



wwPDB X-ray Structure Validation Summary Report

Mar 8, 2026 – 08:06 AM UTC

PDB ID : 4EVN / pdb_00004evn
Title : Crystal Structure of Fab CR6261 (somatic heavy chain with germline-reverted light chain)
Authors : Whittle, J.R.R.
Deposited on : 2012-04-26
Resolution : 2.85 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

<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 : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

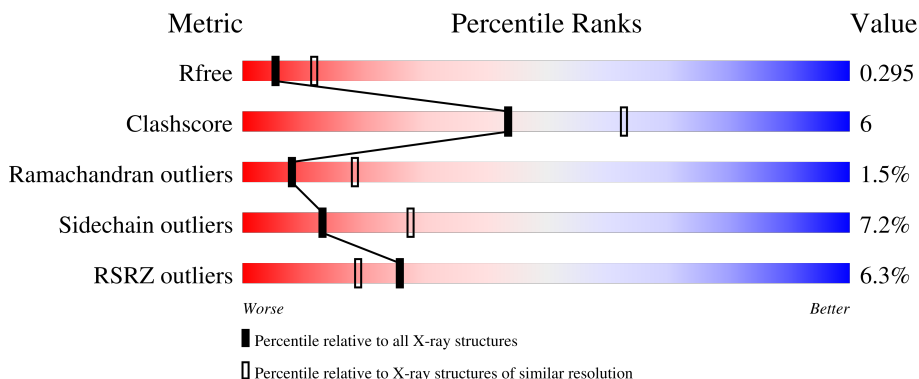
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

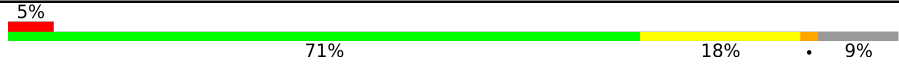
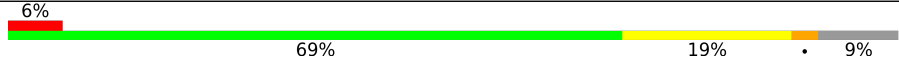



The reported resolution of this entry is 2.85 Å.

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}	180053	1407 (2.88-2.84)
Clashscore	190562	1446 (2.88-2.84)
Ramachandran outliers	187476	1406 (2.88-2.84)
Sidechain outliers	187428	1407 (2.88-2.84)
RSRZ outliers	180081	1408 (2.88-2.84)

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 $\leq 5\%$. 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	242	
1	C	242	
1	E	242	
1	G	242	
1	I	242	

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Mol	Chain	Length	Quality of chain
1	K	242	<p>7% 69% 20% 9%</p>
1	M	242	<p>4% 72% 17% 9%</p>
1	O	242	<p>9% 71% 17% 9%</p>
2	B	217	<p>6% 83% 14% ..</p>
2	D	217	<p>5% 81% 16% ..</p>
2	F	217	<p>5% 82% 14% ..</p>
2	H	217	<p>11% 83% 14% ..</p>
2	J	217	<p>5% 82% 15% ..</p>
2	L	217	<p>3% 81% 16% ..</p>
2	N	217	<p>2% 82% 15% ..</p>
2	P	217	<p>6% 83% 13% ..</p>

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 25293 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 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	C	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	E	221	Total 1625	C 1029	N 269	O 318	S 9	0	0	0
1	G	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	I	221	Total 1625	C 1029	N 269	O 318	S 9	0	0	0
1	K	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	M	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0
1	O	221	Total 1623	C 1028	N 268	O 318	S 9	0	0	0

- Molecule 2 is a protein called Fab Lambda Light Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	213	Total 1541	C 972	N 251	O 314	S 4	0	0	0
2	D	213	Total 1537	C 969	N 250	O 314	S 4	0	0	0
2	F	213	Total 1537	C 969	N 250	O 314	S 4	0	0	0
2	H	213	Total 1537	C 969	N 250	O 314	S 4	0	0	0
2	J	213	Total 1537	C 969	N 250	O 314	S 4	0	0	0
2	L	213	Total 1540	C 970	N 251	O 315	S 4	0	0	0

