wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 07:04 AM JST

PDB ID	:	7XST
EMDB ID	:	EMD-33434
Title	:	Cryo-EM structure of SARS-CoV-2 Omicron spike glycoprotein in complex with three F61 Fab and three D2 Fab
Authors	:	Wang, X.; Li, X.
Deposited on	:	2022-05-15
Resolution	:	3.04 Å(reported)

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

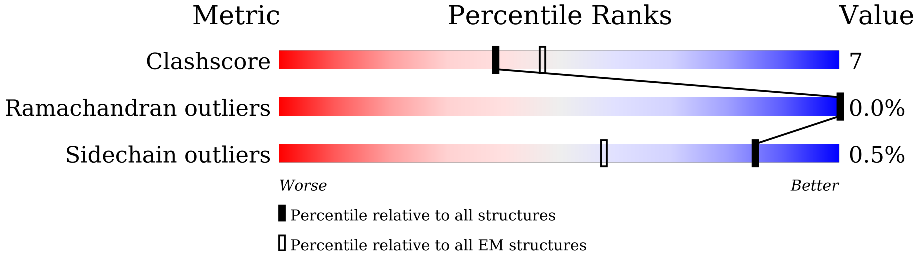
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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

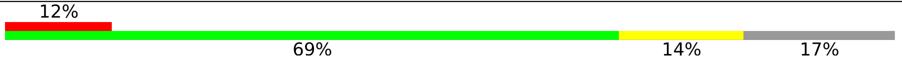
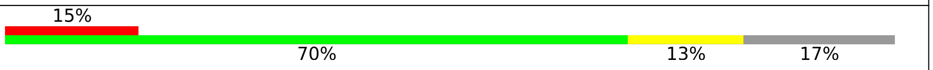
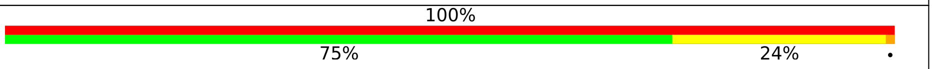
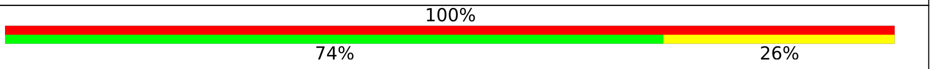
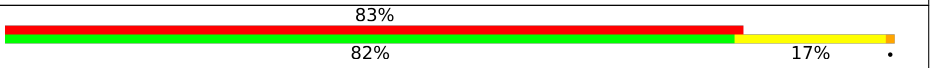
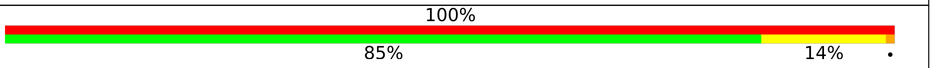
The reported resolution of this entry is 3.04 Å.

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 >=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 <=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	1210	
1	B	1210	
1	C	1210	
2	D	117	
2	H	117	
2	L	117	
3	E	110	
3	I	110	

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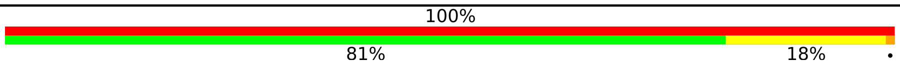
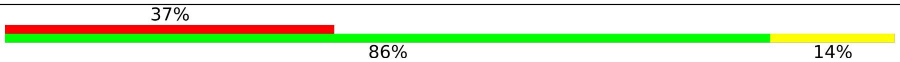
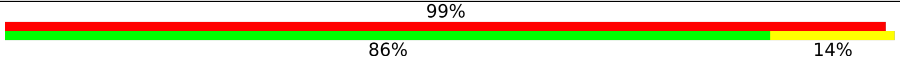
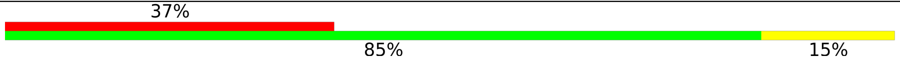
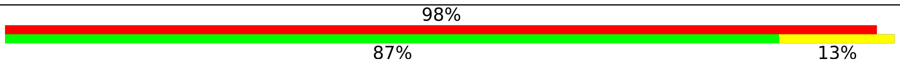
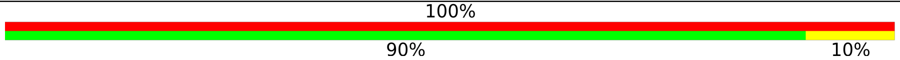
Mol	Chain	Length	Quality of chain
3	M	110	
4	F	123	
4	J	123	
4	N	123	
5	G	110	
5	K	110	
5	O	110	

2 Entry composition ⓘ

There are 6 unique types of molecules in this entry. The entry contains 33532 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1010	7633	4881	1273	1445	34	0	0
1	B	1009	7611	4869	1271	1437	34	0	0
1	C	1008	7638	4894	1275	1435	34	0	0

There are 147 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	conflict	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	conflict	UNP P0DTC2
A	142	ASP	GLY	conflict	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	210A	ILE	-	insertion	UNP P0DTC2
A	210B	VAL	-	insertion	UNP P0DTC2
A	210C	ARG	ASN	conflict	UNP P0DTC2
A	210D	GLU	LEU	conflict	UNP P0DTC2
A	210E	PRO	VAL	conflict	UNP P0DTC2
A	210F	GLU	ARG	conflict	UNP P0DTC2
A	339	ASP	GLY	conflict	UNP P0DTC2
A	371	LEU	SER	conflict	UNP P0DTC2
A	373	PRO	SER	conflict	UNP P0DTC2
A	375	PHE	SER	conflict	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	440	LYS	ASN	conflict	UNP P0DTC2
A	446	SER	GLY	conflict	UNP P0DTC2
A	477	ASN	SER	conflict	UNP P0DTC2
A	478	LYS	THR	conflict	UNP P0DTC2
A	484	ALA	GLU	conflict	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	493	ARG	GLN	conflict	UNP P0DTC2
A	496	SER	GLY	conflict	UNP P0DTC2
A	498	ARG	GLN	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	505	HIS	TYR	conflict	UNP P0DTC2
A	547	LYS	THR	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	655	TYR	HIS	conflict	UNP P0DTC2
A	679	LYS	ASN	conflict	UNP P0DTC2
A	681	HIS	PRO	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	764	LYS	ASN	conflict	UNP P0DTC2
A	796	TYR	ASP	conflict	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	856	LYS	ASN	conflict	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	954	HIS	GLN	conflict	UNP P0DTC2
A	969	LYS	ASN	conflict	UNP P0DTC2
A	981	PHE	LEU	conflict	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	67	VAL	ALA	conflict	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	conflict	UNP P0DTC2
B	142	ASP	GLY	conflict	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	210A	ILE	-	insertion	UNP P0DTC2
B	210B	VAL	-	insertion	UNP P0DTC2
B	210C	ARG	ASN	conflict	UNP P0DTC2
B	210D	GLU	LEU	conflict	UNP P0DTC2
B	210E	PRO	VAL	conflict	UNP P0DTC2
B	210F	GLU	ARG	conflict	UNP P0DTC2
B	339	ASP	GLY	conflict	UNP P0DTC2
B	371	LEU	SER	conflict	UNP P0DTC2
B	373	PRO	SER	conflict	UNP P0DTC2

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Chain	**Residue**	**Modelled**	**Actual**	**Comment**	**Reference**
B	375	PHE	SER	conflict	UNP P0DTC2
B	417	ASN	LYS	conflict	UNP P0DTC2
B	440	LYS	ASN	conflict	UNP P0DTC2
B	446	SER	GLY	conflict	UNP P0DTC2
B	477	ASN	SER	conflict	UNP P0DTC2
B	478	LYS	THR	conflict	UNP P0DTC2
B	484	ALA	GLU	conflict	UNP P0DTC2
B	493	ARG	GLN	conflict	UNP P0DTC2
B	496	SER	GLY	conflict	UNP P0DTC2
B	498	ARG	GLN	conflict	UNP P0DTC2
B	501	TYR	ASN	conflict	UNP P0DTC2
B	505	HIS	TYR	conflict	UNP P0DTC2
B	547	LYS	THR	conflict	UNP P0DTC2
B	614	GLY	ASP	conflict	UNP P0DTC2
B	655	TYR	HIS	conflict	UNP P0DTC2
B	679	LYS	ASN	conflict	UNP P0DTC2
B	681	HIS	PRO	conflict	UNP P0DTC2
B	682	GLY	ARG	conflict	UNP P0DTC2
B	683	SER	ARG	conflict	UNP P0DTC2
B	685	SER	ARG	conflict	UNP P0DTC2
B	764	LYS	ASN	conflict	UNP P0DTC2
B	796	TYR	ASP	conflict	UNP P0DTC2
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	856	LYS	ASN	conflict	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	954	HIS	GLN	conflict	UNP P0DTC2
B	969	LYS	ASN	conflict	UNP P0DTC2
B	981	PHE	LEU	conflict	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	67	VAL	ALA	conflict	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	conflict	UNP P0DTC2
C	142	ASP	GLY	conflict	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	210A	ILE	-	insertion	UNP P0DTC2
C	210B	VAL	-	insertion	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	210C	ARG	ASN	conflict	UNP P0DTC2
C	210D	GLU	LEU	conflict	UNP P0DTC2
C	210E	PRO	VAL	conflict	UNP P0DTC2
C	210F	GLU	ARG	conflict	UNP P0DTC2
C	339	ASP	GLY	conflict	UNP P0DTC2
C	371	LEU	SER	conflict	UNP P0DTC2
C	373	PRO	SER	conflict	UNP P0DTC2
C	375	PHE	SER	conflict	UNP P0DTC2
C	417	ASN	LYS	conflict	UNP P0DTC2
C	440	LYS	ASN	conflict	UNP P0DTC2
C	446	SER	GLY	conflict	UNP P0DTC2
C	477	ASN	SER	conflict	UNP P0DTC2
C	478	LYS	THR	conflict	UNP P0DTC2
C	484	ALA	GLU	conflict	UNP P0DTC2
C	493	ARG	GLN	conflict	UNP P0DTC2
C	496	SER	GLY	conflict	UNP P0DTC2
C	498	ARG	GLN	conflict	UNP P0DTC2
C	501	TYR	ASN	conflict	UNP P0DTC2
C	505	HIS	TYR	conflict	UNP P0DTC2
C	547	LYS	THR	conflict	UNP P0DTC2
C	614	GLY	ASP	conflict	UNP P0DTC2
C	655	TYR	HIS	conflict	UNP P0DTC2
C	679	LYS	ASN	conflict	UNP P0DTC2
C	681	HIS	PRO	conflict	UNP P0DTC2
C	682	GLY	ARG	conflict	UNP P0DTC2
C	683	SER	ARG	conflict	UNP P0DTC2
C	685	SER	ARG	conflict	UNP P0DTC2
C	764	LYS	ASN	conflict	UNP P0DTC2
C	796	TYR	ASP	conflict	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	856	LYS	ASN	conflict	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	954	HIS	GLN	conflict	UNP P0DTC2
C	969	LYS	ASN	conflict	UNP P0DTC2
C	981	PHE	LEU	conflict	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

- Molecule 2 is a protein called F61 heavy chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
2	L	117	Total C N O S 874 545 151 174 4	0	0
2	H	117	Total C N O S 872 543 151 174 4	0	0
2	D	117	Total C N O S 874 545 151 174 4	0	0

- Molecule 3 is a protein called F61 light chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
3	M	110	Total C N O S 803 500 135 166 2	0	0
3	I	110	Total C N O S 803 500 135 166 2	0	0
3	E	110	Total C N O S 803 500 135 166 2	0	0

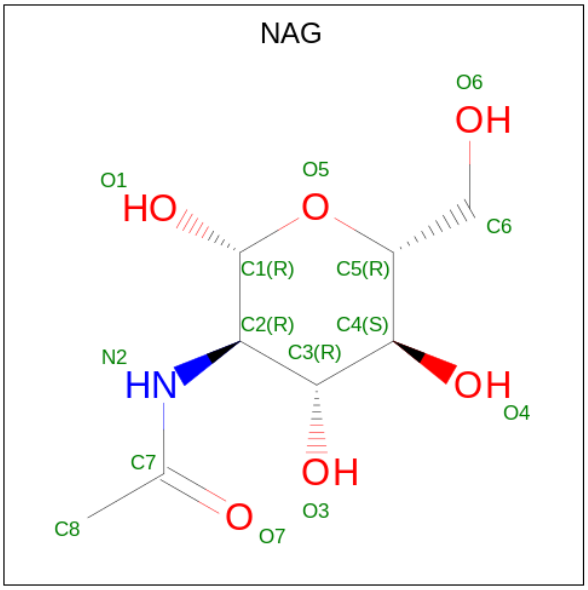
- Molecule 4 is a protein called D2 heavy chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
4	N	123	Total C N O S 943 594 157 188 4	0	0
4	J	123	Total C N O S 943 594 157 188 4	0	0
4	F	123	Total C N O S 943 594 157 188 4	0	0

- Molecule 5 is a protein called D2 light chain.

