



## Full wwPDB EM Validation Report ⓘ

May 13, 2023 – 05:27 pm BST

PDB ID : 7QOI  
EMDB ID : EMD-14091  
Title : Unique vertex of the phicrAss001 virion  
Authors : Bayfield, O.W.; Shkoporov, A.N.; Yutin, N.; Khokhlova, E.V.; Smith, J.L.R.;  
Hawkins, D.E.D.P.; Koonin, E.V.; Hill, C.; Antson, A.A.  
Deposited on : 2021-12-24  
Resolution : 3.62 Å(reported)

This is a Full wwPDB EM Validation 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:

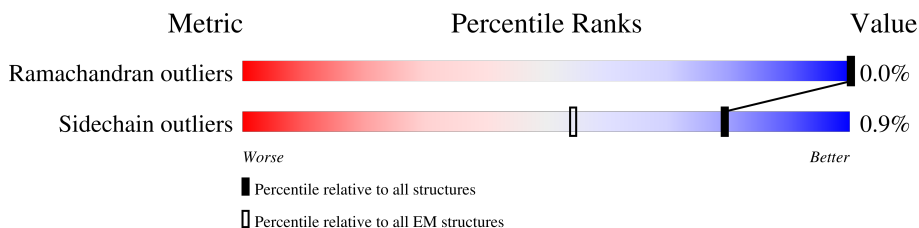
EMDB validation analysis : 0.0.1.dev50  
MolProbity : 4.02b-467  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.32.2

# 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 3.62 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	AA	504	
1	AB	504	
1	AC	504	
1	AD	504	
1	AE	504	
1	AF	504	
1	BA	504	
1	BB	504	
1	BC	504	

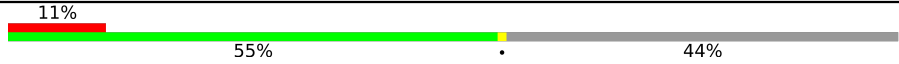
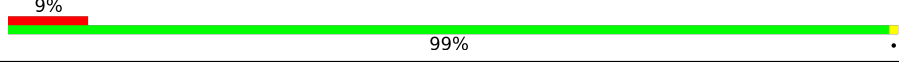
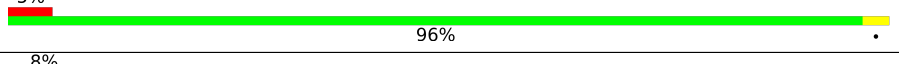
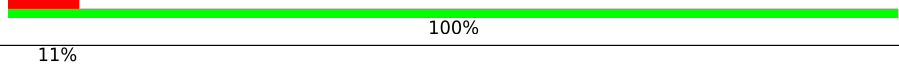

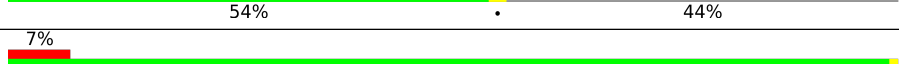
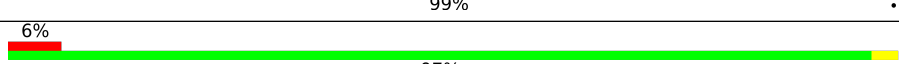
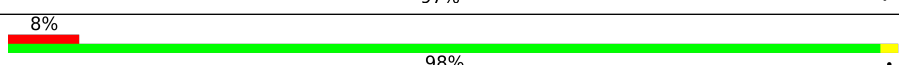
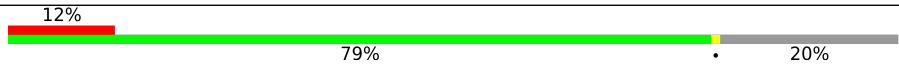

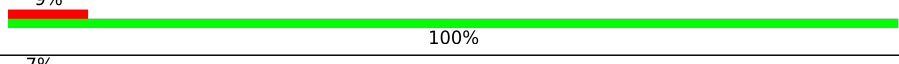
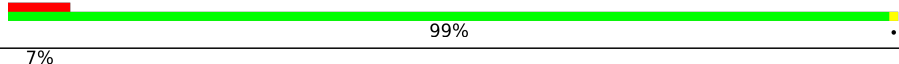
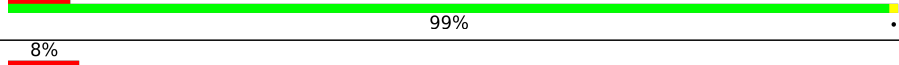

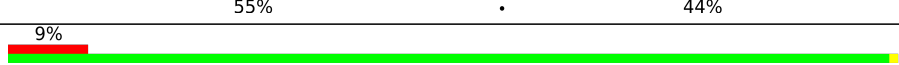
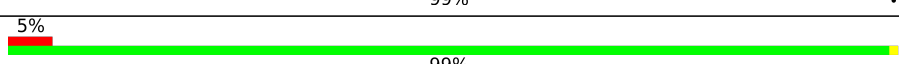
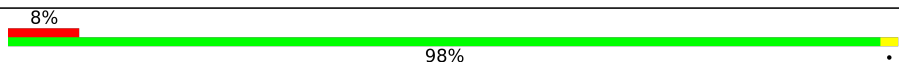








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Mol	Chain	Length	Quality of chain
1	BD	504	90% 10%
1	BE	504	100%
1	BF	504	6% 100%
1	CA	504	5% 95%
1	CB	504	99%
1	CC	504	99%
1	CD	504	89% 11%
1	CE	504	100%
1	CF	504	6% 98%
1	DA	504	6% 94%
1	DB	504	99%
1	DC	504	99%
1	DD	504	90% 10%
1	DE	504	100%
1	DF	504	6% 99%
1	EA	504	6% 96%
1	EB	504	99%
1	EC	504	98%
1	ED	504	90% 10%
1	EE	504	99%
1	EF	504	7% 99%
2	Aa	333	6% 100%
2	Ab	333	5% 98%
2	Ad	333	8% 98%
2	Ae	333	7% 80% 20%




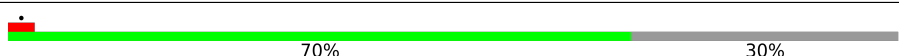
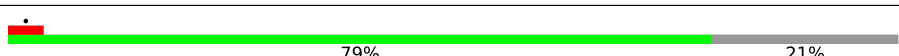
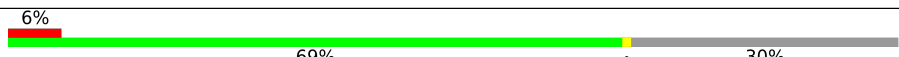
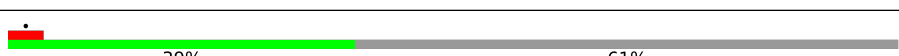




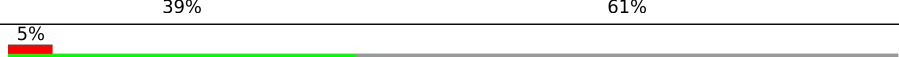

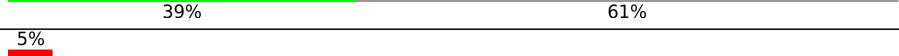
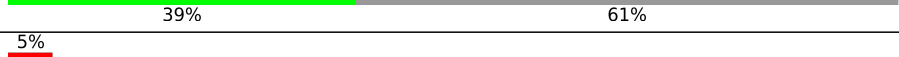






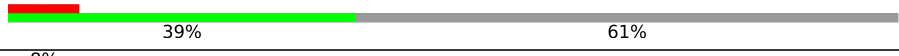



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Mol	Chain	Length	Quality of chain
2	Af	333	
2	Ba	333	
2	Bb	333	
2	Bd	333	
2	Be	333	
2	Bf	333	
2	Ca	333	
2	Cb	333	
2	Cd	333	
2	Ce	333	
2	Cf	333	
2	Da	333	
2	Db	333	
2	Dd	333	
2	De	333	
2	Df	333	
2	Ea	333	
2	Eb	333	
2	Ed	333	
2	Ee	333	
2	Ef	333	
3	Ag	104	
3	Ah	104	
3	Bg	104	
3	Bh	104	

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Mol	Chain	Length	Quality of chain
3	Cg	104	 79% 21%
3	Ch	104	 70% 30%
3	Dg	104	 79% 21%
3	Dh	104	 70% 30%
3	Eg	104	 79% 21%
3	Eh	104	 69% 30%
4	Ai	97	 39% 61%
4	Aj	97	 39% 61%
4	Ak	97	 38% 61%
4	Bi	97	 39% 61%
4	Bj	97	 39% 61%
4	Bk	97	 39% 61%
4	Ci	97	 39% 61%
4	Cj	97	 39% 61%
4	Ck	97	 39% 61%
4	Di	97	 39% 61%
4	Dj	97	 39% 61%
4	Dk	97	 39% 61%
4	Ei	97	 39% 61%
4	Ej	97	 39% 61%
4	Ek	97	 39% 61%
5	FA	806	 84% 15%
5	FB	806	 83% 16%
5	FC	806	 84% 15%
5	FD	806	 86% 13%

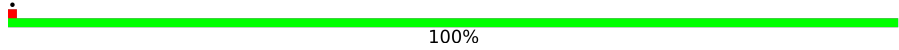
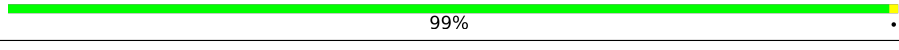
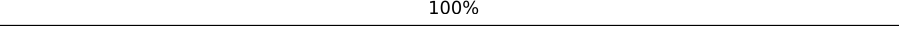
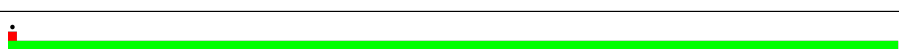
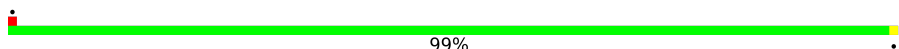
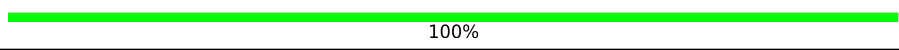
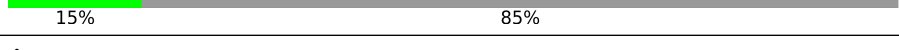
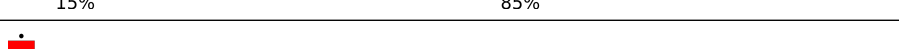



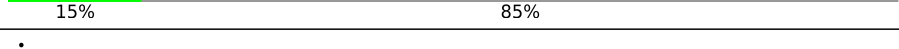




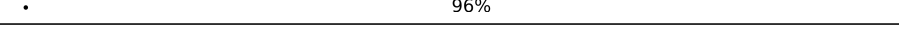

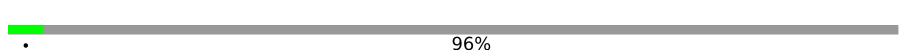
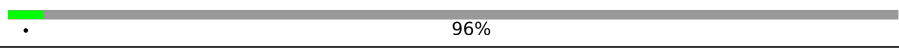
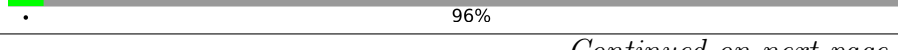



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Mol	Chain	Length	Quality of chain
5	FE	806	7% 81% 18%
5	FF	806	7% 84% 15%
5	FG	806	7% 83% 16%
5	FH	806	7% 83% 15%
5	FI	806	8% 84% 14%
5	FJ	806	8% 86% 13%
5	FK	806	6% 83% 17%
5	FL	806	7% 83% 16%
6	FM	236	94% ..
6	FN	236	93% ... .
6	FO	236	95% ..
6	FP	236	94% ..
6	FQ	236	95% ..
6	FR	236	95% .
6	FS	236	96% ..
6	FT	236	95% ..
6	FU	236	95% .
6	FV	236	94% ..
6	FW	236	94% ..
6	FX	236	94% ..
7	FY	225	100%
7	FZ	225	100%
7	GA	225	99% .
7	GB	225	100%
7	GC	225	100%

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Mol	Chain	Length	Quality of chain
7	GD	225	 100%
7	GE	225	 99%
7	GF	225	 100%
7	GG	225	 100%
7	GH	225	 100%
7	GI	225	 99%
7	GJ	225	 100%
8	GK	842	 15% 85%
8	GL	842	 15% 85%
8	GM	842	 15% 85%
8	GN	842	 15% 85%
8	GO	842	 15% 85%
8	GP	842	 15% 85%
8	GQ	842	 15% 85%
8	GR	842	 15% 85%
8	GS	842	 15% 85%
8	GT	842	 15% 85%
8	GU	842	 15% 85%
8	GV	842	 15% 85%
8	IK	842	 96%
8	IL	842	 96%
8	IM	842	 96%
8	IN	842	 96%
8	IO	842	 96%
8	IP	842	96%

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Mol	Chain	Length	Quality of chain
8	IQ	842	96%
8	IR	842	96%
8	IS	842	96%
8	IT	842	96%
8	IU	842	96%
8	IV	842	96%



## 2 Entry composition i

There are 9 unique types of molecules in this entry. The entry contains 310209 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 Major capsid protein gp32.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	AA	484	3861	2451	668	723	19	0	0
1	AB	503	4012	2552	695	745	20	0	0
1	AC	503	4012	2552	695	745	20	0	0
1	AD	456	3649	2329	631	671	18	0	0
1	AE	503	4012	2552	695	745	20	0	0
1	AF	503	4012	2552	695	745	20	0	0
1	BA	485	3868	2455	669	725	19	0	0
1	BB	503	4012	2552	695	745	20	0	0
1	BC	503	4012	2552	695	745	20	0	0
1	BD	456	3649	2329	631	671	18	0	0
1	BE	503	4012	2552	695	745	20	0	0
1	BF	503	4012	2552	695	745	20	0	0
1	CA	483	3855	2448	667	721	19	0	0
1	CB	503	4012	2552	695	745	20	0	0
1	CC	503	4012	2552	695	745	20	0	0
1	CD	451	3612	2307	623	664	18	0	0
1	CE	503	4012	2552	695	745	20	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	CF	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	DA	485	Total	C	N	O	S	0	0
			3868	2455	669	725	19		
1	DB	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	DC	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	DD	456	Total	C	N	O	S	0	0
			3649	2329	631	671	18		
1	DE	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	DF	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	EA	485	Total	C	N	O	S	0	0
			3868	2455	669	725	19		
1	EB	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	EC	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	ED	456	Total	C	N	O	S	0	0
			3649	2329	631	671	18		
1	EE	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		
1	EF	503	Total	C	N	O	S	0	0
			4012	2552	695	745	20		

- Molecule 2 is a protein called Auxiliary capsid protein gp36.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Aa	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ab	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ad	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		
2	Ae	267	Total	C	N	O	S	0	0
			2077	1335	332	401	9		
2	Af	185	Total	C	N	O	S	0	0
			1434	919	226	283	6		
2	Ba	333	Total	C	N	O	S	0	0
			2542	1624	410	498	10		

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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	Bb	333	2542	1624	410	498	10	0	0
2	Bd	333	2542	1624	410	498	10	0	0
2	Be	266	2070	1330	331	400	9	0	0
2	Bf	185	1434	919	226	283	6	0	0
2	Ca	333	2542	1624	410	498	10	0	0
2	Cb	333	2542	1624	410	498	10	0	0
2	Cd	333	2542	1624	410	498	10	0	0
2	Ce	267	2077	1335	332	401	9	0	0
2	Cf	185	1434	919	226	283	6	0	0
2	Da	333	2542	1624	410	498	10	0	0
2	Db	333	2542	1624	410	498	10	0	0
2	Dd	333	2542	1624	410	498	10	0	0
2	De	267	2077	1335	332	401	9	0	0
2	Df	185	1434	919	226	283	6	0	0
2	Ea	333	2542	1624	410	498	10	0	0
2	Eb	333	2542	1624	410	498	10	0	0
2	Ed	333	2542	1624	410	498	10	0	0
2	Ee	267	2077	1335	332	401	9	0	0
2	Ef	185	1434	919	226	283	6	0	0

- Molecule 3 is a protein called Portal vertex capsid protein gp57.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Ag	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Ah	73	Total	C	N	O	S	0	0
			563	359	91	105	8		
3	Bg	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Bh	73	Total	C	N	O	S	0	0
			563	359	91	105	8		
3	Cg	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Ch	73	Total	C	N	O	S	0	0
			563	359	91	105	8		
3	Dg	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Dh	73	Total	C	N	O	S	0	0
			563	359	91	105	8		
3	Eg	82	Total	C	N	O	S	0	0
			619	392	100	118	9		
3	Eh	73	Total	C	N	O	S	0	0
			563	359	91	105	8		

- Molecule 4 is a protein called Head fiber trimer protein gp21.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	Ai	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Aj	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ak	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Bi	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Bj	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Bk	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ci	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Cj	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ck	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Di	38	Total	C	N	O	S	0	0
			310	201	51	56	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
4	Dj	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Dk	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ei	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ej	38	Total	C	N	O	S	0	0
			310	201	51	56	2		
4	Ek	38	Total	C	N	O	S	0	0
			310	201	51	56	2		

- Molecule 5 is a protein called Portal protein gp20.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	FA	688	Total	C	N	O	S	0	0
			5617	3558	957	1077	25		
5	FB	678	Total	C	N	O	S	0	0
			5545	3519	941	1062	23		
5	FC	684	Total	C	N	O	S	0	0
			5597	3550	951	1072	24		
5	FD	705	Total	C	N	O	S	0	0
			5759	3657	976	1102	24		
5	FE	660	Total	C	N	O	S	0	0
			5400	3426	920	1031	23		
5	FF	684	Total	C	N	O	S	0	0
			5593	3543	952	1074	24		
5	FG	680	Total	C	N	O	S	0	0
			5569	3531	948	1066	24		
5	FH	689	Total	C	N	O	S	0	0
			5618	3558	958	1078	24		
5	FI	694	Total	C	N	O	S	0	0
			5671	3601	961	1085	24		
5	FJ	698	Total	C	N	O	S	0	0
			5699	3613	967	1094	25		
5	FK	669	Total	C	N	O	S	0	0
			5478	3483	929	1043	23		
5	FL	681	Total	C	N	O	S	0	0
			5563	3529	945	1066	23		

- Molecule 6 is a protein called Ring protein 1 gp43.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	FM	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FN	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FO	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FP	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FQ	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FR	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FS	229	Total	C	N	O	S	0	0
			1868	1204	314	341	9		
6	FT	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FU	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FV	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FW	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		
6	FX	226	Total	C	N	O	S	0	0
			1841	1188	308	336	9		

- Molecule 7 is a protein called Ring protein 2 gp40.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	FY	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	FZ	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GA	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GB	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GC	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GD	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GE	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GF	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		

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Mol	Chain	Residues	Atoms					AltConf	Trace
7	GG	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GH	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GI	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		
7	GJ	225	Total	C	N	O	S	0	0
			1841	1180	292	357	12		

- Molecule 8 is a protein called Cargo protein 1 gp45.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	GK	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GL	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GM	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GN	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GO	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GP	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GQ	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GR	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GS	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GT	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GU	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	GV	126	Total	C	N	O	S	0	0
			987	605	179	201	2		
8	IK	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IL	32	Total	C	N	O	S	0	0
			251	157	44	49	1		
8	IM	32	Total	C	N	O	S	0	0
			251	157	44	49	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
8	IN	32	Total 251	C 157	N 44	O 49	S 1	0	0
8	IO	32	Total 251	C 157	N 44	O 49	S 1	0	0
8	IP	32	Total 251	C 157	N 44	O 49	S 1	0	0
8	IQ	32	Total 251	C 157	N 44	O 49	S 1	0	0
8	IR	32	Total 251	C 157	N 44	O 49	S 1	0	0
8	IS	32	Total 251	C 157	N 44	O 49	S 1	0	0
8	IT	32	Total 251	C 157	N 44	O 49	S 1	0	0
8	IU	32	Total 251	C 157	N 44	O 49	S 1	0	0
8	IV	32	Total 251	C 157	N 44	O 49	S 1	0	0

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
9	AB	1	Total 1	Mg 1	0
9	AC	1	Total 1	Mg 1	0
9	AD	1	Total 1	Mg 1	0
9	AE	1	Total 1	Mg 1	0
9	BB	1	Total 1	Mg 1	0
9	BD	1	Total 1	Mg 1	0
9	CB	1	Total 1	Mg 1	0
9	CD	1	Total 1	Mg 1	0
9	CE	1	Total 1	Mg 1	0
9	CF	1	Total 1	Mg 1	0

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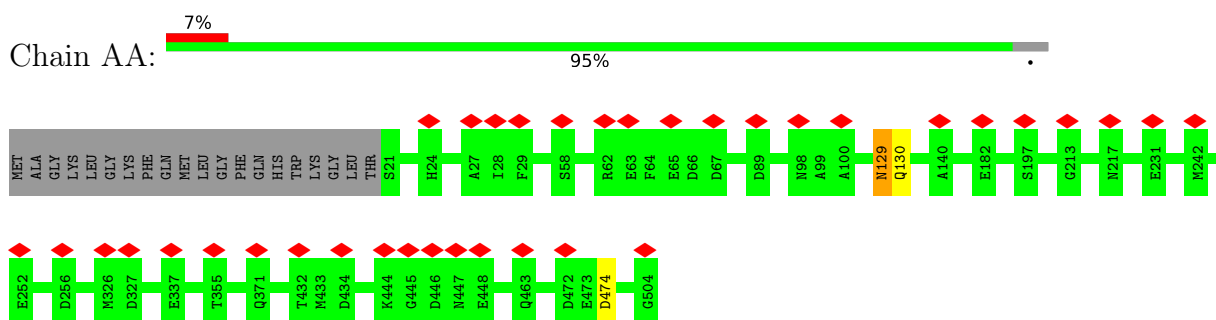
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
9	DB	1	1	1	0
9	DE	1	1	1	0
9	DF	1	1	1	0
9	EB	1	1	1	0
9	ED	1	1	1	0
9	FA	1	1	1	0
9	FB	1	1	1	0
9	FC	1	1	1	0
9	FD	1	1	1	0
9	FE	1	1	1	0
9	FF	1	1	1	0
9	FG	1	1	1	0
9	FH	1	1	1	0
9	FI	1	1	1	0
9	FJ	1	1	1	0
9	FK	1	1	1	0
9	FL	1	1	1	0

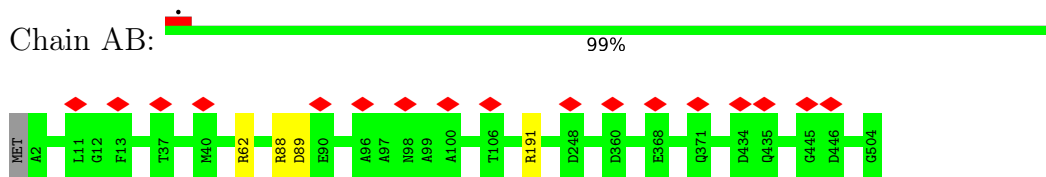
### 3 Residue-property plots [i](#)