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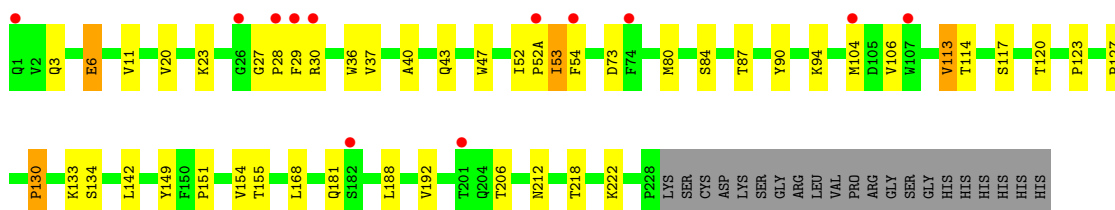
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	213	1537	969	250	314	4	0	0	0
2	P	213	1539	970	251	314	4	0	0	0

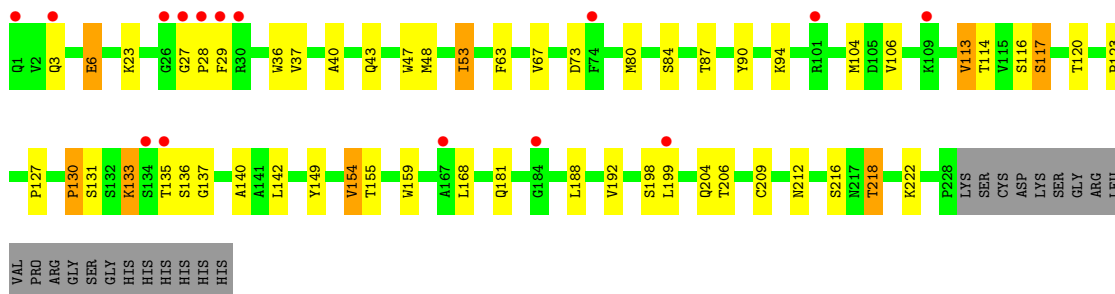
3 Residue-property plots [i](#)

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.