Mol	Chain	Residues	Atoms	AltConf	Trace
5	O	110	Total C N O S 786 490 131 163 2	0	0
5	K	110	Total C N O S 786 490 131 163 2	0	0
5	G	110	Total C N O S 786 490 131 163 2	0	0

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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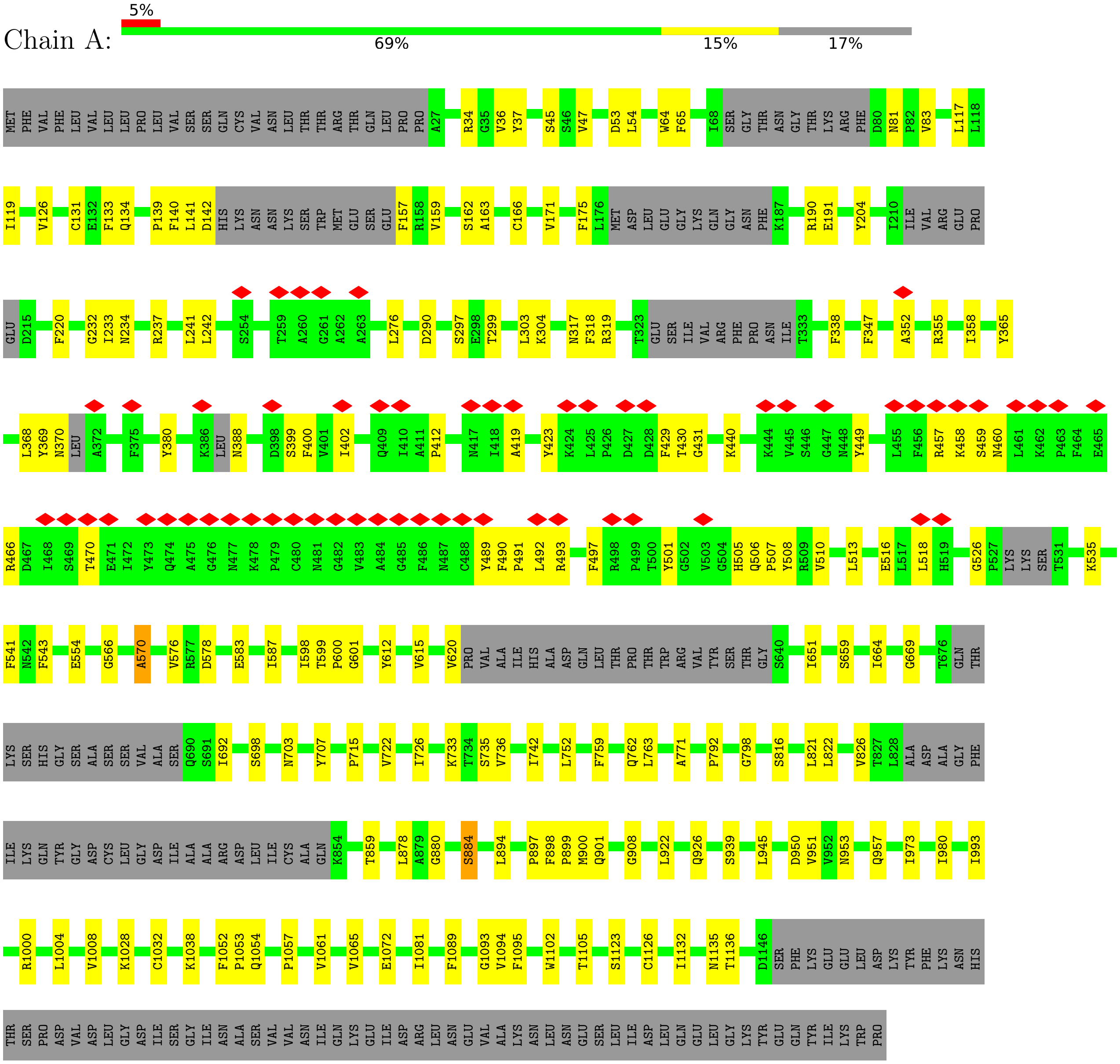
Mol	Chain	Residues	Atoms	AltConf
6	B	1	Total C N O 14 8 1 5	0
6	B	1	Total C N O 14 8 1 5	0
6	B	1	Total C N O 14 8 1 5	0
6	B	1	Total C N O 14 8 1 5	0
6	B	1	Total C N O 14 8 1 5	0
6	B	1	Total C N O 14 8 1 5	0
6	C	1	Total C N O 14 8 1 5	0
6	C	1	Total C N O 14 8 1 5	0
6	C	1	Total C N O 14 8 1 5	0
6	C	1	Total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

3 Residue-property plots ⓘ

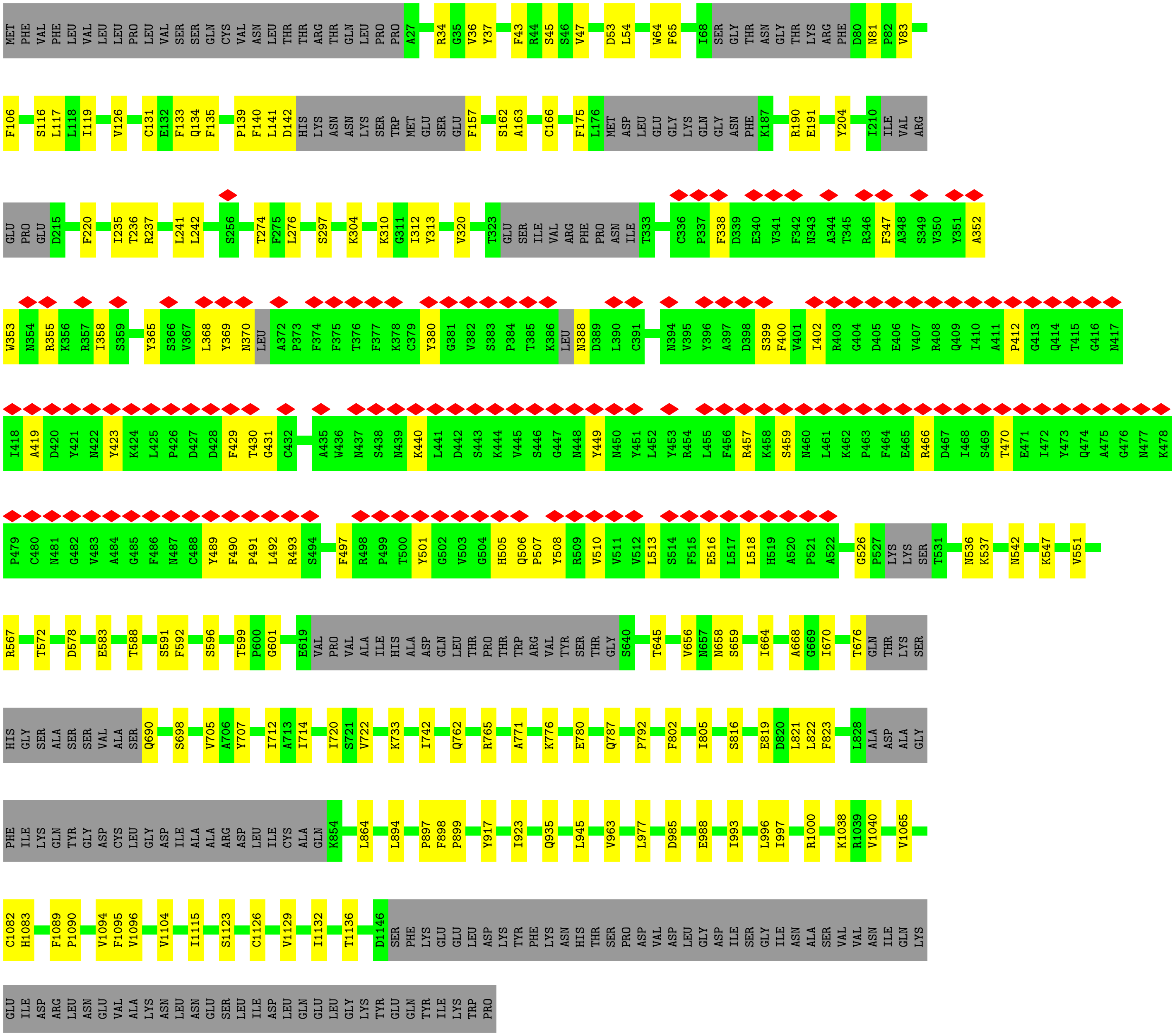
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein



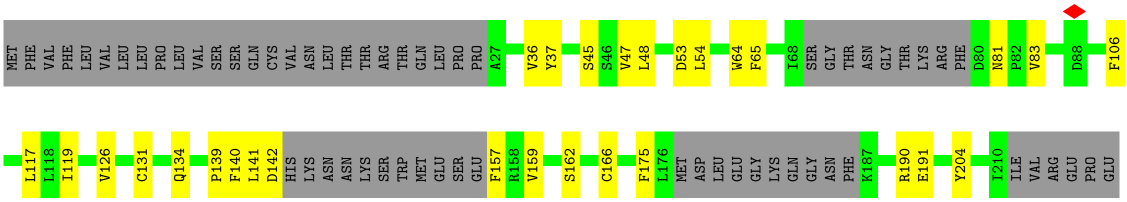
- Molecule 1: Spike glycoprotein

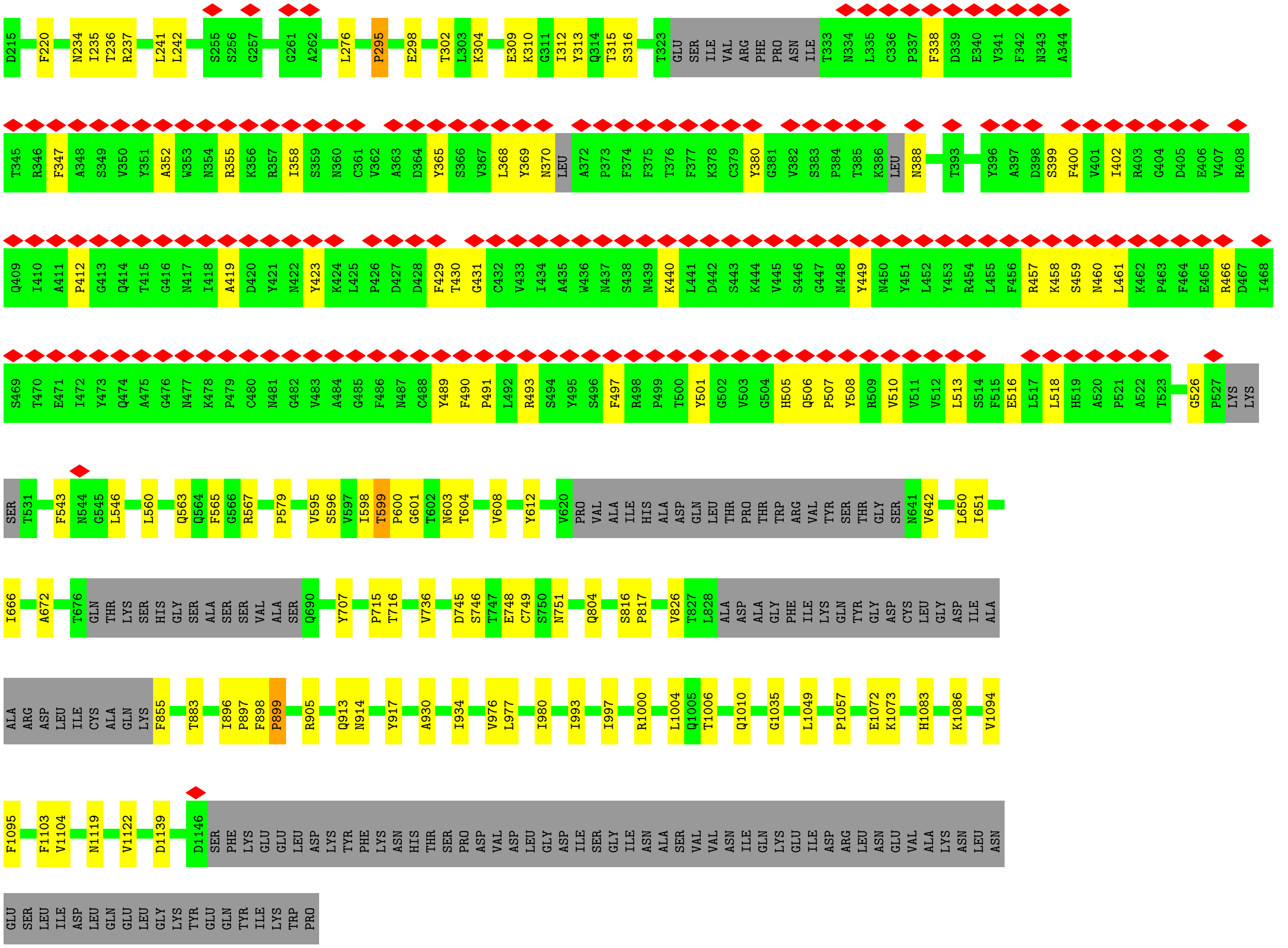
Chain B:



- Molecule 1: Spike glycoprotein

Chain C:



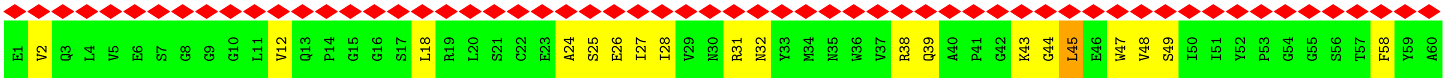


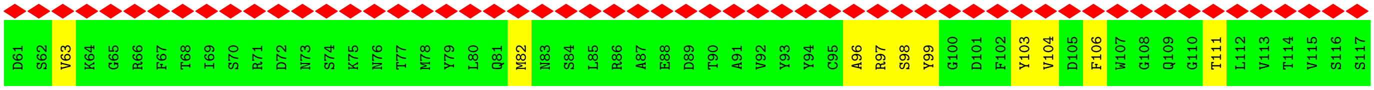
- Molecule 2: F61 heavy chain

Chain L:

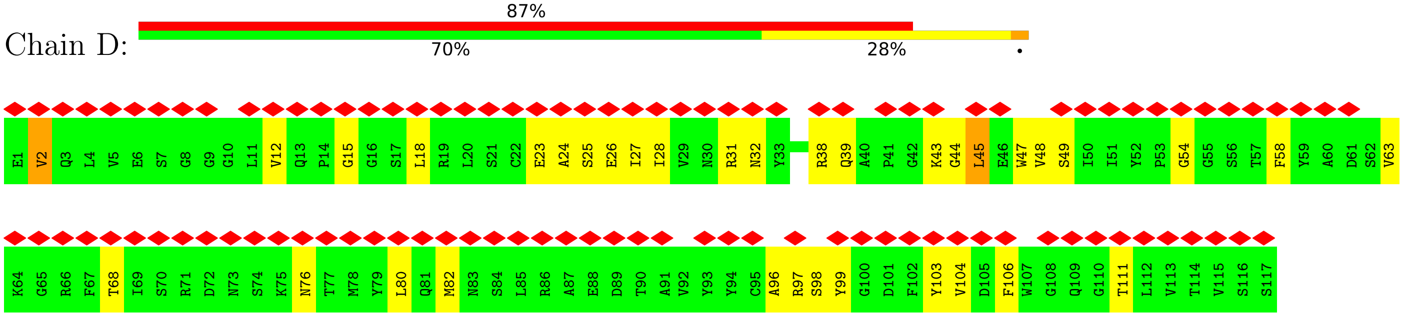
- Molecule 2: F61 heavy chain

Chain H:

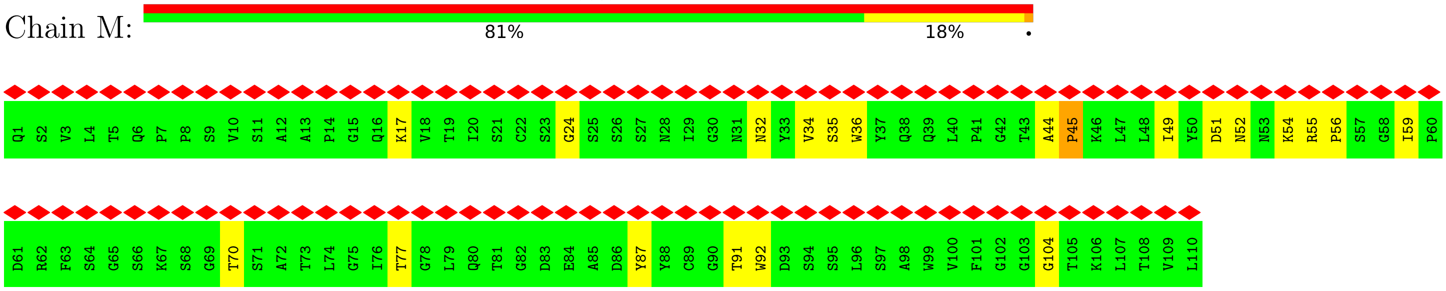




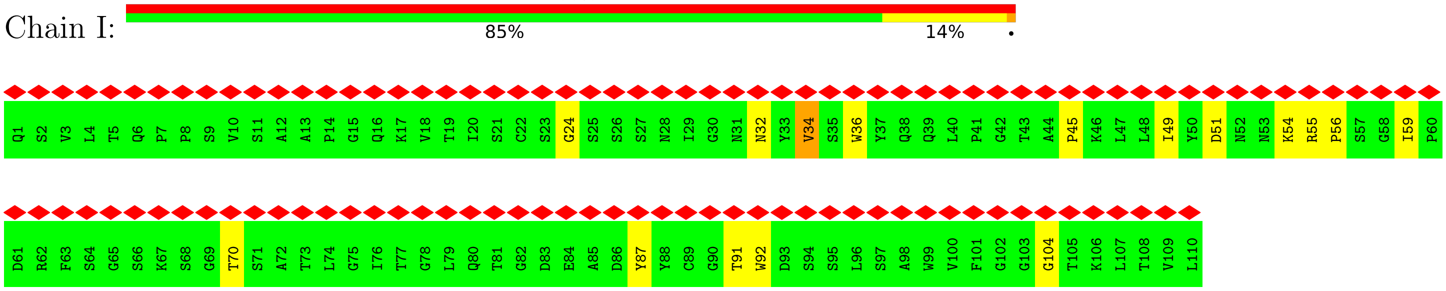
- Molecule 2: F61 heavy chain



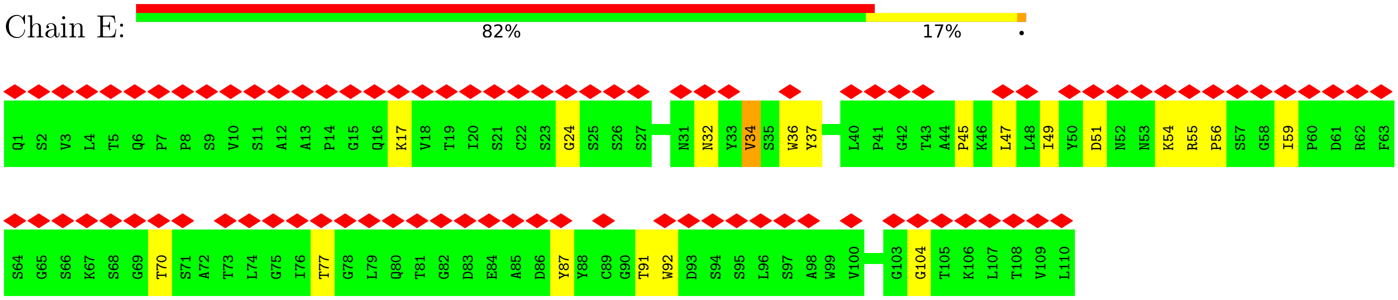
- Molecule 3: F61 light chain



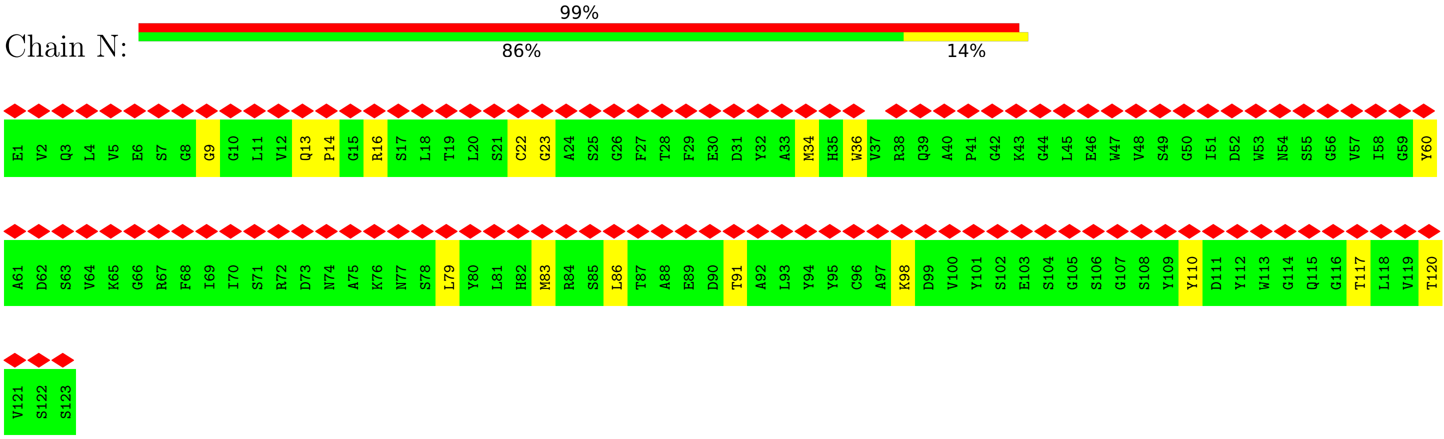
- Molecule 3: F61 light chain



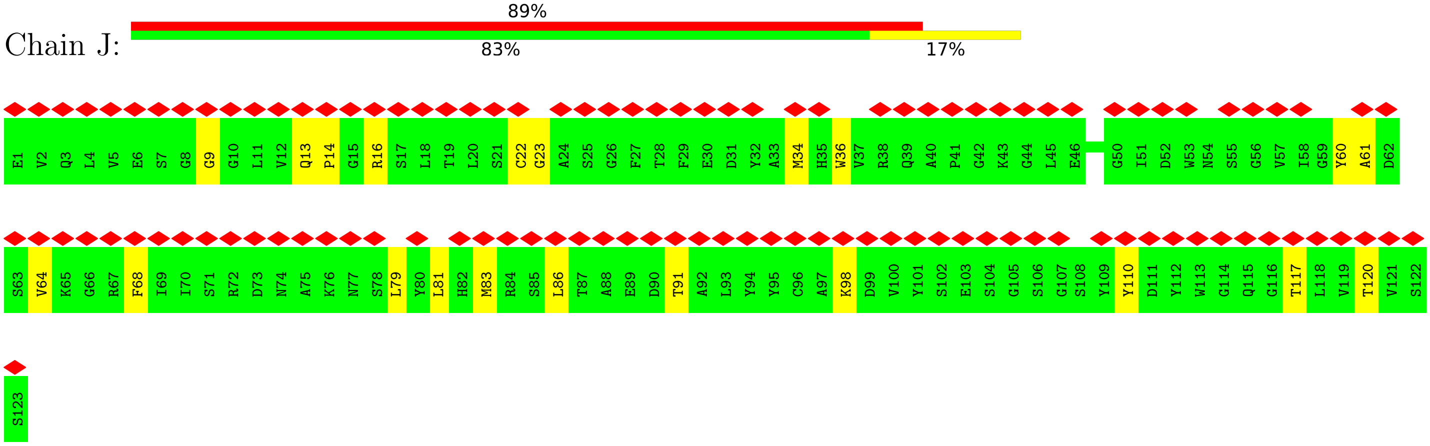
- Molecule 3: F61 light chain



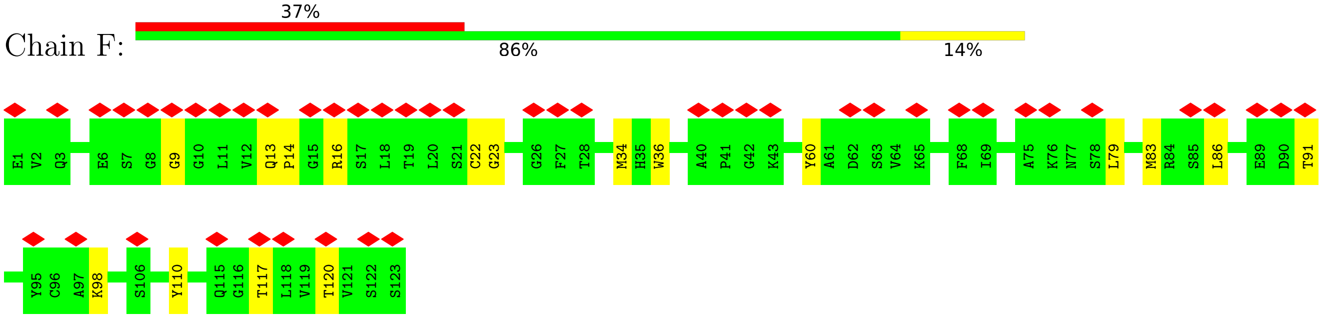
- Molecule 4: D2 heavy chain



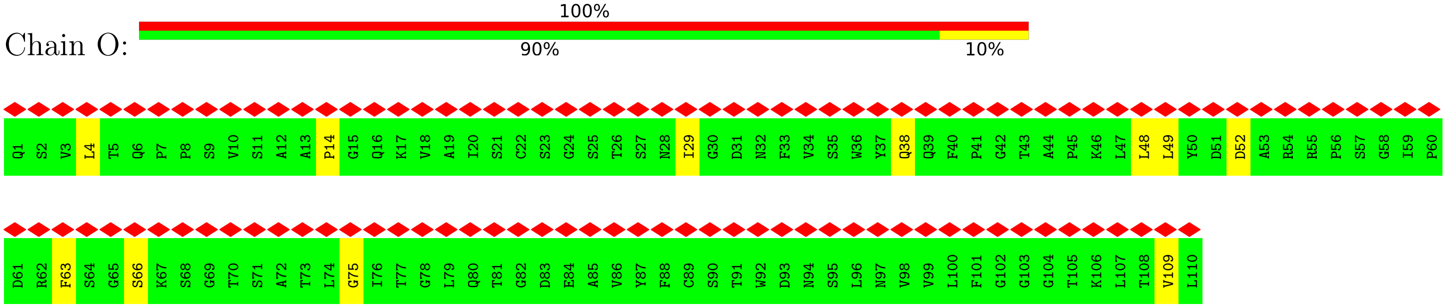
- Molecule 4: D2 heavy chain



- Molecule 4: D2 heavy chain

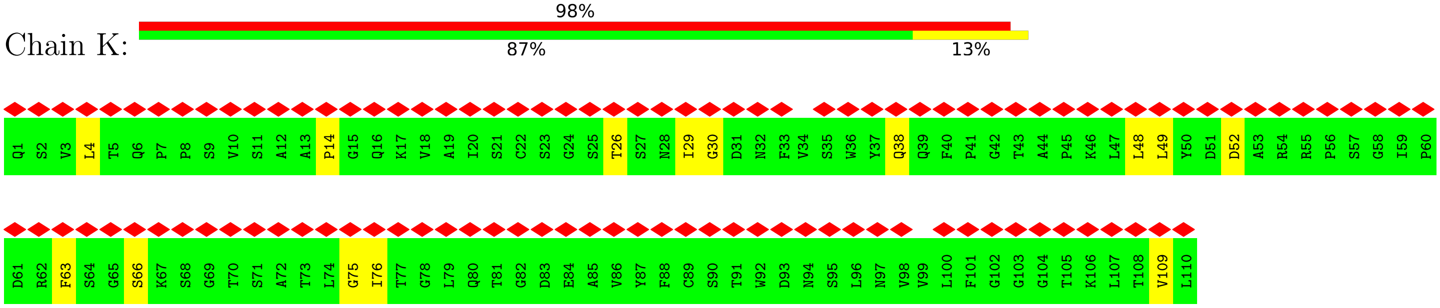


- Molecule 5: D2 light chain



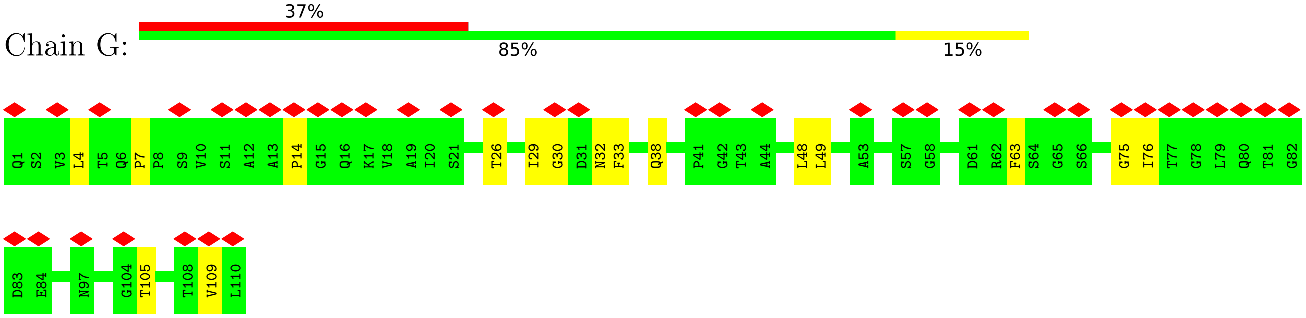
- Molecule 5: D2 light chain

Chain K:



- Molecule 5: D2 light chain

Chain G:



4 Experimental information ⓘ

Property	**Value**	**Source**
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	670525	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{Å}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.291	Depositor
Minimum map value	-2.646	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.078	Depositor
Recommended contour level	0.173	Depositor
Map size (Å)	329.80002, 329.80002, 329.80002	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.97, 0.97, 0.97	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	0.44	4/7812 (0.1%)	0.60	0/10664
1	B	0.42	3/7789 (0.0%)	0.62	2/10633 (0.0%)
1	C	0.48	4/7817 (0.1%)	0.60	4/10665 (0.0%)
2	D	0.55	1/891 (0.1%)	0.88	1/1208 (0.1%)
2	H	0.55	1/889 (0.1%)	0.88	1/1205 (0.1%)
2	L	0.55	1/891 (0.1%)	0.88	1/1208 (0.1%)
3	E	0.40	0/822	0.58	0/1120
3	I	0.40	0/822	0.58	0/1120
3	M	0.82	1/822 (0.1%)	0.60	1/1120 (0.1%)
4	F	0.43	0/966	0.58	0/1308
4	J	0.43	0/966	0.57	0/1308
4	N	0.43	0/966	0.57	0/1308
5	G	0.43	0/803	0.63	1/1097 (0.1%)
5	K	0.43	0/803	0.63	1/1097 (0.1%)
5	O	0.43	0/803	0.63	1/1097 (0.1%)
All	All	0.46	15/33862 (0.0%)	0.63	13/46158 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	D	0	1
2	H	0	1
2	L	0	1
All	All	0	3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	45	PRO	N-CD	-20.47	1.19	1.47
1	C	897	PRO	N-CD	-12.87	1.29	1.47
1	C	899	PRO	N-CD	-12.32	1.30	1.47
1	C	295	PRO	N-CD	-8.32	1.36	1.47
1	A	816	SER	CA-CB	-7.24	1.42	1.52

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	38	ARG	CB-CA-C	-6.05	98.31	110.40
2	D	38	ARG	CB-CA-C	-6.04	98.31	110.40
2	H	38	ARG	CB-CA-C	-6.04	98.32	110.40
3	M	45	PRO	CA-N-CD	5.93	120.00	111.70
1	B	897	PRO	N-CA-CB	-5.71	96.33	102.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	103	TYR	Mainchain
2	H	103	TYR	Mainchain
2	L	103	TYR	Mainchain

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	7633	0	7162	117	0
1	B	7611	0	7143	116	0
1	C	7638	0	7218	109	0
2	D	874	0	810	29	0
2	H	872	0	803	24	0
2	L	874	0	810	27	0
3	E	803	0	766	11	0
3	I	803	0	766	9	0
3	M	803	0	766	13	0
4	F	943	0	882	9	0
4	J	943	0	882	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	N	943	0	882	10	0
5	G	786	0	742	7	0
5	K	786	0	742	6	0
5	O	786	0	742	5	0
6	A	140	0	130	0	0
6	B	140	0	130	0	0
6	C	154	0	143	1	0
All	All	33532	0	31519	464	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 7.

