



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 19, 2024 – 01:35 PM EDT

PDB ID : 8TVD  
Title : Fab 221-11 in complex with OspA  
Authors : Rudolph, M.J.; Mantis, N.  
Deposited on : 2023-08-18  
Resolution : 3.08 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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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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)  
Xtrriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

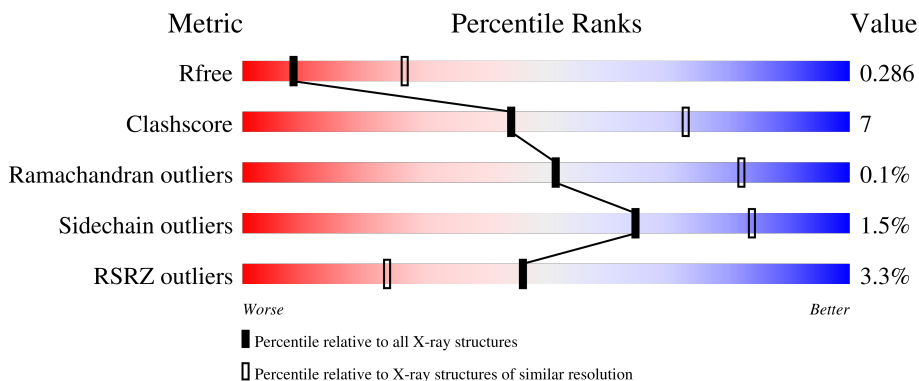
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.08 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.



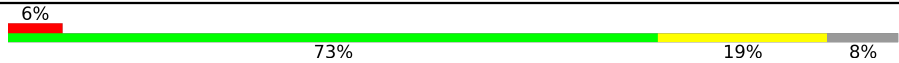
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1447 (3.10-3.06)
Clashscore	141614	1546 (3.10-3.06)
Ramachandran outliers	138981	1487 (3.10-3.06)
Sidechain outliers	138945	1486 (3.10-3.06)
RSRZ outliers	127900	1416 (3.10-3.06)

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  $\leq 5\%$ . 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	212	
1	L	212	
2	B	220	
2	H	220	
3	C	249	

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Mol	Chain	Length	Quality of chain
3	E	249	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a small red segment at the beginning labeled '6%', a large green segment labeled '73%', a yellow segment labeled '19%', and a small grey segment at the end labeled '8%'.</p>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 10103 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 Light chain of Fab 221-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	L	211	Total 1616	C 1015	N 269	O 328	S 4	0	1	0
1	A	212	Total 1613	C 1012	N 269	O 328	S 4	0	0	0

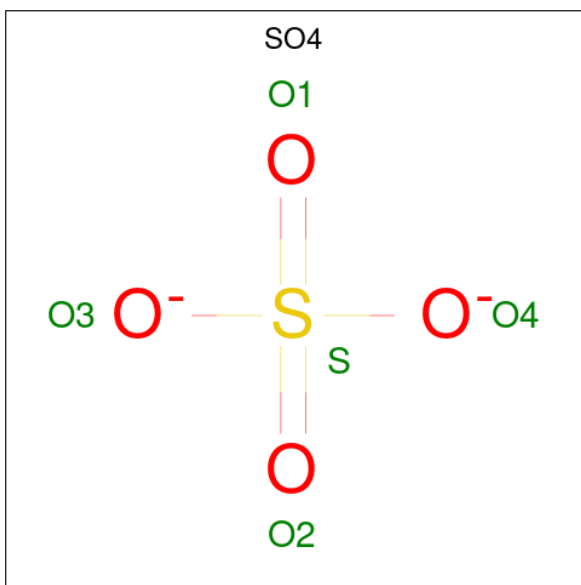
- Molecule 2 is a protein called Heavy chain of Fab 221-11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	H	213	Total 1632	C 1044	N 269	O 312	S 7	0	0	0
2	B	213	Total 1632	C 1044	N 269	O 312	S 7	0	0	0

- Molecule 3 is a protein called Outer surface protein A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	230	Total 1729	C 1069	N 286	O 374		0	0	0
3	C	243	Total 1839	C 1139	N 303	O 396	S 1	0	0	0

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	L	1	Total	O	S	0	0
			5	4	1		
4	E	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	C	1	Total	O	S	0	0
			5	4	1		

