



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 05:33 PM UTC

PDB ID : 8ULF / pdb_00008ulf
Title : Crystal structure of Plasmodium vivax CeLTOS in complex with antibody 7g7
Authors : Tang, W.K.; Tolia, N.H.
Deposited on : 2023-10-16
Resolution : 3.20 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

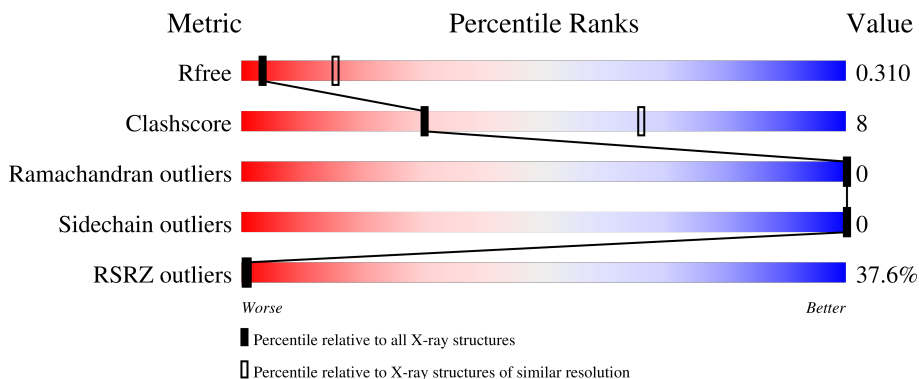
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

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	171	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">19%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 19%, orange 19%, yellow 19%, green 19%, grey 29%);"></div> <div style="text-align: center;">54%</div> <div style="text-align: center;">18%</div> <div style="text-align: center;">29%</div> </div>
1	B	171	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">24%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 24%, orange 24%, yellow 16%, green 56%, grey 29%);"></div> <div style="text-align: center;">56%</div> <div style="text-align: center;">16%</div> <div style="text-align: center;">29%</div> </div>
1	C	171	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">20%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 20%, orange 20%, yellow 17%, green 54%, grey 29%);"></div> <div style="text-align: center;">54%</div> <div style="text-align: center;">17%</div> <div style="text-align: center;">29%</div> </div>
1	D	171	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">22%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 22%, orange 22%, yellow 18%, green 54%, grey 29%);"></div> <div style="text-align: center;">54%</div> <div style="text-align: center;">18%</div> <div style="text-align: center;">29%</div> </div>
2	H	240	<div style="display: flex; justify-content: space-between; align-items: center;"> <div style="text-align: center;">36%</div> <div style="width: 100%; height: 15px; background: linear-gradient(to right, red 36%, orange 36%, yellow 15%, green 77%, grey 8%);"></div> <div style="text-align: center;">77%</div> <div style="text-align: center;">15%</div> <div style="text-align: center;">8%</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	240	<p>38% 75% 17% 8%</p>
2	J	240	<p>39% 74% 18% 8%</p>
2	K	240	<p>35% 73% 19% 8%</p>
3	L	235	<p>36% 72% 17% 11%</p>
3	M	235	<p>36% 75% 14% 11%</p>
3	N	235	<p>31% 77% 12% 11%</p>
3	O	235	<p>35% 74% 14% 11%</p>