The worst 5 of 464 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)
2:H:97:ARG:HG2	2:H:106:PHE:H	1.46	0.81
2:L:97:ARG:HG2	2:L:106:PHE:H	1.46	0.80
2:D:97:ARG:HG2	2:D:106:PHE:H	1.46	0.79
1:B:353:TRP:HZ3	1:B:355:ARG:HE	1.34	0.74
2:H:97:ARG:O	2:H:97:ARG:HG3	1.89	0.73

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 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	986/1210 (82%)	928 (94%)	57 (6%)	1 (0%)	48	79
1	B	985/1210 (81%)	930 (94%)	55 (6%)	0	100	100
1	C	984/1210 (81%)	925 (94%)	59 (6%)	0	100	100
2	D	115/117 (98%)	109 (95%)	6 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	H	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
2	L	115/117 (98%)	109 (95%)	6 (5%)	0	100	100
3	E	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
3	I	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
3	M	108/110 (98%)	100 (93%)	8 (7%)	0	100	100
4	F	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
4	J	121/123 (98%)	110 (91%)	11 (9%)	0	100	100
4	N	121/123 (98%)	111 (92%)	10 (8%)	0	100	100
5	G	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
5	K	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
5	O	108/110 (98%)	102 (94%)	6 (6%)	0	100	100
All	All	4311/5010 (86%)	4048 (94%)	262 (6%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	570	ALA

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	806/1061 (76%)	805 (100%)	1 (0%)	92	97
1	B	801/1061 (76%)	801 (100%)	0	100	100
1	C	808/1061 (76%)	806 (100%)	2 (0%)	92	96
2	D	89/98 (91%)	85 (96%)	4 (4%)	23	54
2	H	88/98 (90%)	86 (98%)	2 (2%)	45	72
2	L	89/98 (91%)	89 (100%)	0	100	100
3	E	88/90 (98%)	86 (98%)	2 (2%)	45	72

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	88/90 (98%)	86 (98%)	2 (2%)	45	72
3	M	88/90 (98%)	88 (100%)	0	100	100
4	F	98/99 (99%)	97 (99%)	1 (1%)	73	87
4	J	98/99 (99%)	97 (99%)	1 (1%)	73	87
4	N	98/99 (99%)	97 (99%)	1 (1%)	73	87
5	G	85/90 (94%)	84 (99%)	1 (1%)	67	84
5	K	85/90 (94%)	84 (99%)	1 (1%)	67	84
5	O	85/90 (94%)	85 (100%)	0	100	100
All	All	3494/4314 (81%)	3476 (100%)	18 (0%)	85	93

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

Mol	Chain	Res	Type
3	E	34	VAL
5	G	76	ILE
4	F	16	ARG
4	J	16	ARG
2	D	111	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 19 such sidechains are listed below:

Mol	Chain	Res	Type
2	H	109	GLN
2	D	109	GLN
3	E	1	GLN
2	D	81	GLN
1	C	913	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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

31 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	$\#\|Z\| > 2$
6	NAG	B	1303	1	14,14,15	0.68	0	17,19,21	1.13	2 (11%)
6	NAG	B	1304	1	14,14,15	0.35	0	17,19,21	1.49	3 (17%)
6	NAG	C	1307	1	14,14,15	0.34	0	17,19,21	0.61	0
6	NAG	C	1309	1	14,14,15	0.41	0	17,19,21	0.82	0
6	NAG	A	1308	1	14,14,15	0.42	0	17,19,21	0.81	0
6	NAG	C	1310	1	14,14,15	0.41	0	17,19,21	0.82	0
6	NAG	B	1309	1	14,14,15	0.33	0	17,19,21	0.66	0
6	NAG	C	1303	1	14,14,15	0.18	0	17,19,21	0.47	0
6	NAG	C	1305	1	14,14,15	0.24	0	17,19,21	0.41	0
6	NAG	C	1311	1	14,14,15	0.28	0	17,19,21	0.61	0
6	NAG	A	1307	1	14,14,15	0.18	0	17,19,21	0.36	0
6	NAG	A	1309	1	14,14,15	0.40	0	17,19,21	0.81	0
6	NAG	C	1306	1	14,14,15	0.39	0	17,19,21	0.63	0
6	NAG	C	1302	1	14,14,15	0.32	0	17,19,21	0.36	0
6	NAG	A	1301	1	14,14,15	0.16	0	17,19,21	0.61	1 (5%)
6	NAG	B	1302	1	14,14,15	0.57	0	17,19,21	0.71	0
6	NAG	B	1307	1	14,14,15	0.39	0	17,19,21	0.57	0
6	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.39	0
6	NAG	A	1303	1	14,14,15	0.37	0	17,19,21	0.52	0
6	NAG	C	1308	1	14,14,15	0.26	0	17,19,21	0.55	0
6	NAG	A	1306	1	14,14,15	0.22	0	17,19,21	0.47	0
6	NAG	A	1304	1	14,14,15	0.18	0	17,19,21	0.42	0
6	NAG	B	1310	1	14,14,15	0.42	0	17,19,21	1.07	2 (11%)
6	NAG	B	1308	1	14,14,15	0.34	0	17,19,21	0.84	1 (5%)
6	NAG	A	1302	1	14,14,15	0.23	0	17,19,21	0.43	0
6	NAG	B	1305	1	14,14,15	0.31	0	17,19,21	0.64	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	NAG	C	1301	1	14,14,15	0.22	0	17,19,21	0.44	0
6	NAG	A	1310	1	14,14,15	0.28	0	17,19,21	0.61	0
6	NAG	B	1301	1	14,14,15	0.56	0	17,19,21	1.30	2 (11%)
6	NAG	A	1305	1	14,14,15	0.25	0	17,19,21	0.49	0
6	NAG	B	1306	1	14,14,15	0.49	0	17,19,21	1.00	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
6	NAG	B	1303	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1307	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
6	NAG	B	1309	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1303	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1307	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1309	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1306	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1307	1	-	0/6/23/26	0/1/1/1
6	NAG	C	1304	1	-	1/6/23/26	0/1/1/1
6	NAG	A	1303	1	-	3/6/23/26	0/1/1/1
6	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
6	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1308	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1305	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1310	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1301	1	-	2/6/23/26	0/1/1/1
6	NAG	A	1305	1	-	1/6/23/26	0/1/1/1
6	NAG	B	1306	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	B	1304	NAG	C2-N2-C7	4.29	129.02	122.90
6	B	1301	NAG	C1-O5-C5	3.24	116.58	112.19
6	B	1310	NAG	C2-N2-C7	-2.80	118.92	122.90
6	B	1304	NAG	C1-O5-C5	2.67	115.81	112.19
6	B	1306	NAG	C1-C2-N2	-2.62	106.01	110.49

There are no chirality outliers.

5 of 47 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1310	NAG	C8-C7-N2-C2
6	A	1310	NAG	O7-C7-N2-C2
6	B	1306	NAG	C8-C7-N2-C2
6	B	1306	NAG	O7-C7-N2-C2
6	B	1308	NAG	C8-C7-N2-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1305	NAG	1	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

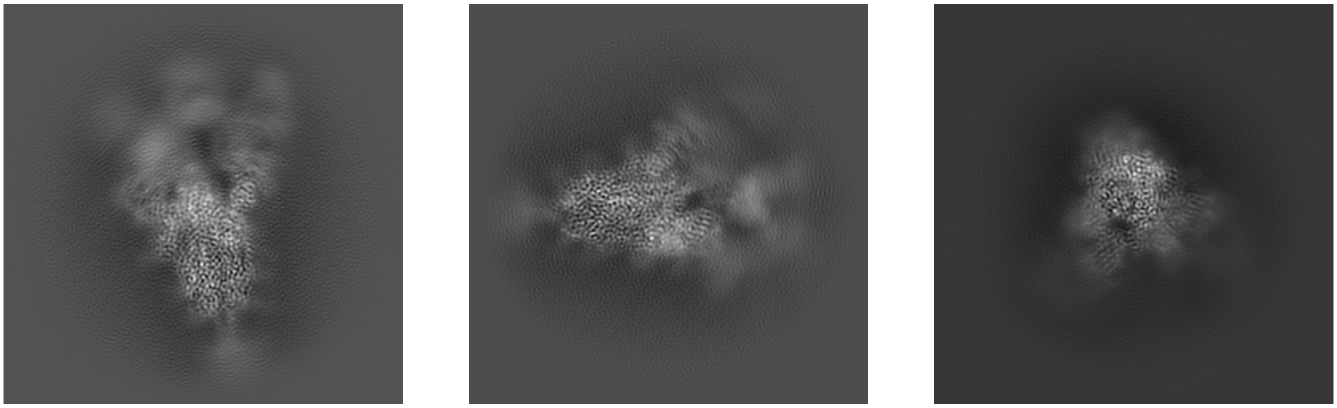
6 Map visualisation ⓘ

This section contains visualisations of the EMDB entry EMD-33434. These allow visual inspection of the internal detail of the map and identification of artifacts.

Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

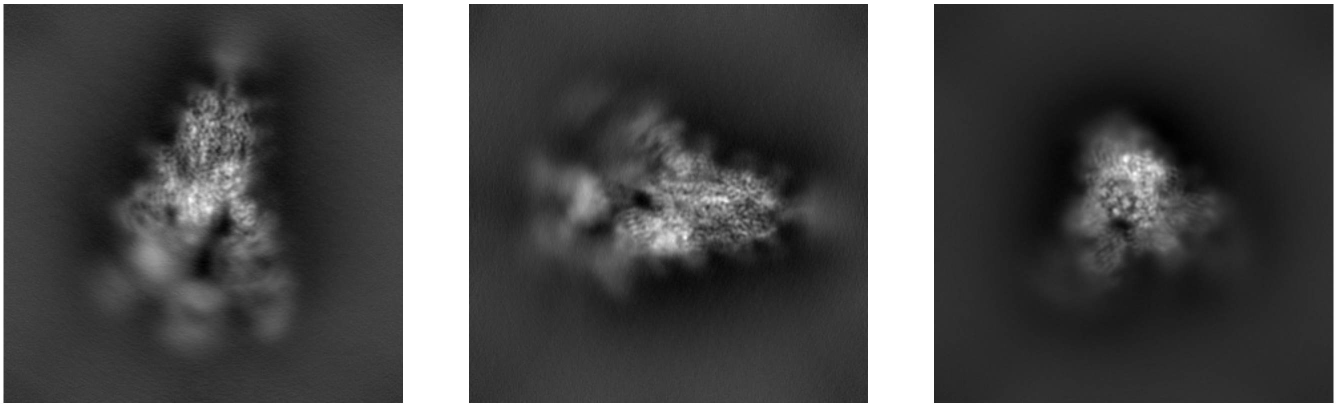
6.1 Orthogonal projections ⓘ

6.1.1 Primary map



X Y Z

6.1.2 Raw map

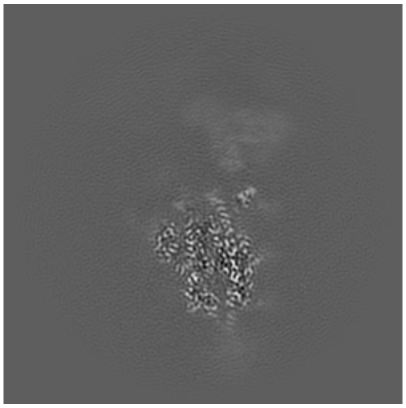


X Y Z

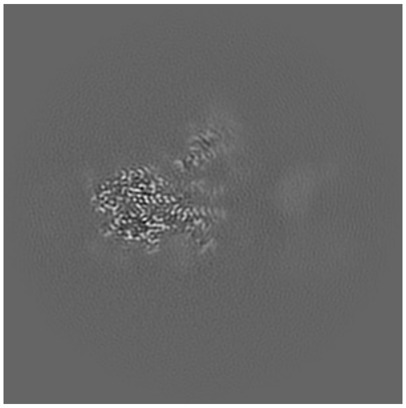
The images above show the map projected in three orthogonal directions.