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

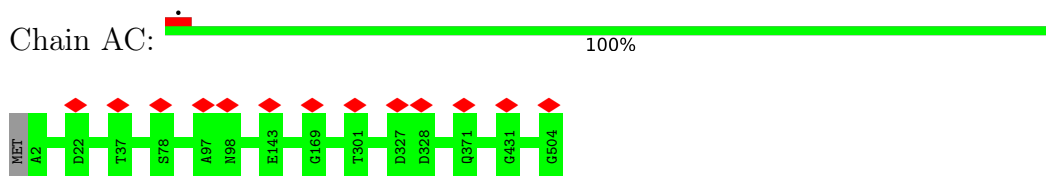
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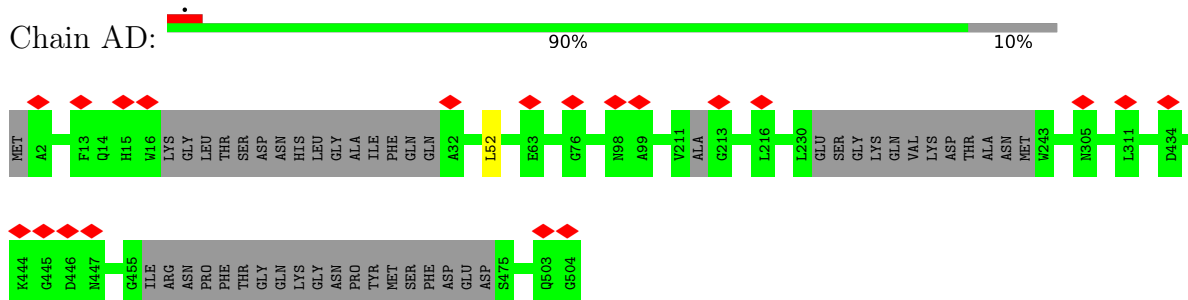
- Molecule 1: Major capsid protein gp32



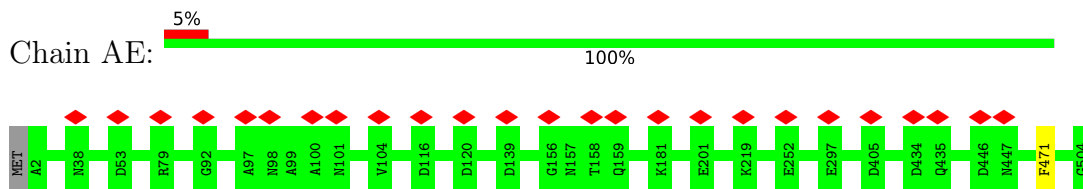
- Molecule 1: Major capsid protein gp32



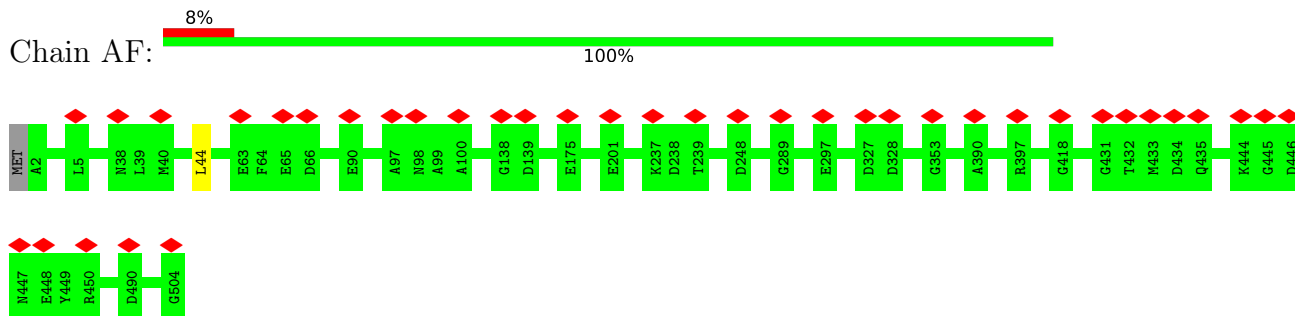
- Molecule 1: Major capsid protein gp32



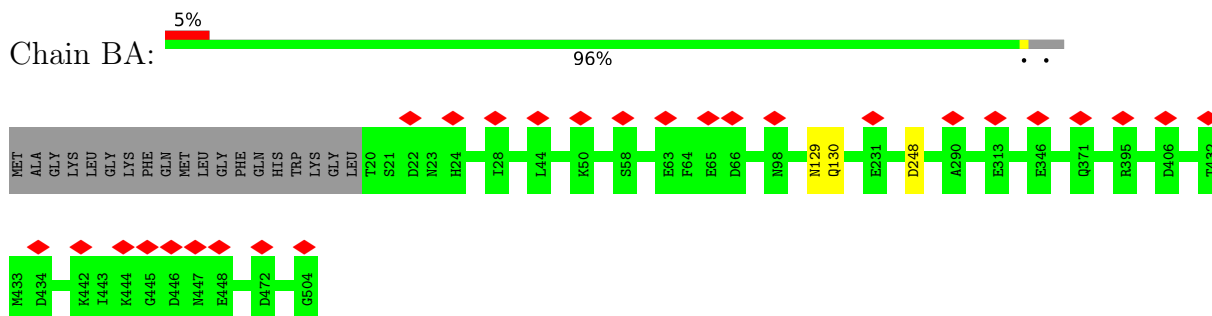
• Molecule 1: Major capsid protein gp32



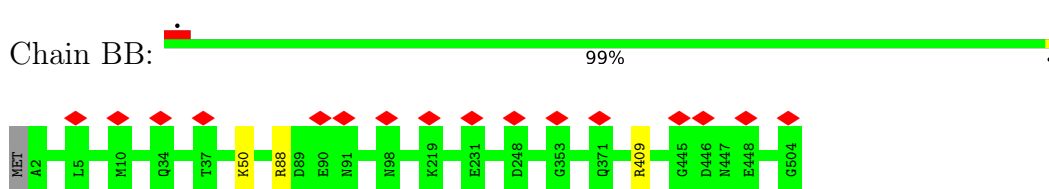
• Molecule 1: Major capsid protein gp32



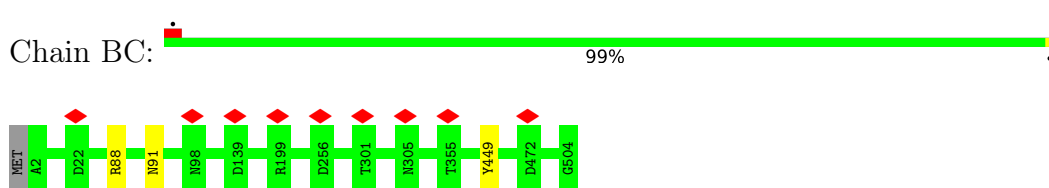
• Molecule 1: Major capsid protein gp32



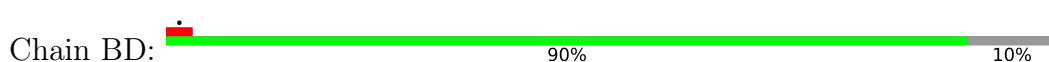
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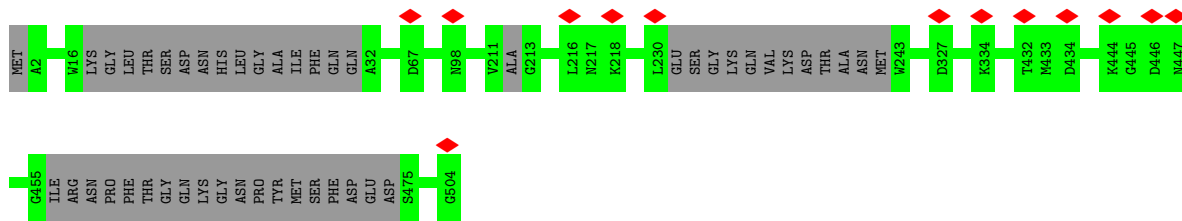


• Molecule 1: Major capsid protein gp32

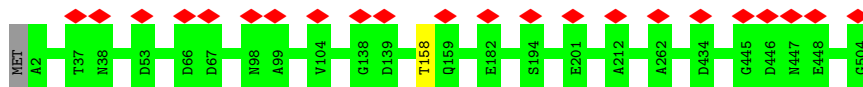


• Molecule 1: Major capsid protein gp32

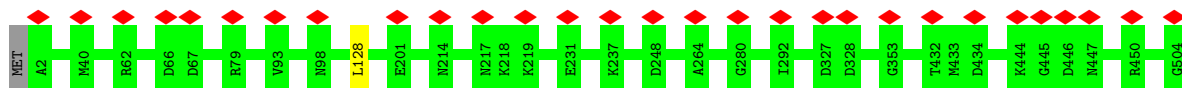




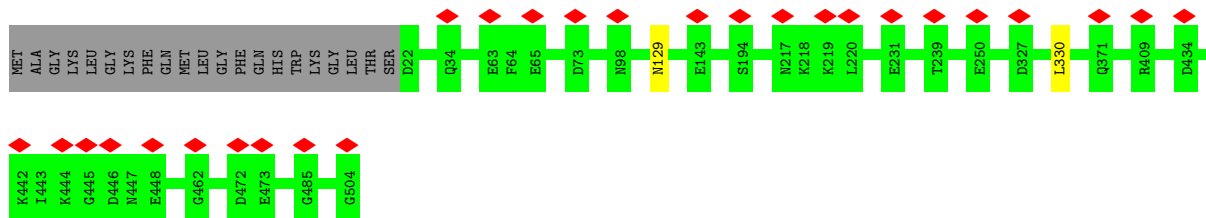
• Molecule 1: Major capsid protein gp32



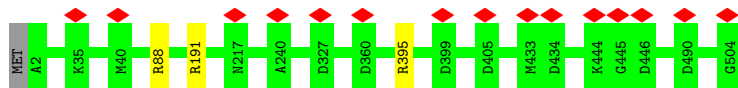
• Molecule 1: Major capsid protein gp32



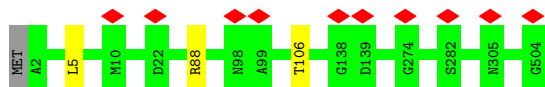
• Molecule 1: Major capsid protein gp32



• Molecule 1: Major capsid protein gp32

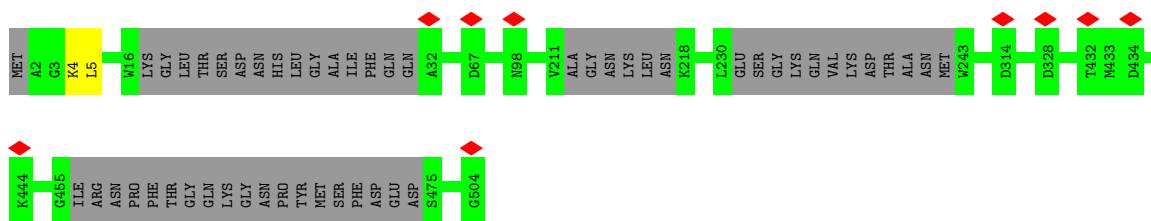


• Molecule 1: Major capsid protein gp32



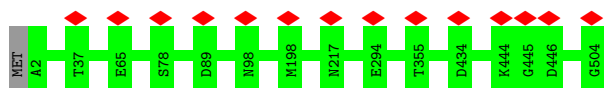
• Molecule 1: Major capsid protein gp32

Chain CD:  89% 11%



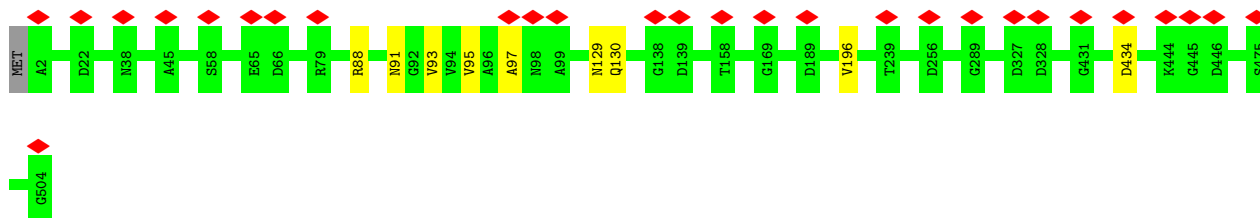
- Molecule 1: Major capsid protein gp32

Chain CE:  100%



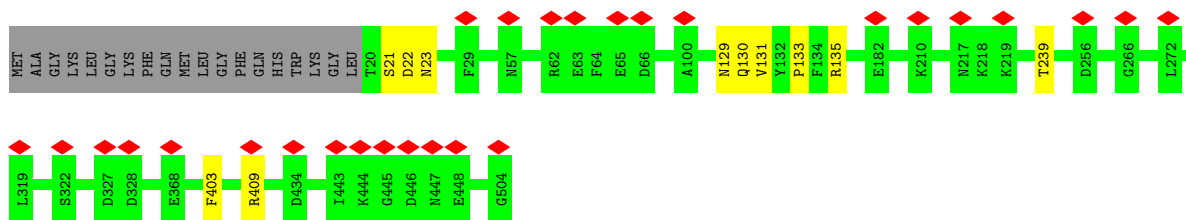
- Molecule 1: Major capsid protein gp32

Chain CF:  98% 6%



- Molecule 1: Major capsid protein gp32

Chain DA:  94% 6%



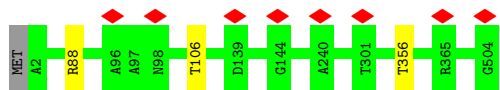
- Molecule 1: Major capsid protein gp32

Chain DB:  99%

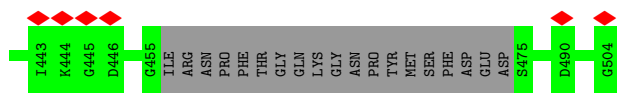
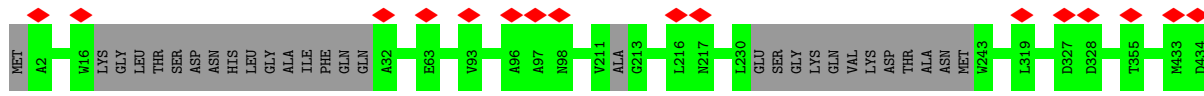


- Molecule 1: Major capsid protein gp32

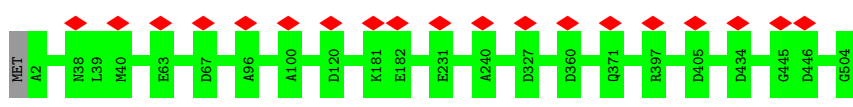
Chain DC:  99%



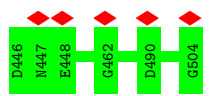
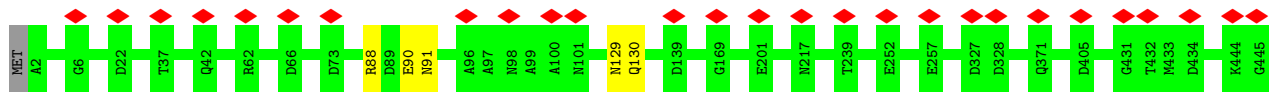
• Molecule 1: Major capsid protein gp32



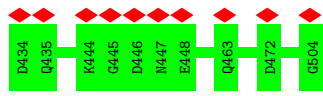
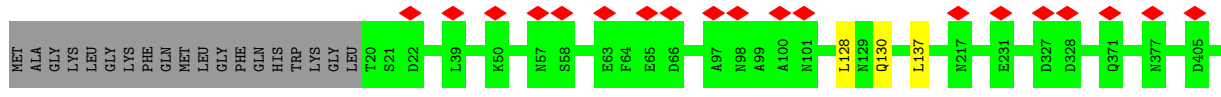
• Molecule 1: Major capsid protein gp32



• Molecule 1: Major capsid protein gp32

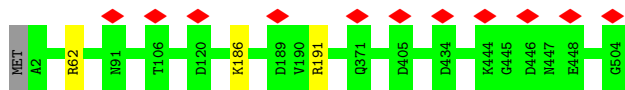


• Molecule 1: Major capsid protein gp32

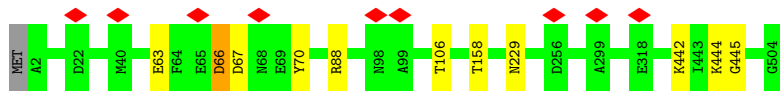


• Molecule 1: Major capsid protein gp32

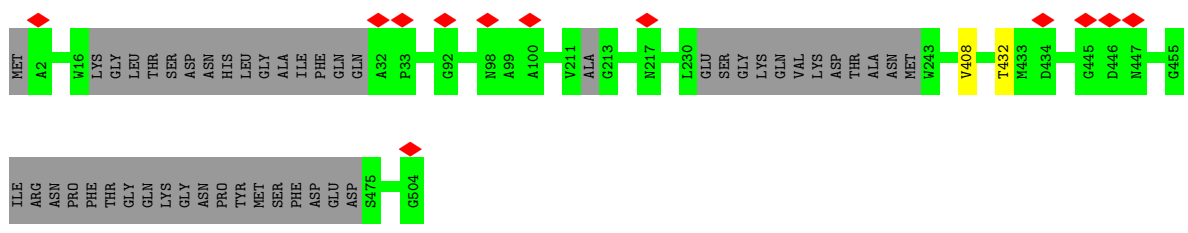
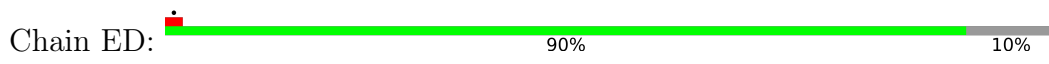




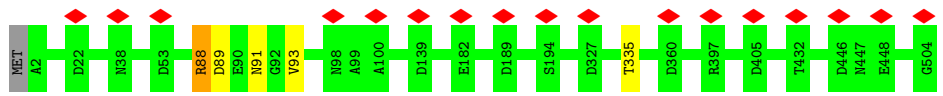
• Molecule 1: Major capsid protein gp32



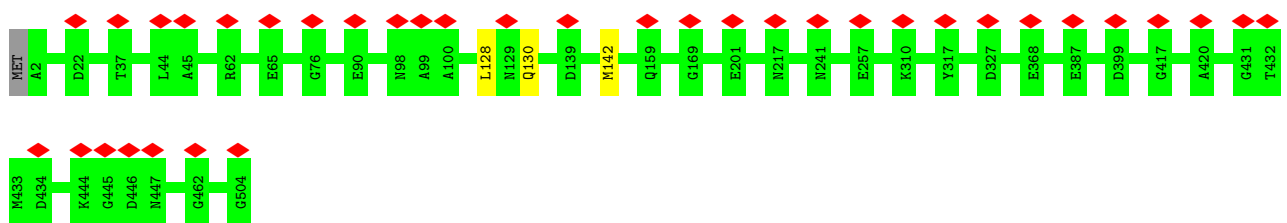
• Molecule 1: Major capsid protein gp32



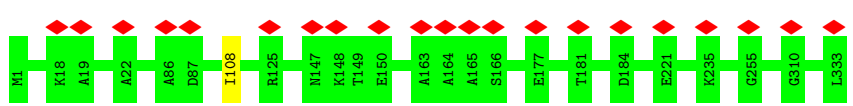
• Molecule 1: Major capsid protein gp32



• Molecule 1: Major capsid protein gp32



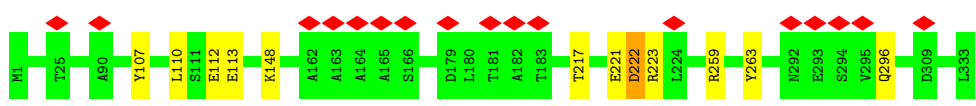
• Molecule 2: Auxiliary capsid protein gp36



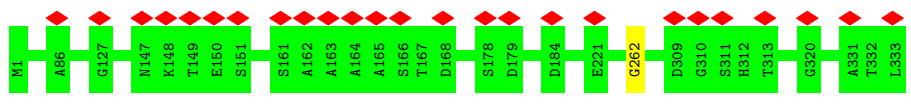
• Molecule 2: Auxiliary capsid protein gp36



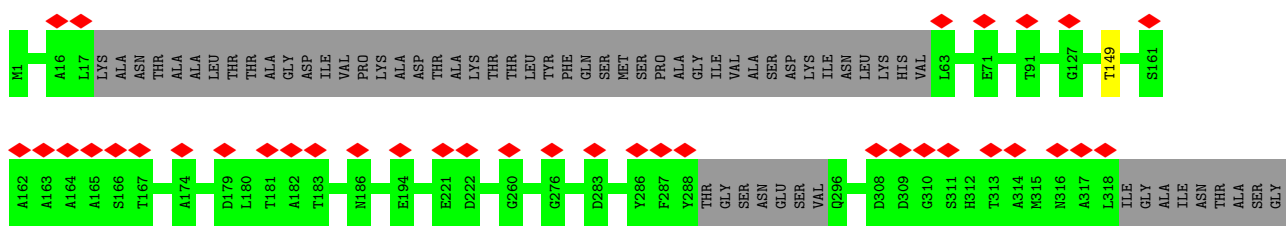
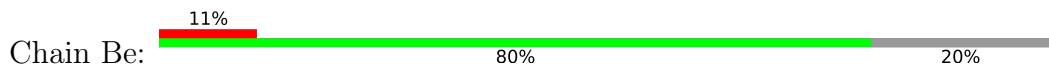




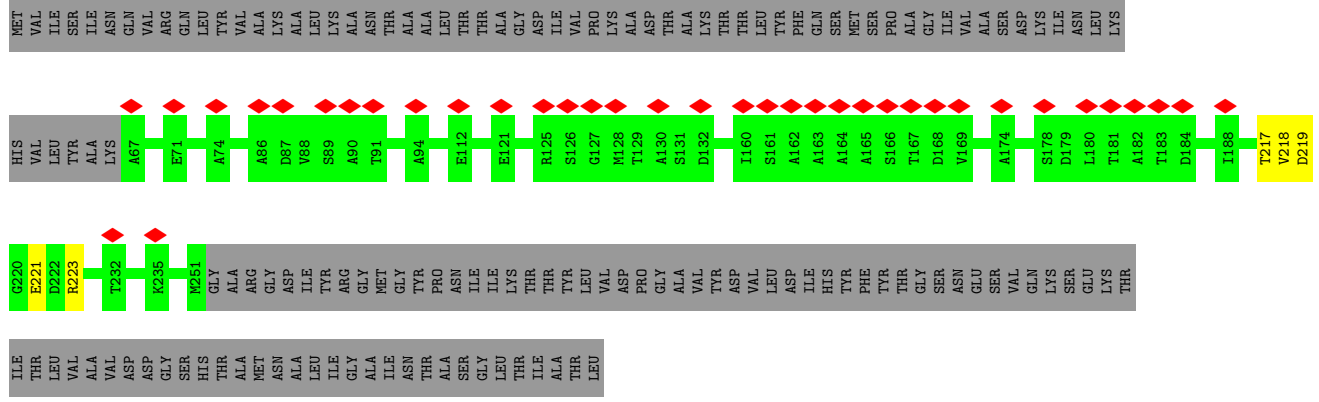
• Molecule 2: Auxiliary capsid protein gp36



