0	100	100
2	E	120/142 (84%)	116 (97%)	4 (3%)	0	100	100
2	H	120/142 (84%)	117 (98%)	3 (2%)	0	100	100
2	K	120/142 (84%)	116 (97%)	4 (3%)	0	100	100
3	C	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
3	F	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	I	105/108 (97%)	103 (98%)	2 (2%)	0	100	100
3	L	105/108 (97%)	102 (97%)	3 (3%)	0	100	100
All	All	1531/1736 (88%)	1482 (97%)	49 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	138/157 (88%)	134 (97%)	4 (3%)	42	62
1	D	138/157 (88%)	132 (96%)	6 (4%)	29	46

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	138/157 (88%)	131 (95%)	7 (5%)	24	39
1	J	139/157 (88%)	134 (96%)	5 (4%)	35	54
2	B	97/103 (94%)	95 (98%)	2 (2%)	53	72
2	E	98/103 (95%)	98 (100%)	0	100	100
2	H	98/103 (95%)	95 (97%)	3 (3%)	40	60
2	K	98/103 (95%)	97 (99%)	1 (1%)	76	88
3	C	91/92 (99%)	91 (100%)	0	100	100
3	F	91/92 (99%)	90 (99%)	1 (1%)	73	87
3	I	91/92 (99%)	89 (98%)	2 (2%)	52	71
3	L	91/92 (99%)	91 (100%)	0	100	100
All	All	1308/1408 (93%)	1277 (98%)	31 (2%)	49	68

5 of 31 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	16	MET
1	G	98	ASP
1	J	64	ASP
1	G	95	GLU
1	G	107	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	J	80	ASN
2	K	15	GLN
3	L	37	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

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	164/184 (89%)	0.17	11 (6%) 17 16	23, 35, 63, 93	0
1	D	164/184 (89%)	0.22	11 (6%) 17 16	19, 39, 65, 82	0
1	G	163/184 (88%)	0.38	17 (10%) 6 6	23, 39, 68, 90	0
1	J	165/184 (89%)	0.10	8 (4%) 30 29	21, 34, 62, 86	0
2	B	121/142 (85%)	-0.44	1 (0%) 86 84	15, 22, 38, 76	0
2	E	122/142 (85%)	-0.49	1 (0%) 86 84	14, 20, 42, 80	0
2	H	122/142 (85%)	-0.35	2 (1%) 72 70	15, 22, 42, 87	0
2	K	122/142 (85%)	-0.46	3 (2%) 57 55	15, 21, 42, 82	0
3	C	107/108 (99%)	-0.41	1 (0%) 84 82	18, 24, 39, 75	0
3	F	107/108 (99%)	-0.52	0 100 100	16, 22, 33, 65	0
3	I	107/108 (99%)	-0.47	0 100 100	17, 24, 36, 58	0
3	L	107/108 (99%)	-0.48	0 100 100	17, 23, 41, 83	0
All	All	1571/1736 (90%)	-0.17	55 (3%) 44 43	14, 27, 60, 93	0

The worst 5 of 55 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	96	GLY	6.7
2	H	3	GLN	5.4
1	G	179	VAL	5.1
1	G	63	VAL	5.0
1	J	179	VAL	4.9

### 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](#)

There are no ligands in this entry.

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

There are no such residues in this entry.