



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 03:42 AM UTC

PDB ID : 8QSY / pdb_00008qsy
EMDB ID : EMD-18642
Title : Portal capsid interface of full Haloferax tailed virus 1.
Authors : Zhang, D.; Daum, B.; Isupov, M.N.; McLaren, M.
Deposited on : 2023-10-11
Resolution : 2.68 Å (reported)
Based on initial model : .

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

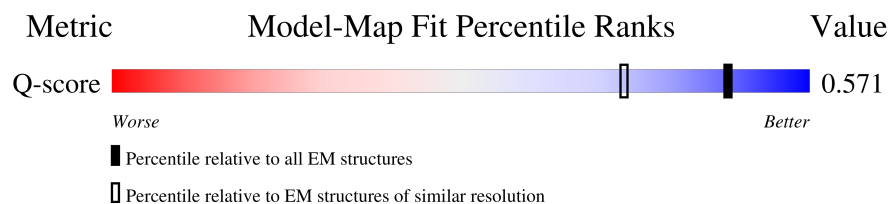
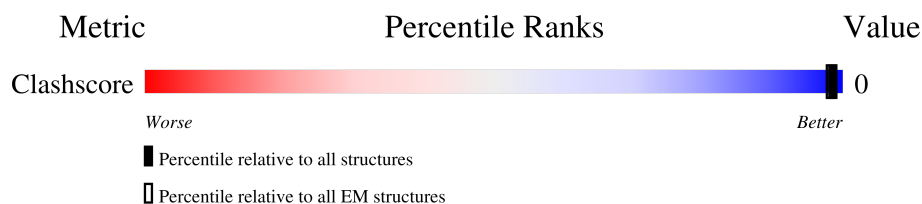
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

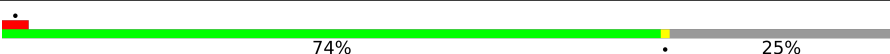
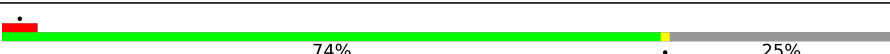
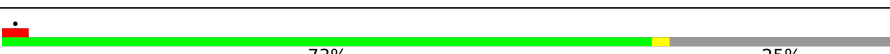
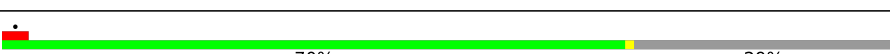
The reported resolution of this entry is 2.68 Å.

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



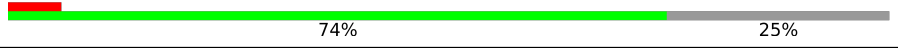
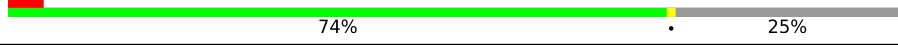
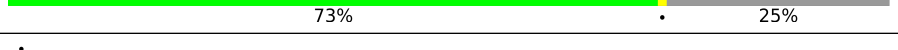
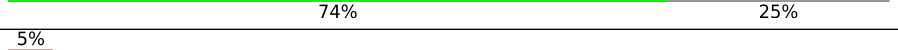
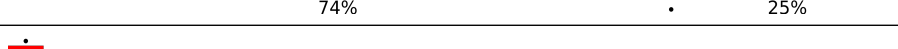
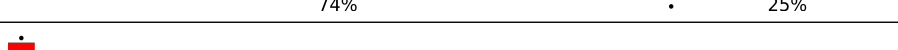
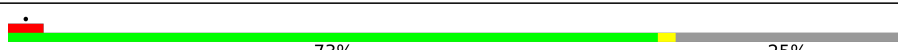
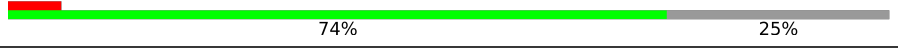
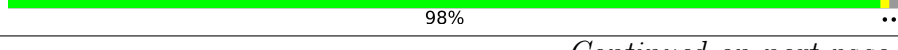
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Q-score	-	25397	9255 (2.18 - 3.18)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	JA	396	 74% 25%
1	JB	396	 74% 25%
1	JC	396	 74% 25%
1	JD	396	 74% 25%
1	JE	396	 73% 25%
1	JF	396	 70% 29%

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Mol	Chain	Length	Quality of chain
1	KA	396	
1	KB	396	
1	KC	396	
1	KD	396	
1	KE	396	
1	KF	396	
1	LA	396	
1	LB	396	
1	LC	396	
1	LD	396	
1	LE	396	
1	LF	396	
1	MA	396	
1	MB	396	
1	MC	396	
1	MD	396	
1	ME	396	
1	MF	396	
1	NA	396	
1	NB	396	
1	NC	396	
1	ND	396	
1	NE	396	
1	NF	396	
2	JI	137	

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Mol	Chain	Length	Quality of chain
2	JJ	137	
2	JK	137	
2	KI	137	
2	KJ	137	
2	KK	137	
2	LI	137	
2	LJ	137	
2	LK	137	
2	MI	137	
2	MJ	137	
2	MK	137	
2	NI	137	
2	NJ	137	
2	NK	137	
3	P5	82	
3	P6	82	
3	P7	82	
3	P8	82	
3	P9	82	
4	PA	675	
4	PB	675	
4	PC	675	
4	PD	675	
4	PE	675	
4	PF	675	

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Mol	Chain	Length	Quality of chain
4	PG	675	
4	PH	675	
4	PI	675	
4	PJ	675	
4	PK	675	
4	PL	675	
5	PM	141	
5	PN	141	
5	PO	141	
5	PP	141	
5	PQ	141	
5	PR	141	
5	PS	141	
5	PT	141	
5	PU	141	
5	PV	141	
5	PW	141	
5	PX	141	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 137239 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 HK97 gp5-like major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	JA	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	JB	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	JC	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	JD	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	JE	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	JF	282	Total 2183	C 1323	N 392	O 462	S 6	0	0
1	KA	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	KB	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	KC	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	KD	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	KE	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	KF	282	Total 2183	C 1323	N 392	O 462	S 6	0	0
1	LA	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	LB	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	LC	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	LD	296	Total 2298	C 1398	N 409	O 485	S 6	0	0
1	LE	296	Total 2298	C 1398	N 409	O 485	S 6	0	0

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Mol	Chain	Residues	Atoms					AltConf	Trace
1	LF	283	Total	C	N	O	S	0	0
			2194	1329	396	463	6		
1	MA	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	MB	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	MC	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	MD	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	ME	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	MF	293	Total	C	N	O	S	0	0
			2277	1383	406	482	6		
1	NA	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	NB	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	NC	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	ND	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	NE	296	Total	C	N	O	S	0	0
			2298	1398	409	485	6		
1	NF	282	Total	C	N	O	S	0	0
			2183	1323	392	462	6		

- Molecule 2 is a protein called Capsid stabilization protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	JI	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	JJ	131	Total	C	N	O	S	0	0
			930	575	144	209	2		
2	JK	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	KI	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	KJ	131	Total	C	N	O	S	0	0
			930	575	144	209	2		
2	KK	136	Total	C	N	O	S	0	0
			967	596	150	219	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
2	LI	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	LJ	129	Total	C	N	O	S	0	0
			917	568	142	205	2		
2	LK	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	MI	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	MJ	130	Total	C	N	O	S	0	0
			926	573	143	208	2		
2	MK	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	NI	136	Total	C	N	O	S	0	0
			967	596	150	219	2		
2	NJ	129	Total	C	N	O	S	0	0
			917	568	142	205	2		
2	NK	136	Total	C	N	O	S	0	0
			967	596	150	219	2		

- Molecule 3 is a protein called Hypothetical protein gp21.

Mol	Chain	Residues	Atoms						AltConf	Trace
3	P5	82	Total 689	C 414	N 132	O 138	P 1	S 4	0	0
3	P6	82	Total 689	C 414	N 132	O 138	P 1	S 4	0	0
3	P7	82	Total 689	C 414	N 132	O 138	P 1	S 4	0	0
3	P8	82	Total 689	C 414	N 132	O 138	P 1	S 4	0	0
3	P9	82	Total 689	C 414	N 132	O 138	P 1	S 4	0	0

- Molecule 4 is a protein called Portal protein.

Mol	Chain	Residues	Atoms						AltConf	Trace
4	PA	404	Total	C	N	O	P	S	0	0
			3175	1968	541	653	3	10		
4	PB	404	Total	C	N	O	P	S	0	0
			3175	1968	541	653	3	10		
4	PC	398	Total	C	N	O	P	S	0	0
			3119	1932	531	643	3	10		

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Mol	Chain	Residues	Atoms						AltConf	Trace
4	PD	396	Total	C	N	O	P	S	0	0
			3108	1925	529	641	3	10		
4	PE	404	Total	C	N	O	P	S	0	0
			3175	1968	541	653	3	10		
4	PF	404	Total	C	N	O	P	S	0	0
			3175	1968	541	653	3	10		
4	PG	404	Total	C	N	O	P	S	0	0
			3175	1968	541	653	3	10		
4	PH	395	Total	C	N	O	P	S	0	0
			3102	1923	527	639	3	10		
4	PI	399	Total	C	N	O	P	S	0	0
			3145	1951	534	648	3	9		
4	PJ	404	Total	C	N	O	P	S	0	0
			3175	1968	541	653	3	10		
4	PK	401	Total	C	N	O	P	S	0	0
			3147	1950	536	648	3	10		
4	PL	398	Total	C	N	O	P	S	0	0
			3119	1932	531	643	3	10		

- Molecule 5 is a protein called HK97 gp6-like/SPP1 gp15-like head-tail connector.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	PM	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PN	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PO	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PP	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PQ	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PR	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PS	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PT	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PU	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PV	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	PW	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		
5	PX	140	Total	C	N	O	S	0	0
			1087	666	184	235	2		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
6	JA	5	Total	Mg	0
			5	5	
6	JB	6	Total	Mg	0
			6	6	
6	JC	6	Total	Mg	0
			6	6	
6	JD	5	Total	Mg	0
			5	5	
6	JE	5	Total	Mg	0
			5	5	
6	JF	5	Total	Mg	0
			5	5	
6	JI	2	Total	Mg	0
			2	2	
6	KA	6	Total	Mg	0
			6	6	
6	KB	5	Total	Mg	0
			5	5	
6	KC	4	Total	Mg	0
			4	4	
6	KD	7	Total	Mg	0
			7	7	
6	KE	5	Total	Mg	0
			5	5	
6	KF	5	Total	Mg	0
			5	5	
6	KI	1	Total	Mg	0
			1	1	
6	LA	6	Total	Mg	0
			6	6	
6	LB	5	Total	Mg	0
			5	5	
6	LC	4	Total	Mg	0
			4	4	

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Mol	Chain	Residues	Atoms		AltConf
6	LD	7	Total 7	Mg 7	0
6	LE	5	Total 5	Mg 5	0
6	LF	4	Total 4	Mg 4	0
6	LI	1	Total 1	Mg 1	0
6	LJ	1	Total 1	Mg 1	0
6	MA	7	Total 7	Mg 7	0
6	MB	5	Total 5	Mg 5	0
6	MC	3	Total 3	Mg 3	0
6	MD	8	Total 8	Mg 8	0
6	ME	4	Total 4	Mg 4	0
6	MF	5	Total 5	Mg 5	0
6	MI	1	Total 1	Mg 1	0
6	NA	5	Total 5	Mg 5	0
6	NB	6	Total 6	Mg 6	0
6	NC	5	Total 5	Mg 5	0
6	ND	7	Total 7	Mg 7	0
6	NE	4	Total 4	Mg 4	0
6	NF	4	Total 4	Mg 4	0
6	NI	1	Total 1	Mg 1	0
6	PM	2	Total 2	Mg 2	0
6	PN	2	Total 2	Mg 2	0

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Mol	Chain	Residues	Atoms		AltConf
6	PO	1	Total 1	Mg 1	0
6	PP	2	Total 2	Mg 2	0
6	PQ	2	Total 2	Mg 2	0
6	PR	1	Total 1	Mg 1	0
6	PS	1	Total 1	Mg 1	0
6	PT	1	Total 1	Mg 1	0
6	PU	1	Total 1	Mg 1	0
6	PV	1	Total 1	Mg 1	0
6	PW	2	Total 2	Mg 2	0
6	PX	2	Total 2	Mg 2	0

- Molecule 7 is POTASSIUM ION (CCD ID: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
7	JI	1	Total 1	K 1	0
7	JJ	1	Total 1	K 1	0
7	JK	1	Total 1	K 1	0
7	KI	1	Total 1	K 1	0
7	KJ	1	Total 1	K 1	0
7	KK	1	Total 1	K 1	0
7	LI	1	Total 1	K 1	0
7	LJ	1	Total 1	K 1	0
7	LK	1	Total 1	K 1	0

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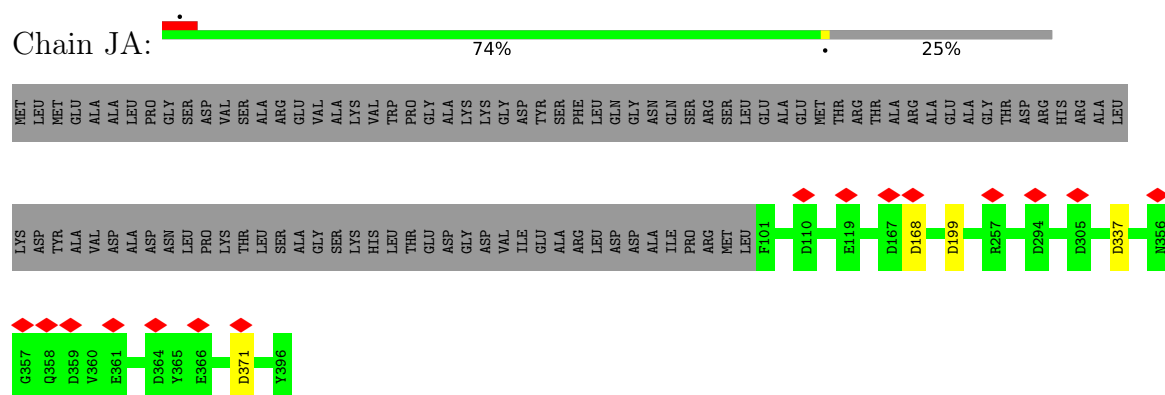
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Mol	Chain	Residues	Atoms		AltConf
7	MI	1	Total 1	K 1	0
7	MJ	2	Total 2	K 2	0
7	MK	1	Total 1	K 1	0
7	NI	1	Total 1	K 1	0
7	NJ	1	Total 1	K 1	0
7	NK	1	Total 1	K 1	0
7	P6	1	Total 1	K 1	0

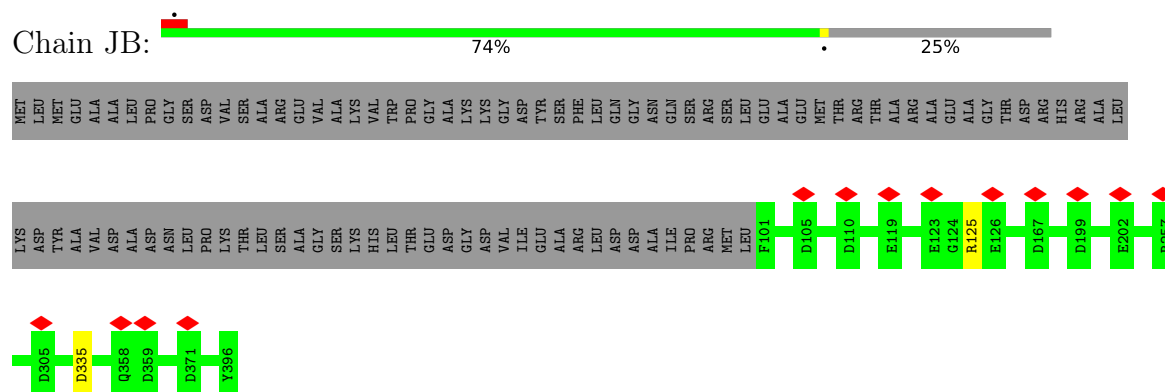
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

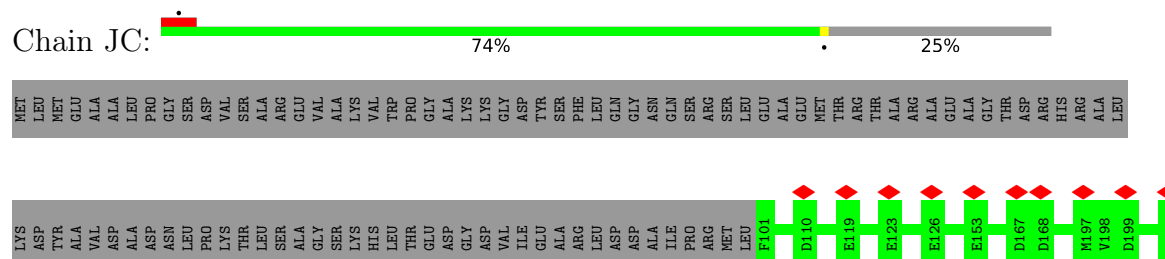
- Molecule 1: HK97 gp5-like major capsid protein

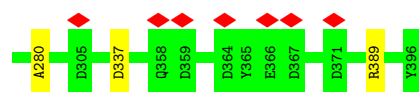


- Molecule 1: HK97 gp5-like major capsid protein



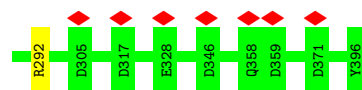
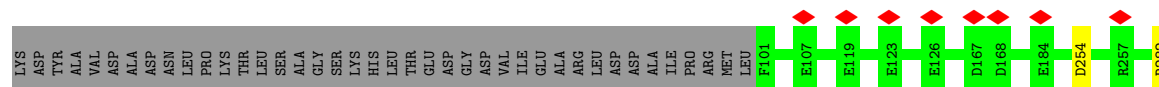
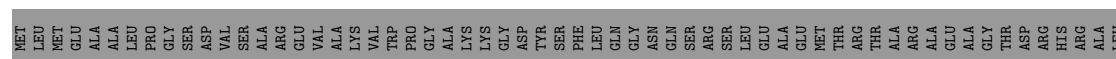
- Molecule 1: HK97 gp5-like major capsid protein





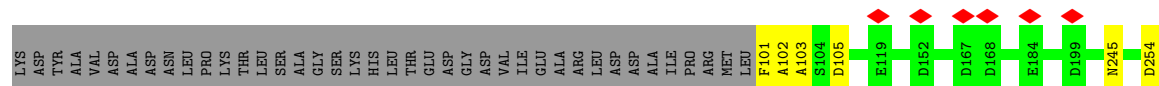
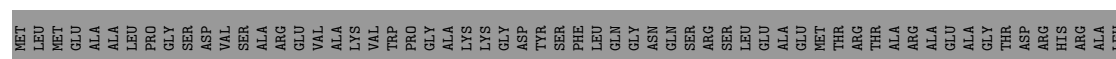
- Molecule 1: HK97 gp5-like major capsid protein

Chain JD: 74% 25%



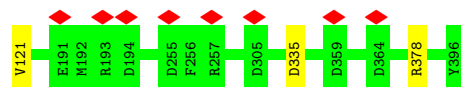
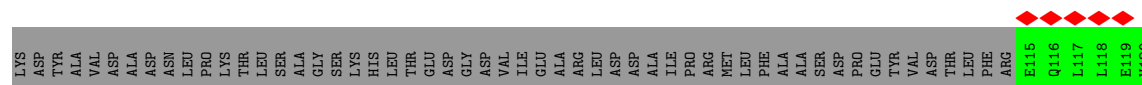
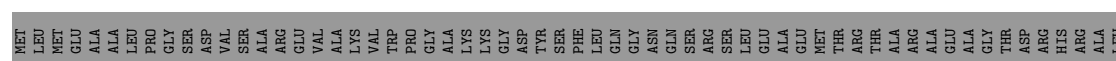
- Molecule 1: HK97 gp5-like major capsid protein

Chain JE: 73% 25%



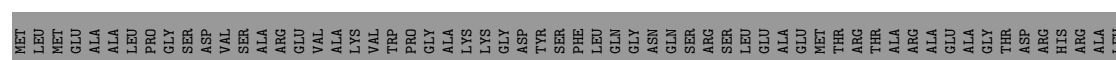
- Molecule 1: HK97 gp5-like major capsid protein

