



wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 17, 2022 – 04:14 PM EST

PDB ID : 7STZ
Title : Crystal Structure of Human E-cadherin EC1-5 bound by mouse monoclonal antibody Fab mAb-1_19A11
Authors : Seattle Structural Genomics Center for Infectious Disease; Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2021-11-15
Resolution : 2.95 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.25
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)	:	2.25

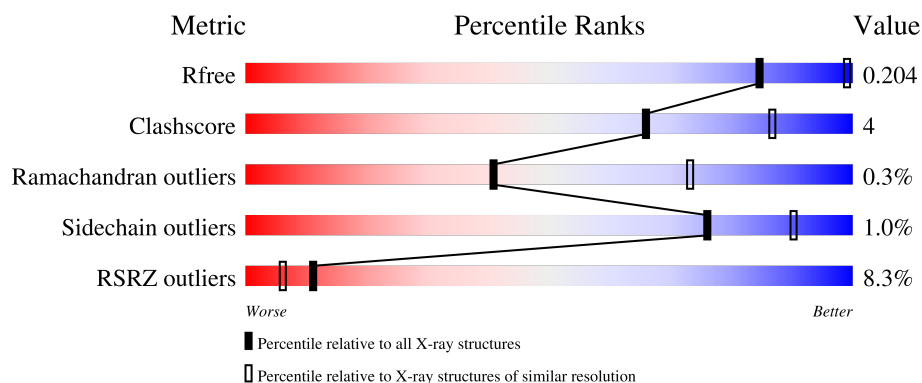
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	590	<div> <div>9%</div> <div>78%</div> <div>13%</div> <div>8%</div> </div>
1	D	590	<div> <div>16%</div> <div>64%</div> <div>8%</div> <div>28%</div> </div>
2	H	246	<div> <div>%</div> <div>81%</div> <div>8%</div> <div>11%</div> </div>
2	I	246	<div> <div>79%</div> <div>8%</div> <div>12%</div> </div>
3	L	240	<div> <div>83%</div> <div>8%</div> <div>8%</div> </div>

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Mol	Chain	Length	Quality of chain
3	M	240	 85% 7% 8%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	H	302	-	-	-	X
6	PG4	C	604	-	-	-	X
7	MAN	C	607	-	-	-	X

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14687 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 Cadherin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	540	Total	C	N	O	S	0	1	0
			4093	2572	660	851	10			
1	D	422	Total	C	N	O	S	0	0	0
			3068	1910	498	656	4			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-15	MET	-	expression tag	UNP P12830
C	-14	PRO	-	expression tag	UNP P12830
C	-13	LEU	-	expression tag	UNP P12830
C	-12	LEU	-	expression tag	UNP P12830
C	-11	LEU	-	expression tag	UNP P12830
C	-10	LEU	-	expression tag	UNP P12830
C	-9	LEU	-	expression tag	UNP P12830
C	-8	PRO	-	expression tag	UNP P12830
C	-7	LEU	-	expression tag	UNP P12830
C	-6	LEU	-	expression tag	UNP P12830
C	-5	TRP	-	expression tag	UNP P12830
C	-4	ALA	-	expression tag	UNP P12830
C	-3	GLY	-	expression tag	UNP P12830
C	-2	ALA	-	expression tag	UNP P12830
C	-1	LEU	-	expression tag	UNP P12830
C	0	ALA	-	expression tag	UNP P12830
D	-15	MET	-	expression tag	UNP P12830
D	-14	PRO	-	expression tag	UNP P12830
D	-13	LEU	-	expression tag	UNP P12830
D	-12	LEU	-	expression tag	UNP P12830
D	-11	LEU	-	expression tag	UNP P12830
D	-10	LEU	-	expression tag	UNP P12830
D	-9	LEU	-	expression tag	UNP P12830
D	-8	PRO	-	expression tag	UNP P12830
D	-7	LEU	-	expression tag	UNP P12830

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-6	LEU	-	expression tag	UNP P12830
D	-5	TRP	-	expression tag	UNP P12830
D	-4	ALA	-	expression tag	UNP P12830
D	-3	GLY	-	expression tag	UNP P12830
D	-2	ALA	-	expression tag	UNP P12830
D	-1	LEU	-	expression tag	UNP P12830
D	0	ALA	-	expression tag	UNP P12830