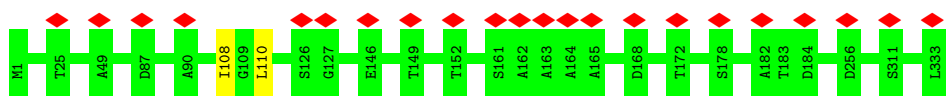
• Molecule 2: Auxiliary capsid protein gp36



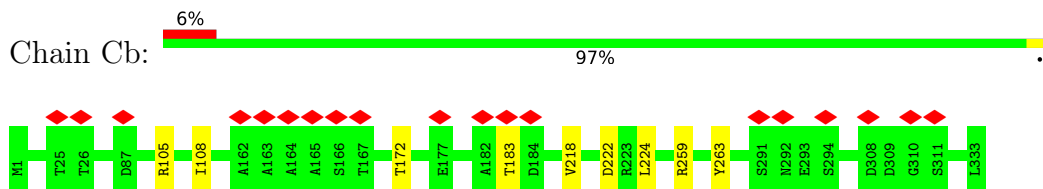
• Molecule 2: Auxiliary capsid protein gp36



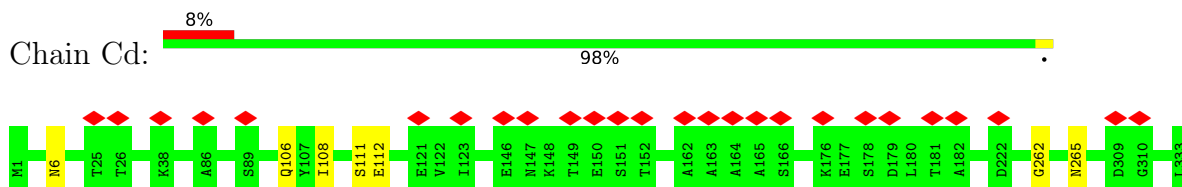
• Molecule 2: Auxiliary capsid protein gp36



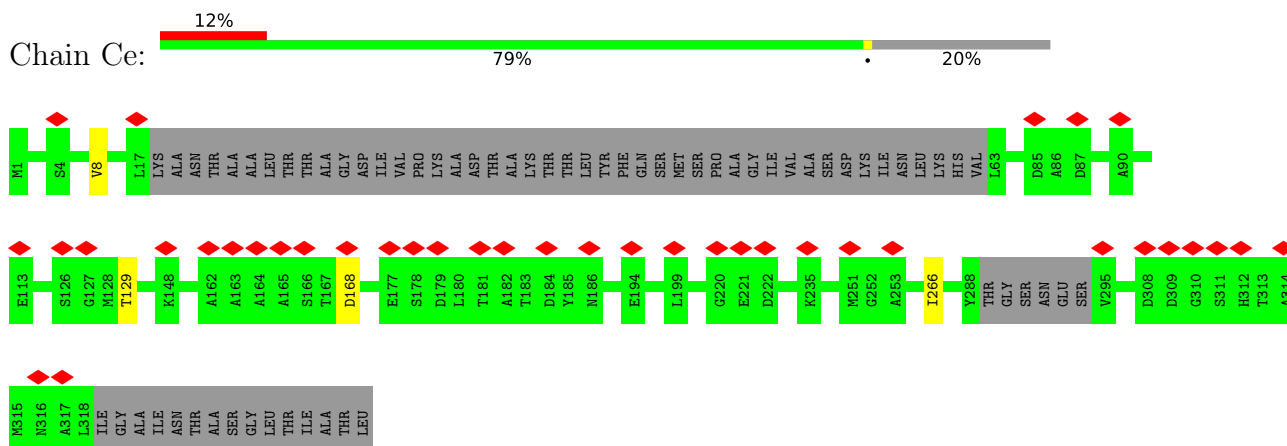
• Molecule 2: Auxiliary capsid protein gp36



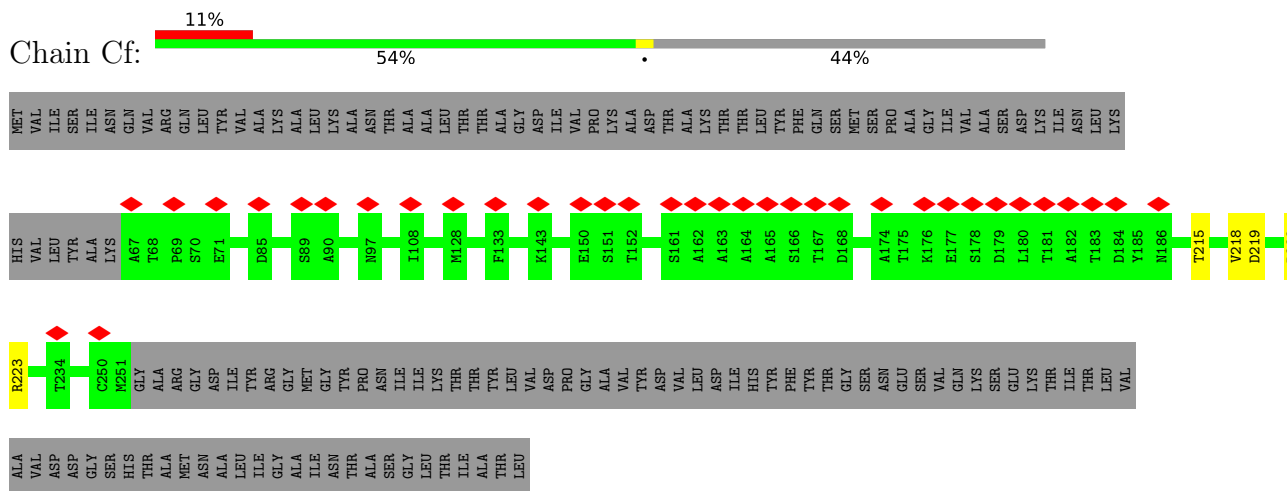
• Molecule 2: Auxiliary capsid protein gp36



• Molecule 2: Auxiliary capsid protein gp36



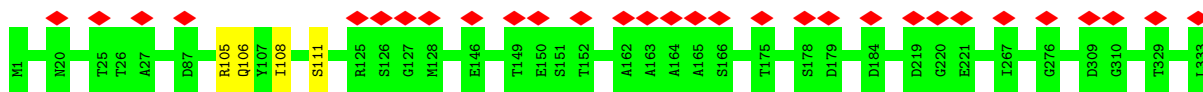
• Molecule 2: Auxiliary capsid protein gp36



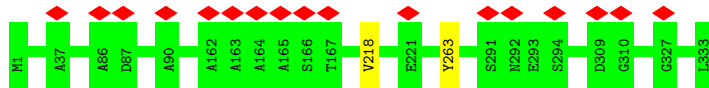
• Molecule 2: Auxiliary capsid protein gp36



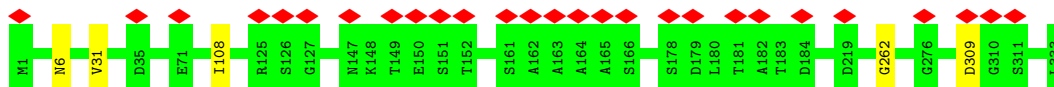




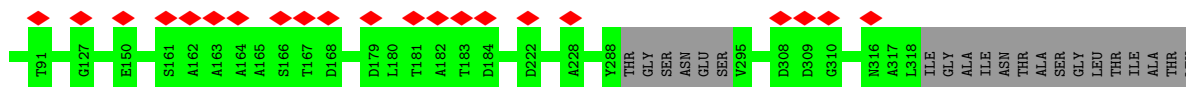
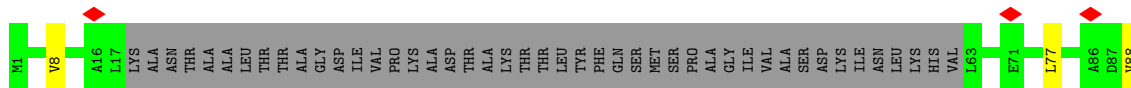
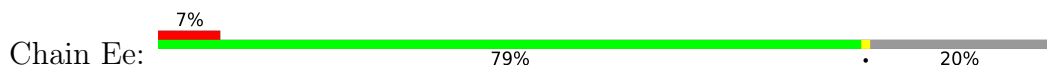
• Molecule 2: Auxiliary capsid protein gp36



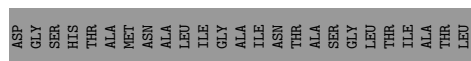
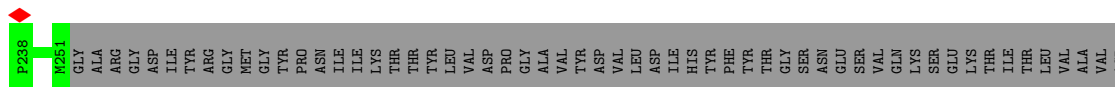
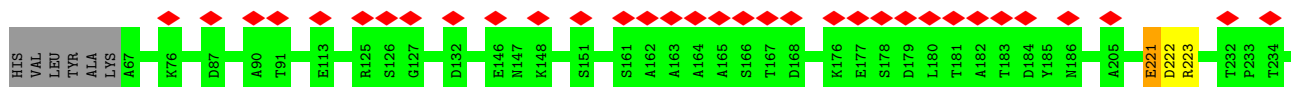
• Molecule 2: Auxiliary capsid protein gp36



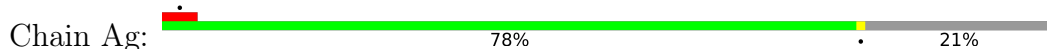
• Molecule 2: Auxiliary capsid protein gp36

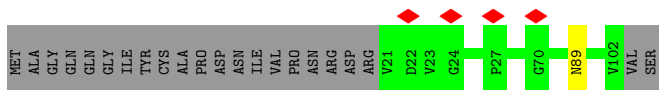


• Molecule 2: Auxiliary capsid protein gp36



• Molecule 3: Portal vertex capsid protein gp57

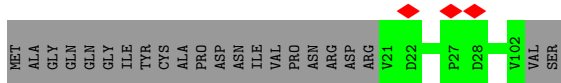
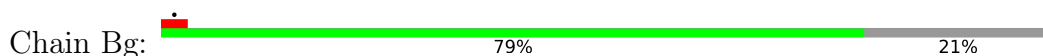




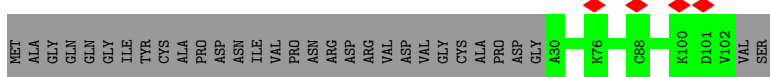
● Molecule 3: Portal vertex capsid protein gp57



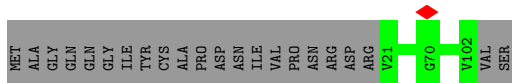
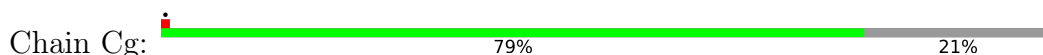
● Molecule 3: Portal vertex capsid protein gp57



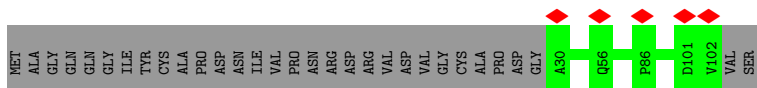
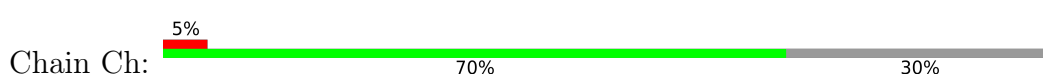
● Molecule 3: Portal vertex capsid protein gp57



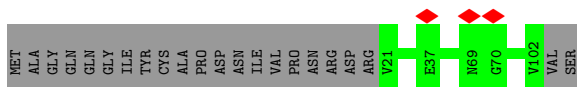
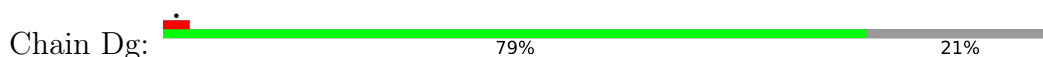
● Molecule 3: Portal vertex capsid protein gp57



● Molecule 3: Portal vertex capsid protein gp57



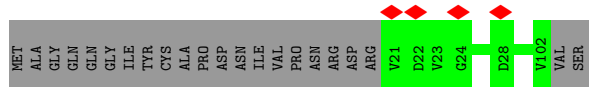
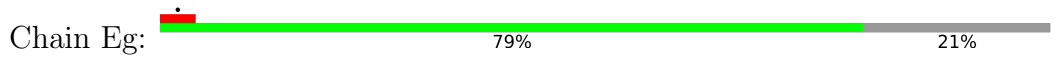
● Molecule 3: Portal vertex capsid protein gp57



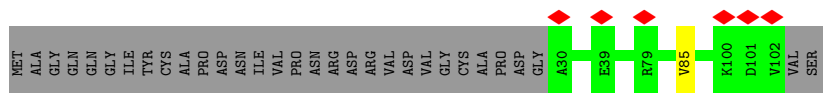
● Molecule 3: Portal vertex capsid protein gp57



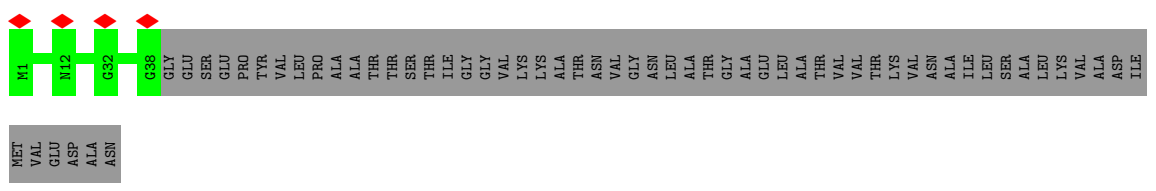
• Molecule 3: Portal vertex capsid protein gp57



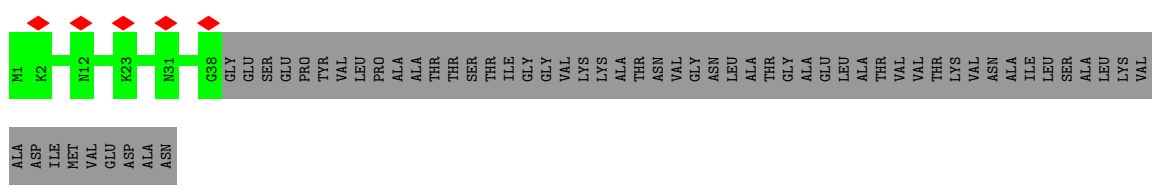
• Molecule 3: Portal vertex capsid protein gp57



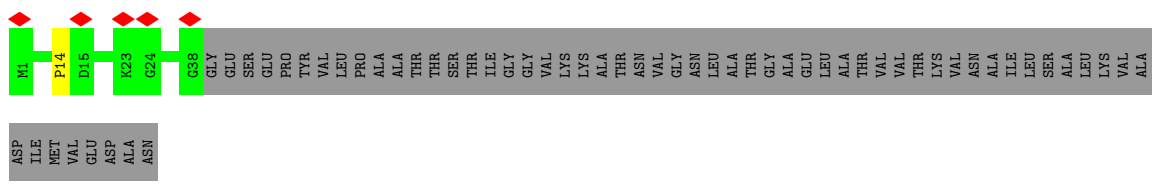
• Molecule 4: Head fiber trimer protein gp21



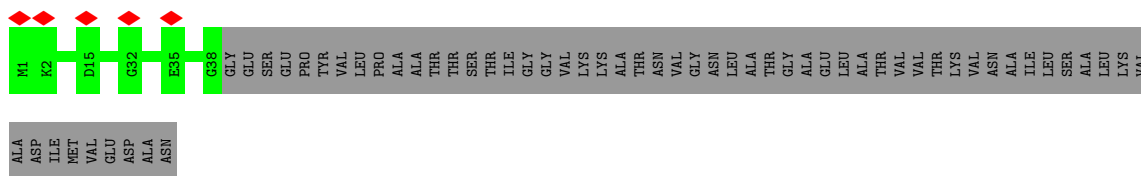
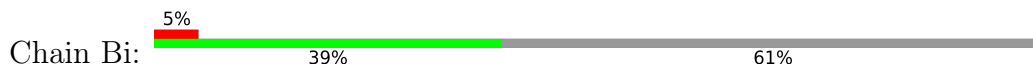
• Molecule 4: Head fiber trimer protein gp21



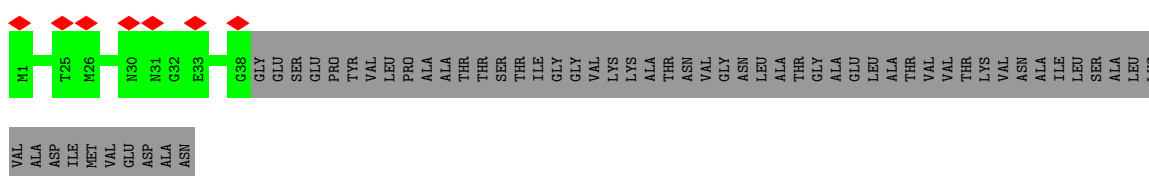
• Molecule 4: Head fiber trimer protein gp21



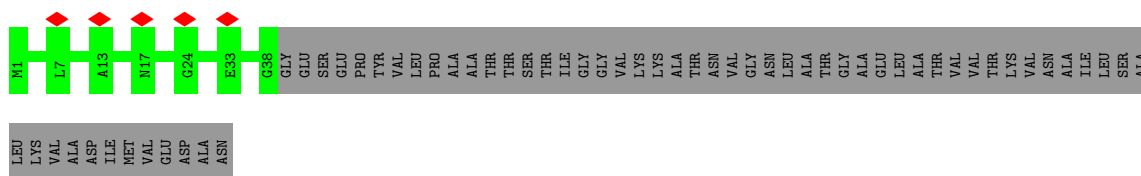
• Molecule 4: Head fiber trimer protein gp21



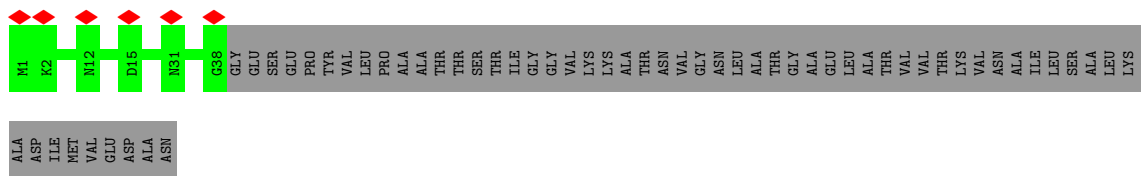
• Molecule 4: Head fiber trimer protein gp21



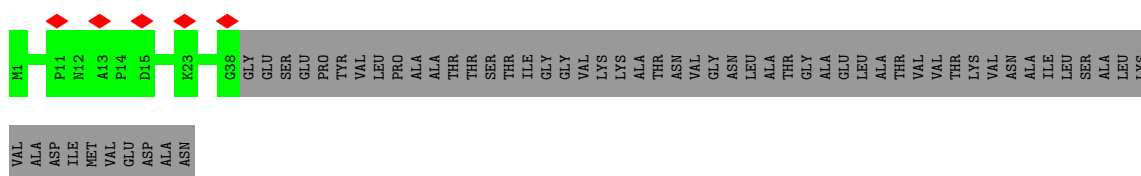
• Molecule 4: Head fiber trimer protein gp21



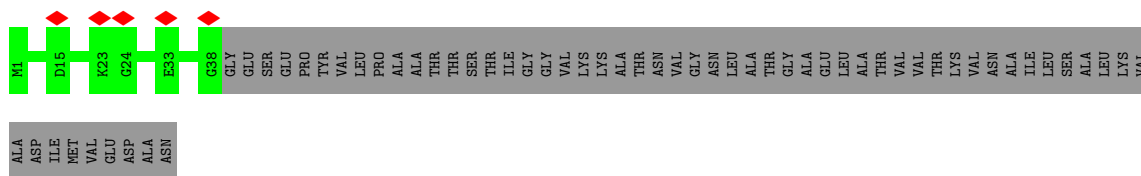
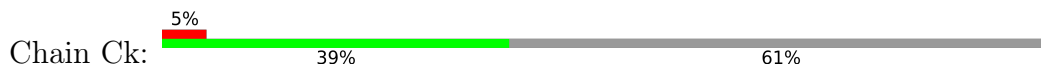
• Molecule 4: Head fiber trimer protein gp21



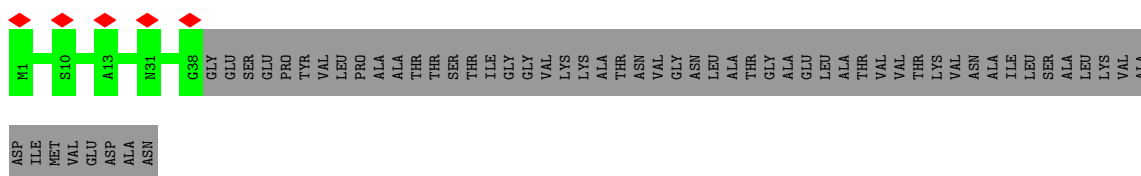
• Molecule 4: Head fiber trimer protein gp21



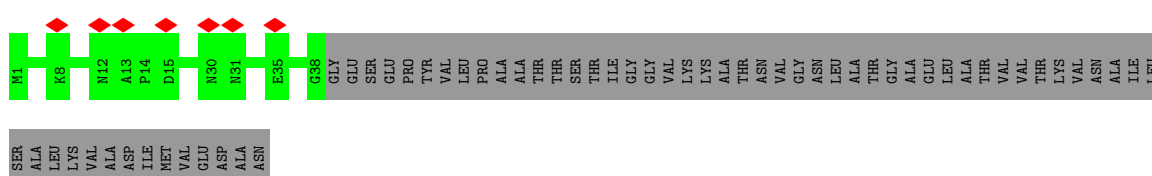
• Molecule 4: Head fiber trimer protein gp21



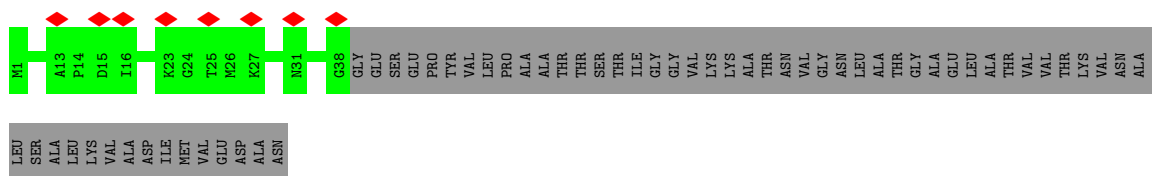
• Molecule 4: Head fiber trimer protein gp21