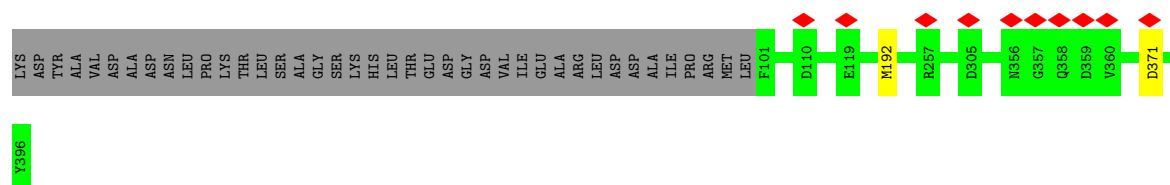
Chain JF: 70% 29%



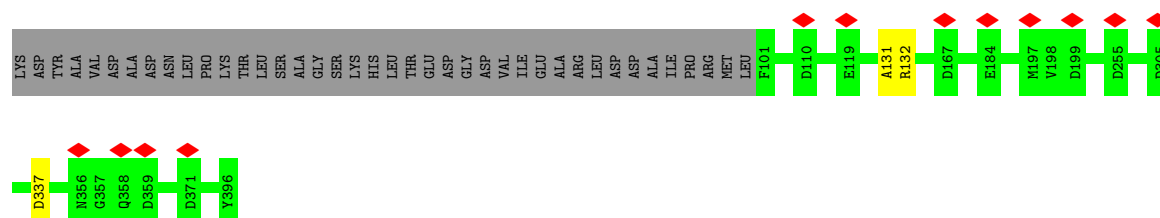
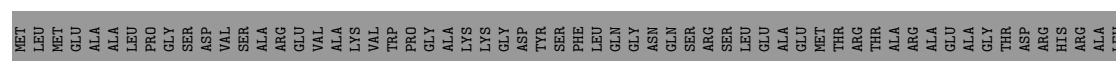
- Molecule 1: HK97 gp5-like major capsid protein

Chain KA: 74% 25%

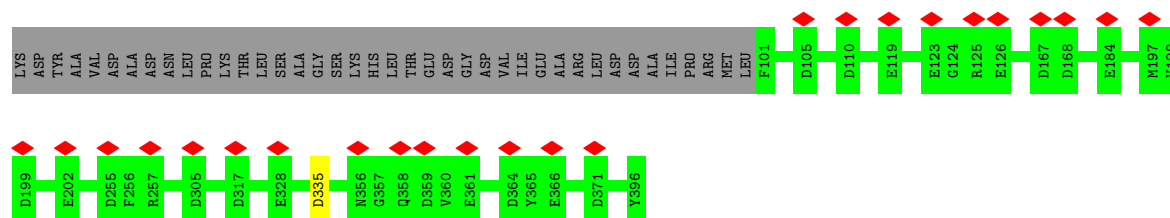
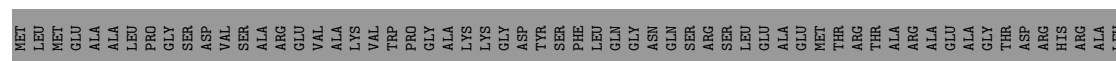
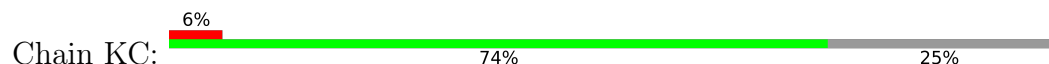




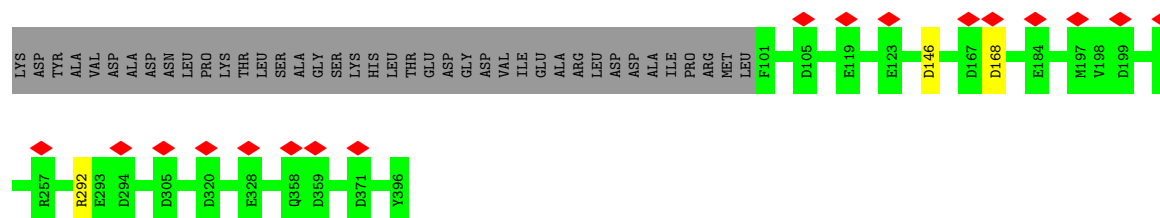
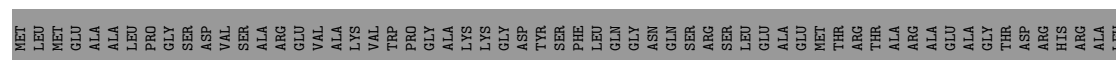
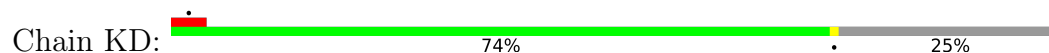
- Molecule 1: HK97 gp5-like major capsid protein



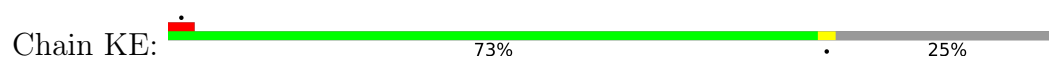
- Molecule 1: HK97 gp5-like major capsid protein



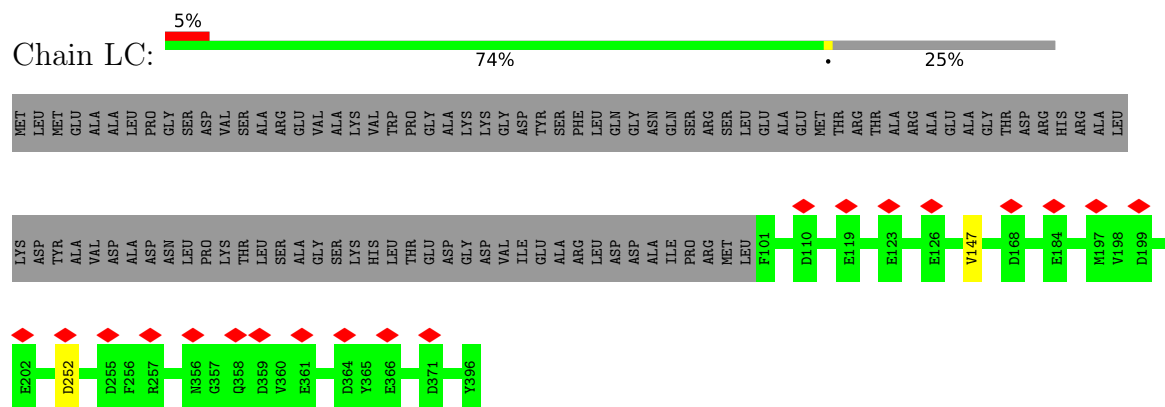
- Molecule 1: HK97 gp5-like major capsid protein



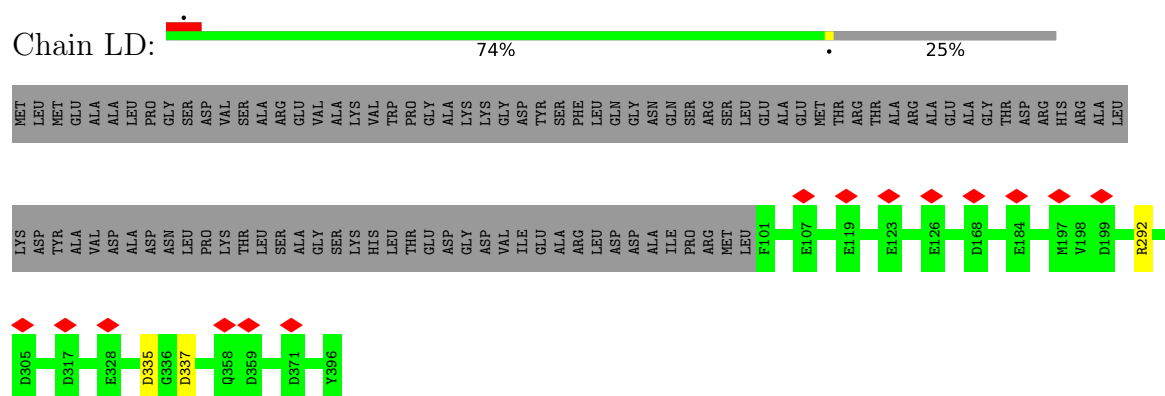
- Molecule 1: HK97 gp5-like major capsid protein



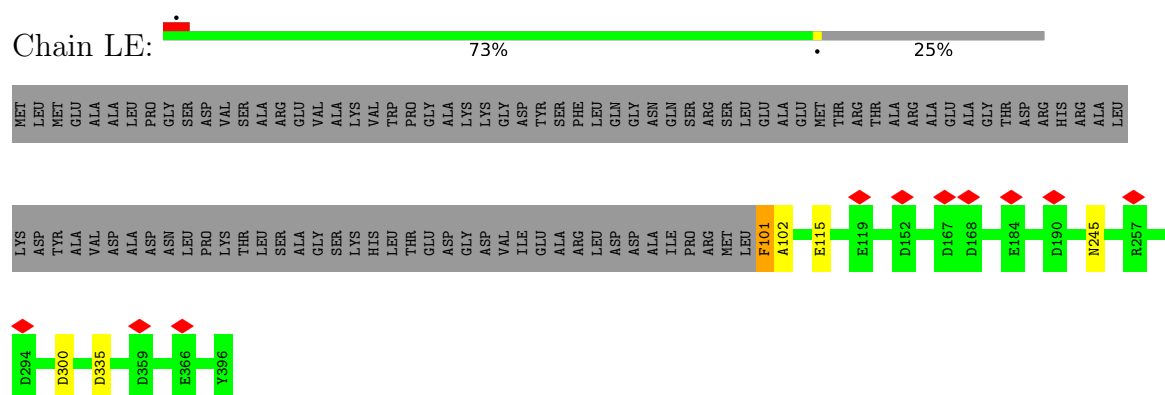
- Molecule 1: HK97 gp5-like major capsid protein



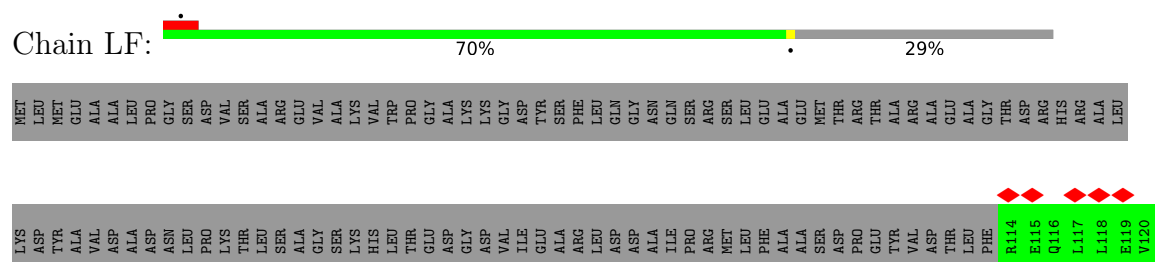
- Molecule 1: HK97 gp5-like major capsid protein

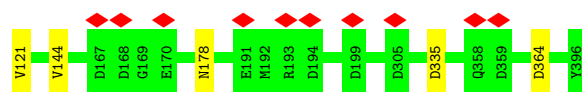


- Molecule 1: HK97 gp5-like major capsid protein



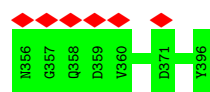
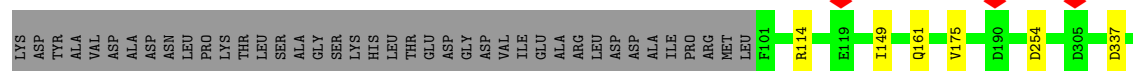
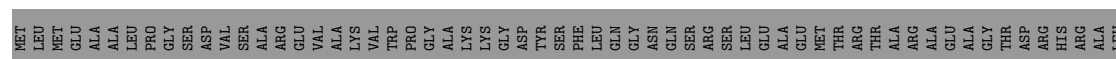
- Molecule 1: HK97 gp5-like major capsid protein





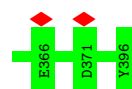
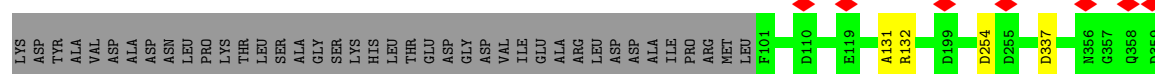
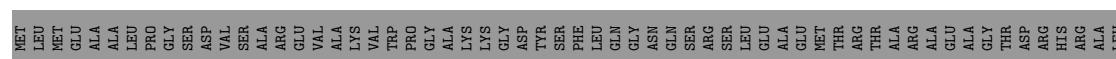
- Molecule 1: HK97 gp5-like major capsid protein

Chain MA: 73% 25%



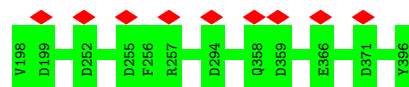
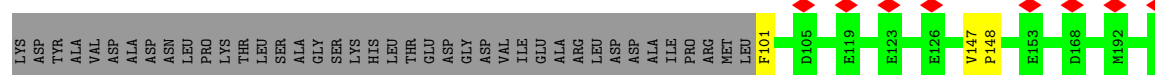
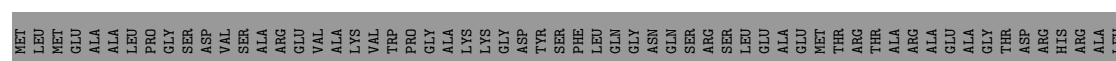
- Molecule 1: HK97 gp5-like major capsid protein

Chain MB: 74% 25%



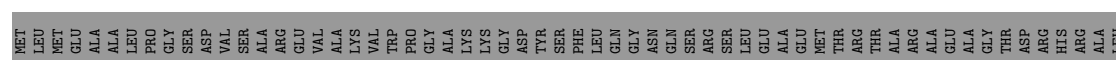
- Molecule 1: HK97 gp5-like major capsid protein

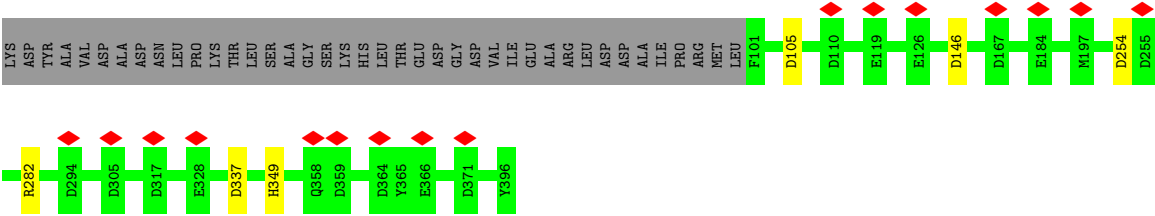
Chain MC: 74% 25%



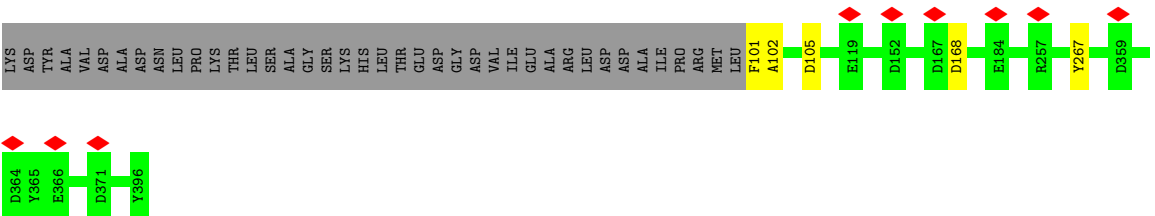
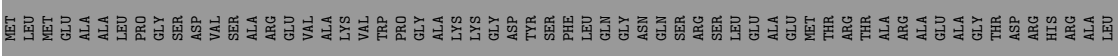
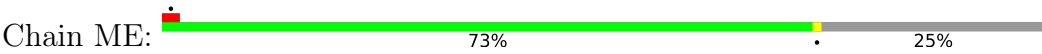
- Molecule 1: HK97 gp5-like major capsid protein

Chain MD: 73% 25%

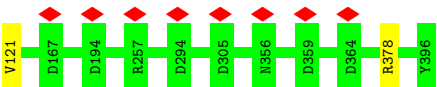
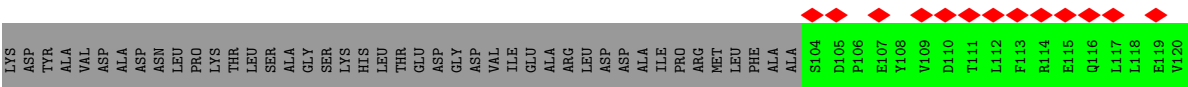
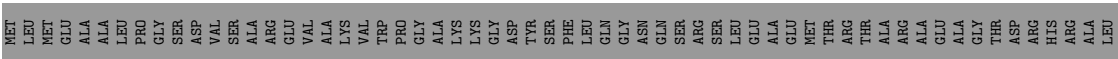
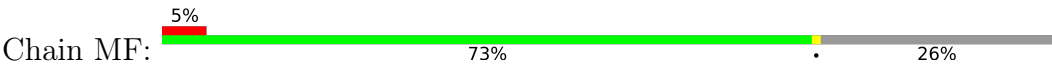




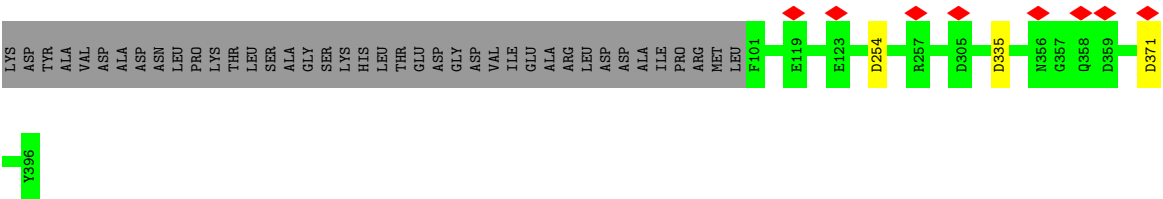
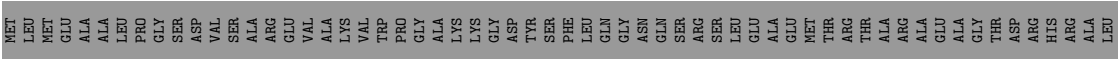
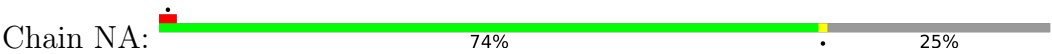
• Molecule 1: HK97 gp5-like major capsid protein



• Molecule 1: HK97 gp5-like major capsid protein

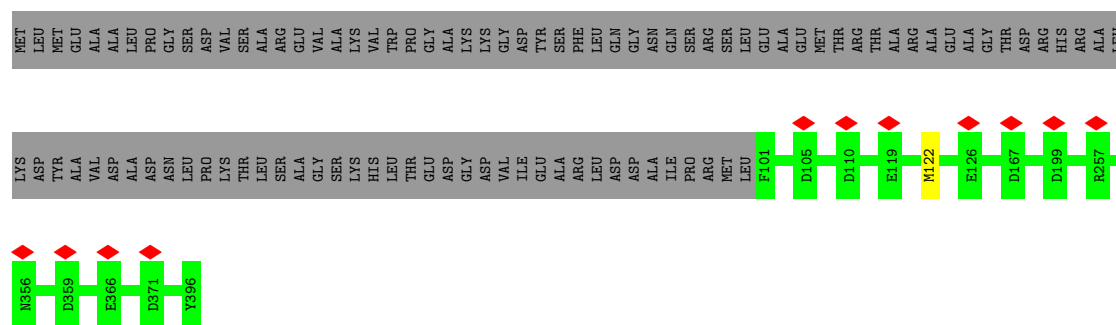


• Molecule 1: HK97 gp5-like major capsid protein



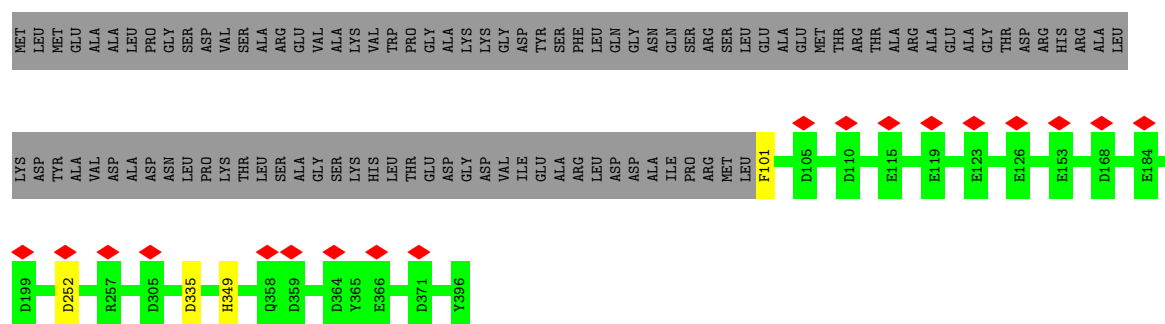
• Molecule 1: HK97 gp5-like major capsid protein

