



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 19, 2018 – 03:14 pm GMT

PDB ID : 5A8H
EMDB ID: : EMD-3096
Title : cryo-ET subtomogram averaging of BG505 SOSIP.664 in complex with sCD4, 17b, and 8ANC195
Authors : Scharf, L.; Wang, H.; Gao, H.; Chen, S.; McDowall, A.; Bjorkman, P.
Deposited on : 2015-07-15
Resolution : 23.00 Å(reported)
Based on PDB ID : 1RZK

This is a wwPDB/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

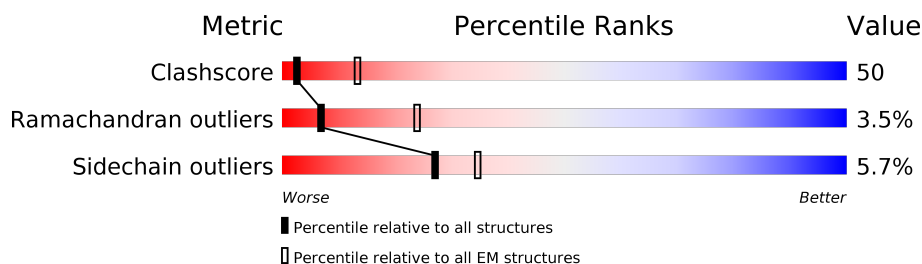
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 23.00 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.




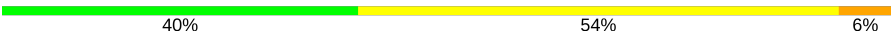
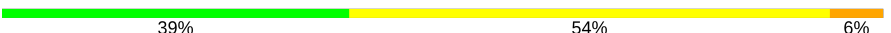






Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	A	313	39% 54% . .
1	G	313	36% 57% . .
1	M	313	34% 59% . .
2	B	185	33% 54% 10% . .
2	H	185	34% 53% 10% . .
2	N	185	34% 53% 9% . .
3	C	214	34% 57% 8% .
3	I	214	34% 57% 8% .
3	O	214	33% 57% 8% .

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Mol	Chain	Length	Quality of chain
4	D	229	
4	J	229	
4	P	229	
5	E	215	
5	K	215	
5	Q	215	
6	F	244	
6	L	244	
6	R	244	

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
7	NAG	A	588	X	-	-	-
7	NAG	A	734	-	-	X	-
7	NAG	A	741	X	-	-	-
7	NAG	A	776	-	-	X	-
7	NAG	G	588	X	-	-	-
7	NAG	G	734	-	-	X	-
7	NAG	G	741	X	-	-	-
7	NAG	M	588	X	-	-	-
7	NAG	M	734	-	-	X	-
7	NAG	M	741	X	-	-	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 31872 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 HIV-1 GP120.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		
1	G	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		
1	M	306	Total	C	N	O	S	0	0
			2385	1494	417	454	20		

- Molecule 2 is a protein called T-CELL SURFACE GLYCOPROTEIN CD4.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		
2	H	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		
2	N	181	Total	C	N	O	S	0	0
			1412	885	247	276	4		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	184	ASN	-	expression tag	UNP P01730
B	185	THR	-	expression tag	UNP P01730
H	184	ASN	-	expression tag	UNP P01730
H	185	THR	-	expression tag	UNP P01730
N	184	ASN	-	expression tag	UNP P01730
N	185	THR	-	expression tag	UNP P01730

- Molecule 3 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		
3	O	214	Total	C	N	O	S	0	0
			1647	1028	282	332	5		

- Molecule 4 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 17B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		
4	J	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		
4	P	229	Total	C	N	O	S	0	0
			1722	1086	289	342	5		

- Molecule 5 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		
5	K	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		
5	Q	214	Total	C	N	O	S	0	0
			1605	1002	273	325	5		

- Molecule 6 is a protein called FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		
6	L	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		
6	R	224	Total	C	N	O	S	0	0
			1643	1046	273	319	5		

- Molecule 7 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: C₈H₁₅NO₆).



Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	
7	A	1	Total	C	N	O	0
			196	112	14	70	

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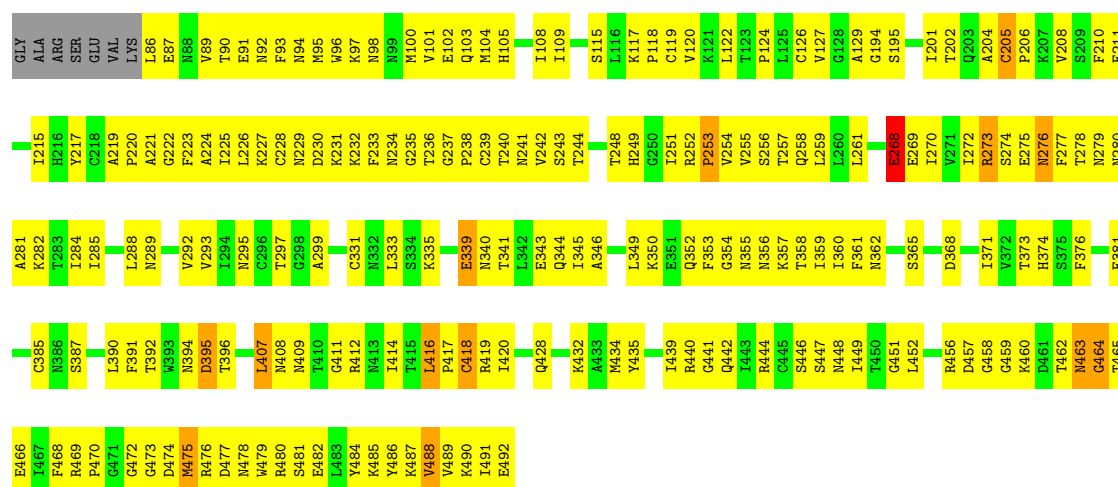
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Mol	Chain	Residues	Atoms				AltConf
7	F	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	G	1	Total 196	C 112	N 14	O 70	0
7	L	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 196	C 112	N 14	O 70	0
7	M	1	Total 196	C 112	N 14	O 70	0
7	M	1	Total 196	C 112	N 14	O 70	0
7	M	1	Total 196	C 112	N 14	O 70	0
7	M	1	Total 196	C 112	N 14	O 70	0

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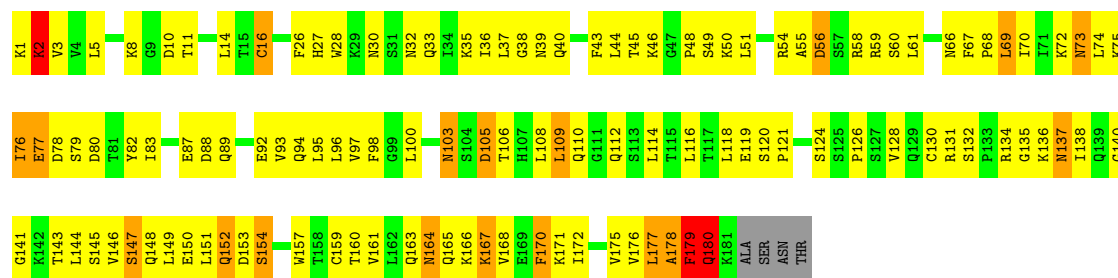
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Mol	Chain	Residues	Atoms				AltConf
7	M	1	Total	C	N	O	0
			196	112	14	70	
7	M	1	Total	C	N	O	0
			196	112	14	70	
7	M	1	Total	C	N	O	0
			196	112	14	70	
7	M	1	Total	C	N	O	0
			196	112	14	70	
7	M	1	Total	C	N	O	0
			196	112	14	70	
7	M	1	Total	C	N	O	0
			196	112	14	70	
7	M	1	Total	C	N	O	0
			196	112	14	70	
7	R	1	Total	C	N	O	0
			14	8	1	5	



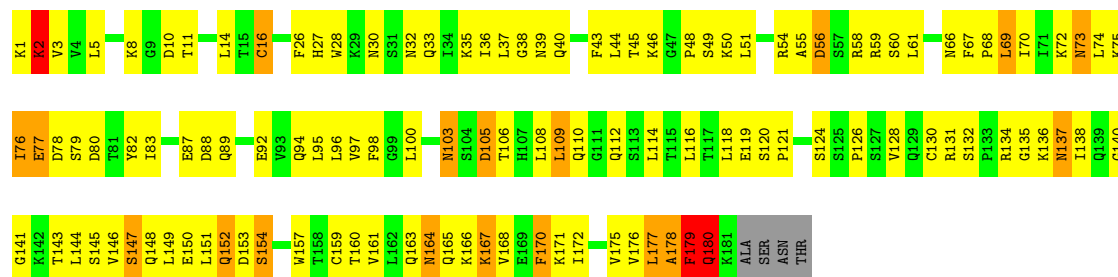
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

Chain B: 33% 54% 10% . .



