



# wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 4, 2022 – 12:31 PM EDT

PDB ID : 7S4G  
Title : Fab fragment bound to the Cter peptide of Ly6G6D  
Authors : Rouge, L.; Lupardus, P.  
Deposited on : 2021-09-08  
Resolution : 2.20 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  
Xtriage (Phenix) : 1.13  
EDS : **FAILED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.27

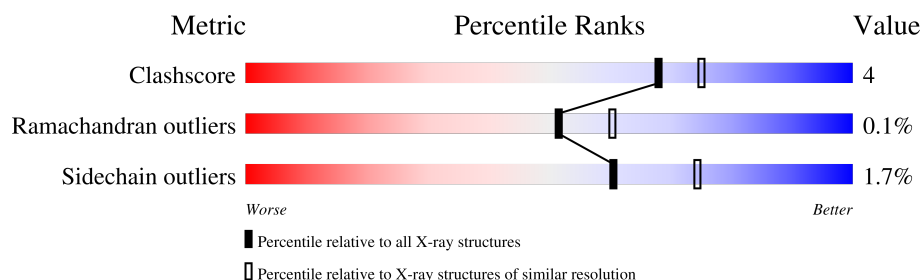
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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))
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)





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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	223	81% 11% 7%
1	C	223	87% 7% 6%
1	E	223	85% 8% 7%
1	H	223	87% 7% 6%
2	B	220	93% 5%
2	D	220	90% 9%
2	F	220	86% 12%
2	L	220	90% 10%

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Mol	Chain	Length	Quality of chain
3	G	9	 67%33%
3	I	9	 100%
3	J	9	 100%
3	K	9	 100%

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 14394 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 heavy chain Fab 1G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1584	1003	267	306	8			
1	C	210	Total	C	N	O	S	0	0	0
			1592	1007	269	308	8			
1	E	208	Total	C	N	O	S	0	0	0
			1583	1002	267	306	8			
1	H	210	Total	C	N	O	S	0	0	0
			1592	1007	269	308	8			

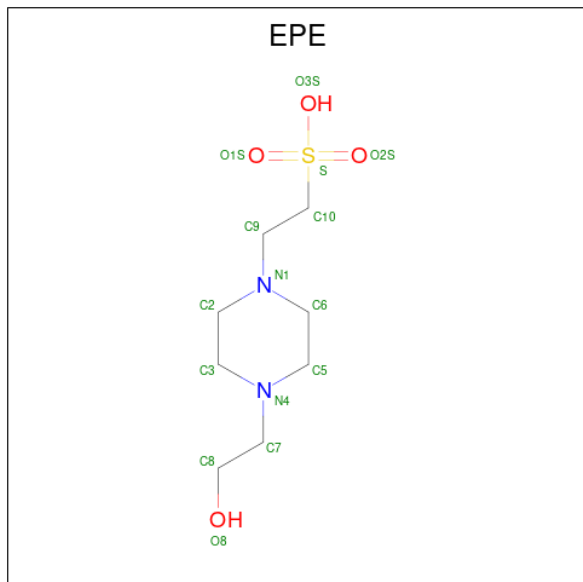
- Molecule 2 is a protein called light chain Fab 1G4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	217	Total	C	N	O	S	0	1	0
			1667	1041	281	340	5			
2	D	218	Total	C	N	O	S	0	0	0
			1666	1040	281	340	5			
2	F	218	Total	C	N	O	S	0	0	0
			1666	1040	281	340	5			
2	L	218	Total	C	N	O	S	0	0	0
			1666	1040	281	340	5			

- Molecule 3 is a protein called Lymphocyte antigen 6 complex locus protein G6d.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	9	Total	C	N	O	S	0	0	0
			68	41	10	15	2			
3	I	9	Total	C	N	O	S	0	0	0
			68	41	10	15	2			
3	J	9	Total	C	N	O	S	0	0	0
			68	41	10	15	2			
3	K	9	Total	C	N	O	S	0	0	0
			68	41	10	15	2			

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula:  $C_8H_{18}N_2O_4S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	D	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	F	1	Total	C	N	O	S	0	0
			15	8	2	4	1		
4	L	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	107	Total	O	0	5
			112	112		
6	B	138	Total	O	0	5
			143	143		
6	C	148	Total	O	0	3
			151	151		
6	D	130	Total	O	0	7
			137	137		
6	E	96	Total	O	0	2
			98	98		
6	F	124	Total	O	0	3
			127	127		
6	G	5	Total	O	0	0
			5	5		
6	I	5	Total	O	0	1
			6	6		
6	J	6	Total	O	0	0
			6	6		
6	K	6	Total	O	0	0
			6	6		