Chain NB: 



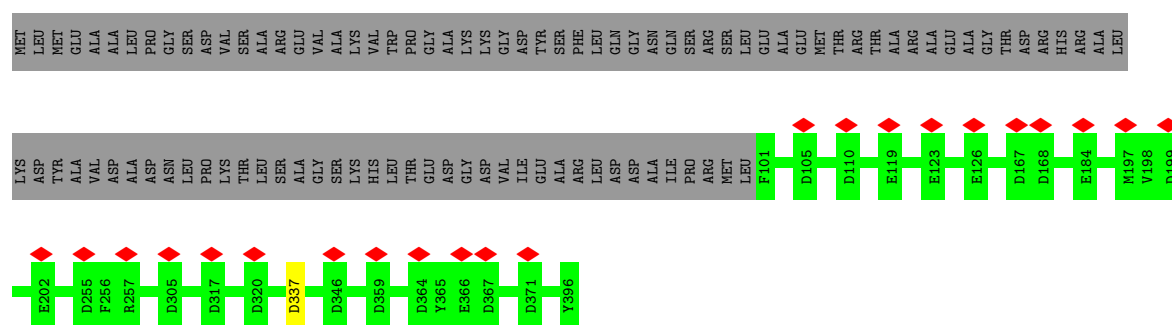
- Molecule 1: HK97 gp5-like major capsid protein

Chain NC: 



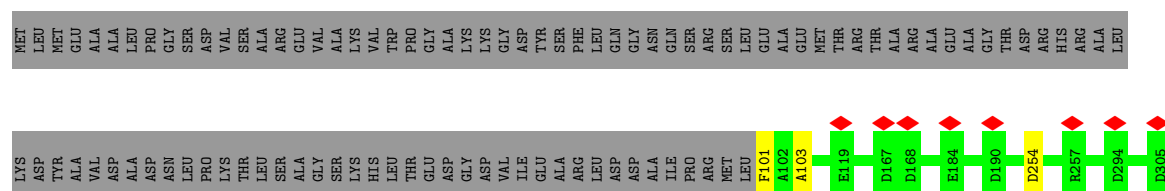
- Molecule 1: HK97 gp5-like major capsid protein

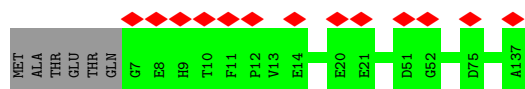
Chain ND: 



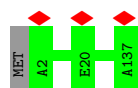
- Molecule 1: HK97 gp5-like major capsid protein

Chain NE: 

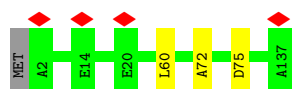




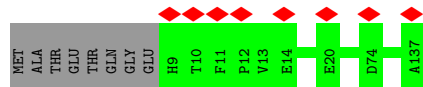
- Molecule 2: Capsid stabilization protein



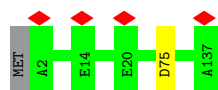
- Molecule 2: Capsid stabilization protein



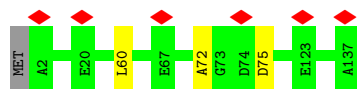
- Molecule 2: Capsid stabilization protein



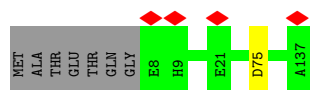
- Molecule 2: Capsid stabilization protein



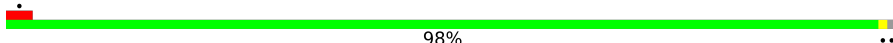
- Molecule 2: Capsid stabilization protein

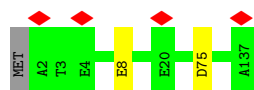


- Molecule 2: Capsid stabilization protein

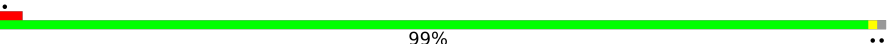


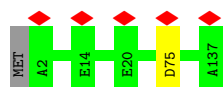
- Molecule 2: Capsid stabilization protein

Chain MK:  98%



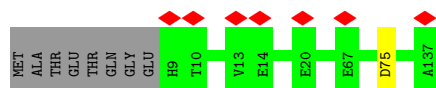
- Molecule 2: Capsid stabilization protein

Chain NI:  99%

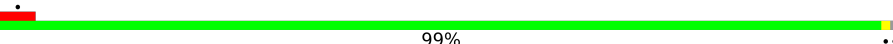


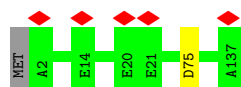
- Molecule 2: Capsid stabilization protein

Chain NJ:  5% 93% 6%

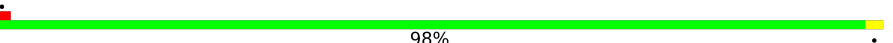


- Molecule 2: Capsid stabilization protein

Chain NK:  99%

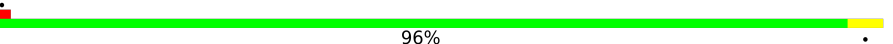


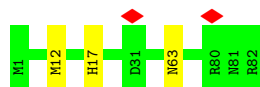
- Molecule 3: Hypothetical protein gp21

Chain P5:  98%

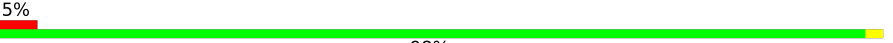


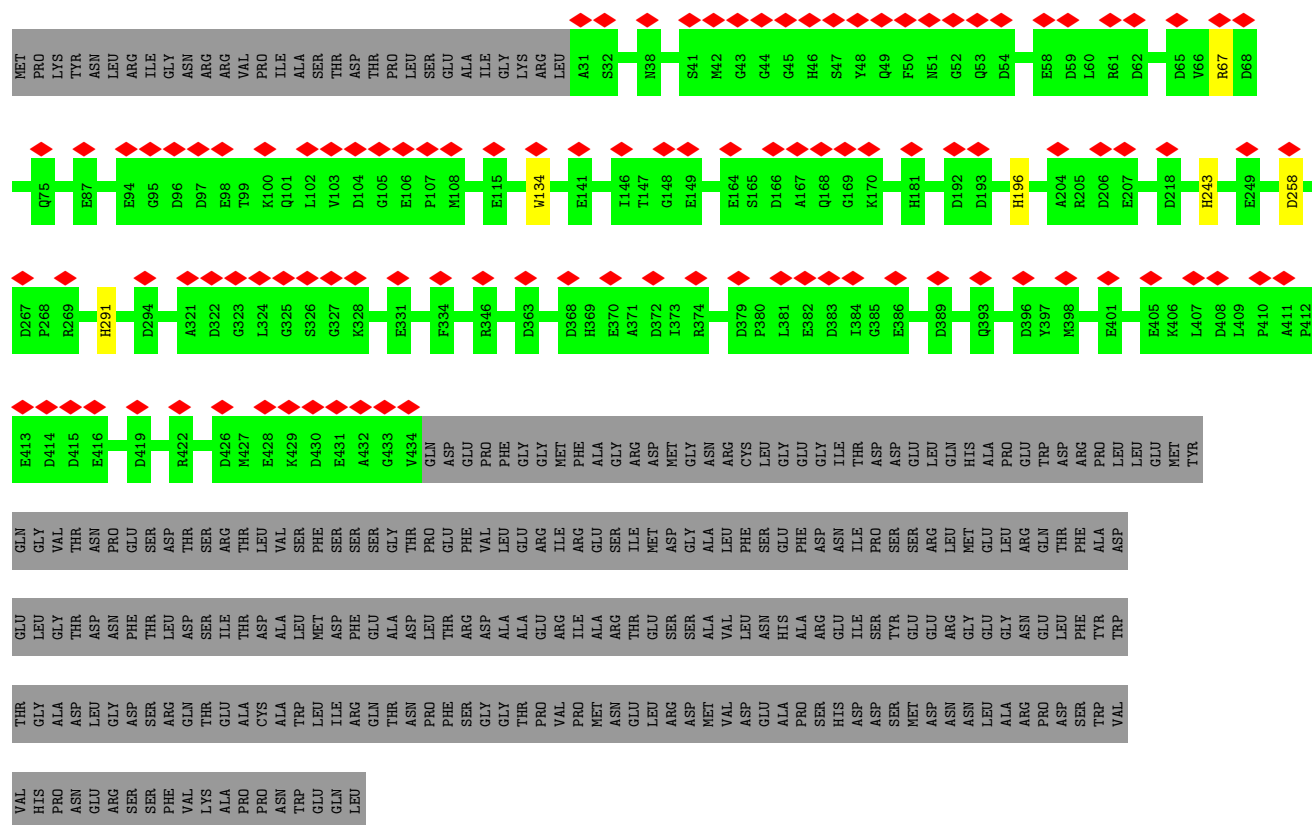
- Molecule 3: Hypothetical protein gp21

Chain P6:  96%

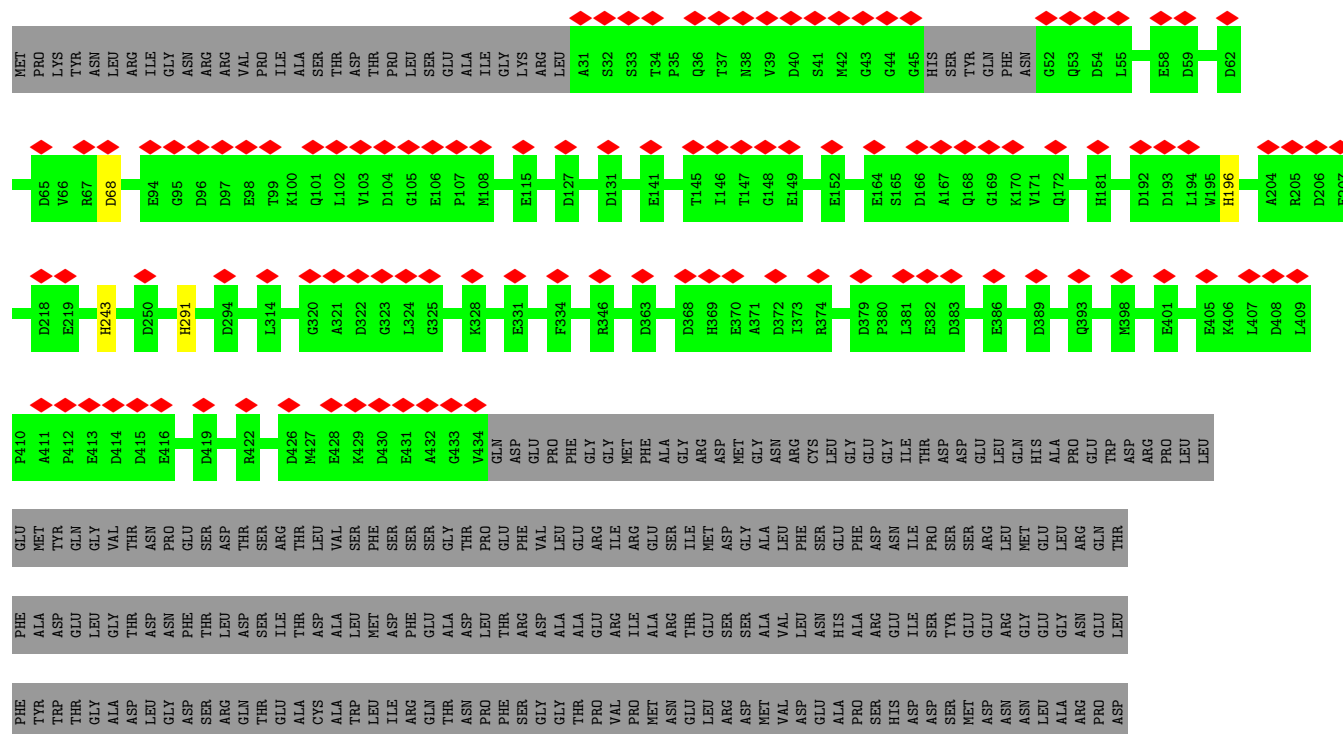


- Molecule 3: Hypothetical protein gp21

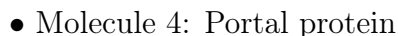
Chain P7:  5% 98%



• Molecule 4: Portal protein

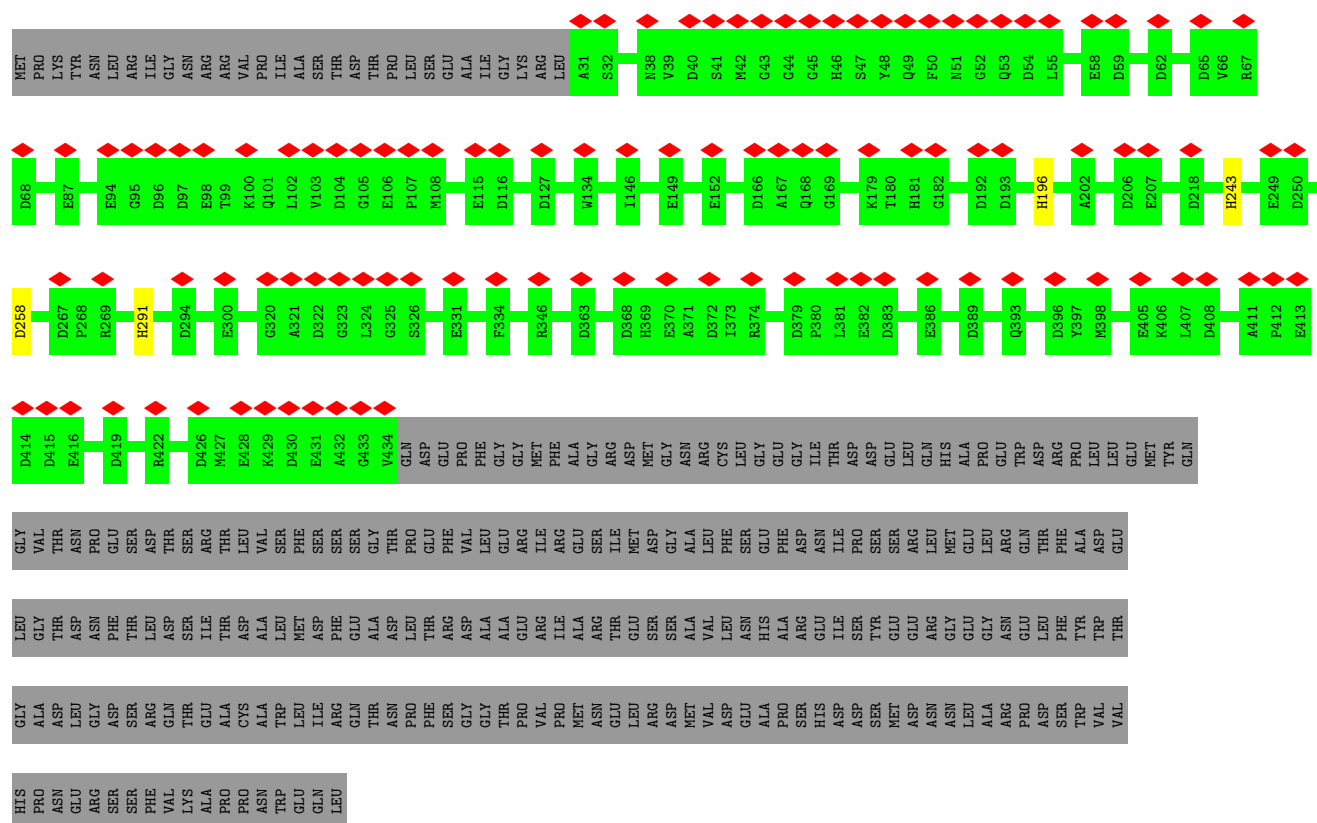


Chain PD:

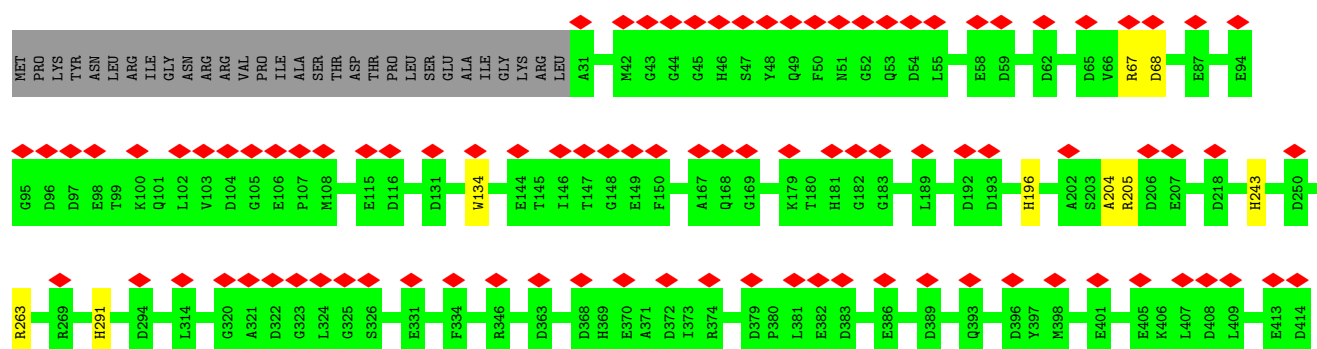


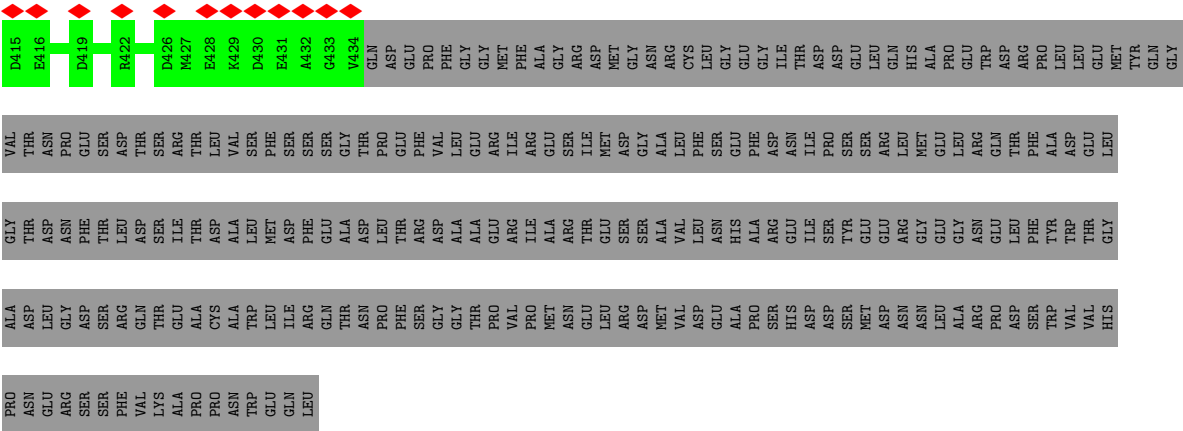
SER	GLY	GLY	THR	PRO	VAL	PRO	MET	ASN	GLU	ARG	ASP	MET	VAL	ASP	GLU	ALA	PRO	SER	HIS	ASP	ASP	ASP	SER	MET	ASP	ASN	ASN	LEU	ALA	ARG	PRO	ASP	ASP	TRP	VAL	VAL	HIS	PRO	ASN	GLU	ARG	SER	SER	PHE	VAL	LYS	ALA	ALA	PRO	PRO	ASN	TRP	TRP	GLU	GLN	LEU
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

Chain PF:

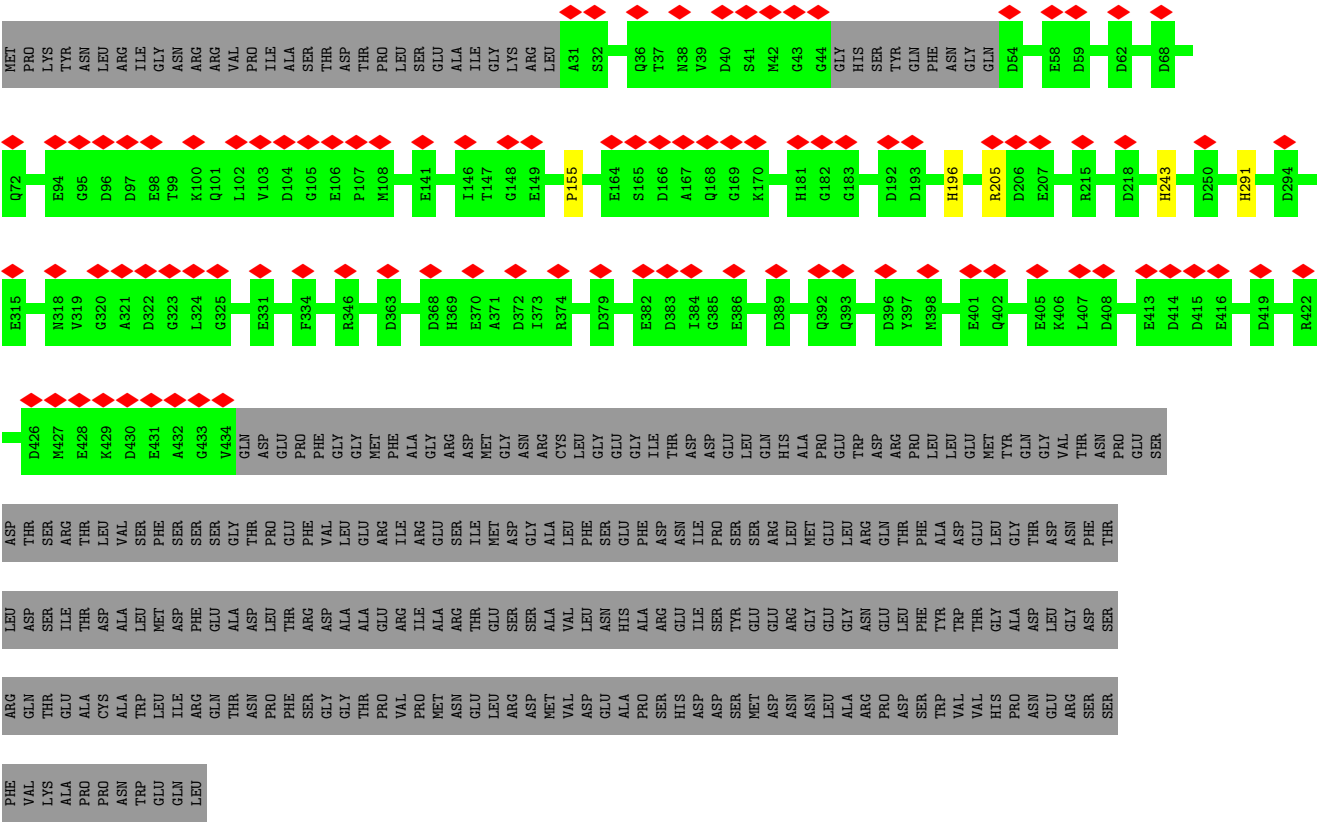


Chain PG:

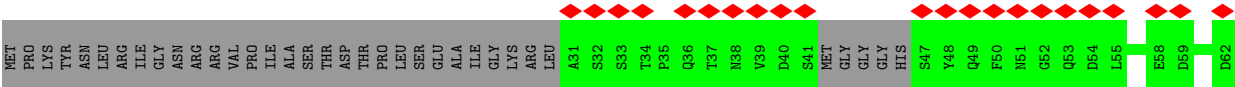


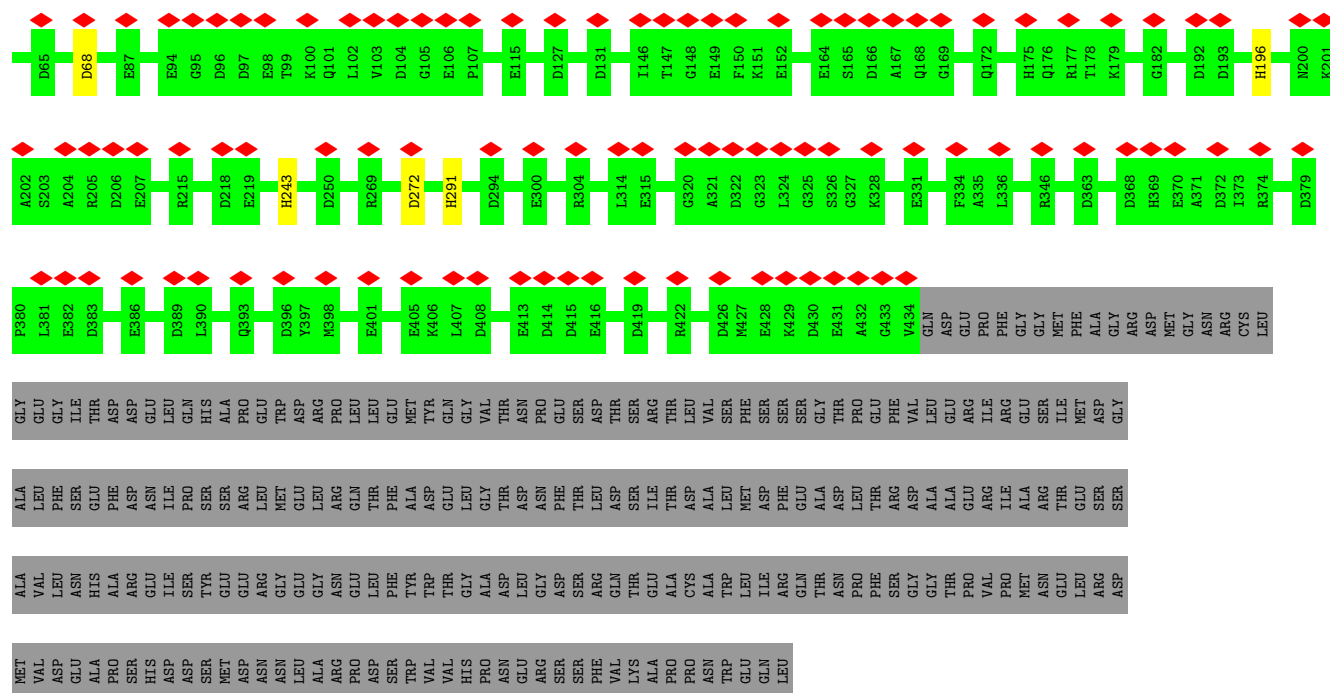


• Molecule 4: Portal protein

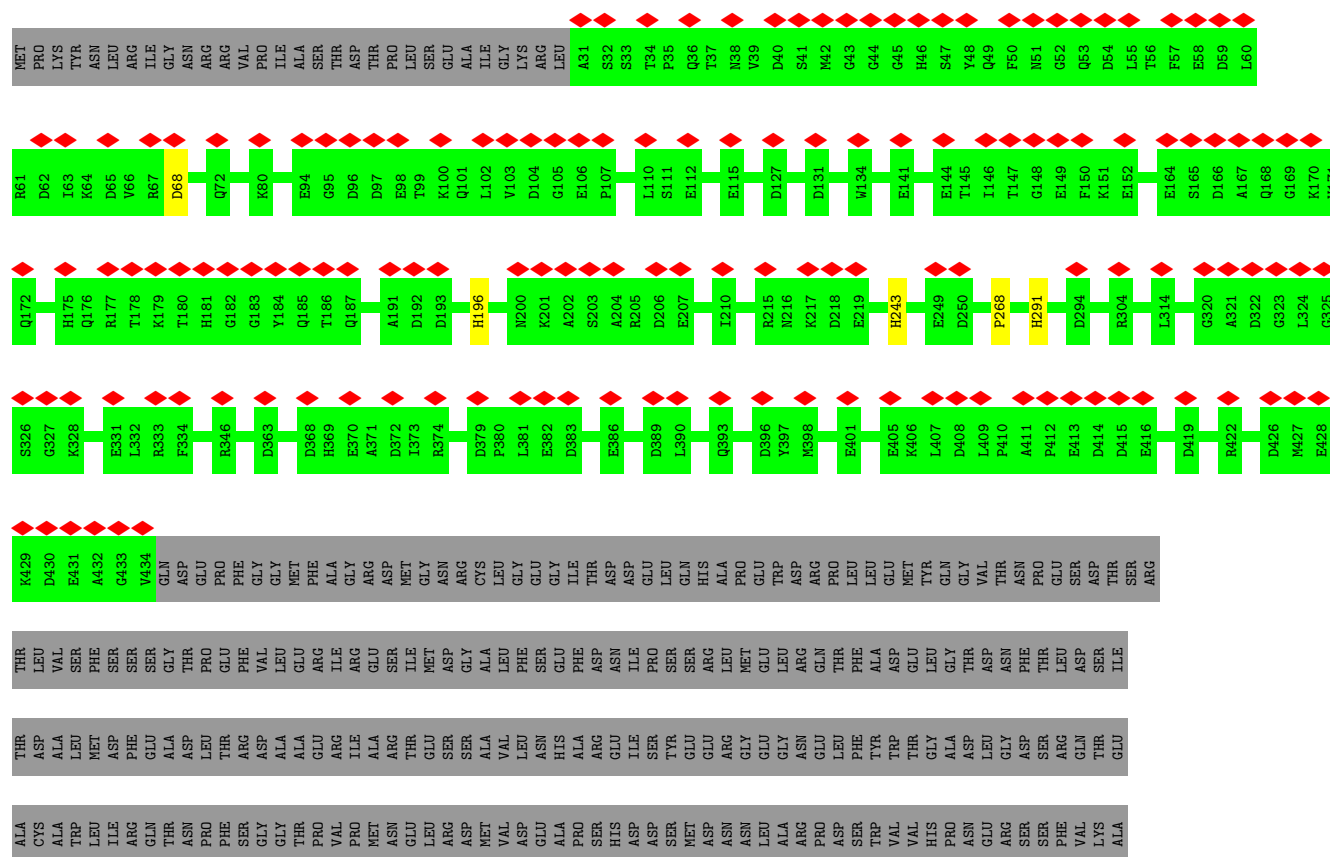


• Molecule 4: Portal protein



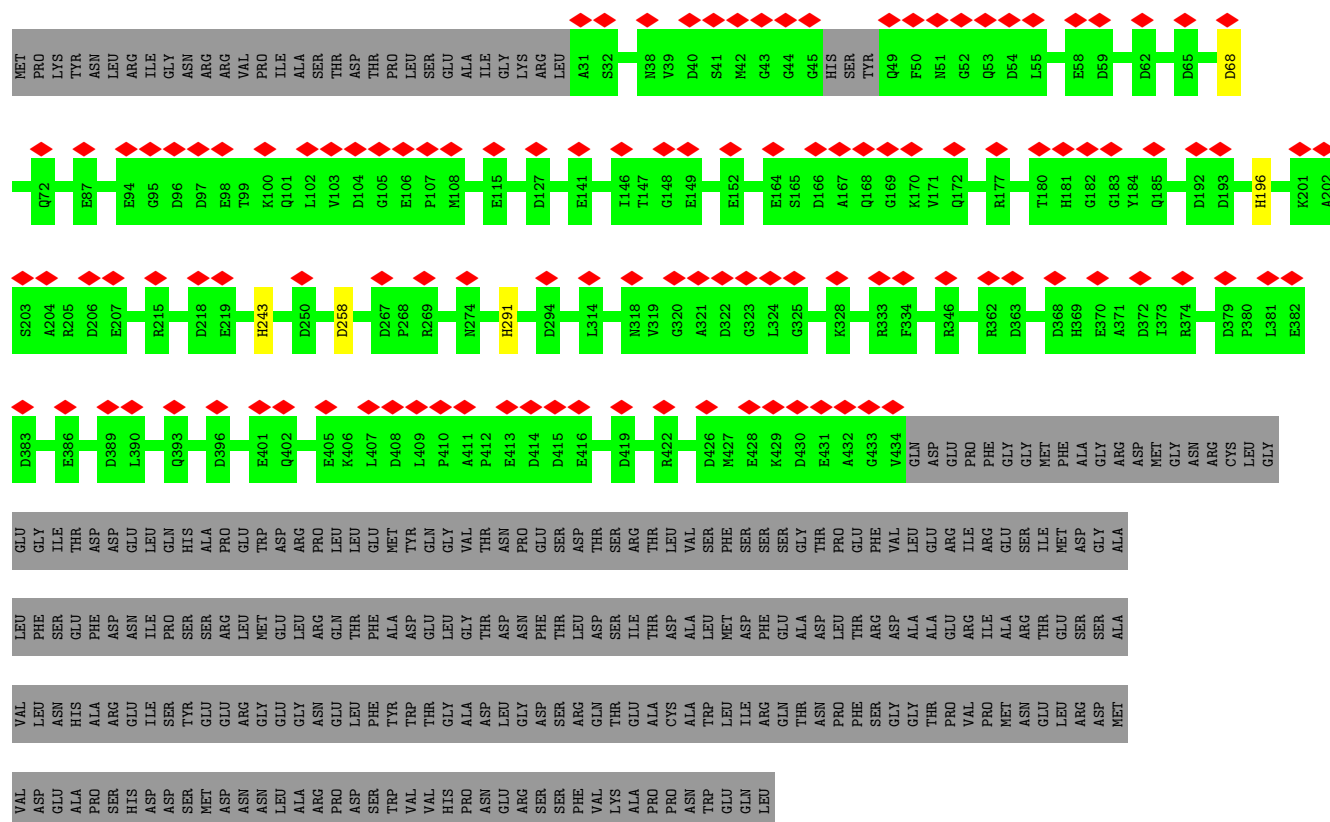


• Molecule 4: Portal protein

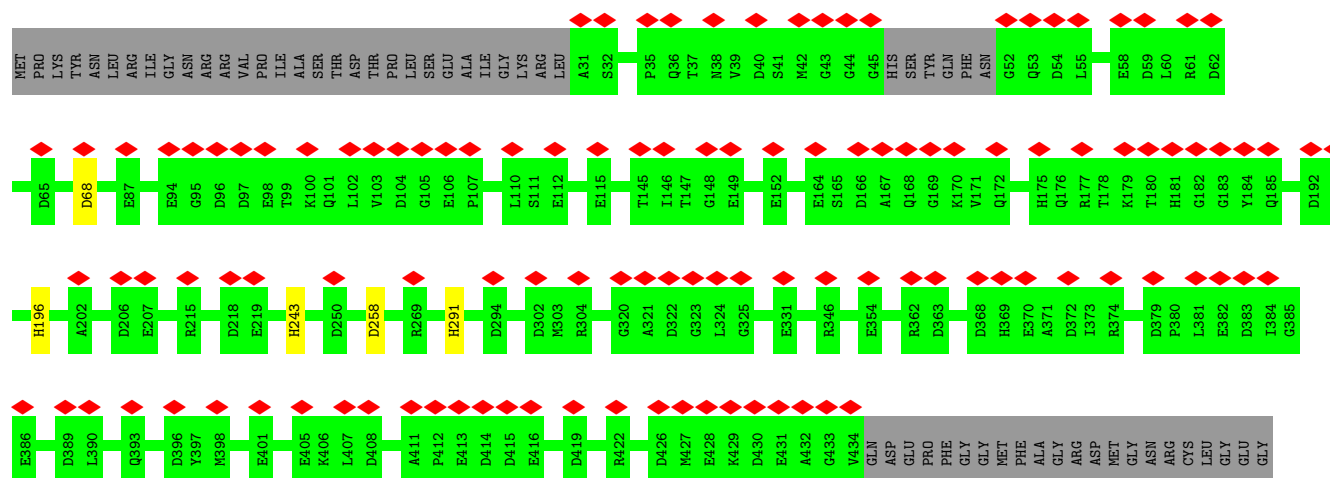


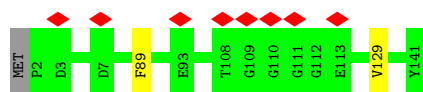
PRO
PRO
ASN
TRP
GLU
GLN
LEU

• Molecule 4: Portal protein

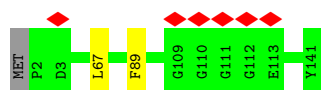


• Molecule 4: Portal protein

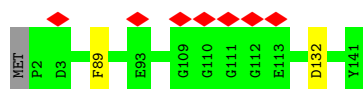




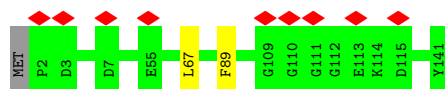
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



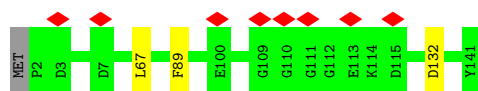
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



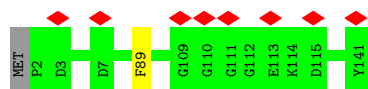
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157388	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50, 54.6	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	TFS FALCON 4i (4k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.057	Depositor
Minimum map value	-0.028	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	412.19202, 412.19202, 412.19202	wwPDB
Map dimensions	352, 352, 352	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.171, 1.171, 1.171	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, HIP, K

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	JA	0.54	0/2335	1.06	3/3172 (0.1%)
1	JB	0.55	0/2335	1.02	1/3172 (0.0%)
1	JC	0.55	0/2335	1.04	3/3172 (0.1%)
1	JD	0.55	0/2335	1.04	2/3172 (0.1%)
1	JE	0.54	0/2335	1.05	3/3172 (0.1%)
1	JF	0.55	0/2216	1.05	1/3009 (0.0%)
1	KA	0.54	0/2335	1.02	0/3172
1	KB	0.55	0/2335	1.05	1/3172 (0.0%)
1	KC	0.55	0/2335	1.05	1/3172 (0.0%)
1	KD	0.56	0/2335	1.06	2/3172 (0.1%)
1	KE	0.54	0/2335	1.04	4/3172 (0.1%)
1	KF	0.54	0/2216	1.04	1/3009 (0.0%)
1	LA	0.55	0/2335	1.07	2/3172 (0.1%)
1	LB	0.55	0/2335	1.05	0/3172
1	LC	0.55	0/2335	1.04	1/3172 (0.0%)
1	LD	0.56	0/2335	1.03	2/3172 (0.1%)
1	LE	0.54	0/2335	1.04	2/3172 (0.1%)
1	LF	0.55	0/2227	1.04	3/3023 (0.1%)
1	MA	0.55	0/2335	1.07	3/3172 (0.1%)
1	MB	0.55	0/2335	1.06	2/3172 (0.1%)
1	MC	0.55	0/2335	1.05	1/3172 (0.0%)
1	MD	0.55	0/2335	1.06	6/3172 (0.2%)
1	ME	0.55	0/2335	1.02	1/3172 (0.0%)
1	MF	0.55	0/2313	1.05	0/3142
1	NA	0.54	0/2335	1.05	2/3172 (0.1%)
1	NB	0.55	0/2335	1.03	1/3172 (0.0%)
1	NC	0.55	0/2335	1.07	3/3172 (0.1%)
1	ND	0.55	0/2335	1.04	1/3172 (0.0%)
1	NE	0.54	0/2335	1.05	1/3172 (0.0%)
1	NF	0.55	0/2216	1.06	1/3009 (0.0%)
2	JI	0.58	0/980	0.94	0/1337
2	JJ	0.59	0/943	0.96	2/1286 (0.2%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	JK	0.57	0/980	0.97	2/1337 (0.1%)
2	KI	0.59	0/980	0.98	1/1337 (0.1%)
2	KJ	0.60	0/943	0.97	0/1286
2	KK	0.58	0/980	0.95	0/1337
2	LI	0.58	0/980	0.95	1/1337 (0.1%)
2	LJ	0.60	0/930	0.96	0/1269
2	LK	0.58	0/980	0.95	1/1337 (0.1%)
2	MI	0.59	0/980	0.94	1/1337 (0.1%)
2	MJ	0.59	0/939	0.96	1/1281 (0.1%)
2	MK	0.57	0/980	0.96	1/1337 (0.1%)
2	NI	0.58	0/980	0.94	1/1337 (0.1%)
2	NJ	0.60	0/930	0.98	1/1269 (0.1%)
2	NK	0.58	0/980	0.95	1/1337 (0.1%)
3	P5	0.53	0/685	1.11	0/918
3	P6	0.54	0/685	1.13	2/918 (0.2%)
3	P7	0.54	0/685	1.10	0/918
3	P8	0.53	0/685	1.09	0/918
3	P9	0.54	0/685	1.12	0/918
4	PA	0.55	0/3190	1.01	1/4326 (0.0%)
4	PB	0.54	0/3190	1.01	0/4326
4	PC	0.54	0/3130	1.00	1/4243 (0.0%)
4	PD	0.55	0/3119	1.02	2/4228 (0.0%)
4	PE	0.55	0/3190	1.01	3/4326 (0.1%)
4	PF	0.54	0/3190	0.99	0/4326
4	PG	0.55	0/3190	1.00	2/4326 (0.0%)
4	PH	0.54	0/3113	1.00	1/4221 (0.0%)
4	PI	0.54	0/3158	1.01	2/4283 (0.0%)
4	PJ	0.55	0/3190	1.00	1/4326 (0.0%)
4	PK	0.55	0/3159	1.01	1/4282 (0.0%)
4	PL	0.54	0/3130	0.98	1/4243 (0.0%)
5	PM	0.56	0/1105	1.08	0/1492
5	PN	0.56	0/1105	1.03	1/1492 (0.1%)
5	PO	0.55	0/1105	1.02	1/1492 (0.1%)
5	PP	0.56	0/1105	1.05	1/1492 (0.1%)
5	PQ	0.58	0/1105	1.07	0/1492
5	PR	0.55	0/1105	1.04	1/1492 (0.1%)
5	PS	0.56	0/1105	1.06	1/1492 (0.1%)
5	PT	0.56	0/1105	1.05	2/1492 (0.1%)
5	PU	0.56	0/1105	1.06	1/1492 (0.1%)
5	PV	0.55	0/1105	1.02	2/1492 (0.1%)
5	PW	0.55	0/1105	1.05	1/1492 (0.1%)
5	PX	0.56	0/1105	1.02	1/1492 (0.1%)
All	All	0.55	0/138682	1.03	96/188203 (0.1%)

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	LE	0	1
1	ME	0	1
1	NE	0	1
All	All	0	3

There are no bond length outliers.

