



# wwPDB X-ray Structure Validation Summary Report ⓘ

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PDB ID : 1Q9K  
Title : S25-2 Fab Unliganded 1  
Authors : Nguyen, H.P.; Seto, N.O.; MacKenzie, C.R.; Brade, L.; Kosma, P.; Brade, H.;  
Evans, S.V.  
Deposited on : 2003-08-25  
Resolution : 1.96 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	:	2.11
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)	:	2.11

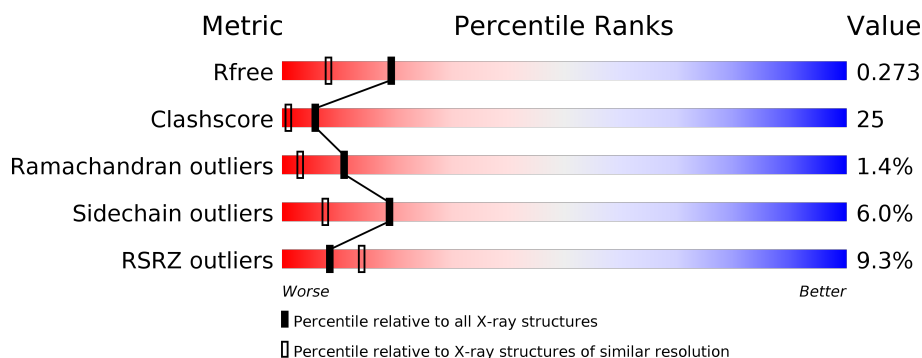
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.96 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	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	219	<div> <div>4%</div> <div>67%</div> <div>31%</div> <div>•</div> </div>
2	B	222	<div> <div>14%</div> <div>61%</div> <div>32%</div> <div>6%</div> <div>•</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3672 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 S25-2 Fab (IgG1k) light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	219	Total	C	N	O	S	0	0	0
			1701	1056	290	347	8			

- Molecule 2 is a protein called S25-2 Fab (IgG1k) heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	222	Total	C	N	O	S	0	0	0
			1698	1075	283	333	7			

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	4	Total	Mg	0	0
			4	4		

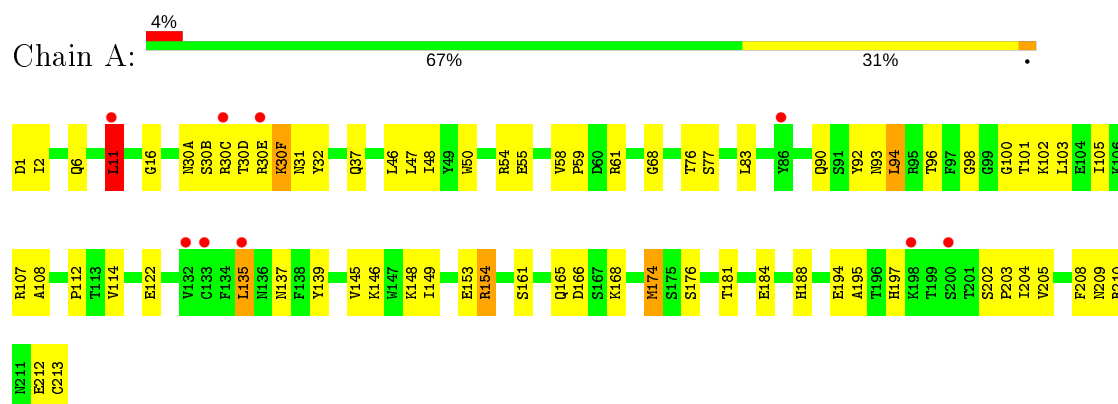
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	157	Total	O	0	0
			157	157		
4	B	112	Total	O	0	0
			112	112		

