



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 04:46 AM UTC

PDB ID : 7S11 / pdb_00007s11
Title : Crystal structure of Fab in complex with mouse CD96 monomer
Authors : Lee, P.S.; Chau, B.; Strop, P.
Deposited on : 2021-08-31
Resolution : 2.58 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:

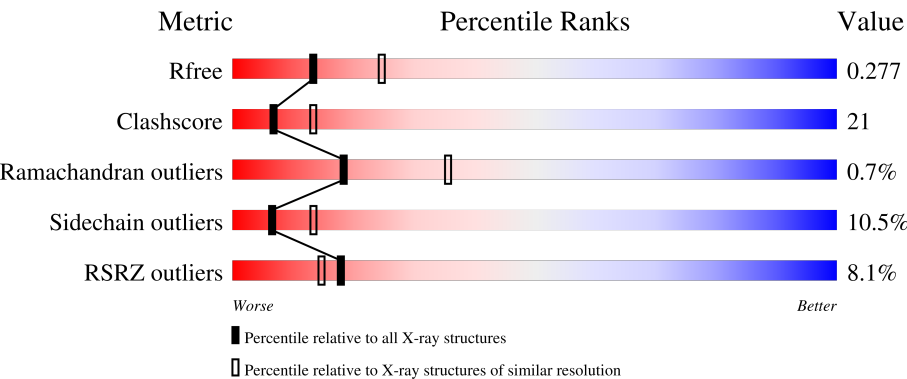
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.58 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	4770 (2.60-2.56)
Clashscore	190562	5124 (2.60-2.56)
Ramachandran outliers	187476	5046 (2.60-2.56)
Sidechain outliers	187428	5046 (2.60-2.56)
RSRZ outliers	180081	4770 (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 $\leq 5\%$. 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	C	122	2% 61% 30% 7%
1	D	122	14% 49% 37% 6% 7%
1	E	122	25% 37% 34% 6% 22%
1	F	122	30% 36% 30% 12% 5% 16%
2	H	229	10% 48% 41% 6% 5%

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Mol	Chain	Length	Quality of chain
2	I	229	59% 31% 2% 7%
2	J	229	61% 27% 4% 8%
2	K	229	51% 38% 6% 5%
3	L	216	62% 29% 4% 6%
3	M	216	59% 32% 4% 6%
3	N	216	59% 36% 6% 2%
3	O	216	69% 23% 4% 6%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 16283 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 T-cell surface protein tactile.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	113	Total	C	N	O	S	0	0	0
			897	572	142	177	6			
1	D	113	Total	C	N	O	S	0	0	0
			897	572	142	177	6			
1	E	95	Total	C	N	O	S	0	0	0
			753	482	119	146	6			
1	F	102	Total	C	N	O	S	0	0	0
			810	517	128	159	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	139	GLY	-	expression tag	UNP Q3U0X8
C	140	HIS	-	expression tag	UNP Q3U0X8
C	141	HIS	-	expression tag	UNP Q3U0X8
C	142	HIS	-	expression tag	UNP Q3U0X8
C	143	HIS	-	expression tag	UNP Q3U0X8
C	144	HIS	-	expression tag	UNP Q3U0X8
C	145	HIS	-	expression tag	UNP Q3U0X8
D	139	GLY	-	expression tag	UNP Q3U0X8
D	140	HIS	-	expression tag	UNP Q3U0X8
D	141	HIS	-	expression tag	UNP Q3U0X8
D	142	HIS	-	expression tag	UNP Q3U0X8
D	143	HIS	-	expression tag	UNP Q3U0X8
D	144	HIS	-	expression tag	UNP Q3U0X8
D	145	HIS	-	expression tag	UNP Q3U0X8
E	139	GLY	-	expression tag	UNP Q3U0X8
E	140	HIS	-	expression tag	UNP Q3U0X8
E	141	HIS	-	expression tag	UNP Q3U0X8
E	142	HIS	-	expression tag	UNP Q3U0X8
E	143	HIS	-	expression tag	UNP Q3U0X8
E	144	HIS	-	expression tag	UNP Q3U0X8
E	145	HIS	-	expression tag	UNP Q3U0X8