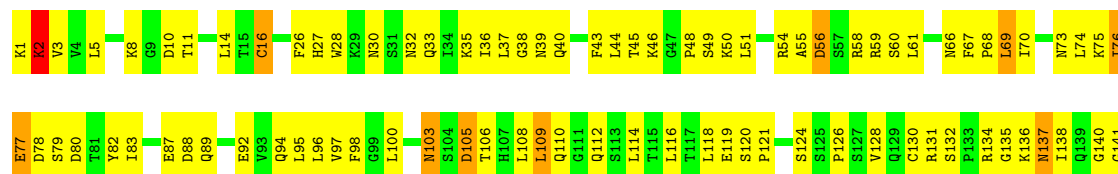
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

Chain H: 34% 53% 10% . .

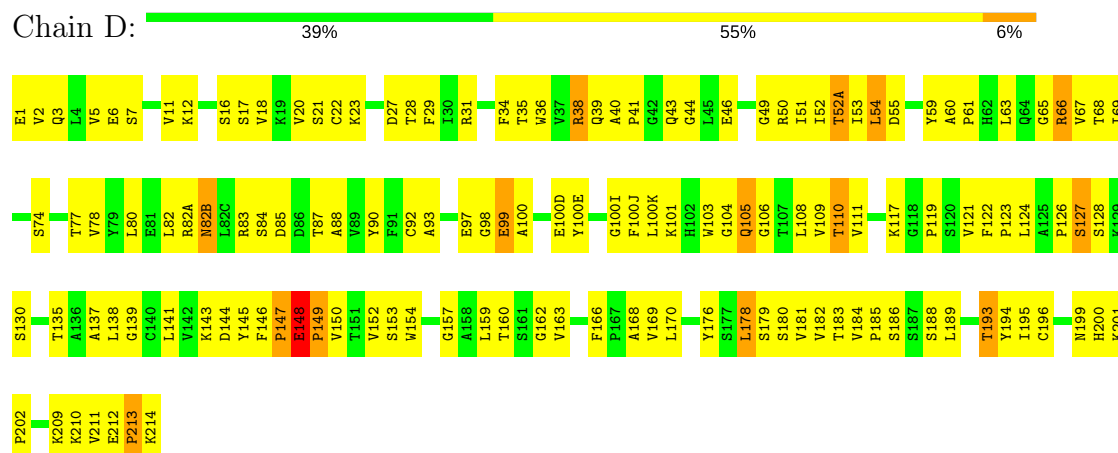


• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

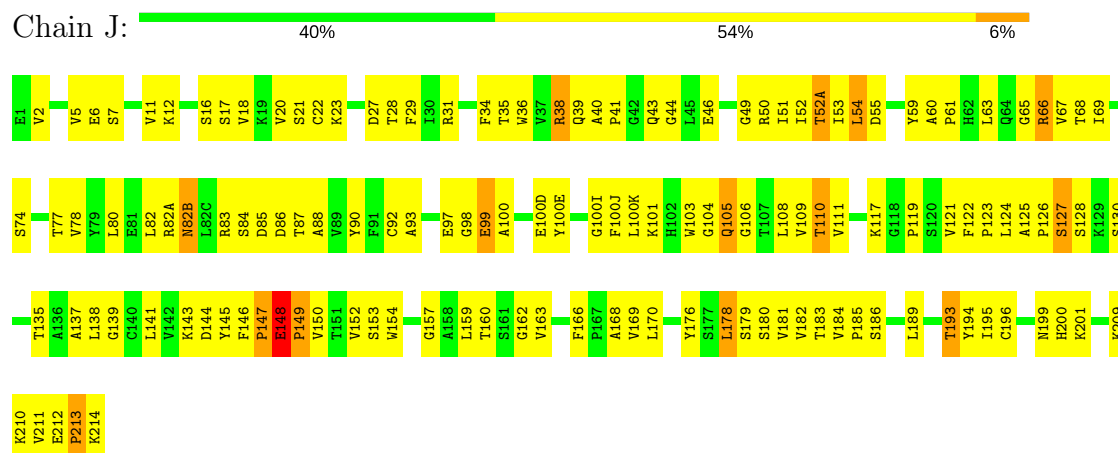
Chain N: 34% 53% 9% . .



