



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2020 – 03:04 PM BST

PDB ID : 6XMI
Title : Structure of Fab4 bound to P22 TerL(1-33)
Authors : Cingolani, G.; Lokareddy, R.; Ko, Y.
Deposited on : 2020-06-30
Resolution : 1.51 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 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	:	2.14.2
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)	:	2.14.2

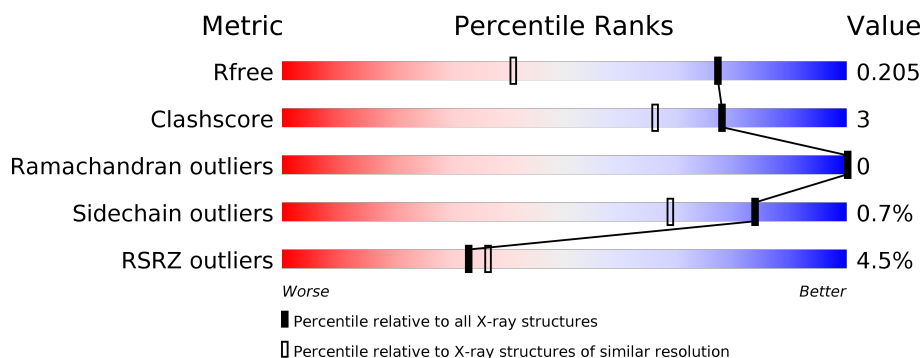
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.51 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	4009 (1.54-1.50)
Clashscore	141614	4249 (1.54-1.50)
Ramachandran outliers	138981	4148 (1.54-1.50)
Sidechain outliers	138945	4146 (1.54-1.50)
RSRZ outliers	127900	3943 (1.54-1.50)

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 ≥ 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	215	<div> <div>3%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
1	D	215	<div> <div>%</div> <div> <div></div> <div>94%</div> <div>5%</div> </div> </div>
2	B	243	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>10%</div> <div>5%</div> </div> </div>
2	E	243	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>• 5%</div> </div> </div>
3	C	33	<div> <div>6%</div> <div> <div></div> <div>79%</div> <div>12%</div> <div>9%</div> </div> </div>
3	F	33	<div> <div>9%</div> <div> <div></div> <div>91%</div> <div>9%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 15049 atoms, of which 6980 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 Fab Light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	214	Total	C	H	N	O	S	0	0	0
			3223	1018	1594	274	331	6			
1	D	214	Total	C	H	N	O	S	0	0	0
			3212	1018	1583	274	331	6			

- Molecule 2 is a protein called Fab Heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	231	Total	C	H	N	O	S	0	0	0
			3385	1104	1651	286	338	6			
2	E	232	Total	C	H	N	O	S	0	0	0
			3430	1113	1683	287	341	6			

- Molecule 3 is a protein called Terminase, large subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	F	33	Total	C	H	N	O	S	0	0	0
			524	167	250	42	64	1			
3	C	30	Total	C	H	N	O	S	0	0	0
			468	153	219	36	59	1			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	206	Total	O	0	0
			206	206		
4	B	166	Total	O	0	0
			166	166		
4	D	190	Total	O	0	0
			190	190		
4	E	197	Total	O	0	0
			197	197		

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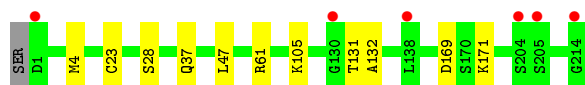
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	F	29	Total	O	0	0
			29	29		
4	C	19	Total	O	0	0
			19	19		

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.

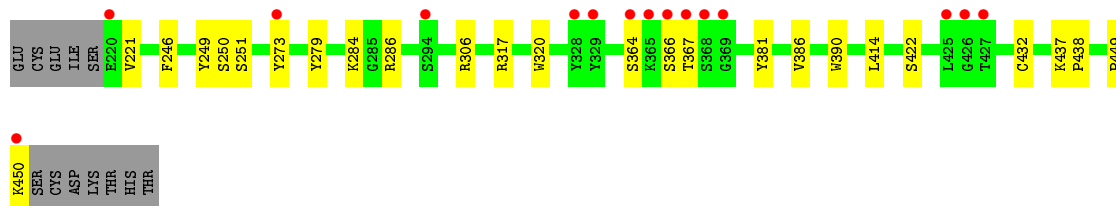
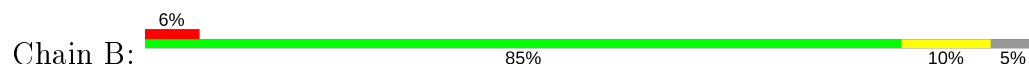
- Molecule 1: Fab Light chain



