



Full wwPDB EM Validation Report ⓘ

Oct 14, 2024 – 05:27 pm BST

PDB ID : 8QSY
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.dev113
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.39

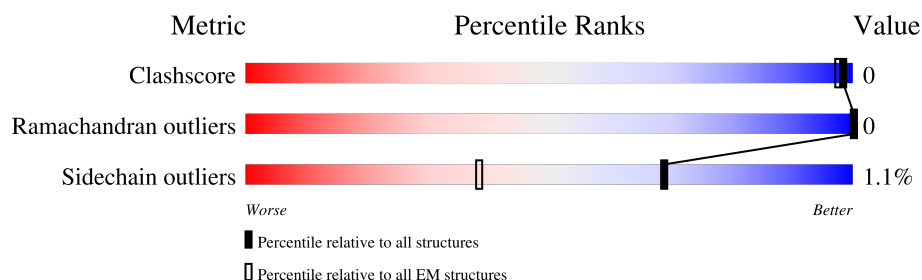
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY






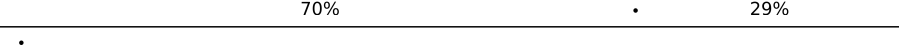
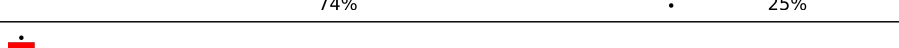

The reported resolution of this entry is 2.68 Å.

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
1	JB	396	
1	JC	396	
1	JD	396	
1	JE	396	
1	JF	396	
1	KA	396	
1	KB	396	

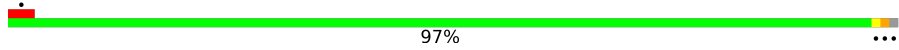
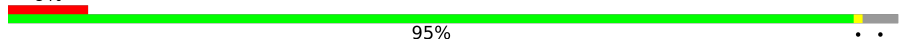
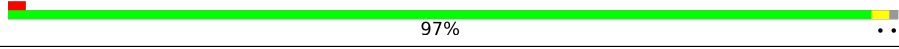
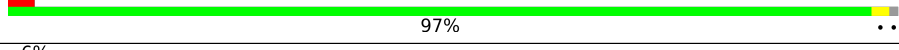
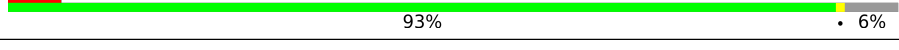
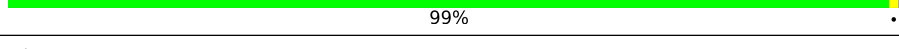
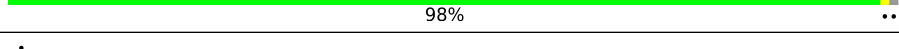
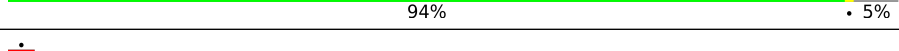
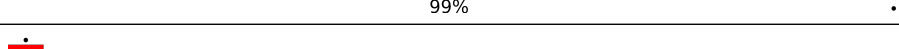
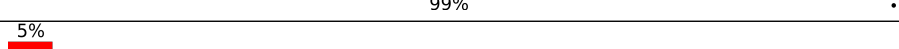
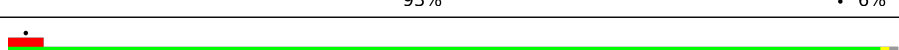
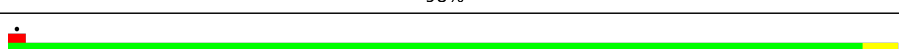
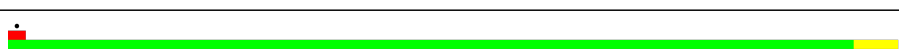
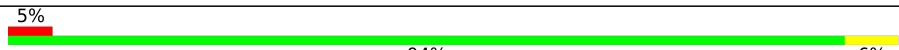
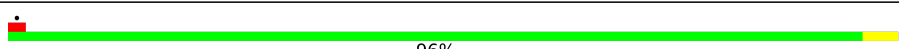
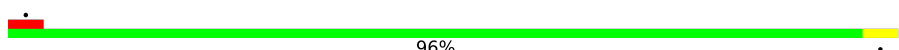