All (96) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	NI	75	ASP	CA-CB-CG	8.10	120.70	112.60
2	MK	75	ASP	CA-CB-CG	7.79	120.39	112.60
2	NJ	75	ASP	CA-CB-CG	7.47	120.07	112.60
4	PI	272	ASP	CA-CB-CG	7.26	119.86	112.60
4	PD	205	ARG	CG-CD-NE	7.23	127.92	112.00
2	JK	75	ASP	CA-CB-CG	7.13	119.73	112.60
2	MI	75	ASP	CA-CB-CG	7.01	119.61	112.60
4	PE	205	ARG	CG-CD-NE	6.89	127.15	112.00
1	MD	105	ASP	CA-CB-CG	6.84	119.44	112.60
2	JJ	75	ASP	CA-CB-CG	6.82	119.42	112.60
2	MJ	75	ASP	CA-CB-CG	6.69	119.29	112.60
1	LF	178	ASN	CA-CB-CG	6.51	119.11	112.60
4	PH	205	ARG	CG-CD-NE	6.29	125.84	112.00
2	LK	75	ASP	CA-CB-CG	6.23	118.83	112.60
4	PG	205	ARG	CG-CD-NE	6.13	125.48	112.00
1	MD	282	ARG	CG-CD-NE	6.04	125.29	112.00
1	LE	335	ASP	CA-CB-CG	5.96	118.56	112.60
1	JA	168	ASP	CA-CB-CG	5.93	118.53	112.60
1	KE	300	ASP	CA-CB-CG	5.93	118.53	112.60
1	KE	335	ASP	CA-CB-CG	5.86	118.45	112.60
1	KB	337	ASP	CA-CB-CG	5.84	118.44	112.60
1	JA	337	ASP	CA-CB-CG	5.80	118.40	112.60
4	PK	68	ASP	CA-CB-CG	5.78	118.38	112.60
1	KE	254	ASP	CA-CB-CG	5.76	118.36	112.60
2	NK	75	ASP	CA-CB-CG	5.70	118.30	112.60
1	LF	335	ASP	CA-CB-CG	5.69	118.29	112.60
4	PI	68	ASP	CA-CB-CG	5.66	118.26	112.60
1	MA	337	ASP	CA-CB-CG	5.62	118.22	112.60
5	PT	89	PHE	CA-CB-CG	5.62	119.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	PE	68	ASP	CA-CB-CG	5.58	118.18	112.60
1	KF	335	ASP	CA-CB-CG	5.58	118.17	112.60
2	LI	75	ASP	CA-CB-CG	5.55	118.15	112.60
4	PG	68	ASP	CA-CB-CG	5.55	118.15	112.60
2	JK	20	GLU	CB-CG-CD	5.55	122.03	112.60
1	MA	254	ASP	CA-CB-CG	5.55	118.15	112.60
1	NE	254	ASP	CA-CB-CG	5.52	118.12	112.60
1	NC	101	PHE	CA-CB-CG	5.49	119.29	113.80
2	JJ	62	ASP	CA-CB-CG	5.48	118.08	112.60
1	JA	199	ASP	CA-CB-CG	5.48	118.08	112.60
5	PR	89	PHE	CA-CB-CG	5.47	119.27	113.80
1	MC	101	PHE	CA-CB-CG	5.44	119.24	113.80
1	KD	168	ASP	CA-CB-CG	5.43	118.03	112.60
1	KC	335	ASP	CA-CB-CG	5.42	118.03	112.60
5	PN	89	PHE	CA-CB-CG	5.42	119.22	113.80
1	MB	337	ASP	CA-CB-CG	5.39	117.99	112.60
1	MD	254	ASP	CA-CB-CG	5.39	117.99	112.60
1	JE	254	ASP	CA-CB-CG	5.39	117.99	112.60
1	LF	364	ASP	CA-CB-CG	5.39	117.99	112.60
4	PL	68	ASP	CA-CB-CG	5.39	117.99	112.60
1	JB	335	ASP	CA-CB-CG	5.36	117.96	112.60
1	JC	337	ASP	CA-CB-CG	5.36	117.96	112.60
1	KD	146	ASP	CA-CB-CG	5.34	117.94	112.60
1	LE	300	ASP	CA-CB-CG	5.34	117.94	112.60
1	LA	378	ARG	NE-CZ-NH2	5.32	123.99	119.20
1	JE	105	ASP	CA-CB-CG	5.30	117.90	112.60
5	PW	89	PHE	CA-CB-CG	5.27	119.07	113.80
1	MD	146	ASP	CA-CB-CG	5.27	117.87	112.60
5	PT	132	ASP	CA-CB-CG	5.26	117.86	112.60
1	NA	335	ASP	CA-CB-CG	5.25	117.85	112.60
1	KE	105	ASP	CA-CB-CG	5.21	117.81	112.60
1	JD	282	ARG	CG-CD-NE	5.19	123.42	112.00
1	ME	168	ASP	CA-CB-CG	5.19	117.79	112.60
1	NC	335	ASP	CA-CB-CG	5.18	117.78	112.60
1	MD	337	ASP	CA-CB-CG	5.18	117.78	112.60
4	PA	205	ARG	CG-CD-NE	5.18	123.39	112.00
1	ND	337	ASP	CA-CB-CG	5.16	117.76	112.60
1	JC	280	ALA	CA-C-N	5.16	128.55	120.82
1	JC	280	ALA	C-N-CA	5.16	128.55	120.82
1	MA	114	ARG	CG-CD-NE	5.15	123.33	112.00
1	LD	337	ASP	CA-CB-CG	5.15	117.75	112.60
5	PV	89	PHE	CA-CB-CG	5.15	118.95	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	JD	254	ASP	CA-CB-CG	5.13	117.73	112.60
1	LD	335	ASP	CA-CB-CG	5.13	117.73	112.60
1	LA	254	ASP	CA-CB-CG	5.11	117.71	112.60
5	PO	89	PHE	CA-CB-CG	5.11	118.91	113.80
4	PC	68	ASP	CA-CB-CG	5.11	117.70	112.60
5	PS	89	PHE	CA-CB-CG	5.11	118.91	113.80
1	NB	335	ASP	CA-CB-CG	5.10	117.70	112.60
5	PP	89	PHE	CA-CB-CG	5.09	118.89	113.80
1	NF	378	ARG	NE-CZ-NH2	5.07	123.76	119.20
4	PD	177	ARG	CG-CD-NE	5.06	123.14	112.00
2	KI	74	ASP	CA-CB-CG	5.06	117.66	112.60
3	P6	63	ASN	CA-C-N	5.06	128.06	120.87
3	P6	63	ASN	C-N-CA	5.06	128.06	120.87
5	PV	132	ASP	CA-CB-CG	5.05	117.65	112.60
1	JE	335	ASP	CA-CB-CG	5.04	117.64	112.60
1	JF	335	ASP	CA-CB-CG	5.04	117.64	112.60
1	NC	252	ASP	CA-CB-CG	5.04	117.64	112.60
1	MD	349	HIS	CA-CB-CG	-5.03	108.77	113.80
1	LC	252	ASP	CA-CB-CG	5.02	117.62	112.60
1	NA	254	ASP	CA-CB-CG	5.02	117.62	112.60
4	PJ	68	ASP	CA-CB-CG	5.01	117.61	112.60
5	PU	89	PHE	CA-CB-CG	5.01	118.81	113.80
1	MB	254	ASP	CA-CB-CG	5.01	117.61	112.60
4	PE	322	ASP	CA-CB-CG	5.01	117.61	112.60
5	PX	89	PHE	CA-CB-CG	5.01	118.81	113.80

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	LE	101	PHE	Peptide
1	ME	267	TYR	Sidechain
1	NE	101	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JA	2298	0	2139	1	0
1	JB	2298	0	2139	1	0
1	JC	2298	0	2139	1	0
1	JD	2298	0	2139	1	0
1	JE	2298	0	2139	3	0
1	JF	2183	0	2036	2	0
1	KA	2298	0	2138	3	0
1	KB	2298	0	2139	1	0
1	KC	2298	0	2139	0	0
1	KD	2298	0	2139	1	0
1	KE	2298	0	2139	2	0
1	KF	2183	0	2036	3	0
1	LA	2298	0	2139	3	0
1	LB	2298	0	2139	1	0
1	LC	2298	0	2139	1	0
1	LD	2298	0	2139	1	0
1	LE	2298	0	2139	3	0
1	LF	2194	0	2049	2	0
1	MA	2298	0	2139	3	0
1	MB	2298	0	2139	1	0
1	MC	2298	0	2139	1	0
1	MD	2298	0	2139	0	0
1	ME	2298	0	2139	3	0
1	MF	2277	0	2120	2	0
1	NA	2298	0	2139	1	0
1	NB	2298	0	2139	1	0
1	NC	2298	0	2139	1	0
1	ND	2298	0	2139	0	0
1	NE	2298	0	2139	1	0
1	NF	2183	0	2036	2	0
2	JI	967	0	894	1	0
2	JJ	930	0	861	0	0
2	JK	967	0	894	0	0
2	KI	967	0	894	1	0
2	KJ	930	0	861	0	0
2	KK	967	0	894	0	0
2	LI	967	0	894	1	0
2	LJ	917	0	852	0	0
2	LK	967	0	894	0	0
2	MI	967	0	894	1	0
2	MJ	926	0	858	0	0
2	MK	967	0	894	1	0
2	NI	967	0	894	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	NJ	917	0	852	0	0
2	NK	967	0	894	0	0
3	P5	689	0	651	1	0
3	P6	689	0	651	2	0
3	P7	689	0	651	2	0
3	P8	689	0	651	3	0
3	P9	689	0	651	1	0
4	PA	3175	0	2999	1	0
4	PB	3175	0	2999	2	0
4	PC	3119	0	2954	0	0
4	PD	3108	0	2941	0	0
4	PE	3175	0	2999	1	0
4	PF	3175	0	2999	1	0
4	PG	3175	0	2999	3	0
4	PH	3102	0	2940	1	0
4	PI	3145	0	2973	0	0
4	PJ	3175	0	2999	1	0
4	PK	3147	0	2977	1	0
4	PL	3119	0	2954	1	0
5	PM	1087	0	1018	1	0
5	PN	1087	0	1018	1	0
5	PO	1087	0	1018	0	0
5	PP	1087	0	1018	0	0
5	PQ	1087	0	1018	0	0
5	PR	1087	0	1018	1	0
5	PS	1087	0	1018	1	0
5	PT	1087	0	1018	0	0
5	PU	1087	0	1018	1	0
5	PV	1087	0	1018	1	0
5	PW	1087	0	1018	0	0
5	PX	1087	0	1018	2	0
6	JA	5	0	0	0	0
6	JB	6	0	0	0	0
6	JC	6	0	0	0	0
6	JD	5	0	0	0	0
6	JE	5	0	0	0	0
6	JF	5	0	0	0	0
6	JI	2	0	0	0	0
6	KA	6	0	0	0	0
6	KB	5	0	0	0	0
6	KC	4	0	0	0	0
6	KD	7	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	KE	5	0	0	0	0
6	KF	5	0	0	0	0
6	KI	1	0	0	0	0
6	LA	6	0	0	0	0
6	LB	5	0	0	0	0
6	LC	4	0	0	0	0
6	LD	7	0	0	0	0
6	LE	5	0	0	0	0
6	LF	4	0	0	0	0
6	LI	1	0	0	0	0
6	LJ	1	0	0	0	0
6	MA	7	0	0	0	0
6	MB	5	0	0	0	0
6	MC	3	0	0	0	0
6	MD	8	0	0	0	0
6	ME	4	0	0	0	0
6	MF	5	0	0	0	0
6	MI	1	0	0	0	0
6	NA	5	0	0	0	0
6	NB	6	0	0	0	0
6	NC	5	0	0	0	0
6	ND	7	0	0	0	0
6	NE	4	0	0	0	0
6	NF	4	0	0	0	0
6	NI	1	0	0	0	0
6	PM	2	0	0	0	0
6	PN	2	0	0	0	0
6	PO	1	0	0	0	0
6	PP	2	0	0	0	0
6	PQ	2	0	0	0	0
6	PR	1	0	0	0	0
6	PS	1	0	0	0	0
6	PT	1	0	0	0	0
6	PU	1	0	0	0	0
6	PV	1	0	0	0	0
6	PW	2	0	0	0	0
6	PX	2	0	0	0	0
7	JI	1	0	0	0	0
7	JJ	1	0	0	0	0
7	JK	1	0	0	0	0
7	KI	1	0	0	0	0
7	KJ	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	KK	1	0	0	0	0
7	LI	1	0	0	0	0
7	LJ	1	0	0	0	0
7	LK	1	0	0	0	0
7	MI	1	0	0	0	0
7	MJ	2	0	0	0	0
7	MK	1	0	0	0	0
7	NI	1	0	0	0	0
7	NJ	1	0	0	0	0
7	NK	1	0	0	0	0
7	P6	1	0	0	0	0
All	All	137239	0	128179	51	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 0.

All (51) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:LE:115:GLU:HG2	1:LF:144:VAL:HG23	1.86	0.58
1:KF:121:VAL:HG22	3:P6:12:MET:HE1	1.88	0.56
1:MF:121:VAL:HG22	3:P8:12:MET:HE1	1.87	0.55
4:PG:263:ARG:HH21	4:PG:263:ARG:HG2	1.76	0.50
3:P6:12:MET:HE2	3:P6:12:MET:HA	1.93	0.50
2:KI:59:ASN:HD22	2:KI:69:VAL:HG23	1.77	0.49
2:MI:60:LEU:HD21	2:MI:72:ALA:HB2	1.95	0.49
1:MA:161:GLN:NE2	1:ME:105:ASP:H	2.11	0.48
4:PB:258:ASP:HA	5:PS:67:LEU:HD21	1.96	0.48
1:JF:121:VAL:CG2	3:P5:12:MET:HE1	2.43	0.48
3:P8:12:MET:HA	3:P8:12:MET:HE2	1.96	0.47
4:PG:67:ARG:HE	4:PG:134:TRP:CD1	2.33	0.47
1:JE:101:PHE:CG	1:JE:102:ALA:N	2.83	0.46
1:KA:192:MET:CE	1:NE:103:ALA:HB1	2.45	0.46
1:JE:103:ALA:HB3	1:LA:188:VAL:HG12	1.98	0.46
4:PK:258:ASP:HA	5:PX:67:LEU:HD21	1.98	0.45
1:MA:161:GLN:HE22	1:ME:105:ASP:H	1.64	0.45
2:JI:60:LEU:HD21	2:JI:72:ALA:HB2	1.97	0.45
1:KA:371:ASP:CG	1:NF:378:ARG:HE	2.25	0.45
3:P7:12:MET:HA	3:P7:12:MET:HE2	1.98	0.45
1:JF:378:ARG:HE	1:LA:371:ASP:CG	2.24	0.45
1:LD:292:ARG:NH2	1:LE:245:ASN:OD1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:KD:292:ARG:NH2	1:KE:245:ASN:OD1	2.51	0.44
1:ME:101:PHE:O	1:ME:102:ALA:C	2.60	0.44
1:JA:371:ASP:CG	1:KF:378:ARG:HE	2.26	0.43
4:PB:67:ARG:HE	4:PB:134:TRP:CD1	2.35	0.43
1:KE:101:PHE:O	1:KE:102:ALA:C	2.62	0.43
1:MF:378:ARG:NH2	1:NA:371:ASP:OD1	2.52	0.43
3:P9:12:MET:HA	3:P9:12:MET:HE2	2.00	0.43
5:PR:129:VAL:HG12	5:PR:129:VAL:O	2.19	0.43
1:JD:292:ARG:NH2	1:JE:245:ASN:OD1	2.52	0.43
4:PL:258:ASP:HA	5:PU:67:LEU:HD21	2.01	0.43
1:LB:122:MET:HE2	1:LC:147:VAL:HG21	2.01	0.42
1:LA:388:GLY:H	2:MK:8:GLU:CD	2.26	0.42
4:PA:258:ASP:HA	5:PV:67:LEU:HD21	2.01	0.42
1:LF:121:VAL:CG2	3:P7:12:MET:HE1	2.50	0.42
4:PF:258:ASP:HA	5:PM:67:LEU:HD21	2.02	0.42
1:LE:101:PHE:CG	1:LE:102:ALA:N	2.88	0.42
3:P8:22:ARG:HD3	5:PN:141:TYR:HB2	2.01	0.42
4:PE:67:ARG:HA	4:PE:134:TRP:CH2	2.55	0.42
2:LI:60:LEU:HD21	2:LI:72:ALA:HB2	2.02	0.41
1:MB:131:ALA:O	1:MB:132:ARG:HB2	2.20	0.41
4:PG:204:ALA:HB3	4:PH:155:PRO:HG2	2.01	0.41
1:JB:125:ARG:HD3	1:JC:389:ARG:NH1	2.35	0.41
1:KB:131:ALA:O	1:KB:132:ARG:HB2	2.21	0.41
1:KF:136:ASN:HD22	1:KF:349:HIS:CD2	2.38	0.41
1:KA:371:ASP:OD2	1:NF:181:LYS:NZ	2.54	0.40
1:NB:122:MET:HE1	1:NC:349:HIS:CE1	2.56	0.40
4:PJ:268:PRO:HD2	5:PX:140:THR:HG21	2.03	0.40
1:MA:149:ILE:CD1	1:MA:175:VAL:HG23	2.51	0.40
1:MC:147:VAL:HA	1:MC:148:PRO:HD3	1.99	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