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

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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	1	Total	O	0	0
			1	1		
6	H	3	Total	O	0	0
			3	3		

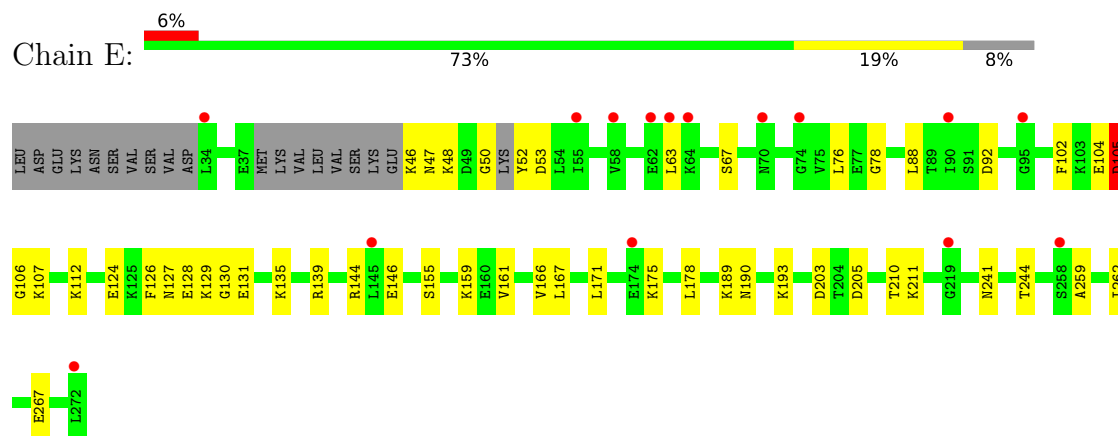
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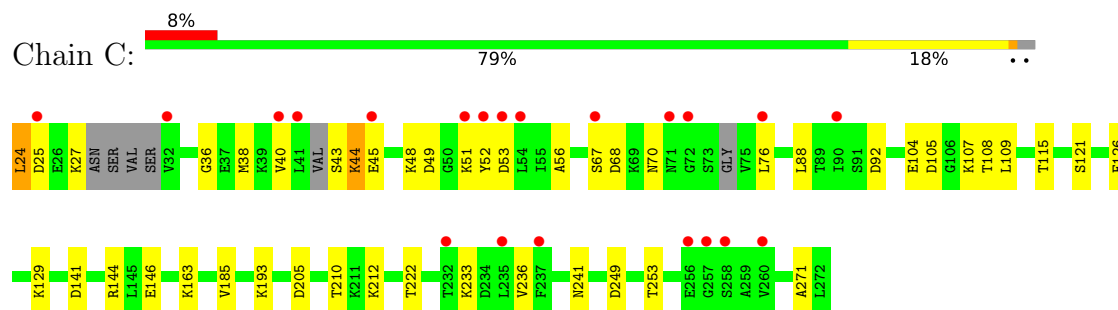
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	E	1	Total O 1 1	0	0
6	A	3	Total O 3 3	0	0
6	B	1	Total O 1 1	0	0
6	C	2	Total O 2 2	0	0



- Molecule 3: Outer surface protein A



- Molecule 3: Outer surface protein A





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.81Å 107.81Å 316.85Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.73 – 3.08 48.73 – 3.08	Depositor EDS
% Data completeness (in resolution range)	99.0 (48.73-3.08) 99.1 (48.73-3.08)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.64 (at 3.07Å)	Xtrriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, $R_{free}$	0.234 , 0.286 0.234 , 0.286	Depositor DCC
$R_{free}$ test set	1736 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	79.0	Xtrriage
Anisotropy	0.299	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.42$ , $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	10103	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	99.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.46% 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: CL, SO4

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	0.25	0/1648	0.47	0/2237
1	L	0.25	0/1651	0.45	0/2241
2	B	0.25	0/1677	0.47	0/2286
2	H	0.25	0/1677	0.48	0/2286
3	C	0.24	0/1845	0.48	0/2470
3	E	0.25	0/1736	0.49	0/2328
All	All	0.25	0/10234	0.47	0/13848

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	H	0	1
3	E	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	104	GLU	Peptide
2	H	54	GLY	Peptide

## 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	1613	0	1568	8	0
1	L	1616	0	1569	23	0
2	B	1632	0	1596	30	0
2	H	1632	0	1596	23	0
3	C	1839	0	1907	28	0
3	E	1729	0	1783	33	0
4	A	5	0	0	0	0
4	B	10	0	0	0	0
4	C	5	0	0	0	0
4	E	5	0	0	0	0
4	L	5	0	0	0	0
5	B	1	0	0	0	0
6	A	3	0	0	0	0
6	B	1	0	0	0	0
6	C	2	0	0	0	0
6	E	1	0	0	1	0
6	H	3	0	0	0	0
6	L	1	0	0	0	0
All	All	10103	0	10019	133	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 7.

