



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 05:01 AM UTC

PDB ID : 8H08 / pdb_00008h08
EMDB ID : EMD-34411
Title : SARS-CoV-2 BA.1 variants S ectodomain trimer in complex with neutralizing antibody 10-5B and 6-2C
Authors : Wang, X.; Wang, Z.
Deposited on : 2022-09-28
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

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

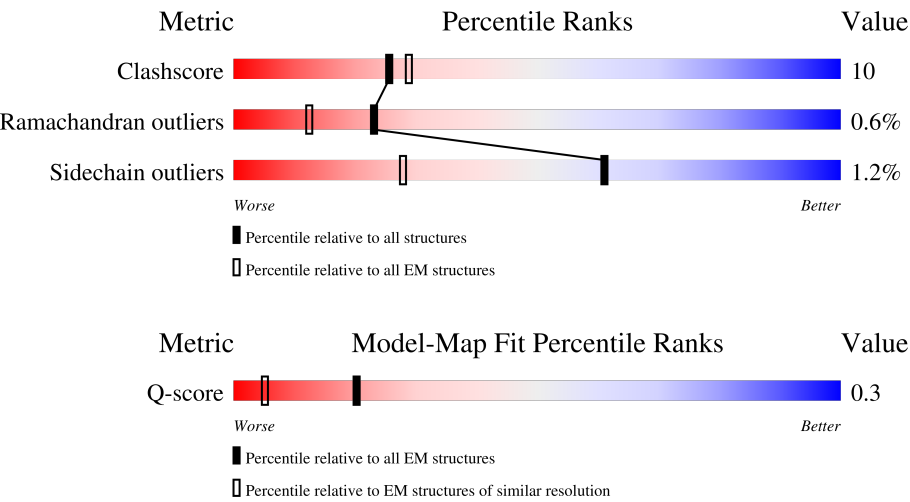
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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 $\leq 5\%$. 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	1300	5% 55% 16% • 27%
1	B	1300	• 56% 14% • 28%
1	C	1300	5% 58% 13% • 27%
2	D	117	79% 70% 29% •

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Mol	Chain	Length	Quality of chain
2	F	117	
2	L	117	
3	H	107	
3	J	107	
3	P	107	
4	I	122	
4	N	122	
4	Q	122	
5	K	107	
5	O	107	
5	R	107	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 31277 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
1	A	948	Total	C	N	O	S	0	0
			7138	4564	1203	1344	27		
1	B	933	Total	C	N	O	S	0	0
			7024	4476	1194	1329	25		
1	C	948	Total	C	N	O	S	0	0
			7125	4544	1200	1355	26		

There are 141 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	VAL	ALA	variant	UNP P0DTC2
A	?	-	HIS	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	95	ILE	THR	variant	UNP P0DTC2
A	?	-	GLY	deletion	UNP P0DTC2
A	?	-	VAL	deletion	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	145	ASP	TYR	variant	UNP P0DTC2
A	212	ILE	LEU	variant	UNP P0DTC2
A	214A	GLU	-	insertion	UNP P0DTC2
A	214B	PRO	-	insertion	UNP P0DTC2
A	214C	GLU	-	insertion	UNP P0DTC2
A	339	ASP	GLY	variant	UNP P0DTC2
A	371	LEU	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	446	SER	GLY	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	493	ARG	GLN	variant	UNP P0DTC2
A	496	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	547	LYS	THR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	682	GLY	ARG	engineered mutation	UNP P0DTC2
A	683	SER	ARG	engineered mutation	UNP P0DTC2
A	685	SER	ARG	engineered mutation	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	856	LYS	ASN	variant	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
A	981	PHE	LEU	variant	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
B	69	VAL	ALA	variant	UNP P0DTC2
B	?	-	HIS	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	95	ILE	THR	variant	UNP P0DTC2
B	?	-	GLY	deletion	UNP P0DTC2
B	?	-	VAL	deletion	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	145	ASP	TYR	variant	UNP P0DTC2
B	212	ILE	LEU	variant	UNP P0DTC2
B	214A	GLU	-	insertion	UNP P0DTC2
B	214B	PRO	-	insertion	UNP P0DTC2
B	214C	GLU	-	insertion	UNP P0DTC2
B	339	ASP	GLY	variant	UNP P0DTC2
B	371	LEU	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	446	SER	GLY	variant	UNP P0DTC2

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Chain	Residue	Modelled	Actual	Comment	Reference
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	493	ARG	GLN	variant	UNP P0DTC2
B	496	SER	GLY	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	547	LYS	THR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	682	GLY	ARG	engineered mutation	UNP P0DTC2
B	683	SER	ARG	engineered mutation	UNP P0DTC2
B	685	SER	ARG	engineered mutation	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	817	PRO	PHE	conflict	UNP P0DTC2
B	856	LYS	ASN	variant	UNP P0DTC2
B	892	PRO	ALA	conflict	UNP P0DTC2
B	899	PRO	ALA	conflict	UNP P0DTC2
B	942	PRO	ALA	conflict	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
B	981	PHE	LEU	variant	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	69	VAL	ALA	variant	UNP P0DTC2
C	?	-	HIS	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	95	ILE	THR	variant	UNP P0DTC2
C	?	-	GLY	deletion	UNP P0DTC2
C	?	-	VAL	deletion	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	145	ASP	TYR	variant	UNP P0DTC2
C	212	ILE	LEU	variant	UNP P0DTC2
C	214A	GLU	-	insertion	UNP P0DTC2
C	214B	PRO	-	insertion	UNP P0DTC2
C	214C	GLU	-	insertion	UNP P0DTC2
C	339	ASP	GLY	variant	UNP P0DTC2
C	371	LEU	SER	variant	UNP P0DTC2

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

- Molecule 2 is a protein called 10-5B H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	D	116	Total	C	N	O	S	0	0
			839	519	150	166	4		
2	F	116	Total	C	N	O	S	0	0
			839	519	150	166	4		
2	L	116	Total	C	N	O	S	0	0
			839	519	150	166	4		

- Molecule 3 is a protein called 10-5B L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	J	104	Total	C	N	O	S	0	0
			738	453	130	152	3		
3	H	104	Total	C	N	O	S	0	0
			738	453	130	152	3		
3	P	104	Total	C	N	O	S	0	0
			738	453	130	152	3		

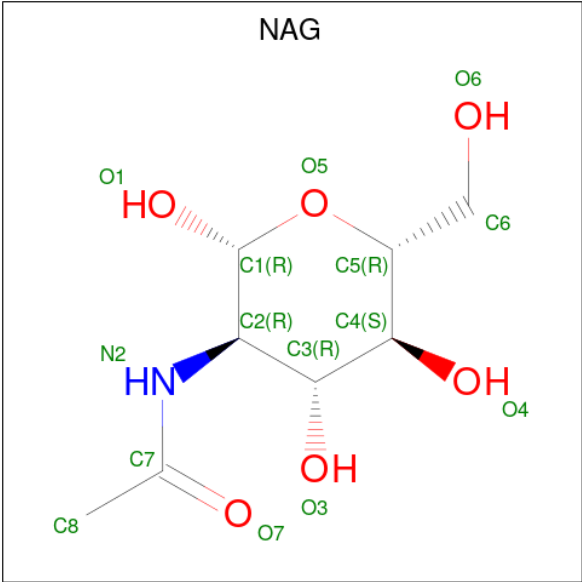
- Molecule 4 is a protein called 6-2C H chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	N	122	Total	C	N	O	S	0	0
			945	597	165	181	2		
4	I	122	Total	C	N	O	S	0	0
			945	597	165	181	2		
4	Q	122	Total	C	N	O	S	0	0
			945	597	165	181	2		

- Molecule 5 is a protein called 6-2C L chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	O	106	Total	C	N	O	S	0	0
			794	506	133	153	2		
5	K	106	Total	C	N	O	S	0	0
			794	506	133	153	2		
5	R	106	Total	C	N	O	S	0	0
			794	506	133	153	2		

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆) (labeled as "Ligand of Interest" by depositor).

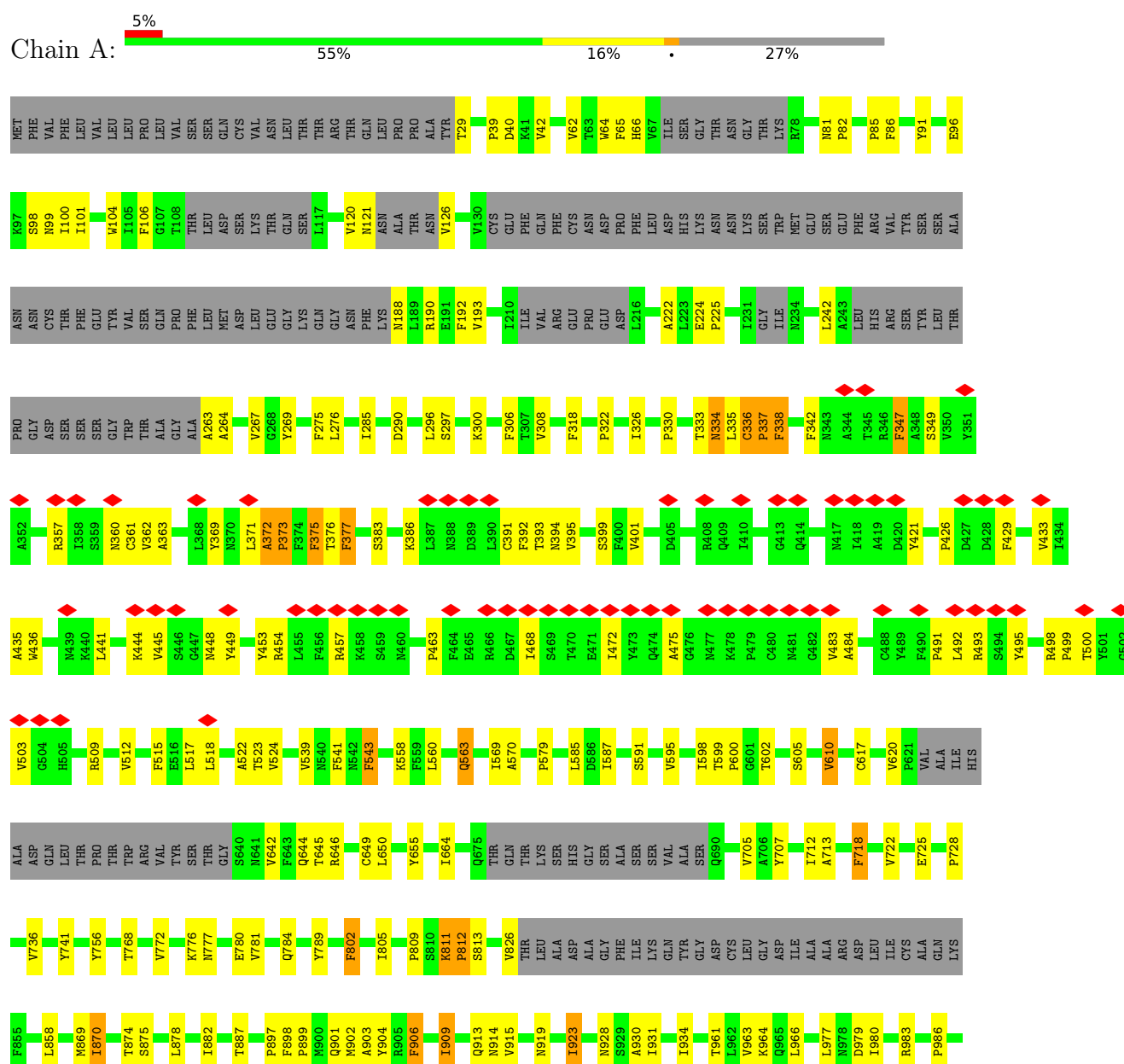


Mol	Chain	Residues	Atoms				AltConf
6	A	1	Total	C	N	O	0
			14	8	1	5	
6	B	1	Total	C	N	O	0
			14	8	1	5	
6	C	1	Total	C	N	O	0
			14	8	1	5	

