



# wwPDB EM Validation Summary Report ⓘ

Oct 28, 2024 – 09:32 am 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 initial model : 1RZK

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

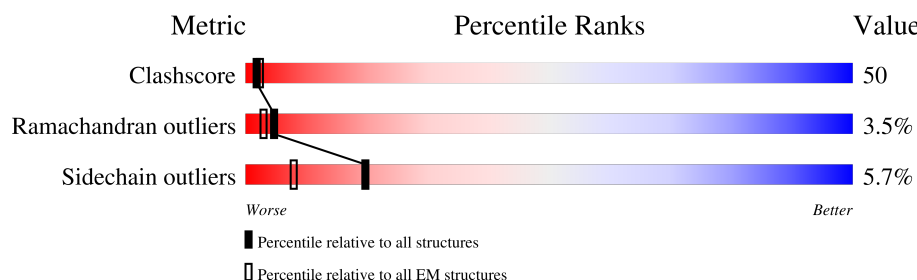
# 1 Overall quality at a glance

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.



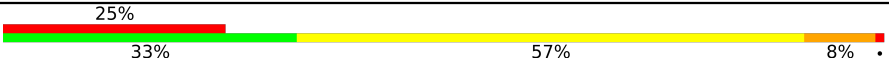

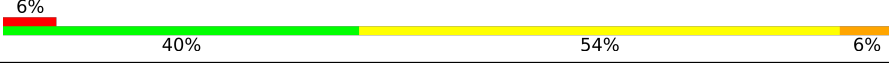
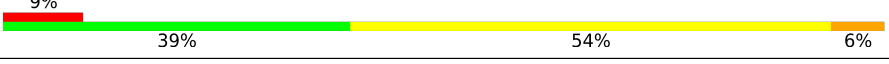

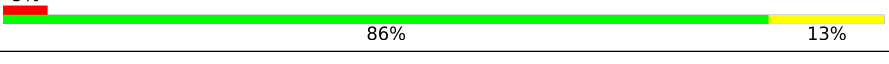
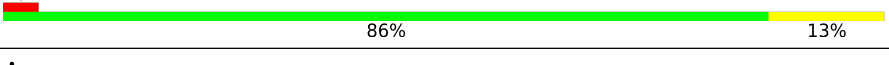

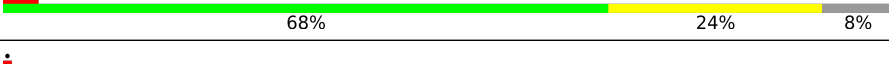

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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 EM map (all-atom inclusion  $< 40\%$ ). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	313	<div> <div>11%</div> <div>39%</div> <div>54%</div> <div>• •</div> </div>
1	G	313	<div> <div>•</div> <div>36%</div> <div>57%</div> <div>• •</div> </div>
1	M	313	<div> <div>•</div> <div>34%</div> <div>59%</div> <div>• •</div> </div>
2	B	185	<div> <div>28%</div> <div>33%</div> <div>54%</div> <div>10% • •</div> </div>
2	H	185	<div> <div>47%</div> <div>34%</div> <div>53%</div> <div>10% • •</div> </div>
2	N	185	<div> <div>49%</div> <div>34%</div> <div>53%</div> <div>9% • •</div> </div>
3	C	214	<div> <div>13%</div> <div>34%</div> <div>57%</div> <div>8% •</div> </div>
3	I	214	<div> <div>27%</div> <div>34%</div> <div>57%</div> <div>8% •</div> </div>

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Mol	Chain	Length	Quality of chain
3	O	214	
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 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

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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 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	G	1	Total 14	C 8	N 1	O 5	0
7	L	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0

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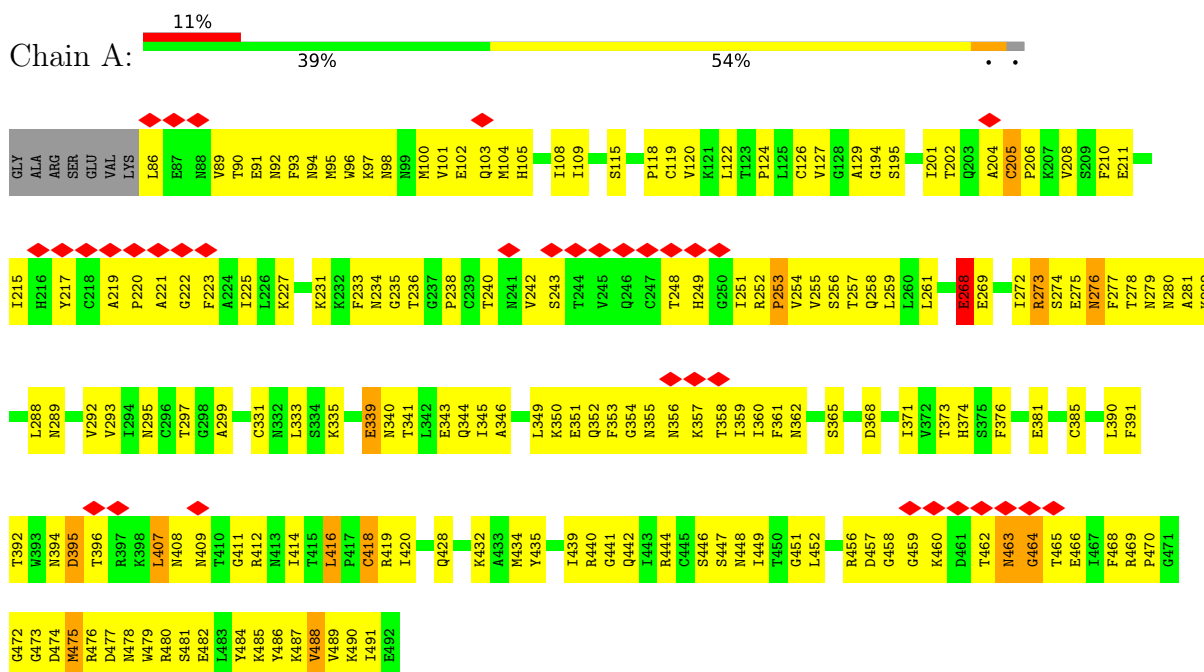
Mol	Chain	Residues	Atoms				AltConf
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	M	1	Total 14	C 8	N 1	O 5	0
7	R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



### 3 Residue-property plots

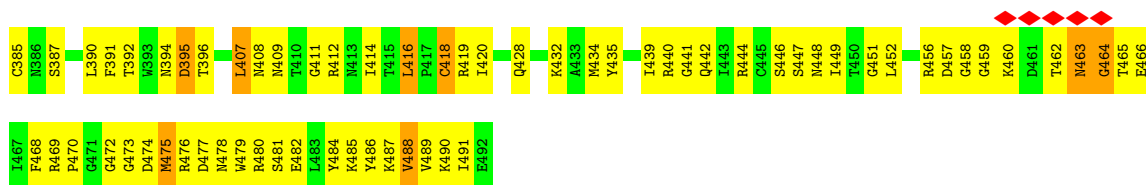
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: HIV-1 GP120