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Chain	Residue	Modelled	Actual	Comment	Reference
F	139	GLY	-	expression tag	UNP Q3U0X8
F	140	HIS	-	expression tag	UNP Q3U0X8
F	141	HIS	-	expression tag	UNP Q3U0X8
F	142	HIS	-	expression tag	UNP Q3U0X8
F	143	HIS	-	expression tag	UNP Q3U0X8
F	144	HIS	-	expression tag	UNP Q3U0X8
F	145	HIS	-	expression tag	UNP Q3U0X8

- Molecule 2 is a protein called Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	218	Total	C	N	O	S	0	0	0
			1630	1027	273	322	8			
2	I	214	Total	C	N	O	S	0	0	0
			1603	1012	268	315	8			
2	J	219	Total	C	N	O	S	0	0	0
			1636	1030	274	324	8			
2	K	218	Total	C	N	O	S	0	0	0
			1630	1027	273	322	8			

- Molecule 3 is a protein called Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	212	Total	C	N	O	S	0	0	0
			1591	996	268	323	4			
3	M	211	Total	C	N	O	S	0	0	0
			1582	991	266	321	4			
3	N	215	Total	C	N	O	S	0	0	0
			1614	1009	272	329	4			
3	O	211	Total	C	N	O	S	0	0	0
			1582	991	267	320	4			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

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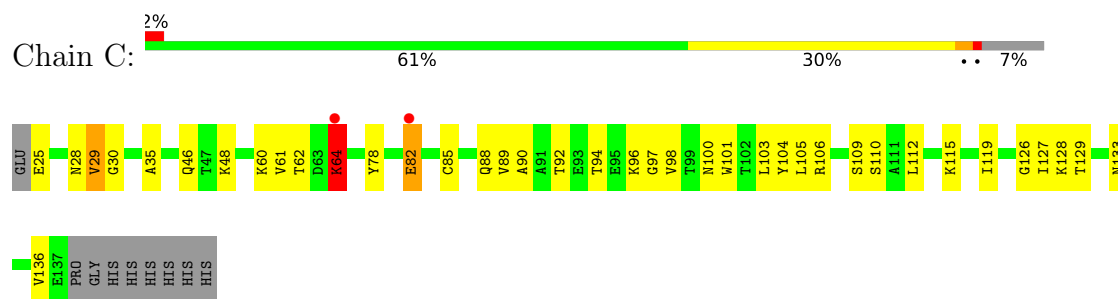
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	D	1	Total	O	S	0	0
			5	4	1		
5	D	1	Total	O	S	0	0
			5	4	1		
5	N	1	Total	O	S	0	0
			5	4	1		
5	K	1	Total	O	S	0	0
			5	4	1		

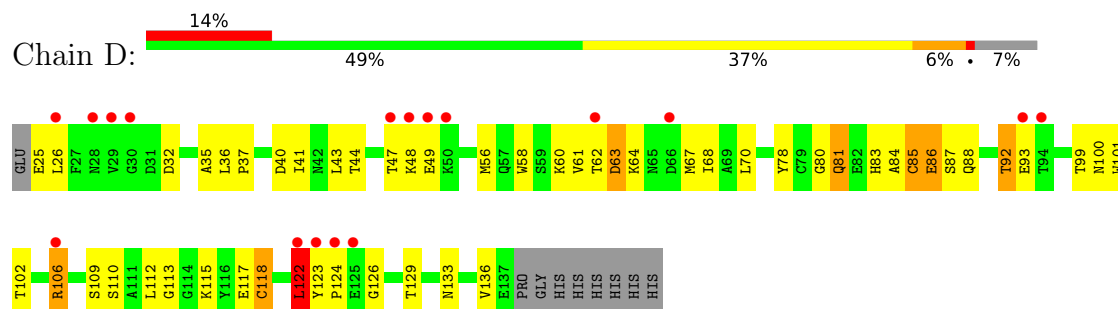
3 Residue-property plots [i](#)

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.