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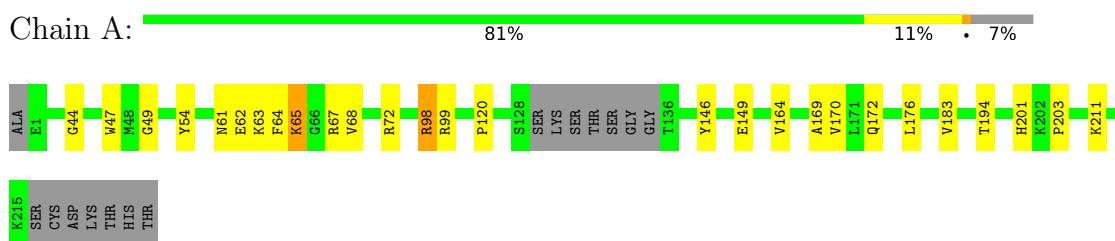
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	H	113	Total 116	O 116	0	3
6	L	125	Total 127	O 127	0	2

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

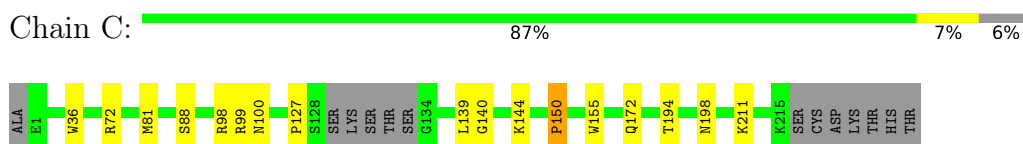
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS failed to run properly.

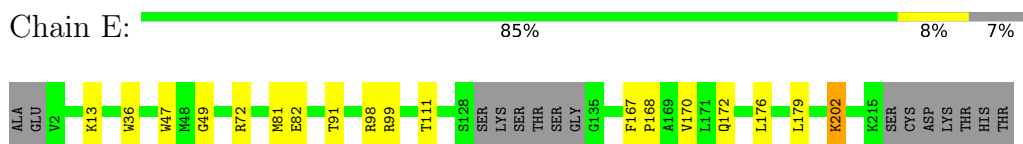
- Molecule 1: heavy chain Fab 1G4



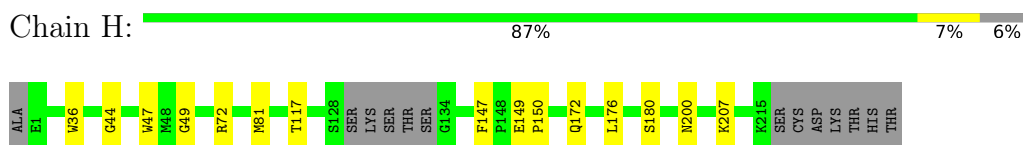
- Molecule 1: heavy chain Fab 1G4



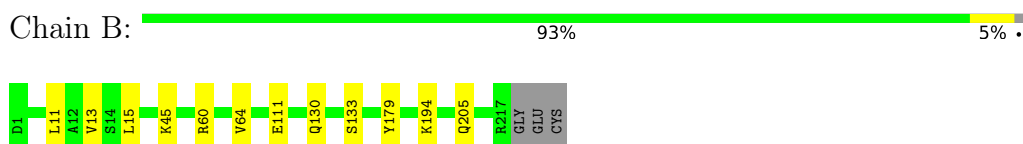
- Molecule 1: heavy chain Fab 1G4



- Molecule 1: heavy chain Fab 1G4



- Molecule 2: light chain Fab 1G4






- Molecule 2: light chain Fab 1G4

Chain D:  90% 9%




- Molecule 2: light chain Fab 1G4

Chain F:  86% 12%



- Molecule 2: light chain Fab 1G4

Chain L:  90% 10%



- Molecule 3: Lymphocyte antigen 6 complex locus protein G6d

Chain G:  67% 33%



- Molecule 3: Lymphocyte antigen 6 complex locus protein G6d

Chain I:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Lymphocyte antigen 6 complex locus protein G6d

Chain J:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Lymphocyte antigen 6 complex locus protein G6d

Chain K:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	69.29Å 133.39Å 100.04Å 90.00° 90.03° 90.00°	Depositor
Resolution (Å)	35.05 – 2.20	Depositor
% Data completeness (in resolution range)	96.9 (35.05-2.20)	Depositor
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.72 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.192 , 0.235	Depositor
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.491	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.117 for h,-k,-l	Xtriage
Total number of atoms	14394	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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, EPE