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



A989	LEU	LYS	TRP
E996	ASP	SER	HIS
R1000	PHE	PRO	GLN
L1001	LYS	GLN	TYR
L1004	GLU	ILE	LYS
Q1011	LEU	TRP	LYS
L1024	ASP	GLY	GLY
T1027	ASP	GLY	GLY
K1028	ASN	LYS	TYR
M1029	HIS	ILE	GLY
S1030	THR	PRO	GLY
E1031	SER	ALA	GLY
C1032	PRO	ARG	GLY
G1035	ASP	ASP	SER
L1049	VAL	GLY	GLN
F1052	GLY	ALA	GLY
P1053	ASP	ASP	GLY
P1057	ILE	ILE	GLY
F1062	ASN	GLY	GLY
L1063	ALA	CYS	GLY
H1064	SER	TRP	VAL
Y1067	VAL	VAL	VAL
E1072	ASN	ILE	VAL
A1080	GLU	THR	THR
I1081	ILE	LEU	LEU
F1089	ASP	GLY	GLY
P1090	ARG	SER	ARG
V1094	LEU	LEU	GLY
F1095	VAL	VAL	VAL
V1096	ALA	PHE	LEU
Q1106	LYS	GLN	GLY
F1109	ASN	PRO	PRO
I1114	GLU	GLY	HIS
I1115	SER	HIS	HIS
F1121	LEU	HIS	HIS
L1141	ASP	HIS	HIS
GLN	GLN	HIS	HIS
PRO	GLU	HIS	HIS
GLY	LEU	SER	GLY

• Molecule 1: Spike glycoprotein



Y170	ARG	Y265	D389	S494	TVR	V772	ALA	P986	LYS
Q173	SER	Y266	D391	Y495	SER	E773	GLN	E990	TYR
F107	ASN	Y267	F392	R498	THR	Q774	GLY	I993	PHE
G107	PRO	G268	F393	P499	THR	S640	LYS	L1004	ASN
T108	LEU	F275	R394	T500	GLY	G648	ASN	L1006	HIS
THR	THR	F276	R395	V503	ASP	G648	THR	Q1006	THR
GLN	GLN	F277	V399	R509	SER	T651	GLY	T1006	SER
S116	ASN	F278	F401	V512	SER	Y655	GLY	Q1010	ASP
L117	GLY	F279	V401	V515	GLY	Y656	GLY	M1029	ASP
N121	GLY	F280	Y421	F515	THR	Y657	THR	Y873	LEU
ASN	GLY	F281	P426	L518	ALA	Y658	ALA	T874	GLY
ALA	THR	F282	F429	V524	ALA	P665	THR	S875	ASP
V130	CYS	F283	V433	C525	ALA	G667	GLN	L877	ASP
GLU	GLY	F284	V434	G526	ALA	C671	THR	F1042	SER
PHE	THR	F285	V435	P527	ALA	Q675	LYS	G1043	GLY
GLN	GLN	F286	V436	C538	ALA	GLN	GLN	G1044	ILE
Y28	ASP	F287	V441	V539	ALA	THR	LYS	L1049	ASN
Y37	CYS	F288	V444	V551	ALA	LYS	HIS	A1056	SER
ASN	ASN	F289	V445	L560	ALA	SER	GLY	P1057	VAL
V62	ASP	F290	V448	V569	ALA	ALA	ALA	H1058	ASN
T63	PRO	F291	V449	A570	ALA	SER	ALA	G1059	ILE
W64	PHE	F292	V453	D571	ALA	VAL	VAL	F1062	GLN
F65	LEU	F293	R454	T572	ALA	ALA	ALA	Y1067	GLY
HIS	ASP	F294	R457	V573	SER	LEU	LEU	C1082	ASP
VAL	ASP	F295	P463	D574	ALA	ALA	ALA	F1089	ASN
ILE	LEU	F296	V468	D586	SER	ASP	ASP	V1104	LEU
THR	LEU	F297	S469	Y612	THR	GLY	GLY	Q1106	ASN
GLY	GLY	F298	T470	T618	THR	ILE	ILE	T1116	SER
THR	THR	F299	E471	E619	THR	ALA	ALA	T1117	LEU
GLY	GLY	F300	V472	V620	THR	ALA	ALA	T1120	ASP
TRP	TRP	F301	V473	P621	THR	ALA	ALA	F1121	LEU
GLY	GLY	F302	Q474	V475	THR	ALA	ALA	S939	GLN
MET	GLY	F303	A475	A475	THR	ALA	ALA	Y1138	LEU
GLY	GLY	F304	G476	G476	THR	ALA	ALA	L1141	GLY
ASN	ASN	F305	L371	L371	THR	ALA	ALA	D1146	SER
ARG	ARG	F306	A372	A372	THR	ALA	ALA	A944	PHE
PRO	PRO	F307	P373	P373	THR	ALA	ALA	L945	GLY
VAL	VAL	F308	F374	F374	THR	ALA	ALA	L948	THR
ASP	ASP	F309	F375	F375	THR	ALA	ALA	T961	ILE
ASN	ASN	F310	F376	F376	THR	ALA	ALA	Q965	TRP
ASN	ASN	F311	F377	F377	THR	ALA	ALA	ASP	PRO
GLY	GLY	F312	S383	S383	THR	ALA	ALA		
GLY	GLY	F313	K386	K386	THR	ALA	ALA		
GLY	GLY	F314	P491	P491	THR	ALA	ALA		
GLY	GLY	F315	L492	L492	THR	ALA	ALA		
GLY	GLY	F316	R493	R493	THR	ALA	ALA		

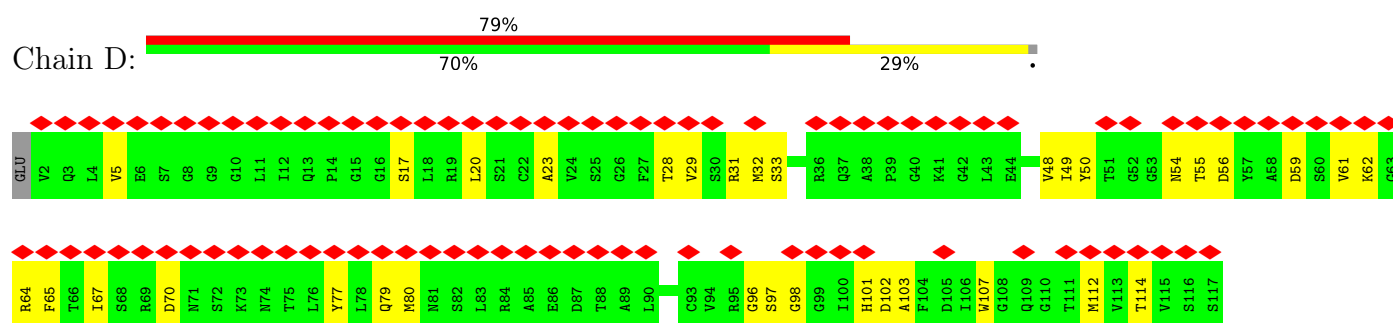
GLY	SER	GLY	GLY	TYR	GLY	ILE	PRO	GLU	ALA	GLY	PRO	GLY	ARG	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLY	GLY	VAL	ASP	ASP	ASP	ASP	LYS
GLY	GLY	SER	GLY	TYR	GLY	GLY	PRO	GLU	ALA	SER	GLY	ARG	ASP	GLY	GLN	ALA	TYR	VAL	ARG	LYS	ASP	GLY	GLY	GLY	VAL	ASP	ASP	ASP	ASP	LYS	

• Molecule 1: Spike glycoprotein

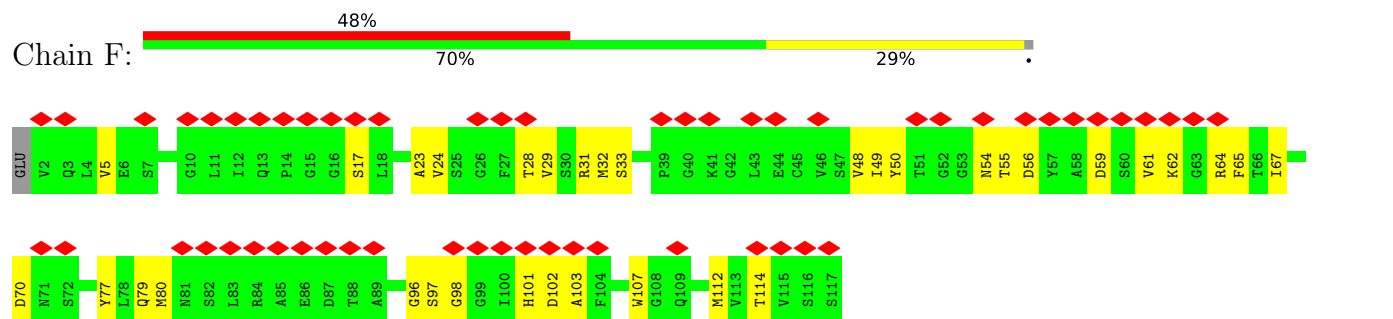


MET	PHE	VAL	PHE	LEU	VAL	LEU	LEU	PRO	LEU	THR	VAL	SER	GLN	CYS	VAL	ASN	THR	LEU	GLN	THR	ARG	PRO	P26	T29	N30	S31	F32	T33	P39	T51	F58	H66	VAL	ILE	SER	GLY	THR	GLY	THR	ASN	GLY	PHE	LYS	ARG	ALA	SER	TRP	D80	N81	P82	V83	L84	Y91	I95		
GLU	LYS	SER	ASN	I101	I105	F106	G107	THR	THR	LEU	ASP	SER	LYS	VAL	THR	GLN	SER	LEU	THR	ARG	PRO	V130	CYS	GLU	PHE	GLN	PHE	CYS	ASN	ASP	PRO	PHE	ASN	LYS	VAL	SER	TRP	MET	GLY	THR	ASN	GLY	PHE	VAL	THR	VAL	TYR	SER	TRP	D80	N81	P82	V83	L84	Y91	I95
PRO	PHE	LEU	MET	ASP	LEU	GLY	GLN	GLY	ASN	PHE	ASN	ASN	THR	GLN	THR	PRO	ILE	VAL	ARG	GLU	PRO	GLU	D215	P230	ILE	GLY	ASN	ILE	ASN	ILE	T236	L242	ALA	LEU	HIS	ARG	SER	TRP	TYR	LEU	THR	PRO	GLY	ASP	SER	SER	SER	GLY	TRP	ALA	THR	ALA	A263	F168		
V267	F275	G283	V289	L296	T299	K300	C301	F306	K386	L387	N388	D389	L390	C391	T393	N394	V395	S399	F400	V401	D405	E406	Q409	I410	G413	Q414	T415	L492	R493	S494	Y495	R498	P499	T500	V503	G504	H505	R509	V510	V511	V512	F515	L518	H519	A520	T523	V524	C525	G526							
L371	A372	P373	F374	T376	F377	S383	K386	L387	N388	D389	L390	C391	T393	N394	V395	S399	F400	V401	D405	E406	Q409	I410	G413	Q414	T415	L492	R493	S494	Y495	R498	P499	T500	V503	G504	H505	R509	V510	V511	V512	F515	L518	H519	A520	T523	V524	C525	G526									
Y453	R454	R457	P463	R466	D467	I468	S469	T470	E471	I472	Y473	Q474	A475	G476	H477	K478	P479	C480	N481	G482	V483	A484	C488	Y489	F490	P491	L492	R493	S494	Y495	R498	P499	T500	V503	G504	H505	R509	V510	V511	V512	F515	L518	H519	A520	T523	V524	C525	G526								
P527	S530	T531	V534	N542	F543	K558	I569	A570	P579	C590	V608	V620	P621	VAL	ILE	HIS	ALA	ASP	GLN	LEU	THR	PRO	THR	TRP	ARG	VAL	TYR	SER	THR	GLY	SER	H641	C649	G675	THR	GLN	THR	LYS	GLY	HIS	ASP	ALA	SER	GLY	ALA	SER	VAL	ALA								
SER	GLN	S691	N703	Y707	T716	N717	F718	S721	E725	L726	P728	W729	V736	L754	L767	I770	Q774	K776	N777	L778	P779	F780	V781	F782	A783	F802	I805	P809	R814	S815	S816	V826	T827	LEU	ALA	ALA	ASP	ALA	ASP	ALA	GLY	PHE	ILE	GLN												
TYR	GLY	ASP	CYS	GLY	ASP	ILE	ALA	ARG	ASP	LEU	ILE	CYS	GLN	LYS	F855	K856	I870	L878	T881	L882	S883	L894	K895	L896	P897	F898	Q901	Y904	R905	F906	T907	I909	Y917	E918	N919	L922	Y923	Q926	S940	T941	P942	L945	G946	K947												
L948	V963	L966	P986	V1008	N1023	T1027	G1035	V1040	D1041	F1042	G1043	G1044	Y1047	L1048	L1049	F1052	P1053	P1057	H1068	G1069	G1059	V1060	F1061	F1062	T1066	Y1067	K1073	N1074	F1075	T1076	T1077	F1089	N919	V1094	N1108	F1121	L1141	L1145	ASP	SER	PHE	LYS														
GLU	GLU	LEU	ASP	LYS	THR	SER	PRO	ASP	VAL	GLY	ASP	ILE	SER	GLY	ASN	VAL	VAL	ASN	ILE	GLN	LYS	GLY	LEU	THR	PHE	LEU	GLY	ILE	ARG	SER	LEU	ASN	GLY	ASN	GLY	THR	ASP	GLN	GLY	THR	ASP	GLY	THR	ASP	GLY	THR	ASP	GLY	THR							
ILE	LYS	TRP	PRO	GLY	GLY	SER	GLY	TYR	GLY	ILE	PRO	ARG	ASP	ASP	GLY	ALA	GLY	ASP	TYR	VAL	ARG	LYS	GLY	GLY	TRP	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL						
PHE	GLU	LYS	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY						