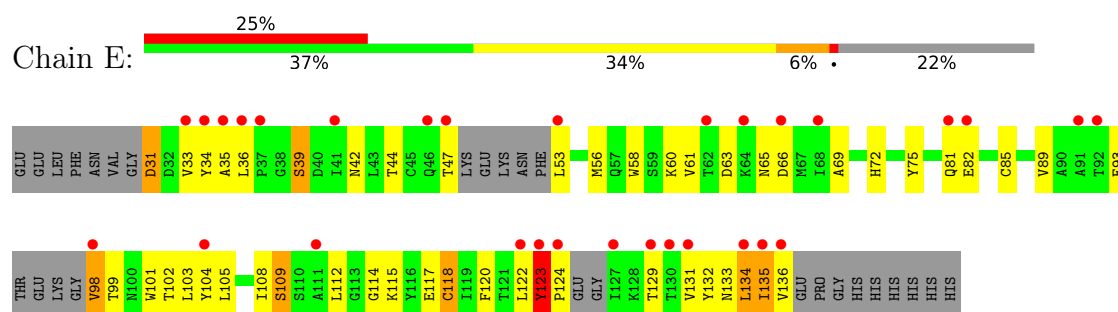
- Molecule 1: T-cell surface protein tactile



- Molecule 1: T-cell surface protein tactile

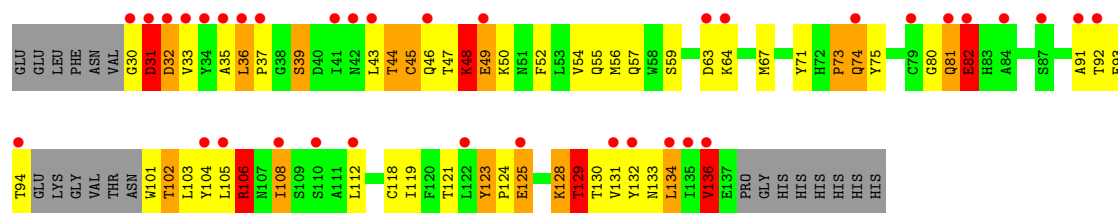


- Molecule 1: T-cell surface protein tactile

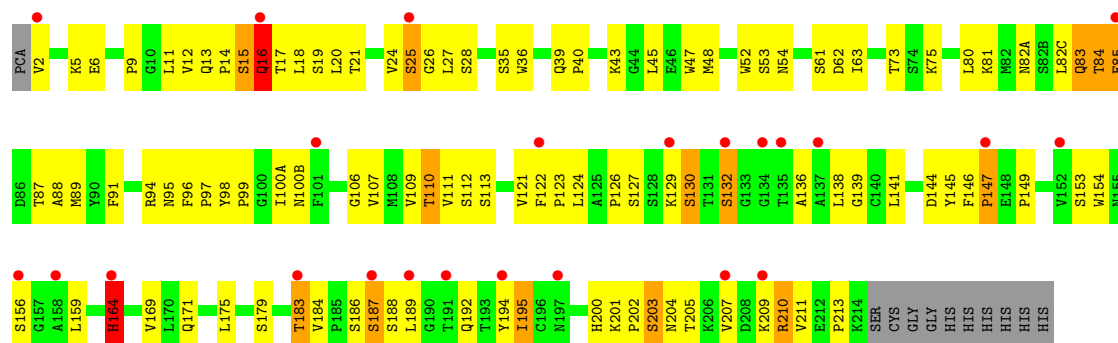


- Molecule 1: T-cell surface protein tactile

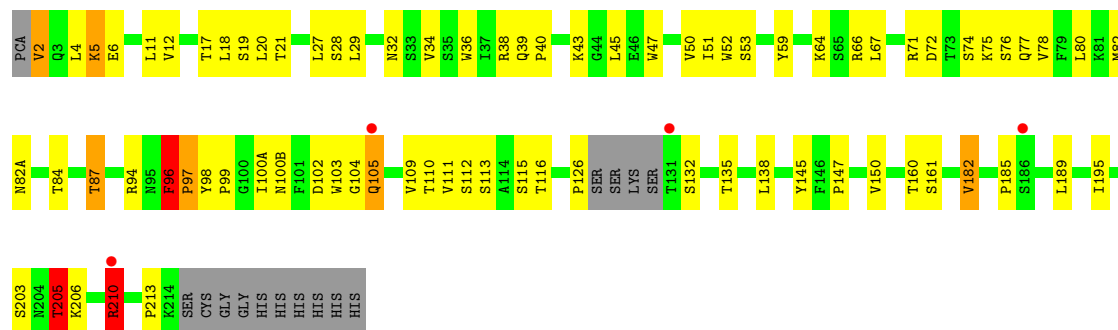




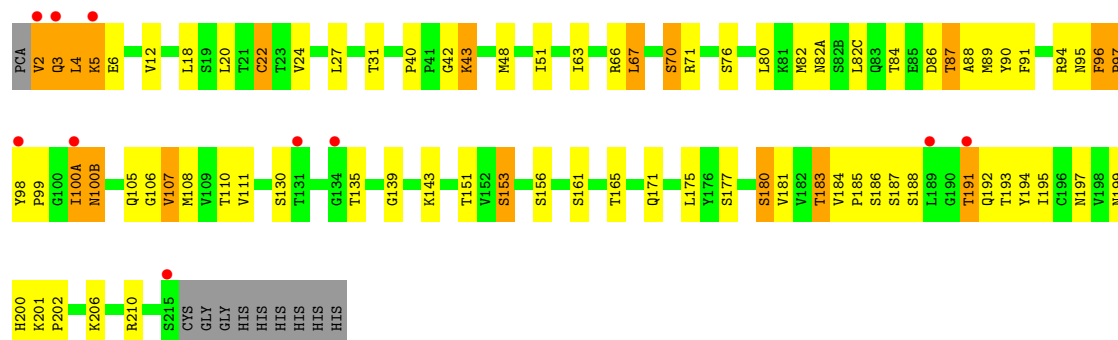
• Molecule 2: Fab heavy chain



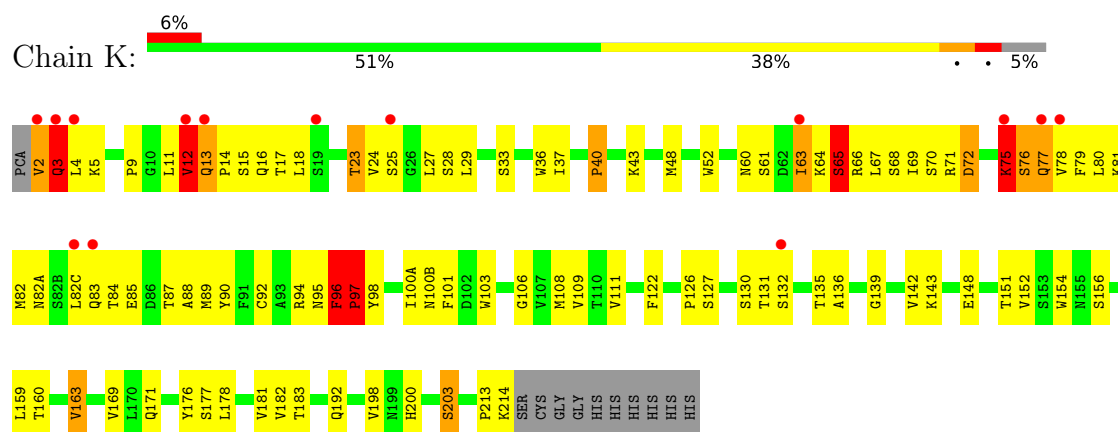
• Molecule 2: Fab heavy chain



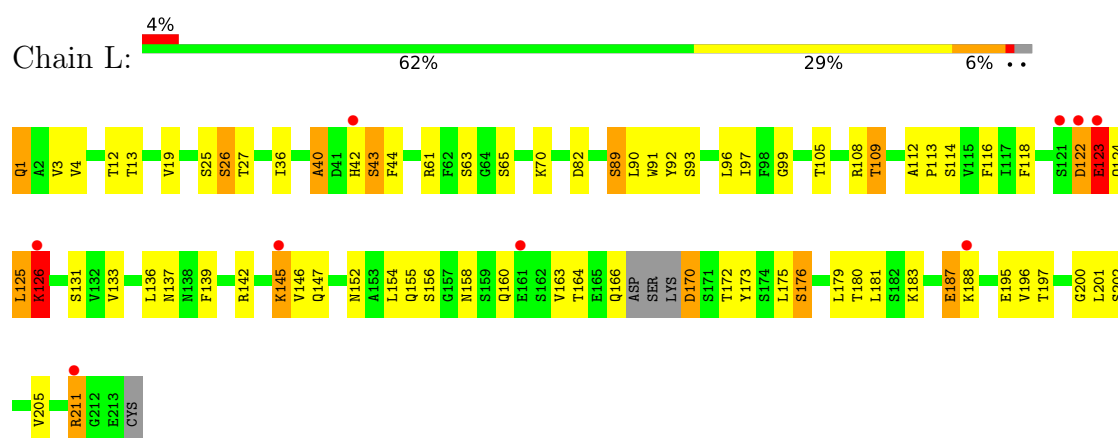
• Molecule 2: Fab heavy chain



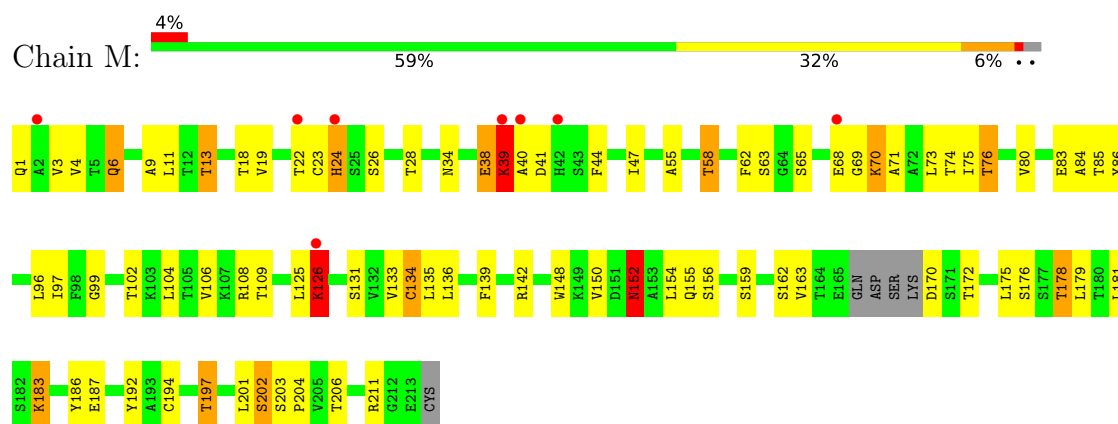
- Molecule 2: Fab heavy chain



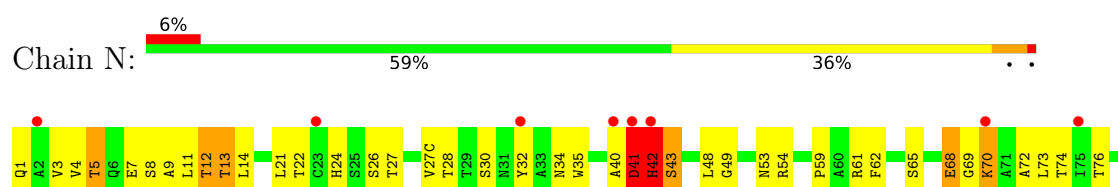
- Molecule 3: Fab light chain

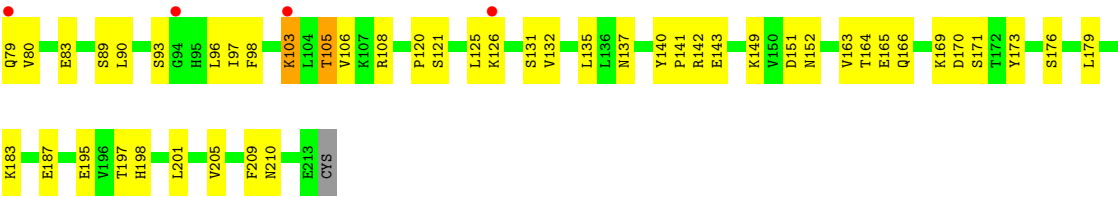


- Molecule 3: Fab light chain

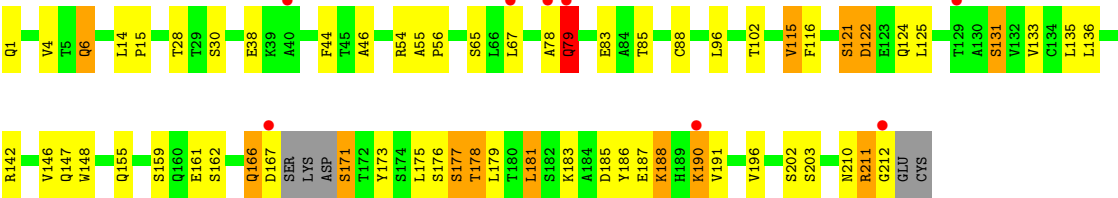


- Molecule 3: Fab light chain





● Molecule 3: Fab light chain