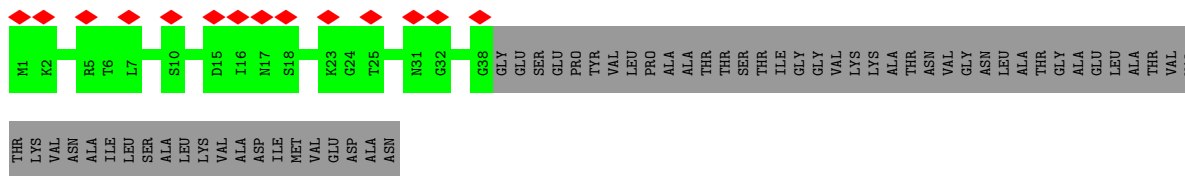
• Molecule 4: Head fiber trimer protein gp21



• Molecule 4: Head fiber trimer protein gp21

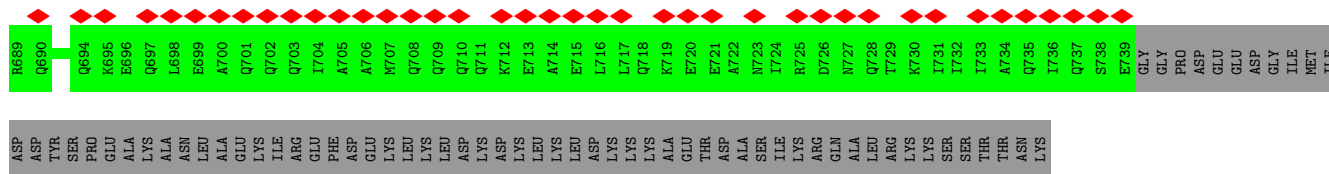


• Molecule 4: Head fiber trimer protein gp21

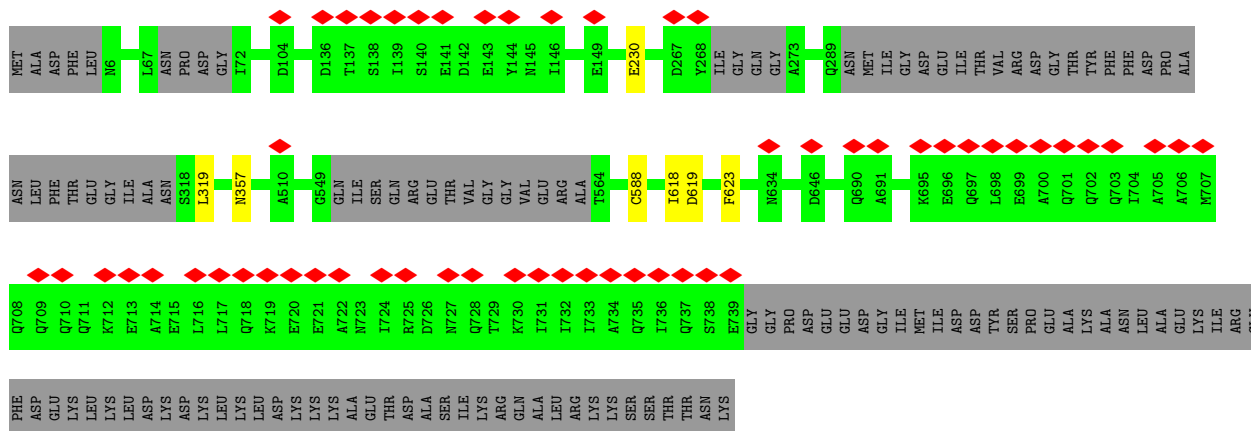
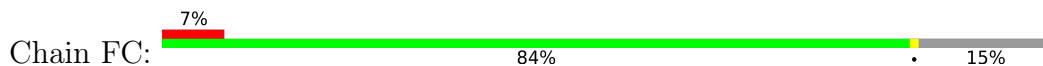




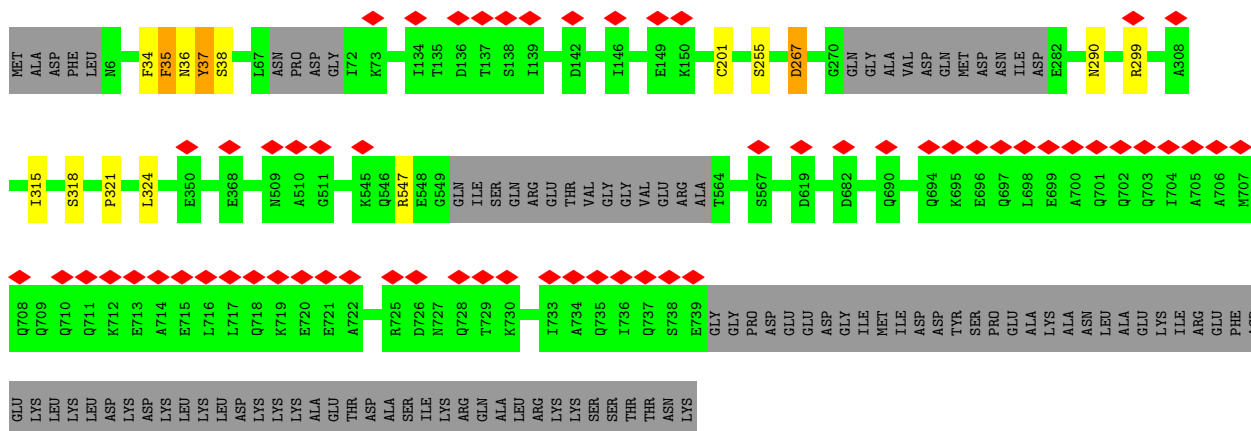
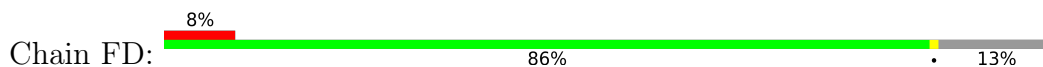




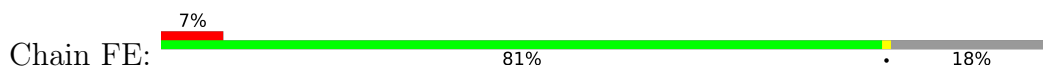
• Molecule 5: Portal protein gp20



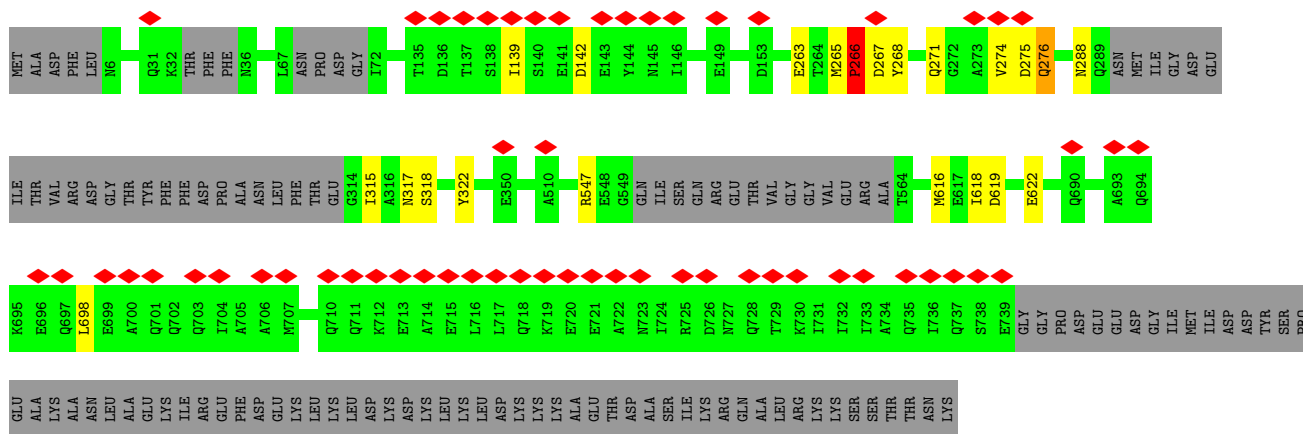
• Molecule 5: Portal protein gp20



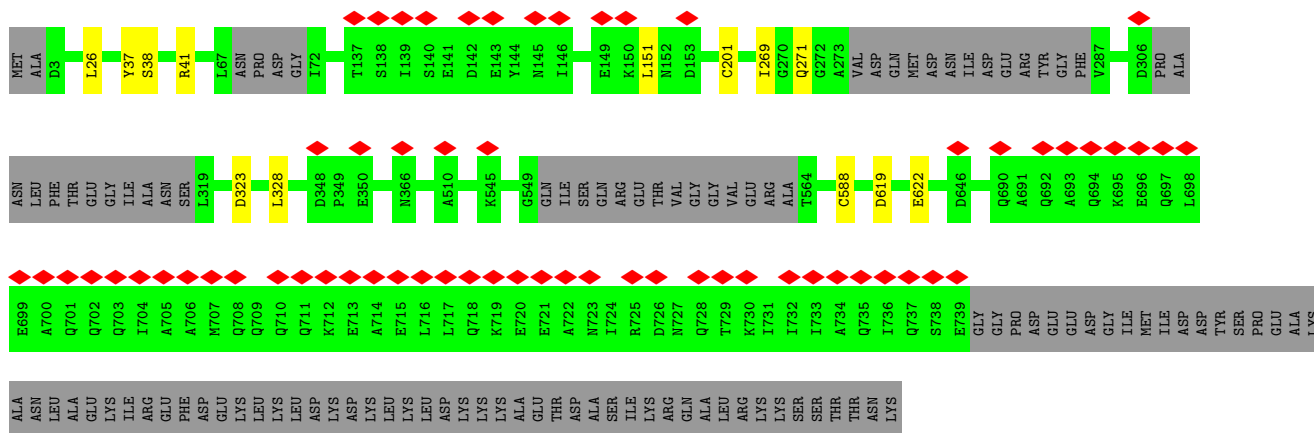
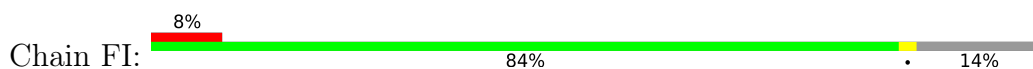
• Molecule 5: Portal protein gp20



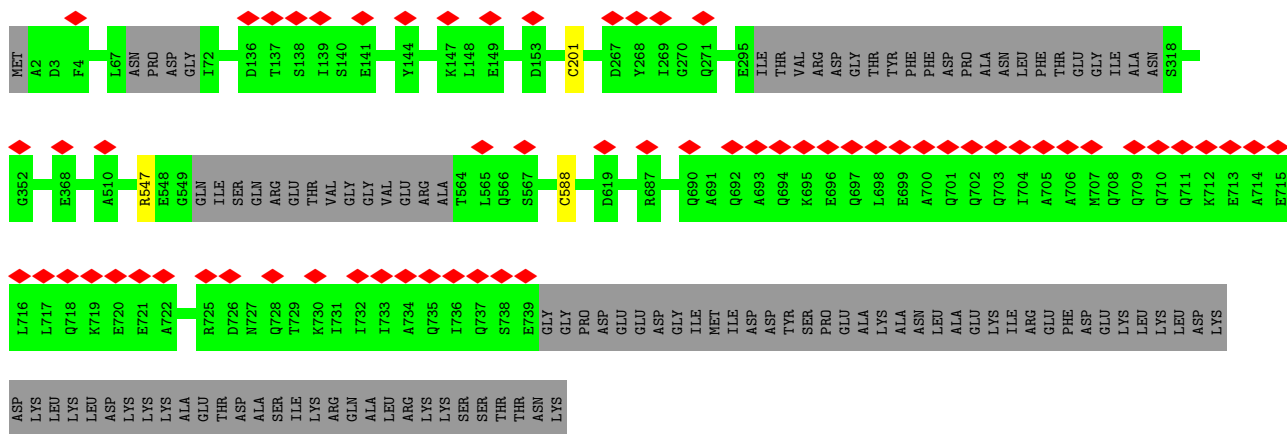
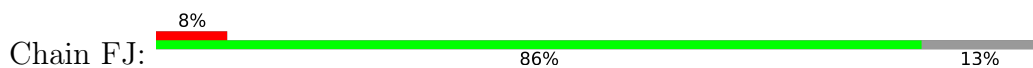




• Molecule 5: Portal protein gp20



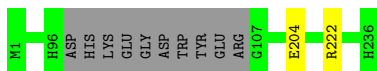
• Molecule 5: Portal protein gp20



• Molecule 5: Portal protein gp20

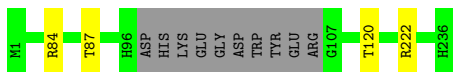


Chain FO:  95%  ..



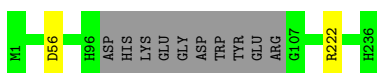
- Molecule 6: Ring protein 1 gp43

Chain FP:  94%  ..



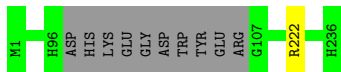
- Molecule 6: Ring protein 1 gp43

Chain FQ:  95%  ..



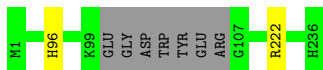
- Molecule 6: Ring protein 1 gp43

Chain FR:  95%  .



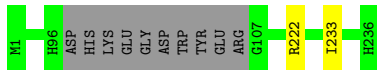
- Molecule 6: Ring protein 1 gp43

Chain FS:  96%  ..



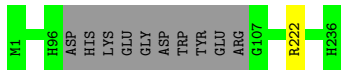
- Molecule 6: Ring protein 1 gp43

Chain FT:  95%  ..

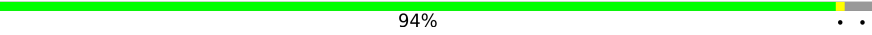


- Molecule 6: Ring protein 1 gp43

Chain FU:  95%  .



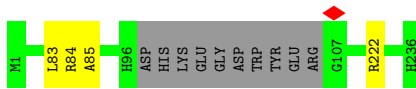
- Molecule 6: Ring protein 1 gp43

Chain FV:  94%



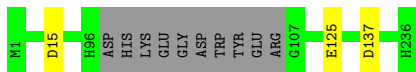
- Molecule 6: Ring protein 1 gp43

Chain FW:  94%



- Molecule 6: Ring protein 1 gp43

Chain FX:  94%



- Molecule 7: Ring protein 2 gp40

Chain FY:  100%



- Molecule 7: Ring protein 2 gp40

Chain FZ:  100%



- Molecule 7: Ring protein 2 gp40

Chain GA:  99%



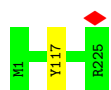
- Molecule 7: Ring protein 2 gp40

Chain GB:  100%



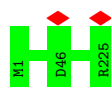
- Molecule 7: Ring protein 2 gp40

Chain GC:  100%



- Molecule 7: Ring protein 2 gp40

Chain GD:  100%




- Molecule 7: Ring protein 2 gp40

Chain GE:  99%



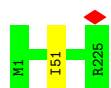
- Molecule 7: Ring protein 2 gp40

Chain GF:  100%



- Molecule 7: Ring protein 2 gp40

Chain GG:  100%



- Molecule 7: Ring protein 2 gp40

Chain GH:  100%



- Molecule 7: Ring protein 2 gp40

Chain GI:  99%











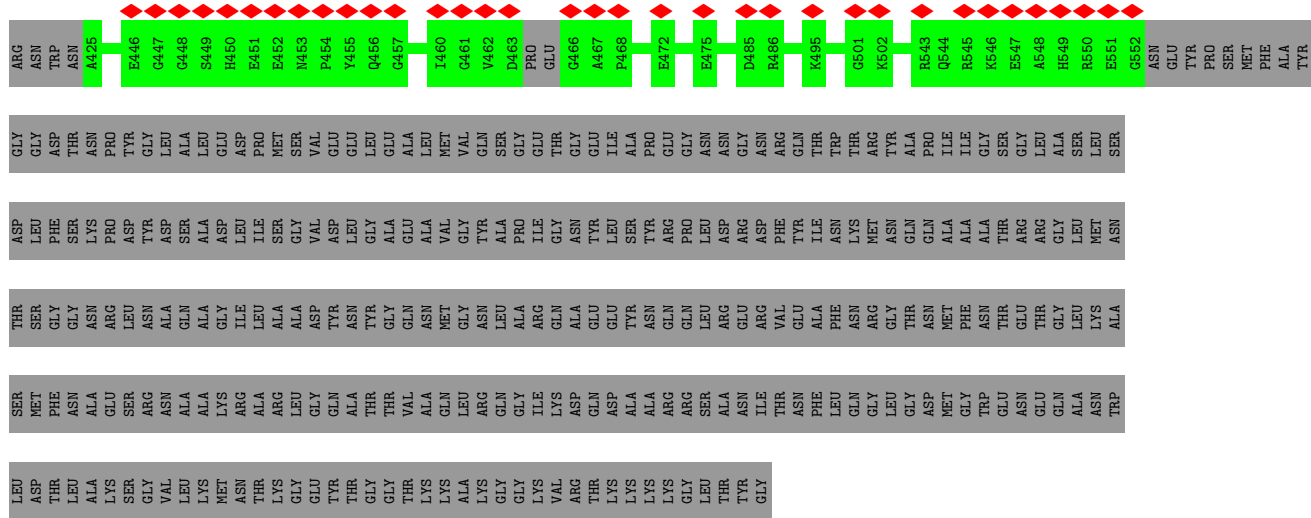




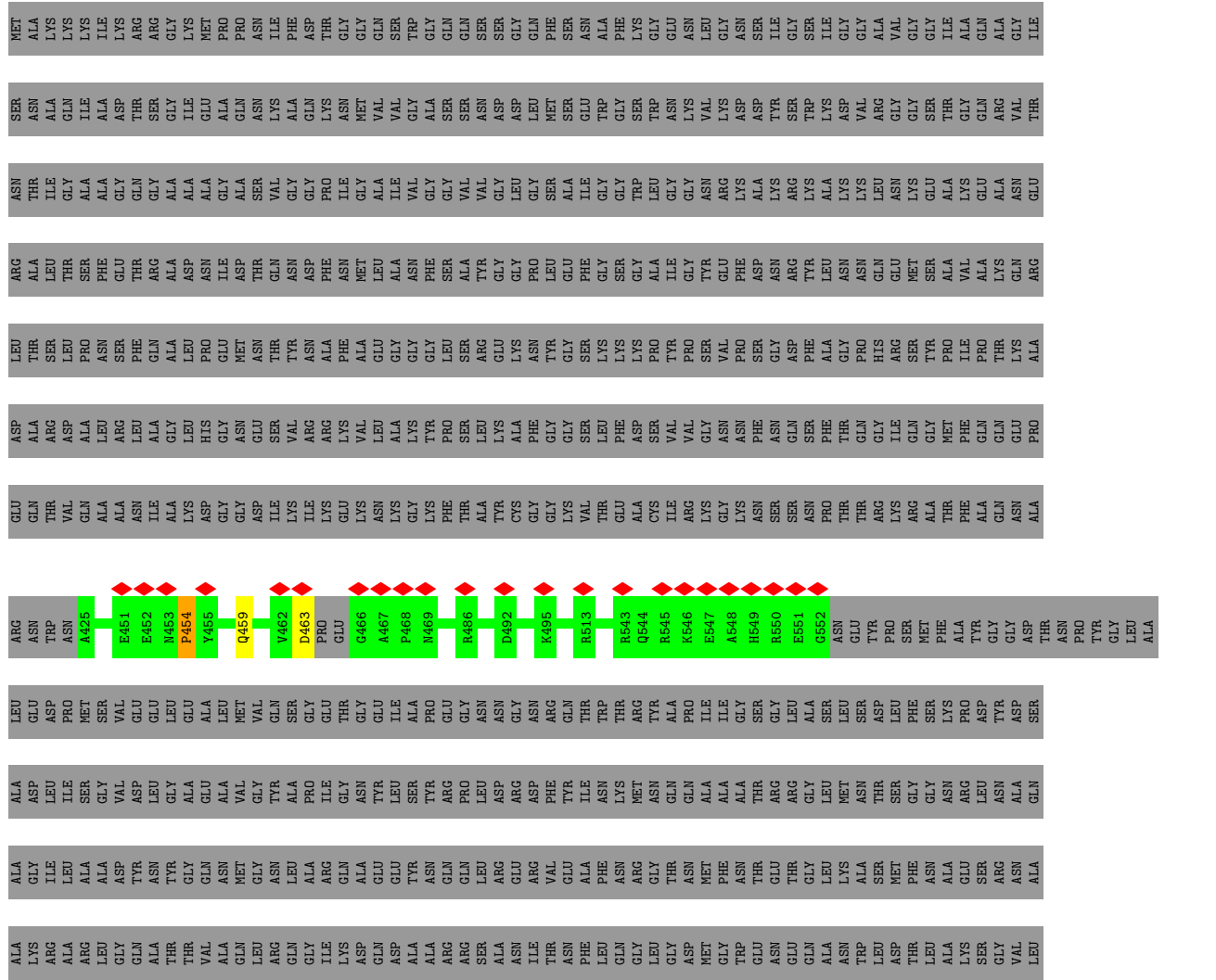








• Molecule 8: Cargo protein 1 gp45

























## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	122709	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	51	Depositor
Minimum defocus (nm)	300	Depositor
Maximum defocus (nm)	1500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.628	Depositor
Minimum map value	-0.478	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.036	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	398.71204, 398.71204, 398.71204	wwPDB
Map dimensions	286, 286, 286	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.394098, 1.394098, 1.394098	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