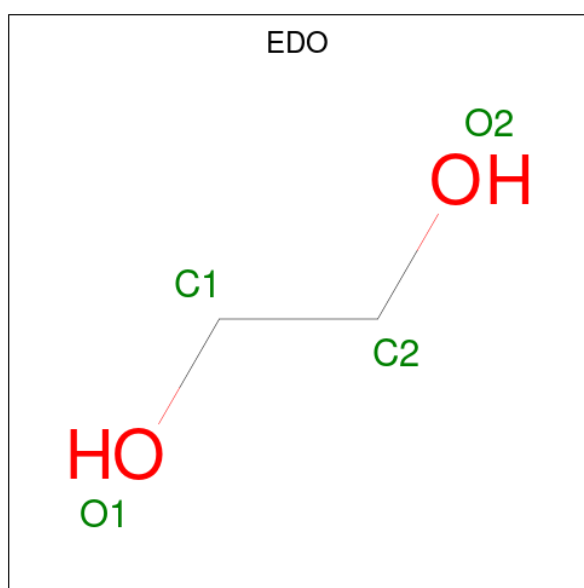
- Molecule 2 is a protein called mAb-1_19A11 Heavy Chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	219	Total	C	N	O	S	0	5	0
			1643	1042	268	322	11			
2	I	216	Total	C	N	O	S	0	6	0
			1646	1041	273	322	10			

- Molecule 3 is a protein called mAb-1_19A11 Light Chain.

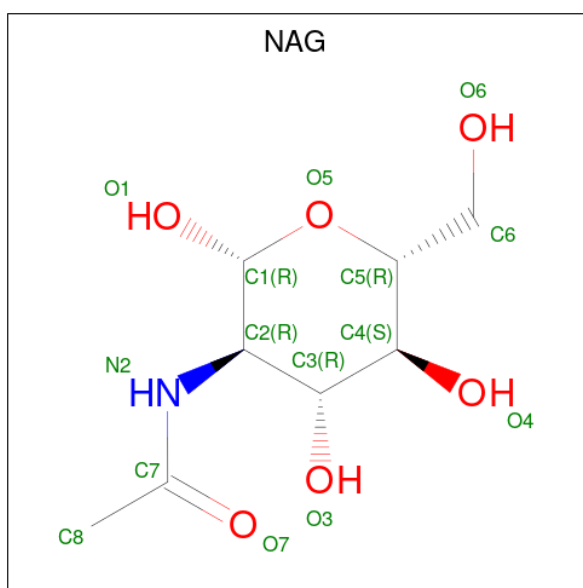
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	L	220	Total	C	N	O	S	0	2	0
			1703	1060	289	345	9			
3	M	220	Total	C	N	O	S	0	2	0
			1712	1066	293	345	8			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



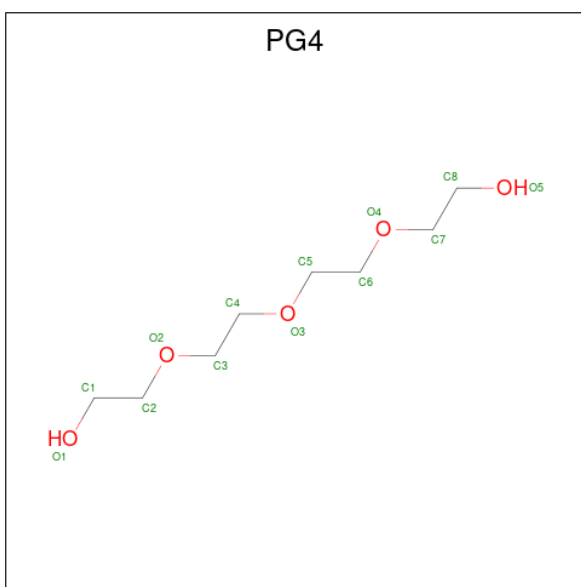
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	H	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		
4	I	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