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	124.93Å 154.89Å 306.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	61.20 – 2.58 61.20 – 2.58	Depositor EDS
% Data completeness (in resolution range)	63.8 (61.20-2.58) 63.9 (61.20-2.58)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.49 (at 2.58Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.226 , 0.279 0.226 , 0.277	Depositor DCC
R_{free} test set	2923 reflections (3.12%)	wwPDB-VP
Wilson B-factor (Å ²)	55.2	Xtriage
Anisotropy	0.064	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 39.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	16283	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.03% 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 ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: NAG, SO4, PCA

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	C	0.57	0/916	0.86	2/1245 (0.2%)
1	D	0.63	0/916	1.34	9/1245 (0.7%)
1	E	0.38	0/767	0.63	0/1043
1	F	0.69	0/827	1.88	37/1123 (3.3%)
2	H	0.69	1/1669 (0.1%)	1.13	13/2276 (0.6%)
2	I	0.64	0/1641	1.06	16/2238 (0.7%)
2	J	0.55	0/1675	1.04	13/2284 (0.6%)
2	K	0.78	6/1669 (0.4%)	1.19	20/2276 (0.9%)
3	L	0.71	5/1616 (0.3%)	1.11	11/2201 (0.5%)
3	M	0.72	3/1607 (0.2%)	1.23	17/2189 (0.8%)
3	N	0.58	1/1640 (0.1%)	0.97	11/2234 (0.5%)
3	O	0.50	0/1607	0.93	8/2189 (0.4%)
All	All	0.64	16/16550 (0.1%)	1.13	157/22543 (0.7%)

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	D	0	2
1	E	0	2
1	F	1	4
2	H	0	3
2	I	0	3
2	J	0	2
2	K	0	4
3	L	0	3
3	M	0	4
3	N	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	O	0	1
All	All	1	31

The worst 5 of 16 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	K	77	GLN	CA-CB	11.89	1.73	1.53
2	K	40	PRO	CA-C	-9.89	1.46	1.51
2	K	75	LYS	CG-CD	-9.10	1.25	1.52
3	M	126	LYS	CD-CE	8.83	1.78	1.52
3	L	126	LYS	CE-NZ	8.05	1.73	1.49