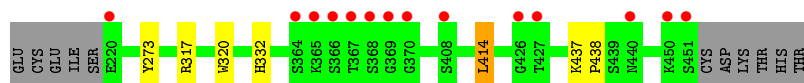
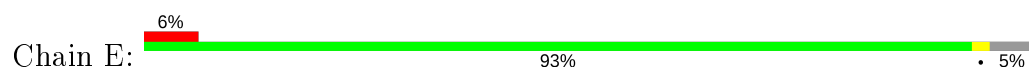
- Molecule 1: Fab Light chain



- Molecule 2: Fab Heavy chain

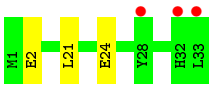


- Molecule 2: Fab Heavy chain

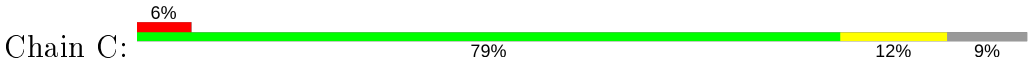


- Molecule 3: Terminase, large subunit





● Molecule 3: Terminase, large subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	74.18Å 86.39Å 86.15Å 90.00° 97.72° 90.00°	Depositor
Resolution (Å)	14.98 – 1.51 14.98 – 1.51	Depositor EDS
% Data completeness (in resolution range)	94.5 (14.98-1.51) 95.5 (14.98-1.51)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.91 (at 1.51Å)	Xtriage
Refinement program	PHENIX 1.16	Depositor
R, R_{free}	0.167 , 0.203 0.171 , 0.205	Depositor DCC
R_{free} test set	1994 reflections (1.23%)	wwPDB-VP
Wilson B-factor (Å ²)	22.8	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	15049	wwPDB-VP
Average B, all atoms (Å ²)	37.0	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 22.22 % 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 5.9586e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

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	0.57	0/1663	0.69	0/2257
1	D	0.59	0/1663	0.70	0/2257
2	B	0.57	0/1784	0.68	0/2436
2	E	0.57	0/1798	0.70	0/2455
3	C	0.70	0/249	0.73	0/335
3	F	0.65	0/275	0.63	0/371
All	All	0.58	0/7432	0.69	0/10111

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

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	1629	1594	1596	8	0
1	D	1629	1583	1596	8	0
2	B	1734	1651	1675	18	0
2	E	1747	1683	1687	4	0
3	C	249	219	230	5	0
3	F	274	250	250	3	0
4	A	206	0	0	0	0
4	B	166	0	0	4	0
4	C	19	0	0	1	0
4	D	190	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	197	0	0	1	0
4	F	29	0	0	0	0
All	All	8069	6980	7034	41	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 3.

All (41) 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:D:192:LYS:NZ	4:D:301:HOH:O	2.20	0.75
1:D:89:GLN:NE2	1:D:98:LEU:HD23	2.09	0.68
2:B:251:SER:N	4:B:501:HOH:O	2.27	0.66
2:E:320:TRP:CH2	3:F:2:GLU:HG2	2.34	0.62
2:B:320:TRP:HB2	4:B:501:HOH:O	2.01	0.61
1:A:105:LYS:HD3	1:A:105:LYS:N	2.20	0.56
2:B:449:PRO:O	2:B:450:LYS:HB2	2.07	0.55
2:B:320:TRP:CH2	3:C:2:GLU:HG2	2.43	0.53
2:B:250:SER:C	4:B:501:HOH:O	2.45	0.52
1:A:37:GLN:HB2	1:A:47:LEU:HD11	1.94	0.50
1:A:169:ASP:OD1	1:A:171:LYS:HG2	2.11	0.50
2:B:320:TRP:CZ2	3:C:2:GLU:HG2	2.47	0.49
1:D:201:GLN:HA	3:C:28:TYR:O	2.12	0.49
2:E:332:HIS:CD2	4:E:635:HOH:O	2.65	0.48
2:B:279:TYR:HB2	2:B:284:LYS:HG3	1.96	0.48
2:E:414:LEU:HD12	2:E:414:LEU:C	2.34	0.48
2:B:306:ARG:NH2	4:B:505:HOH:O	2.46	0.47
3:F:21:LEU:O	3:F:24:GLU:HG2	2.15	0.47
1:D:4:MET:HB3	1:D:23:CYS:SG	2.55	0.47
2:E:437:LYS:N	2:E:438:PRO:CD	2.79	0.46
1:D:20:THR:HG23	1:D:72:THR:HG23	1.98	0.46
1:A:4:MET:HB3	1:A:23:CYS:SG	2.57	0.45
3:C:26:GLU:OE2	4:C:101:HOH:O	2.21	0.44
1:A:169:ASP:OD1	1:A:171:LYS:CG	2.66	0.43
2:B:286:ARG:NH1	2:B:306:ARG:HD2	2.34	0.43
2:B:414:LEU:C	2:B:414:LEU:HD12	2.39	0.43
1:D:20:THR:HG23	1:D:72:THR:CG2	2.47	0.43
2:B:381:TYR:CE2	2:B:386:VAL:HG13	2.53	0.43
2:B:221:VAL:HG13	2:B:246:PHE:CD1	2.54	0.43
2:B:364:SER:O	2:B:366:SER:N	2.43	0.42
2:B:437:LYS:N	2:B:438:PRO:CD	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:250:SER:OG	2:B:320:TRP:HB3	2.20	0.42
1:D:182:THR:HB	4:D:428:HOH:O	2.20	0.41
1:A:61:ARG:HG3	1:A:61:ARG:NH1	2.35	0.41
2:B:390:TRP:CH2	2:B:432:CYS:HB3	2.56	0.41
1:A:28:SER:HB2	3:C:27:ASN:HD22	1.86	0.41
2:B:250:SER:HG	2:B:320:TRP:HB3	1.87	0.40
1:D:40:PRO:CB	1:D:167:GLU:HG3	2.52	0.40
1:A:131:THR:HG22	1:A:132:ALA:N	2.36	0.40
2:B:367:THR:O	2:B:422:SER:CB	2.69	0.40
3:F:21:LEU:HA	3:F:24:GLU:HG2	2.03	0.40