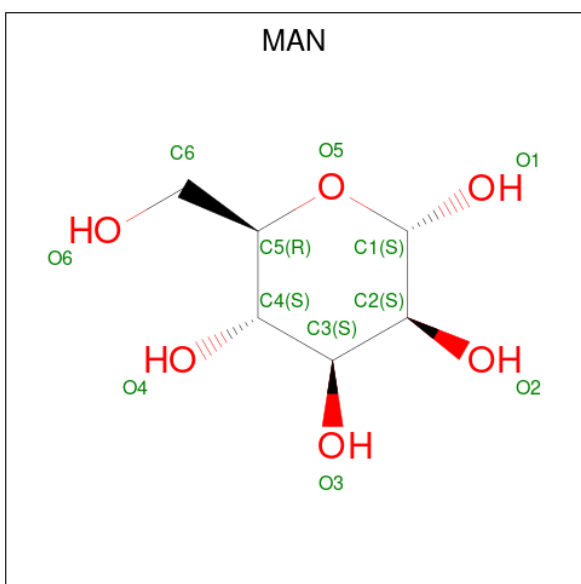
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



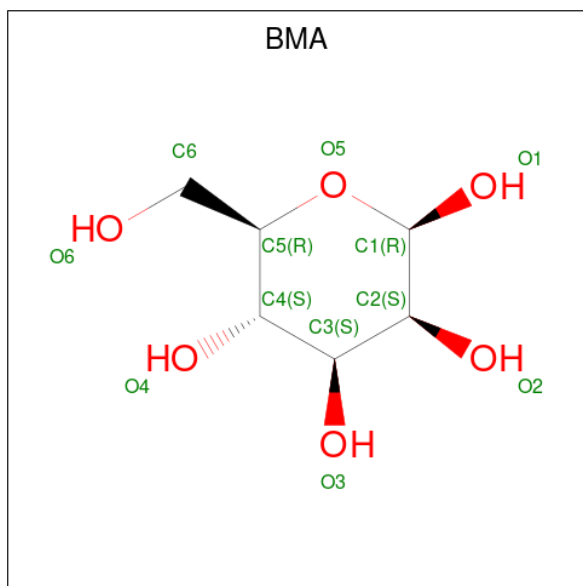
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		
6	H	1	Total	C	O	0	0
			13	8	5		
6	D	1	Total	C	O	0	0
			13	8	5		
6	I	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is alpha-D-mannopyranose (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is beta-D-mannopyranose (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	C	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		
8	D	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	12	Total	Ca	0	0
			12	12		
9	D	11	Total	Ca	0	0
			11	11		
9	M	1	Total	Ca	0	0
			1	1		

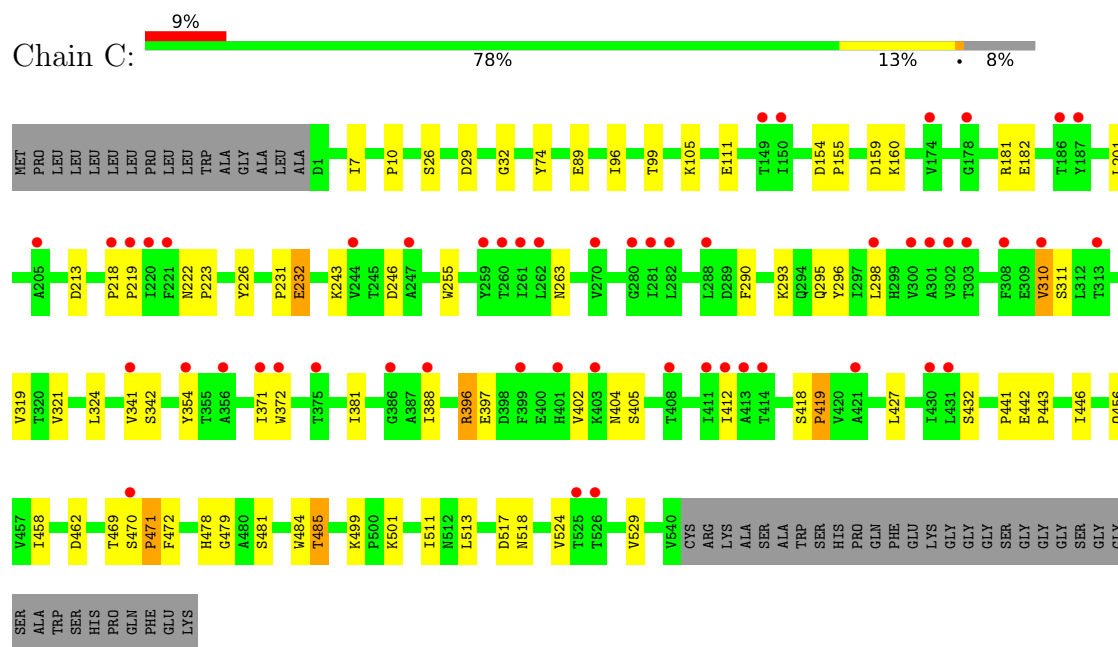
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	C	81	Total	O	0	0
			81	81		
10	H	76	Total	O	0	0
			76	76		
10	L	107	Total	O	0	0
			107	107		
10	D	62	Total	O	0	0
			62	62		
10	I	103	Total	O	0	0
			103	103		
10	M	105	Total	O	0	0
			105	105		