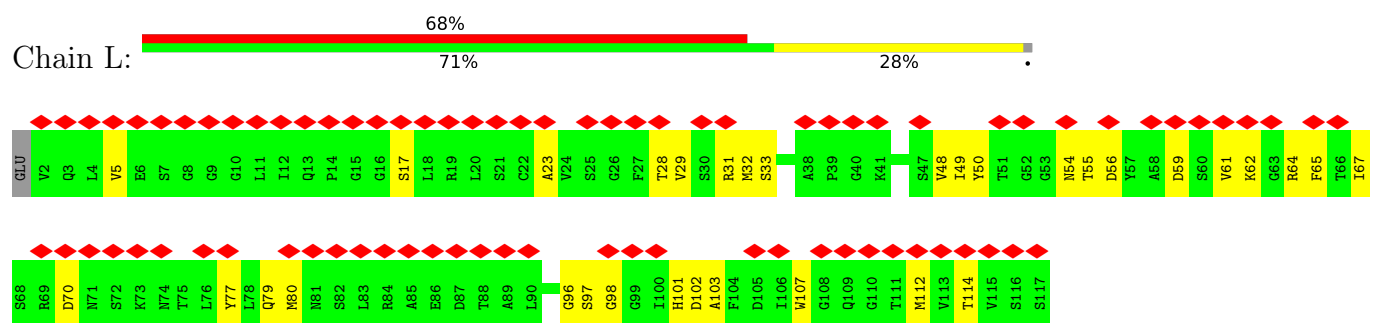
• Molecule 2: 10-5B H chain



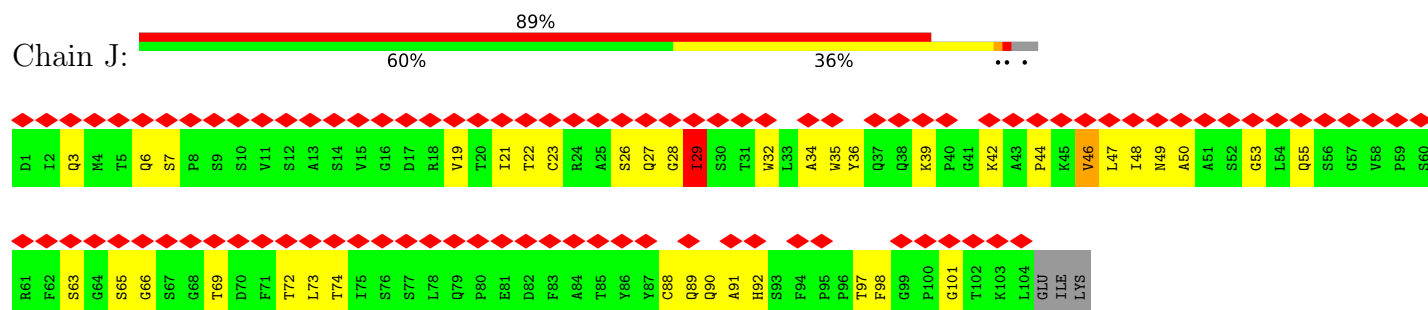
- Molecule 2: 10-5B H chain



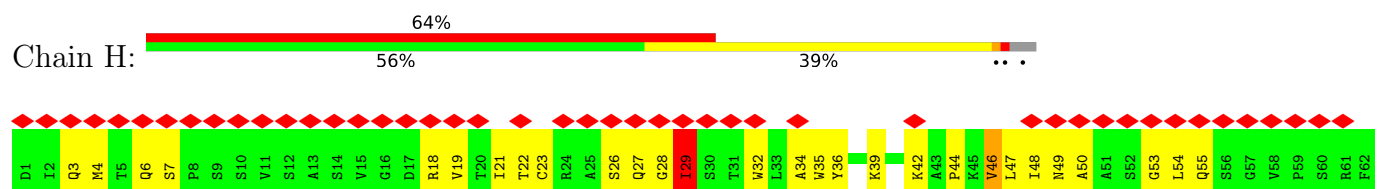
- Molecule 2: 10-5B H chain

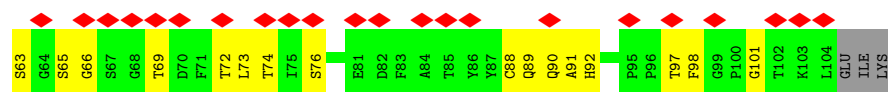


- Molecule 3: 10-5B L chain

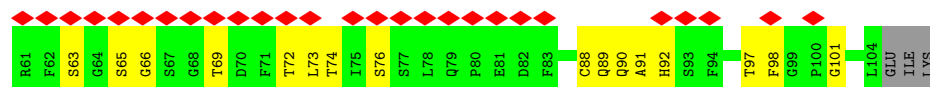
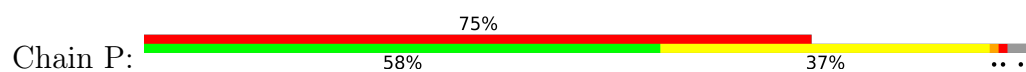


- Molecule 3: 10-5B L chain

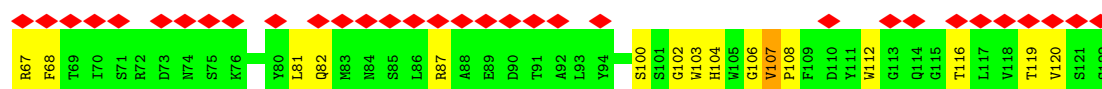
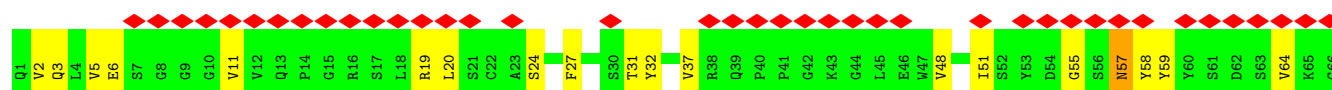
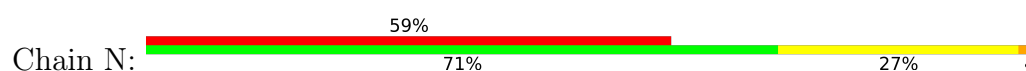




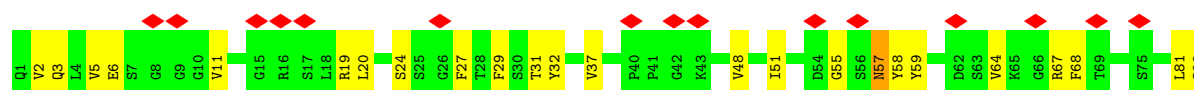
• Molecule 3: 10-5B L chain



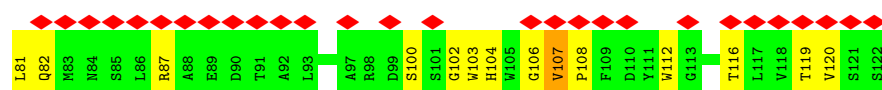
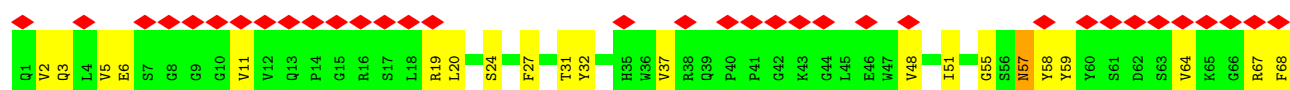
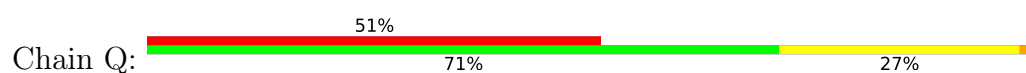
• Molecule 4: 6-2C H chain



