



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 19, 2016 – 07:32 PM GMT

PDB ID : 4R7D
Title : Fab Hu 15C1
Authors : Loyau, J.; Didelot, G.; Malinge, P.; Ravn, U.; Magistrelli, G.; Depoisier, J.F.;
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Deposited on : 2014-08-27
Resolution : 2.75 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
A user guide is available at
<http://wwpdb.org/validation/2016/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
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

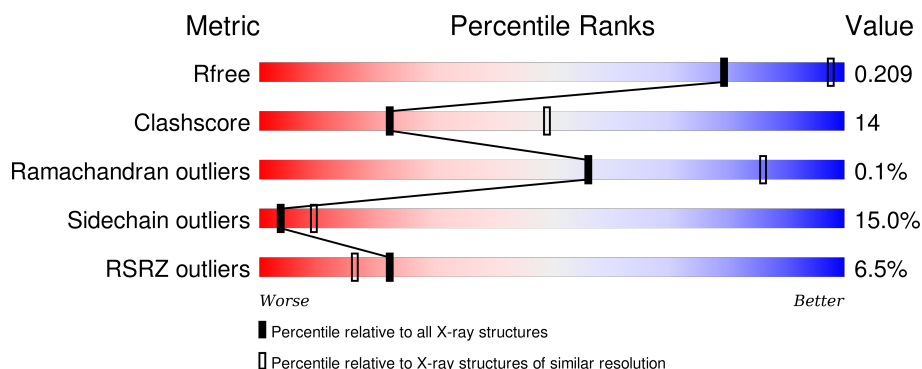
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	91344	3340 (2.80-2.72)
Clashscore	102246	3829 (2.80-2.72)
Ramachandran outliers	100387	3767 (2.80-2.72)
Sidechain outliers	100360	3770 (2.80-2.72)
RSRZ outliers	91569	3352 (2.80-2.72)

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. 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	225	
1	C	225	
1	E	225	
1	G	225	
1	I	225	

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Mol	Chain	Length	Quality of chain
1	K	225	
1	M	225	
1	O	225	
2	B	214	
2	D	214	
2	F	214	
2	H	214	
2	J	214	
2	L	214	
2	N	214	
2	P	214	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 26033 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 Fab Hu 15C1 Heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	218	Total	C	N	O	S	0	0	0
			1641	1042	272	322	5			
1	C	210	Total	C	N	O	S	0	0	0
			1593	1016	263	309	5			
1	E	209	Total	C	N	O	S	0	0	0
			1584	1011	261	307	5			
1	G	190	Total	C	N	O	S	0	0	0
			1445	927	236	277	5			
1	I	218	Total	C	N	O	S	0	0	0
			1641	1042	272	322	5			
1	K	201	Total	C	N	O	S	0	0	0
			1533	980	253	295	5			
1	M	201	Total	C	N	O	S	0	0	0
			1533	980	253	295	5			
1	O	209	Total	C	N	O	S	0	0	0
			1584	1011	261	307	5			

- Molecule 2 is a protein called Fab Hu 15C1 Light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	211	Total	C	N	O	S	0	0	0
			1631	1023	275	329	4			
2	D	211	Total	C	N	O	S	0	0	0
			1626	1020	275	327	4			
2	F	211	Total	C	N	O	S	0	0	0
			1626	1020	275	327	4			
2	H	212	Total	C	N	O	S	0	0	0
			1635	1025	276	330	4			
2	J	212	Total	C	N	O	S	0	0	0
			1635	1025	276	330	4			
2	L	211	Total	C	N	O	S	0	0	0
			1631	1023	275	329	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	211	Total	C	N	O	S	0	0	0
			1626	1020	275	327	4			
2	P	211	Total	C	N	O	S	0	0	0
			1626	1020	275	327	4			