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 33061 atoms, of which 16149 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 Pv cell-traversal protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	H	N	O			
1	A	122	1905	605	964	150	186	0	0	0
1	B	122	1905	605	964	150	186	0	0	0
1	C	122	1905	605	964	150	186	0	0	0
1	D	122	1906	605	965	150	186	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	34	MET	-	initiating methionine	UNP Q53UB7
A	35	GLY	-	expression tag	UNP Q53UB7
A	197	LEU	-	expression tag	UNP Q53UB7
A	198	GLU	-	expression tag	UNP Q53UB7
A	199	HIS	-	expression tag	UNP Q53UB7
A	200	HIS	-	expression tag	UNP Q53UB7
A	201	HIS	-	expression tag	UNP Q53UB7
A	202	HIS	-	expression tag	UNP Q53UB7
A	203	HIS	-	expression tag	UNP Q53UB7
A	204	HIS	-	expression tag	UNP Q53UB7
B	34	MET	-	initiating methionine	UNP Q53UB7
B	35	GLY	-	expression tag	UNP Q53UB7
B	197	LEU	-	expression tag	UNP Q53UB7
B	198	GLU	-	expression tag	UNP Q53UB7
B	199	HIS	-	expression tag	UNP Q53UB7
B	200	HIS	-	expression tag	UNP Q53UB7
B	201	HIS	-	expression tag	UNP Q53UB7
B	202	HIS	-	expression tag	UNP Q53UB7
B	203	HIS	-	expression tag	UNP Q53UB7
B	204	HIS	-	expression tag	UNP Q53UB7
C	34	MET	-	initiating methionine	UNP Q53UB7

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Chain	Residue	Modelled	Actual	Comment	Reference
C	35	GLY	-	expression tag	UNP Q53UB7
C	197	LEU	-	expression tag	UNP Q53UB7
C	198	GLU	-	expression tag	UNP Q53UB7
C	199	HIS	-	expression tag	UNP Q53UB7
C	200	HIS	-	expression tag	UNP Q53UB7
C	201	HIS	-	expression tag	UNP Q53UB7
C	202	HIS	-	expression tag	UNP Q53UB7
C	203	HIS	-	expression tag	UNP Q53UB7
C	204	HIS	-	expression tag	UNP Q53UB7
D	34	MET	-	initiating methionine	UNP Q53UB7
D	35	GLY	-	expression tag	UNP Q53UB7
D	197	LEU	-	expression tag	UNP Q53UB7
D	198	GLU	-	expression tag	UNP Q53UB7
D	199	HIS	-	expression tag	UNP Q53UB7
D	200	HIS	-	expression tag	UNP Q53UB7
D	201	HIS	-	expression tag	UNP Q53UB7
D	202	HIS	-	expression tag	UNP Q53UB7
D	203	HIS	-	expression tag	UNP Q53UB7
D	204	HIS	-	expression tag	UNP Q53UB7

- Molecule 2 is a protein called 7g7 heavy chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	H	221	3231	1071	1546	276	331	7	0	0	0
2	I	221	3231	1071	1546	276	331	7	0	0	0
2	J	221	3231	1071	1546	276	331	7	0	0	0
2	K	221	3231	1071	1546	276	331	7	0	0	0

- Molecule 3 is a protein called 7g7 light chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	L	209	3128	1000	1527	264	329	8	0	2	0
3	M	209	3128	1000	1527	264	329	8	0	2	0
3	N	209	3128	1000	1527	264	329	8	0	2	0

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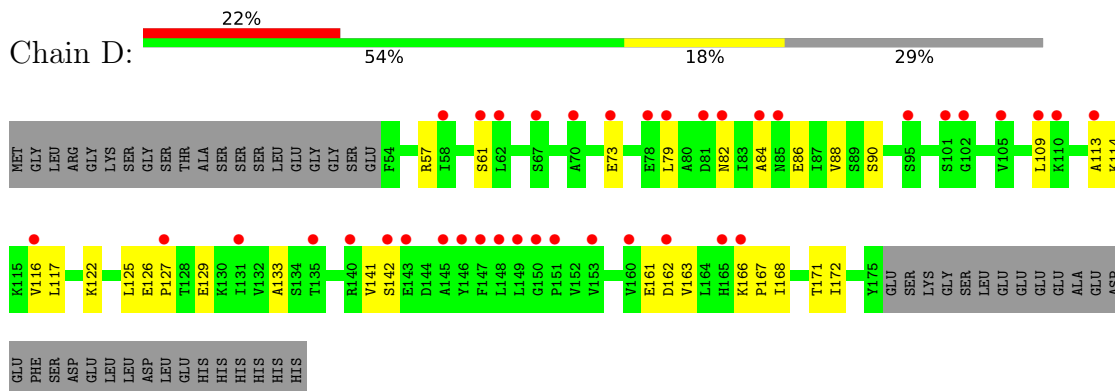
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace	
			Total	C	H	N	O				S
3	O	209	3128	1000	1527	264	329	8	0	2	0