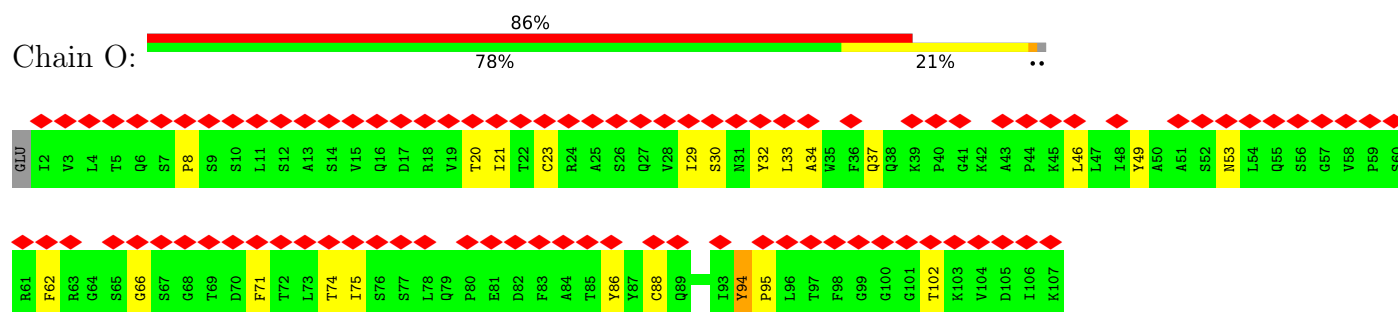
• Molecule 4: 6-2C H chain



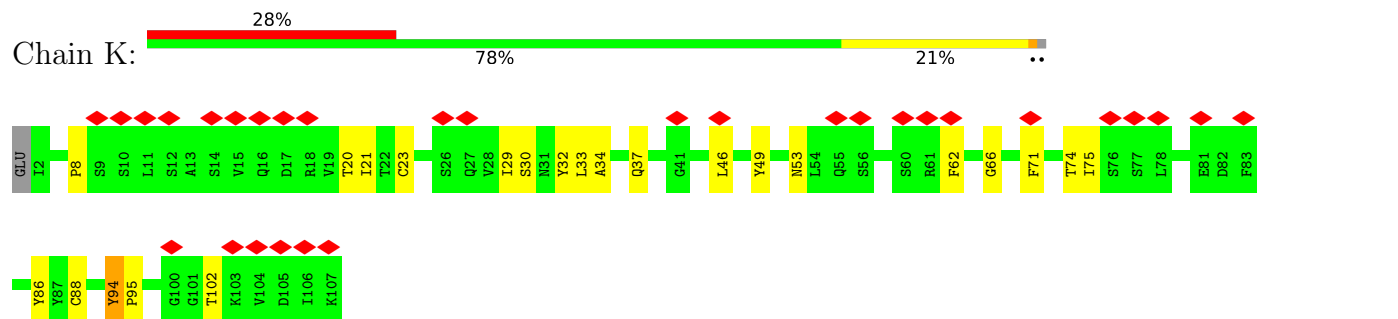
• Molecule 4: 6-2C H chain



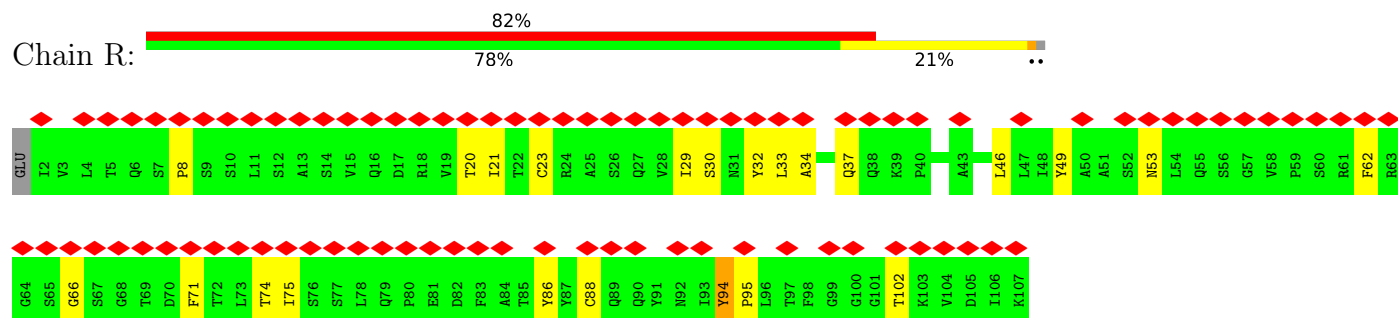
• Molecule 5: 6-2C L chain



● Molecule 5: 6-2C L chain



● Molecule 5: 6-2C L chain



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	372377	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 ($e^-/\text{\AA}^2$)	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	2.588	Depositor
Minimum map value	-1.650	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.054	Depositor
Recommended contour level	0.15	Depositor
Map size ($\text{\AA}$)	329.80002, 329.80002, 329.80002	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	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	1.01	4/7307 (0.1%)	1.50	59/9967 (0.6%)
1	B	1.02	7/7181 (0.1%)	1.49	57/9777 (0.6%)
1	C	1.02	5/7293 (0.1%)	1.50	51/9944 (0.5%)
2	D	0.91	0/853	1.27	1/1152 (0.1%)
2	F	0.91	0/853	1.27	1/1152 (0.1%)
2	L	0.91	0/853	1.27	1/1152 (0.1%)
3	H	1.01	0/756	1.38	4/1032 (0.4%)
3	J	1.02	0/756	1.37	4/1032 (0.4%)
3	P	1.01	0/756	1.37	4/1032 (0.4%)
4	I	1.06	2/975 (0.2%)	1.36	8/1326 (0.6%)
4	N	1.06	2/975 (0.2%)	1.37	8/1326 (0.6%)
4	Q	1.06	2/975 (0.2%)	1.37	8/1326 (0.6%)
5	K	0.97	0/812	1.46	4/1104 (0.4%)
5	O	0.97	0/812	1.46	4/1104 (0.4%)
5	R	0.97	0/812	1.46	4/1104 (0.4%)
All	All	1.01	22/31969 (0.1%)	1.46	218/43530 (0.5%)

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	I	57	ASN	C-N	11.71	1.49	1.33
4	N	57	ASN	C-N	11.70	1.49	1.33
4	Q	57	ASN	C-N	11.63	1.48	1.33
4	N	58	TYR	C-N	9.79	1.48	1.33
4	Q	58	TYR	C-N	9.79	1.48	1.33

The worst 5 of 218 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	812	PRO	N-CA-C	-12.91	95.01	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	909	ILE	N-CA-C	-8.73	104.63	113.10
3	P	29	ILE	CA-C-N	-8.72	110.53	122.30
3	P	29	ILE	C-N-CA	-8.72	110.53	122.30
1	A	337	PRO	N-CA-C	8.72	124.25	112.48

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	7138	0	6670	152	0
1	B	7024	0	6549	120	0
1	C	7125	0	6607	113	0
2	D	839	0	779	25	0
2	F	839	0	779	25	0
2	L	839	0	779	23	0
3	H	738	0	671	37	0
3	J	738	0	671	34	0
3	P	738	0	671	35	0
4	I	945	0	834	25	0
4	N	945	0	834	22	0
4	Q	945	0	834	24	0
5	K	794	0	768	15	0
5	O	794	0	768	15	0
5	R	794	0	768	15	0
6	A	14	0	13	0	0
6	B	14	0	13	0	0
6	C	14	0	13	0	0
All	All	31277	0	29021	622	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 10.

The worst 5 of 622 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:A:722:VAL:CG2	1:A:934:ILE:HG13	1.67	1.24
1:A:722:VAL:HG21	1:A:934:ILE:HG13	1.37	1.05
1:A:722:VAL:CG2	1:A:934:ILE:CG1	2.38	1.01
1:C:483:VAL:CG1	2:D:54:ASN:OD1	2.11	0.99
1:B:483:VAL:CG1	2:F:54:ASN:OD1	2.11	0.99

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	926/1300 (71%)	875 (94%)	47 (5%)	4 (0%)	30	62
1	B	903/1300 (70%)	852 (94%)	47 (5%)	4 (0%)	30	62
1	C	924/1300 (71%)	867 (94%)	49 (5%)	8 (1%)	14	47
2	D	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
2	F	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
2	L	114/117 (97%)	110 (96%)	4 (4%)	0	100	100
3	H	102/107 (95%)	95 (93%)	4 (4%)	3 (3%)	3	24
3	J	102/107 (95%)	95 (93%)	4 (4%)	3 (3%)	3	24
3	P	102/107 (95%)	95 (93%)	4 (4%)	3 (3%)	3	24
4	I	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
4	N	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
4	Q	120/122 (98%)	110 (92%)	10 (8%)	0	100	100
5	K	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
5	O	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
5	R	104/107 (97%)	100 (96%)	4 (4%)	0	100	100
All	All	4073/5259 (77%)	3839 (94%)	209 (5%)	25 (1%)	23	56

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	811	LYS
1	C	946	GLY
1	C	1057	PRO
1	B	325	SER
1	C	530	SER

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	738/1130 (65%)	725 (98%)	13 (2%)	51	74
1	B	723/1130 (64%)	719 (99%)	4 (1%)	78	84
1	C	734/1130 (65%)	723 (98%)	11 (2%)	57	76
2	D	83/95 (87%)	82 (99%)	1 (1%)	63	79
2	F	83/95 (87%)	82 (99%)	1 (1%)	63	79
2	L	83/95 (87%)	82 (99%)	1 (1%)	63	79
3	H	76/89 (85%)	75 (99%)	1 (1%)	61	78
3	J	76/89 (85%)	75 (99%)	1 (1%)	61	78
3	P	76/89 (85%)	75 (99%)	1 (1%)	61	78
4	I	92/104 (88%)	91 (99%)	1 (1%)	65	79
4	N	92/104 (88%)	91 (99%)	1 (1%)	65	79
4	Q	92/104 (88%)	91 (99%)	1 (1%)	65	79
5	K	85/92 (92%)	85 (100%)	0	100	100
5	O	85/92 (92%)	85 (100%)	0	100	100
5	R	85/92 (92%)	85 (100%)	0	100	100
All	All	3203/4530 (71%)	3166 (99%)	37 (1%)	61	79

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	D	56	ASP
3	P	46	VAL
3	J	46	VAL
3	H	46	VAL
1	A	858	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 52 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	282	ASN
1	C	926	GLN
2	L	81	ASN
1	C	317	ASN
1	C	658	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	A	1401	1	14,14,15	0.50	0	17,19,21	0.76	1 (5%)
6	NAG	B	1401	1	14,14,15	0.51	0	17,19,21	0.77	1 (5%)
6	NAG	C	1401	1	14,14,15	0.52	0	17,19,21	0.77	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	A	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	B	1401	1	-	2/6/23/26	0/1/1/1
6	NAG	C	1401	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	NAG	C1-O5-C5	2.34	115.33	112.19
6	A	1401	NAG	C1-O5-C5	2.31	115.28	112.19
6	B	1401	NAG	C1-O5-C5	2.30	115.27	112.19

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

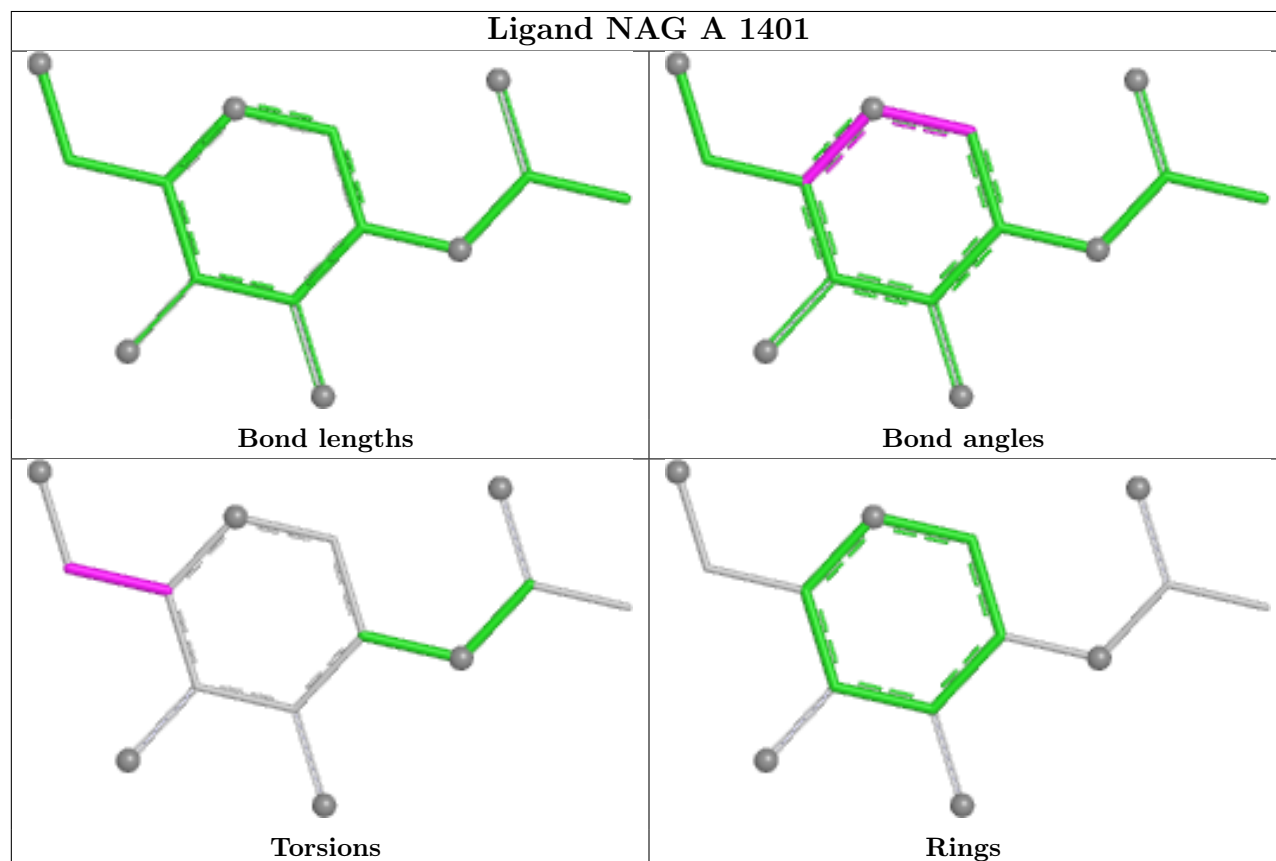
Mol	Chain	Res	Type	Atoms
6	A	1401	NAG	O5-C5-C6-O6
6	B	1401	NAG	O5-C5-C6-O6
6	C	1401	NAG	O5-C5-C6-O6
6	B	1401	NAG	C4-C5-C6-O6
6	C	1401	NAG	C4-C5-C6-O6