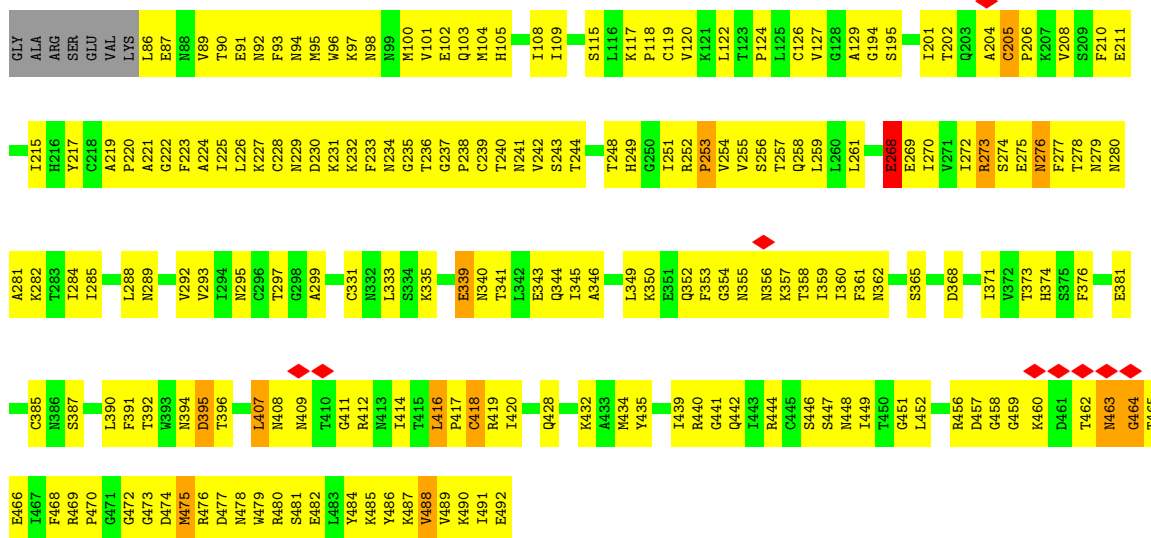
#### • Molecule 1: HIV-1 GP120





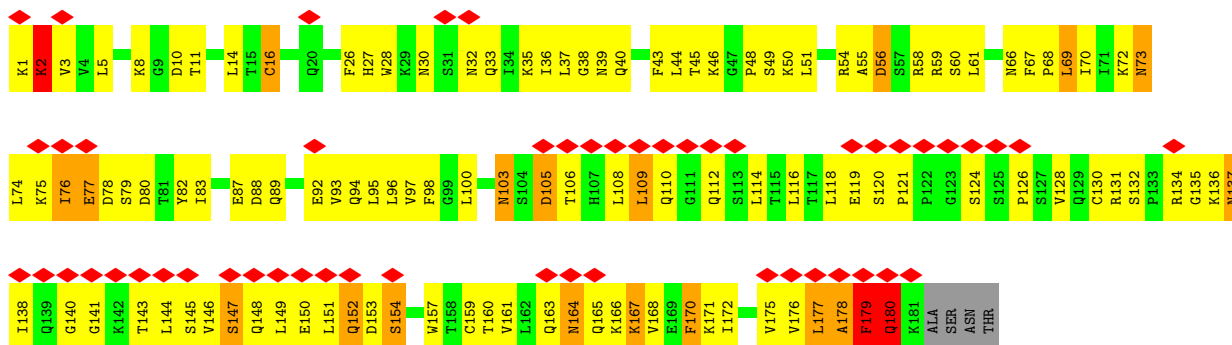
• Molecule 1: HIV-1 GP120

Chain M: 34% 59%



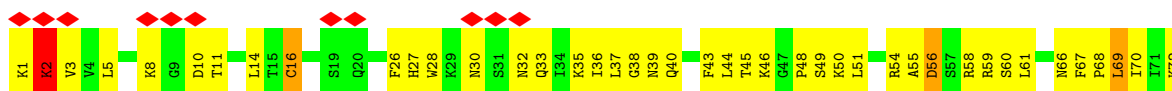
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

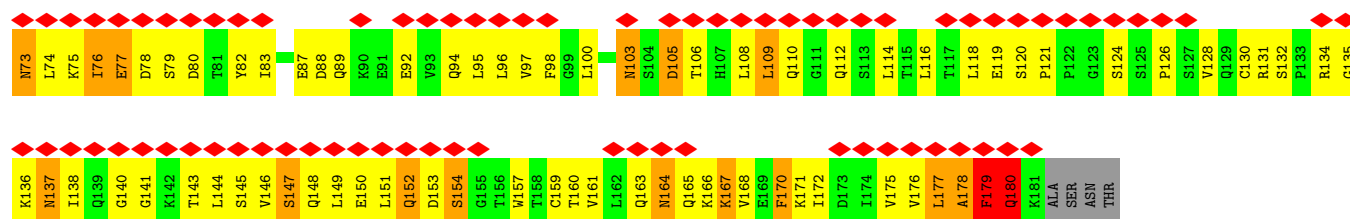
Chain B: 28% 33% 54% 10%



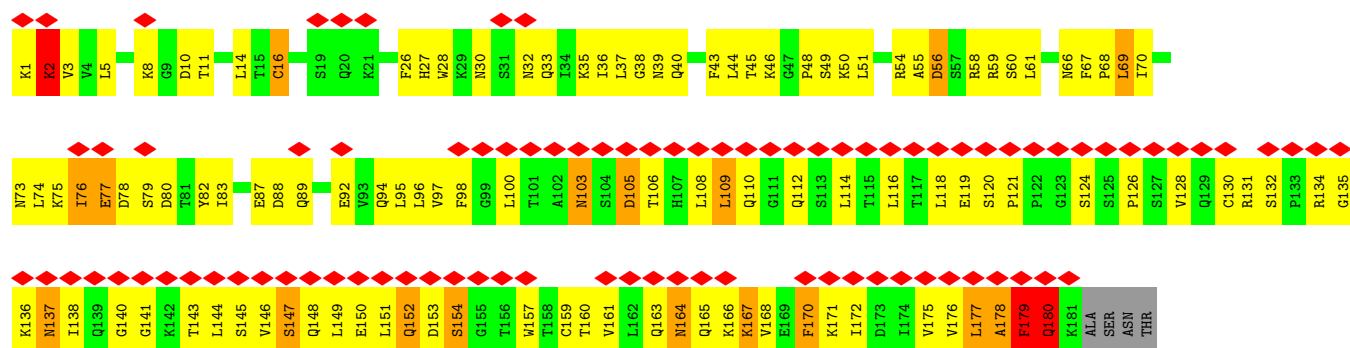
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