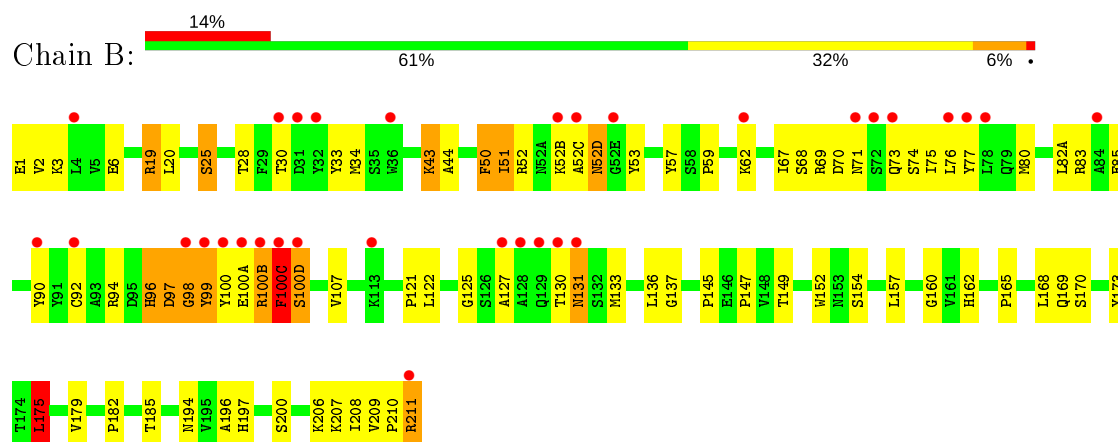
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: S25-2 Fab (IgG1k) light chain



- Molecule 2: S25-2 Fab (IgG1k) heavy chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 <sub>1</sub> 2 <sub>1</sub> 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	96.80 Å   112.20 Å   41.50 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	19.74 – 1.96 19.74 – 1.96	Depositor EDS
% Data completeness (in resolution range)	90.3 (19.74-1.96) 90.3 (19.74-1.96)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.51 (at 1.96 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.228   ,   0.278 0.222   ,   0.273	Depositor DCC
$R_{free}$ test set	2995 reflections (9.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	30.3	Xtriage
Anisotropy	0.667	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 54.3	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	0.95	EDS
Total number of atoms	3672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: MG

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	0.53	0/1736	0.76	1/2351 (0.0%)
2	B	0.49	0/1744	0.73	1/2381 (0.0%)
All	All	0.51	0/3480	0.74	2/4732 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	11	LEU	CA-CB-CG	6.17	129.49	115.30
2	B	175	LEU	CA-CB-CG	5.53	128.02	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	90	TYR	Sidechain

### 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	1701	0	1649	77	1
2	B	1698	0	1648	100	0
3	A	4	0	0	0	0
4	A	157	0	0	3	0
4	B	112	0	0	0	0
All	All	3672	0	3297	168	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 25.

The worst 5 of 168 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:90:GLN:HE21	1:A:96:THR:HG22	1.03	1.14
1:A:194:GLU:HG2	1:A:205:VAL:HG22	1.44	0.98
2:B:1:GLU:HG3	2:B:1:GLU:O	1.60	0.98
1:A:90:GLN:NE2	1:A:96:THR:HG22	1.88	0.89
2:B:211:ARG:HH11	2:B:211:ARG:HG3	1.37	0.88

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:1:ASP:OD1	1:A:1:ASP:OD1[2_445]	1.43	0.77

## 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.

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	217/219 (99%)	206 (95%)	11 (5%)	0	100	100
2	B	220/222 (99%)	201 (91%)	13 (6%)	6 (3%)	5	1
All	All	437/441 (99%)	407 (93%)	24 (6%)	6 (1%)	11	3

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	97	ASP
2	B	100(B)	ARG
2	B	100(C)	PHE
2	B	98	GLY
2	B	131	ASN

### 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	195/195 (100%)	189 (97%)	6 (3%)	40	28
2	B	190/190 (100%)	173 (91%)	17 (9%)	9	2
All	All	385/385 (100%)	362 (94%)	23 (6%)	19	8

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	43	LYS
2	B	51	ILE
2	B	175	LEU
2	B	50	PHE
2	B	52(D)	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:



Mol	Chain	Res	Type
1	A	165	GLN
2	B	197	HIS
2	B	162	HIS
1	A	42	GLN
2	B	71	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 carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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](#)

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	219/219 (100%)	0.39	9 (4%) 37 46	24, 34, 52, 66	0
2	B	222/222 (100%)	0.86	32 (14%) 2 4	24, 38, 70, 97	0
All	All	441/441 (100%)	0.62	41 (9%) 8 14	24, 36, 63, 97	0

The worst 5 of 41 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	130	THR	10.8
2	B	128	ALA	6.5
2	B	99	TYR	6.3
2	B	100	TYR	5.2
2	B	129	GLN	5.1

### 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 carbohydrates 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	MG	A	216	1/1	0.92	0.20	45,45,45,45	0
3	MG	A	215	1/1	0.93	0.17	58,58,58,58	0
3	MG	A	217	1/1	0.96	0.35	18,18,18,18	0
3	MG	A	214	1/1	0.99	0.09	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.