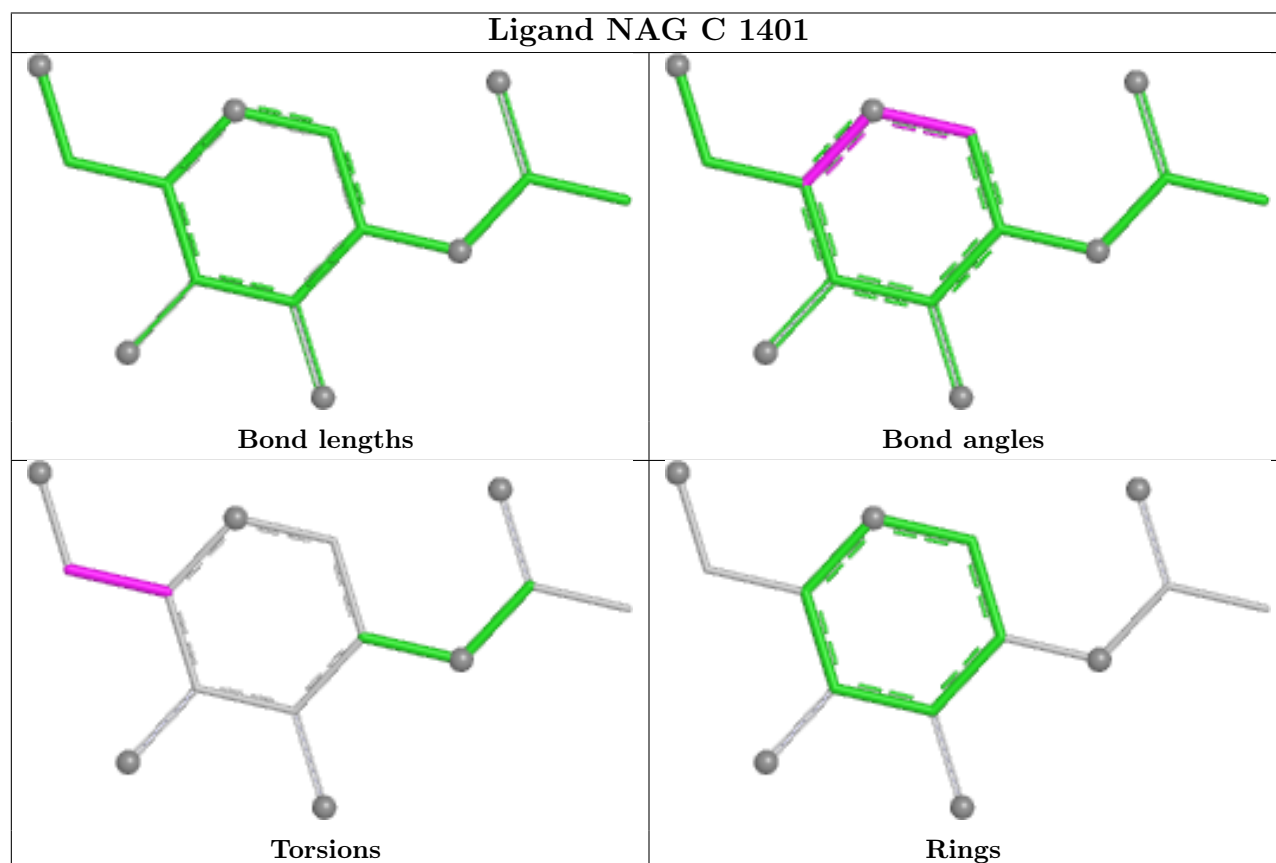
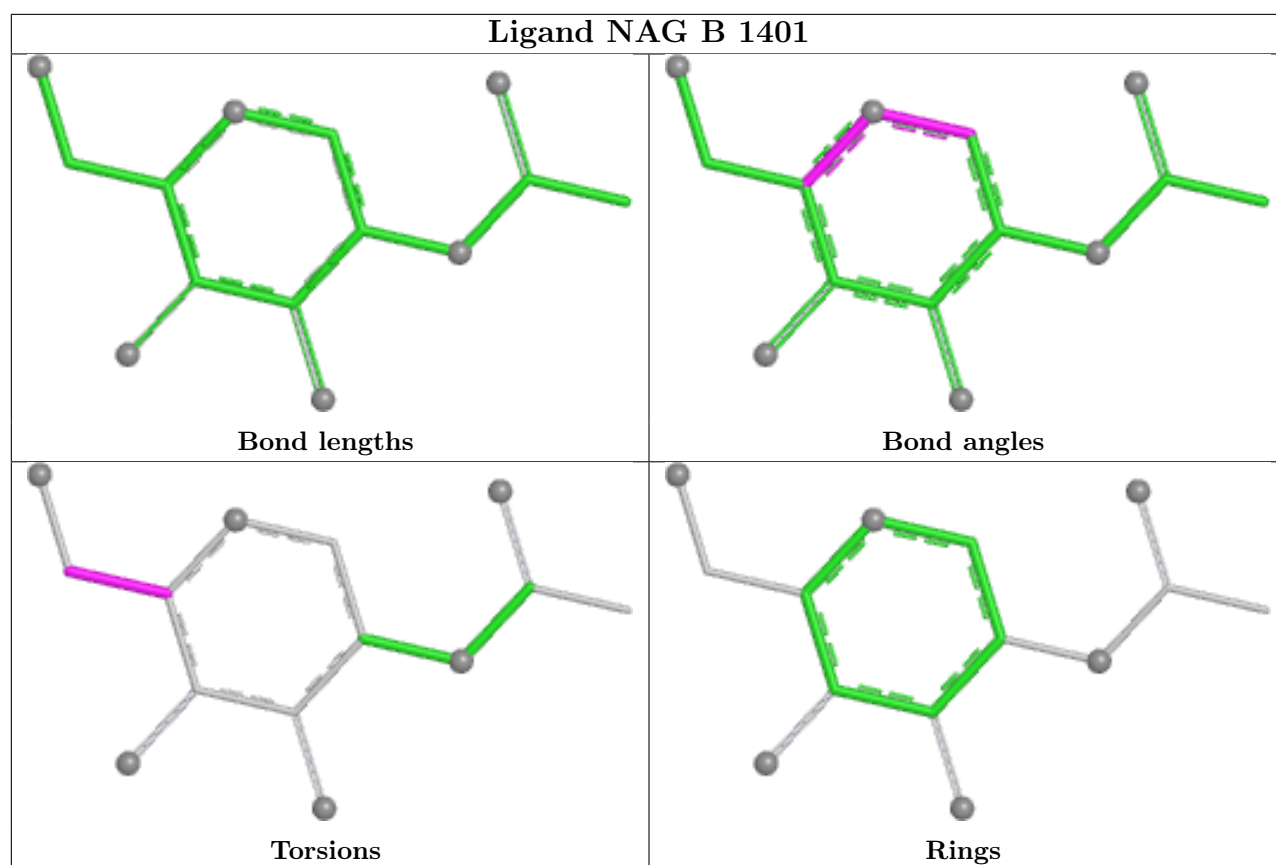
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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.

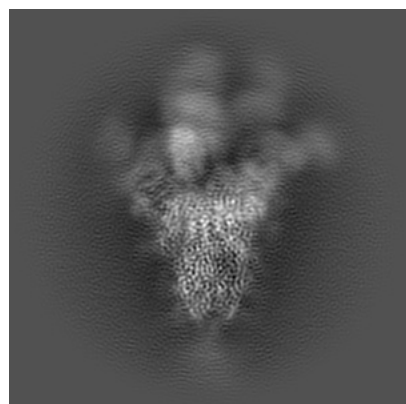
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-34411. These allow visual inspection of the internal detail of the map and identification of artifacts.

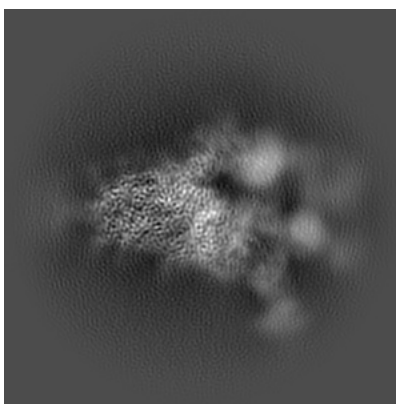
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

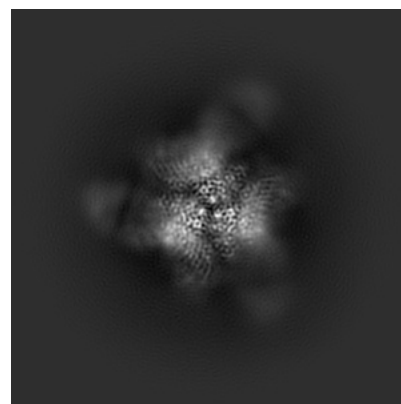
6.1.1 Primary map



X

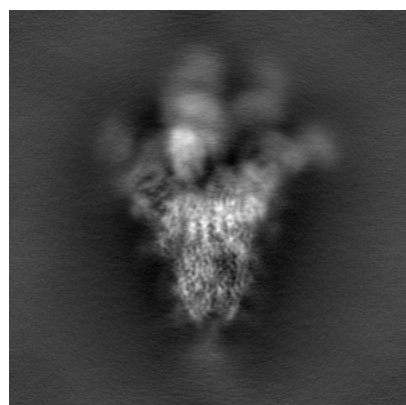


Y

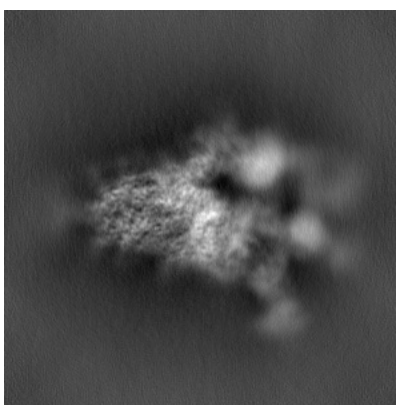


Z

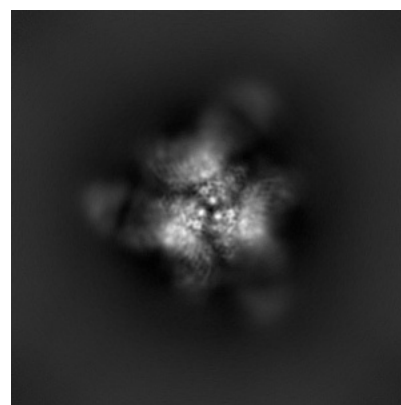
6.1.2 Raw map



X



Y

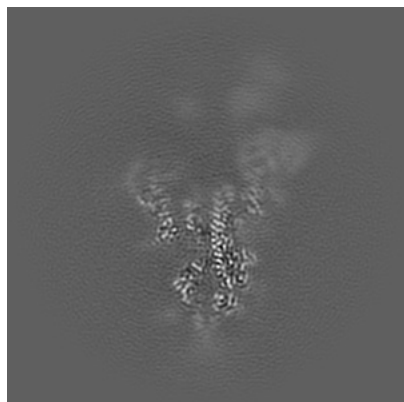


Z

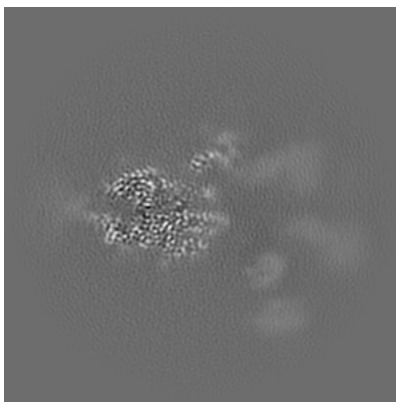
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