Chain H: 34% 47% 53% 10%

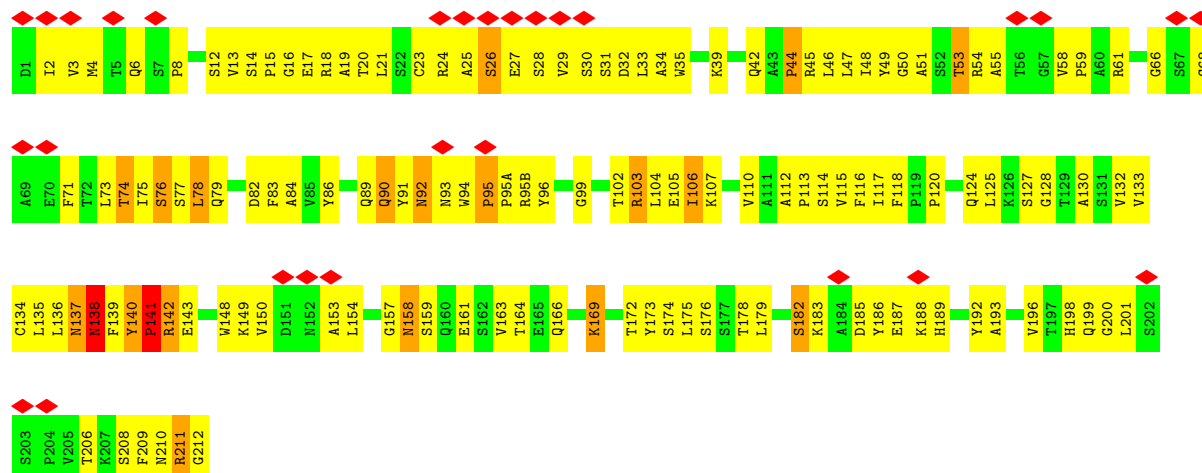




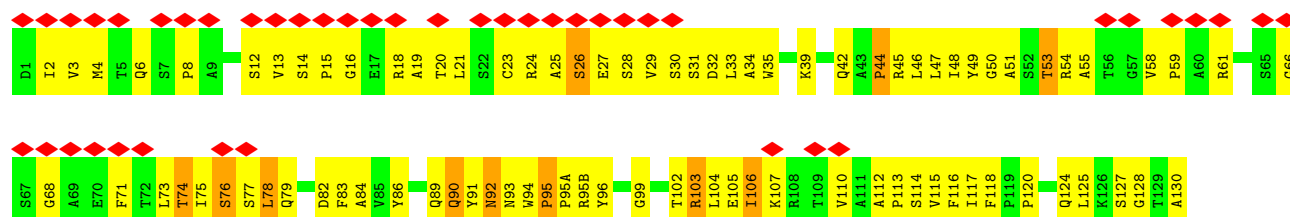
• Molecule 2: T-CELL SURFACE GLYCOPROTEIN CD4

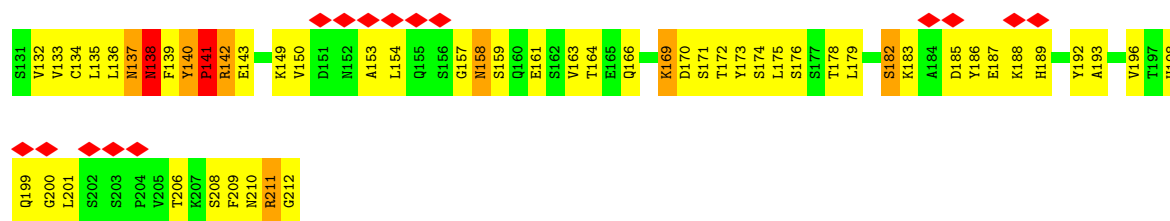


• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

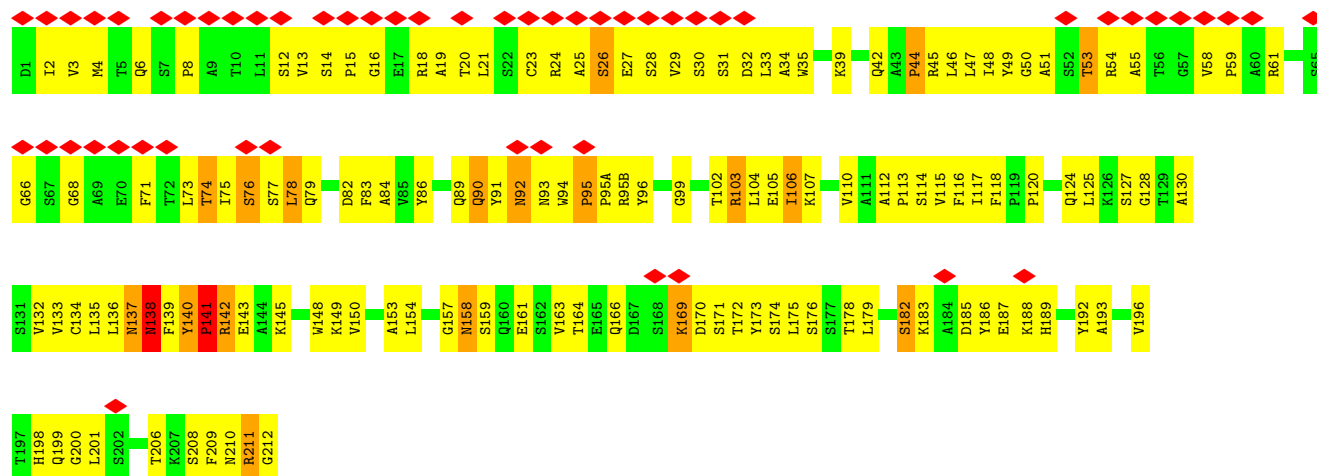


• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

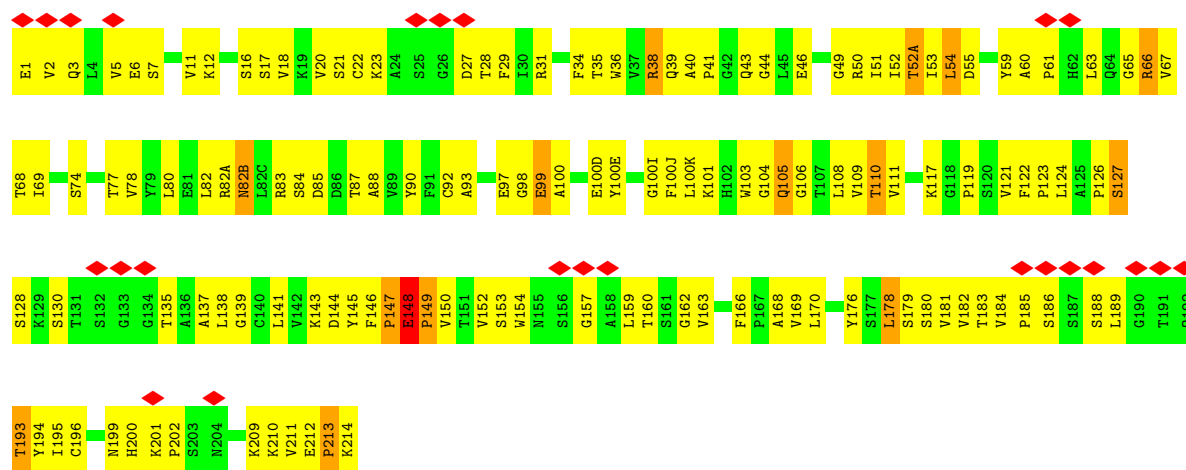




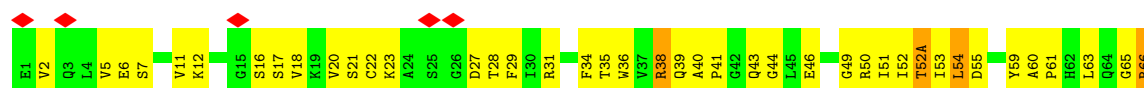
• Molecule 3: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