The worst 5 of 133 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:L:6:GLN:NE2	1:L:86:TYR:O	2.14	0.79
2:B:6:GLN:H	2:B:113:GLN:HE22	1.32	0.78
3:E:102:PHE:HB3	3:E:106:GLY:HA2	1.68	0.76
2:H:102:ARG:NH2	3:E:107:LYS:O	2.23	0.72
3:C:76:LEU:HB2	3:C:88:LEU:HB3	1.72	0.71

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	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
1	L	210/212 (99%)	204 (97%)	6 (3%)	0	100	100
2	B	209/220 (95%)	200 (96%)	9 (4%)	0	100	100
2	H	209/220 (95%)	198 (95%)	11 (5%)	0	100	100
3	C	235/249 (94%)	228 (97%)	7 (3%)	0	100	100
3	E	224/249 (90%)	214 (96%)	9 (4%)	1 (0%)	34	66
All	All	1297/1362 (95%)	1248 (96%)	48 (4%)	1 (0%)	51	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	105	ASP

### 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	183/183 (100%)	181 (99%)	2 (1%)	73	88
1	L	184/183 (100%)	183 (100%)	1 (0%)	88	94
2	B	182/188 (97%)	181 (100%)	1 (0%)	88	94
2	H	182/188 (97%)	176 (97%)	6 (3%)	38	68
3	C	213/218 (98%)	208 (98%)	5 (2%)	50	75
3	E	199/218 (91%)	197 (99%)	2 (1%)	76	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1143/1178 (97%)	1126 (98%)	17 (2%)	65 84

5 of 17 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	45	GLU
3	C	104	GLU
3	E	92	ASP
3	E	105	ASP
1	A	53	SER

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

Mol	Chain	Res	Type
1	L	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](#)

Of 7 ligands modelled in this entry, 1 is monoatomic - leaving 6 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
4	SO4	C	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	A	301	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	B	302	-	4,4,4	0.14	0	6,6,6	0.05	0
4	SO4	E	301	-	4,4,4	0.13	0	6,6,6	0.08	0
4	SO4	L	301	-	4,4,4	0.14	0	6,6,6	0.05	0

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	212/212 (100%)	0.09	5 (2%) 59 35	58, 93, 150, 191	0
1	L	211/212 (99%)	-0.01	0 100 100	54, 86, 125, 155	0
2	B	213/220 (96%)	-0.05	0 100 100	53, 83, 117, 149	0
2	H	213/220 (96%)	-0.03	2 (0%) 84 68	57, 82, 115, 135	0
3	C	243/249 (97%)	0.24	21 (8%) 10 4	60, 102, 152, 232	0
3	E	230/249 (92%)	0.26	15 (6%) 18 7	85, 124, 177, 197	0
All	All	1322/1362 (97%)	0.09	43 (3%) 46 24	53, 94, 151, 232	0

The worst 5 of 43 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	257	GLY	4.8
3	C	52	TYR	4.7
3	E	64	LYS	4.6
3	E	74	GLY	4.3
3	C	258	SER	4.2

### 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(Å <sup>2</sup> )	Q<0.9
4	SO4	L	301	5/5	0.86	0.18	127,138,143,145	0
5	CL	B	303	1/1	0.86	0.10	82,82,82,82	0
4	SO4	C	301	5/5	0.92	0.29	163,167,170,171	0
4	SO4	A	301	5/5	0.93	0.16	123,134,140,143	0
4	SO4	B	302	5/5	0.93	0.19	128,129,132,138	0
4	SO4	E	301	5/5	0.94	0.14	118,122,129,132	0
4	SO4	B	301	5/5	0.97	0.12	93,96,99,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.