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

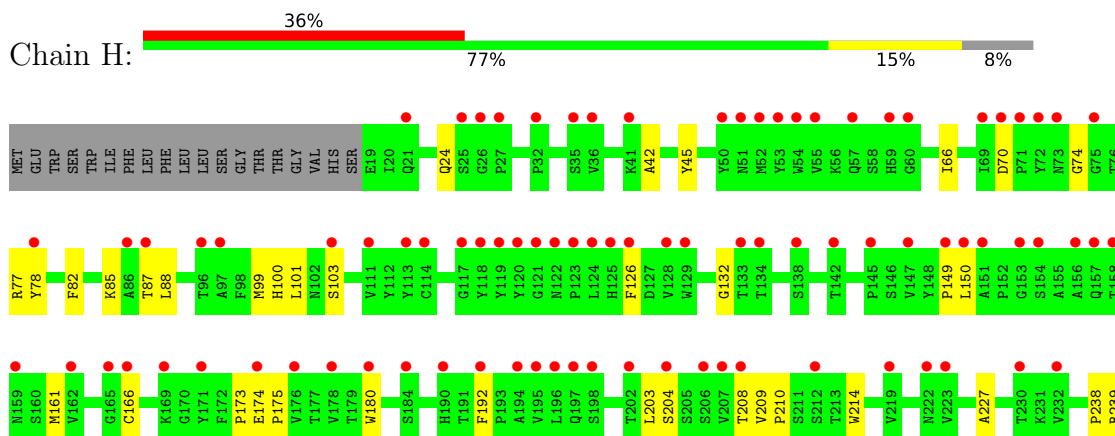
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Na 1	0	0
4	B	1	Total 1	Na 1	0	0
4	C	1	Total 1	Na 1	0	0
4	D	1	Total 1	Na 1	0	0