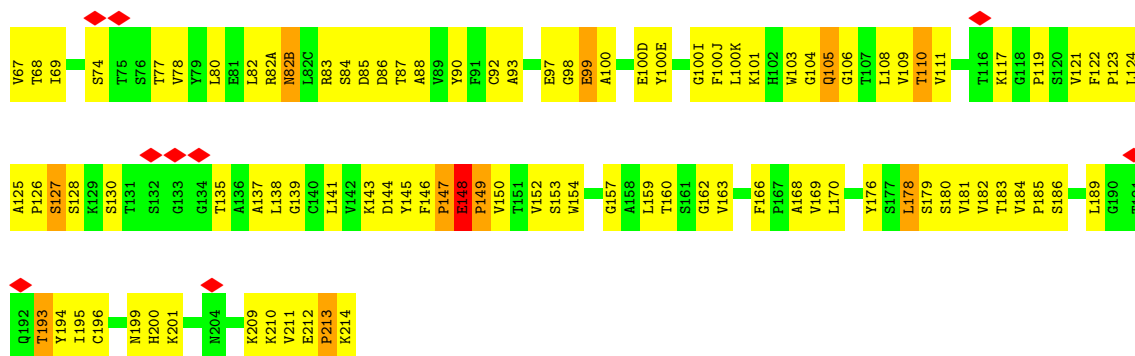


• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

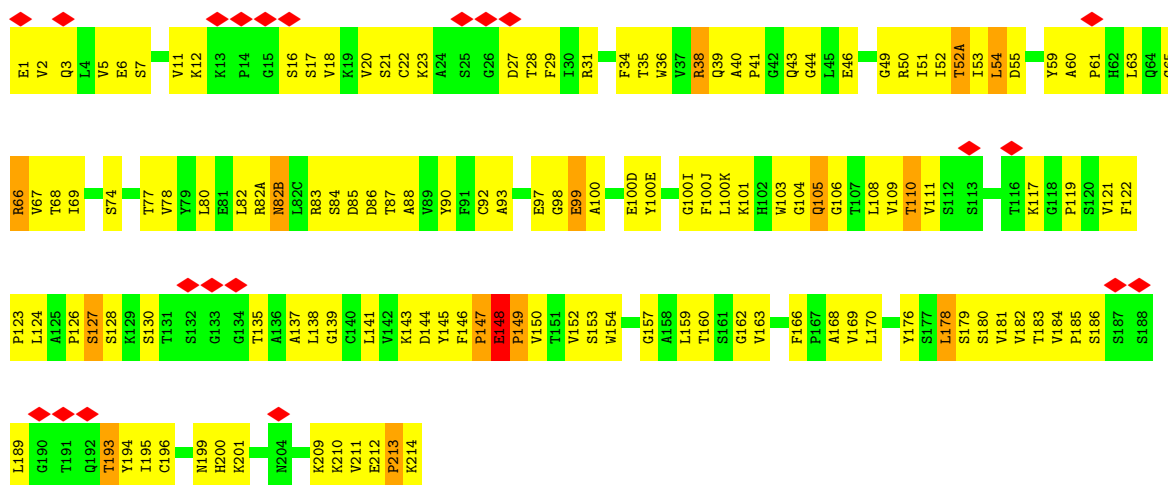


• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B

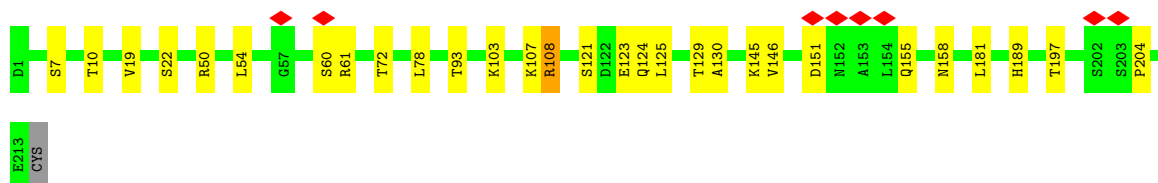
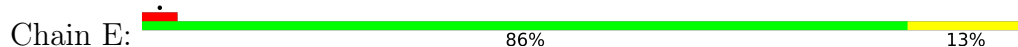




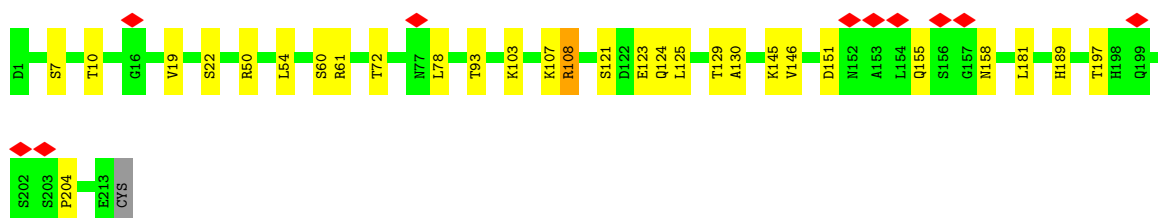
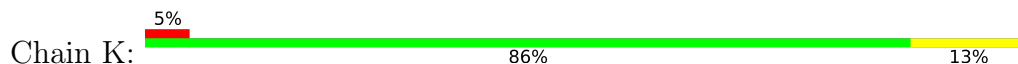
• Molecule 4: FAB OF BROADLY NEUTRALIZING ANTIBODY 17B



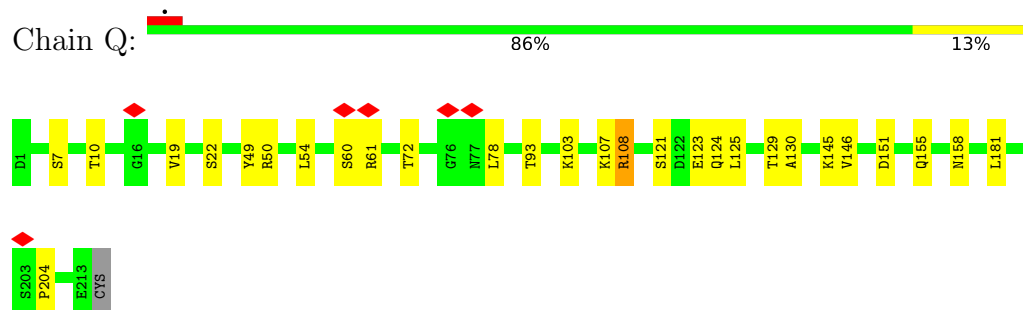
• Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5



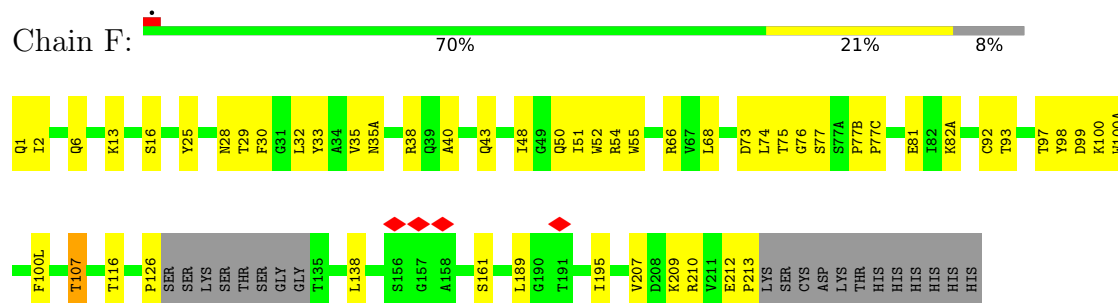
• Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5



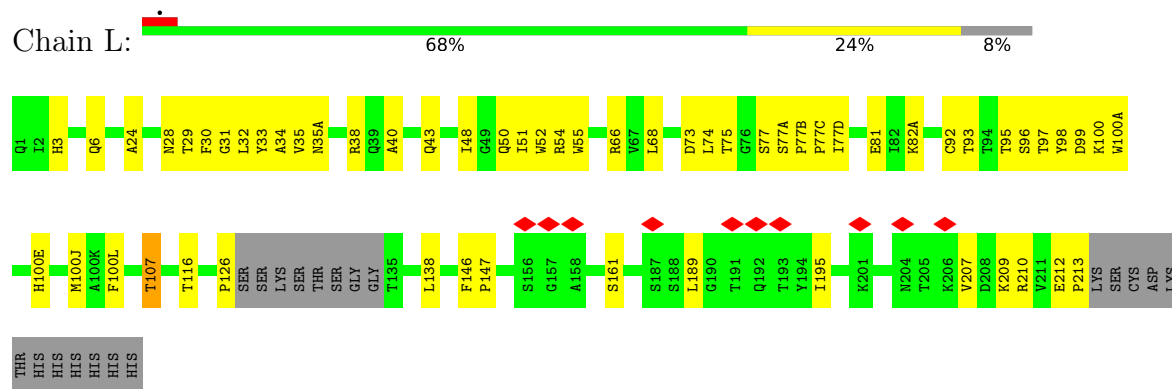
• Molecule 5: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5