The worst 5 of 157 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	106	ARG	CB-CG-CD	-25.30	53.10	111.30
3	M	68	GLU	CA-CB-CG	-23.39	67.33	114.10
2	K	75	LYS	CB-CA-C	-16.50	83.34	110.74
3	L	126	LYS	CB-CG-CD	-14.97	76.86	111.30
2	K	3	GLN	CA-CB-CG	14.80	143.69	114.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	F	121	THR	CB

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	64	LYS	Peptide
2	H	147	PRO	Peptide
2	H	164	HIS	Sidechain
2	H	25	SER	Peptide
3	L	40	ALA	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	C	897	0	862	30	0
1	D	897	0	862	37	0
1	E	753	0	725	38	0
1	F	810	0	777	55	0
2	H	1630	0	1613	83	0
2	I	1603	0	1584	52	0
2	J	1636	0	1618	82	0
2	K	1630	0	1612	112	0
3	L	1591	0	1544	83	0
3	M	1582	0	1536	61	0
3	N	1614	0	1567	74	0
3	O	1582	0	1538	40	0
4	C	14	0	13	0	0
4	D	14	0	13	0	0
5	C	5	0	0	1	0
5	D	10	0	0	0	0
5	K	5	0	0	1	0
5	L	5	0	0	1	0
5	N	5	0	0	0	0
All	All	16283	0	15864	689	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 21.