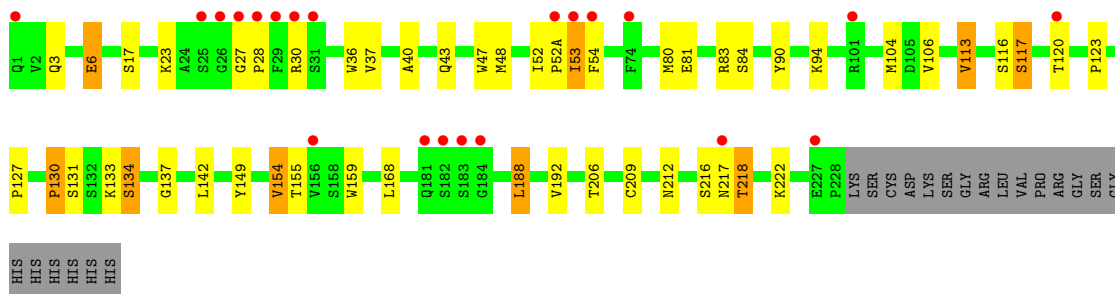
- Molecule 1: Fab Heavy Chain



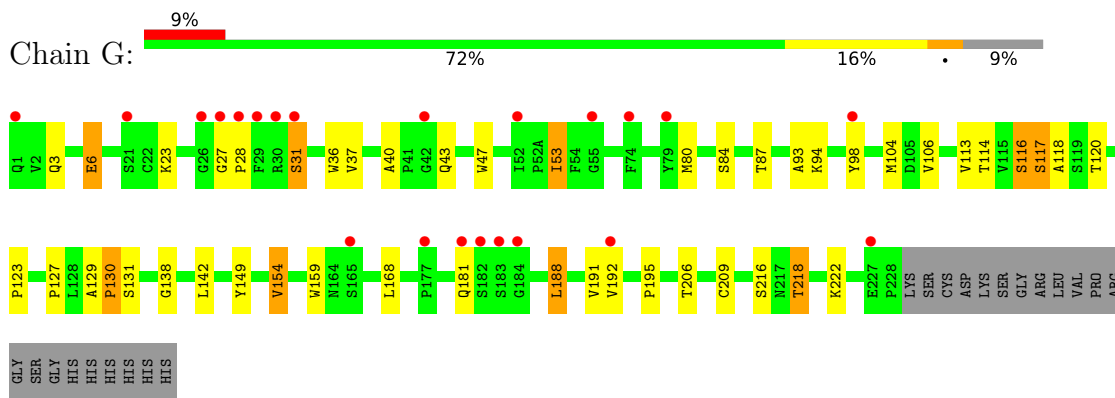
- Molecule 1: Fab Heavy Chain



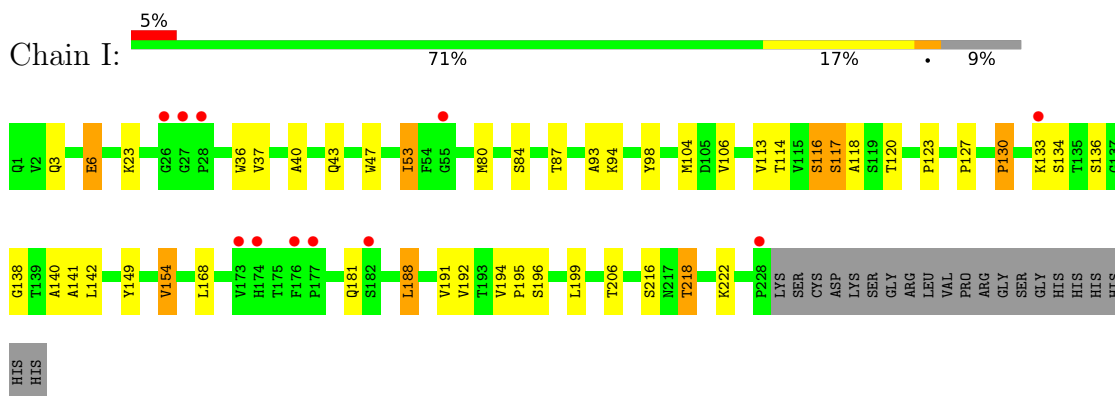
- Molecule 1: Fab Heavy Chain