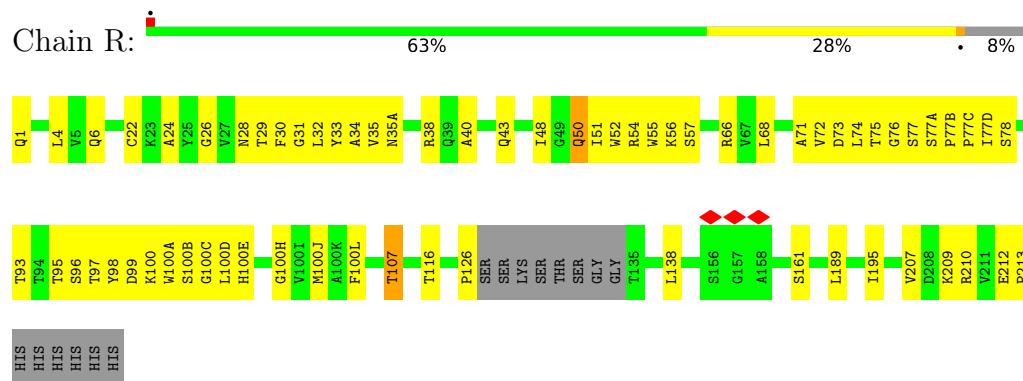
• Molecule 6: FAB OF BROADLY NEUTRALIZING ANTIBODY 8ANC195 VARIANT G52K5



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



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



## 4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of tilted images used	1745	Depositor
Resolution determination method	Not provided	
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	
Maximum defocus (nm)	Not provided	
Magnification	41000	Depositor
Image detector	GATAN K2 (4k x 4k)	Depositor
Maximum voxel value	178.420	Depositor
Minimum voxel value	167.490	Depositor
Average voxel value	171.431	Depositor
Voxel value standard deviation	0.982	Depositor
Recommended contour level	173	Depositor
Tomogram size ( $\text{\AA}$ )	260.0, 260.0, 260.0	wwPDB
Tomogram dimensions	50, 50, 50	wwPDB
Tomogram angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Grid spacing ( $\text{\AA}$ )	5.2, 5.2, 5.2	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  > 5$	RMSZ	# $ Z  > 5$
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	17
1	G	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	2	17
1	M	304/313 (97%)	242 (80%)	48 (16%)	14 (5%)	2	17
2	B	179/185 (97%)	127 (71%)	38 (21%)	14 (8%)	1	10
2	H	179/185 (97%)	127 (71%)	38 (21%)	14 (8%)	1	10
2	N	179/185 (97%)	126 (70%)	39 (22%)	14 (8%)	1	10
3	C	212/214 (99%)	171 (81%)	28 (13%)	13 (6%)	1	13
3	I	212/214 (99%)	170 (80%)	29 (14%)	13 (6%)	1	13
3	O	212/214 (99%)	171 (81%)	28 (13%)	13 (6%)	1	13
4	D	227/229 (99%)	185 (82%)	35 (15%)	7 (3%)	3	22
4	J	227/229 (99%)	184 (81%)	36 (16%)	7 (3%)	3	22
4	P	227/229 (99%)	184 (81%)	36 (16%)	7 (3%)	3	22

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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%)	5	20

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%)	19	40
1	G	271/276 (98%)	257 (95%)	14 (5%)	19	40
1	M	271/276 (98%)	257 (95%)	14 (5%)	19	40
2	B	164/167 (98%)	149 (91%)	15 (9%)	7	24
2	H	164/167 (98%)	149 (91%)	15 (9%)	7	24
2	N	164/167 (98%)	149 (91%)	15 (9%)	7	24
3	C	184/184 (100%)	174 (95%)	10 (5%)	18	40
3	I	184/184 (100%)	174 (95%)	10 (5%)	18	40
3	O	184/184 (100%)	174 (95%)	10 (5%)	18	40
4	D	193/193 (100%)	183 (95%)	10 (5%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	J	193/193 (100%)	183 (95%)	10 (5%)	19	40
4	P	193/193 (100%)	183 (95%)	10 (5%)	19	40
5	E	174/182 (96%)	164 (94%)	10 (6%)	17	38
5	K	174/182 (96%)	164 (94%)	10 (6%)	17	38
5	Q	174/182 (96%)	164 (94%)	10 (6%)	17	38
6	F	183/210 (87%)	175 (96%)	8 (4%)	24	45
6	L	183/210 (87%)	175 (96%)	8 (4%)	24	45
6	R	183/210 (87%)	175 (96%)	8 (4%)	24	45
All	All	3507/3636 (96%)	3306 (94%)	201 (6%)	20	38

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

Mol	Chain	Res	Type
4	J	178	LEU
1	M	418	CYS
6	R	207	VAL
5	K	61	ARG
6	L	116	THR

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

Mol	Chain	Res	Type
2	N	110	GLN
3	O	100	GLN
4	P	200	HIS
1	G	246	GLN
1	G	114	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