6.2 Central slices

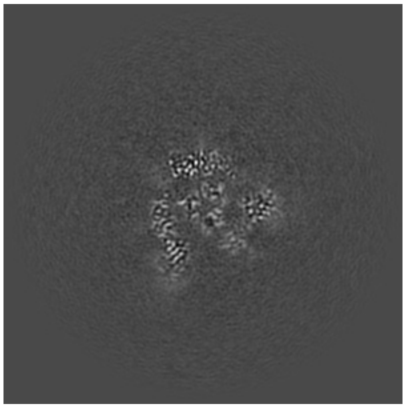
6.2.1 Primary map



X Index: 170

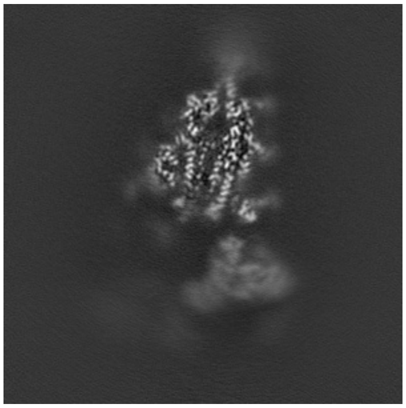


Y Index: 170

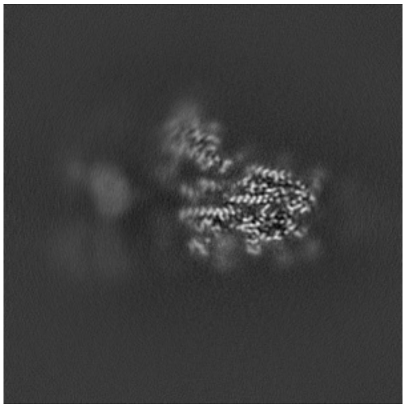


Z Index: 170

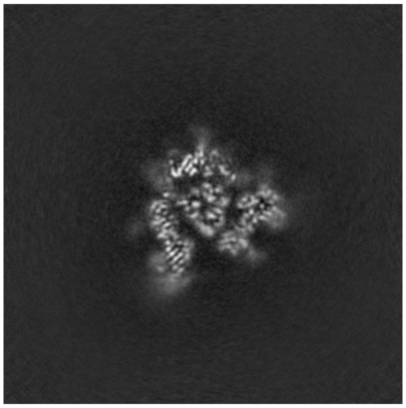
6.2.2 Raw map



X Index: 170



Y Index: 170

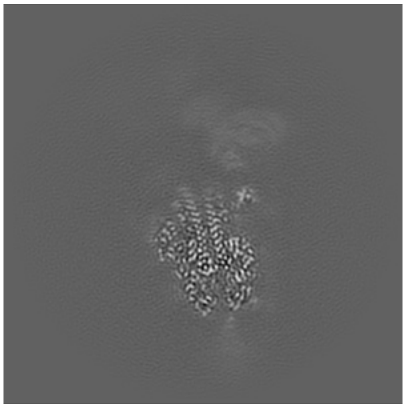


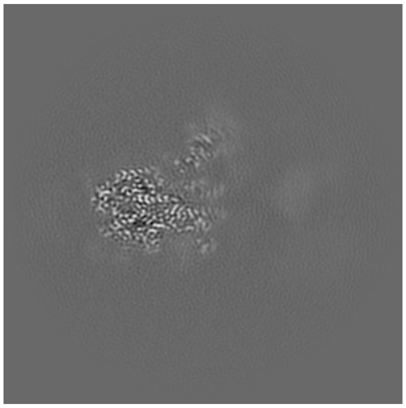
Z Index: 170

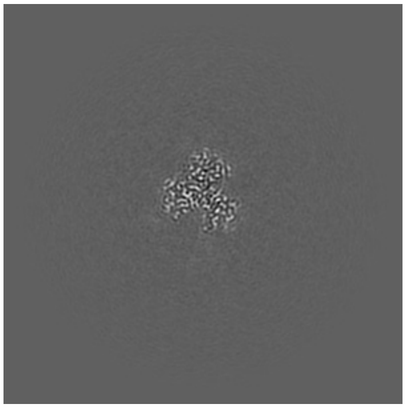
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices ⓘ

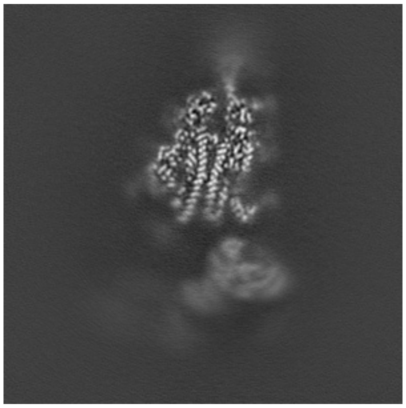
6.3.1 Primary map

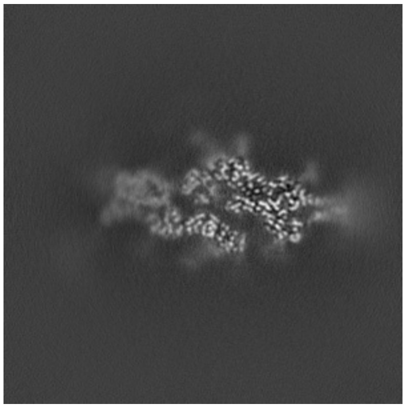

X Index: 174

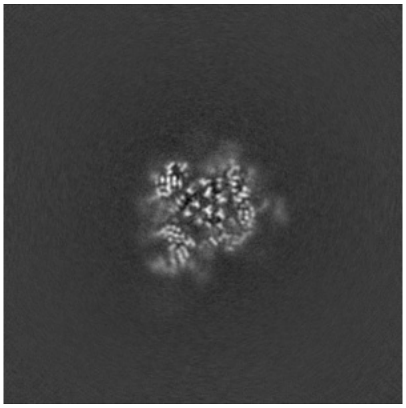

Y Index: 171


Z Index: 118

6.3.2 Raw map


X Index: 173

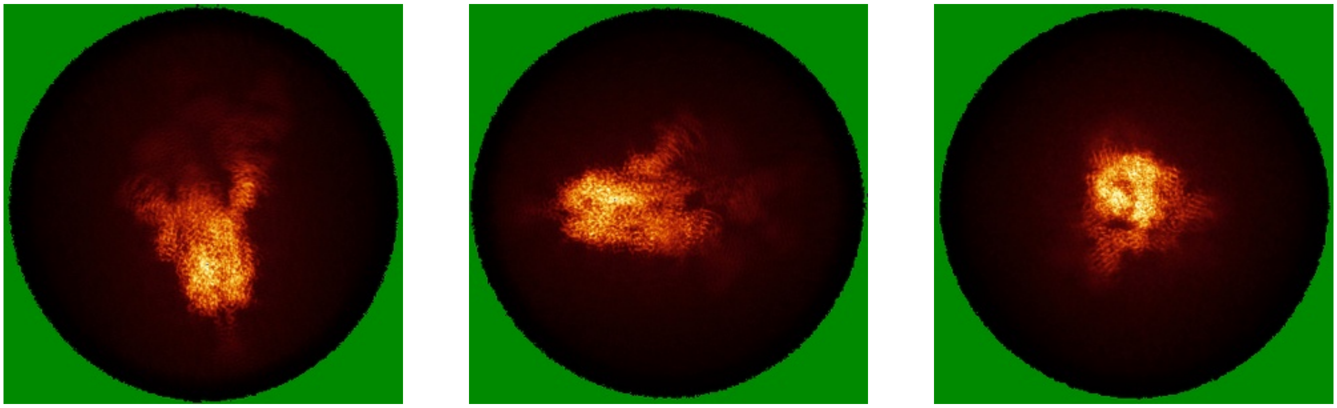

Y Index: 195


Z Index: 183

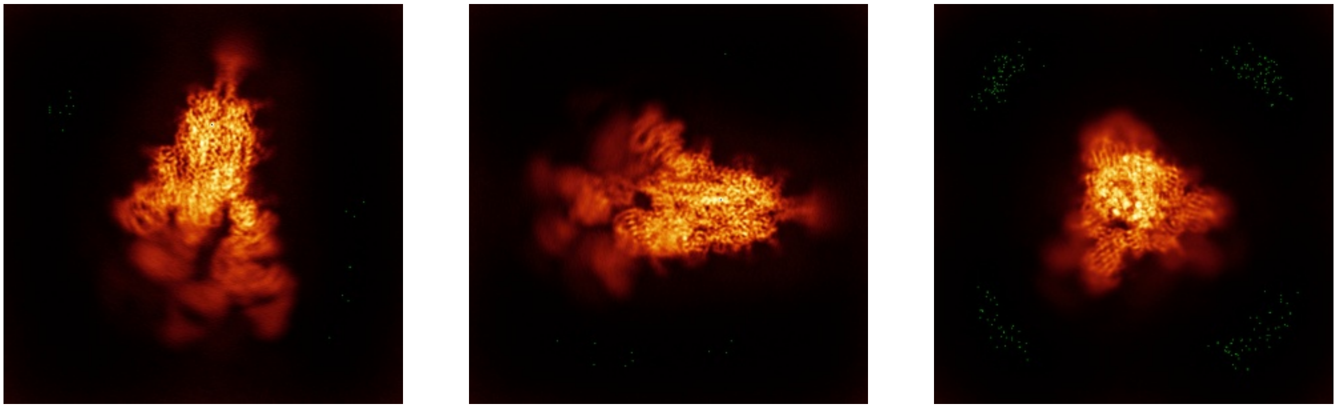
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

6.4.1 Primary map


X Y Z

6.4.2 Raw map


X Y Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views

6.5.1 Primary map

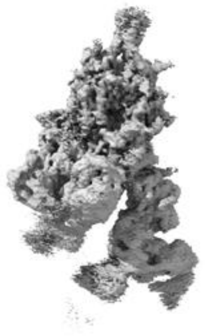

X

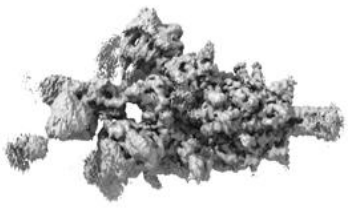

Y


Z

The images above show the 3D surface view of the map at the recommended contour level 0.173. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map