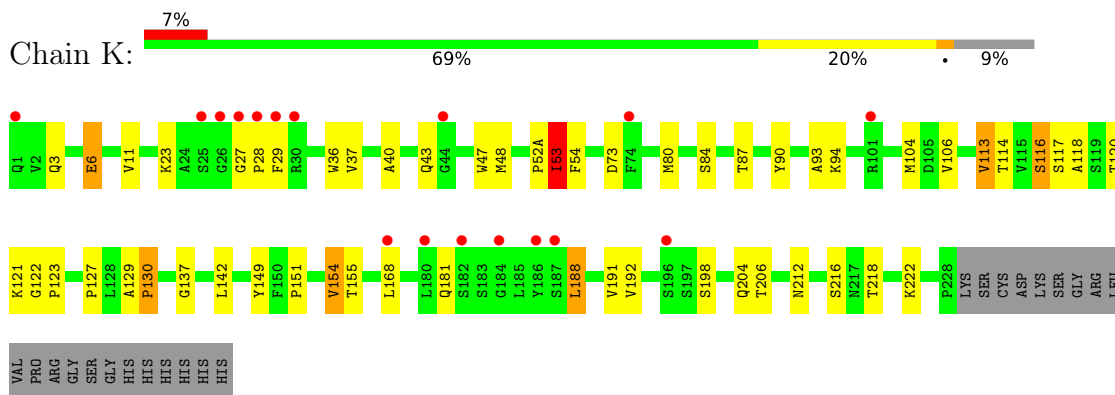
- Molecule 1: Fab Heavy Chain



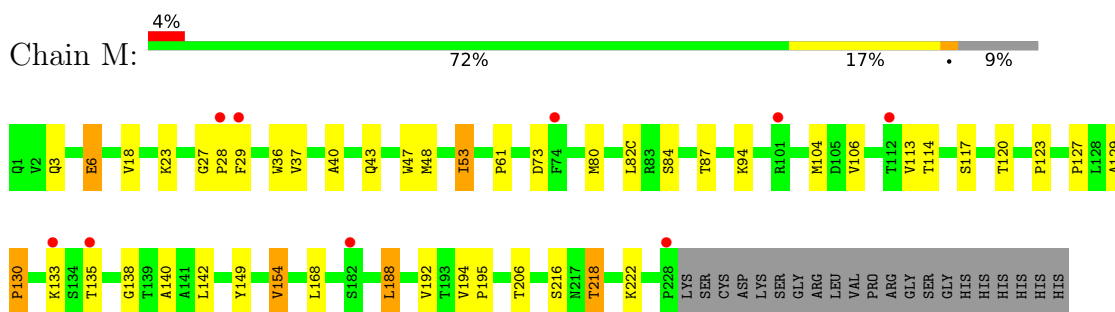
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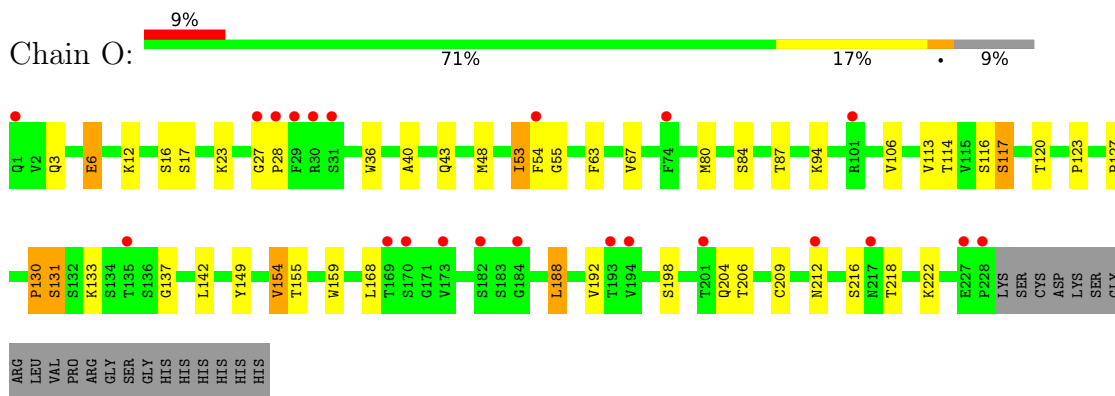
- Molecule 1: Fab Heavy Chain