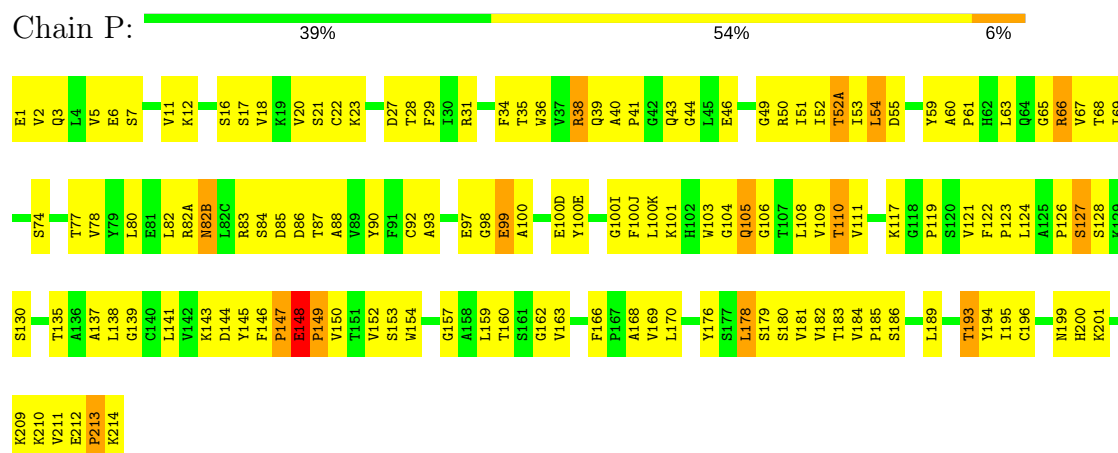




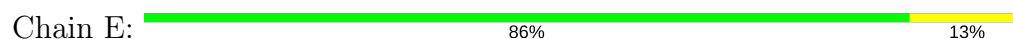
• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

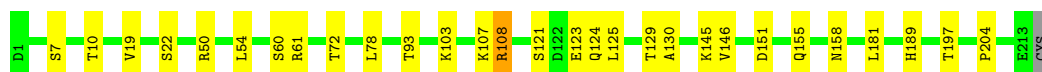


• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B



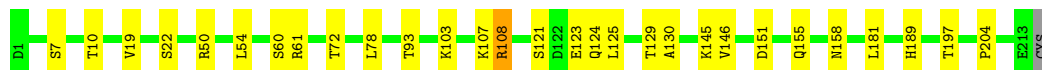
• Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5





- Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5

Chain K: 86% 13%



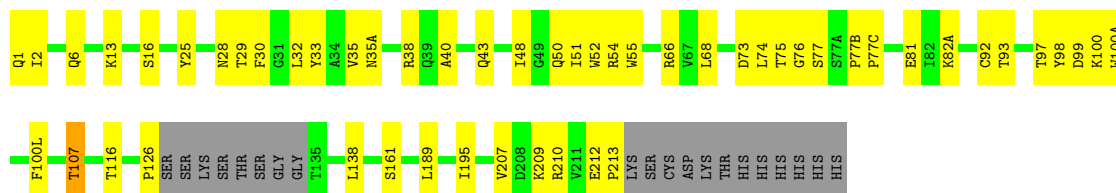
- Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5

Chain Q: 86% 13%



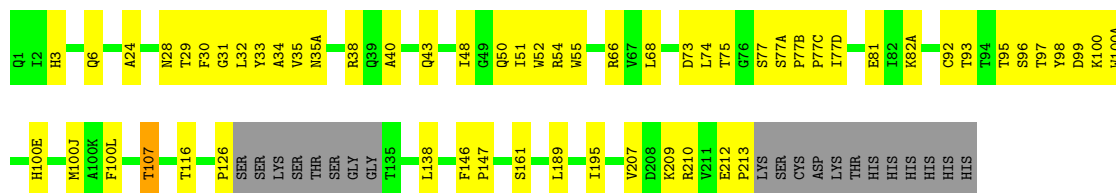
- Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5