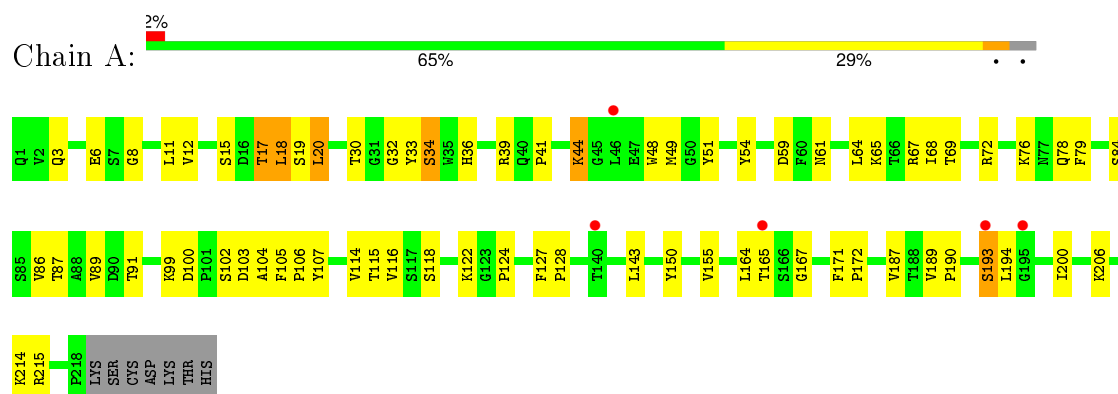
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total	O	0	0
			35	35		
3	B	25	Total	O	0	0
			25	25		
3	C	29	Total	O	0	0
			29	29		
3	D	23	Total	O	0	0
			23	23		
3	E	18	Total	O	0	0
			18	18		
3	F	22	Total	O	0	0
			22	22		
3	G	42	Total	O	0	0
			42	42		
3	H	21	Total	O	0	0
			21	21		
3	I	37	Total	O	0	0
			37	37		
3	J	28	Total	O	0	0
			28	28		
3	K	33	Total	O	0	0
			33	33		
3	L	24	Total	O	0	0
			24	24		
3	M	29	Total	O	0	0
			29	29		
3	N	32	Total	O	0	0
			32	32		
3	O	19	Total	O	0	0
			19	19		
3	P	26	Total	O	0	0
			26	26		

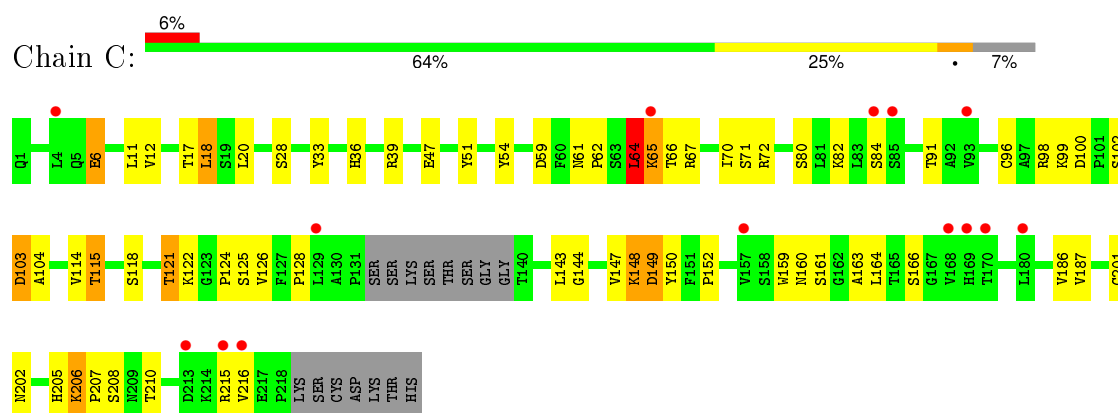
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

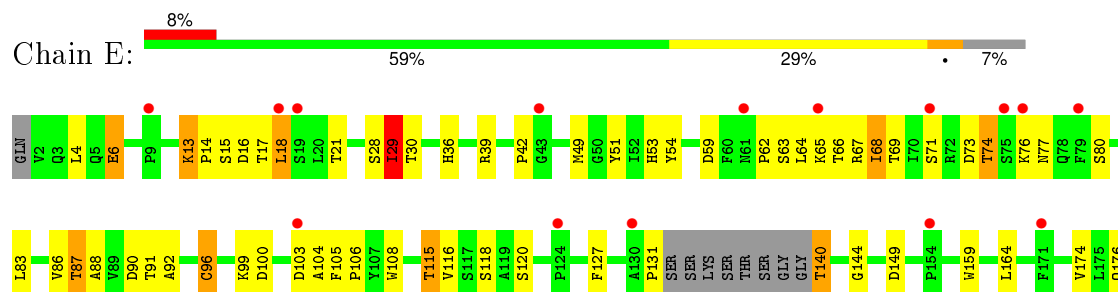
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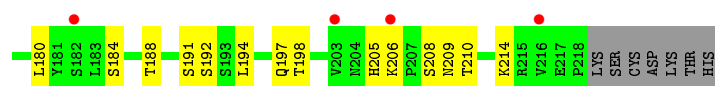