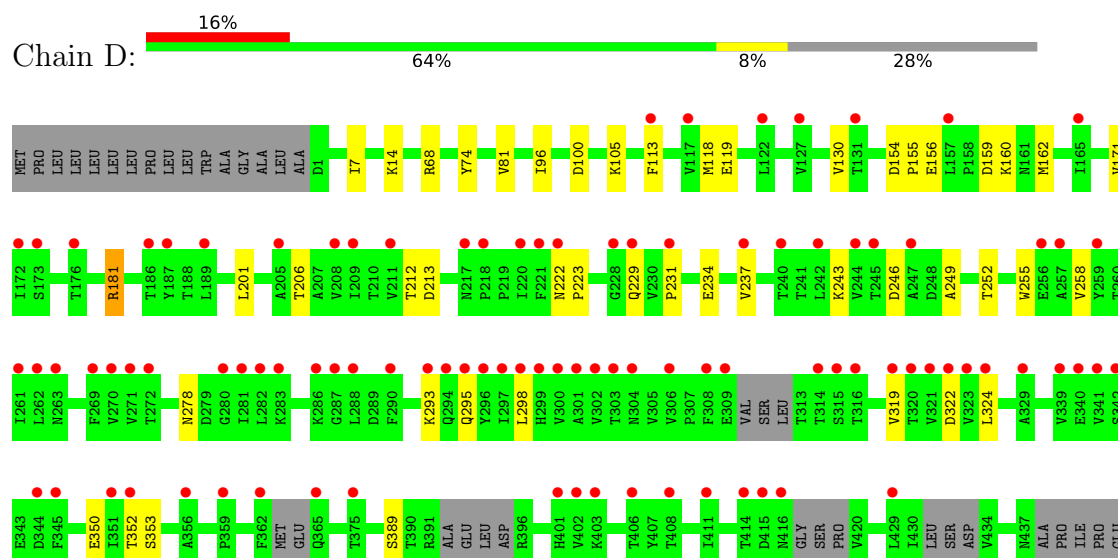
3 Residue-property plots [i](#)

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.

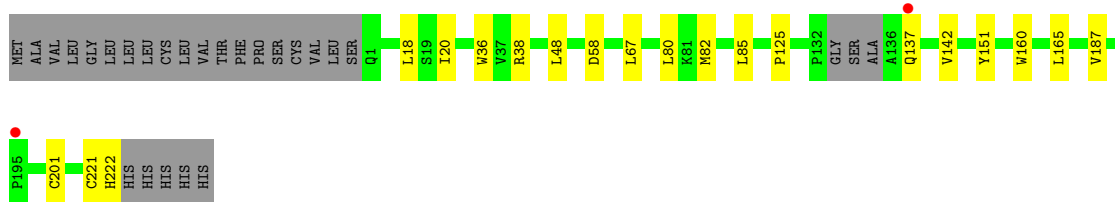
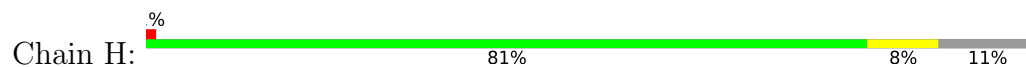
• Molecule 1: Cadherin-1