41 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	HIP	PB	196	4	10,14,15	1.36	3 (30%)	4,20,22	1.24	1 (25%)
3	HIP	P8	17	3	10,14,15	1.45	3 (30%)	4,20,22	1.31	1 (25%)
4	HIP	PC	243	4	10,14,15	1.46	3 (30%)	4,20,22	1.43	1 (25%)
4	HIP	PI	243	4	10,14,15	1.61	3 (30%)	4,20,22	1.47	1 (25%)
4	HIP	PF	243	4	10,14,15	1.42	3 (30%)	4,20,22	1.45	1 (25%)
4	HIP	PC	196	4	10,14,15	1.39	2 (20%)	4,20,22	1.33	1 (25%)
4	HIP	PI	291	4	10,14,15	1.35	2 (20%)	4,20,22	1.49	1 (25%)
4	HIP	PJ	243	4	10,14,15	1.51	3 (30%)	4,20,22	1.54	1 (25%)
4	HIP	PG	196	4	10,14,15	1.41	3 (30%)	4,20,22	1.26	1 (25%)
4	HIP	PH	243	4	10,14,15	1.54	3 (30%)	4,20,22	1.54	1 (25%)
4	HIP	PE	243	4	10,14,15	1.55	3 (30%)	4,20,22	1.48	1 (25%)
4	HIP	PF	291	4	10,14,15	1.32	1 (10%)	4,20,22	1.44	1 (25%)
4	HIP	PA	196	4	10,14,15	1.44	2 (20%)	4,20,22	1.38	1 (25%)
4	HIP	PJ	291	4	10,14,15	1.34	1 (10%)	4,20,22	1.41	1 (25%)
3	HIP	P6	17	3	10,14,15	1.51	3 (30%)	4,20,22	1.21	1 (25%)
4	HIP	PE	291	4	10,14,15	1.38	2 (20%)	4,20,22	1.56	1 (25%)
4	HIP	PI	196	4	10,14,15	1.36	3 (30%)	4,20,22	1.41	1 (25%)
4	HIP	PA	243	4	10,14,15	1.61	3 (30%)	4,20,22	1.55	1 (25%)
4	HIP	PL	243	4	10,14,15	1.56	3 (30%)	4,20,22	1.48	1 (25%)
4	HIP	PF	196	4	10,14,15	1.33	3 (30%)	4,20,22	1.35	1 (25%)
4	HIP	PL	196	4	10,14,15	1.43	2 (20%)	4,20,22	1.30	1 (25%)
4	HIP	PJ	196	4	10,14,15	1.40	3 (30%)	4,20,22	1.25	1 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	HIP	PK	291	4	10,14,15	1.39	2 (20%)	4,20,22	1.47	1 (25%)
4	HIP	PH	196	4	10,14,15	1.35	2 (20%)	4,20,22	1.41	1 (25%)
4	HIP	PB	291	4	10,14,15	1.43	2 (20%)	4,20,22	1.47	1 (25%)
4	HIP	PD	291	4	10,14,15	1.97	3 (30%)	4,20,22	1.56	1 (25%)
4	HIP	PA	291	4	10,14,15	1.26	1 (10%)	4,20,22	2.06	2 (50%)
4	HIP	PG	291	4	10,14,15	1.34	1 (10%)	4,20,22	1.41	1 (25%)
4	HIP	PL	291	4	10,14,15	1.35	2 (20%)	4,20,22	1.48	1 (25%)
4	HIP	PC	291	4	10,14,15	1.32	1 (10%)	4,20,22	1.45	1 (25%)
4	HIP	PE	196	4	10,14,15	1.28	3 (30%)	4,20,22	1.43	1 (25%)
4	HIP	PK	243	4	10,14,15	1.51	3 (30%)	4,20,22	1.53	1 (25%)
4	HIP	PD	196	4	10,14,15	1.27	2 (20%)	4,20,22	1.35	1 (25%)
4	HIP	PK	196	4	10,14,15	1.41	3 (30%)	4,20,22	1.39	1 (25%)
3	HIP	P5	17	3	10,14,15	1.36	2 (20%)	4,20,22	1.36	1 (25%)
3	HIP	P7	17	3	10,14,15	1.44	2 (20%)	4,20,22	1.21	1 (25%)
4	HIP	PD	243	4	10,14,15	1.56	3 (30%)	4,20,22	1.49	1 (25%)
3	HIP	P9	17	3	10,14,15	1.44	2 (20%)	4,20,22	1.34	1 (25%)
4	HIP	PH	291	4	10,14,15	1.25	2 (20%)	4,20,22	2.20	2 (50%)
4	HIP	PB	243	4	10,14,15	1.58	3 (30%)	4,20,22	1.46	1 (25%)
4	HIP	PG	243	4	10,14,15	1.45	3 (30%)	4,20,22	1.39	1 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HIP	PB	196	4	-	2/5/12/14	0/1/1/1
3	HIP	P8	17	3	-	0/5/12/14	0/1/1/1
4	HIP	PC	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PI	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PF	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PC	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PI	291	4	-	3/5/12/14	0/1/1/1
4	HIP	PJ	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PG	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PH	243	4	-	2/5/12/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HIP	PE	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PF	291	4	-	2/5/12/14	0/1/1/1
4	HIP	PA	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PJ	291	4	-	2/5/12/14	0/1/1/1
3	HIP	P6	17	3	-	0/5/12/14	0/1/1/1
4	HIP	PE	291	4	-	3/5/12/14	0/1/1/1
4	HIP	PI	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PA	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PL	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PF	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PL	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PJ	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PK	291	4	-	3/5/12/14	0/1/1/1
4	HIP	PH	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PB	291	4	-	3/5/12/14	0/1/1/1
4	HIP	PD	291	4	-	2/5/12/14	0/1/1/1
4	HIP	PA	291	4	-	1/5/12/14	0/1/1/1
4	HIP	PG	291	4	-	3/5/12/14	0/1/1/1
4	HIP	PL	291	4	-	3/5/12/14	0/1/1/1
4	HIP	PC	291	4	-	2/5/12/14	0/1/1/1
4	HIP	PE	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PK	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PD	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PK	196	4	-	2/5/12/14	0/1/1/1
3	HIP	P5	17	3	-	0/5/12/14	0/1/1/1
3	HIP	P7	17	3	-	0/5/12/14	0/1/1/1
4	HIP	PD	243	4	-	2/5/12/14	0/1/1/1
3	HIP	P9	17	3	-	0/5/12/14	0/1/1/1
4	HIP	PH	291	4	-	0/5/12/14	0/1/1/1
4	HIP	PB	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PG	243	4	-	2/5/12/14	0/1/1/1

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	PD	291	HIP	P-O1P	4.45	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	PK	291	HIP	P-O3P	-3.33	1.48	1.56
4	PB	291	HIP	P-O3P	-3.32	1.48	1.56
4	PE	291	HIP	P-O3P	-3.28	1.48	1.56
4	PF	291	HIP	P-O3P	-3.20	1.48	1.56
4	PI	291	HIP	P-O3P	-3.20	1.48	1.56
4	PG	291	HIP	P-O3P	-3.18	1.48	1.56
4	PJ	291	HIP	P-O3P	-3.12	1.48	1.56
4	PC	291	HIP	P-O3P	-3.11	1.48	1.56
4	PL	291	HIP	P-O3P	-3.11	1.48	1.56
4	PB	243	HIP	P-O3P	-3.07	1.48	1.56
4	PD	291	HIP	P-O3P	-3.07	1.48	1.56
4	PA	243	HIP	P-O3P	-3.04	1.48	1.56
3	P6	17	HIP	P-O1P	3.02	1.50	1.46
4	PI	243	HIP	P-O3P	-2.99	1.48	1.56
4	PH	243	HIP	P-O3P	-2.91	1.49	1.56
4	PL	243	HIP	P-O3P	-2.90	1.49	1.56
4	PF	243	HIP	P-O3P	-2.88	1.49	1.56
4	PJ	243	HIP	P-O3P	-2.87	1.49	1.56
4	PA	291	HIP	P-O3P	-2.84	1.49	1.56
4	PA	196	HIP	P-O1P	2.84	1.50	1.46
4	PD	291	HIP	P-O2P	-2.82	1.49	1.56
4	PC	243	HIP	P-O3P	-2.81	1.49	1.56
4	PE	243	HIP	P-O3P	-2.79	1.49	1.56
4	PL	196	HIP	P-O1P	2.78	1.50	1.46
4	PE	243	HIP	P-O1P	2.78	1.50	1.46
4	PD	243	HIP	P-O3P	-2.78	1.49	1.56
4	PA	243	HIP	P-O1P	2.76	1.50	1.46
4	PK	243	HIP	P-O3P	-2.75	1.49	1.56
4	PI	243	HIP	P-O1P	2.75	1.50	1.46
4	PD	243	HIP	P-O2P	-2.73	1.49	1.56
4	PG	243	HIP	P-O3P	-2.73	1.49	1.56
3	P7	17	HIP	P-O1P	2.72	1.50	1.46
3	P9	17	HIP	P-O1P	2.72	1.50	1.46
4	PK	196	HIP	P-O1P	2.71	1.50	1.46
4	PH	243	HIP	P-O2P	-2.70	1.49	1.56
4	PA	196	HIP	P-O2P	-2.70	1.49	1.56
4	PJ	243	HIP	P-O2P	-2.69	1.49	1.56
3	P6	17	HIP	P-O3P	-2.69	1.49	1.56
4	PA	243	HIP	P-O2P	-2.68	1.49	1.56
4	PG	196	HIP	P-O2P	-2.68	1.49	1.56
4	PC	196	HIP	P-O2P	-2.68	1.49	1.56
4	PD	196	HIP	P-O2P	-2.67	1.49	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	PL	196	HIP	P-O2P	-2.67	1.49	1.56
3	P9	17	HIP	P-O3P	-2.67	1.49	1.56
4	PB	196	HIP	P-O2P	-2.67	1.49	1.56
4	PL	243	HIP	P-O1P	2.67	1.50	1.46
4	PJ	196	HIP	P-O2P	-2.66	1.49	1.56
4	PH	196	HIP	P-O2P	-2.65	1.49	1.56
4	PI	243	HIP	P-O2P	-2.64	1.49	1.56
4	PB	243	HIP	P-O2P	-2.64	1.49	1.56
4	PE	196	HIP	P-O2P	-2.63	1.49	1.56
3	P7	17	HIP	P-O3P	-2.62	1.49	1.56
4	PD	243	HIP	P-O1P	2.62	1.50	1.46
4	PL	243	HIP	P-O2P	-2.61	1.49	1.56
4	PF	196	HIP	P-O2P	-2.61	1.49	1.56
4	PK	243	HIP	P-O2P	-2.61	1.49	1.56
3	P8	17	HIP	P-O1P	2.61	1.50	1.46
4	PG	196	HIP	P-O1P	2.60	1.50	1.46
4	PH	291	HIP	P-O3P	-2.60	1.49	1.56
4	PC	196	HIP	P-O1P	2.59	1.50	1.46
3	P8	17	HIP	P-O3P	-2.56	1.50	1.56
4	PJ	196	HIP	P-O1P	2.56	1.50	1.46
4	PK	196	HIP	P-O2P	-2.53	1.50	1.56
4	PI	196	HIP	P-O2P	-2.50	1.50	1.56
3	P5	17	HIP	P-O1P	2.48	1.49	1.46
4	PK	243	HIP	P-O1P	2.48	1.49	1.46
4	PE	243	HIP	P-O2P	-2.48	1.50	1.56
4	PB	243	HIP	P-O1P	2.48	1.49	1.46
3	P5	17	HIP	P-O3P	-2.46	1.50	1.56
4	PC	243	HIP	P-O2P	-2.45	1.50	1.56
4	PG	243	HIP	P-O1P	2.44	1.49	1.46
4	PH	196	HIP	P-O1P	2.44	1.49	1.46
4	PH	243	HIP	P-O1P	2.42	1.49	1.46
4	PI	196	HIP	P-O1P	2.38	1.49	1.46
4	PB	196	HIP	P-O1P	2.36	1.49	1.46
4	PI	196	HIP	P-O3P	-2.34	1.50	1.56
4	PC	243	HIP	P-O1P	2.31	1.49	1.46
4	PG	243	HIP	P-O2P	-2.30	1.50	1.56
4	PJ	243	HIP	P-O1P	2.28	1.49	1.46
3	P8	17	HIP	P-O2P	-2.26	1.50	1.56
4	PF	243	HIP	P-O2P	-2.26	1.50	1.56
4	PK	196	HIP	P-O3P	-2.23	1.50	1.56
4	PF	196	HIP	P-O1P	2.20	1.49	1.46
4	PF	196	HIP	P-O3P	-2.19	1.51	1.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	PJ	196	HIP	P-O3P	-2.18	1.51	1.56
4	PB	291	HIP	P-O1P	2.17	1.49	1.46
4	PF	243	HIP	P-O1P	2.13	1.49	1.46
4	PE	291	HIP	P-O1P	2.12	1.49	1.46
4	PG	196	HIP	P-O3P	-2.12	1.51	1.56
4	PB	196	HIP	P-O3P	-2.10	1.51	1.56
3	P6	17	HIP	P-O2P	-2.08	1.51	1.56
4	PD	196	HIP	P-O3P	-2.07	1.51	1.56
4	PL	291	HIP	P-O1P	2.04	1.49	1.46
4	PK	291	HIP	P-O1P	2.03	1.49	1.46
4	PE	196	HIP	P-O3P	-2.03	1.51	1.56
4	PI	291	HIP	P-O1P	2.02	1.49	1.46
4	PH	291	HIP	P-O1P	2.02	1.49	1.46
4	PE	196	HIP	P-O1P	2.00	1.49	1.46

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	PH	291	HIP	O3P-P-O1P	3.19	120.81	112.95
4	PA	291	HIP	O3P-P-O1P	2.98	120.27	112.95
4	PH	291	HIP	CD2-NE2-CE1	2.79	108.89	105.24
4	PI	291	HIP	CD2-NE2-CE1	2.78	108.88	105.24
4	PA	291	HIP	CD2-NE2-CE1	2.74	108.83	105.24
4	PF	291	HIP	CD2-NE2-CE1	2.71	108.79	105.24
4	PE	291	HIP	CD2-NE2-CE1	2.70	108.78	105.24
4	PD	291	HIP	CD2-NE2-CE1	2.68	108.75	105.24
4	PK	291	HIP	CD2-NE2-CE1	2.67	108.73	105.24
4	PH	243	HIP	CD2-NE2-CE1	2.67	108.73	105.24
4	PB	291	HIP	CD2-NE2-CE1	2.65	108.71	105.24
4	PA	243	HIP	CD2-NE2-CE1	2.64	108.69	105.24
4	PG	291	HIP	CD2-NE2-CE1	2.64	108.69	105.24
4	PC	291	HIP	CD2-NE2-CE1	2.63	108.68	105.24
4	PJ	291	HIP	CD2-NE2-CE1	2.63	108.68	105.24
4	PJ	243	HIP	CD2-NE2-CE1	2.63	108.67	105.24
4	PL	291	HIP	CD2-NE2-CE1	2.61	108.65	105.24
4	PD	243	HIP	CD2-NE2-CE1	2.56	108.59	105.24
4	PE	196	HIP	CD2-NE2-CE1	2.56	108.59	105.24
4	PI	243	HIP	CD2-NE2-CE1	2.55	108.58	105.24
4	PL	243	HIP	CD2-NE2-CE1	2.55	108.58	105.24
4	PC	243	HIP	CD2-NE2-CE1	2.52	108.54	105.24
4	PH	196	HIP	CD2-NE2-CE1	2.52	108.54	105.24
4	PK	196	HIP	CD2-NE2-CE1	2.51	108.52	105.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P5	17	HIP	CD2-NE2-CE1	2.51	108.52	105.24
4	PB	243	HIP	CD2-NE2-CE1	2.51	108.52	105.24
4	PK	243	HIP	CD2-NE2-CE1	2.51	108.52	105.24
4	PA	196	HIP	CD2-NE2-CE1	2.50	108.51	105.24
4	PC	196	HIP	CD2-NE2-CE1	2.49	108.50	105.24
4	PF	243	HIP	CD2-NE2-CE1	2.49	108.50	105.24
4	PI	196	HIP	CD2-NE2-CE1	2.48	108.49	105.24
3	P9	17	HIP	CD2-NE2-CE1	2.47	108.48	105.24
4	PD	196	HIP	CD2-NE2-CE1	2.47	108.47	105.24
4	PE	243	HIP	CD2-NE2-CE1	2.44	108.43	105.24
4	PL	196	HIP	CD2-NE2-CE1	2.41	108.39	105.24
4	PJ	196	HIP	CD2-NE2-CE1	2.40	108.38	105.24
4	PG	243	HIP	CD2-NE2-CE1	2.40	108.38	105.24
3	P8	17	HIP	CD2-NE2-CE1	2.39	108.37	105.24
4	PG	196	HIP	CD2-NE2-CE1	2.39	108.36	105.24
4	PF	196	HIP	CD2-NE2-CE1	2.38	108.35	105.24
4	PB	196	HIP	CD2-NE2-CE1	2.32	108.28	105.24
3	P6	17	HIP	CD2-NE2-CE1	2.26	108.20	105.24
3	P7	17	HIP	CD2-NE2-CE1	2.22	108.14	105.24

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	PA	243	HIP	O-C-CA-CB
4	PB	243	HIP	O-C-CA-CB
4	PB	291	HIP	O-C-CA-CB
4	PB	291	HIP	CA-CB-CG-ND1
4	PC	243	HIP	O-C-CA-CB
4	PC	291	HIP	CA-CB-CG-ND1
4	PD	243	HIP	O-C-CA-CB
4	PD	291	HIP	CA-CB-CG-ND1
4	PE	243	HIP	O-C-CA-CB
4	PE	291	HIP	O-C-CA-CB
4	PE	291	HIP	CA-CB-CG-ND1
4	PF	243	HIP	O-C-CA-CB
4	PG	243	HIP	O-C-CA-CB
4	PG	291	HIP	O-C-CA-CB
4	PH	243	HIP	O-C-CA-CB
4	PI	243	HIP	O-C-CA-CB
4	PI	291	HIP	O-C-CA-CB
4	PJ	243	HIP	O-C-CA-CB

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Mol	Chain	Res	Type	Atoms
4	PK	243	HIP	O-C-CA-CB
4	PK	291	HIP	O-C-CA-CB
4	PK	291	HIP	CA-CB-CG-ND1
4	PL	243	HIP	O-C-CA-CB
4	PL	291	HIP	O-C-CA-CB
4	PL	291	HIP	CA-CB-CG-ND1
4	PA	196	HIP	N-CA-CB-CG
4	PB	196	HIP	N-CA-CB-CG
4	PC	196	HIP	N-CA-CB-CG
4	PD	196	HIP	N-CA-CB-CG
4	PE	196	HIP	N-CA-CB-CG
4	PF	196	HIP	N-CA-CB-CG
4	PG	196	HIP	N-CA-CB-CG
4	PH	196	HIP	N-CA-CB-CG
4	PI	196	HIP	N-CA-CB-CG
4	PJ	196	HIP	N-CA-CB-CG
4	PK	196	HIP	N-CA-CB-CG
4	PL	196	HIP	N-CA-CB-CG
4	PG	291	HIP	CA-CB-CG-ND1
4	PJ	291	HIP	CA-CB-CG-ND1
4	PA	243	HIP	CA-CB-CG-CD2
4	PB	243	HIP	CA-CB-CG-CD2
4	PB	291	HIP	CA-CB-CG-CD2
4	PC	243	HIP	CA-CB-CG-CD2
4	PC	291	HIP	CA-CB-CG-CD2
4	PD	243	HIP	CA-CB-CG-CD2
4	PD	291	HIP	CA-CB-CG-CD2
4	PE	243	HIP	CA-CB-CG-CD2
4	PE	291	HIP	CA-CB-CG-CD2
4	PF	243	HIP	CA-CB-CG-CD2
4	PF	291	HIP	CA-CB-CG-CD2
4	PG	243	HIP	CA-CB-CG-CD2
4	PG	291	HIP	CA-CB-CG-CD2
4	PH	243	HIP	CA-CB-CG-CD2
4	PI	243	HIP	CA-CB-CG-CD2
4	PI	291	HIP	CA-CB-CG-CD2
4	PJ	243	HIP	CA-CB-CG-CD2
4	PJ	291	HIP	CA-CB-CG-CD2
4	PK	243	HIP	CA-CB-CG-CD2
4	PK	291	HIP	CA-CB-CG-CD2
4	PL	243	HIP	CA-CB-CG-CD2
4	PL	291	HIP	CA-CB-CG-CD2

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Mol	Chain	Res	Type	Atoms
4	PA	196	HIP	C-CA-CB-CG
4	PB	196	HIP	C-CA-CB-CG
4	PC	196	HIP	C-CA-CB-CG
4	PD	196	HIP	C-CA-CB-CG
4	PE	196	HIP	C-CA-CB-CG
4	PF	196	HIP	C-CA-CB-CG
4	PG	196	HIP	C-CA-CB-CG
4	PH	196	HIP	C-CA-CB-CG
4	PI	196	HIP	C-CA-CB-CG
4	PJ	196	HIP	C-CA-CB-CG
4	PK	196	HIP	C-CA-CB-CG
4	PL	196	HIP	C-CA-CB-CG
4	PF	291	HIP	CA-CB-CG-ND1
4	PI	291	HIP	CA-CB-CG-ND1
4	PA	291	HIP	CA-CB-CG-CD2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 200 ligands modelled in this entry, 200 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 ⓘ

There are no chain breaks in this entry.

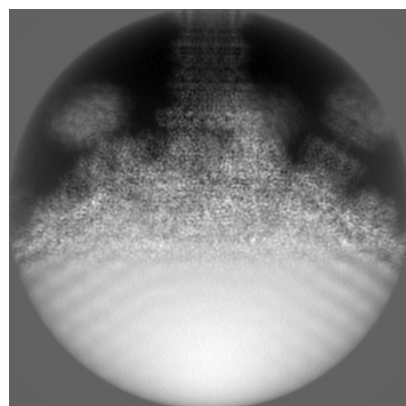
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-18642. These allow visual inspection of the internal detail of the map and identification of artifacts.