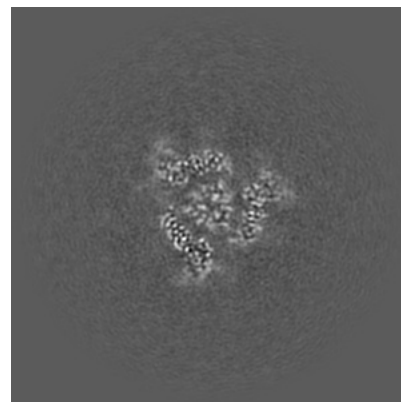
6.2.1 Primary map



X Index: 170

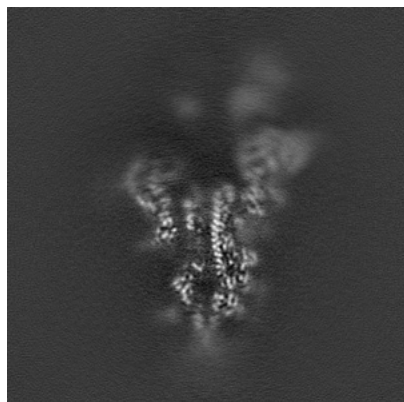


Y Index: 170

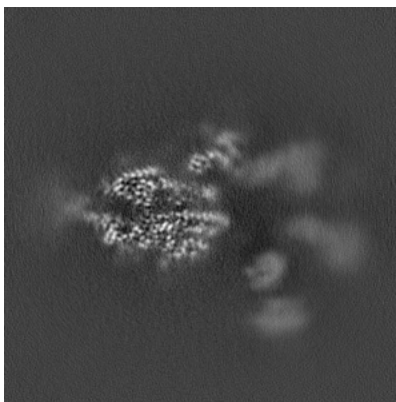


Z Index: 170

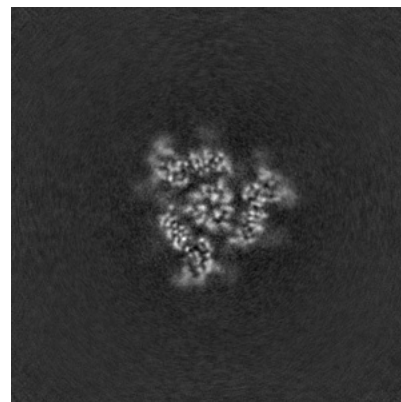
6.2.2 Raw map



X Index: 170



Y Index: 170

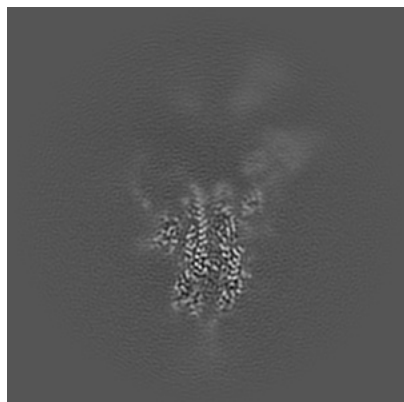


Z Index: 170

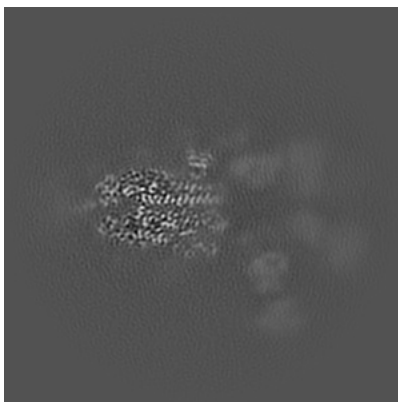
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

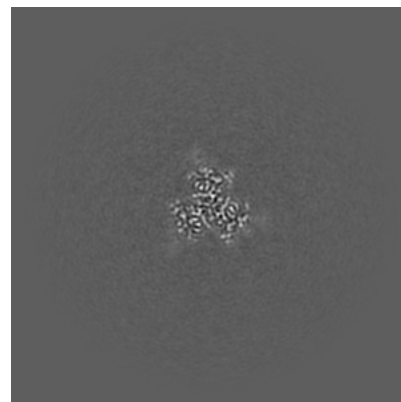
6.3.1 Primary map



X Index: 176

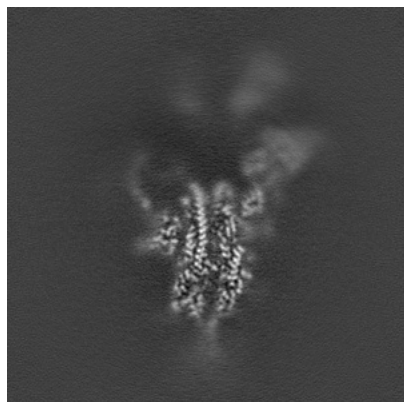


Y Index: 164

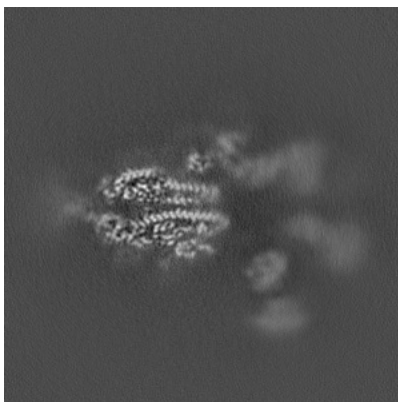


Z Index: 119

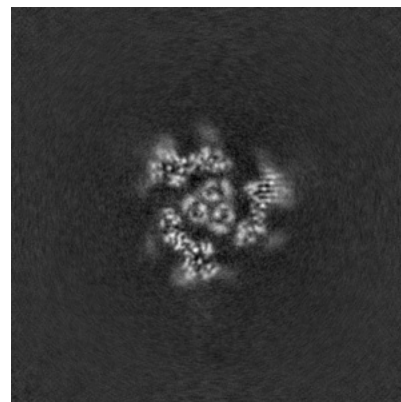
6.3.2 Raw map



X Index: 176



Y Index: 168

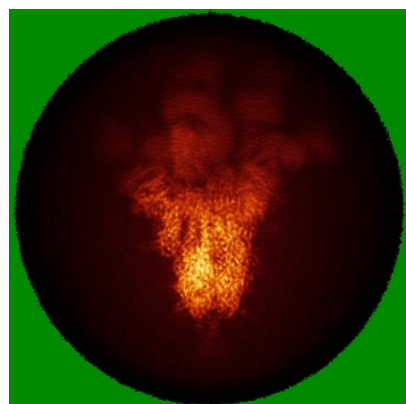


Z Index: 175

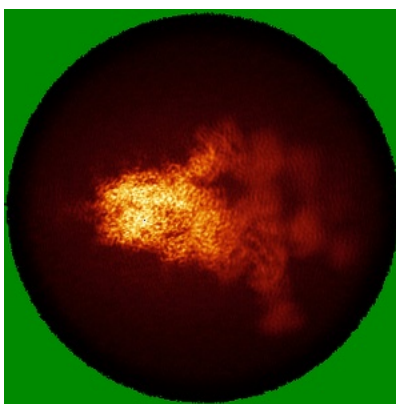
The images above show the largest variance slices of the map in three orthogonal directions.

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

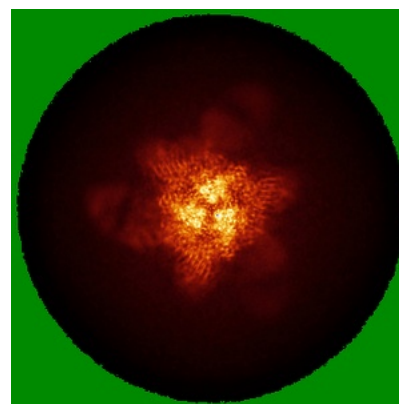
6.4.1 Primary map



X

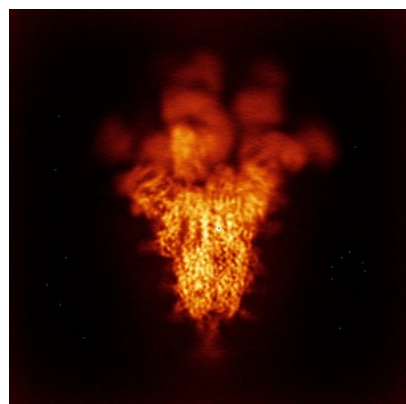


Y

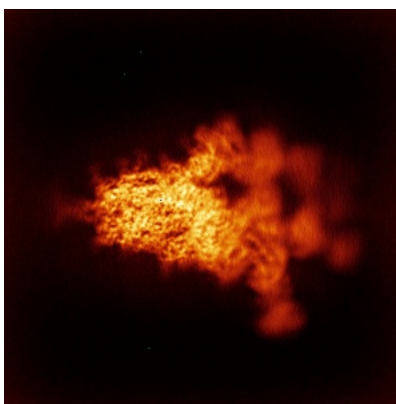


Z

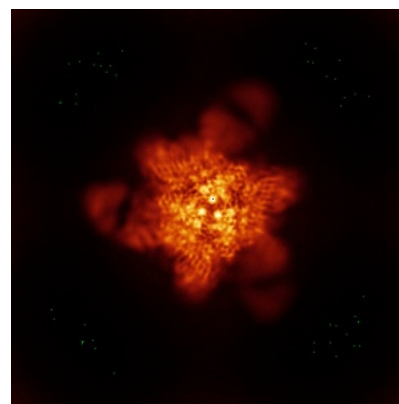
6.4.2 Raw map



X



Y

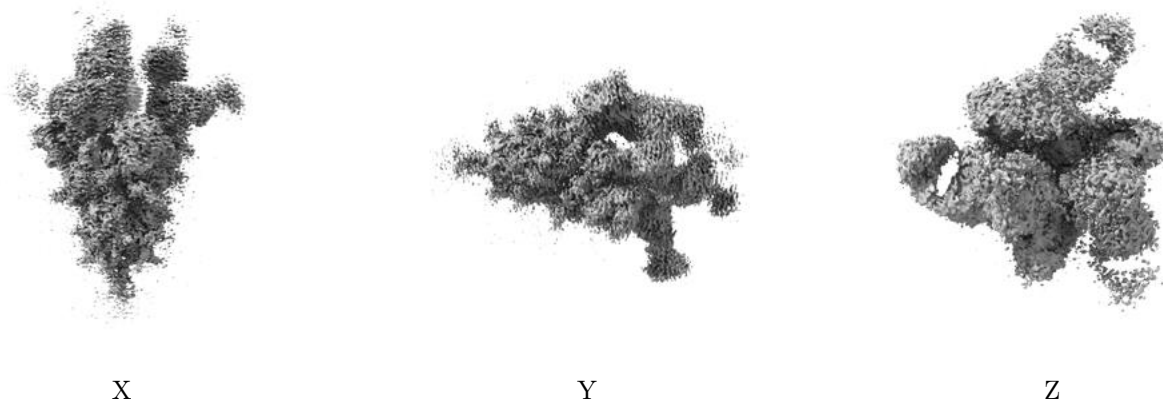


Z

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 [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.15. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