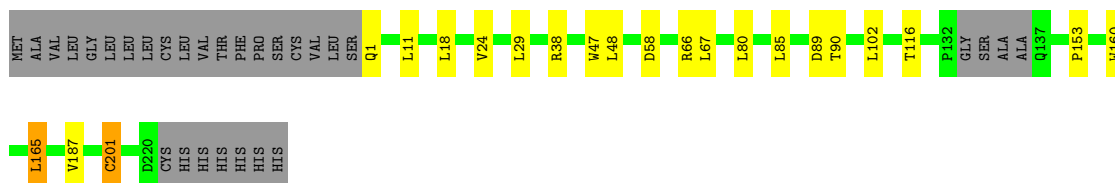
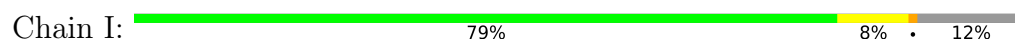
• Molecule 1: Cadherin-1



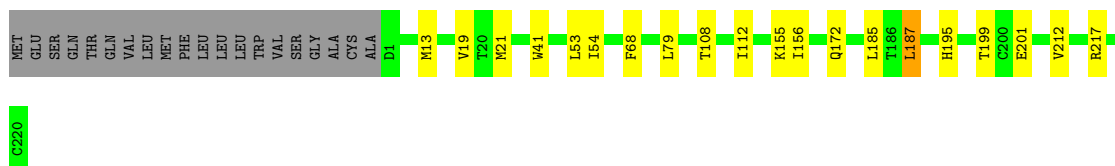
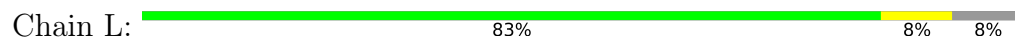
● Molecule 2: mAb-1 19A11 Heavy Chain



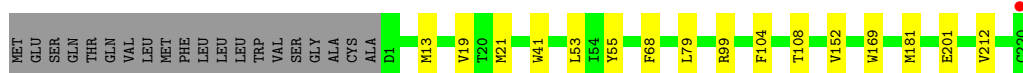
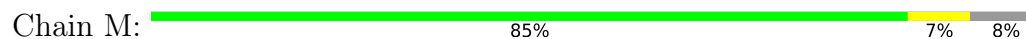
- Molecule 2: mAb-1_19A11 Heavy Chain



- Molecule 3: mAb-1_19A11 Light Chain



- Molecule 3: mAb-1_19A11 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	85.34Å 131.62Å 201.76Å 90.00° 100.86° 90.00°	Depositor
Resolution (Å)	49.54 – 2.95 49.54 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.54-2.95) 95.6 (49.54-2.95)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.99 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.20rc3-4406	Depositor
R, R_{free}	0.182 , 0.208 0.183 , 0.204	Depositor DCC
R_{free} test set	2000 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.524	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 72.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14687	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, MAN, BMA, NAG, PG4, EDO

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	0.25	0/4181	0.48	0/5745
1	D	0.24	0/3121	0.45	0/4293
2	H	0.25	0/1701	0.48	0/2328
2	I	0.26	0/1707	0.51	0/2334
3	L	0.26	0/1752	0.52	1/2376 (0.0%)
3	M	0.26	0/1755	0.51	0/2379
All	All	0.25	0/14217	0.49	1/19455 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	187	LEU	CA-CB-CG	6.13	129.41	115.30

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	C	4093	0	3897	45	0
1	D	3068	0	2794	24	0
2	H	1643	0	1596	10	0
2	I	1646	0	1602	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	1703	0	1633	10	0
3	M	1712	0	1650	12	0
4	C	4	0	6	0	0
4	H	8	0	10	0	0
4	I	8	0	12	0	0
5	C	14	0	13	0	0
6	C	26	0	36	3	0
6	D	13	0	18	0	0
6	H	13	0	18	0	0
6	I	13	0	18	3	0
7	C	33	0	30	0	0
8	C	66	0	60	0	0
8	D	66	0	60	1	0
9	C	12	0	0	0	0
9	D	11	0	0	0	0
9	M	1	0	0	0	0
10	C	81	0	0	0	0
10	D	62	0	0	0	0
10	H	76	0	0	0	0
10	I	103	0	0	0	0
10	L	107	0	0	0	0
10	M	105	0	0	0	0
All	All	14687	0	13453	111	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 4.