X


Y


Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

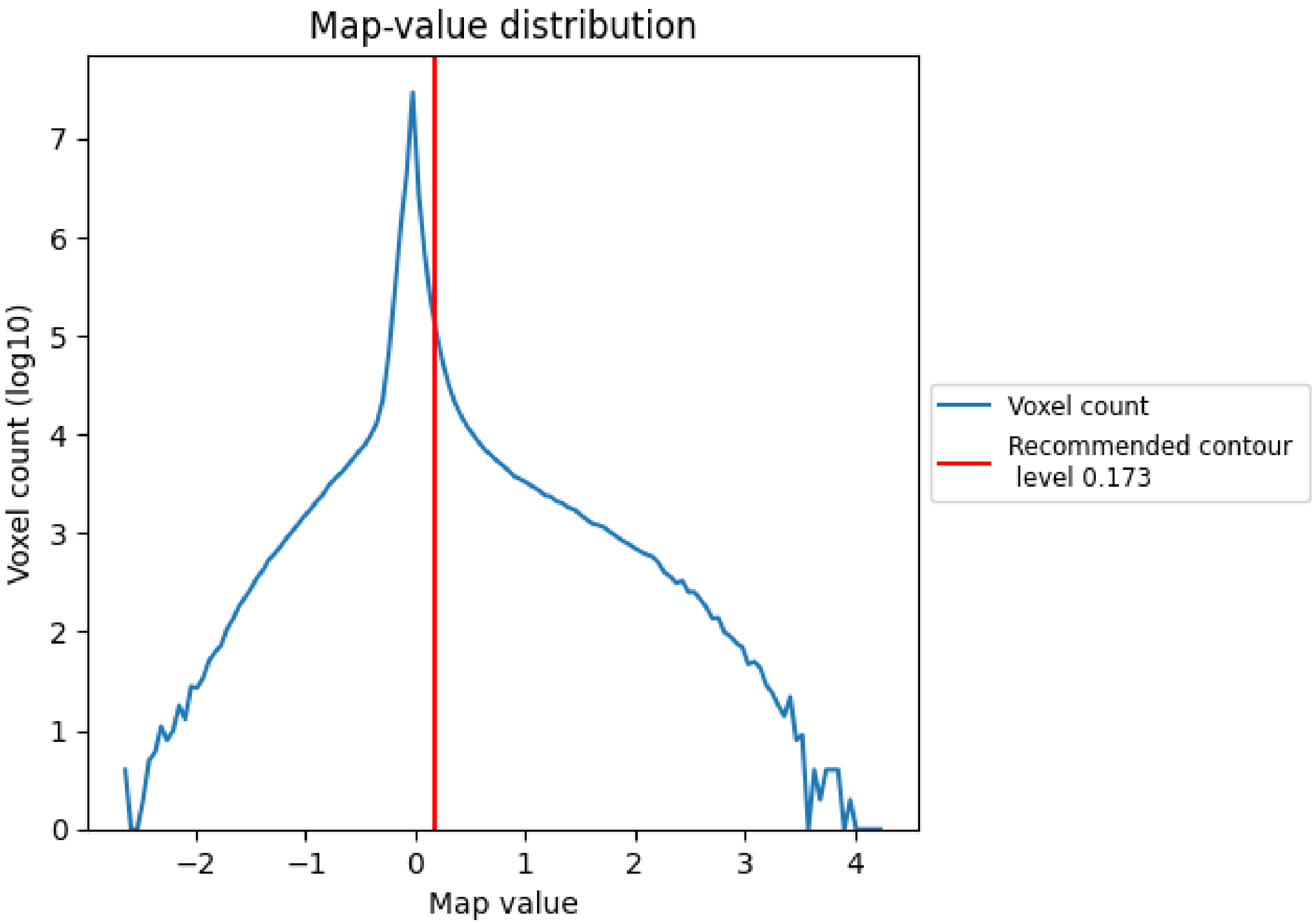
6.6 Mask visualisation

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

7 Map analysis ⓘ

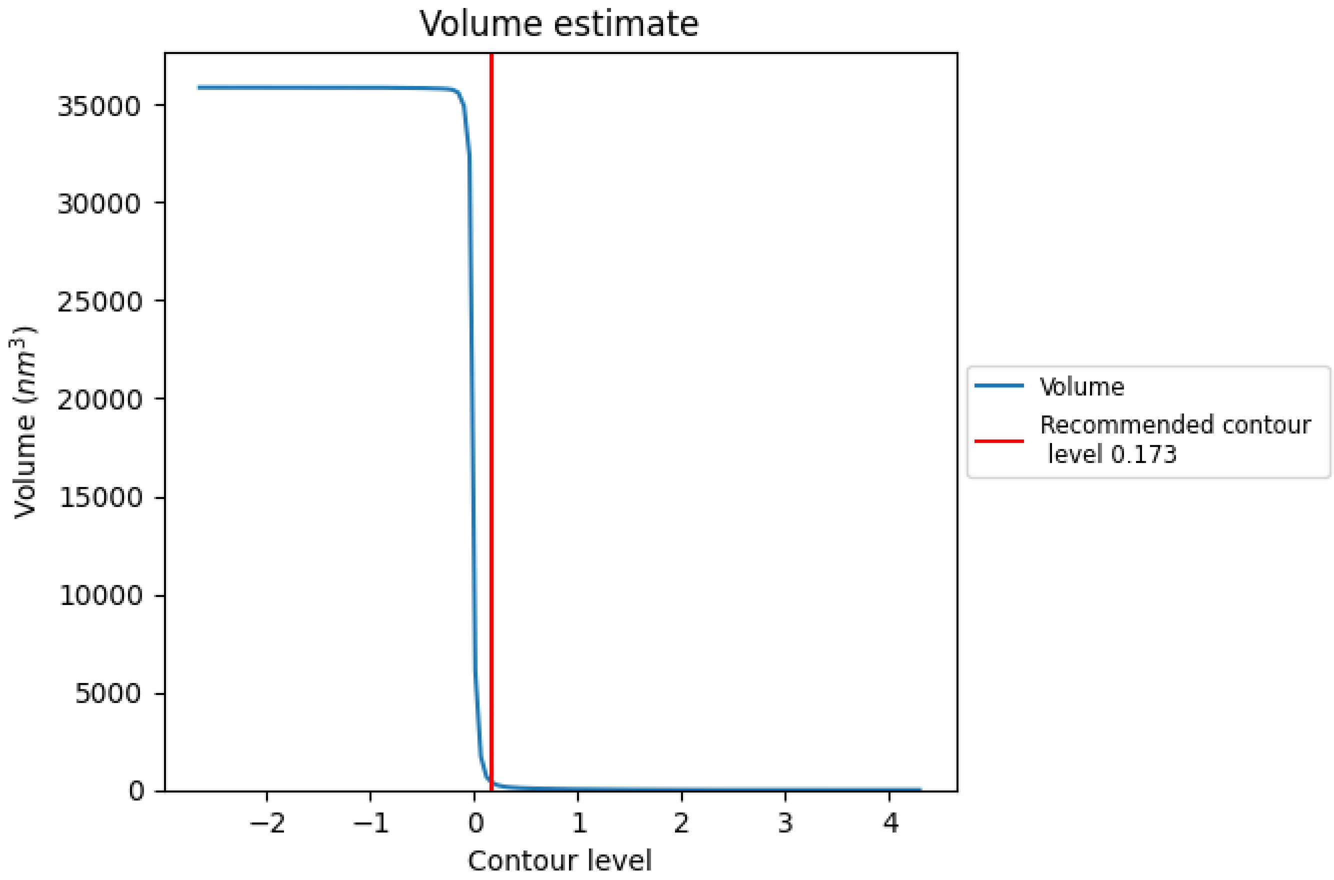
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution ⓘ



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

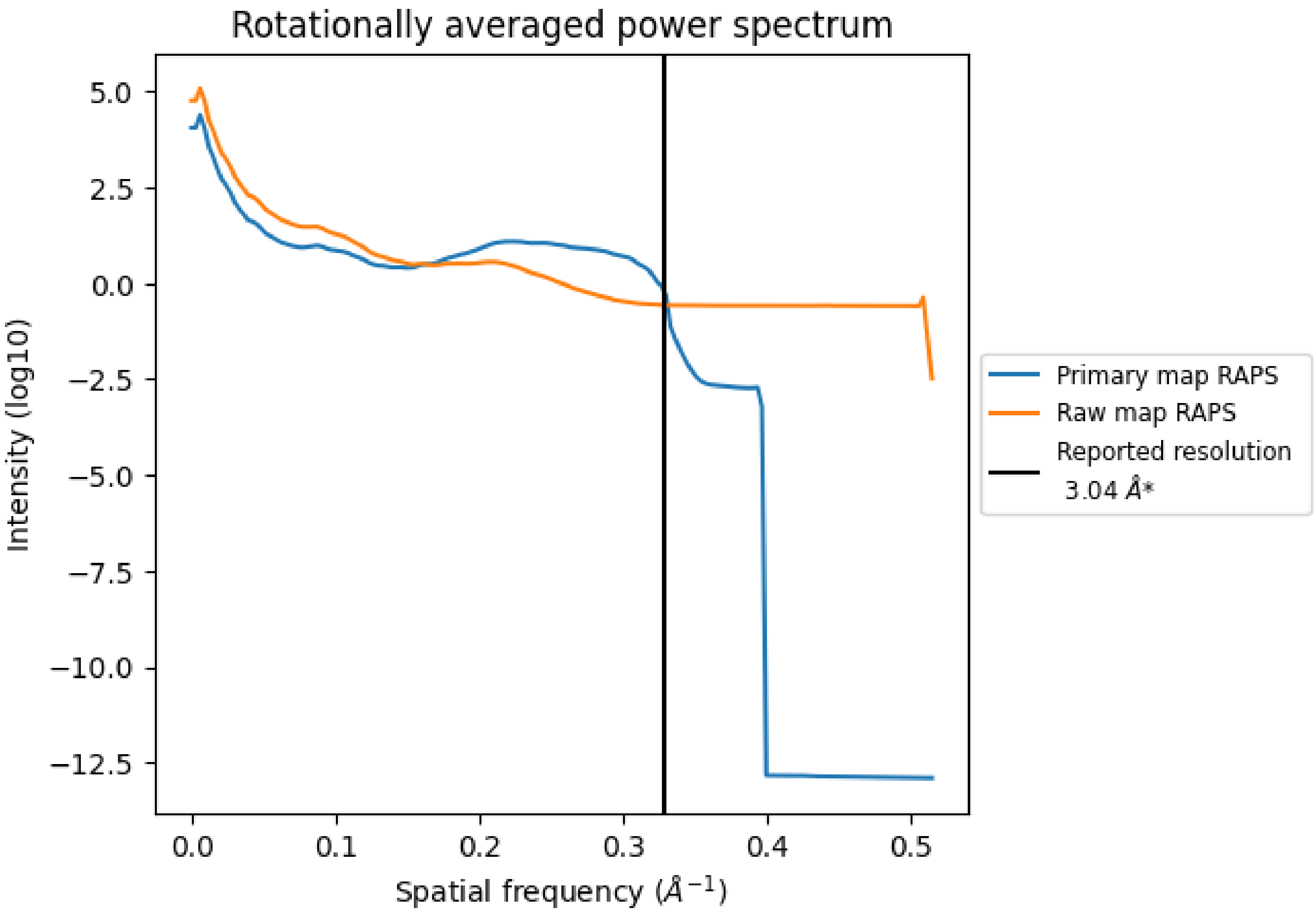
7.2 Volume estimate ⓘ



The volume at the recommended contour level is 360 nm^3; this corresponds to an approximate mass of 325 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