Chain F: 70% 21% 8%



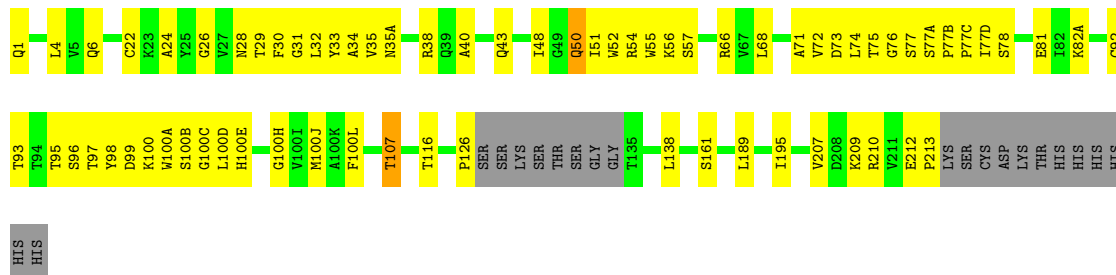
- Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5

Chain L: 68% 24% 8%



- Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5

Chain R: 63% 28% 8%



HIS
HIS

4 Experimental information

Property	Value	Source
Reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	1745	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	EACH MICROGRAPH	Depositor
Microscope	FEI TECNAI F30	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	120	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	41000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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 > 2$	RMSZ	# $ Z > 2$
1	A	0.45	0/2432	0.66	0/3296
1	G	0.45	0/2432	0.66	0/3296
1	M	0.45	0/2432	0.66	0/3296
2	B	0.41	0/1432	0.72	2/1930 (0.1%)
2	H	0.41	0/1432	0.72	2/1930 (0.1%)
2	N	0.41	0/1432	0.72	2/1930 (0.1%)
3	C	0.43	0/1684	0.86	3/2288 (0.1%)
3	I	0.43	0/1684	0.86	3/2288 (0.1%)
3	O	0.43	0/1684	0.86	3/2288 (0.1%)
4	D	0.42	0/1762	0.64	0/2399
4	J	0.42	0/1762	0.64	0/2399
4	P	0.42	0/1762	0.64	0/2399
5	E	0.51	0/1640	0.60	0/2232
5	K	0.51	0/1640	0.60	0/2232
5	Q	0.51	0/1640	0.60	0/2232
6	F	0.54	1/1687 (0.1%)	0.60	1/2310 (0.0%)
6	L	0.54	1/1687 (0.1%)	0.61	1/2310 (0.0%)
6	R	0.54	1/1687 (0.1%)	0.60	1/2310 (0.0%)
All	All	0.46	3/31911 (0.0%)	0.68	18/43365 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	213	PRO	N-CD	5.16	1.55	1.47
6	F	213	PRO	N-CD	5.15	1.55	1.47
6	R	213	PRO	N-CD	5.11	1.54	1.47

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	140	TYR	C-N-CD	-21.38	73.57	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	140	TYR	C-N-CD	-21.37	73.58	120.60
3	O	140	TYR	C-N-CD	-21.37	73.59	120.60
3	I	140	TYR	C-N-CA	13.74	179.73	122.00
3	C	140	TYR	C-N-CA	13.73	179.67	122.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2385	0	2322	376	0
1	G	2385	0	2321	467	0
1	M	2385	0	2300	819	0
2	B	1412	0	1444	147	0
2	H	1412	0	1444	150	0
2	N	1412	0	1444	146	0
3	C	1647	0	1593	171	0
3	I	1647	0	1593	169	0
3	O	1647	0	1593	171	0
4	D	1722	0	1691	154	0
4	J	1722	0	1691	152	0
4	P	1722	0	1691	149	0
5	E	1605	0	1521	14	0
5	K	1605	0	1521	14	0
5	Q	1605	0	1521	15	0
6	F	1643	0	1578	218	0
6	L	1643	0	1574	309	0
6	R	1643	0	1567	644	0
7	A	196	0	172	50	0
7	F	14	0	13	0	0
7	G	196	0	176	51	0
7	L	14	0	13	0	0
7	M	196	0	177	29	0
7	R	14	0	13	0	0
All	All	31872	0	30973	3148	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 50.

The worst 5 of 3148 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:M:488:VAL:HG23	6:R:98:TYR:CE2	1.16	1.65
1:G:89:VAL:CA	6:L:52:TRP:HZ2	1.02	1.65
1:M:96:TRP:CD1	6:R:77(B):PRO:HA	1.28	1.64
1:M:285:ILE:HD12	6:R:75:THR:CG2	1.29	1.62
1:A:353:PHE:CZ	6:F:75:THR:HG23	1.17	1.61

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 PDB entries followed by that with respect to all EM entries.

