Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2023 – 10:40 PM EDT

PDB ID	:	7S8G
Title	:	Structure of anti-LASV Fab 25.10C with FNQI mutation
Authors	:	Hastie, K.M.; Enriquez, A.S.
Deposited on	:	2021-09-17
Resolution	:	2.57 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *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.

The following versions of software and data (see references ⓘ) were used in the production of this report:

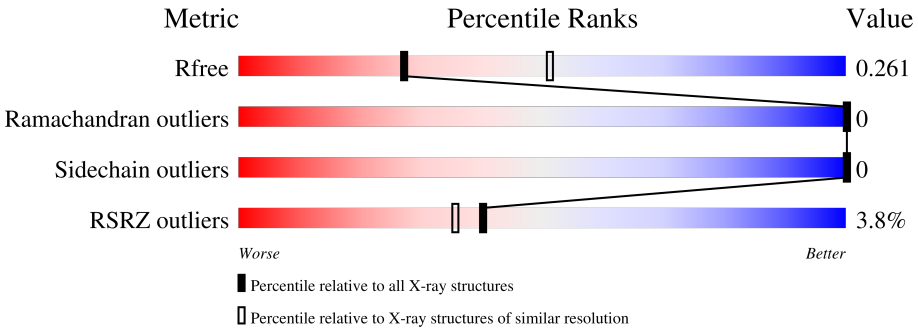
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.57 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	3676 (2.60-2.56)
Ramachandran outliers	138981	3979 (2.60-2.56)
Sidechain outliers	138945	3979 (2.60-2.56)
RSRZ outliers	127900	3614 (2.60-2.56)

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 >=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 <=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	H	227	4% 93% 7%
1	h	227	5% 92% 8%
2	L	210	4% 100%
2	l	210	% 100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12612 atoms, of which 6158 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 25.10C-FNQI Fab Heavy Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	H	212	Total	C	H	N	O	S	0	1	0
			3210	1024	1591	281	308	6			
1	h	208	Total	C	H	N	O	S	0	0	0
			3031	981	1476	267	301	6			

- Molecule 2 is a protein called 25.10C-FNQI Fab Light Chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	L	209	Total	C	H	N	O	S	0	0	0
			3136	995	1544	270	322	5			
2	l	209	Total	C	H	N	O	S	0	0	0
			3140	995	1547	270	323	5			

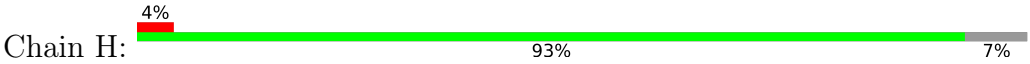
- Molecule 3 is water.

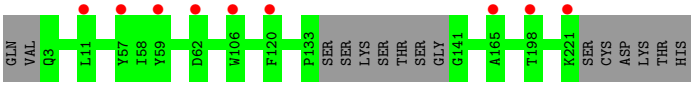
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	H	18	Total	O	0	0
			18	18		
3	L	15	Total	O	0	0
			15	15		
3	h	29	Total	O	0	0
			29	29		
3	l	33	Total	O	0	0
			33	33		

3 Residue-property plots (i)

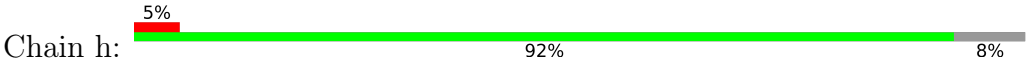
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

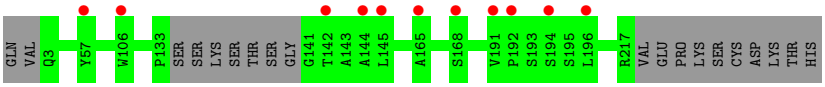
• Molecule 1: 25.10C-FNQI Fab Heavy Chain



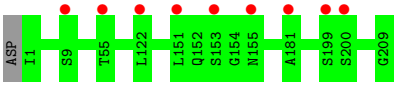


• Molecule 1: 25.10C-FNQI Fab Heavy Chain

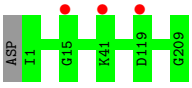




• Molecule 2: 25.10C-FNQI Fab Light Chain



• Molecule 2: 25.10C-FNQI Fab Light Chain



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.60Å 72.72Å 90.01Å 90.00° 113.27° 90.00°	Depositor
Resolution (Å)	65.78 – 2.57 65.78 – 2.57	Depositor EDS
% Data completeness (in resolution range)	98.8 (65.78-2.57) 98.1 (65.78-2.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.83 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.220 , 0.263 0.221 , 0.261	Depositor DCC
R_{free} test set	1354 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	55.6	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 28.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Estimated twinning fraction	0.378 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	12612	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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

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	H	0.25	0/1665	0.50	0/2264
1	h	0.26	0/1592	0.52	0/2173
2	L	0.27	0/1624	0.51	0/2206
2	l	0.29	0/1625	0.50	0/2207
All	All	0.27	0/6506	0.51	0/8850

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

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	H	209/227 (92%)	207 (99%)	2 (1%)	0	100	100
1	h	204/227 (90%)	200 (98%)	4 (2%)	0	100	100
2	L	207/210 (99%)	202 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	l	207/210 (99%)	199 (96%)	8 (4%)	0	100	100
All	All	827/874 (95%)	808 (98%)	19 (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	H	180/194 (93%)	180 (100%)	0	100	100
1	h	167/194 (86%)	167 (100%)	0	100	100
2	L	180/184 (98%)	180 (100%)	0	100	100
2	l	181/184 (98%)	181 (100%)	0	100	100
All	All	708/756 (94%)	708 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

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

6.1 Protein, DNA and RNA chains

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^{th} 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^2)	Q<0.9
1	H	212/227 (93%)	0.32	9 (4%)	36	32	40, 62, 80, 102	0
1	h	208/227 (91%)	0.50	11 (5%)	26	22	42, 65, 100, 126	0
2	L	209/210 (99%)	0.39	9 (4%)	35	31	39, 63, 95, 127	0
2	l	209/210 (99%)	0.21	3 (1%)	75	73	39, 54, 81, 99	0
All	All	838/874 (95%)	0.36	32 (3%)	40	36	39, 62, 93, 127	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	H	59	TYR	4.3
1	h	57	TYR	4.0
1	H	120	PHE	3.6
1	h	145	LEU	3.5
2	L	199	SER	3.2
1	H	221	LYS	3.1
1	h	196	LEU	3.0
1	h	168	SER	2.8
2	L	55	THR	2.7
1	h	144	ALA	2.7
1	H	57	TYR	2.7
1	h	142	THR	2.6
2	L	181	ALA	2.6
1	H	11	LEU	2.6
1	h	165	ALA	2.6
2	l	41	LYS	2.5
2	l	119	ASP	2.5
2	L	9	SER	2.4
2	l	15	GLY	2.4
1	h	194	SER	2.4
1	H	198	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	h	191	VAL	2.3
2	L	122	LEU	2.3
1	h	106	TRP	2.3
1	h	192	PRO	2.2
2	L	151	LEU	2.2
1	H	106	TRP	2.2
2	L	153	SER	2.2
1	H	165	ALA	2.2
2	L	155	ASN	2.2
2	L	200	SER	2.1
1	H	62	ASP	2.0

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.