• Molecule 1: Fab Hu 15C1 Heavy chain

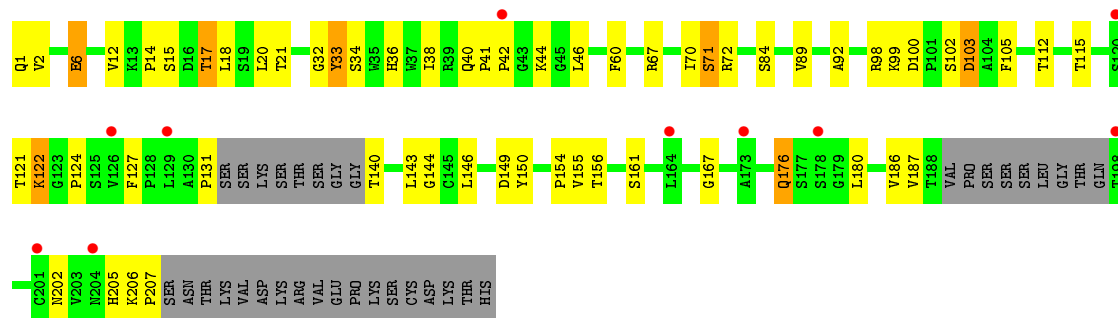


• Molecule 1: Fab Hu 15C1 Heavy chain

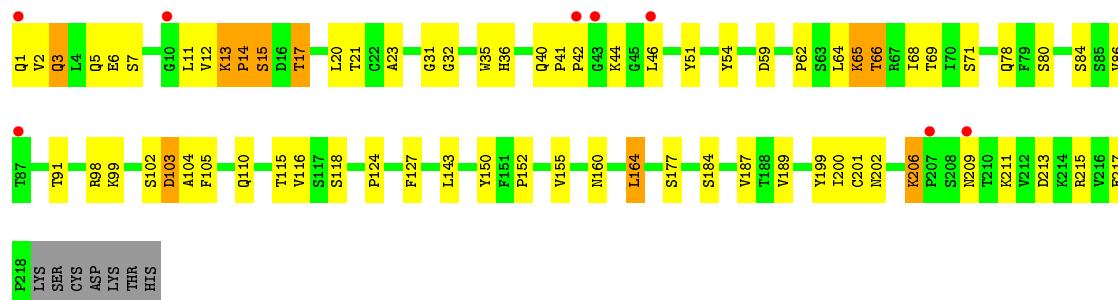




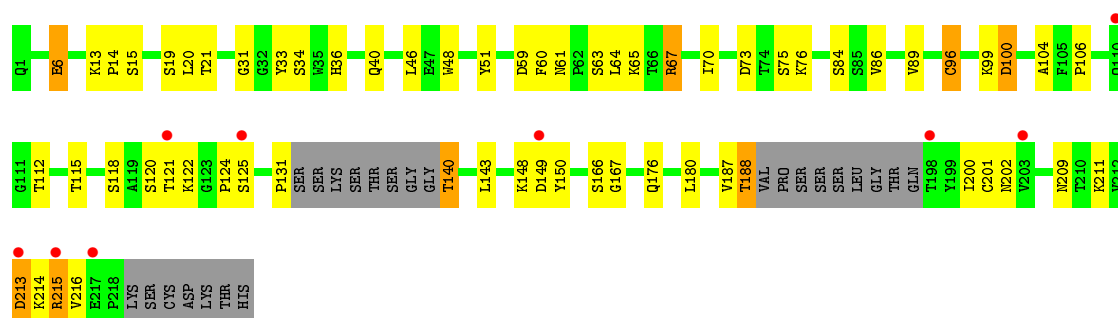
• Molecule 1: Fab Hu 15C1 Heavy chain



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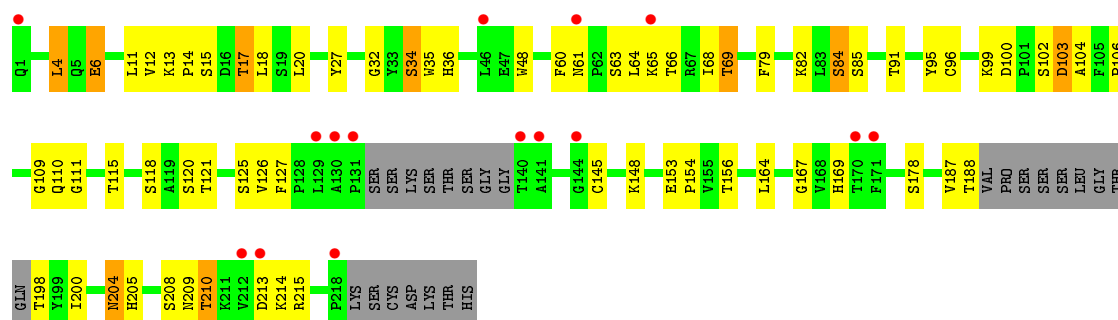