The worst 5 of 111 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:470:SER:HB3	1:C:471:PRO:HD2	1.51	0.91
3:M:13:MET:HG3	3:M:19:VAL:HG22	1.71	0.72
1:C:441:PRO:HD3	1:C:524:VAL:HG21	1.76	0.67
1:C:501:LYS:HG3	6:C:604:PG4:H52	1.79	0.64
3:L:13:MET:HG3	3:L:19:VAL:HG22	1.80	0.64

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	539/590 (91%)	504 (94%)	30 (6%)	5 (1%)	17	51
1	D	410/590 (70%)	387 (94%)	23 (6%)	0	100	100
2	H	220/246 (89%)	213 (97%)	7 (3%)	0	100	100
2	I	218/246 (89%)	213 (98%)	5 (2%)	0	100	100
3	L	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
3	M	220/240 (92%)	217 (99%)	3 (1%)	0	100	100
All	All	1827/2152 (85%)	1751 (96%)	71 (4%)	5 (0%)	41	73

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	310	VAL
1	C	471	PRO
1	C	472	PHE
1	C	232	GLU
1	C	419	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	C	455/507 (90%)	449 (99%)	6 (1%)	69	87
1	D	323/507 (64%)	318 (98%)	5 (2%)	65	85
2	H	188/214 (88%)	186 (99%)	2 (1%)	73	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	189/214 (88%)	185 (98%)	4 (2%)	53	80
3	L	196/214 (92%)	195 (100%)	1 (0%)	88	95
3	M	196/214 (92%)	196 (100%)	0	100	100
All	All	1547/1870 (83%)	1529 (99%)	18 (1%)	76	88

5 of 18 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	58[A]	ASP
2	I	201	CYS
2	I	165	LEU
3	L	187	LEU
1	D	258	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 50 ligands modelled in this entry, 24 are monoatomic - leaving 26 for Mogul analysis.

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	$\# Z > 2$
6	PG4	C	604	-	12,12,12	0.15	0	11,11,11	0.61	0
7	MAN	C	611	1	11,11,12	0.76	0	15,15,17	1.26	3 (20%)
7	MAN	C	605	1	11,11,12	0.83	1 (9%)	15,15,17	1.05	2 (13%)
6	PG4	D	601	-	12,12,12	0.13	0	11,11,11	0.62	0
6	PG4	C	603	-	12,12,12	0.13	0	11,11,11	0.61	0
6	PG4	I	303	-	12,12,12	0.13	0	11,11,11	0.66	0
8	BMA	C	609	-	11,11,12	0.92	0	15,15,17	1.22	2 (13%)
7	MAN	C	607	1	11,11,12	0.69	0	15,15,17	1.08	2 (13%)
4	EDO	I	301	-	3,3,3	0.49	0	2,2,2	0.31	0
8	BMA	D	605	-	11,11,12	0.67	0	15,15,17	1.07	2 (13%)
8	BMA	D	603	-	11,11,12	0.81	0	15,15,17	1.33	2 (13%)
8	BMA	C	608	-	11,11,12	0.75	0	15,15,17	1.41	3 (20%)
8	BMA	C	606	-	11,11,12	0.93	1 (9%)	15,15,17	1.04	2 (13%)
8	BMA	C	613	-	11,11,12	0.84	0	15,15,17	1.37	3 (20%)
8	BMA	D	607	-	11,11,12	0.83	0	15,15,17	1.45	3 (20%)
8	BMA	C	612	-	11,11,12	0.86	0	15,15,17	1.61	3 (20%)
4	EDO	C	601	-	3,3,3	0.50	0	2,2,2	0.26	0
8	BMA	D	604	-	11,11,12	0.67	0	15,15,17	1.11	2 (13%)
4	EDO	H	301	-	3,3,3	0.48	0	2,2,2	0.28	0
5	NAG	C	602	1	14,14,15	0.27	0	17,19,21	0.43	0
8	BMA	D	606	-	11,11,12	0.85	0	15,15,17	1.22	3 (20%)
4	EDO	H	302	-	3,3,3	0.50	0	2,2,2	0.28	0
4	EDO	I	302	-	3,3,3	0.47	0	2,2,2	0.29	0
8	BMA	D	602	-	11,11,12	0.79	0	15,15,17	1.05	1 (6%)
6	PG4	H	303	-	12,12,12	0.14	0	11,11,11	0.63	0
8	BMA	C	610	-	11,11,12	0.75	0	15,15,17	1.06	2 (13%)