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	734	1	14,14,15	0.62	0	17,19,21	0.51	0
7	NAG	A	908	1	14,14,15	0.63	0	17,19,21	0.60	0
7	NAG	G	776	1	14,14,15	0.59	0	17,19,21	0.78	0
7	NAG	M	734	1	14,14,15	0.63	0	17,19,21	0.52	0
7	NAG	G	697	1	14,14,15	0.65	0	17,19,21	0.65	0
7	NAG	M	795	1	14,14,15	0.52	0	17,19,21	0.73	0
7	NAG	A	795	1	14,14,15	0.52	0	17,19,21	0.74	0
7	NAG	A	789	1	14,14,15	0.64	0	17,19,21	0.88	0
7	NAG	A	963	1	14,14,15	0.75	0	17,19,21	0.65	0
7	NAG	A	886	1	14,14,15	0.66	0	17,19,21	1.05	2 (11%)
7	NAG	M	588	1	14,14,15	0.63	0	17,19,21	0.79	0
7	NAG	G	886	1	14,14,15	0.67	0	17,19,21	1.04	2 (11%)
7	NAG	M	776	1	14,14,15	0.60	0	17,19,21	0.79	0
7	NAG	G	588	1	14,14,15	0.63	0	17,19,21	0.79	0
7	NAG	G	856	1	14,14,15	0.77	0	17,19,21	0.71	0
7	NAG	A	588	1	14,14,15	0.63	0	17,19,21	0.78	0
7	NAG	M	789	1	14,14,15	0.65	0	17,19,21	0.88	0
7	NAG	M	741	1	14,14,15	0.56	0	17,19,21	0.60	0
7	NAG	M	963	1	14,14,15	0.75	0	17,19,21	0.66	0
7	NAG	G	894	1	14,14,15	0.66	0	17,19,21	0.74	1 (5%)
7	NAG	M	894	1	14,14,15	0.66	0	17,19,21	0.74	1 (5%)
7	NAG	G	948	1	14,14,15	0.91	1 (7%)	17,19,21	0.94	1 (5%)
7	NAG	M	948	1	14,14,15	0.89	1 (7%)	17,19,21	0.95	1 (5%)
7	NAG	L	1000	6	14,14,15	1.67	1 (7%)	17,19,21	1.38	1 (5%)
7	NAG	G	734	1	14,14,15	0.63	0	17,19,21	0.51	0
7	NAG	M	697	1	14,14,15	0.65	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NAG	G	908	1	14,14,15	0.63	0	17,19,21	0.60	0
7	NAG	M	908	1	14,14,15	0.61	0	17,19,21	0.60	0
7	NAG	M	886	1	14,14,15	0.66	0	17,19,21	1.04	2 (11%)
7	NAG	A	741	1	14,14,15	0.57	0	17,19,21	0.61	0
7	NAG	G	795	1	14,14,15	0.52	0	17,19,21	0.73	0
7	NAG	A	948	1	14,14,15	0.90	1 (7%)	17,19,21	0.96	1 (5%)
7	NAG	A	856	1	14,14,15	0.77	0	17,19,21	0.71	0
7	NAG	A	697	1	14,14,15	0.64	0	17,19,21	0.64	0
7	NAG	G	789	1	14,14,15	0.64	0	17,19,21	0.88	0
7	NAG	A	894	1	14,14,15	0.65	0	17,19,21	0.74	1 (5%)
7	NAG	G	963	1	14,14,15	0.75	0	17,19,21	0.66	0
7	NAG	A	762	1	14,14,15	0.61	0	17,19,21	0.72	1 (5%)
7	NAG	F	1000	6	14,14,15	1.67	1 (7%)	17,19,21	1.38	1 (5%)
7	NAG	G	741	1	14,14,15	0.56	0	17,19,21	0.60	0
7	NAG	M	856	1	14,14,15	0.78	0	17,19,21	0.71	0
7	NAG	A	776	1	14,14,15	0.59	0	17,19,21	0.79	0
7	NAG	R	1000	6	14,14,15	1.66	1 (7%)	17,19,21	1.38	1 (5%)
7	NAG	M	762	1	14,14,15	0.63	0	17,19,21	0.73	1 (5%)
7	NAG	G	762	1	14,14,15	0.62	0	17,19,21	0.73	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	734	1	-	5/6/23/26	0/1/1/1
7	NAG	A	908	1	-	2/6/23/26	0/1/1/1
7	NAG	G	776	1	-	2/6/23/26	0/1/1/1
7	NAG	M	734	1	-	5/6/23/26	0/1/1/1
7	NAG	G	697	1	-	5/6/23/26	0/1/1/1
7	NAG	M	795	1	-	2/6/23/26	0/1/1/1
7	NAG	A	795	1	-	2/6/23/26	0/1/1/1
7	NAG	A	789	1	-	4/6/23/26	0/1/1/1
7	NAG	A	963	1	-	5/6/23/26	0/1/1/1
7	NAG	A	886	1	-	4/6/23/26	0/1/1/1
7	NAG	M	588	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	G	886	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	M	776	1	-	2/6/23/26	0/1/1/1
7	NAG	G	588	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	G	856	1	-	4/6/23/26	0/1/1/1
7	NAG	A	588	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	M	789	1	-	4/6/23/26	0/1/1/1
7	NAG	M	741	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	M	963	1	-	5/6/23/26	0/1/1/1
7	NAG	G	894	1	-	4/6/23/26	0/1/1/1
7	NAG	M	894	1	-	4/6/23/26	0/1/1/1
7	NAG	G	948	1	-	4/6/23/26	0/1/1/1
7	NAG	M	948	1	-	4/6/23/26	0/1/1/1
7	NAG	L	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	G	734	1	-	5/6/23/26	0/1/1/1
7	NAG	M	697	1	-	5/6/23/26	0/1/1/1
7	NAG	G	908	1	-	2/6/23/26	0/1/1/1
7	NAG	M	908	1	-	2/6/23/26	0/1/1/1
7	NAG	M	886	1	-	4/6/23/26	0/1/1/1
7	NAG	A	741	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	G	795	1	-	2/6/23/26	0/1/1/1
7	NAG	A	948	1	-	4/6/23/26	0/1/1/1
7	NAG	A	856	1	-	4/6/23/26	0/1/1/1
7	NAG	A	697	1	-	5/6/23/26	0/1/1/1
7	NAG	G	789	1	-	4/6/23/26	0/1/1/1
7	NAG	A	894	1	-	4/6/23/26	0/1/1/1
7	NAG	G	963	1	-	5/6/23/26	0/1/1/1
7	NAG	G	741	1	1/1/5/7	4/6/23/26	0/1/1/1
7	NAG	A	762	1	-	6/6/23/26	0/1/1/1
7	NAG	F	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	M	856	1	-	4/6/23/26	0/1/1/1
7	NAG	A	776	1	-	2/6/23/26	0/1/1/1
7	NAG	R	1000	6	-	0/6/23/26	0/1/1/1
7	NAG	M	762	1	-	6/6/23/26	0/1/1/1
7	NAG	G	762	1	-	6/6/23/26	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	-5.92	1.34	1.43
7	L	1000	NAG	O5-C1	-5.92	1.34	1.43
7	R	1000	NAG	O5-C1	-5.88	1.34	1.43
7	A	948	NAG	C1-C2	2.60	1.56	1.52
7	G	948	NAG	C1-C2	2.58	1.56	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	1000	NAG	C1-O5-C5	-4.74	105.77	112.19
7	F	1000	NAG	C1-O5-C5	-4.73	105.78	112.19
7	R	1000	NAG	C1-O5-C5	-4.73	105.78	112.19
7	A	886	NAG	C2-N2-C7	-2.70	119.06	122.90
7	G	886	NAG	C2-N2-C7	-2.69	119.07	122.90

5 of 6 chirality outliers are listed below:

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

5 of 165 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	588	NAG	C8-C7-N2-C2
7	A	588	NAG	O7-C7-N2-C2
7	A	697	NAG	C1-C2-N2-C7
7	A	697	NAG	C8-C7-N2-C2
7	A	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	908	NAG	3	0
7	G	776	NAG	5	0
7	M	734	NAG	9	0
7	A	789	NAG	5	0

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

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

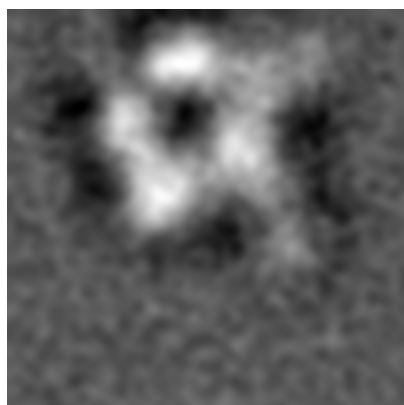
## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

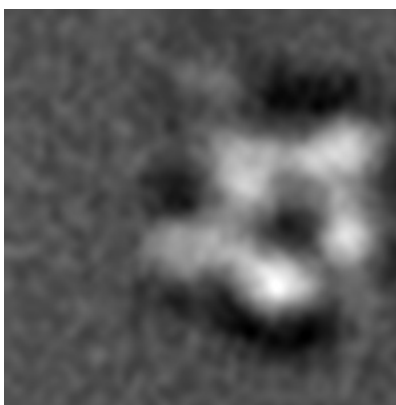
## 6 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-3096. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

### 6.1 Orthogonal projections [i](#)



X



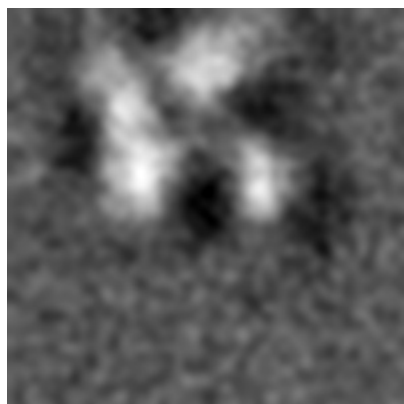
Y



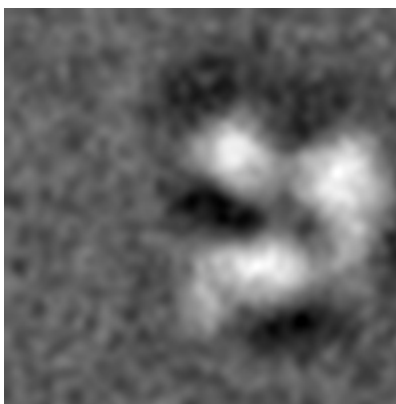
Z

The images above show the tomogram projected in three orthogonal directions.