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	0.56	0/1623	0.65	0/2210
1	C	0.50	0/1631	0.61	0/2220
1	E	0.60	0/1622	0.63	0/2208
1	H	0.75	0/1631	0.66	0/2220
2	B	0.59	0/1705	0.62	0/2318
2	D	0.58	0/1701	0.66	0/2312
2	F	0.52	0/1701	0.58	0/2312
2	L	0.63	0/1701	0.64	0/2312
3	G	0.61	0/68	0.75	0/91
3	I	0.59	0/68	0.90	0/91
3	J	1.42	0/68	1.02	0/91
3	K	0.47	0/68	0.65	0/91
All	All	0.60	0/13587	0.64	0/18476

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 [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	1584	0	1551	16	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	1592	0	1557	8	0
1	E	1583	0	1549	18	0
1	H	1592	0	1557	10	0
2	B	1667	0	1623	8	0
2	D	1666	0	1620	10	0
2	F	1666	0	1620	30	0
2	L	1666	0	1620	12	0
3	G	68	0	55	2	0
3	I	68	0	55	0	0
3	J	68	0	55	0	0
3	K	68	0	55	0	0
4	B	15	0	17	0	0
4	D	15	0	17	0	0
4	F	15	0	17	1	0
4	L	15	0	18	1	0
5	D	6	0	8	1	0
5	L	6	0	8	2	0
6	A	112	0	0	0	0
6	B	143	0	0	3	0
6	C	151	0	0	1	0
6	D	137	0	0	2	0
6	E	98	0	0	1	0
6	F	127	0	0	1	0
6	G	5	0	0	0	0
6	H	116	0	0	1	0
6	I	6	0	0	0	0
6	J	6	0	0	0	0
6	K	6	0	0	0	0
6	L	127	0	0	1	0
All	All	14394	0	13002	101	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 4.

The worst 5 of 101 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:F:164:ASN:O	2:F:185:LEU:HD12	1.68	0.93
2:B:194:LYS:HE2	6:B:488:HOH:O	1.68	0.93
2:F:167:GLU:OE1	6:F:401[B]:HOH:O	1.90	0.87
1:A:64:PHE:O	1:A:68:VAL:HG12	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:170:VAL:CG1	2:F:166:GLN:NE2	2.40	0.84

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	204/223 (92%)	192 (94%)	11 (5%)	1 (0%)	29	31
1	C	206/223 (92%)	201 (98%)	5 (2%)	0	100	100
1	E	204/223 (92%)	201 (98%)	3 (2%)	0	100	100
1	H	206/223 (92%)	200 (97%)	6 (3%)	0	100	100
2	B	216/220 (98%)	208 (96%)	8 (4%)	0	100	100
2	D	216/220 (98%)	210 (97%)	6 (3%)	0	100	100
2	F	216/220 (98%)	208 (96%)	7 (3%)	1 (0%)	29	31
2	L	216/220 (98%)	209 (97%)	7 (3%)	0	100	100
3	G	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	I	7/9 (78%)	6 (86%)	1 (14%)	0	100	100
3	J	7/9 (78%)	7 (100%)	0	0	100	100
3	K	7/9 (78%)	7 (100%)	0	0	100	100
All	All	1712/1808 (95%)	1655 (97%)	55 (3%)	2 (0%)	51	60

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
2	F	165	SER

### 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	177/191 (93%)	173 (98%)	4 (2%)	50	63
1	C	177/191 (93%)	173 (98%)	4 (2%)	50	63
1	E	177/191 (93%)	173 (98%)	4 (2%)	50	63
1	H	177/191 (93%)	175 (99%)	2 (1%)	73	85
2	B	191/192 (100%)	190 (100%)	1 (0%)	88	94
2	D	190/192 (99%)	186 (98%)	4 (2%)	53	67
2	F	190/192 (99%)	189 (100%)	1 (0%)	88	94
2	L	190/192 (99%)	185 (97%)	5 (3%)	46	58
3	G	8/8 (100%)	8 (100%)	0	100	100
3	I	8/8 (100%)	8 (100%)	0	100	100
3	J	8/8 (100%)	8 (100%)	0	100	100
3	K	8/8 (100%)	8 (100%)	0	100	100
All	All	1501/1564 (96%)	1476 (98%)	25 (2%)	60	74

5 of 25 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	82	GLU
2	F	208	SER
2	L	208	SER
1	E	202	LYS
1	H	72	ARG

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

Mol	Chain	Res	Type
2	F	166	GLN

### 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](#)

6 ligands are modelled in this entry.

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.

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](#)

EDS failed to run properly - this section is therefore empty.

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.