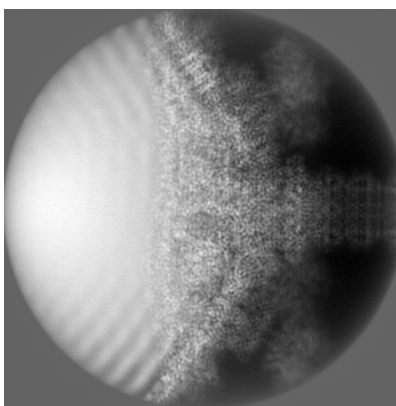
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

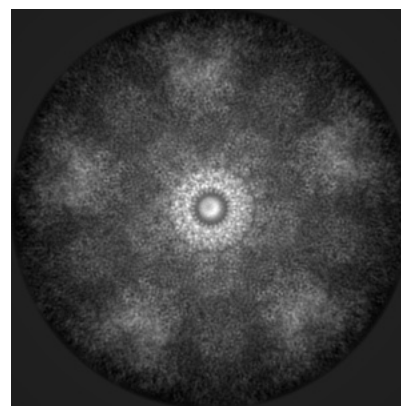
6.1.1 Primary map



X

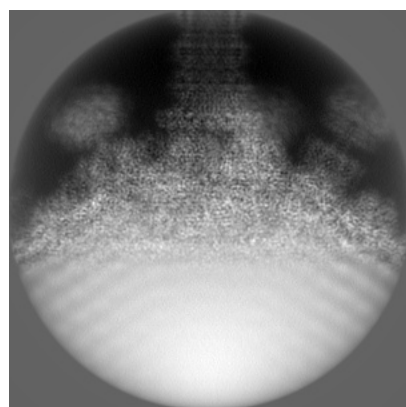


Y

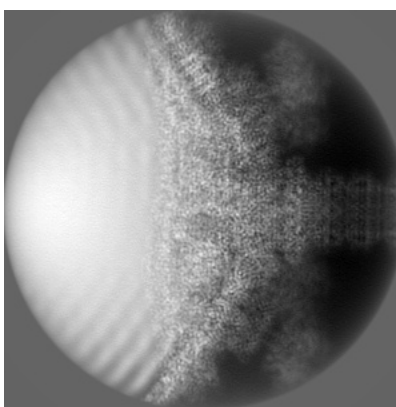


Z

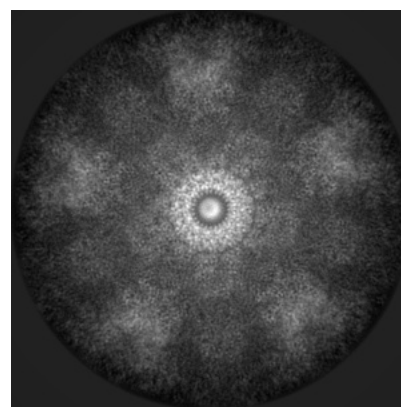
6.1.2 Raw map



X



Y

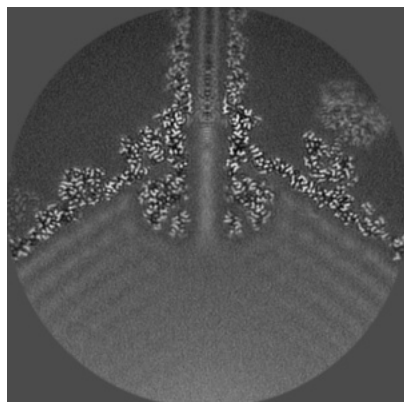


Z

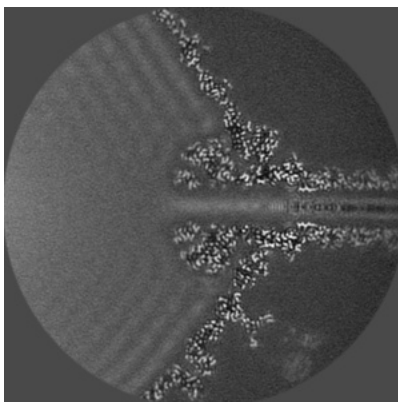
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

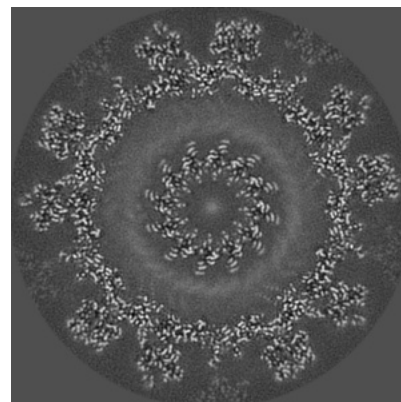
6.2.1 Primary map



X Index: 176

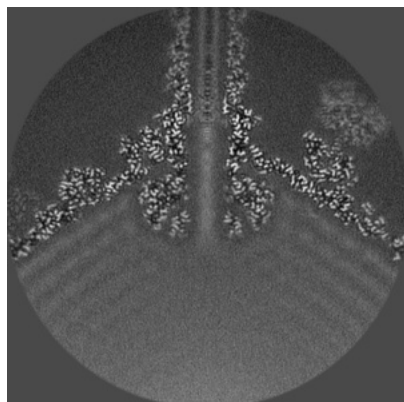


Y Index: 176

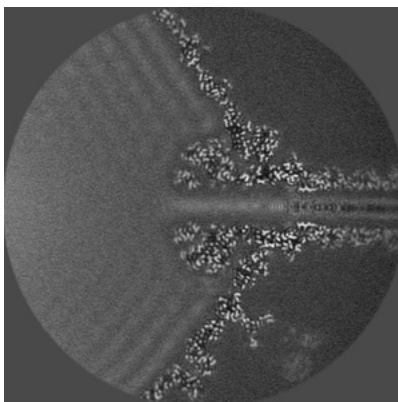


Z Index: 176

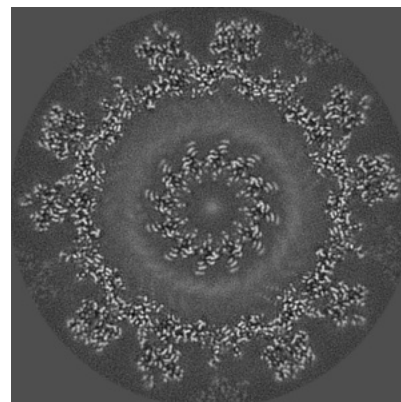
6.2.2 Raw map



X Index: 176



Y Index: 176

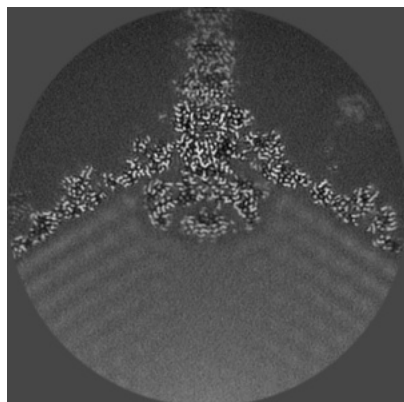


Z Index: 176

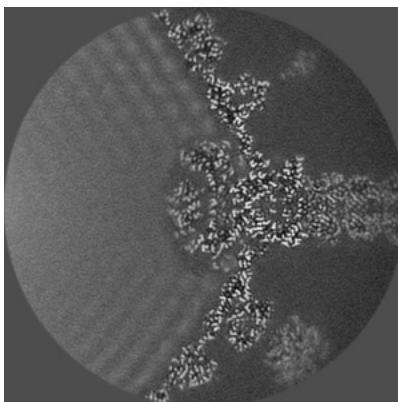
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

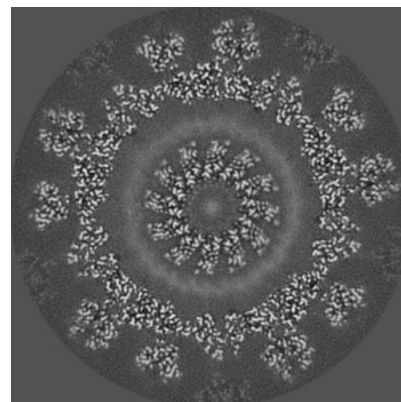
6.3.1 Primary map



X Index: 199

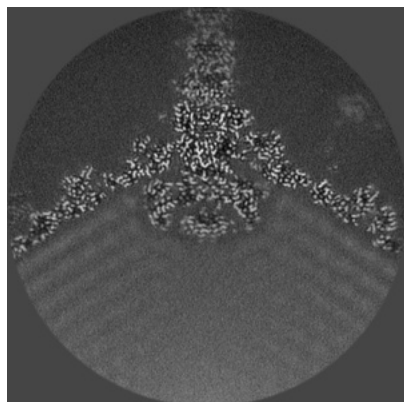


Y Index: 194

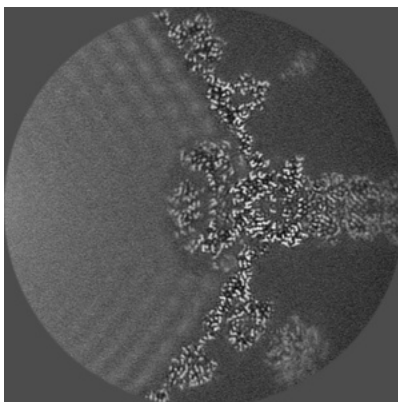


Z Index: 180

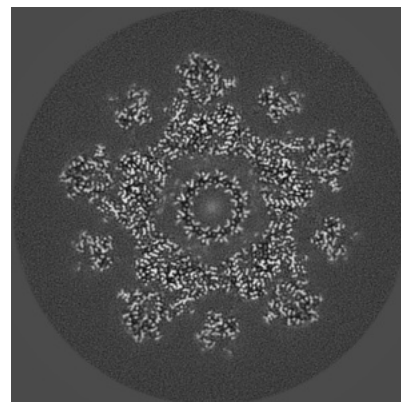
6.3.2 Raw map



X Index: 199



Y Index: 194

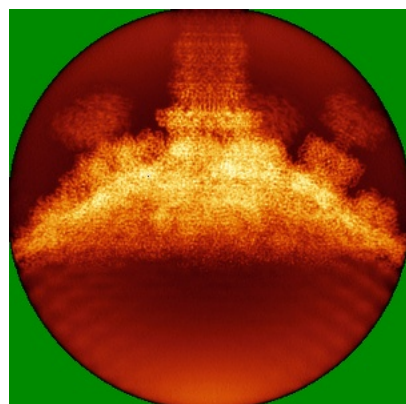


Z Index: 206

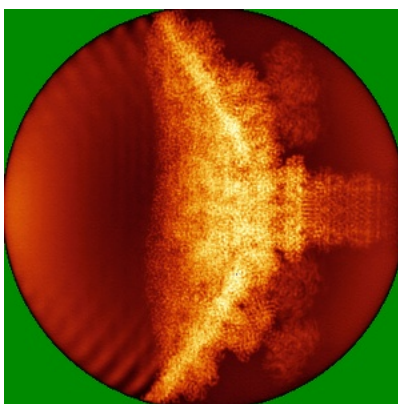
The images above show the largest variance slices of the map in three orthogonal directions.

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

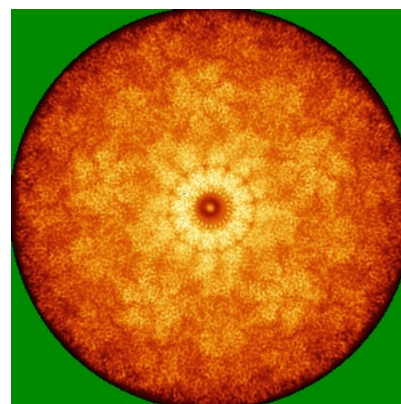
6.4.1 Primary map



X

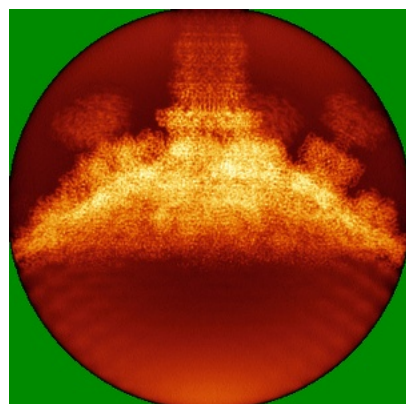


Y

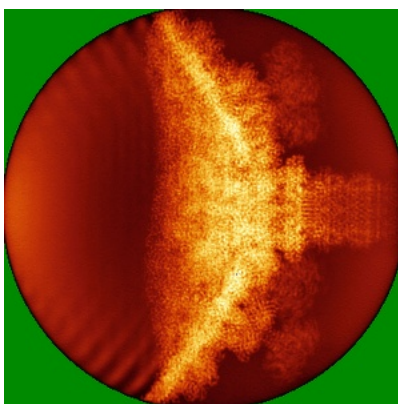


Z

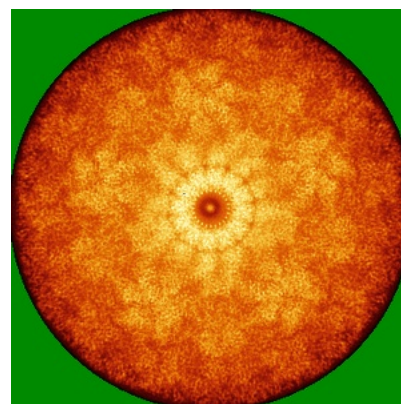
6.4.2 Raw map



X



Y

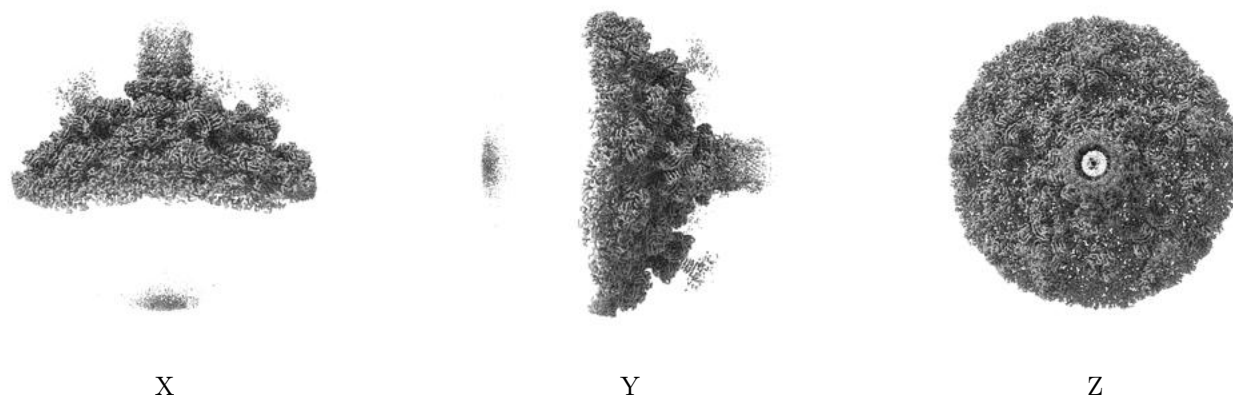


Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.015. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

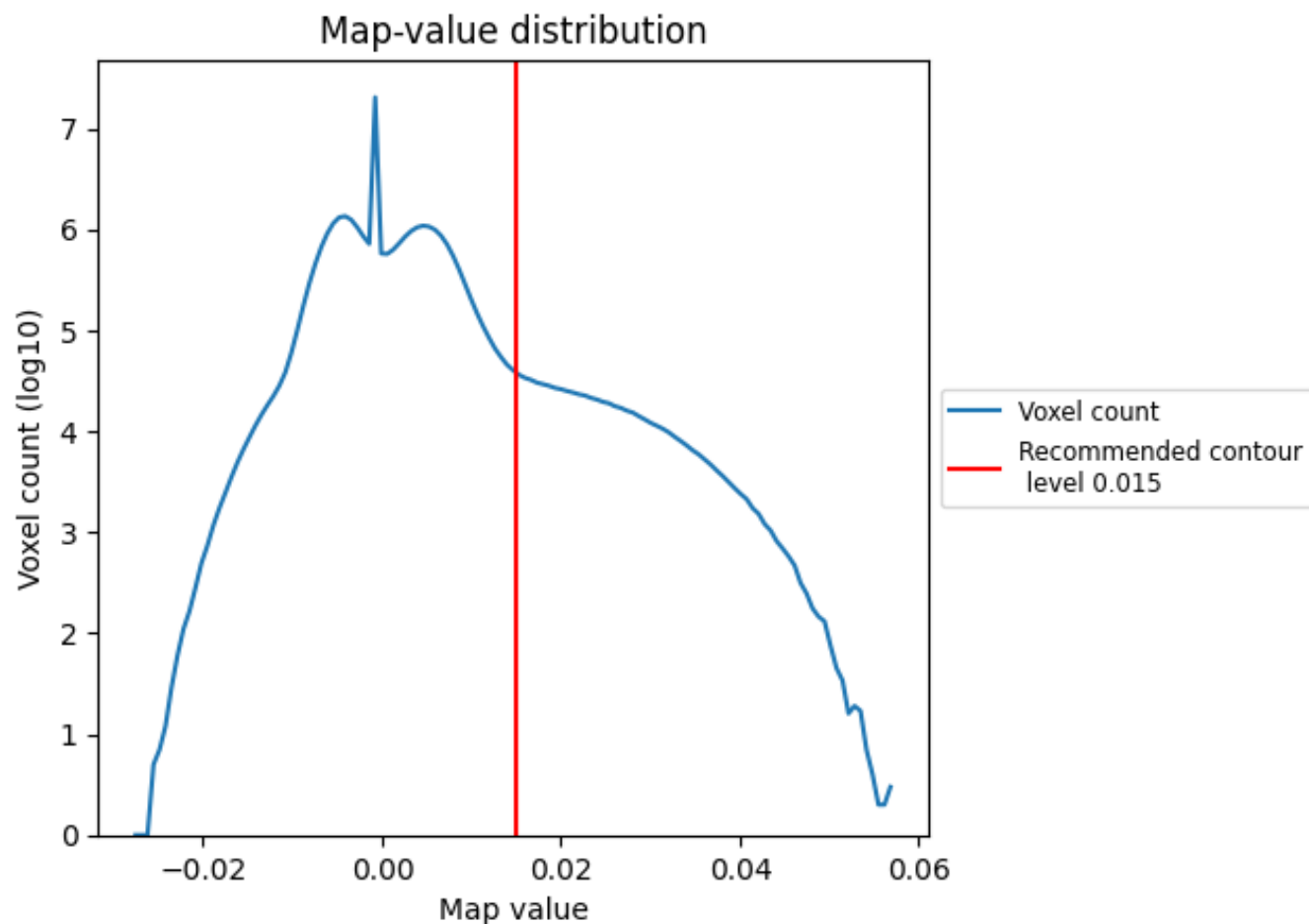
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

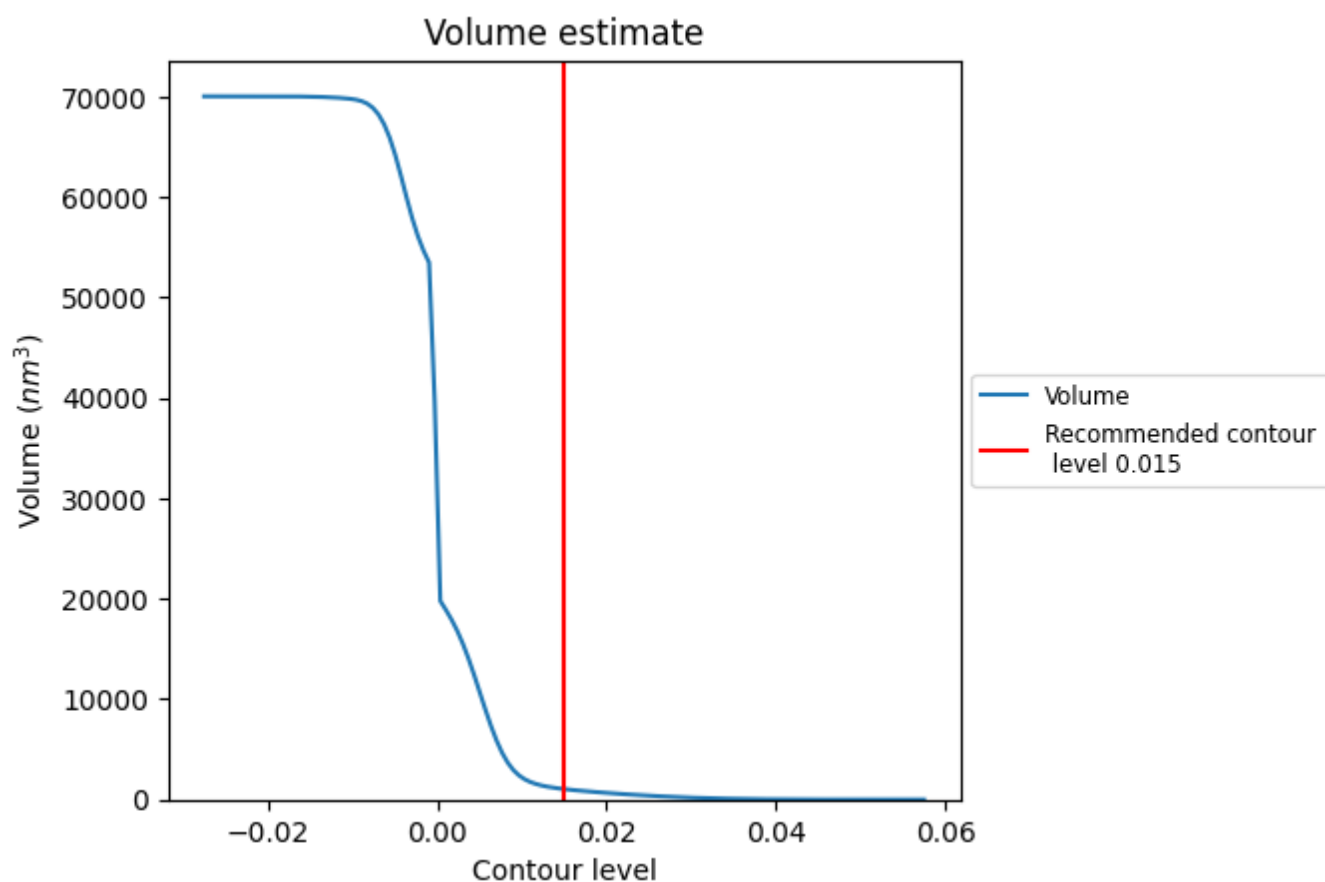
This section contains the results of statistical analysis of the map.