• Molecule 1: Fab Hu 15C1 Heavy chain

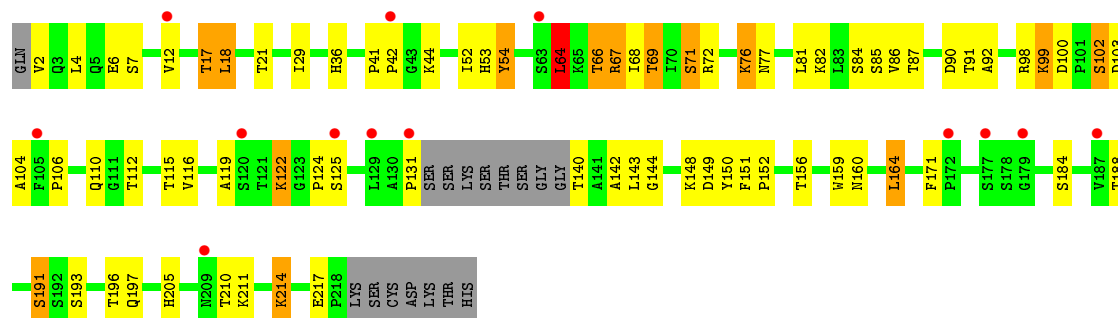


• Molecule 1: Fab Hu 15C1 Heavy chain

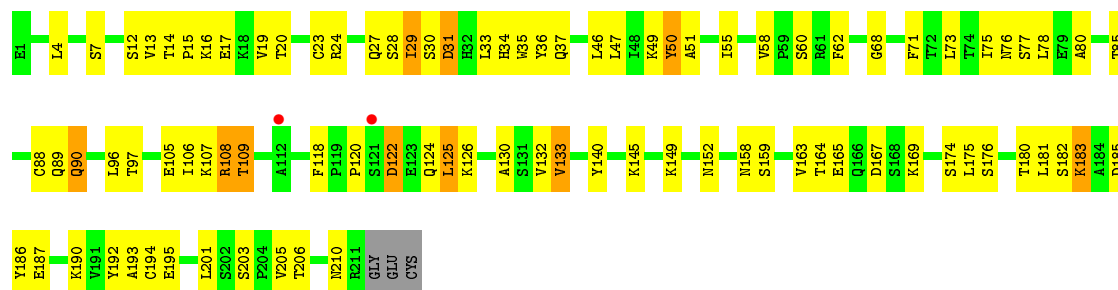




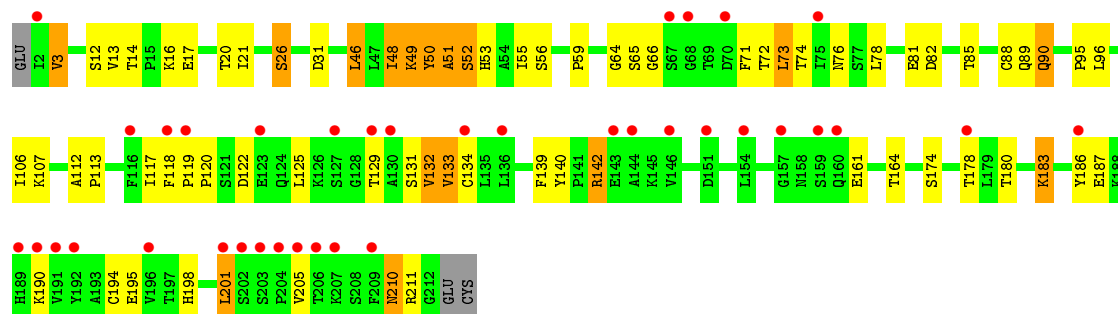
• Molecule 1: Fab Hu 15C1 Heavy chain



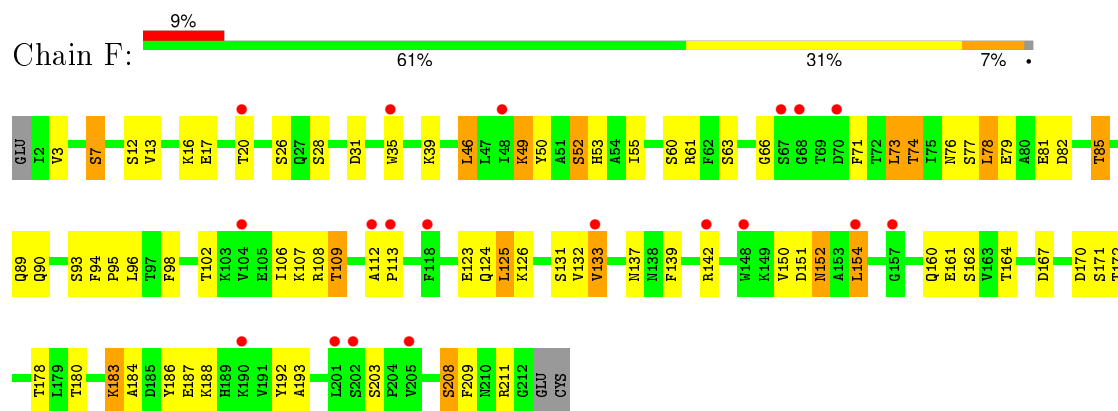
• Molecule 2: Fab Hu 15C1 Light chain



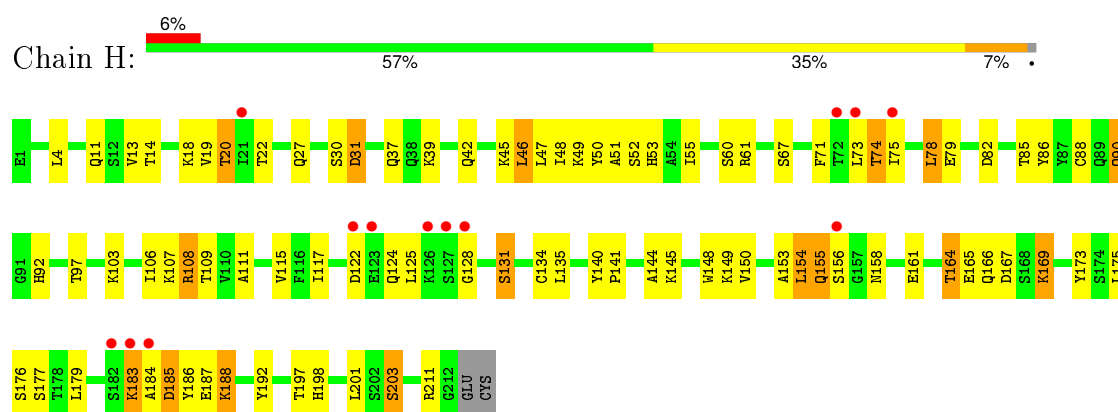
• Molecule 2: Fab Hu 15C1 Light chain



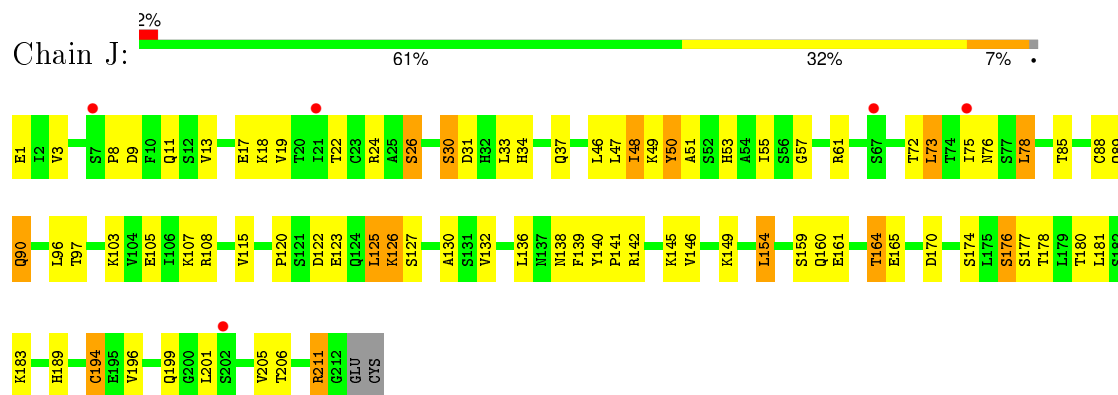
- Molecule 2: Fab Hu 15C1 Light chain



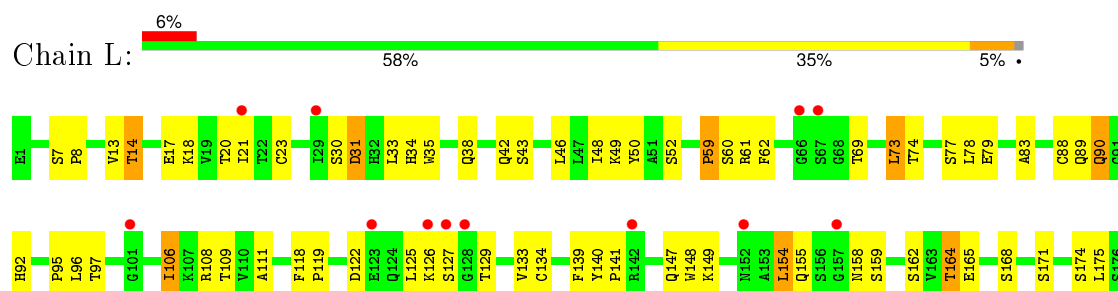
- Molecule 2: Fab Hu 15C1 Light chain

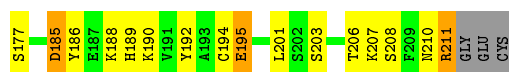


- Molecule 2: Fab Hu 15C1 Light chain

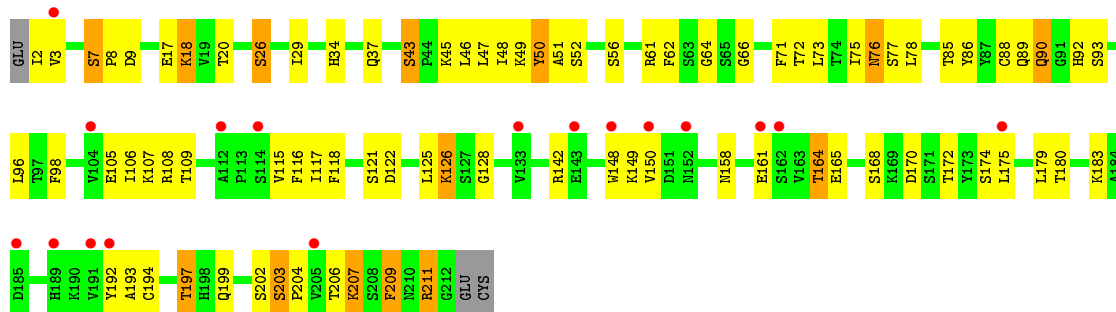


- Molecule 2: Fab Hu 15C1 Light chain

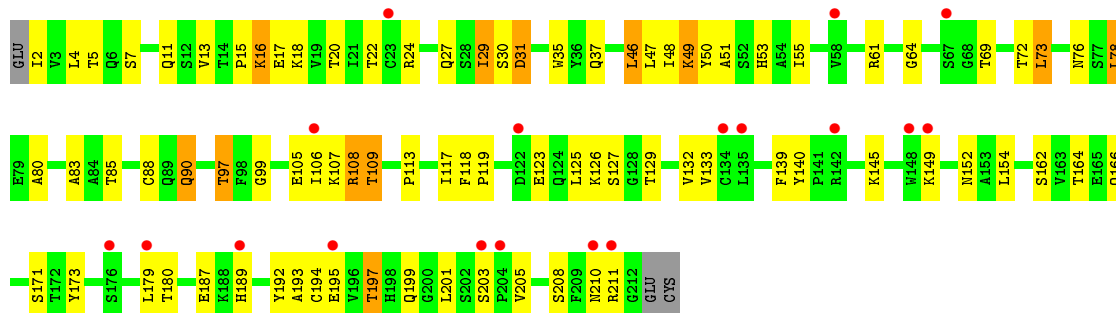




• Molecule 2: Fab Hu 15C1 Light chain



• Molecule 2: Fab Hu 15C1 Light chain



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.82Å 82.51Å 261.57Å 90.00° 101.21° 90.00°	Depositor