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

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	AA	0.30	0/3950	0.54	1/5346 (0.0%)
1	AB	0.31	0/4106	0.53	1/5553 (0.0%)
1	AC	0.33	0/4106	0.54	0/5553
1	AD	0.32	0/3732	0.54	1/5044 (0.0%)
1	AE	0.31	0/4106	0.53	0/5553
1	AF	0.31	0/4106	0.53	0/5553
1	BA	0.31	0/3957	0.53	0/5356
1	BB	0.31	0/4106	0.52	0/5553
1	BC	0.34	0/4106	0.56	0/5553
1	BD	0.33	0/3732	0.54	0/5044
1	BE	0.30	0/4106	0.52	0/5553
1	BF	0.29	0/4106	0.52	0/5553
1	CA	0.31	0/3944	0.52	1/5338 (0.0%)
1	CB	0.32	0/4106	0.54	0/5553
1	CC	0.35	0/4106	0.56	2/5553 (0.0%)
1	CD	0.32	0/3695	0.53	1/4995 (0.0%)
1	CE	0.30	0/4106	0.51	0/5553
1	CF	0.32	0/4106	0.57	2/5553 (0.0%)
1	DA	0.31	0/3957	0.53	1/5356 (0.0%)
1	DB	0.31	0/4106	0.53	0/5553
1	DC	0.33	0/4106	0.52	1/5553 (0.0%)
1	DD	0.32	0/3732	0.54	0/5044
1	DE	0.30	0/4106	0.52	0/5553
1	DF	0.30	0/4106	0.53	0/5553
1	EA	0.31	0/3957	0.53	1/5356 (0.0%)
1	EB	0.31	0/4106	0.51	0/5553
1	EC	0.36	0/4106	0.63	5/5553 (0.1%)
1	ED	0.32	0/3732	0.53	0/5044
1	EE	0.31	0/4106	0.54	1/5553 (0.0%)
1	EF	0.30	0/4106	0.53	0/5553
2	Aa	0.29	0/2591	0.54	0/3533
2	Ab	0.35	0/2591	0.58	1/3533 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
2	Ad	0.33	0/2591	0.57	1/3533 (0.0%)
2	Ae	0.29	0/2119	0.54	1/2887 (0.0%)
2	Af	0.30	0/1465	0.54	0/2001
2	Ba	0.30	0/2591	0.58	2/3533 (0.1%)
2	Bb	0.37	0/2591	0.61	2/3533 (0.1%)
2	Bd	0.32	0/2591	0.55	0/3533
2	Be	0.29	0/2112	0.53	0/2877
2	Bf	0.30	0/1465	0.55	0/2001
2	Ca	0.30	0/2591	0.56	1/3533 (0.0%)
2	Cb	0.35	0/2591	0.59	0/3533
2	Cd	0.32	0/2591	0.54	0/3533
2	Ce	0.29	0/2119	0.52	0/2887
2	Cf	0.31	0/1465	0.60	0/2001
2	Da	0.29	0/2591	0.55	0/3533
2	Db	0.35	1/2591 (0.0%)	0.57	0/3533
2	Dd	0.32	0/2591	0.56	0/3533
2	De	0.29	0/2119	0.53	0/2887
2	Df	0.30	0/1465	0.54	0/2001
2	Ea	0.31	0/2591	0.54	0/3533
2	Eb	0.34	0/2591	0.58	0/3533
2	Ed	0.33	0/2591	0.56	0/3533
2	Ee	0.29	0/2119	0.51	0/2887
2	Ef	0.31	0/1465	0.57	1/2001 (0.0%)
3	Ag	0.34	0/629	0.55	0/852
3	Ah	0.35	0/572	0.59	0/773
3	Bg	0.33	0/629	0.54	0/852
3	Bh	0.35	0/572	0.59	0/773
3	Cg	0.33	0/629	0.54	0/852
3	Ch	0.35	0/572	0.61	0/773
3	Dg	0.36	0/629	0.55	0/852
3	Dh	0.36	0/572	0.62	0/773
3	Eg	0.35	0/629	0.53	0/852
3	Eh	0.37	0/572	0.60	0/773
4	Ai	0.29	0/318	0.50	0/430
4	Aj	0.28	0/318	0.50	0/430
4	Ak	0.29	0/318	0.54	0/430
4	Bi	0.28	0/318	0.47	0/430
4	Bj	0.29	0/318	0.52	0/430
4	Bk	0.27	0/318	0.53	0/430
4	Ci	0.31	0/318	0.59	0/430
4	Cj	0.28	0/318	0.52	0/430
4	Ck	0.33	0/318	0.62	0/430
4	Di	0.31	0/318	0.54	0/430

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
4	Dj	0.28	0/318	0.52	0/430
4	Dk	0.27	0/318	0.54	0/430
4	Ei	0.27	0/318	0.50	0/430
4	Ej	0.30	0/318	0.54	0/430
4	Ek	0.29	0/318	0.53	0/430
5	FA	0.41	0/5718	0.61	3/7713 (0.0%)
5	FB	0.40	0/5646	0.57	0/7616
5	FC	0.41	0/5700	0.58	2/7690 (0.0%)
5	FD	0.44	2/5868 (0.0%)	0.65	6/7920 (0.1%)
5	FE	0.40	0/5500	0.60	3/7419 (0.0%)
5	FF	0.40	0/5697	0.58	3/7687 (0.0%)
5	FG	0.40	0/5670	0.60	3/7645 (0.0%)
5	FH	0.43	0/5719	0.64	4/7715 (0.1%)
5	FI	0.43	0/5776	0.64	5/7793 (0.1%)
5	FJ	0.40	0/5804	0.57	0/7831
5	FK	0.40	0/5581	0.57	0/7531
5	FL	0.41	0/5664	0.60	2/7640 (0.0%)
6	FM	0.45	0/1881	0.60	1/2548 (0.0%)
6	FN	0.41	0/1881	0.64	2/2548 (0.1%)
6	FO	0.43	0/1881	0.56	0/2548
6	FP	0.45	0/1881	0.61	0/2548
6	FQ	0.42	0/1881	0.57	0/2548
6	FR	0.40	0/1881	0.56	0/2548
6	FS	0.42	0/1909	0.57	0/2585
6	FT	0.41	0/1881	0.59	0/2548
6	FU	0.41	0/1881	0.55	0/2548
6	FV	0.46	0/1881	0.61	1/2548 (0.0%)
6	FW	0.44	0/1881	0.61	1/2548 (0.0%)
6	FX	0.42	0/1881	0.54	0/2548
7	FY	0.44	0/1886	0.57	0/2552
7	FZ	0.45	0/1886	0.55	0/2552
7	GA	0.43	0/1886	0.54	0/2552
7	GB	0.43	0/1886	0.55	0/2552
7	GC	0.43	0/1886	0.54	0/2552
7	GD	0.45	0/1886	0.55	0/2552
7	GE	0.44	0/1886	0.54	0/2552
7	GF	0.44	0/1886	0.55	0/2552
7	GG	0.47	0/1886	0.55	0/2552
7	GH	0.44	0/1886	0.55	0/2552
7	GI	0.46	0/1886	0.53	0/2552
7	GJ	0.45	0/1886	0.54	0/2552
8	GK	0.33	0/1003	0.59	0/1347
8	GL	0.31	0/1003	0.58	0/1347

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	GM	0.32	0/1003	0.59	0/1347
8	GN	0.32	0/1003	0.57	0/1347
8	GO	0.33	0/1003	0.60	0/1347
8	GP	0.33	0/1003	0.59	0/1347
8	GQ	0.34	0/1003	0.61	0/1347
8	GR	0.32	0/1003	0.59	0/1347
8	GS	0.31	0/1003	0.56	0/1347
8	GT	0.32	0/1003	0.59	0/1347
8	GU	0.32	0/1003	0.59	0/1347
8	GV	0.34	0/1003	0.61	1/1347 (0.1%)
8	IK	0.34	0/255	0.58	0/342
8	IL	0.34	0/255	0.53	0/342
8	IM	0.32	0/255	0.53	0/342
8	IN	0.32	0/255	0.58	0/342
8	IO	0.32	0/255	0.56	0/342
8	IP	0.31	0/255	0.54	0/342
8	IQ	0.32	0/255	0.53	0/342
8	IR	0.32	0/255	0.54	0/342
8	IS	0.57	1/255 (0.4%)	0.84	2/342 (0.6%)
8	IT	0.29	0/255	0.53	0/342
8	IU	0.32	0/255	0.55	0/342
8	IV	0.30	0/255	0.50	0/342
All	All	0.36	4/316732 (0.0%)	0.56	66/428688 (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
1	BF	0	1
2	Ab	0	1
2	Ad	0	2
2	Bb	0	2
2	Bd	0	1
2	Cb	0	1
2	Cd	0	2
2	Db	0	1
2	Dd	0	1
2	Eb	0	1
2	Ed	0	2
3	Ah	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	Eh	0	1
6	FS	0	1
All	All	0	18

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	IS	243	SER	CA-CB	-5.64	1.44	1.52
5	FD	38	SER	CA-CB	-5.61	1.44	1.52
5	FD	255	SER	CA-CB	-5.32	1.45	1.52
2	Db	111	SER	CA-CB	-5.03	1.45	1.52

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	EC	66	ASP	CB-CA-C	-11.62	87.17	110.40
6	FN	95	THR	CB-CA-C	-11.40	80.82	111.60
5	FD	37	TYR	CB-CA-C	10.73	131.86	110.40
1	EC	67	ASP	CB-CA-C	10.19	130.77	110.40
5	FE	266	PRO	N-CA-C	10.03	138.19	112.10
5	FH	266	PRO	CA-N-CD	-9.30	98.48	111.50
5	FA	621	ASP	CB-CA-C	-9.12	92.16	110.40
5	FG	282	GLU	CB-CA-C	-8.83	92.73	110.40
2	Ba	107	TYR	CB-CA-C	8.72	127.84	110.40
5	FD	35	PHE	CB-CA-C	8.63	127.66	110.40
2	Ad	112	GLU	CB-CA-C	8.32	127.03	110.40
5	FA	619	ASP	CB-CA-C	-8.30	93.79	110.40
1	EC	106	THR	C-N-CA	8.09	141.92	121.70
5	FL	324	LEU	CA-CB-CG	7.89	133.44	115.30
5	FD	36	ASN	CB-CA-C	7.44	125.28	110.40
5	FI	323	ASP	CB-CA-C	-7.12	96.16	110.40
5	FF	319	LEU	CA-CB-CG	7.06	131.53	115.30
5	FD	34	PHE	N-CA-C	-7.04	91.98	111.00
6	FW	85	ALA	N-CA-CB	-6.97	100.34	110.10
1	AA	129	ASN	CB-CA-C	-6.79	96.82	110.40
1	EC	444	LYS	CB-CA-C	6.71	123.82	110.40
1	CF	129	ASN	CB-CA-C	-6.68	97.04	110.40
1	CF	434	ASP	CB-CG-OD1	6.65	124.29	118.30
6	FN	94	PRO	N-CA-CB	-6.62	95.31	102.60
8	IS	245	PRO	CB-CA-C	-6.56	95.60	112.00
8	IS	245	PRO	N-CA-CB	-6.55	95.39	102.60
5	FI	26	LEU	CB-CG-CD1	-6.49	99.96	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	FI	269	ILE	N-CA-C	-6.41	93.70	111.00
1	CC	106	THR	C-N-CA	6.18	137.15	121.70
1	EA	137	LEU	CA-CB-CG	6.04	129.19	115.30
5	FC	319	LEU	CA-CB-CG	6.00	129.11	115.30
1	DA	135	ARG	CB-CA-C	-5.92	98.55	110.40
2	Ae	242	LEU	CA-CB-CG	5.87	128.81	115.30
5	FD	34	PHE	CB-CA-C	-5.84	98.72	110.40
5	FG	283	ARG	CB-CA-C	5.84	122.08	110.40
1	DC	106	THR	C-N-CA	5.73	136.03	121.70
5	FI	271	GLN	CB-CA-C	5.71	121.82	110.40
2	Bb	112	GLU	CB-CA-C	5.67	121.75	110.40
1	EC	445	GLY	N-CA-C	-5.57	99.17	113.10
2	Ca	110	LEU	C-N-CA	-5.54	107.85	121.70
8	GV	454	PRO	CB-CA-C	-5.51	98.23	112.00
1	CD	4	LYS	CB-CA-C	-5.46	99.48	110.40
2	Ab	107	TYR	CB-CA-C	5.46	121.32	110.40
6	FM	85	ALA	N-CA-CB	-5.45	102.47	110.10
5	FH	322	TYR	CB-CA-C	5.43	121.25	110.40
2	Ef	221	GLU	CB-CA-C	5.39	121.18	110.40
1	AD	52	LEU	CA-CB-CG	5.36	127.63	115.30
5	FH	698	LEU	CA-CB-CG	5.28	127.44	115.30
5	FC	623	PHE	CB-CA-C	5.26	120.93	110.40
1	AB	89	ASP	CB-CG-OD1	5.26	123.03	118.30
1	CA	330	LEU	CA-CB-CG	5.23	127.33	115.30
5	FH	266	PRO	N-CA-CB	-5.21	96.86	102.60
6	FV	84	ARG	CB-CA-C	-5.20	100.00	110.40
5	FL	623	PHE	CB-CA-C	5.18	120.76	110.40
5	FF	206	GLY	C-N-CA	5.17	134.63	121.70
1	EE	88	ARG	CB-CA-C	5.15	120.71	110.40
5	FA	223	SER	N-CA-C	-5.14	97.13	111.00
5	FF	717	LEU	CA-CB-CG	5.14	127.11	115.30
5	FE	267	ASP	CB-CA-C	-5.11	100.18	110.40
2	Bb	222	ASP	CB-CA-C	5.07	120.54	110.40
5	FD	321	PRO	CB-CA-C	-5.07	99.33	112.00
5	FE	574	LEU	CA-CB-CG	5.06	126.94	115.30
5	FG	284	TYR	N-CA-C	-5.02	97.44	111.00
1	CC	5	LEU	CA-CB-CG	5.02	126.85	115.30
2	Ba	145	LEU	CB-CG-CD2	-5.01	102.49	111.00
5	FI	151	LEU	CA-CB-CG	5.00	126.81	115.30

There are no chirality outliers.

All (18) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	Ab	263	TYR	Peptide
2	Ad	262	GLY	Peptide
2	Ad	6	ASN	Peptide
3	Ah	85	VAL	Peptide
1	BF	128	LEU	Peptide
2	Bb	263	TYR	Peptide
2	Bb	296	GLN	Peptide
2	Bd	262	GLY	Peptide
2	Cb	263	TYR	Peptide
2	Cd	262	GLY	Peptide
2	Cd	6	ASN	Peptide
2	Db	263	TYR	Peptide
2	Dd	262	GLY	Peptide
2	Eb	263	TYR	Peptide
2	Ed	262	GLY	Peptide
2	Ed	6	ASN	Peptide
3	Eh	85	VAL	Peptide
6	FS	96	HIS	Peptide

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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	AA	482/504 (96%)	466 (97%)	16 (3%)	0	100	100
1	AB	501/504 (99%)	479 (96%)	22 (4%)	0	100	100
1	AC	501/504 (99%)	484 (97%)	17 (3%)	0	100	100
1	AD	446/504 (88%)	426 (96%)	20 (4%)	0	100	100
1	AE	501/504 (99%)	488 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	AF	501/504 (99%)	485 (97%)	16 (3%)	0	100	100
1	BA	483/504 (96%)	472 (98%)	11 (2%)	0	100	100
1	BB	501/504 (99%)	478 (95%)	23 (5%)	0	100	100
1	BC	501/504 (99%)	482 (96%)	19 (4%)	0	100	100
1	BD	446/504 (88%)	427 (96%)	19 (4%)	0	100	100
1	BE	501/504 (99%)	488 (97%)	13 (3%)	0	100	100
1	BF	501/504 (99%)	481 (96%)	20 (4%)	0	100	100
1	CA	481/504 (95%)	473 (98%)	8 (2%)	0	100	100
1	CB	501/504 (99%)	478 (95%)	23 (5%)	0	100	100
1	CC	501/504 (99%)	480 (96%)	21 (4%)	0	100	100
1	CD	441/504 (88%)	421 (96%)	20 (4%)	0	100	100
1	CE	501/504 (99%)	486 (97%)	15 (3%)	0	100	100
1	CF	501/504 (99%)	482 (96%)	18 (4%)	1 (0%)	47	79
1	DA	483/504 (96%)	469 (97%)	13 (3%)	1 (0%)	47	79
1	DB	501/504 (99%)	476 (95%)	25 (5%)	0	100	100
1	DC	501/504 (99%)	486 (97%)	15 (3%)	0	100	100
1	DD	446/504 (88%)	426 (96%)	20 (4%)	0	100	100
1	DE	501/504 (99%)	482 (96%)	19 (4%)	0	100	100
1	DF	501/504 (99%)	485 (97%)	16 (3%)	0	100	100
1	EA	483/504 (96%)	467 (97%)	16 (3%)	0	100	100
1	EB	501/504 (99%)	482 (96%)	19 (4%)	0	100	100
1	EC	501/504 (99%)	474 (95%)	27 (5%)	0	100	100
1	ED	446/504 (88%)	427 (96%)	19 (4%)	0	100	100
1	EE	501/504 (99%)	486 (97%)	15 (3%)	0	100	100
1	EF	501/504 (99%)	483 (96%)	18 (4%)	0	100	100
2	Aa	331/333 (99%)	315 (95%)	16 (5%)	0	100	100
2	Ab	331/333 (99%)	308 (93%)	23 (7%)	0	100	100
2	Ad	331/333 (99%)	313 (95%)	18 (5%)	0	100	100
2	Ae	261/333 (78%)	248 (95%)	13 (5%)	0	100	100
2	Af	183/333 (55%)	175 (96%)	8 (4%)	0	100	100
2	Ba	331/333 (99%)	310 (94%)	21 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	Bb	331/333 (99%)	313 (95%)	17 (5%)	1 (0%)	41	74
2	Bd	331/333 (99%)	309 (93%)	22 (7%)	0	100	100
2	Be	260/333 (78%)	249 (96%)	11 (4%)	0	100	100
2	Bf	183/333 (55%)	173 (94%)	10 (6%)	0	100	100
2	Ca	331/333 (99%)	315 (95%)	16 (5%)	0	100	100
2	Cb	331/333 (99%)	311 (94%)	20 (6%)	0	100	100
2	Cd	331/333 (99%)	311 (94%)	20 (6%)	0	100	100
2	Ce	261/333 (78%)	247 (95%)	14 (5%)	0	100	100
2	Cf	183/333 (55%)	174 (95%)	9 (5%)	0	100	100
2	Da	331/333 (99%)	313 (95%)	18 (5%)	0	100	100
2	Db	331/333 (99%)	313 (95%)	18 (5%)	0	100	100
2	Dd	331/333 (99%)	316 (96%)	15 (4%)	0	100	100
2	De	261/333 (78%)	249 (95%)	12 (5%)	0	100	100
2	Df	183/333 (55%)	174 (95%)	9 (5%)	0	100	100
2	Ea	331/333 (99%)	314 (95%)	17 (5%)	0	100	100
2	Eb	331/333 (99%)	308 (93%)	23 (7%)	0	100	100
2	Ed	331/333 (99%)	315 (95%)	16 (5%)	0	100	100
2	Ee	261/333 (78%)	247 (95%)	14 (5%)	0	100	100
2	Ef	183/333 (55%)	171 (93%)	12 (7%)	0	100	100
3	Ag	80/104 (77%)	76 (95%)	4 (5%)	0	100	100
3	Ah	71/104 (68%)	64 (90%)	7 (10%)	0	100	100
3	Bg	80/104 (77%)	75 (94%)	5 (6%)	0	100	100
3	Bh	71/104 (68%)	67 (94%)	4 (6%)	0	100	100
3	Cg	80/104 (77%)	77 (96%)	3 (4%)	0	100	100
3	Ch	71/104 (68%)	66 (93%)	5 (7%)	0	100	100
3	Dg	80/104 (77%)	76 (95%)	4 (5%)	0	100	100
3	Dh	71/104 (68%)	67 (94%)	4 (6%)	0	100	100
3	Eg	80/104 (77%)	77 (96%)	3 (4%)	0	100	100
3	Eh	71/104 (68%)	66 (93%)	5 (7%)	0	100	100
4	Ai	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Aj	36/97 (37%)	34 (94%)	2 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	Ak	36/97 (37%)	32 (89%)	3 (8%)	1 (3%)	5	34
4	Bi	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Bj	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Bk	36/97 (37%)	34 (94%)	2 (6%)	0	100	100
4	Ci	36/97 (37%)	34 (94%)	2 (6%)	0	100	100
4	Cj	36/97 (37%)	34 (94%)	2 (6%)	0	100	100
4	Ck	36/97 (37%)	31 (86%)	5 (14%)	0	100	100
4	Di	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Dj	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Dk	36/97 (37%)	33 (92%)	3 (8%)	0	100	100
4	Ei	36/97 (37%)	34 (94%)	2 (6%)	0	100	100
4	Ej	36/97 (37%)	35 (97%)	1 (3%)	0	100	100
4	Ek	36/97 (37%)	33 (92%)	3 (8%)	0	100	100
5	FA	678/806 (84%)	657 (97%)	21 (3%)	0	100	100
5	FB	666/806 (83%)	647 (97%)	19 (3%)	0	100	100
5	FC	674/806 (84%)	658 (98%)	16 (2%)	0	100	100
5	FD	697/806 (86%)	662 (95%)	34 (5%)	1 (0%)	51	83
5	FE	652/806 (81%)	634 (97%)	18 (3%)	0	100	100
5	FF	676/806 (84%)	658 (97%)	18 (3%)	0	100	100
5	FG	668/806 (83%)	643 (96%)	25 (4%)	0	100	100
5	FH	679/806 (84%)	656 (97%)	21 (3%)	2 (0%)	41	74
5	FI	684/806 (85%)	669 (98%)	15 (2%)	0	100	100
5	FJ	690/806 (86%)	672 (97%)	18 (3%)	0	100	100
5	FK	661/806 (82%)	636 (96%)	25 (4%)	0	100	100
5	FL	669/806 (83%)	645 (96%)	24 (4%)	0	100	100
6	FM	222/236 (94%)	215 (97%)	7 (3%)	0	100	100
6	FN	222/236 (94%)	208 (94%)	14 (6%)	0	100	100
6	FO	222/236 (94%)	211 (95%)	11 (5%)	0	100	100
6	FP	222/236 (94%)	212 (96%)	10 (4%)	0	100	100
6	FQ	222/236 (94%)	208 (94%)	14 (6%)	0	100	100
6	FR	222/236 (94%)	209 (94%)	13 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	FS	225/236 (95%)	214 (95%)	11 (5%)	0	100	100
6	FT	222/236 (94%)	211 (95%)	11 (5%)	0	100	100
6	FU	222/236 (94%)	210 (95%)	12 (5%)	0	100	100
6	FV	222/236 (94%)	213 (96%)	9 (4%)	0	100	100
6	FW	222/236 (94%)	210 (95%)	12 (5%)	0	100	100
6	FX	222/236 (94%)	214 (96%)	8 (4%)	0	100	100
7	FY	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
7	FZ	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
7	GA	223/225 (99%)	210 (94%)	13 (6%)	0	100	100
7	GB	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
7	GC	223/225 (99%)	217 (97%)	6 (3%)	0	100	100
7	GD	223/225 (99%)	219 (98%)	4 (2%)	0	100	100
7	GE	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
7	GF	223/225 (99%)	214 (96%)	9 (4%)	0	100	100
7	GG	223/225 (99%)	216 (97%)	7 (3%)	0	100	100
7	GH	223/225 (99%)	213 (96%)	10 (4%)	0	100	100
7	GI	223/225 (99%)	217 (97%)	6 (3%)	0	100	100
7	GJ	223/225 (99%)	210 (94%)	13 (6%)	0	100	100
8	GK	122/842 (14%)	117 (96%)	5 (4%)	0	100	100
8	GL	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GM	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GN	122/842 (14%)	112 (92%)	10 (8%)	0	100	100
8	GO	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GP	122/842 (14%)	120 (98%)	1 (1%)	1 (1%)	19	58
8	GQ	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GR	122/842 (14%)	112 (92%)	10 (8%)	0	100	100
8	GS	122/842 (14%)	117 (96%)	5 (4%)	0	100	100
8	GT	122/842 (14%)	116 (95%)	6 (5%)	0	100	100
8	GU	122/842 (14%)	114 (93%)	8 (7%)	0	100	100
8	GV	122/842 (14%)	115 (94%)	7 (6%)	0	100	100
8	IK	30/842 (4%)	25 (83%)	5 (17%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	IL	30/842 (4%)	29 (97%)	1 (3%)	0	100	100
8	IM	30/842 (4%)	25 (83%)	5 (17%)	0	100	100
8	IN	30/842 (4%)	27 (90%)	3 (10%)	0	100	100
8	IO	30/842 (4%)	26 (87%)	4 (13%)	0	100	100
8	IP	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
8	IQ	30/842 (4%)	26 (87%)	4 (13%)	0	100	100
8	IR	30/842 (4%)	27 (90%)	3 (10%)	0	100	100
8	IS	30/842 (4%)	29 (97%)	1 (3%)	0	100	100
8	IT	30/842 (4%)	28 (93%)	2 (7%)	0	100	100
8	IU	30/842 (4%)	27 (90%)	3 (10%)	0	100	100
8	IV	30/842 (4%)	27 (90%)	3 (10%)	0	100	100
All	All	38397/61352 (63%)	36786 (96%)	1603 (4%)	8 (0%)	100	100