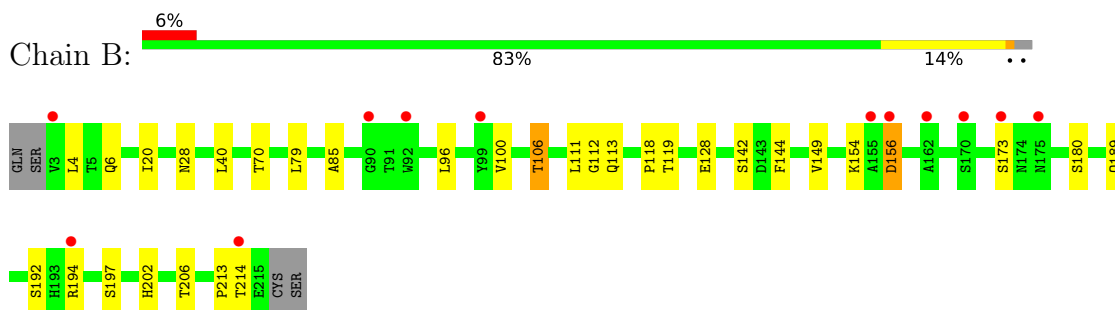
- Molecule 1: Fab Heavy Chain



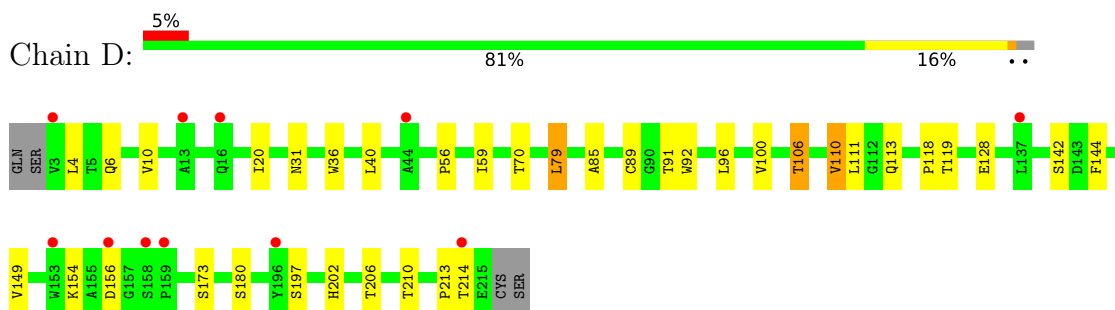
- Molecule 1: Fab Heavy Chain



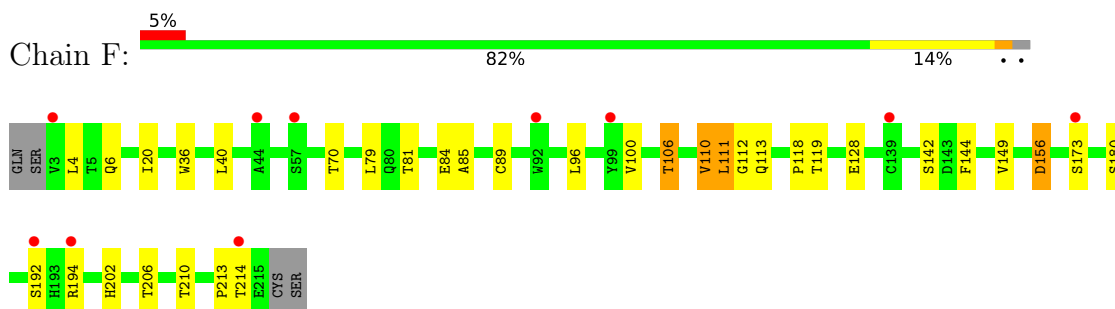
- Molecule 2: Fab Lambda Light Chain



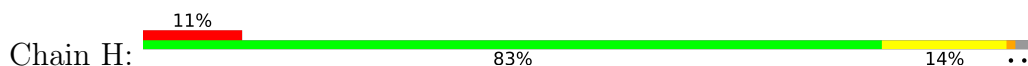
- Molecule 2: Fab Lambda Light Chain

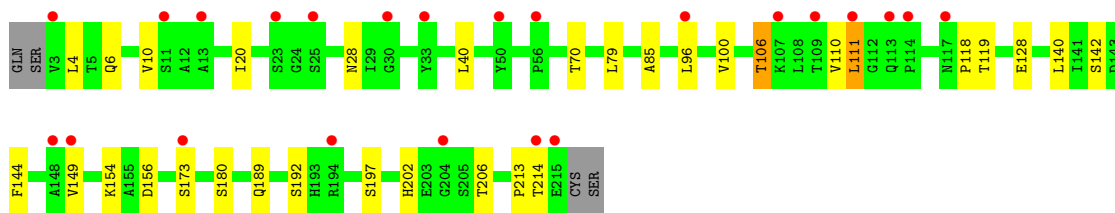


- Molecule 2: Fab Lambda Light Chain

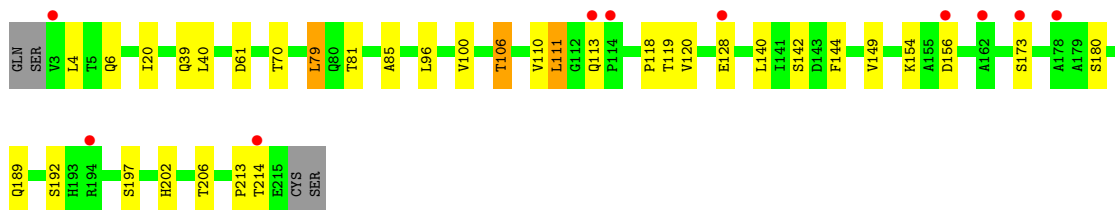
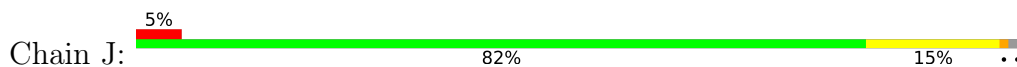