Resolution (Å)	15.00 – 2.75 49.74 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.8 (15.00-2.75) 98.8 (49.74-2.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.54 (at 2.77Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.177 , 0.209 0.179 , 0.209	Depositor DCC
R_{free} test set	5474 reflections (5.00%)	DCC
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.445	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 6.6	EDS
Estimated twinning fraction	0.377 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Outliers	0 of 109500 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	26033	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.11% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.58	0/1687	0.68	0/2307
1	C	0.50	0/1638	0.66	1/2241 (0.0%)
1	E	0.50	0/1629	0.69	1/2229 (0.0%)
1	G	0.55	1/1487 (0.1%)	0.69	1/2034 (0.0%)
1	I	0.57	0/1687	0.72	1/2307 (0.0%)
1	K	0.56	0/1576	0.72	2/2154 (0.1%)
1	M	0.49	0/1576	0.66	0/2154
1	O	0.50	0/1629	0.67	0/2229
2	B	0.48	0/1668	0.64	0/2265
2	D	0.47	0/1663	0.66	1/2258 (0.0%)
2	F	0.44	0/1663	0.63	0/2258
2	H	0.46	0/1672	0.64	1/2270 (0.0%)
2	J	0.64	0/1672	0.74	0/2270
2	L	0.48	0/1668	0.64	0/2265
2	N	0.53	0/1663	0.69	0/2258
2	P	0.48	0/1663	0.67	0/2258
All	All	0.52	1/26241 (0.0%)	0.67	8/35757 (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
1	C	0	1
1	O	0	1
2	D	0	2
All	All	0	4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	33	TYR	CE1-CZ	-5.35	1.31	1.38

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	18	LEU	CA-CB-CG	6.80	130.95	115.30
2	H	31	ASP	CB-CG-OD1	5.92	123.62	118.30
1	K	13	LYS	C-N-CD	5.85	140.68	128.40
1	E	13	LYS	C-N-CD	5.73	140.44	128.40
2	D	52	SER	N-CA-C	5.72	126.43	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	64	LEU	Peptide
2	D	50	TYR	Peptide
2	D	51	ALA	Peptide
1	O	64	LEU	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	1641	0	1609	44	0
1	C	1593	0	1562	38	0
1	E	1584	0	1551	46	0
1	G	1445	0	1409	29	0
1	I	1641	0	1609	43	0