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	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	2	27
1	G	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	2	27
1	M	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	2	27
2	B	179/185 (97%)	127 (71%)	38 (21%)	14 (8%)	1	17
2	H	179/185 (97%)	127 (71%)	38 (21%)	14 (8%)	1	17
2	N	179/185 (97%)	126 (70%)	39 (22%)	14 (8%)	1	17
3	C	212/214 (99%)	171 (81%)	28 (13%)	13 (6%)	1	22
3	I	212/214 (99%)	170 (80%)	29 (14%)	13 (6%)	1	22
3	O	212/214 (99%)	171 (81%)	28 (13%)	13 (6%)	1	22
4	D	227/229 (99%)	185 (82%)	35 (15%)	7 (3%)	4	35
4	J	227/229 (99%)	184 (81%)	36 (16%)	7 (3%)	4	35
4	P	227/229 (99%)	184 (81%)	36 (16%)	7 (3%)	4	35

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	E	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
5	K	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
5	Q	212/215 (99%)	211 (100%)	1 (0%)	0	100	100
6	F	220/244 (90%)	219 (100%)	1 (0%)	0	100	100
6	L	220/244 (90%)	219 (100%)	1 (0%)	0	100	100
6	R	220/244 (90%)	219 (100%)	1 (0%)	0	100	100
All	All	4062/4200 (97%)	3461 (85%)	457 (11%)	144 (4%)	7	32

5 of 144 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	268	GLU
1	A	409	ASN
1	A	475	MET
2	B	109	LEU
2	B	165	GLN

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 PDB entries followed by that with respect to all EM entries.

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	271/276 (98%)	257 (95%)	14 (5%)	25	56
1	G	271/276 (98%)	257 (95%)	14 (5%)	25	56
1	M	271/276 (98%)	257 (95%)	14 (5%)	25	56
2	B	164/167 (98%)	149 (91%)	15 (9%)	10	35
2	H	164/167 (98%)	149 (91%)	15 (9%)	10	35
2	N	164/167 (98%)	149 (91%)	15 (9%)	10	35
3	C	184/184 (100%)	174 (95%)	10 (5%)	24	55
3	I	184/184 (100%)	174 (95%)	10 (5%)	24	55
3	O	184/184 (100%)	174 (95%)	10 (5%)	24	55
4	D	193/193 (100%)	183 (95%)	10 (5%)	25	56

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	193/193 (100%)	183 (95%)	10 (5%)	25	56
4	P	193/193 (100%)	183 (95%)	10 (5%)	25	56
5	E	174/182 (96%)	164 (94%)	10 (6%)	23	53
5	K	174/182 (96%)	164 (94%)	10 (6%)	23	53
5	Q	174/182 (96%)	164 (94%)	10 (6%)	23	53
6	F	183/210 (87%)	175 (96%)	8 (4%)	31	60
6	L	183/210 (87%)	175 (96%)	8 (4%)	31	60
6	R	183/210 (87%)	175 (96%)	8 (4%)	31	60
All	All	3507/3636 (96%)	3306 (94%)	201 (6%)	27	53

5 of 201 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	137	ASN
4	J	110	THR
5	Q	50	ARG
2	H	167	LYS
3	I	137	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	103	ASN
4	J	82(B)	ASN
4	P	200	HIS
2	H	110	GLN
3	I	147	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