- Molecule 2: Fab Lambda Light Chain

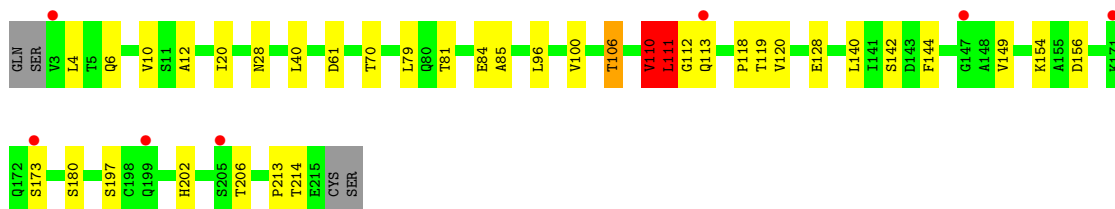
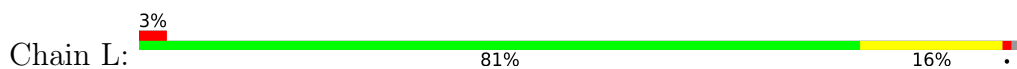




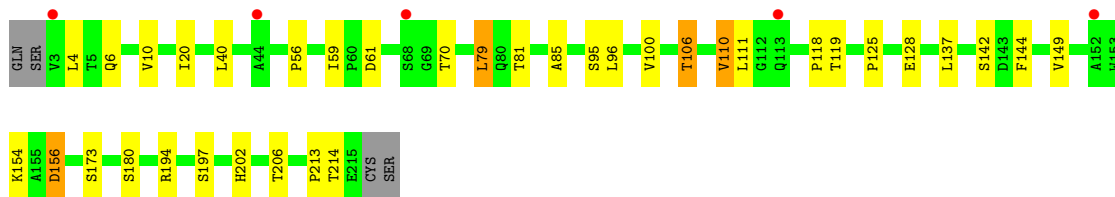
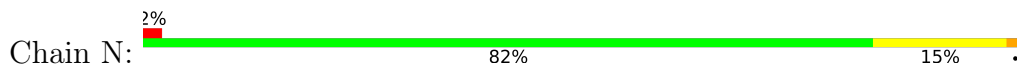
- Molecule 2: Fab Lambda Light Chain



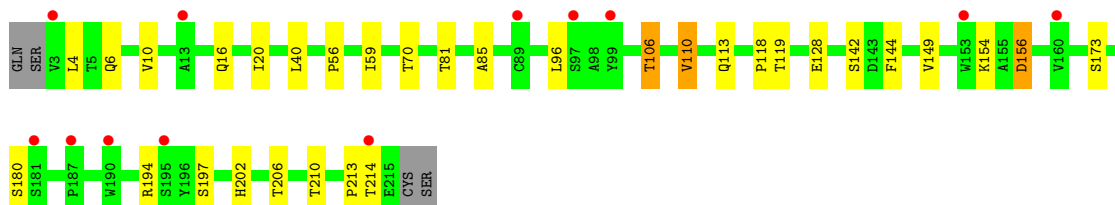
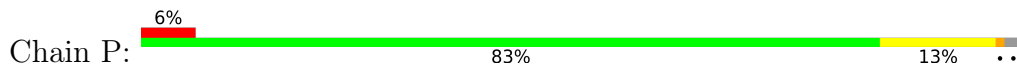
- Molecule 2: Fab Lambda Light Chain