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	212/215 (99%)	206 (97%)	6 (3%)	0	100	100
1	D	212/215 (99%)	207 (98%)	5 (2%)	0	100	100
2	B	229/243 (94%)	224 (98%)	5 (2%)	0	100	100
2	E	230/243 (95%)	225 (98%)	5 (2%)	0	100	100
3	C	28/33 (85%)	28 (100%)	0	0	100	100
3	F	31/33 (94%)	31 (100%)	0	0	100	100
All	All	942/982 (96%)	921 (98%)	21 (2%)	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	188/189 (100%)	188 (100%)	0	100	100
1	D	188/189 (100%)	188 (100%)	0	100	100
2	B	192/205 (94%)	189 (98%)	3 (2%)	62	35
2	E	194/205 (95%)	191 (98%)	3 (2%)	65	38
3	C	28/32 (88%)	28 (100%)	0	100	100
3	F	31/32 (97%)	31 (100%)	0	100	100
All	All	821/852 (96%)	815 (99%)	6 (1%)	84	69

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	249	TYR
2	B	273	TYR
2	B	317	ARG
2	E	273	TYR
2	E	317	ARG
2	E	414	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	89	GLN
2	E	435	ASN

5.3.3 RNA ⓘ

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, 95th 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	A	214/215 (99%)	0.05	6 (2%) 53 58	20, 29, 46, 61	0
1	D	214/215 (99%)	0.05	3 (1%) 75 79	18, 29, 49, 64	0
2	B	231/243 (95%)	0.37	15 (6%) 18 20	21, 33, 63, 104	0
2	E	232/243 (95%)	0.20	14 (6%) 21 24	20, 30, 57, 90	0
3	C	30/33 (90%)	0.40	2 (6%) 17 19	27, 40, 54, 93	0
3	F	33/33 (100%)	0.63	3 (9%) 9 10	25, 35, 61, 91	0
All	All	954/982 (97%)	0.19	43 (4%) 33 36	18, 30, 54, 104	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	33	LEU	15.5
2	B	366	SER	9.3
2	E	369	GLY	6.8
2	E	427	THR	6.5
2	B	367	THR	6.4
2	E	367	THR	6.1
3	C	29	ARG	5.7
2	B	329	TYR	5.2
2	E	408	SER	5.0
2	E	451	SER	5.0
1	D	214	GLY	4.8
2	B	368	SER	4.5
3	C	30	ASN	4.5
2	E	364	SER	4.2
2	E	368	SER	4.1
2	B	364	SER	4.1
2	E	365	LYS	3.8
2	B	365	LYS	3.7
1	A	214	GLY	3.6

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Mol	Chain	Res	Type	RSRZ
2	B	427	THR	3.4
2	B	220	GLU	3.3
2	B	273	TYR	3.2
2	B	450	LYS	3.2
1	A	1	ASP	3.1
1	D	128	LYS	3.1
2	E	370	GLY	3.0
2	B	328	TYR	2.9
2	E	366	SER	2.9
2	B	369	GLY	2.8
2	B	426	GLY	2.8
1	A	204	SER	2.6
2	E	426	GLY	2.6
2	E	220	GLU	2.6
1	D	204	SER	2.6
2	E	450	LYS	2.5
3	F	28	TYR	2.4
1	A	205	SER	2.4
3	F	32	HIS	2.3
2	B	425	LEU	2.3
1	A	138	LEU	2.2
2	B	294	SER	2.1
1	A	130	GLY	2.1
2	E	440	ASN	2.1

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 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.