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	CF	97	ALA
5	FH	266	PRO
5	FH	276	GLN
5	FD	267	ASP
2	Bb	107	TYR
8	GP	426	PHE
1	DA	133	PRO
4	Ak	14	PRO

### 5.3.2 Protein sidechains [i](#)

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	AA	412/427 (96%)	409 (99%)	3 (1%)	84	92
1	AB	426/427 (100%)	423 (99%)	3 (1%)	84	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	AC	426/427 (100%)	426 (100%)	0	100	100
1	AD	387/427 (91%)	387 (100%)	0	100	100
1	AE	426/427 (100%)	425 (100%)	1 (0%)	93	98
1	AF	426/427 (100%)	425 (100%)	1 (0%)	93	98
1	BA	413/427 (97%)	410 (99%)	3 (1%)	84	92
1	BB	426/427 (100%)	423 (99%)	3 (1%)	84	92
1	BC	426/427 (100%)	423 (99%)	3 (1%)	84	92
1	BD	387/427 (91%)	387 (100%)	0	100	100
1	BE	426/427 (100%)	425 (100%)	1 (0%)	93	98
1	BF	426/427 (100%)	426 (100%)	0	100	100
1	CA	411/427 (96%)	410 (100%)	1 (0%)	93	98
1	CB	426/427 (100%)	423 (99%)	3 (1%)	84	92
1	CC	426/427 (100%)	425 (100%)	1 (0%)	93	98
1	CD	383/427 (90%)	382 (100%)	1 (0%)	92	97
1	CE	426/427 (100%)	426 (100%)	0	100	100
1	CF	426/427 (100%)	420 (99%)	6 (1%)	67	84
1	DA	413/427 (97%)	404 (98%)	9 (2%)	52	77
1	DB	426/427 (100%)	421 (99%)	5 (1%)	71	86
1	DC	426/427 (100%)	424 (100%)	2 (0%)	88	95
1	DD	387/427 (91%)	387 (100%)	0	100	100
1	DE	426/427 (100%)	426 (100%)	0	100	100
1	DF	426/427 (100%)	421 (99%)	5 (1%)	71	86
1	EA	413/427 (97%)	411 (100%)	2 (0%)	88	95
1	EB	426/427 (100%)	423 (99%)	3 (1%)	84	92
1	EC	426/427 (100%)	419 (98%)	7 (2%)	62	82
1	ED	387/427 (91%)	385 (100%)	2 (0%)	88	95
1	EE	426/427 (100%)	421 (99%)	5 (1%)	71	86
1	EF	426/427 (100%)	423 (99%)	3 (1%)	84	92
2	Aa	275/275 (100%)	274 (100%)	1 (0%)	91	96
2	Ab	275/275 (100%)	272 (99%)	3 (1%)	73	87
2	Ad	275/275 (100%)	270 (98%)	5 (2%)	59	81

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	Ae	225/275 (82%)	224 (100%)	1 (0%)	91	96
2	Af	157/275 (57%)	154 (98%)	3 (2%)	57	80
2	Ba	275/275 (100%)	273 (99%)	2 (1%)	84	92
2	Bb	275/275 (100%)	267 (97%)	8 (3%)	42	71
2	Bd	275/275 (100%)	275 (100%)	0	100	100
2	Be	224/275 (82%)	223 (100%)	1 (0%)	91	96
2	Bf	157/275 (57%)	152 (97%)	5 (3%)	39	69
2	Ca	275/275 (100%)	274 (100%)	1 (0%)	91	96
2	Cb	275/275 (100%)	267 (97%)	8 (3%)	42	71
2	Cd	275/275 (100%)	270 (98%)	5 (2%)	59	81
2	Ce	225/275 (82%)	221 (98%)	4 (2%)	59	81
2	Cf	157/275 (57%)	152 (97%)	5 (3%)	39	69
2	Da	275/275 (100%)	275 (100%)	0	100	100
2	Db	275/275 (100%)	273 (99%)	2 (1%)	84	92
2	Dd	275/275 (100%)	272 (99%)	3 (1%)	73	87
2	De	225/275 (82%)	225 (100%)	0	100	100
2	Df	157/275 (57%)	155 (99%)	2 (1%)	69	86
2	Ea	275/275 (100%)	271 (98%)	4 (2%)	65	83
2	Eb	275/275 (100%)	274 (100%)	1 (0%)	91	96
2	Ed	275/275 (100%)	272 (99%)	3 (1%)	73	87
2	Ee	225/275 (82%)	222 (99%)	3 (1%)	69	86
2	Ef	157/275 (57%)	154 (98%)	3 (2%)	57	80
3	Ag	68/86 (79%)	67 (98%)	1 (2%)	65	83
3	Ah	62/86 (72%)	62 (100%)	0	100	100
3	Bg	68/86 (79%)	68 (100%)	0	100	100
3	Bh	62/86 (72%)	62 (100%)	0	100	100
3	Cg	68/86 (79%)	68 (100%)	0	100	100
3	Ch	62/86 (72%)	62 (100%)	0	100	100
3	Dg	68/86 (79%)	68 (100%)	0	100	100
3	Dh	62/86 (72%)	62 (100%)	0	100	100
3	Eg	68/86 (79%)	68 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	Eh	62/86 (72%)	62 (100%)	0	100	100
4	Ai	34/78 (44%)	34 (100%)	0	100	100
4	Aj	34/78 (44%)	34 (100%)	0	100	100
4	Ak	34/78 (44%)	34 (100%)	0	100	100
4	Bi	34/78 (44%)	34 (100%)	0	100	100
4	Bj	34/78 (44%)	34 (100%)	0	100	100
4	Bk	34/78 (44%)	34 (100%)	0	100	100
4	Ci	34/78 (44%)	34 (100%)	0	100	100
4	Cj	34/78 (44%)	34 (100%)	0	100	100
4	Ck	34/78 (44%)	34 (100%)	0	100	100
4	Di	34/78 (44%)	34 (100%)	0	100	100
4	Dj	34/78 (44%)	34 (100%)	0	100	100
4	Dk	34/78 (44%)	34 (100%)	0	100	100
4	Ei	34/78 (44%)	34 (100%)	0	100	100
4	Ej	34/78 (44%)	34 (100%)	0	100	100
4	Ek	34/78 (44%)	34 (100%)	0	100	100
5	FA	615/714 (86%)	608 (99%)	7 (1%)	73	87
5	FB	607/714 (85%)	602 (99%)	5 (1%)	81	91
5	FC	613/714 (86%)	608 (99%)	5 (1%)	81	91
5	FD	629/714 (88%)	619 (98%)	10 (2%)	62	82
5	FE	591/714 (83%)	586 (99%)	5 (1%)	81	91
5	FF	612/714 (86%)	605 (99%)	7 (1%)	73	87
5	FG	610/714 (85%)	600 (98%)	10 (2%)	62	82
5	FH	614/714 (86%)	594 (97%)	20 (3%)	38	69
5	FI	620/714 (87%)	612 (99%)	8 (1%)	69	86
5	FJ	623/714 (87%)	620 (100%)	3 (0%)	88	95
5	FK	600/714 (84%)	598 (100%)	2 (0%)	92	97
5	FL	608/714 (85%)	598 (98%)	10 (2%)	62	82
6	FM	206/215 (96%)	203 (98%)	3 (2%)	65	83
6	FN	206/215 (96%)	199 (97%)	7 (3%)	37	68
6	FO	206/215 (96%)	204 (99%)	2 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	FP	206/215 (96%)	202 (98%)	4 (2%)	57	80
6	FQ	206/215 (96%)	204 (99%)	2 (1%)	76	88
6	FR	206/215 (96%)	205 (100%)	1 (0%)	88	95
6	FS	209/215 (97%)	208 (100%)	1 (0%)	88	95
6	FT	206/215 (96%)	204 (99%)	2 (1%)	76	88
6	FU	206/215 (96%)	205 (100%)	1 (0%)	88	95
6	FV	206/215 (96%)	203 (98%)	3 (2%)	65	83
6	FW	206/215 (96%)	203 (98%)	3 (2%)	65	83
6	FX	206/215 (96%)	203 (98%)	3 (2%)	65	83
7	FY	208/208 (100%)	208 (100%)	0	100	100
7	FZ	208/208 (100%)	208 (100%)	0	100	100
7	GA	208/208 (100%)	206 (99%)	2 (1%)	76	88
7	GB	208/208 (100%)	208 (100%)	0	100	100
7	GC	208/208 (100%)	207 (100%)	1 (0%)	88	95
7	GD	208/208 (100%)	208 (100%)	0	100	100
7	GE	208/208 (100%)	206 (99%)	2 (1%)	76	88
7	GF	208/208 (100%)	208 (100%)	0	100	100
7	GG	208/208 (100%)	207 (100%)	1 (0%)	88	95
7	GH	208/208 (100%)	207 (100%)	1 (0%)	88	95
7	GI	208/208 (100%)	206 (99%)	2 (1%)	76	88
7	GJ	208/208 (100%)	208 (100%)	0	100	100
8	GK	100/644 (16%)	97 (97%)	3 (3%)	41	71
8	GL	100/644 (16%)	100 (100%)	0	100	100
8	GM	100/644 (16%)	100 (100%)	0	100	100
8	GN	100/644 (16%)	99 (99%)	1 (1%)	76	88
8	GO	100/644 (16%)	97 (97%)	3 (3%)	41	71
8	GP	100/644 (16%)	99 (99%)	1 (1%)	76	88
8	GQ	100/644 (16%)	99 (99%)	1 (1%)	76	88
8	GR	100/644 (16%)	100 (100%)	0	100	100
8	GS	100/644 (16%)	100 (100%)	0	100	100
8	GT	100/644 (16%)	99 (99%)	1 (1%)	76	88

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	GU	100/644 (16%)	100 (100%)	0	100	100
8	GV	100/644 (16%)	97 (97%)	3 (3%)	41	71
8	IK	26/644 (4%)	26 (100%)	0	100	100
8	IL	26/644 (4%)	26 (100%)	0	100	100
8	IM	26/644 (4%)	26 (100%)	0	100	100
8	IN	26/644 (4%)	26 (100%)	0	100	100
8	IO	26/644 (4%)	25 (96%)	1 (4%)	33	65
8	IP	26/644 (4%)	26 (100%)	0	100	100
8	IQ	26/644 (4%)	26 (100%)	0	100	100
8	IR	26/644 (4%)	26 (100%)	0	100	100
8	IS	26/644 (4%)	24 (92%)	2 (8%)	13	44
8	IT	26/644 (4%)	26 (100%)	0	100	100
8	IU	26/644 (4%)	26 (100%)	0	100	100
8	IV	26/644 (4%)	26 (100%)	0	100	100
All	All	33532/50815 (66%)	33236 (99%)	296 (1%)	79	89

All (296) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	AA	129	ASN
1	AA	130	GLN
1	AA	474	ASP
1	AB	62	ARG
1	AB	88	ARG
1	AB	191	ARG
1	AE	471	PHE
1	AF	44	LEU
2	Aa	108	ILE
2	Ab	219	ASP
2	Ab	221	GLU
2	Ab	329	THR
2	Ad	106	GLN
2	Ad	108	ILE
2	Ad	110	LEU
2	Ad	112	GLU
2	Ad	172	THR
2	Ae	222	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	Af	219	ASP
2	Af	221	GLU
2	Af	222	ASP
3	Ag	89	ASN
1	BA	129	ASN
1	BA	130	GLN
1	BA	248	ASP
1	BB	50	LYS
1	BB	88	ARG
1	BB	409	ARG
1	BC	88	ARG
1	BC	91	ASN
1	BC	449	TYR
1	BE	158	THR
2	Ba	107	TYR
2	Ba	108	ILE
2	Bb	110	LEU
2	Bb	113	GLU
2	Bb	148	LYS
2	Bb	217	THR
2	Bb	221	GLU
2	Bb	222	ASP
2	Bb	223	ARG
2	Bb	259	ARG
2	Be	149	THR
2	Bf	217	THR
2	Bf	218	VAL
2	Bf	219	ASP
2	Bf	221	GLU
2	Bf	223	ARG
1	CA	129	ASN
1	CB	88	ARG
1	CB	191	ARG
1	CB	395	ARG
1	CC	88	ARG
1	CD	5	LEU
1	CF	88	ARG
1	CF	91	ASN
1	CF	93	VAL
1	CF	95	VAL
1	CF	130	GLN
1	CF	196	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	Ca	108	ILE
2	Cb	105	ARG
2	Cb	108	ILE
2	Cb	172	THR
2	Cb	183	THR
2	Cb	218	VAL
2	Cb	222	ASP
2	Cb	224	LEU
2	Cb	259	ARG
2	Cd	106	GLN
2	Cd	108	ILE
2	Cd	111	SER
2	Cd	112	GLU
2	Cd	265	ASN
2	Ce	8	VAL
2	Ce	129	THR
2	Ce	168	ASP
2	Ce	266	ILE
2	Cf	215	THR
2	Cf	218	VAL
2	Cf	219	ASP
2	Cf	222	ASP
2	Cf	223	ARG
1	DA	21	SER
1	DA	22	ASP
1	DA	23	ASN
1	DA	129	ASN
1	DA	130	GLN
1	DA	131	VAL
1	DA	239	THR
1	DA	403	PHE
1	DA	409	ARG
1	DB	62	ARG
1	DB	88	ARG
1	DB	191	ARG
1	DB	239	THR
1	DB	405	ASP
1	DC	88	ARG
1	DC	356	THR
1	DF	88	ARG
1	DF	90	GLU
1	DF	91	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	DF	129	ASN
1	DF	130	GLN
2	Db	111	SER
2	Db	268	LYS
2	Dd	110	LEU
2	Dd	111	SER
2	Dd	172	THR
2	Df	218	VAL
2	Df	222	ASP
1	EA	128	LEU
1	EA	130	GLN
1	EB	62	ARG
1	EB	186	LYS
1	EB	191	ARG
1	EC	63	GLU
1	EC	66	ASP
1	EC	70	TYR
1	EC	88	ARG
1	EC	158	THR
1	EC	229	ASN
1	EC	442	LYS
1	ED	408	VAL
1	ED	432	THR
1	EE	88	ARG
1	EE	89	ASP
1	EE	91	ASN
1	EE	93	VAL
1	EE	335	THR
1	EF	128	LEU
1	EF	130	GLN
1	EF	142	MET
2	Ea	105	ARG
2	Ea	106	GLN
2	Ea	108	ILE
2	Ea	111	SER
2	Eb	218	VAL
2	Ed	31	VAL
2	Ed	108	ILE
2	Ed	309	ASP
2	Ee	8	VAL
2	Ee	77	LEU
2	Ee	88	VAL

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	Ef	221	GLU
2	Ef	222	ASP
2	Ef	223	ARG
5	FA	223	SER
5	FA	226	SER
5	FA	398	ARG
5	FA	547	ARG
5	FA	619	ASP
5	FA	622	GLU
5	FA	712	LYS
5	FB	39	LEU
5	FB	142	ASP
5	FB	201	CYS
5	FB	253	VAL
5	FB	588	CYS
5	FC	230	GLU
5	FC	357	ASN
5	FC	588	CYS
5	FC	618	ILE
5	FC	619	ASP
5	FD	35	PHE
5	FD	37	TYR
5	FD	201	CYS
5	FD	267	ASP
5	FD	290	ASN
5	FD	299	ARG
5	FD	315	ILE
5	FD	318	SER
5	FD	324	LEU
5	FD	547	ARG
5	FE	201	CYS
5	FE	257	LYS
5	FE	260	LYS
5	FE	265	MET
5	FE	588	CYS
5	FF	39	LEU
5	FF	237	LEU
5	FF	432	ASP
5	FF	547	ARG
5	FF	616	MET
5	FF	619	ASP
5	FF	622	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	FG	4	PHE
5	FG	5	LEU
5	FG	9	ARG
5	FG	57	ARG
5	FG	59	HIS
5	FG	65	LEU
5	FG	66	VAL
5	FG	282	GLU
5	FG	283	ARG
5	FG	286	PHE
5	FH	139	ILE
5	FH	142	ASP
5	FH	263	GLU
5	FH	265	MET
5	FH	266	PRO
5	FH	267	ASP
5	FH	268	TYR
5	FH	271	GLN
5	FH	274	VAL
5	FH	275	ASP
5	FH	276	GLN
5	FH	288	ASN
5	FH	315	ILE
5	FH	317	ASN
5	FH	318	SER
5	FH	547	ARG
5	FH	616	MET
5	FH	618	ILE
5	FH	619	ASP
5	FH	622	GLU
5	FI	37	TYR
5	FI	38	SER
5	FI	41	ARG
5	FI	201	CYS
5	FI	328	LEU
5	FI	588	CYS
5	FI	619	ASP
5	FI	622	GLU
5	FJ	201	CYS
5	FJ	547	ARG
5	FJ	588	CYS
5	FK	5	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	FK	332	ARG
5	FL	201	CYS
5	FL	269	ILE
5	FL	297	THR
5	FL	299	ARG
5	FL	320	LEU
5	FL	517	THR
5	FL	588	CYS
5	FL	617	GLU
5	FL	619	ASP
5	FL	712	LYS
6	FM	83	LEU
6	FM	84	ARG
6	FM	222	ARG
6	FN	8	VAL
6	FN	83	LEU
6	FN	93	TYR
6	FN	94	PRO
6	FN	95	THR
6	FN	96	HIS
6	FN	222	ARG
6	FO	204	GLU
6	FO	222	ARG
6	FP	84	ARG
6	FP	87	THR
6	FP	120	THR
6	FP	222	ARG
6	FQ	56	ASP
6	FQ	222	ARG
6	FR	222	ARG
6	FS	222	ARG
6	FT	222	ARG
6	FT	233	ILE
6	FU	222	ARG
6	FV	84	ARG
6	FV	87	THR
6	FV	222	ARG
6	FW	83	LEU
6	FW	84	ARG
6	FW	222	ARG
6	FX	15	ASP
6	FX	125	GLU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
6	FX	137	ASP
7	GA	130	CYS
7	GA	170	CYS
7	GC	117	TYR
7	GE	147	PHE
7	GE	170	CYS
7	GG	51	ILE
7	GH	204	ARG
7	GI	130	CYS
7	GI	147	PHE
8	GK	459	GLN
8	GK	521	ASP
8	GK	546	LYS
8	GN	502	LYS
8	GO	459	GLN
8	GO	460	ILE
8	GO	546	LYS
8	GP	426	PHE
8	GQ	459	GLN
8	GT	521	ASP
8	GV	454	PRO
8	GV	459	GLN
8	GV	463	ASP
8	IO	242	THR
8	IS	243	SER
8	IS	245	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (413) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AA	57	ASN
1	AA	101	ASN
1	AA	235	GLN
1	AA	278	ASN
1	AA	361	ASN
1	AA	377	ASN
1	AA	458	ASN
1	AA	463	GLN
1	AB	271	ASN
1	AB	295	GLN
1	AB	410	ASN
1	AB	458	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	AC	168	GLN
1	AC	254	GLN
1	AC	273	ASN
1	AC	284	ASN
1	AC	410	ASN
1	AC	414	HIS
1	AC	435	GLN
1	AD	98	ASN
1	AD	167	GLN
1	AD	200	ASN
1	AD	214	ASN
1	AD	217	ASN
1	AD	254	GLN
1	AD	295	GLN
1	AD	361	ASN
1	AD	377	ASN
1	AD	410	ASN
1	AD	435	GLN
1	AE	9	GLN
1	AE	14	GLN
1	AE	214	ASN
1	AE	261	ASN
1	AE	361	ASN
1	AE	384	GLN
1	AE	410	ASN
1	AF	24	HIS
1	AF	57	ASN
1	AF	159	GLN
1	AF	168	GLN
1	AF	463	GLN
2	Aa	7	GLN
2	Aa	115	GLN
2	Ab	147	ASN
2	Ab	195	GLN
2	Ad	7	GLN
2	Ae	97	ASN
2	Af	204	GLN
3	Ag	56	GLN
4	Ai	12	ASN
1	BA	38	ASN
1	BA	42	GLN
1	BA	57	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	BA	68	ASN
1	BA	278	ASN
1	BA	284	ASN
1	BA	392	ASN
1	BB	31	GLN
1	BB	235	GLN
1	BB	271	ASN
1	BB	284	ASN
1	BB	361	ASN
1	BB	377	ASN
1	BB	392	ASN
1	BC	57	ASN
1	BC	91	ASN
1	BC	168	GLN
1	BC	229	ASN
1	BC	361	ASN
1	BC	414	HIS
1	BC	479	HIS
1	BC	503	GLN
1	BD	245	HIS
1	BD	254	GLN
1	BE	14	GLN
1	BE	98	ASN
1	BE	200	ASN
1	BE	229	ASN
1	BE	245	HIS
1	BE	384	GLN
1	BE	410	ASN
1	BF	57	ASN
1	BF	278	ASN
1	BF	284	ASN
1	BF	392	ASN
1	BF	414	HIS
1	BF	435	GLN
2	Ba	7	GLN
2	Ba	115	GLN
2	Ba	204	GLN
2	Bd	316	ASN
2	Bd	323	ASN
2	Be	187	GLN
2	Bf	97	ASN
3	Bg	89	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	Bh	82	GLN
4	Bi	12	ASN
4	Bk	17	ASN
1	CA	57	ASN
1	CA	200	ASN
1	CA	278	ASN
1	CA	414	HIS
1	CA	479	HIS
1	CB	159	GLN
1	CB	295	GLN
1	CB	392	ASN
1	CB	410	ASN
1	CB	447	ASN
1	CB	458	ASN
1	CB	466	ASN
1	CB	503	GLN
1	CC	31	GLN
1	CC	42	GLN
1	CC	157	ASN
1	CC	168	GLN
1	CC	214	ASN
1	CC	261	ASN
1	CC	342	GLN
1	CC	410	ASN
1	CC	414	HIS
1	CC	479	HIS
1	CD	38	ASN
1	CD	167	GLN
1	CD	273	ASN
1	CD	361	ASN
1	CD	410	ASN
1	CE	9	GLN
1	CE	14	GLN
1	CE	34	GLN
1	CE	129	ASN
1	CE	273	ASN
1	CE	295	GLN
1	CE	371	GLN
1	CE	384	GLN
1	CE	458	ASN
1	CF	91	ASN
1	CF	101	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	CF	130	GLN
1	CF	235	GLN
1	CF	261	ASN
1	CF	278	ASN
1	CF	414	HIS
2	Ca	96	GLN
2	Ca	115	GLN
2	Ca	187	GLN
2	Ca	204	GLN
2	Cb	292	ASN
2	Cd	156	ASN
2	Cd	285	HIS
2	Cd	292	ASN
2	Cd	323	ASN
2	Ce	97	ASN
2	Ce	204	GLN
2	Cf	144	ASN
2	Cf	204	GLN
3	Cg	89	ASN
3	Ch	57	GLN
3	Ch	82	GLN
3	Ch	89	ASN
4	Ci	12	ASN
4	Ci	31	ASN
1	DA	342	GLN
1	DB	271	ASN
1	DB	284	ASN
1	DB	295	GLN
1	DB	362	ASN
1	DB	410	ASN
1	DB	435	GLN
1	DC	129	ASN
1	DC	130	GLN
1	DC	168	GLN
1	DC	261	ASN
1	DC	342	GLN
1	DC	414	HIS
1	DC	447	ASN
1	DD	159	GLN
1	DD	167	GLN
1	DD	214	ASN
1	DD	217	ASN