- Molecule 2: Fab Lambda Light Chain



- Molecule 2: Fab Lambda 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	70.11Å 159.27Å 176.44Å 90.00° 89.73° 90.00°	Depositor
Resolution (Å)	55.01 – 2.85 55.01 – 2.85	Depositor EDS
% Data completeness (in resolution range)	96.3 (55.01-2.85) 93.4 (55.01-2.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.17	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.79 (at 2.86Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.230 , 0.293 0.227 , 0.295	Depositor DCC
R_{free} test set	2024 reflections (2.33%)	wwPDB-VP
Wilson B-factor (Å ²)	53.9	Xtrriage
Anisotropy	0.454	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 58.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.069 for h,-k,-l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	25293	wwPDB-VP
Average B, all atoms (Å ²)	75.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 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	0.60	0/1664	0.88	0/2270
1	C	0.70	3/1664 (0.2%)	0.94	0/2270
1	E	0.73	2/1666 (0.1%)	0.96	0/2272
1	G	0.63	1/1664 (0.1%)	0.89	2/2270 (0.1%)
1	I	0.67	2/1666 (0.1%)	0.90	1/2272 (0.0%)
1	K	0.67	1/1664 (0.1%)	0.93	1/2270 (0.0%)
1	M	0.61	0/1664	0.86	0/2270
1	O	0.69	2/1664 (0.1%)	0.92	1/2270 (0.0%)
2	B	0.61	1/1580 (0.1%)	0.90	1/2168 (0.0%)
2	D	0.64	0/1576	0.91	2/2164 (0.1%)
2	F	0.63	0/1576	0.91	1/2164 (0.0%)
2	H	0.60	1/1576 (0.1%)	0.85	0/2164
2	J	0.61	0/1576	0.91	1/2164 (0.0%)
2	L	0.62	1/1579 (0.1%)	0.91	3/2168 (0.1%)
2	N	0.60	0/1576	0.85	0/2164
2	P	0.59	0/1578	0.88	1/2166 (0.0%)
All	All	0.64	14/25933 (0.1%)	0.90	14/35486 (0.0%)

The worst 5 of 14 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLN	CD-NE2	7.46	1.49	1.33
1	E	116	SER	CA-C	7.24	1.61	1.52
2	L	28	ASN	CA-C	6.51	1.56	1.52
1	O	116	SER	CA-C	6.24	1.60	1.52
2	H	28	ASN	CA-C	6.23	1.56	1.52

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	113	GLN	N-CA-C	-7.74	95.69	108.23
2	F	113	GLN	N-CA-C	-6.47	101.98	110.39
2	J	120	VAL	N-CA-C	6.01	116.52	107.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	110	VAL	CB-CA-C	-6.01	104.74	111.23
1	G	116	SER	CA-C-O	5.92	126.89	120.32

There are no chirality outliers.

There are no planarity outliers.

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	1623	0	1580	22	0
1	C	1623	0	1580	25	0
1	E	1625	0	1587	35	0
1	G	1623	0	1580	31	0
1	I	1625	0	1587	26	0
1	K	1623	0	1580	32	0
1	M	1623	0	1580	21	1
1	O	1623	0	1580	25	0
2	B	1541	0	1444	11	0
2	D	1537	0	1433	18	0
2	F	1537	0	1433	15	0
2	H	1537	0	1433	11	0
2	J	1537	0	1433	16	0
2	L	1540	0	1437	16	0
2	N	1537	0	1433	18	0
2	P	1539	0	1440	12	1
All	All	25293	0	24140	303	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 6.

The worst 5 of 303 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)
2:B:192:SER:HB2	2:P:96:LEU:HD12	1.49	0.94
1:E:81:GLU:OE2	1:O:12:LYS:NZ	2.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:81:THR:HA	2:P:110:VAL:HG21	1.52	0.91
1:I:138:GLY:O	1:I:196:SER:N	2.06	0.89
2:D:96:LEU:HD12	2:F:192:SER:HB2	1.51	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:M:61:PRO:O	2:P:16:GLN:NE2[2_555]	2.08	0.12

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	219/242 (90%)	211 (96%)	6 (3%)	2 (1%)	14	28
1	C	219/242 (90%)	210 (96%)	6 (3%)	3 (1%)	9	19
1	E	219/242 (90%)	207 (94%)	9 (4%)	3 (1%)	9	19
1	G	219/242 (90%)	207 (94%)	10 (5%)	2 (1%)	14	28
1	I	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	9	19
1	K	219/242 (90%)	209 (95%)	7 (3%)	3 (1%)	9	19
1	M	219/242 (90%)	209 (95%)	8 (4%)	2 (1%)	14	28
1	O	219/242 (90%)	208 (95%)	7 (3%)	4 (2%)	6	15
2	B	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	6	14
2	D	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	9	19
2	F	211/217 (97%)	201 (95%)	7 (3%)	3 (1%)	9	19
2	H	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	6	14
2	J	211/217 (97%)	200 (95%)	7 (3%)	4 (2%)	6	14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	211/217 (97%)	199 (94%)	7 (3%)	5 (2%)	4	10
2	N	211/217 (97%)	199 (94%)	8 (4%)	4 (2%)	6	14
2	P	211/217 (97%)	202 (96%)	6 (3%)	3 (1%)	9	19
All	All	3440/3672 (94%)	3272 (95%)	116 (3%)	52 (2%)	8	18