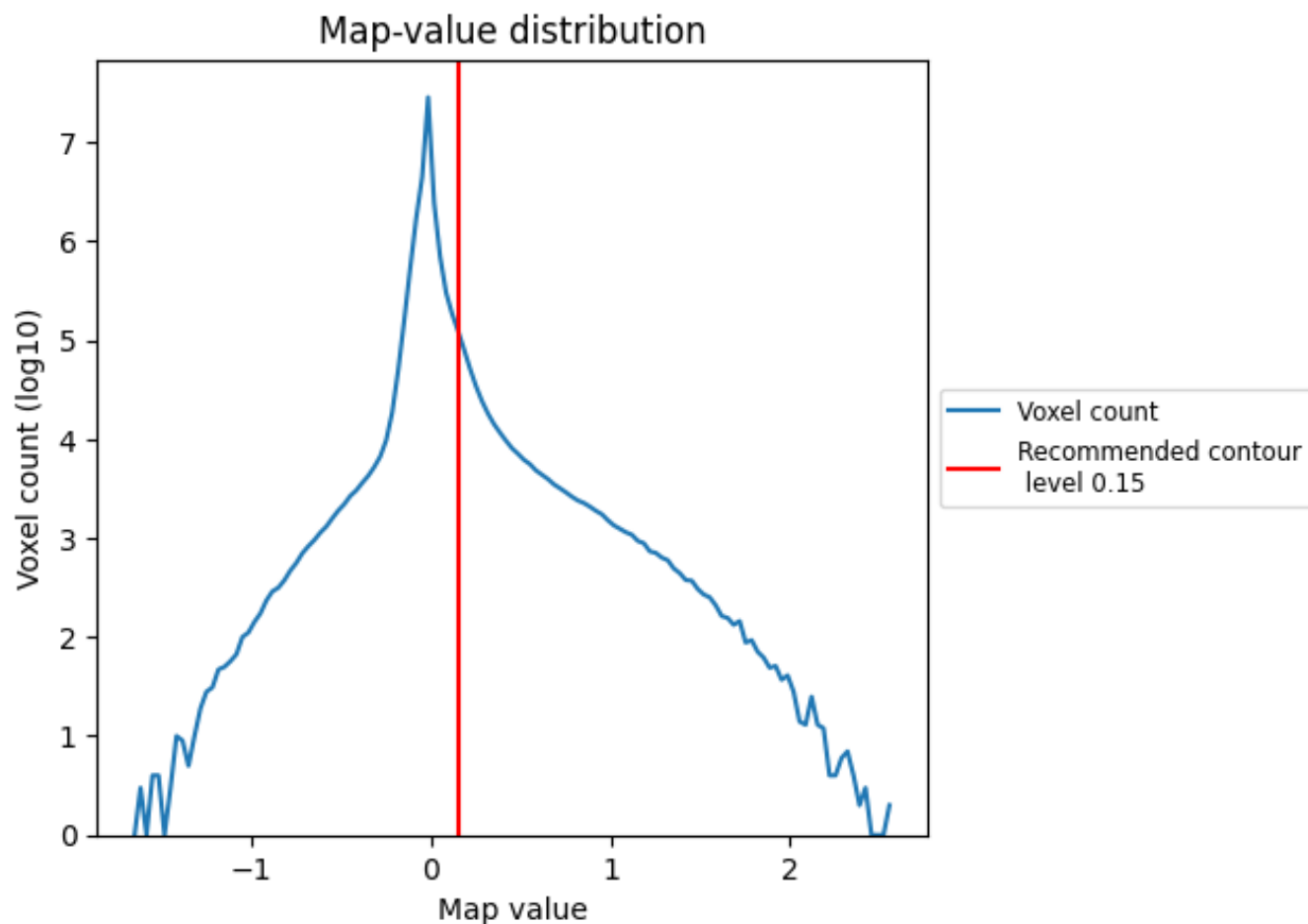
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

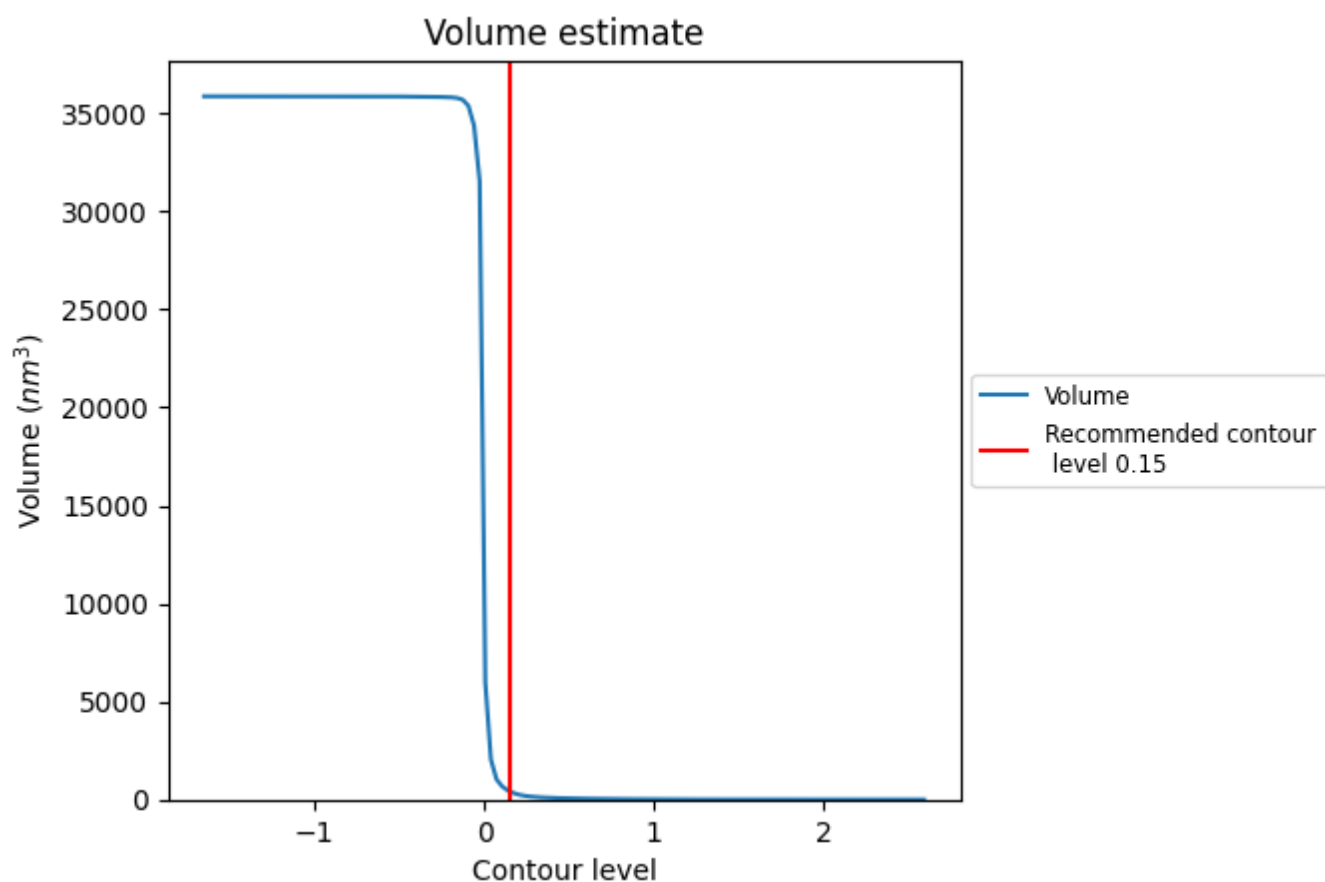
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

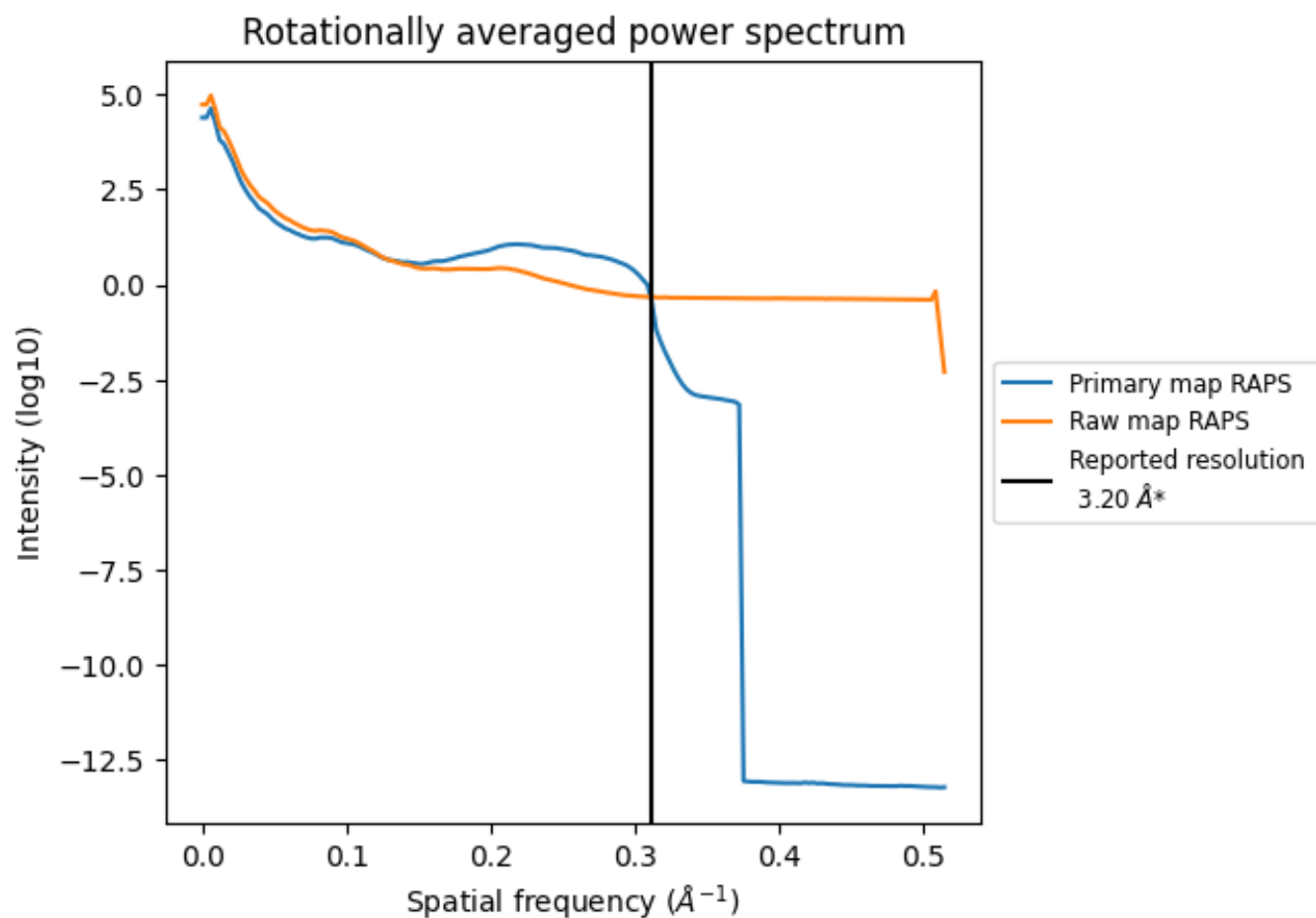
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 419 nm³; this corresponds to an approximate mass of 378 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 ⓘ