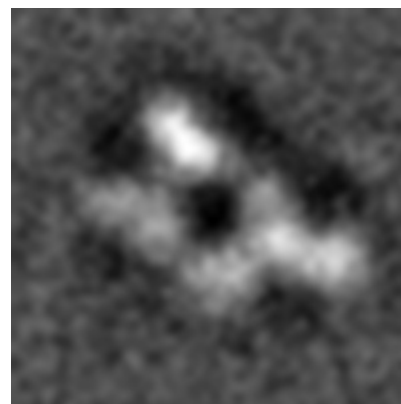
### 6.2 Central slices [i](#)



X Index: 25



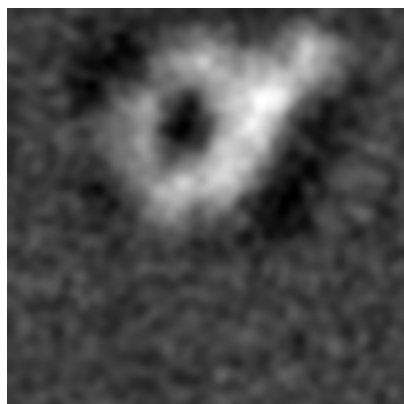
Y Index: 25



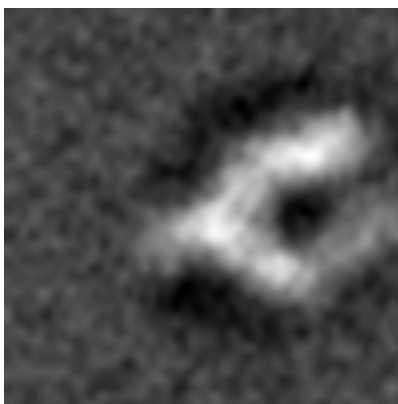
Z Index: 25

The images above show central slices of the tomogram in three orthogonal directions.

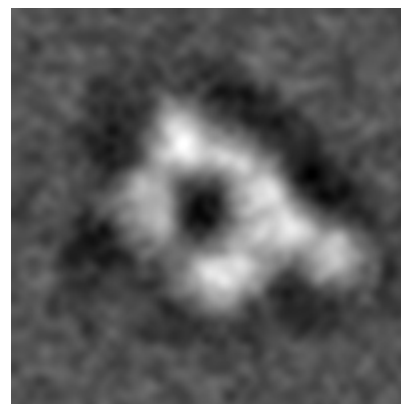
### 6.3 Largest variance slices [i](#)



X Index: 31



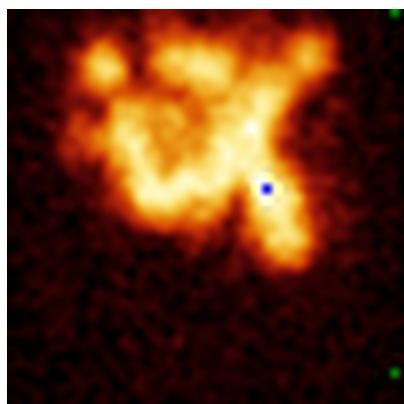
Y Index: 31



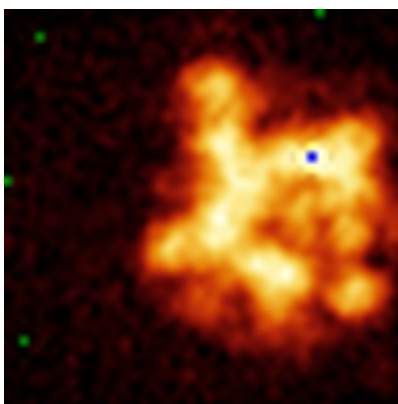
Z Index: 28

The images above show the largest variance slices of the tomogram in three orthogonal directions.

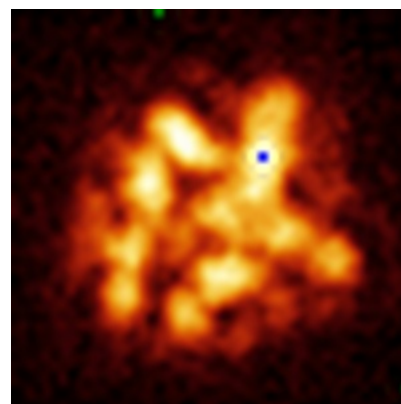
### 6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

The images above show the tomogram projected in three orthogonal directions.

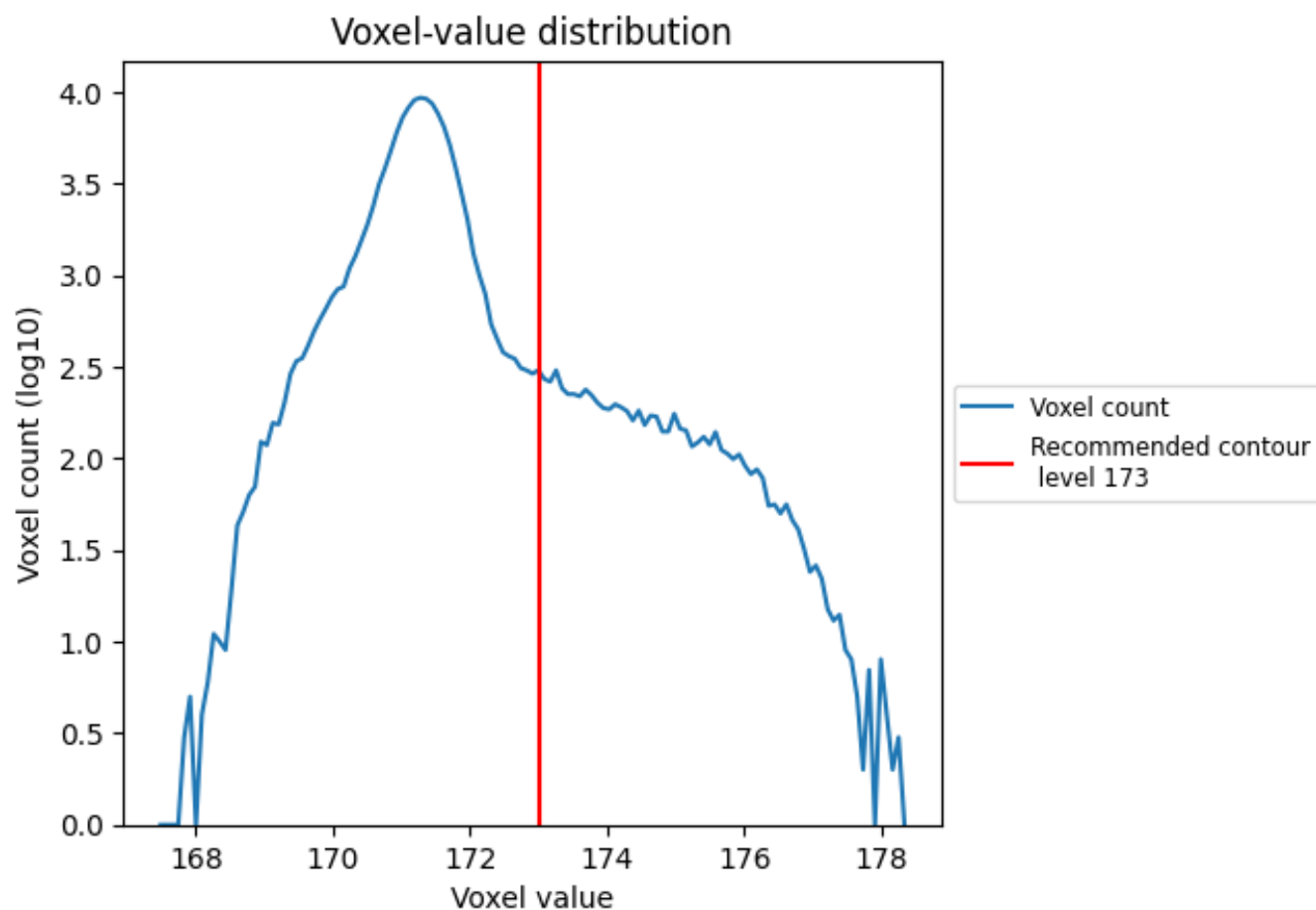
### 6.5 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

## 7 Tomogram analysis [i](#)

This section contains the results of statistical analysis of the tomogram.