*Continued on next page...*



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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	DD	229	ASN
1	DD	254	GLN
1	DD	271	ASN
1	DD	278	ASN
1	DE	14	GLN
1	DE	23	ASN
1	DE	34	GLN
1	DE	38	ASN
1	DE	127	ASN
1	DE	129	ASN
1	DE	361	ASN
1	DE	384	GLN
1	DE	458	ASN
1	DF	101	ASN
1	DF	278	ASN
1	DF	377	ASN
1	DF	392	ASN
2	Da	187	GLN
2	Da	316	ASN
2	Db	316	ASN
2	Dd	292	ASN
2	De	212	GLN
2	Df	204	GLN
3	Dg	89	ASN
3	Dh	82	GLN
4	Di	12	ASN
4	Di	30	ASN
1	EA	24	HIS
1	EA	34	GLN
1	EA	57	ASN
1	EA	101	ASN
1	EA	168	GLN
1	EA	214	ASN
1	EA	254	GLN
1	EA	260	ASN
1	EA	261	ASN
1	EA	295	GLN
1	EA	300	ASN
1	EA	435	GLN
1	EA	463	GLN
1	EB	57	ASN
1	EB	91	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	EB	168	GLN
1	EB	361	ASN
1	EB	410	ASN
1	EC	168	GLN
1	EC	217	ASN
1	EC	261	ASN
1	EC	271	ASN
1	EC	362	ASN
1	EC	414	HIS
1	EC	447	ASN
1	ED	167	GLN
1	ED	217	ASN
1	ED	284	ASN
1	ED	362	ASN
1	EE	9	GLN
1	EE	14	GLN
1	EE	81	ASN
1	EE	157	ASN
1	EE	300	ASN
1	EE	384	GLN
1	EE	410	ASN
1	EE	458	ASN
1	EF	68	ASN
1	EF	129	ASN
1	EF	159	GLN
1	EF	245	HIS
1	EF	254	GLN
1	EF	278	ASN
1	EF	295	GLN
1	EF	392	ASN
1	EF	410	ASN
1	EF	414	HIS
1	EF	463	GLN
2	Ea	7	GLN
2	Ea	106	GLN
2	Ea	115	GLN
2	Ea	187	GLN
2	Eb	156	ASN
2	Eb	265	ASN
2	Ed	156	ASN
2	Ed	186	ASN
2	Ed	316	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	Ed	323	ASN
2	Ee	106	GLN
2	Ee	144	ASN
2	Ef	186	ASN
2	Ef	204	GLN
3	Eg	54	ASN
3	Eg	89	ASN
3	Eh	32	GLN
3	Eh	82	GLN
4	Ei	12	ASN
4	Ei	17	ASN
4	Ej	30	ASN
4	Ek	17	ASN
5	FA	82	GLN
5	FA	185	ASN
5	FA	639	GLN
5	FA	650	GLN
5	FA	676	GLN
5	FB	152	ASN
5	FB	168	ASN
5	FB	200	GLN
5	FB	401	GLN
5	FB	406	ASN
5	FB	634	ASN
5	FB	639	GLN
5	FB	676	GLN
5	FB	685	GLN
5	FB	723	ASN
5	FC	10	GLN
5	FC	128	GLN
5	FC	200	GLN
5	FC	357	ASN
5	FC	508	ASN
5	FC	634	ASN
5	FC	639	GLN
5	FC	718	GLN
5	FD	172	ASN
5	FD	200	GLN
5	FD	309	ASN
5	FD	317	ASN
5	FD	518	ASN
5	FD	676	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	FD	685	GLN
5	FD	703	GLN
5	FD	709	GLN
5	FD	727	ASN
5	FE	10	GLN
5	FE	31	GLN
5	FE	145	ASN
5	FE	172	ASN
5	FE	200	GLN
5	FE	401	GLN
5	FE	546	GLN
5	FE	676	GLN
5	FE	685	GLN
5	FE	697	GLN
5	FE	735	GLN
5	FF	6	ASN
5	FF	317	ASN
5	FF	401	GLN
5	FF	406	ASN
5	FF	438	ASN
5	FF	634	ASN
5	FF	709	GLN
5	FF	723	ASN
5	FF	727	ASN
5	FG	10	GLN
5	FG	82	GLN
5	FG	200	GLN
5	FG	401	GLN
5	FG	546	GLN
5	FG	566	GLN
5	FG	569	HIS
5	FG	634	ASN
5	FG	639	GLN
5	FG	676	GLN
5	FH	30	ASN
5	FH	200	GLN
5	FH	288	ASN
5	FH	317	ASN
5	FH	389	ASN
5	FH	546	GLN
5	FH	676	GLN
5	FH	723	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
5	FI	10	GLN
5	FI	31	GLN
5	FI	406	ASN
5	FI	676	GLN
5	FI	697	GLN
5	FI	701	GLN
5	FJ	10	GLN
5	FJ	30	ASN
5	FJ	31	GLN
5	FJ	152	ASN
5	FJ	650	GLN
5	FJ	690	GLN
5	FJ	727	ASN
5	FJ	737	GLN
5	FK	185	ASN
5	FK	200	GLN
5	FK	650	GLN
5	FK	676	GLN
5	FK	723	ASN
5	FL	31	GLN
5	FL	36	ASN
5	FL	200	GLN
5	FL	327	ASN
5	FL	701	GLN
5	FL	702	GLN
5	FL	728	GLN
6	FM	3	ASN
6	FN	178	ASN
6	FN	182	GLN
6	FO	46	ASN
6	FO	96	HIS
6	FR	46	ASN
6	FT	192	ASN
6	FU	114	GLN
6	FV	77	HIS
6	FV	190	GLN
6	FW	3	ASN
6	FW	147	ASN
6	FX	190	GLN
7	GC	50	GLN
7	GE	57	GLN
7	GG	104	GLN

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Mol	Chain	Res	Type
7	GI	57	GLN
8	GL	456	GLN
8	GL	459	GLN
8	GO	459	GLN
8	GP	469	ASN
8	GP	529	GLN
8	GR	453	ASN
8	GR	539	GLN
8	GS	450	HIS
8	GS	544	GLN
8	GT	473	GLN
8	GU	459	GLN
8	GU	544	GLN
8	GV	459	GLN
8	IK	229	ASN
8	IK	231	GLN
8	IM	231	GLN
8	IN	231	GLN
8	IQ	231	GLN
8	IR	239	GLN
8	IT	231	GLN
8	IU	231	GLN
8	IV	231	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 [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 27 ligands modelled in this entry, 27 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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.

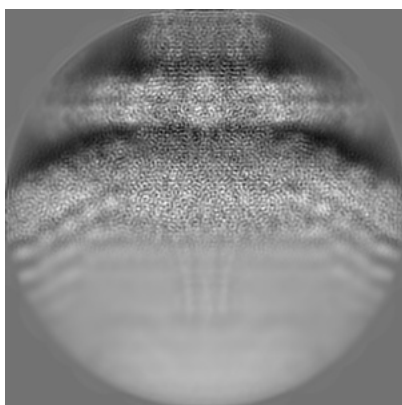
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14091. These allow visual inspection of the internal detail of the map and identification of artifacts.

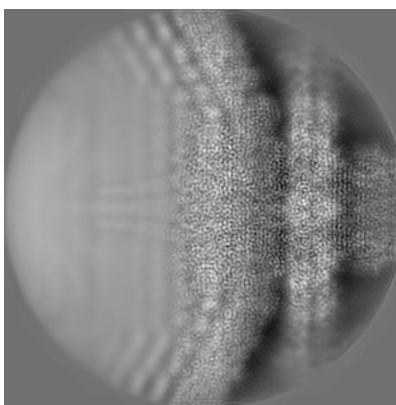
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

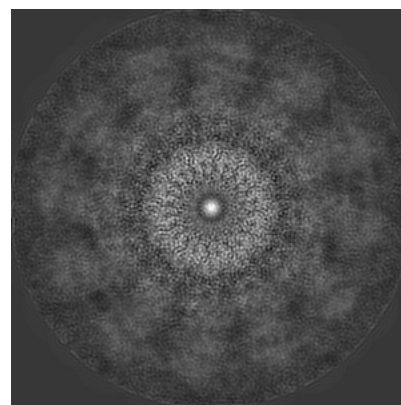
#### 6.1.1 Primary map



X



Y

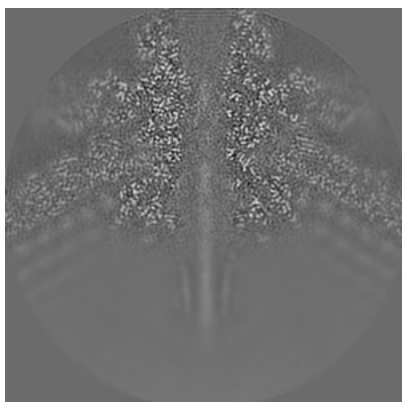


Z

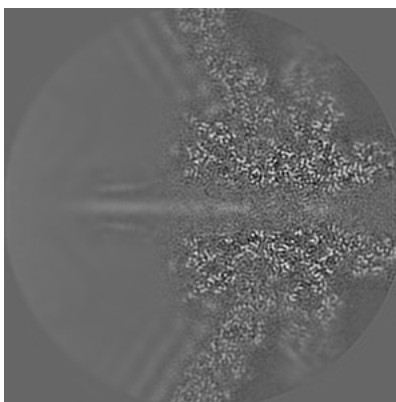
The images above show the map projected in three orthogonal directions.

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

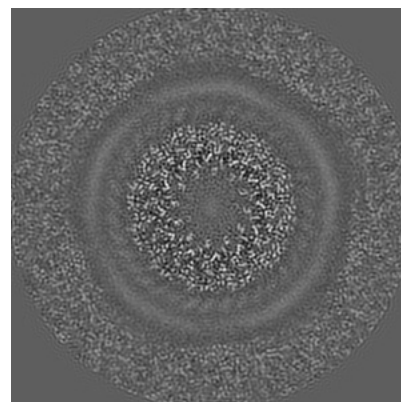
#### 6.2.1 Primary map



X Index: 143



Y Index: 143



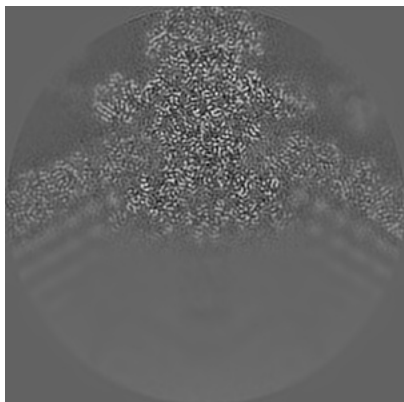
Z Index: 143



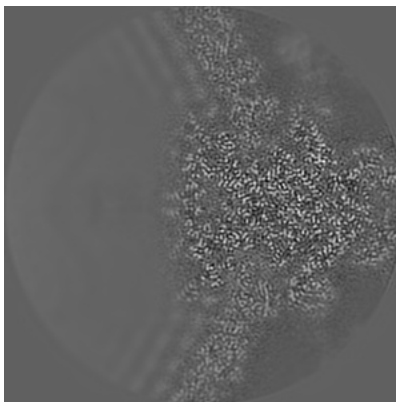
The images above show central slices of the map in three orthogonal directions.

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

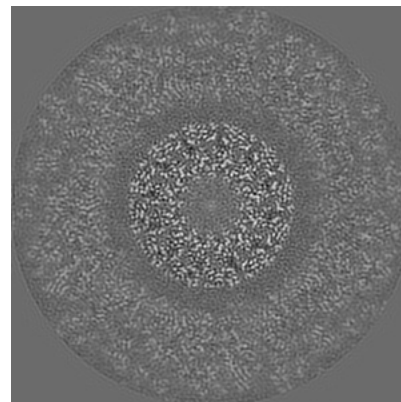
### 6.3.1 Primary map



X Index: 166



Y Index: 121

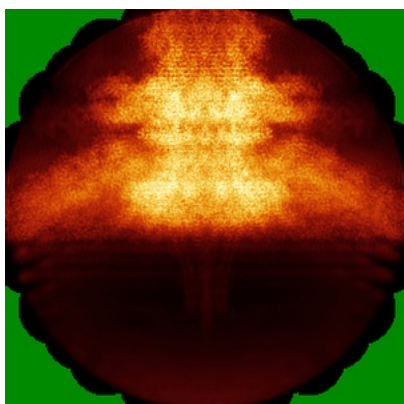


Z Index: 158

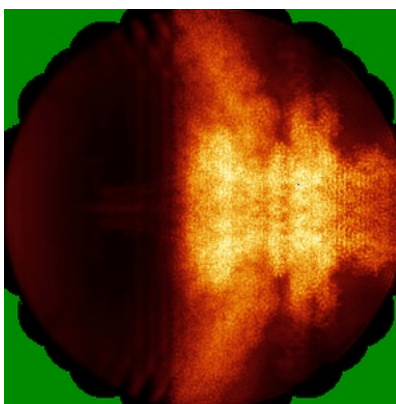
The images above show the largest variance slices of the map in three orthogonal directions.

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

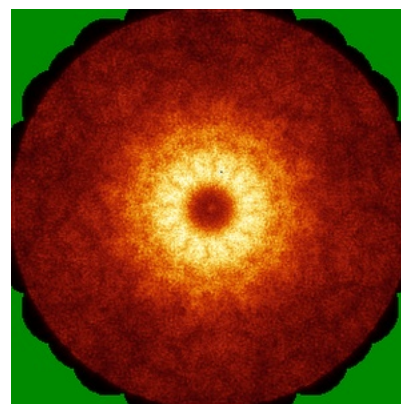
### 6.4.1 Primary map



X



Y

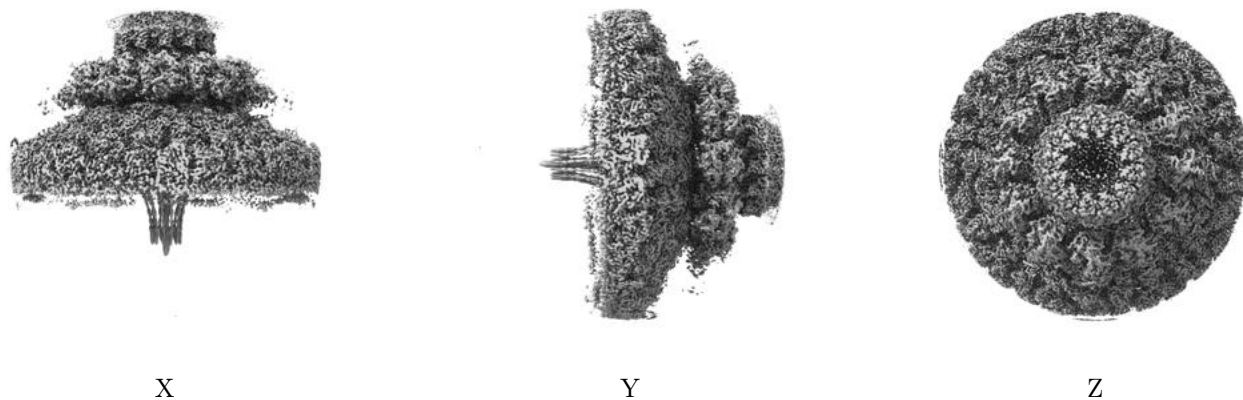


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

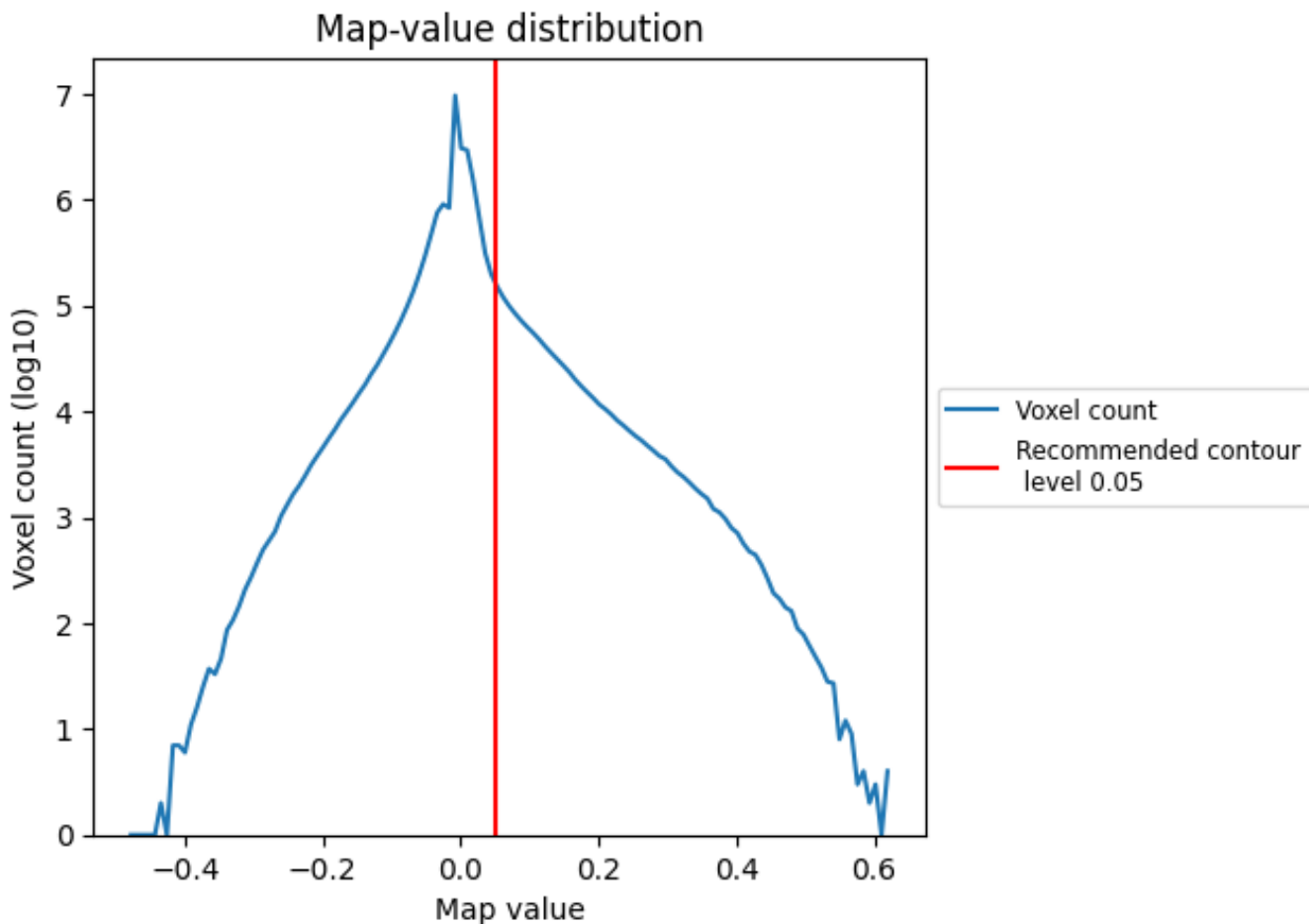
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

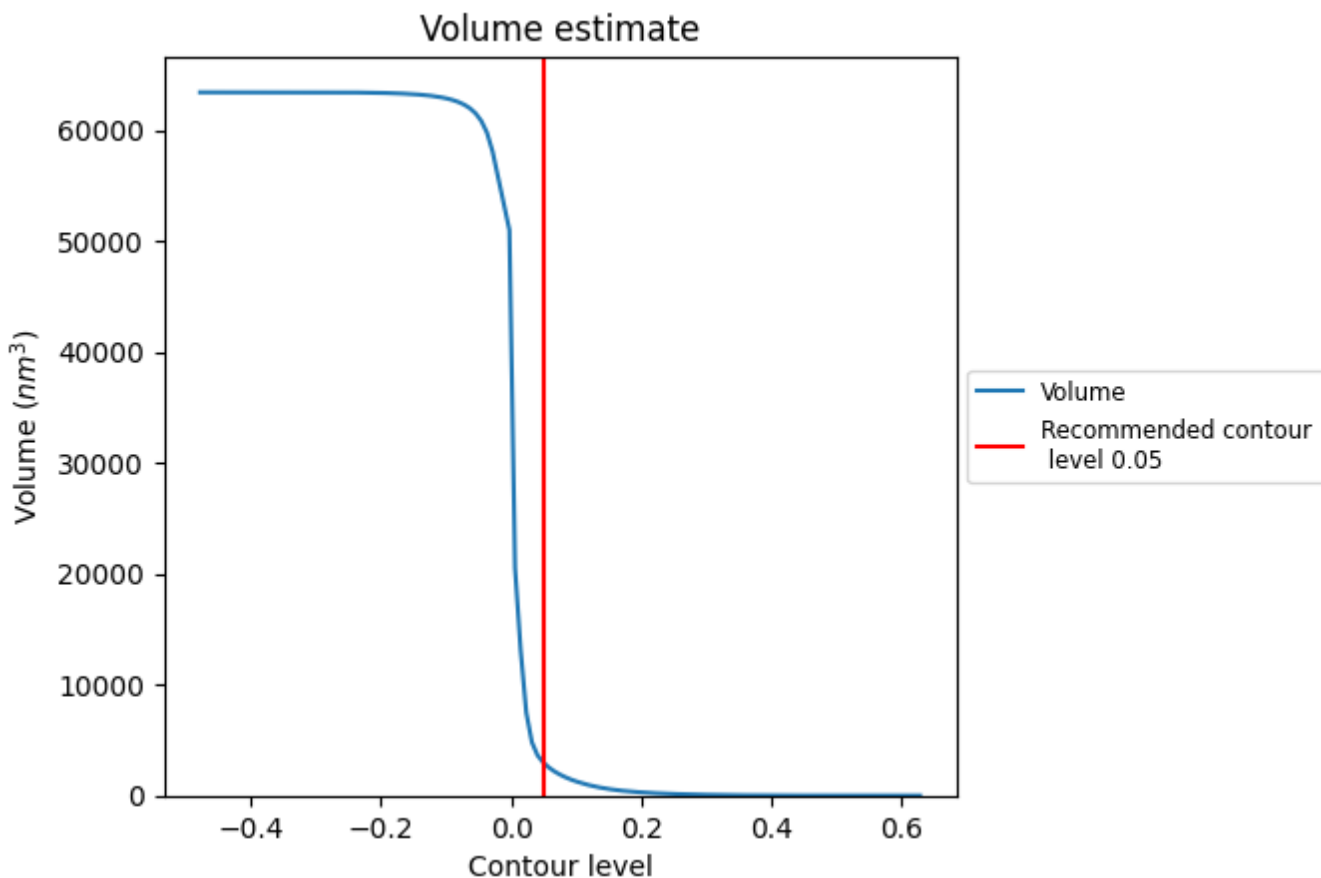
This section contains the results of statistical analysis of the map.