LEU
ASP
LEU
GLU
GLU
HIS
HIS
HIS
HIS
HIS

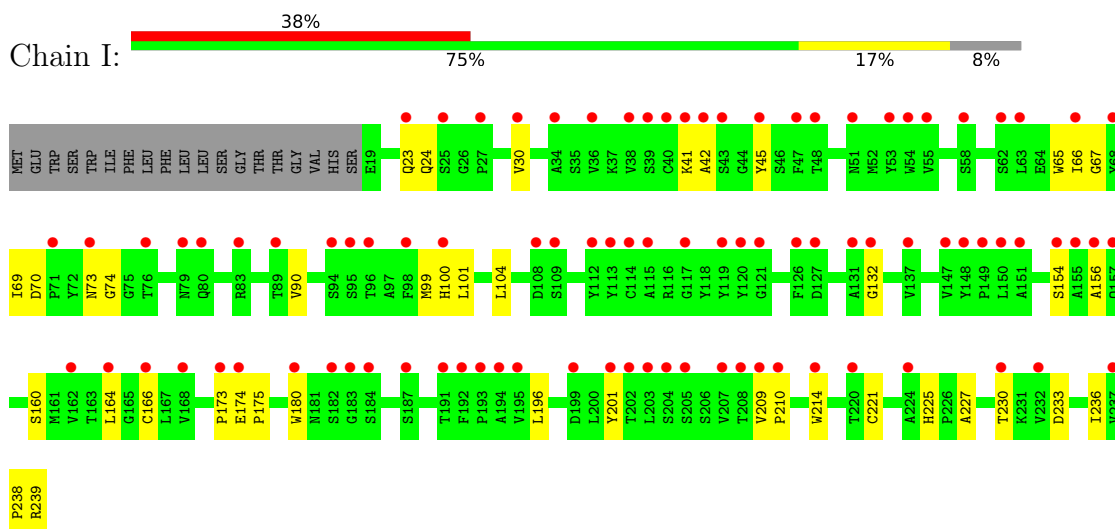
- Molecule 1: Pv cell-traversal protein



- Molecule 2: 7g7 heavy chain

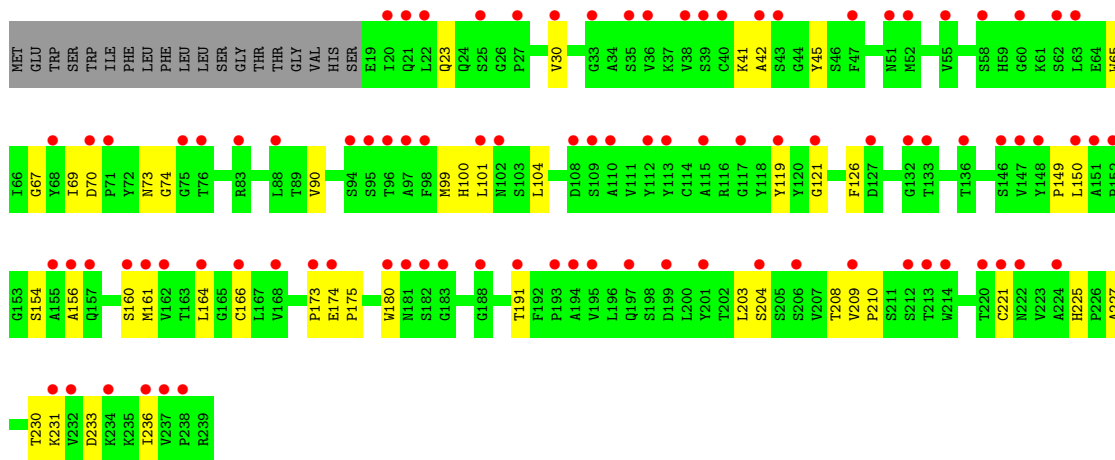


- Molecule 2: 7g7 heavy chain



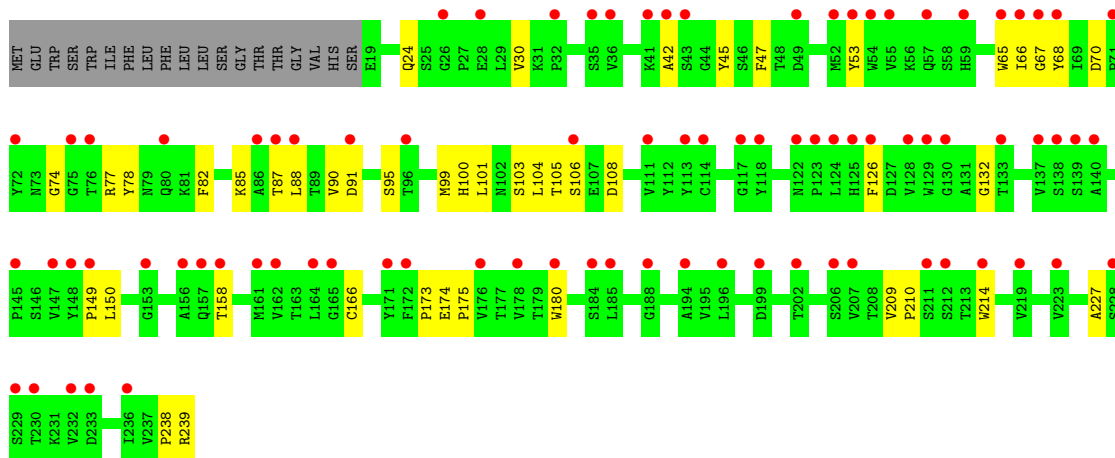
- Molecule 2: 7g7 heavy chain

Chain J:



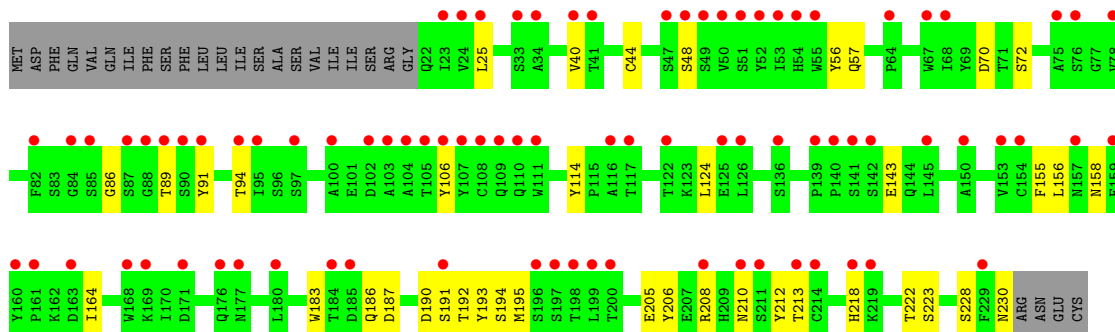
• Molecule 2: 7g7 heavy chain

Chain K:

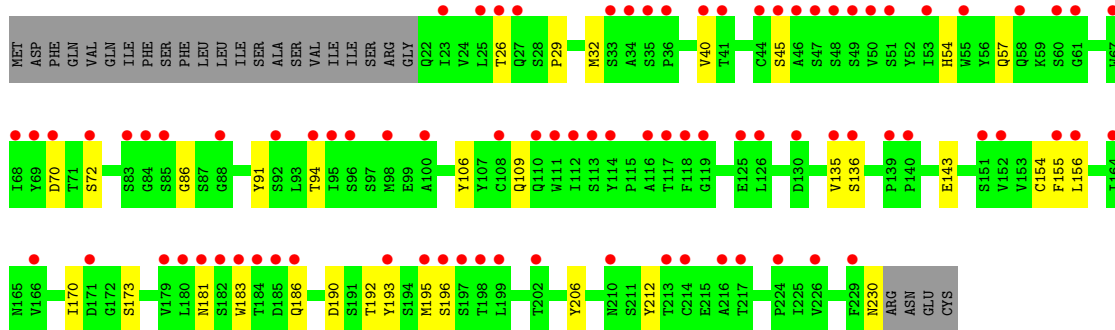
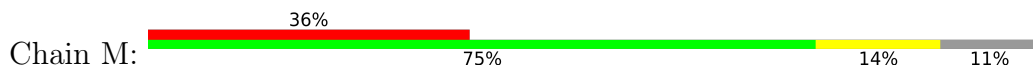


• Molecule 3: 7g7 light chain

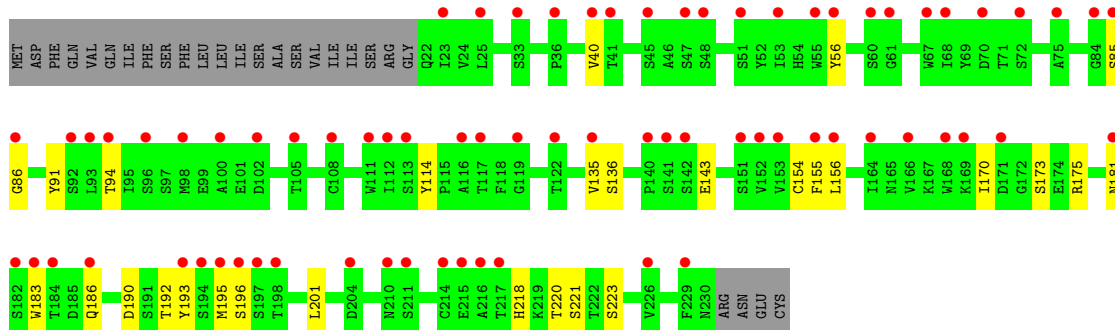
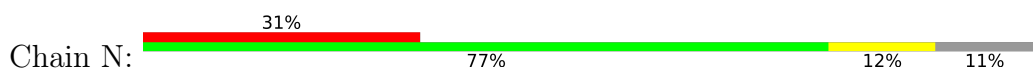
Chain L:



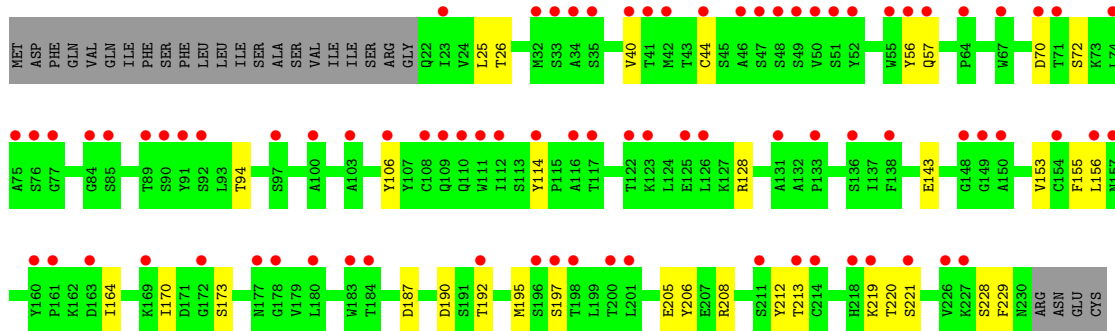
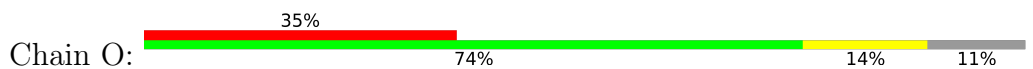
• Molecule 3: 7g7 light chain



• Molecule 3: 7g7 light chain



• Molecule 3: 7g7 light chain



4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	182.89Å 78.62Å 47.32Å 90.03° 95.37° 89.88°	Depositor
Resolution (Å)	48.00 – 3.20 48.00 – 3.20	Depositor EDS
% Data completeness (in resolution range)	90.6 (48.00-3.20) 90.1 (48.00-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.275 , 0.295 0.279 , 0.310	Depositor DCC
R_{free} test set	1962 reflections (4.58%)	wwPDB-VP
Wilson B-factor (Å ²)	109.8	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 600.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l 0.428 for -h,k,-l 0.000 for h+1,-k,-l	Xtriage
F_o, F_c correlation	0.82	EDS
Total number of atoms	33061	wwPDB-VP
Average B, all atoms (Å ²)	151.0	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 99.51 % 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 4.2588e-13. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NA

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	0.16	0/957	0.34	0/1298
1	B	0.16	0/957	0.33	0/1298
1	C	0.17	0/957	0.33	0/1298
1	D	0.16	0/957	0.33	0/1298
2	H	0.17	0/1734	0.34	0/2372
2	I	0.17	0/1734	0.37	0/2372
2	J	0.17	0/1734	0.39	0/2372
2	K	0.17	0/1734	0.35	0/2372
3	L	0.17	0/1640	0.35	0/2229
3	M	0.17	0/1640	0.35	0/2229
3	N	0.16	0/1640	0.32	0/2229
3	O	0.18	0/1640	0.35	0/2229
All	All	0.17	0/17324	0.35	0/23596

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 [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	941	964	963	21	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	941	964	963	21	0
1	C	941	964	963	24	0
1	D	941	965	963	21	0
2	H	1685	1546	1628	28	0
2	I	1685	1546	1628	29	0
2	J	1685	1546	1628	30	0
2	K	1685	1546	1628	30	0
3	L	1601	1527	1525	28	0
3	M	1601	1527	1525	20	0
3	N	1601	1527	1525	19	0
3	O	1601	1527	1525	22	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
All	All	16912	16149	16464	280	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 8.

The worst 5 of 280 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:C:57:ARG:NH2	1:C:86:GLU:OE1	2.15	0.80
1:C:88:VAL:HG22	1:C:109:LEU:HD23	1.65	0.77
2:H:85:LYS:NZ	2:H:103:SER:O	2.18	0.77
3:N:221:SER:OG	3:N:223:SER:O	2.01	0.77
1:B:57:ARG:NH2	1:B:86:GLU:OE1	2.20	0.75

There are no symmetry-related clashes.