### 7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

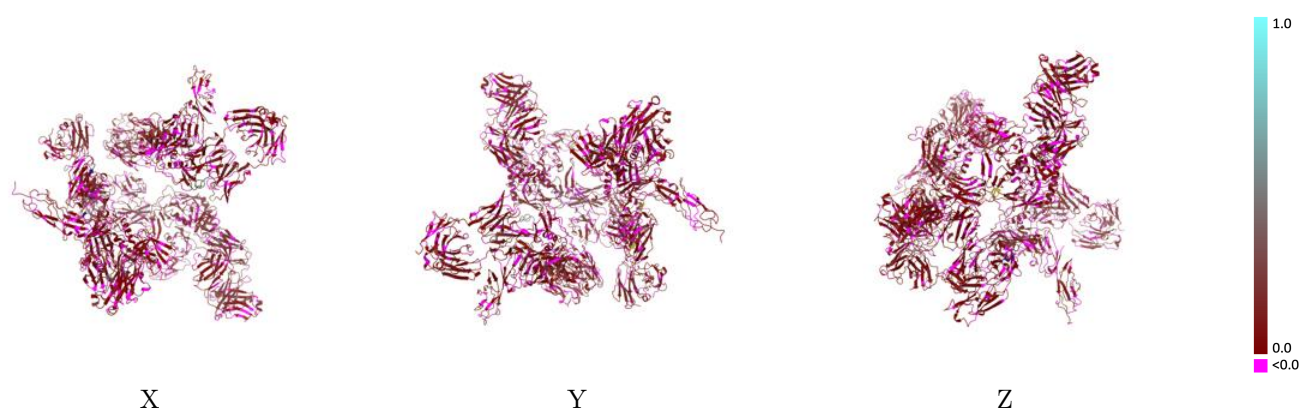
## 8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-3096 and PDB model 5A8H. Per-residue inclusion information can be found in section 3 on page 9.

### 8.1 Map-model overlay [i](#)

This section was not generated.

### 8.2 Q-score mapped to coordinate model [i](#)

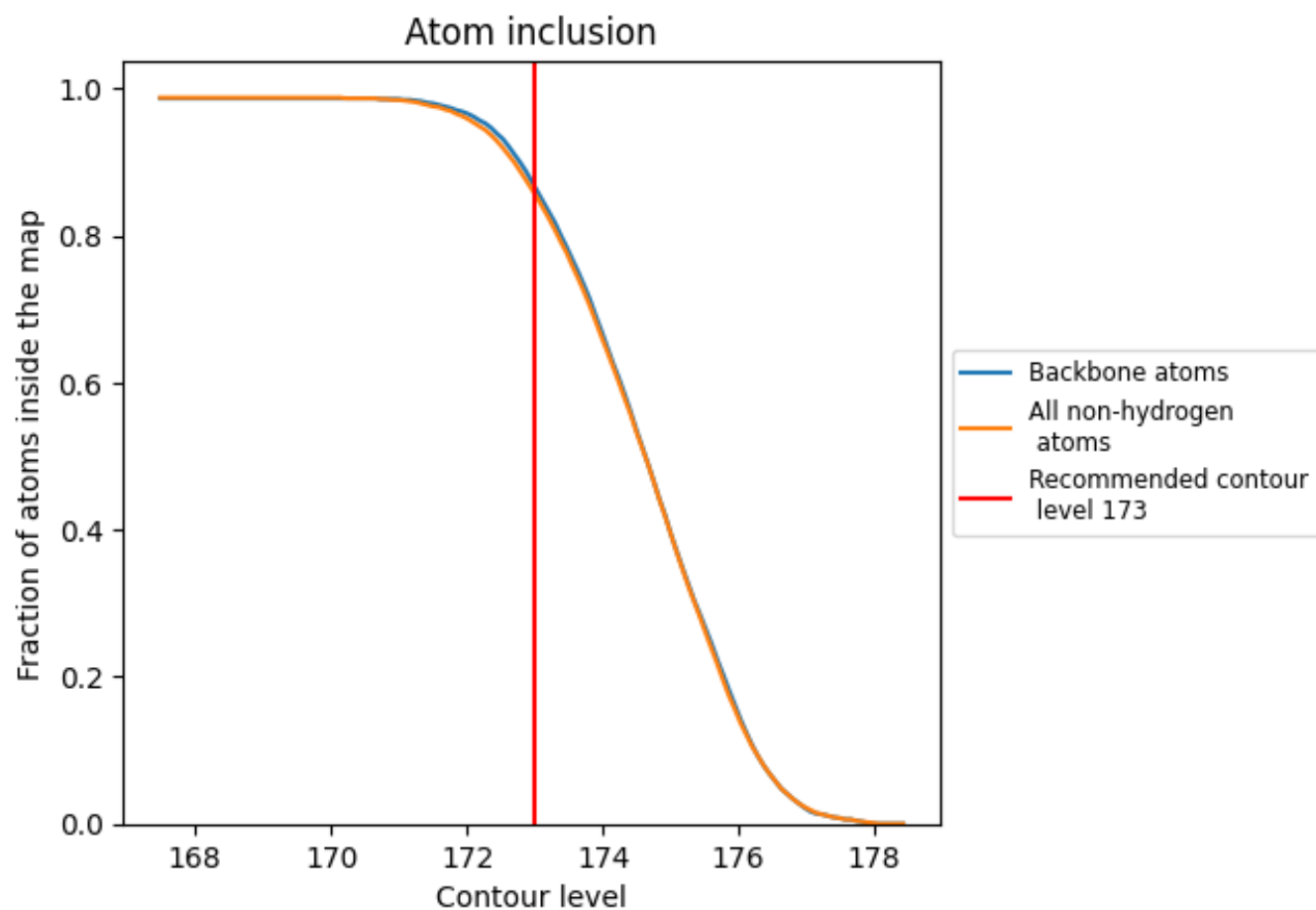


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

### 8.3 Atom inclusion mapped to coordinate model [i](#)

This section was not generated.







































## 8.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 86% of all non-hydrogen atoms, are inside the map.

## 8.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8570	 0.0600
A	 0.8610	 0.0630
B	 0.6950	 0.0620
C	 0.8470	 0.0640
D	 0.8970	 0.0690
E	 0.9610	 0.0500
F	 0.9710	 0.0840
G	 0.9460	 0.0590
H	 0.5040	 0.0410
I	 0.7320	 0.0610
J	 0.9320	 0.0590
K	 0.9440	 0.0580
L	 0.9450	 0.0640
M	 0.9560	 0.0520
N	 0.4850	 0.0420
O	 0.7110	 0.0580
P	 0.8980	 0.0710
Q	 0.9520	 0.0610
R	 0.9590	 0.0530