### 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.

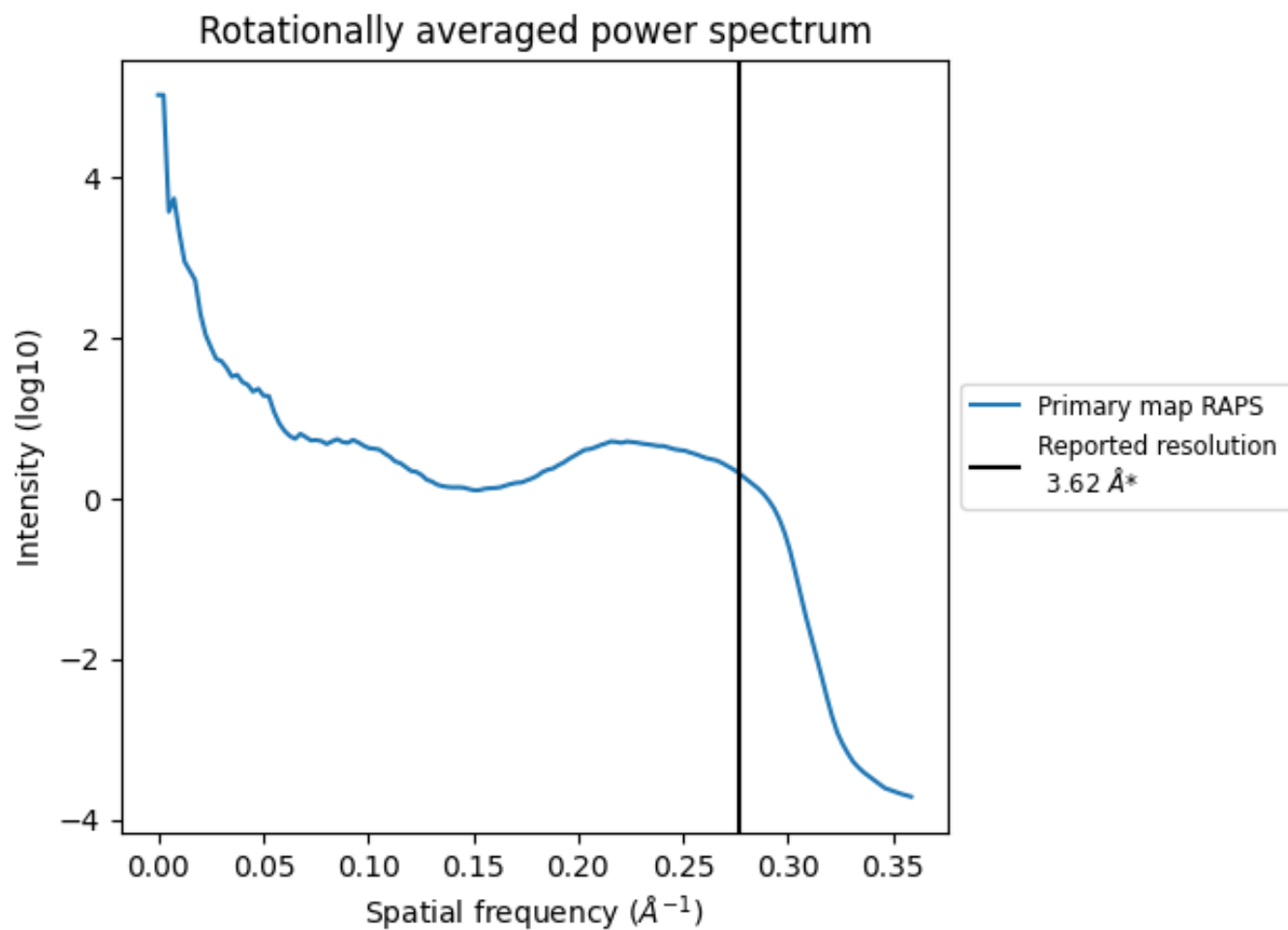
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 2949 nm<sup>3</sup>; this corresponds to an approximate mass of 2664 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 [i](#)

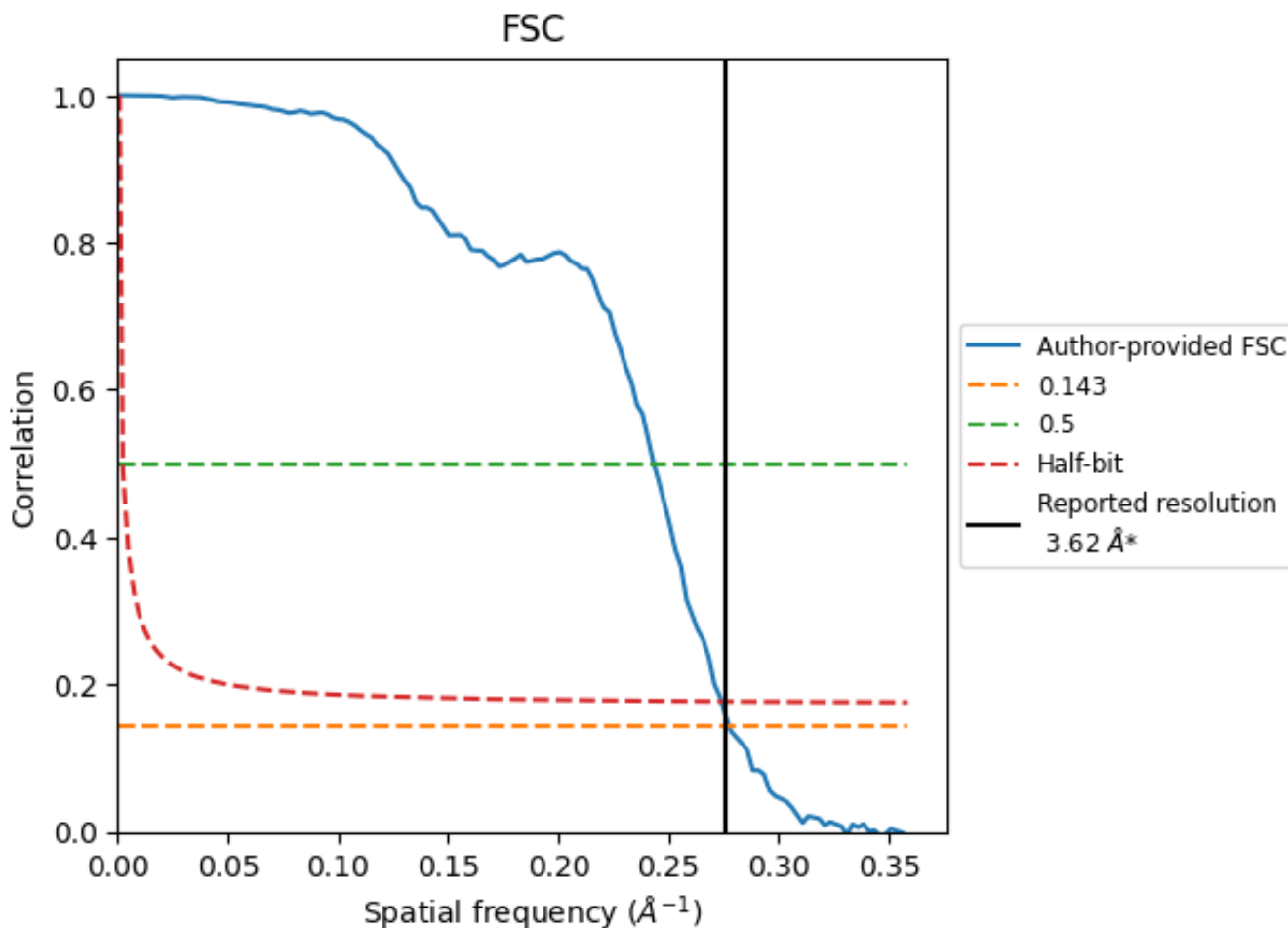


\*Reported resolution corresponds to spatial frequency of 0.276 Å<sup>-1</sup>

## 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 0.276 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

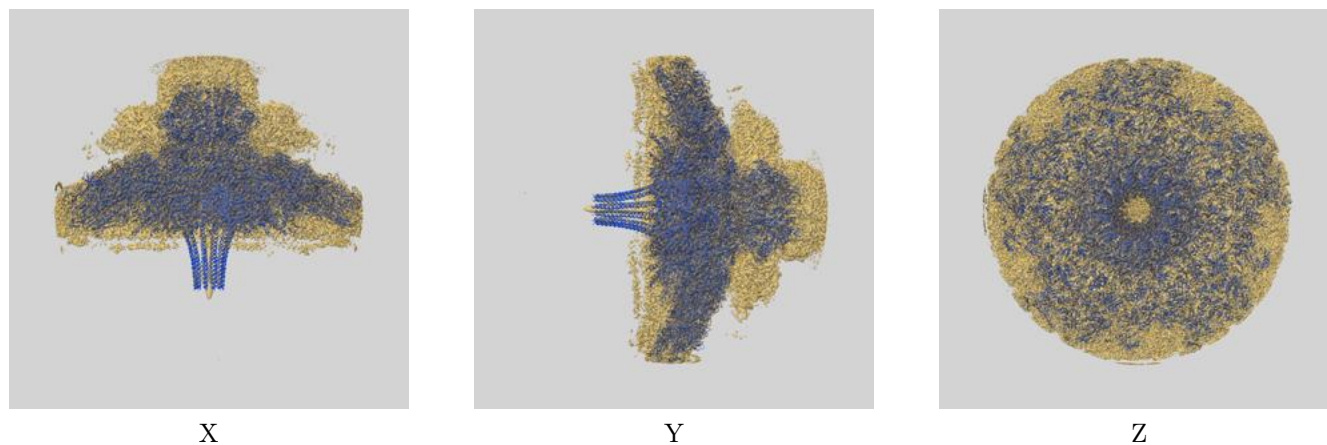
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.62	-	-
Author-provided FSC curve	3.60	4.11	3.65
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

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

This section contains information regarding the fit between EMDB map EMD-14091 and PDB model 7QOI. Per-residue inclusion information can be found in section 3 on page 18.

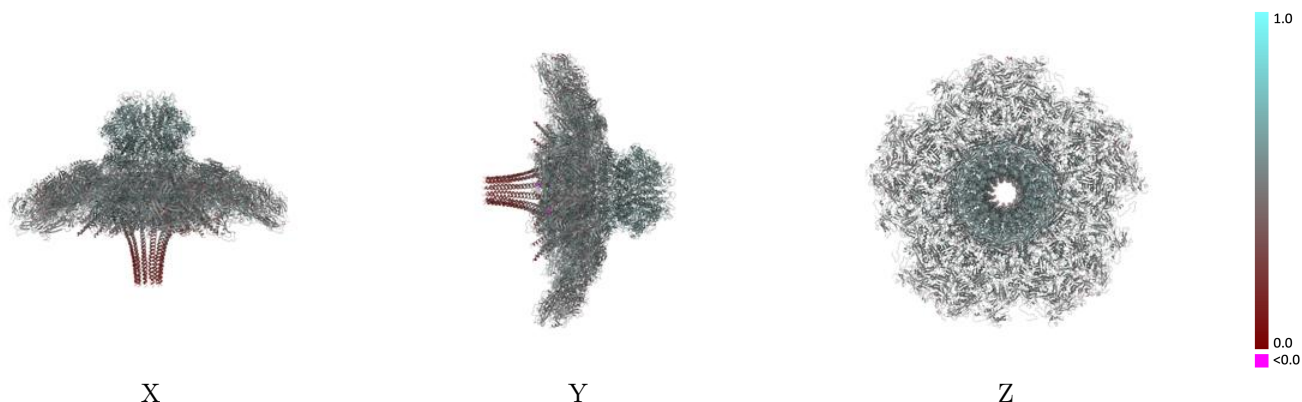
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

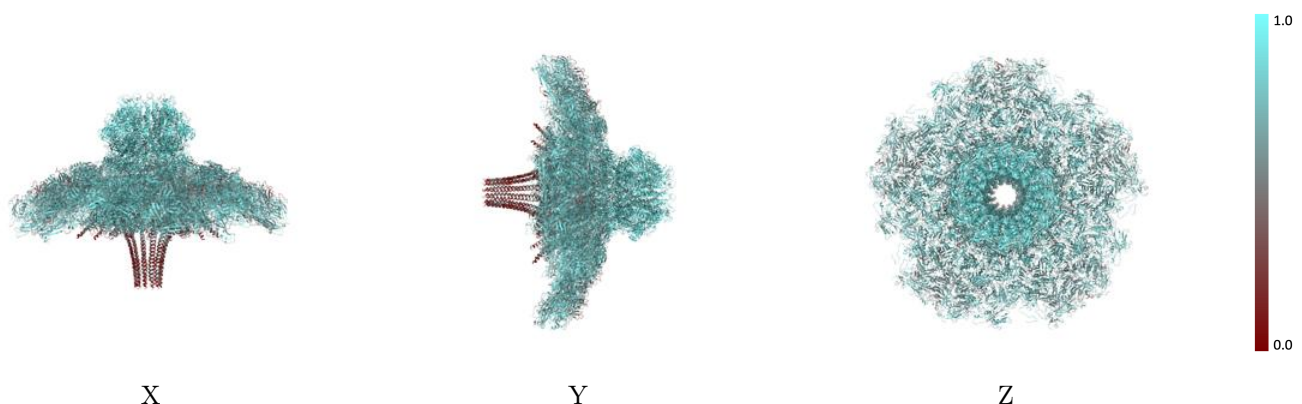


## 9.2 Q-score mapped to coordinate model [i](#)



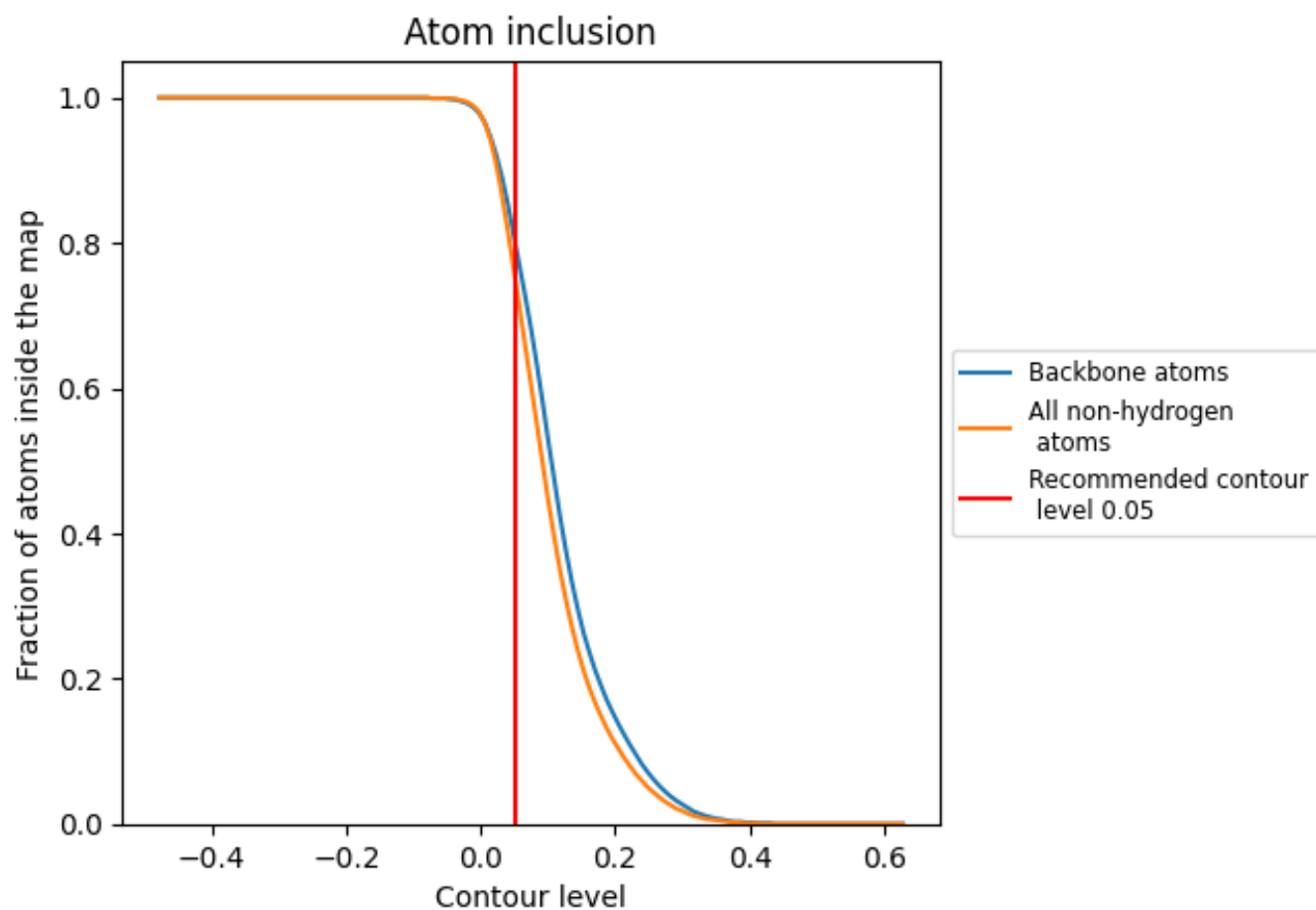
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 81% of all backbone atoms, 76% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.5050
AA	 0.7010	 0.4810
AB	 0.7480	 0.5010
AC	 0.7830	 0.5100
AD	 0.7680	 0.4980
AE	 0.7460	 0.4960
AF	 0.6950	 0.4760
Aa	 0.7240	 0.4850
Ab	 0.7370	 0.4910
Ad	 0.7280	 0.4950
Ae	 0.6870	 0.4820
Af	 0.5810	 0.4460
Ag	 0.7510	 0.4960
Ah	 0.7410	 0.4970
Ai	 0.6480	 0.4900
Aj	 0.6220	 0.4830
Ak	 0.6120	 0.4880
BA	 0.7130	 0.4870
BB	 0.7580	 0.5050
BC	 0.7880	 0.5130
BD	 0.7660	 0.5010
BE	 0.7430	 0.4960
BF	 0.7000	 0.4820
Ba	 0.7040	 0.4860
Bb	 0.7530	 0.5030
Bd	 0.7310	 0.4950
Be	 0.6590	 0.4590
Bf	 0.6070	 0.4570
Bg	 0.7760	 0.5030
Bh	 0.7330	 0.4980
Bi	 0.6580	 0.4920
Bj	 0.5620	 0.4810
Bk	 0.6150	 0.4780
CA	 0.7180	 0.4900
CB	 0.7610	 0.5010























































































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Chain	Atom inclusion	Q-score
CC	 0.7860	 0.5080
CD	 0.7660	 0.5030
CE	 0.7450	 0.5020
CF	 0.7030	 0.4830
Ca	 0.7100	 0.4860
Cb	 0.7470	 0.5020
Cd	 0.7260	 0.4910
Ce	 0.6490	 0.4730
Cf	 0.6140	 0.4430
Cg	 0.7610	 0.5020
Ch	 0.7460	 0.5030
Ci	 0.5790	 0.4840
Cj	 0.6220	 0.4810
Ck	 0.5950	 0.4710
DA	 0.7080	 0.4910
DB	 0.7510	 0.5010
DC	 0.7880	 0.5100
DD	 0.7520	 0.4960
DE	 0.7480	 0.4990
DF	 0.7140	 0.4890
Da	 0.6930	 0.4840
Db	 0.7350	 0.5020
Dd	 0.7200	 0.4880
De	 0.6810	 0.4800
Df	 0.6250	 0.4580
Dg	 0.7500	 0.4920
Dh	 0.7480	 0.4860
Di	 0.6120	 0.4720
Dj	 0.5790	 0.4800
Dk	 0.5790	 0.4860
EA	 0.7230	 0.4910
EB	 0.7710	 0.5030
EC	 0.7870	 0.5080
ED	 0.7830	 0.5040
EE	 0.7510	 0.5010
EF	 0.7000	 0.4780
Ea	 0.6960	 0.4830
Eb	 0.7530	 0.5040
Ed	 0.7370	 0.4940
Ee	 0.6820	 0.4790
Ef	 0.6090	 0.4530
Eg	 0.7640	 0.4950













































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Chain	Atom inclusion	Q-score
Eh	 0.7550	 0.4960
Ei	 0.5130	 0.4500
Ej	 0.4700	 0.4560
Ek	 0.5660	 0.4720
FA	 0.7890	 0.5170
FB	 0.7830	 0.5150
FC	 0.7830	 0.5170
FD	 0.7810	 0.5120
FE	 0.7820	 0.5120
FF	 0.7890	 0.5180
FG	 0.7840	 0.5140
FH	 0.7880	 0.5180
FI	 0.7870	 0.5180
FJ	 0.7820	 0.5160
FK	 0.7980	 0.5180
FL	 0.7850	 0.5110
FM	 0.9040	 0.5640
FN	 0.8910	 0.5560
FO	 0.8790	 0.5540
FP	 0.8830	 0.5570
FQ	 0.8920	 0.5610
FR	 0.8910	 0.5620
FS	 0.8970	 0.5610
FT	 0.8920	 0.5630
FU	 0.8810	 0.5560
FV	 0.8870	 0.5590
FW	 0.8990	 0.5630
FX	 0.8950	 0.5580
FY	 0.8710	 0.5470
FZ	 0.8860	 0.5540
GA	 0.8860	 0.5510
GB	 0.8830	 0.5500
GC	 0.8880	 0.5550
GD	 0.8770	 0.5510
GE	 0.8830	 0.5510
GF	 0.8850	 0.5520
GG	 0.8820	 0.5510
GH	 0.8840	 0.5500
GI	 0.8810	 0.5510
GJ	 0.8770	 0.5460
GK	 0.6080	 0.4640
GL	 0.6380	 0.4750

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Chain	Atom inclusion	Q-score
GM	 0.6270	 0.4660
GN	 0.6050	 0.4620
GO	 0.5980	 0.4550
GP	 0.5950	 0.4650
GQ	 0.6120	 0.4620
GR	 0.5980	 0.4720
GS	 0.6160	 0.4700
GT	 0.5950	 0.4580
GU	 0.5770	 0.4550
GV	 0.6220	 0.4760
IK	 0.7310	 0.5020
IL	 0.7220	 0.5000
IM	 0.7390	 0.4880
IN	 0.7220	 0.5140
IO	 0.7140	 0.5060
IP	 0.7350	 0.5050
IQ	 0.7220	 0.5080
IR	 0.7960	 0.5280
IS	 0.8330	 0.5290
IT	 0.7430	 0.5040
IU	 0.7550	 0.4960
IV	 0.7630	 0.5020