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.

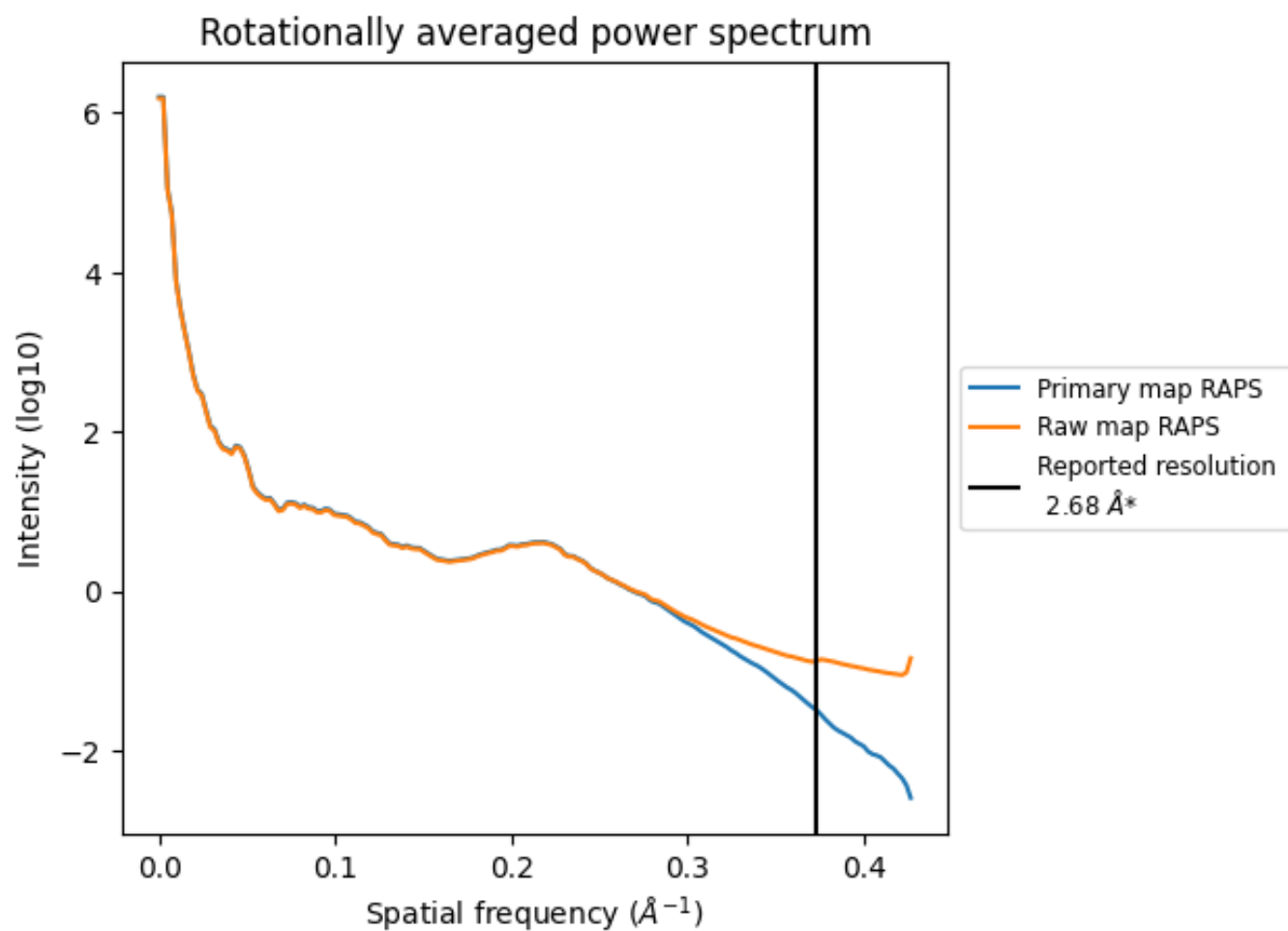
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1041 nm³; this corresponds to an approximate mass of 941 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ

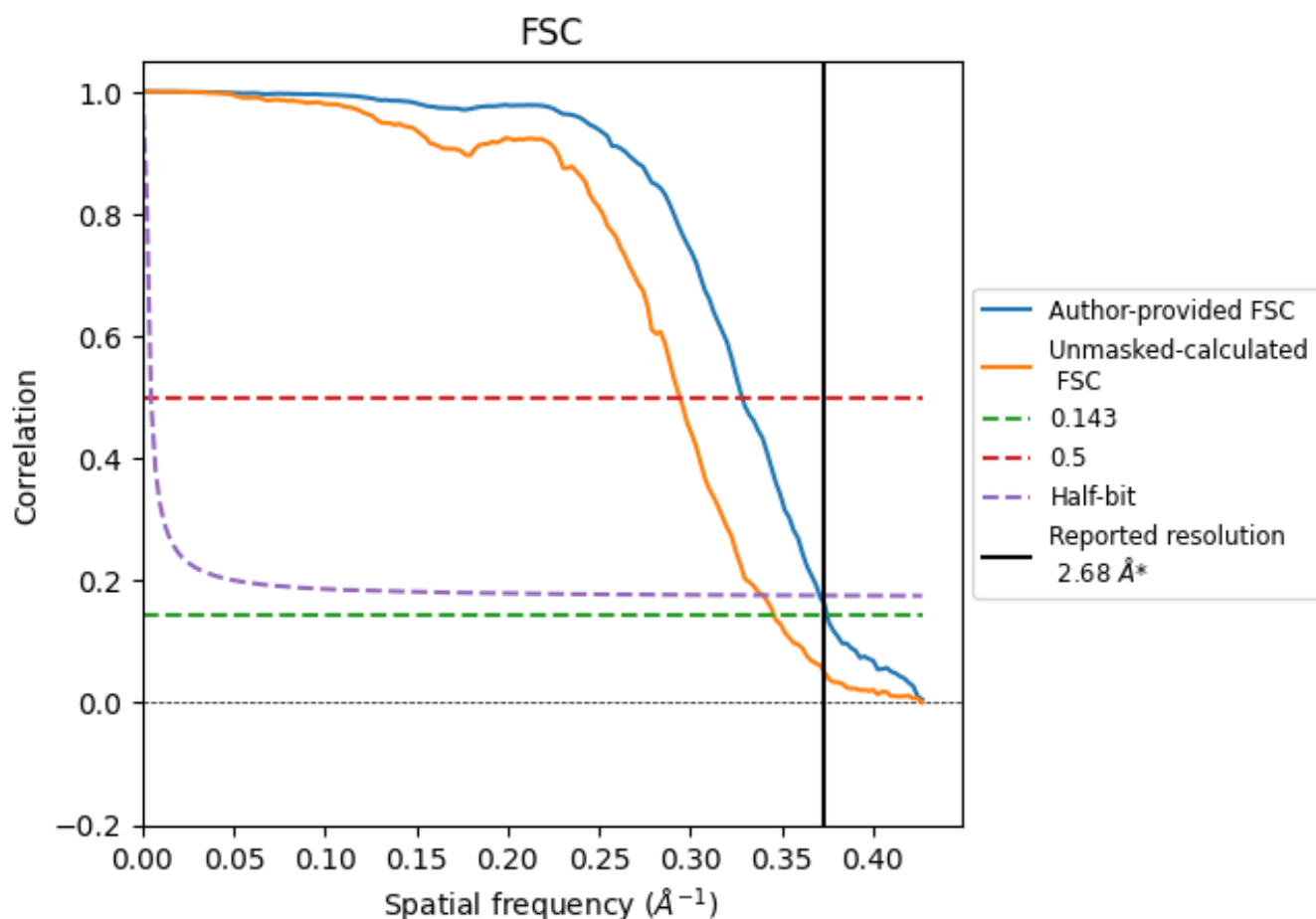


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.373 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

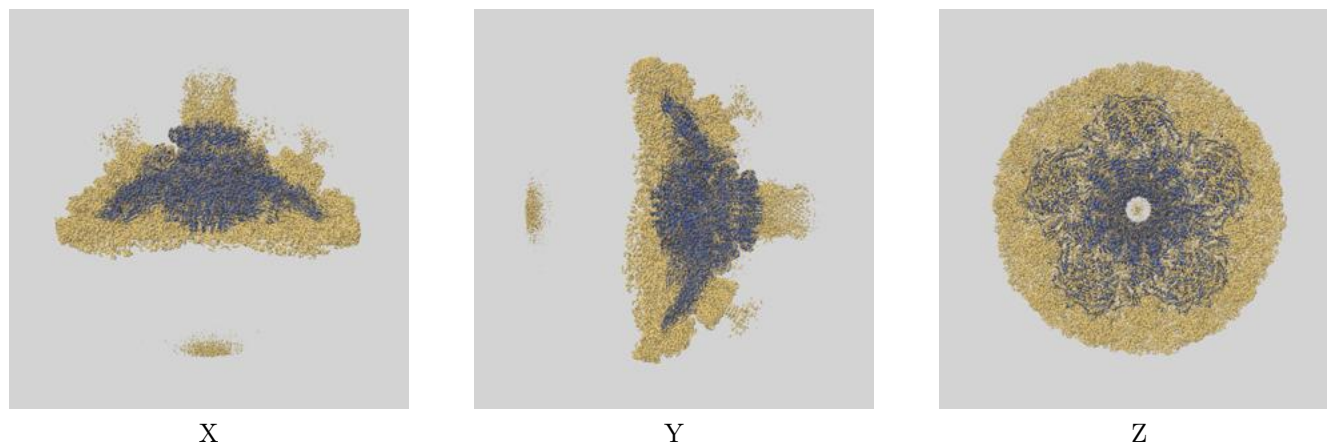
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.67	3.04	2.70
Unmasked-calculated*	2.89	3.40	2.94

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

9 Map-model fit [i](#)

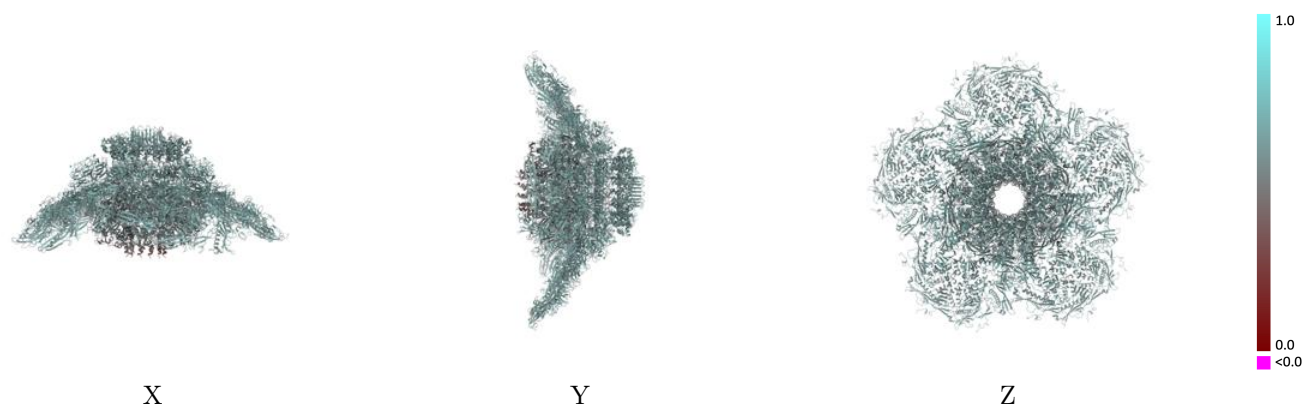
This section contains information regarding the fit between EMDB map EMD-18642 and PDB model 8QSY. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



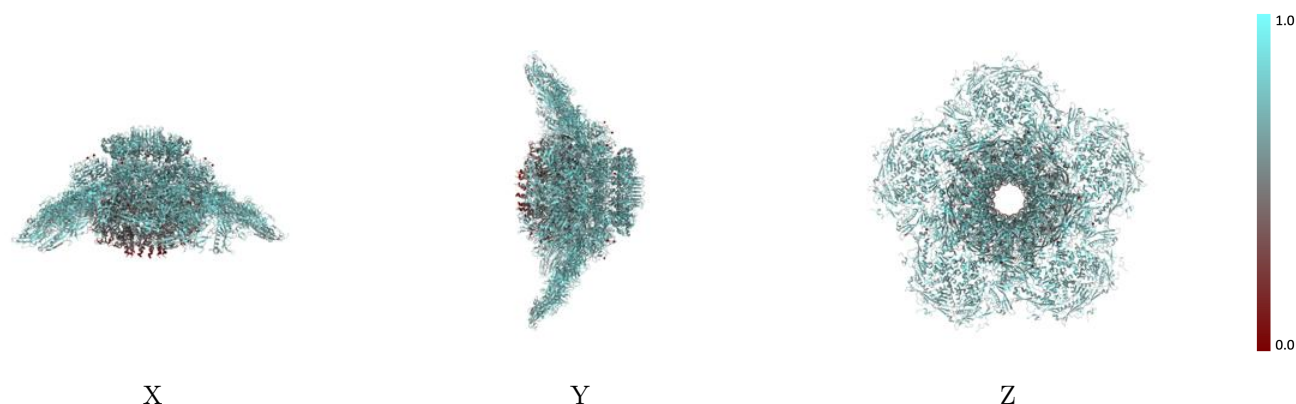
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



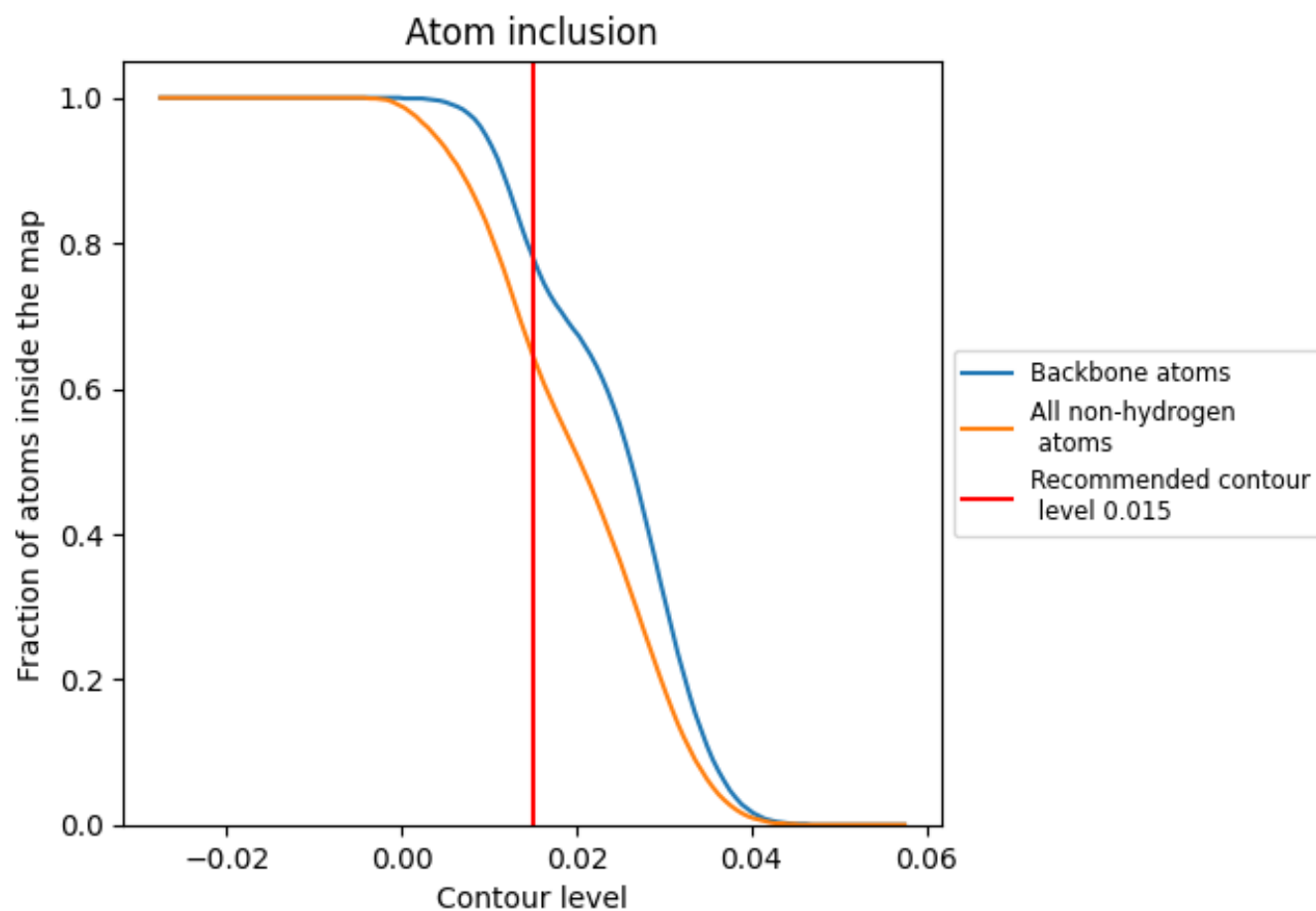
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 78% of all backbone atoms, 65% 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 (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6460	 0.5710
JA	 0.7210	 0.5940
JB	 0.7090	 0.5940
JC	 0.6730	 0.5820
JD	 0.6710	 0.5800
JE	 0.7020	 0.5870
JF	 0.7110	 0.5940
JI	 0.6770	 0.5990
JJ	 0.6520	 0.5770
JK	 0.6780	 0.5990
KA	 0.7160	 0.5930
KB	 0.7090	 0.5930
KC	 0.6710	 0.5830
KD	 0.6660	 0.5780
KE	 0.6950	 0.5890
KF	 0.7110	 0.5940
KI	 0.6730	 0.5960
KJ	 0.6530	 0.5750
KK	 0.6920	 0.6040
LA	 0.7240	 0.5960
LB	 0.7070	 0.5930
LC	 0.6730	 0.5850
LD	 0.6700	 0.5840
LE	 0.6990	 0.5890
LF	 0.7100	 0.5910
LI	 0.6700	 0.5950
LJ	 0.6550	 0.5860
LK	 0.6860	 0.6010
MA	 0.7180	 0.5950
MB	 0.7040	 0.5930
MC	 0.6760	 0.5820
MD	 0.6760	 0.5800
ME	 0.6970	 0.5890
MF	 0.6820	 0.5880
MI	 0.6800	 0.5990



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Chain	Atom inclusion	Q-score
MJ	 0.6880	 0.6000
MK	 0.6980	 0.6040
NA	 0.7280	 0.5980
NB	 0.7040	 0.5890
NC	 0.6710	 0.5830
ND	 0.6710	 0.5810
NE	 0.6930	 0.5880
NF	 0.7020	 0.5910
NI	 0.6710	 0.6020
NJ	 0.6750	 0.5970
NK	 0.6970	 0.6070
P5	 0.7090	 0.5890
P6	 0.6930	 0.5820
P7	 0.7150	 0.5870
P8	 0.7210	 0.5890
P9	 0.7080	 0.5850
PA	 0.5050	 0.5100
PB	 0.5260	 0.5250
PC	 0.5290	 0.5300
PD	 0.5170	 0.5160
PE	 0.5490	 0.5350
PF	 0.5430	 0.5280
PG	 0.5340	 0.5310
PH	 0.5460	 0.5380
PI	 0.5140	 0.5250
PJ	 0.4780	 0.5090
PK	 0.5110	 0.5230
PL	 0.5120	 0.5230
PM	 0.7090	 0.5940
PN	 0.7150	 0.5940
PO	 0.7200	 0.5900
PP	 0.7060	 0.5840
PQ	 0.6980	 0.5820
PR	 0.7050	 0.5910
PS	 0.6800	 0.5850
PT	 0.6950	 0.5820
PU	 0.6920	 0.5840
PV	 0.6990	 0.5840
PW	 0.6940	 0.5850
PX	 0.6800	 0.5830