The worst 5 of 689 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)
3:M:126:LYS:CE	3:M:126:LYS:CD	1.78	1.59
3:L:126:LYS:NZ	3:L:126:LYS:CE	1.73	1.50
3:M:126:LYS:CE	3:M:126:LYS:CG	2.21	1.19
2:K:75:LYS:NZ	2:K:77:GLN:O	1.75	1.17
2:K:75:LYS:CD	2:K:77:GLN:HE21	1.60	1.13

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	C	111/122 (91%)	103 (93%)	7 (6%)	1 (1%)	14	29
1	D	111/122 (91%)	103 (93%)	6 (5%)	2 (2%)	6	13
1	E	87/122 (71%)	77 (88%)	10 (12%)	0	100	100
1	F	98/122 (80%)	90 (92%)	6 (6%)	2 (2%)	6	11
2	H	216/229 (94%)	207 (96%)	7 (3%)	2 (1%)	14	29
2	I	210/229 (92%)	204 (97%)	5 (2%)	1 (0%)	24	44
2	J	217/229 (95%)	205 (94%)	11 (5%)	1 (0%)	24	44
2	K	216/229 (94%)	208 (96%)	7 (3%)	1 (0%)	24	44
3	L	208/216 (96%)	194 (93%)	12 (6%)	2 (1%)	12	26
3	M	207/216 (96%)	196 (95%)	9 (4%)	2 (1%)	12	26
3	N	213/216 (99%)	198 (93%)	15 (7%)	0	100	100
3	O	207/216 (96%)	197 (95%)	9 (4%)	1 (0%)	24	44
All	All	2101/2268 (93%)	1982 (94%)	104 (5%)	15 (1%)	18	36

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	L	126	LYS
1	D	81	GLN
1	D	85	CYS
2	I	97	PRO
3	M	41	ASP

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	C	99/107 (92%)	95 (96%)	4 (4%)	28	52
1	D	99/107 (92%)	94 (95%)	5 (5%)	21	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	84/107 (78%)	73 (87%)	11 (13%)	4	7
1	F	89/107 (83%)	71 (80%)	18 (20%)	1	2
2	H	191/199 (96%)	166 (87%)	25 (13%)	4	7
2	I	187/199 (94%)	172 (92%)	15 (8%)	11	24
2	J	192/199 (96%)	171 (89%)	21 (11%)	6	12
2	K	191/199 (96%)	168 (88%)	23 (12%)	5	9
3	L	175/179 (98%)	162 (93%)	13 (7%)	13	27
3	M	174/179 (97%)	150 (86%)	24 (14%)	3	6
3	N	178/179 (99%)	164 (92%)	14 (8%)	11	24
3	O	174/179 (97%)	155 (89%)	19 (11%)	6	12
All	All	1833/1940 (94%)	1641 (90%)	192 (10%)	6	13

5 of 192 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	J	186	SER
1	F	106	ARG
3	N	5	THR
3	N	105	THR
2	K	2	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
2	K	82(A)	ASN
3	O	37	GLN
2	I	16	GLN
1	D	88	GLN
3	O	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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
3	PCA	N	1	3	7,8,9	1.92	1 (14%)	9,10,12	1.91	3 (33%)
3	PCA	M	1	3	7,8,9	2.24	1 (14%)	9,10,12	1.99	4 (44%)
3	PCA	L	1	3	7,8,9	1.91	1 (14%)	9,10,12	2.01	4 (44%)
3	PCA	O	1	3	7,8,9	2.04	1 (14%)	9,10,12	2.05	3 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PCA	N	1	3	-	0/0/11/13	0/1/1/1
3	PCA	M	1	3	-	0/0/11/13	0/1/1/1
3	PCA	L	1	3	-	0/0/11/13	0/1/1/1
3	PCA	O	1	3	-	0/0/11/13	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	1	PCA	CD-N	5.65	1.48	1.34
3	O	1	PCA	CD-N	5.18	1.47	1.34
3	N	1	PCA	CD-N	4.88	1.46	1.34
3	L	1	PCA	CD-N	4.86	1.46	1.34