1	K	1533	0	1501	34	0
1	M	1533	0	1501	38	0
1	O	1584	0	1551	44	0
2	B	1631	0	1586	47	0
2	D	1626	0	1580	45	0
2	F	1626	0	1580	46	0
2	H	1635	0	1589	52	0
2	J	1635	0	1587	66	0
2	L	1631	0	1586	46	0
2	N	1626	0	1580	54	0
2	P	1626	0	1580	50	1
3	A	35	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	25	0	0	2	0
3	C	29	0	0	3	0
3	D	23	0	0	4	0
3	E	18	0	0	4	0
3	F	22	0	0	4	0
3	G	42	0	0	4	0
3	H	21	0	0	4	1
3	I	37	0	0	4	0
3	J	28	0	0	6	0
3	K	33	0	0	5	0
3	L	24	0	0	4	0
3	M	29	0	0	3	0
3	N	32	0	0	6	0
3	O	19	0	0	6	0
3	P	26	0	0	4	0
All	All	26033	0	24961	698	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 14.

The worst 5 of 698 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:E:28:SER:O	1:E:77:ASN:ND2	1.65	1.30
1:O:149:ASP:OD2	3:O:304:HOH:O	1.76	1.04
1:M:6:GLU:OE2	1:M:109:GLY:HA3	1.66	0.96
1:I:32:GLY:HA3	1:I:54:TYR:HB3	1.48	0.95
1:O:99:LYS:HD2	1:O:103:ASP:HB2	1.45	0.95

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)
2:P:17:GLU:OE2	3:H:303:HOH:O[1_455]	2.01	0.19