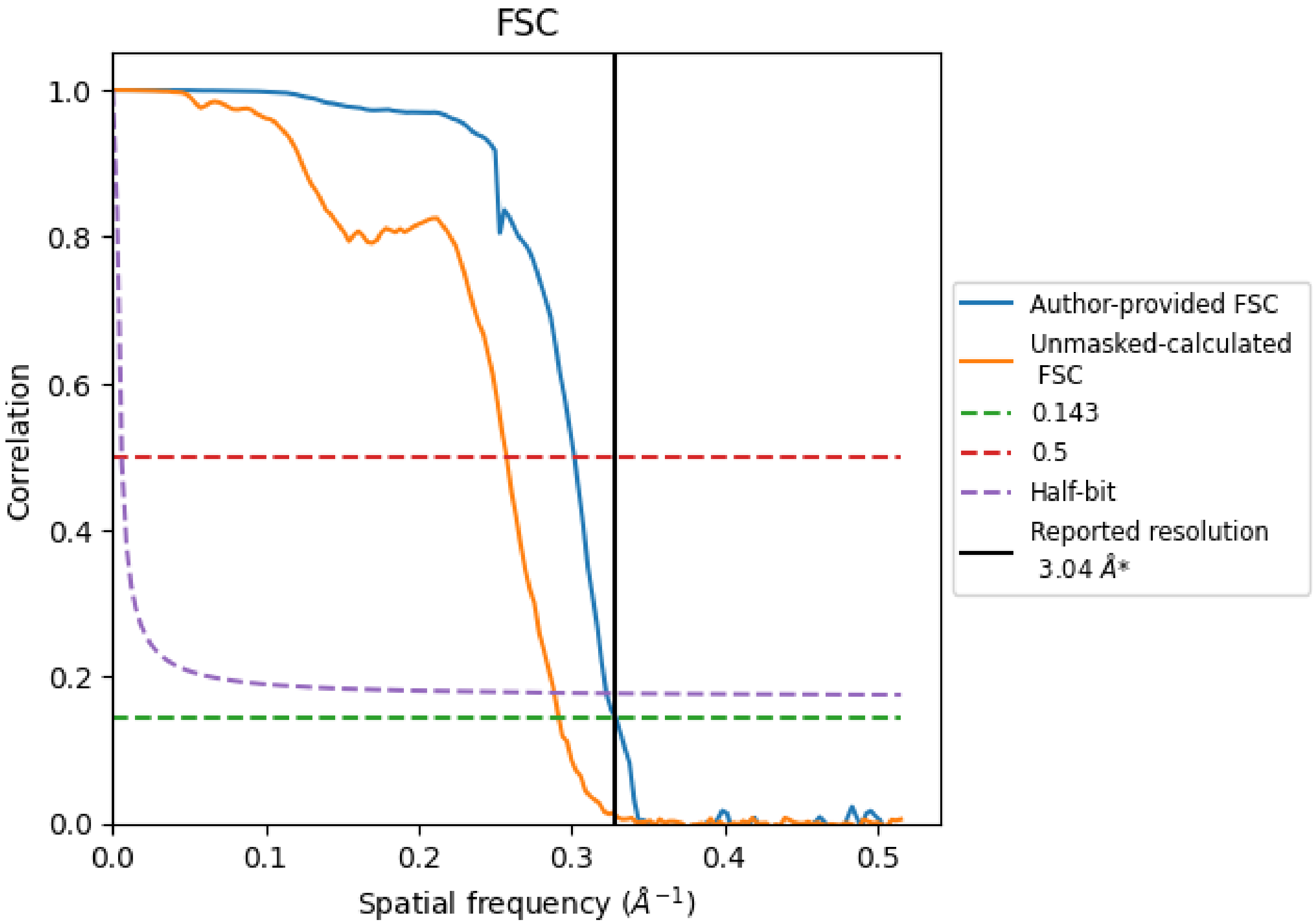


*Reported resolution corresponds to spatial frequency of 0.329 Å^{-1}

8 Fourier-Shell correlation ⓘ

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC ⓘ



*Reported resolution corresponds to spatial frequency of 0.329 Å^{-1}

8.2 Resolution estimates ⓘ

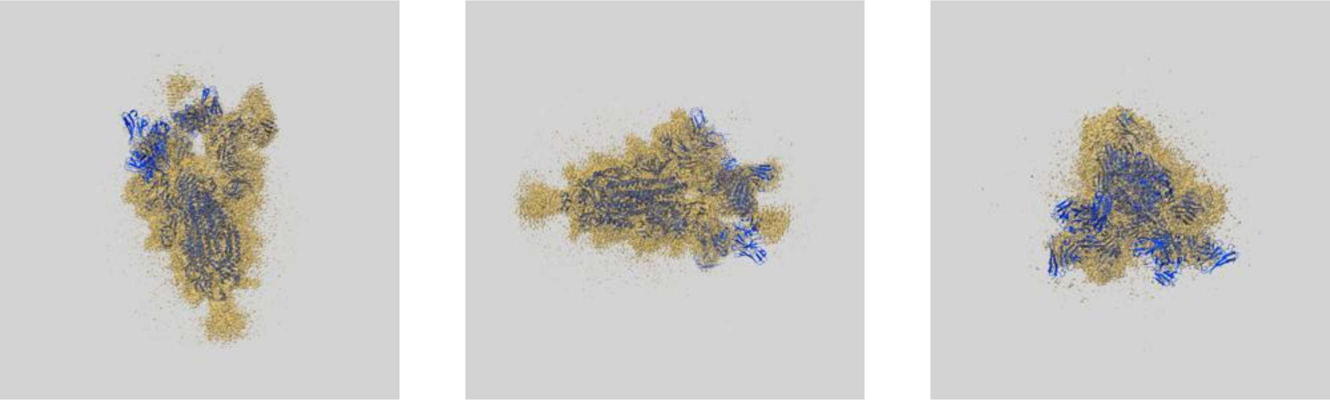
Resolution estimate (Å)	**Estimation criterion (FSC cut-off)**		
	0.143	0.5	Half-bit
Reported by author	3.04	-	-
Author-provided FSC curve	3.04	3.31	3.10
Unmasked-calculated*	3.43	3.88	3.46

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.43 differs from the reported value 3.04 by more than 10 %

9 Map-model fit ⓘ

This section contains information regarding the fit between EMDB map EMD-33434 and PDB model 7XST. Per-residue inclusion information can be found in section 3 on page 11.

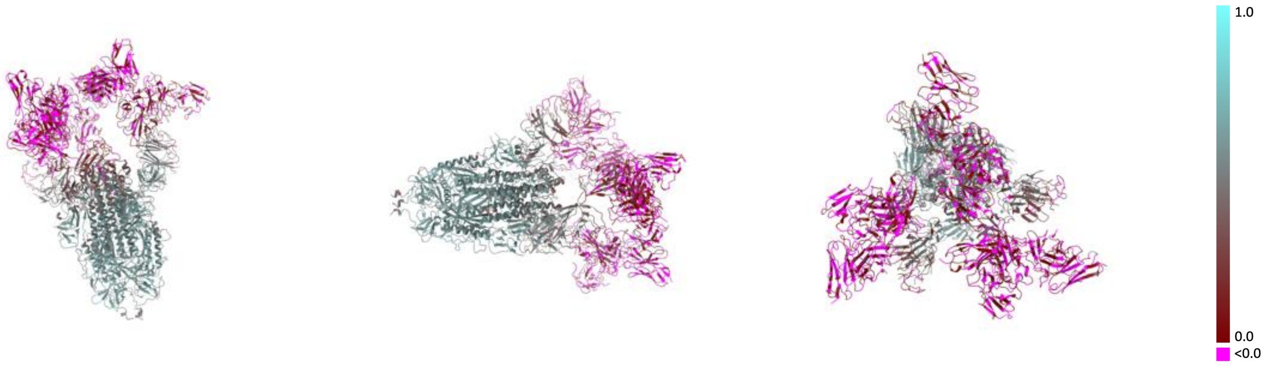
9.1 Map-model overlay ⓘ



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.173 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

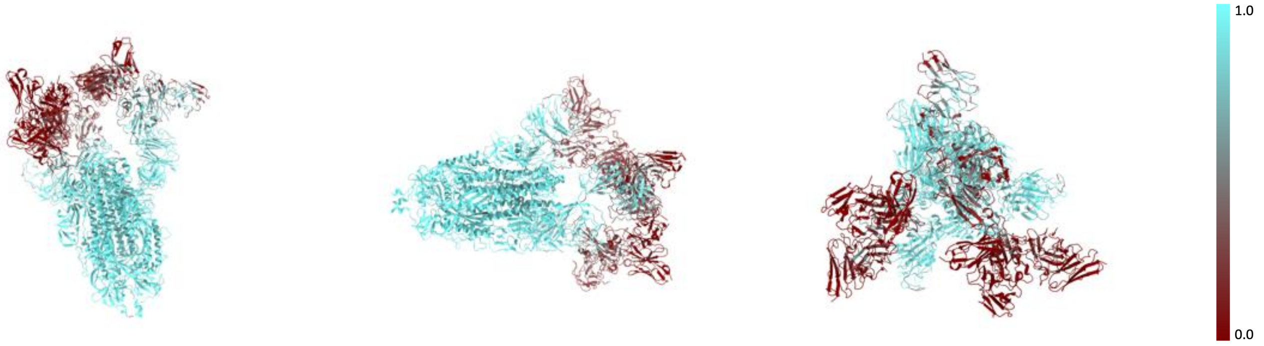
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

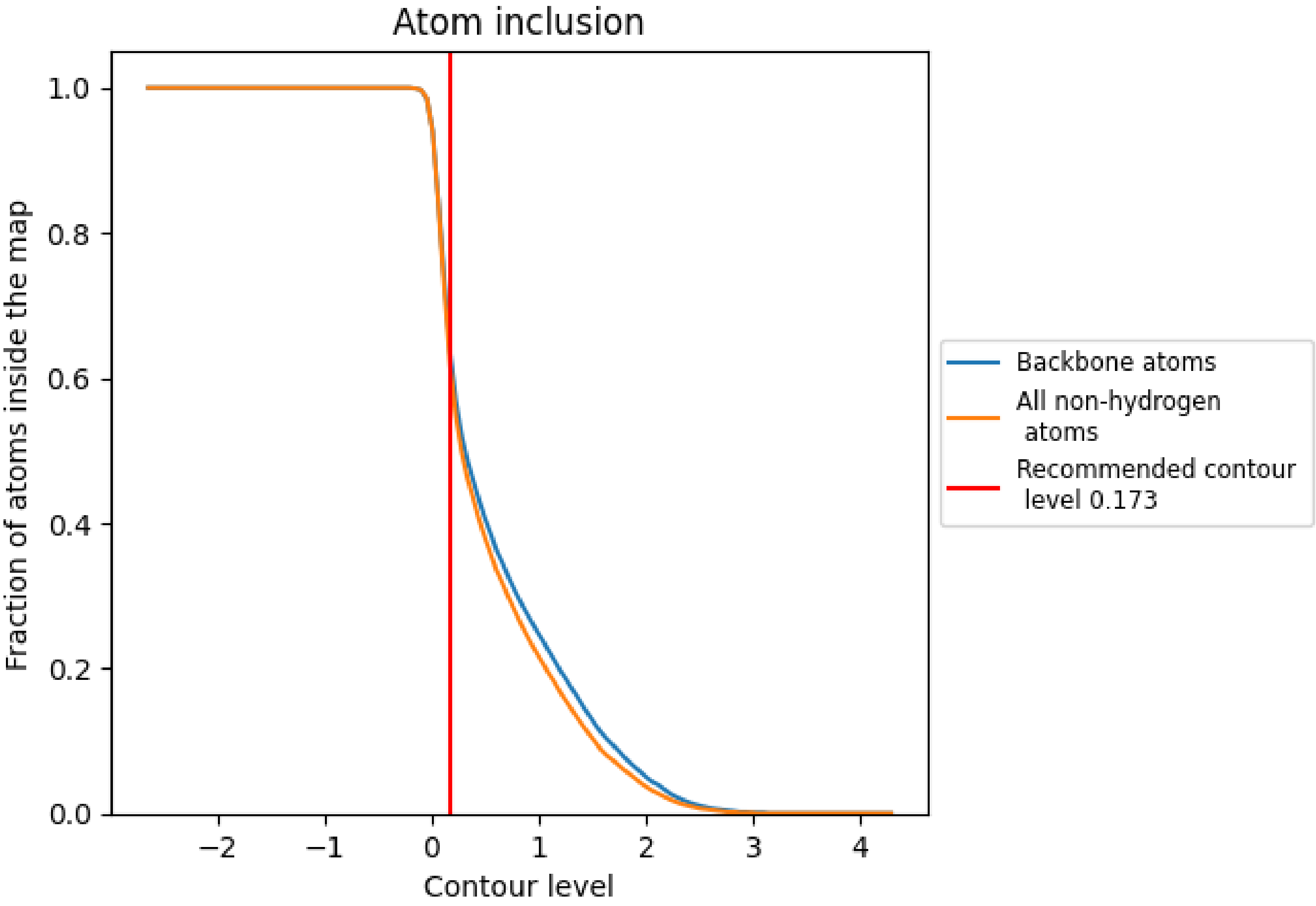
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.173).

9.4 Atom inclusion ⓘ



At the recommended contour level, 63% of all backbone atoms, 62% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6160	0.2990
A	0.8660	0.4230
B	0.8100	0.4230
C	0.7800	0.4020
D	0.2200	0.0310
E	0.1970	0.0170
F	0.5210	0.0900
G	0.5080	0.0780
H	0.0180	0.0410
I	0.0110	-0.0130
J	0.1620	0.0200
K	0.0600	0.0100
L	0.0130	0.0370
M	0.0050	0.0080
N	0.0740	0.0360
O	0.0120	0.0100