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	1	PCA	OE-CD-CG	-3.41	120.64	126.72
3	N	1	PCA	CB-CA-N	3.23	112.13	103.24
3	O	1	PCA	CB-CA-N	3.19	112.01	103.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	1	PCA	CA-N-CD	-2.95	103.48	113.58
3	L	1	PCA	CB-CA-N	2.89	111.20	103.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	L	1	PCA	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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	$\# Z > 2$
5	SO4	L	301	-	4,4,4	0.35	0	6,6,6	0.23	0
5	SO4	K	301	-	4,4,4	0.38	0	6,6,6	0.22	0
5	SO4	D	202	-	4,4,4	0.42	0	6,6,6	0.18	0
4	NAG	D	201	1	14,14,15	0.37	0	17,19,21	0.61	0
5	SO4	C	202	-	4,4,4	0.36	0	6,6,6	0.38	0
5	SO4	N	301	-	4,4,4	0.20	0	6,6,6	0.42	0
4	NAG	C	201	1	14,14,15	0.45	0	17,19,21	0.48	0
5	SO4	D	203	-	4,4,4	0.34	0	6,6,6	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	201	1	-	0/6/23/26	0/1/1/1
4	NAG	D	201	1	-	0/6/23/26	0/1/1/1

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.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	301	SO4	1	0
5	K	301	SO4	1	0
5	C	202	SO4	1	0

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	C	113/122 (92%)	0.41	2 (1%) 67 64	31, 40, 53, 59	0
1	D	113/122 (92%)	0.99	17 (15%) 5 4	37, 50, 73, 77	0
1	E	95/122 (77%)	1.83	30 (31%) 1 1	60, 82, 91, 95	0
1	F	102/122 (83%)	1.81	36 (35%) 1 1	58, 80, 97, 102	0
2	H	218/229 (95%)	0.86	24 (11%) 10 8	33, 55, 83, 90	0
2	I	214/229 (93%)	0.22	4 (1%) 66 62	29, 37, 57, 64	0
2	J	219/229 (95%)	0.40	10 (4%) 37 33	31, 48, 59, 62	0
2	K	218/229 (95%)	0.70	14 (6%) 25 21	36, 54, 71, 77	0
3	L	211/216 (97%)	0.53	9 (4%) 40 35	33, 46, 68, 77	0
3	M	210/216 (97%)	0.40	8 (3%) 44 39	33, 41, 54, 61	0
3	N	214/216 (99%)	0.60	12 (5%) 30 25	30, 49, 68, 76	0
3	O	210/216 (97%)	0.38	8 (3%) 44 39	37, 44, 55, 66	0
All	All	2137/2268 (94%)	0.65	174 (8%) 18 15	29, 47, 82, 102	0

The worst 5 of 174 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	122	LEU	5.7
2	K	13	GLN	5.3
1	E	41	ILE	5.0
1	F	36	LEU	4.9
1	E	47	THR	4.9

6.2 Non-standard residues in protein, DNA, RNA chains [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, 95th 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 ²)	Q<0.9
3	PCA	N	1	8/9	0.44	0.21	82,84,85,85	0
3	PCA	M	1	8/9	0.56	0.27	68,73,74,74	0
3	PCA	O	1	8/9	0.80	0.16	58,61,64,64	0
3	PCA	L	1	8/9	0.87	0.12	46,49,50,51	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th 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 ²)	Q<0.9
5	SO4	D	202	5/5	0.68	0.21	76,79,82,86	0
4	NAG	C	201	14/15	0.74	0.14	55,61,64,65	0
5	SO4	L	301	5/5	0.78	0.17	77,81,85,86	0
4	NAG	D	201	14/15	0.79	0.13	63,69,73,74	0
5	SO4	K	301	5/5	0.84	0.18	77,77,77,77	0
5	SO4	N	301	5/5	0.94	0.07	40,41,42,42	0
5	SO4	D	203	5/5	0.96	0.08	50,54,54,54	0
5	SO4	C	202	5/5	0.97	0.06	45,45,45,47	0

6.5 Other polymers [i](#)

There are no such residues in this entry.