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	120/171 (70%)	116 (97%)	4 (3%)	0	100	100
1	B	120/171 (70%)	115 (96%)	5 (4%)	0	100	100
1	C	120/171 (70%)	115 (96%)	5 (4%)	0	100	100
1	D	120/171 (70%)	118 (98%)	2 (2%)	0	100	100
2	H	219/240 (91%)	211 (96%)	8 (4%)	0	100	100
2	I	219/240 (91%)	209 (95%)	10 (5%)	0	100	100
2	J	219/240 (91%)	210 (96%)	9 (4%)	0	100	100
2	K	219/240 (91%)	211 (96%)	8 (4%)	0	100	100
3	L	207/235 (88%)	199 (96%)	8 (4%)	0	100	100
3	M	207/235 (88%)	198 (96%)	9 (4%)	0	100	100
3	N	207/235 (88%)	200 (97%)	7 (3%)	0	100	100
3	O	207/235 (88%)	197 (95%)	10 (5%)	0	100	100
All	All	2184/2584 (84%)	2099 (96%)	85 (4%)	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	A	107/148 (72%)	107 (100%)	0	100	100
1	B	107/148 (72%)	107 (100%)	0	100	100
1	C	107/148 (72%)	107 (100%)	0	100	100
1	D	107/148 (72%)	107 (100%)	0	100	100
2	H	191/208 (92%)	191 (100%)	0	100	100
2	I	191/208 (92%)	191 (100%)	0	100	100
2	J	191/208 (92%)	191 (100%)	0	100	100
2	K	191/208 (92%)	191 (100%)	0	100	100
3	L	182/206 (88%)	182 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	182/206 (88%)	182 (100%)	0	100	100
3	N	182/206 (88%)	182 (100%)	0	100	100
3	O	182/206 (88%)	182 (100%)	0	100	100
All	All	1920/2248 (85%)	1920 (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. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	165	HIS
2	K	190	HIS
3	O	218	HIS
1	C	77	ASN
2	J	125	HIS

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](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

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.

No monomer is involved in short contacts.

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	122/171 (71%)	1.41	33 (27%)	1 1	126, 190, 246, 292	0
1	B	122/171 (71%)	1.72	41 (33%)	1 1	129, 186, 315, 337	0
1	C	122/171 (71%)	1.64	35 (28%)	1 1	129, 188, 312, 346	0
1	D	122/171 (71%)	1.54	38 (31%)	1 1	130, 188, 252, 284	0
2	H	221/240 (92%)	1.78	87 (39%)	1 1	86, 127, 185, 202	0
2	I	221/240 (92%)	1.86	92 (41%)	0 1	86, 122, 170, 209	0
2	J	221/240 (92%)	1.88	94 (42%)	0 1	83, 120, 170, 200	0
2	K	221/240 (92%)	1.78	85 (38%)	1 1	87, 127, 183, 200	0
3	L	209/235 (88%)	1.82	85 (40%)	0 1	88, 144, 195, 242	0
3	M	209/235 (88%)	1.85	85 (40%)	0 1	95, 148, 217, 240	1 (0%)
3	N	209/235 (88%)	1.74	73 (34%)	1 1	93, 150, 216, 239	1 (0%)
3	O	209/235 (88%)	1.89	83 (39%)	1 1	89, 143, 194, 233	0
All	All	2208/2584 (85%)	1.77	831 (37%)	1 1	83, 145, 229, 346	2 (0%)

The worst 5 of 831 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	L	90	SER	9.6
3	O	122	THR	8.8
2	H	86	ALA	7.3
3	L	89	THR	7.3
3	O	90	SER	6.9

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](#)

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
4	NA	A	301	1/1	0.94	0.10	110,110,110,110	0
4	NA	C	301	1/1	0.94	0.17	101,101,101,101	0
4	NA	D	301	1/1	0.94	0.12	107,107,107,107	0
4	NA	B	301	1/1	0.97	0.22	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.