45 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	$\# Z > 2$
7	NAG	A	588	1	14,14,15	0.62	0	17,19,21	0.83	0
7	NAG	A	697	1	14,14,15	0.65	0	17,19,21	0.65	0
7	NAG	A	734	1	14,14,15	0.62	0	17,19,21	0.53	0
7	NAG	A	741	1	14,14,15	0.56	0	17,19,21	0.63	0
7	NAG	A	762	1	14,14,15	0.61	0	17,19,21	0.73	1 (5%)
7	NAG	A	776	1	14,14,15	0.58	0	17,19,21	0.82	0
7	NAG	A	789	1	14,14,15	0.65	0	17,19,21	0.89	0
7	NAG	A	795	1	14,14,15	0.52	0	17,19,21	0.74	0
7	NAG	A	856	1	14,14,15	0.77	0	17,19,21	0.72	0
7	NAG	A	886	1	14,14,15	0.66	0	17,19,21	1.04	2 (11%)
7	NAG	A	894	1	14,14,15	0.65	0	17,19,21	0.75	1 (5%)
7	NAG	A	908	1	14,14,15	0.62	0	17,19,21	0.63	0
7	NAG	A	948	1	14,14,15	0.92	1 (7%)	17,19,21	0.95	1 (5%)
7	NAG	A	963	1	14,14,15	0.76	0	17,19,21	0.66	0
7	NAG	F	1000	6	14,14,15	1.65	1 (7%)	17,19,21	1.37	1 (5%)
7	NAG	G	588	1	14,14,15	0.62	0	17,19,21	0.83	0
7	NAG	G	697	1	14,14,15	0.65	0	17,19,21	0.65	0
7	NAG	G	734	1	14,14,15	0.63	0	17,19,21	0.54	0
7	NAG	G	741	1	14,14,15	0.55	0	17,19,21	0.62	0
7	NAG	G	762	1	14,14,15	0.61	0	17,19,21	0.75	1 (5%)
7	NAG	G	776	1	14,14,15	0.58	0	17,19,21	0.82	0
7	NAG	G	789	1	14,14,15	0.65	0	17,19,21	0.89	0
7	NAG	G	795	1	14,14,15	0.51	0	17,19,21	0.74	0
7	NAG	G	856	1	14,14,15	0.77	0	17,19,21	0.72	0
7	NAG	G	886	1	14,14,15	0.67	0	17,19,21	1.04	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NAG	G	894	1	14,14,15	0.67	0	17,19,21	0.75	1 (5%)
7	NAG	G	908	1	14,14,15	0.63	0	17,19,21	0.63	0
7	NAG	G	948	1	14,14,15	0.93	1 (7%)	17,19,21	0.94	0
7	NAG	G	963	1	14,14,15	0.75	0	17,19,21	0.66	0
7	NAG	L	1000	6	14,14,15	1.65	1 (7%)	17,19,21	1.38	1 (5%)
7	NAG	M	588	1	14,14,15	0.62	0	17,19,21	0.83	0
7	NAG	M	697	1	14,14,15	0.65	0	17,19,21	0.64	0
7	NAG	M	734	1	14,14,15	0.63	0	17,19,21	0.55	0
7	NAG	M	741	1	14,14,15	0.55	0	17,19,21	0.62	0
7	NAG	M	762	1	14,14,15	0.62	0	17,19,21	0.74	1 (5%)
7	NAG	M	776	1	14,14,15	0.58	0	17,19,21	0.82	0
7	NAG	M	789	1	14,14,15	0.65	0	17,19,21	0.89	0
7	NAG	M	795	1	14,14,15	0.52	0	17,19,21	0.74	0
7	NAG	M	856	1	14,14,15	0.78	0	17,19,21	0.71	0
7	NAG	M	886	1	14,14,15	0.66	0	17,19,21	1.03	2 (11%)
7	NAG	M	894	1	14,14,15	0.66	0	17,19,21	0.76	1 (5%)
7	NAG	M	908	1	14,14,15	0.61	0	17,19,21	0.64	0
7	NAG	M	948	1	14,14,15	0.91	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	M	963	1	14,14,15	0.75	0	17,19,21	0.66	0
7	NAG	R	1000	6	14,14,15	1.64	1 (7%)	17,19,21	1.37	1 (5%)