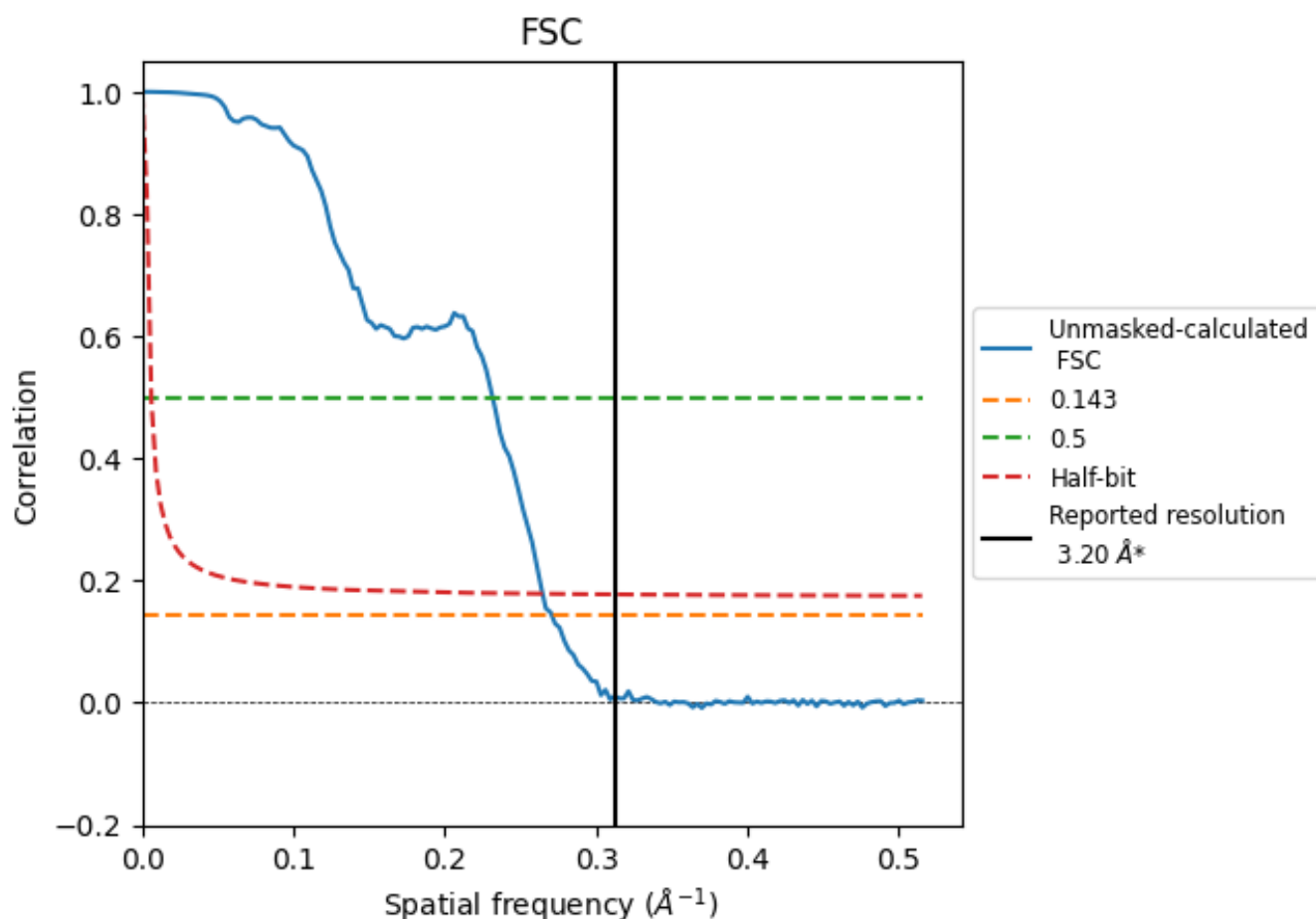


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

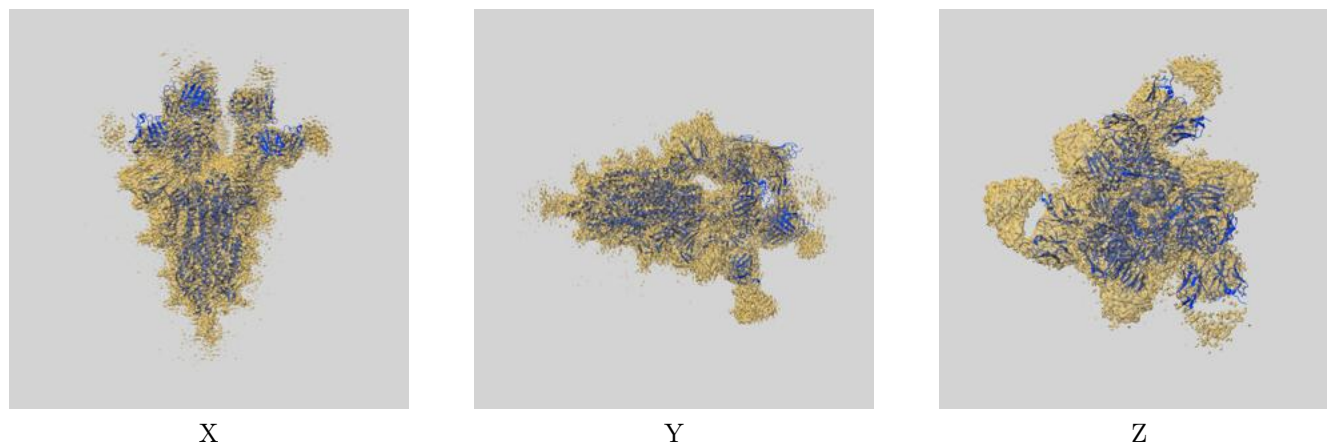
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	4.32	3.78

*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 3.69 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

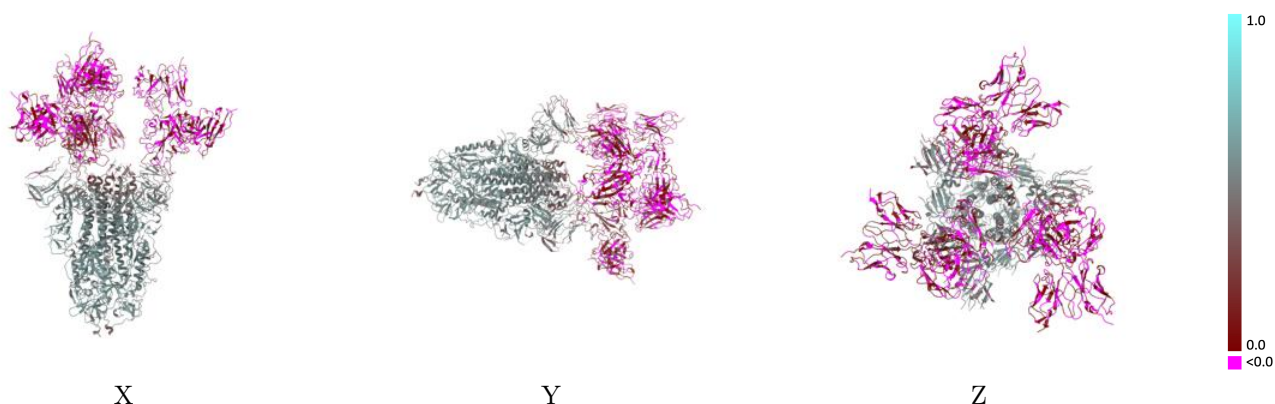
This section contains information regarding the fit between EMDB map EMD-34411 and PDB model 8H08. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

9.1 Map-model overlay [i](#)



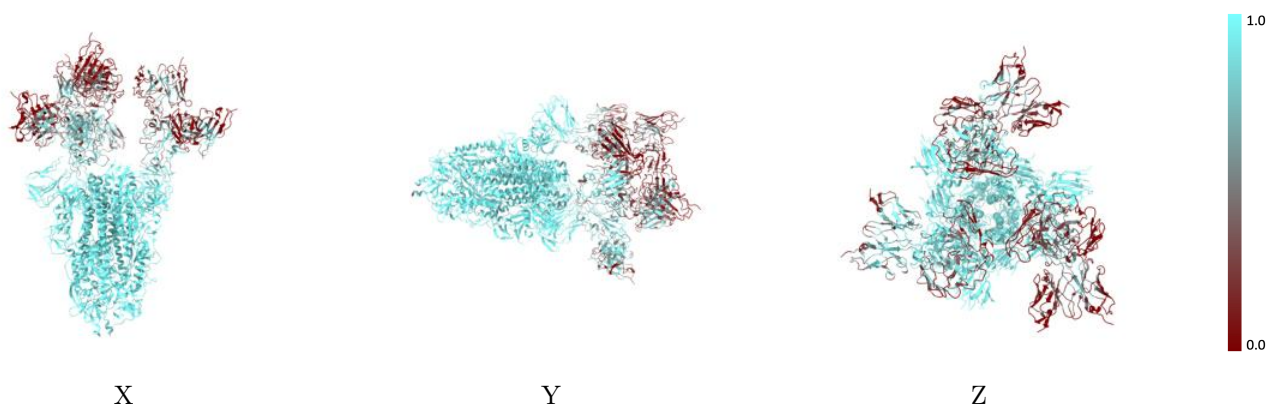
The images above show the 3D surface view of the map at the recommended contour level 0.15 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



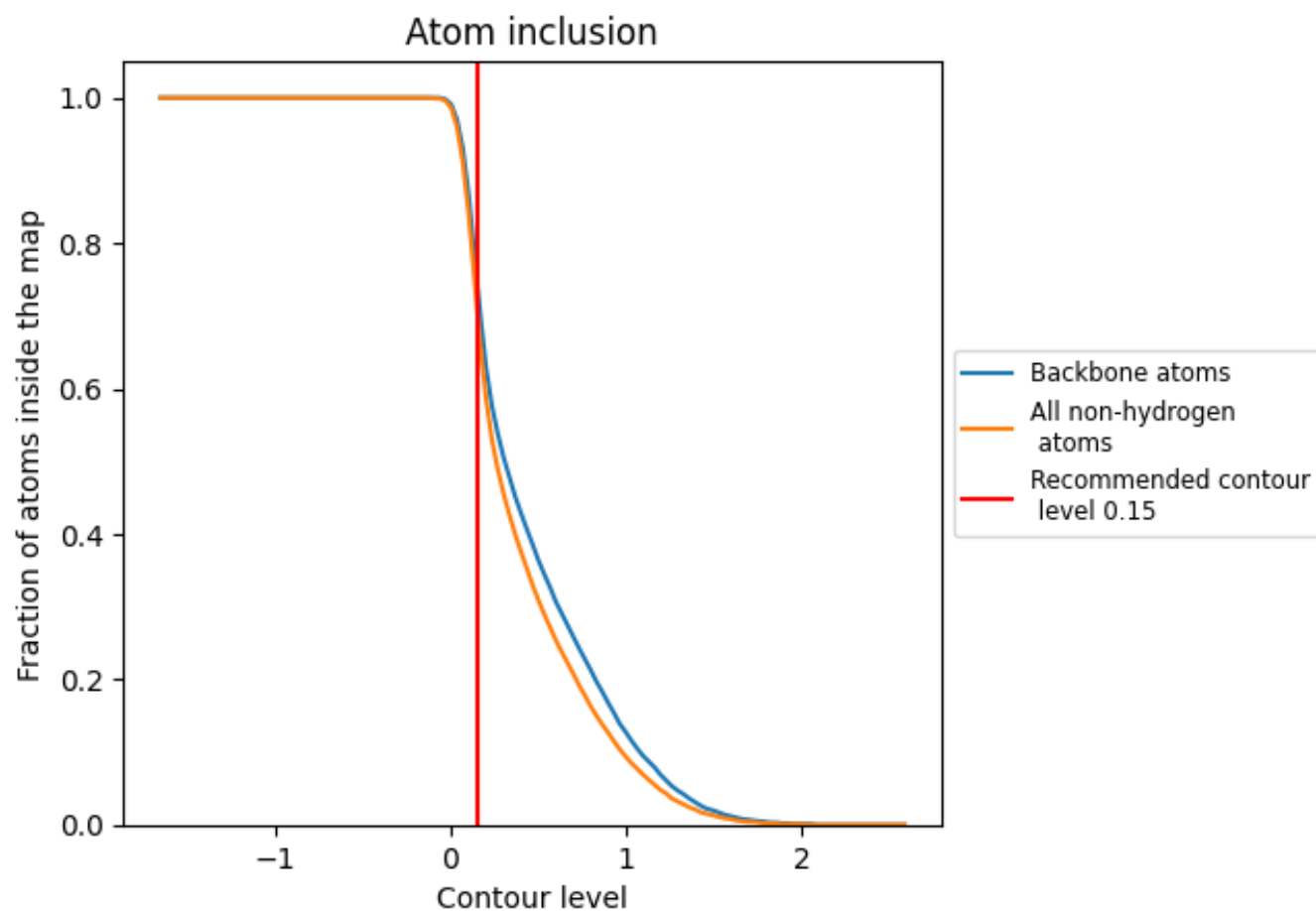
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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 (0.15).

9.4 Atom inclusion [i](#)



At the recommended contour level, 76% of all backbone atoms, 72% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7190	 0.3000
A	 0.8760	 0.4160
B	 0.9170	 0.4410
C	 0.8730	 0.4210
D	 0.1820	 -0.0010
F	 0.4510	 0.0240
H	 0.3300	 0.0390
I	 0.6750	 0.1020
J	 0.1310	 0.0150
K	 0.5760	 0.0820
L	 0.3310	 0.0100
N	 0.3720	 0.0000
O	 0.1940	 0.0240
P	 0.2500	 0.0290
Q	 0.4400	 0.0180
R	 0.1940	 0.0280