5 of 52 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	130	PRO
2	J	111	LEU
2	L	111	LEU
2	N	111	LEU
2	B	214	THR

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	178/202 (88%)	164 (92%)	14 (8%)	11	24
1	C	178/202 (88%)	165 (93%)	13 (7%)	13	27
1	E	179/202 (89%)	165 (92%)	14 (8%)	11	25
1	G	178/202 (88%)	166 (93%)	12 (7%)	15	31
1	I	179/202 (89%)	165 (92%)	14 (8%)	11	25
1	K	178/202 (88%)	167 (94%)	11 (6%)	16	34
1	M	178/202 (88%)	164 (92%)	14 (8%)	11	24
1	O	178/202 (88%)	166 (93%)	12 (7%)	15	31
2	B	164/182 (90%)	153 (93%)	11 (7%)	15	31
2	D	163/182 (90%)	152 (93%)	11 (7%)	15	31
2	F	163/182 (90%)	151 (93%)	12 (7%)	13	26
2	H	163/182 (90%)	150 (92%)	13 (8%)	11	24
2	J	163/182 (90%)	153 (94%)	10 (6%)	17	35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	L	164/182 (90%)	151 (92%)	13 (8%)	11	24
2	N	163/182 (90%)	151 (93%)	12 (7%)	13	26
2	P	164/182 (90%)	152 (93%)	12 (7%)	13	27
All	All	2733/3072 (89%)	2535 (93%)	198 (7%)	13	28

5 of 198 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	70	THR
2	L	128	GLU
2	J	128	GLU
1	K	117	SER
1	M	23	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
2	J	32	ASN
2	L	38	GLN
2	L	32	ASN
1	M	43	GLN
1	E	43	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 oligosaccharides 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 [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, 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	221/242 (91%)	0.34	12 (5%) 31 23	35, 65, 111, 200	0
1	C	221/242 (91%)	0.30	15 (6%) 23 17	32, 60, 132, 231	0
1	E	221/242 (91%)	0.50	21 (9%) 14 11	24, 57, 123, 199	0
1	G	221/242 (91%)	0.63	22 (9%) 12 10	52, 75, 130, 200	0
1	I	221/242 (91%)	0.37	11 (4%) 34 27	38, 72, 122, 200	0
1	K	221/242 (91%)	0.55	17 (7%) 19 14	31, 64, 111, 198	0
1	M	221/242 (91%)	0.44	9 (4%) 41 32	48, 76, 133, 200	0
1	O	221/242 (91%)	0.53	22 (9%) 12 10	28, 68, 146, 199	0
2	B	213/217 (98%)	0.45	12 (5%) 30 22	38, 75, 107, 163	0
2	D	213/217 (98%)	0.35	11 (5%) 33 25	30, 64, 104, 165	0
2	F	213/217 (98%)	0.36	10 (4%) 36 28	31, 65, 105, 162	0
2	H	213/217 (98%)	0.93	23 (10%) 11 8	55, 92, 141, 207	0
2	J	213/217 (98%)	0.52	10 (4%) 36 28	42, 76, 114, 161	0
2	L	213/217 (98%)	0.38	7 (3%) 49 40	34, 71, 118, 163	0
2	N	213/217 (98%)	0.34	5 (2%) 61 52	40, 77, 113, 183	0
2	P	213/217 (98%)	0.52	12 (5%) 30 22	32, 73, 114, 164	0
All	All	3472/3672 (94%)	0.47	219 (6%) 26 19	24, 72, 123, 231	0

The worst 5 of 219 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	29	PHE	5.4
2	J	173	SER	5.1
1	C	29	PHE	5.0
1	K	28	PRO	4.9
1	O	29	PHE	4.8

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 oligosaccharides 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.