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
7	NAG	A	588	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	A	697	1	-	1/6/23/26	0/1/1/1
7	NAG	A	734	1	-	0/6/23/26	0/1/1/1
7	NAG	A	741	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	A	762	1	-	0/6/23/26	0/1/1/1
7	NAG	A	776	1	-	0/6/23/26	0/1/1/1
7	NAG	A	789	1	-	1/6/23/26	0/1/1/1
7	NAG	A	795	1	-	0/6/23/26	0/1/1/1
7	NAG	A	856	1	-	0/6/23/26	0/1/1/1
7	NAG	A	886	1	-	0/6/23/26	0/1/1/1
7	NAG	A	894	1	-	0/6/23/26	0/1/1/1
7	NAG	A	908	1	-	0/6/23/26	0/1/1/1
7	NAG	A	948	1	-	0/6/23/26	0/1/1/1
7	NAG	A	963	1	-	1/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	F	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	G	588	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	G	697	1	-	1/6/23/26	0/1/1/1
7	NAG	G	734	1	-	0/6/23/26	0/1/1/1
7	NAG	G	741	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	G	762	1	-	0/6/23/26	0/1/1/1
7	NAG	G	776	1	-	0/6/23/26	0/1/1/1
7	NAG	G	789	1	-	1/6/23/26	0/1/1/1
7	NAG	G	795	1	-	0/6/23/26	0/1/1/1
7	NAG	G	856	1	-	0/6/23/26	0/1/1/1
7	NAG	G	886	1	-	0/6/23/26	0/1/1/1
7	NAG	G	894	1	-	0/6/23/26	0/1/1/1
7	NAG	G	908	1	-	0/6/23/26	0/1/1/1
7	NAG	G	948	1	-	0/6/23/26	0/1/1/1
7	NAG	G	963	1	-	1/6/23/26	0/1/1/1
7	NAG	L	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	M	588	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	M	697	1	-	1/6/23/26	0/1/1/1
7	NAG	M	734	1	-	0/6/23/26	0/1/1/1
7	NAG	M	741	1	1/1/5/7	0/6/23/26	0/1/1/1
7	NAG	M	762	1	-	0/6/23/26	0/1/1/1
7	NAG	M	776	1	-	0/6/23/26	0/1/1/1
7	NAG	M	789	1	-	1/6/23/26	0/1/1/1
7	NAG	M	795	1	-	0/6/23/26	0/1/1/1
7	NAG	M	856	1	-	0/6/23/26	0/1/1/1
7	NAG	M	886	1	-	0/6/23/26	0/1/1/1
7	NAG	M	894	1	-	0/6/23/26	0/1/1/1
7	NAG	M	908	1	-	0/6/23/26	0/1/1/1
7	NAG	M	948	1	-	0/6/23/26	0/1/1/1
7	NAG	M	963	1	-	1/6/23/26	0/1/1/1
7	NAG	R	1000	6	-	0/6/23/26	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	F	1000	NAG	O5-C1	-5.82	1.34	1.43
7	L	1000	NAG	O5-C1	-5.82	1.34	1.43
7	R	1000	NAG	O5-C1	-5.78	1.34	1.43
7	M	948	NAG	C1-C2	2.67	1.56	1.52
7	G	948	NAG	C1-C2	2.72	1.56	1.52

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1000	NAG	C1-O5-C5	-4.67	105.77	112.19
7	R	1000	NAG	C1-O5-C5	-4.66	105.78	112.19
7	F	1000	NAG	C1-O5-C5	-4.66	105.78	112.19
7	A	886	NAG	C2-N2-C7	-2.66	119.06	122.94
7	G	886	NAG	C2-N2-C7	-2.66	119.07	122.94

5 of 6 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	A	588	NAG	C1
7	M	741	NAG	C1
7	A	741	NAG	C1
7	G	588	NAG	C1
7	M	588	NAG	C1

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	G	963	NAG	O7-C7-N2-C2
7	A	963	NAG	O7-C7-N2-C2
7	M	963	NAG	O7-C7-N2-C2
7	M	697	NAG	O7-C7-N2-C2
7	G	697	NAG	O7-C7-N2-C2

There are no ring outliers.

31 monomers are involved in 130 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	734	NAG	20	0
7	A	741	NAG	1	0
7	A	762	NAG	1	0
7	A	776	NAG	11	0
7	A	789	NAG	5	0
7	A	856	NAG	1	0
7	A	894	NAG	3	0
7	A	908	NAG	3	0
7	A	948	NAG	3	0
7	A	963	NAG	2	0
7	G	588	NAG	4	0
7	G	734	NAG	24	0
7	G	741	NAG	1	0
7	G	762	NAG	1	0
7	G	776	NAG	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	G	789	NAG	5	0
7	G	856	NAG	1	0
7	G	894	NAG	3	0
7	G	908	NAG	3	0
7	G	948	NAG	3	0
7	G	963	NAG	1	0
7	M	734	NAG	9	0
7	M	741	NAG	1	0
7	M	762	NAG	1	0
7	M	776	NAG	1	0
7	M	789	NAG	5	0
7	M	856	NAG	1	0
7	M	894	NAG	3	0
7	M	908	NAG	4	0
7	M	948	NAG	3	0
7	M	963	NAG	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.