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
6	PG4	C	604	-	-	3/10/10/10	-
7	MAN	C	611	1	-	0/2/19/22	0/1/1/1
7	MAN	C	605	1	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	D	601	-	-	5/10/10/10	-
6	PG4	C	603	-	-	2/10/10/10	-
6	PG4	I	303	-	-	8/10/10/10	-
8	BMA	C	609	-	-	2/2/19/22	1/1/1/1
7	MAN	C	607	1	-	2/2/19/22	0/1/1/1
4	EDO	I	301	-	-	0/1/1/1	-
8	BMA	D	605	-	-	0/2/19/22	0/1/1/1
8	BMA	D	603	-	-	0/2/19/22	1/1/1/1
8	BMA	C	608	-	-	2/2/19/22	0/1/1/1
8	BMA	C	606	-	-	2/2/19/22	0/1/1/1
8	BMA	C	613	-	-	1/2/19/22	0/1/1/1
8	BMA	D	607	-	-	1/2/19/22	0/1/1/1
8	BMA	C	612	-	-	2/2/19/22	0/1/1/1
4	EDO	C	601	-	-	0/1/1/1	-
8	BMA	D	604	-	-	2/2/19/22	0/1/1/1
4	EDO	H	301	-	-	0/1/1/1	-
5	NAG	C	602	1	-	2/6/23/26	0/1/1/1
8	BMA	D	606	-	-	2/2/19/22	0/1/1/1
4	EDO	H	302	-	-	0/1/1/1	-
4	EDO	I	302	-	-	0/1/1/1	-
8	BMA	D	602	-	-	0/2/19/22	0/1/1/1
6	PG4	H	303	-	-	6/10/10/10	-
8	BMA	C	610	-	-	2/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	606	BMA	O5-C1	-2.23	1.40	1.43
7	C	605	MAN	O5-C1	-2.11	1.40	1.43

The worst 5 of 35 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	612	BMA	C1-O5-C5	4.25	117.94	112.19
8	D	607	BMA	C1-O5-C5	3.81	117.35	112.19
8	C	608	BMA	C1-O5-C5	3.75	117.27	112.19
8	D	603	BMA	C1-O5-C5	3.72	117.23	112.19
8	C	613	BMA	C1-O5-C5	3.61	117.09	112.19

There are no chirality outliers.

5 of 44 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	612	BMA	O5-C5-C6-O6
8	C	608	BMA	O5-C5-C6-O6
7	C	607	MAN	O5-C5-C6-O6
8	C	609	BMA	C4-C5-C6-O6
8	D	604	BMA	C4-C5-C6-O6

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	603	BMA	C1-C2-C3-C4-C5-O5
8	C	609	BMA	C1-C2-C3-C4-C5-O5

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	604	PG4	3	0
6	I	303	PG4	3	0
8	D	606	BMA	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	540/590 (91%)	0.45	52 (9%) 8 4	35, 99, 146, 213	0
1	D	422/590 (71%)	1.00	97 (22%) 0 0	36, 134, 179, 224	0
2	H	219/246 (89%)	-0.14	2 (0%) 84 71	34, 60, 131, 179	0
2	I	216/246 (87%)	-0.13	0 100 100	29, 46, 82, 182	0
3	L	220/240 (91%)	-0.14	0 100 100	32, 52, 96, 154	0
3	M	220/240 (91%)	-0.11	1 (0%) 91 81	29, 46, 85, 140	0
All	All	1837/2152 (85%)	0.30	152 (8%) 11 6	29, 65, 161, 224	0

The worst 5 of 152 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	300	VAL	7.8
1	D	321	VAL	7.0
1	D	269	PHE	6.9
1	C	301	ALA	6.0
1	D	298	LEU	5.8

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 monosaccharides in this entry.