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	216/225 (96%)	205 (95%)	11 (5%)	0	100	100
1	C	206/225 (92%)	192 (93%)	13 (6%)	1 (0%)	34	67
1	E	205/225 (91%)	194 (95%)	10 (5%)	1 (0%)	34	67
1	G	184/225 (82%)	172 (94%)	12 (6%)	0	100	100
1	I	216/225 (96%)	203 (94%)	13 (6%)	0	100	100
1	K	195/225 (87%)	183 (94%)	12 (6%)	0	100	100
1	M	195/225 (87%)	185 (95%)	10 (5%)	0	100	100
1	O	205/225 (91%)	193 (94%)	12 (6%)	0	100	100
2	B	209/214 (98%)	202 (97%)	7 (3%)	0	100	100
2	D	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
2	F	209/214 (98%)	194 (93%)	15 (7%)	0	100	100
2	H	210/214 (98%)	199 (95%)	11 (5%)	0	100	100
2	J	210/214 (98%)	198 (94%)	12 (6%)	0	100	100
2	L	209/214 (98%)	197 (94%)	11 (5%)	1 (0%)	34	67
2	N	209/214 (98%)	196 (94%)	13 (6%)	0	100	100
2	P	209/214 (98%)	200 (96%)	9 (4%)	0	100	100
All	All	3296/3512 (94%)	3113 (94%)	180 (6%)	3 (0%)	56	86

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	29	ILE
1	C	207	PRO
2	L	59	PRO

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	188/195 (96%)	165 (88%)	23 (12%)	6	16
1	C	182/195 (93%)	162 (89%)	20 (11%)	8	21
1	E	181/195 (93%)	153 (84%)	28 (16%)	3	8
1	G	163/195 (84%)	147 (90%)	16 (10%)	10	26
1	I	188/195 (96%)	159 (85%)	29 (15%)	3	9
1	K	174/195 (89%)	150 (86%)	24 (14%)	4	11
1	M	174/195 (89%)	148 (85%)	26 (15%)	4	9
1	O	181/195 (93%)	149 (82%)	32 (18%)	2	6
2	B	187/189 (99%)	154 (82%)	33 (18%)	2	6
2	D	186/189 (98%)	157 (84%)	29 (16%)	3	8
2	F	186/189 (98%)	151 (81%)	35 (19%)	2	5
2	H	187/189 (99%)	159 (85%)	28 (15%)	3	9
2	J	187/189 (99%)	162 (87%)	25 (13%)	5	12
2	L	187/189 (99%)	154 (82%)	33 (18%)	2	6
2	N	186/189 (98%)	158 (85%)	28 (15%)	3	9
2	P	186/189 (98%)	157 (84%)	29 (16%)	3	8
All	All	2923/3072 (95%)	2485 (85%)	438 (15%)	3	9

5 of 438 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	108	ARG
2	J	48	ILE
1	O	191	SER
2	H	155	GLN
1	I	65	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	90	GLN
2	H	124	GLN
2	J	90	GLN
1	G	3	GLN
2	H	11	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 carbohydrates 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	218/225 (96%)	0.09	5 (2%) 64 57	29, 42, 55, 64	0
1	C	210/225 (93%)	0.46	14 (6%) 21 15	38, 55, 84, 97	0
1	E	209/225 (92%)	0.63	19 (9%) 11 8	43, 58, 70, 80	0
1	G	190/225 (84%)	0.32	10 (5%) 30 23	28, 43, 71, 81	0
1	I	218/225 (96%)	0.20	8 (3%) 45 38	27, 42, 53, 68	0
1	K	201/225 (89%)	0.22	9 (4%) 37 30	30, 45, 62, 76	0
1	M	201/225 (89%)	0.45	15 (7%) 17 12	36, 54, 74, 85	0
1	O	209/225 (92%)	0.41	13 (6%) 24 18	41, 56, 68, 74	0
2	B	211/214 (98%)	0.14	2 (0%) 85 82	36, 49, 66, 78	0
2	D	211/214 (98%)	0.94	37 (17%) 2 1	36, 56, 75, 83	0
2	F	211/214 (98%)	0.53	19 (9%) 12 8	39, 52, 69, 79	0
2	H	212/214 (99%)	0.36	13 (6%) 25 18	32, 52, 78, 84	0
2	J	212/214 (99%)	0.23	5 (2%) 62 56	34, 48, 66, 72	0
2	L	211/214 (98%)	0.27	12 (5%) 27 21	32, 52, 74, 82	0
2	N	211/214 (98%)	0.50	17 (8%) 15 9	33, 54, 71, 81	0
2	P	211/214 (98%)	0.44	18 (8%) 13 8	35, 49, 67, 75	0
All	All	3346/3512 (95%)	0.39	216 (6%) 22 16	27, 51, 72, 97	0

The worst 5 of 216 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	205	VAL	6.9
1	I	42	PRO	6.7
1	M	213	ASP	6.7
2	L	128	GLY	6.5
2	D	118	PHE	6.2

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 carbohydrates 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.