6.4 Ligands ⓘ

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	EDO	H	302	4/4	0.39	0.42	105,108,110,142	0
9	CA	D	618	1/1	0.69	0.05	207,207,207,207	0
6	PG4	C	604	13/13	0.75	0.55	66,84,102,105	0
7	MAN	C	607	11/12	0.78	0.45	135,156,174,174	0
8	BMA	D	606	11/12	0.81	0.42	127,135,144,147	0
8	BMA	D	602	11/12	0.81	0.31	85,124,137,143	0
8	BMA	D	603	11/12	0.83	0.29	99,120,129,136	0
8	BMA	D	605	11/12	0.83	0.42	123,156,166,171	0
4	EDO	C	601	4/4	0.84	0.39	60,70,73,87	0
8	BMA	D	604	11/12	0.85	0.72	153,158,171,176	0
6	PG4	C	603	13/13	0.85	0.29	80,94,116,137	0
5	NAG	C	602	14/15	0.86	0.20	78,111,123,125	0
8	BMA	C	609	11/12	0.86	0.29	109,122,141,152	0
8	BMA	D	607	11/12	0.86	0.38	130,149,159,160	0
8	BMA	C	612	11/12	0.86	0.52	122,132,143,145	0
9	CA	D	615	1/1	0.88	0.20	159,159,159,159	0
9	CA	D	616	1/1	0.88	0.04	124,124,124,124	0
6	PG4	D	601	13/13	0.88	0.24	76,88,101,117	0
8	BMA	C	610	11/12	0.89	0.34	133,147,151,152	0
7	MAN	C	611	11/12	0.89	0.31	96,122,130,141	0
8	BMA	C	613	11/12	0.89	0.22	112,128,153,160	0
4	EDO	I	302	4/4	0.89	0.35	70,75,75,79	0
4	EDO	H	301	4/4	0.90	0.37	66,67,75,76	0
7	MAN	C	605	11/12	0.90	0.28	93,109,117,123	0
9	CA	C	621	1/1	0.90	0.06	87,87,87,87	0
9	CA	D	609	1/1	0.91	0.06	135,135,135,135	0
9	CA	C	618	1/1	0.91	0.11	118,118,118,118	0
9	CA	C	624	1/1	0.91	0.08	116,116,116,116	0
9	CA	D	608	1/1	0.91	0.10	173,173,173,173	0
9	CA	M	301	1/1	0.91	0.15	99,99,99,99	0
6	PG4	H	303	13/13	0.92	0.19	24,85,105,107	0
8	BMA	C	606	11/12	0.92	0.28	93,109,133,136	0
8	BMA	C	608	11/12	0.92	0.27	130,134,146,148	0
9	CA	D	614	1/1	0.92	0.05	135,135,135,135	0
9	CA	D	610	1/1	0.93	0.14	152,152,152,152	0
4	EDO	I	301	4/4	0.93	0.17	48,48,55,62	0
6	PG4	I	303	13/13	0.93	0.26	5,76,106,121	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
9	CA	C	622	1/1	0.94	0.11	106,106,106,106	0
9	CA	C	620	1/1	0.94	0.09	73,73,73,73	0
9	CA	C	623	1/1	0.95	0.06	113,113,113,113	0
9	CA	C	625	1/1	0.95	0.10	133,133,133,133	0
9	CA	C	619	1/1	0.96	0.10	135,135,135,135	0
9	CA	D	617	1/1	0.97	0.17	169,169,169,169	0
9	CA	D	611	1/1	0.97	0.23	49,49,49,49	0
9	CA	C	617	1/1	0.97	0.06	109,109,109,109	0
9	CA	C	615	1/1	0.98	0.24	53,53,53,53	0
9	CA	C	614	1/1	0.99	0.17	43,43,43,43	0
9	CA	D	612	1/1	0.99	0.13	44,44,44,44	0
9	CA	D	613	1/1	0.99	0.13	53,53,53,53	0
9	CA	C	616	1/1	1.00	0.14	42,42,42,42	0

6.5 Other polymers ⓘ

There are no such residues in this entry.