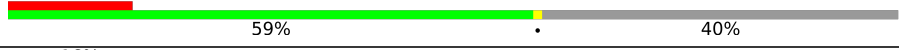
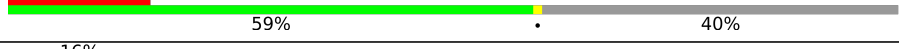



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Mol	Chain	Length	Quality of chain
1	KC	396	
1	KD	396	
1	KE	396	
1	KF	396	
1	LA	396	
1	LB	396	
1	LC	396	
1	LD	396	
1	LE	396	
1	LF	396	
1	MA	396	
1	MB	396	
1	MC	396	
1	MD	396	
1	ME	396	
1	MF	396	
1	NA	396	
1	NB	396	
1	NC	396	
1	ND	396	
1	NE	396	
1	NF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

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Mol	Chain	Length	Quality of chain
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	
4	PG	675	
4	PH	675	

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Mol	Chain	Length	Quality of chain
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 (three-letter code: 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

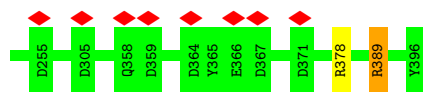
- Molecule 7 is POTASSIUM ION (three-letter code: K) (formula: K) (labeled as "Ligand of Interest" by depositor).

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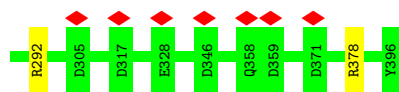
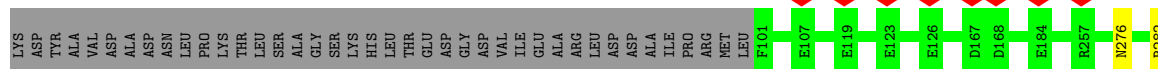
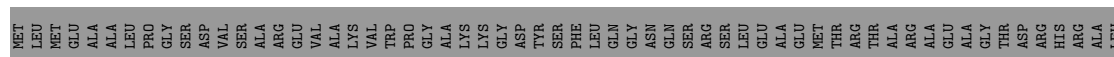
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Mol	Chain	Residues	Atoms		AltConf
7	MI	1	Total 1	K 1	0
7	MJ	2	Total 2	K 2	0
7	MK	1	Total 1	K 1	0
7	NI	1	Total 1	K 1	0
7	NJ	1	Total 1	K 1	0
7	NK	1	Total 1	K 1	0
7	P6	1	Total 1	K 1	0



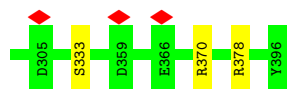
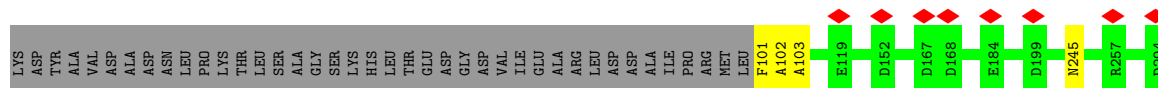
- Molecule 1: HK97 gp5-like major capsid protein

Chain JD: 74% 25%



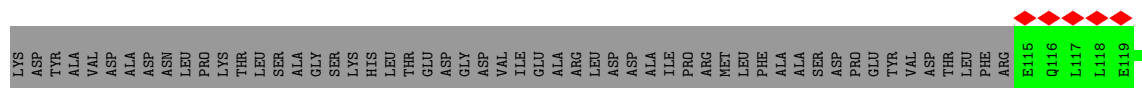
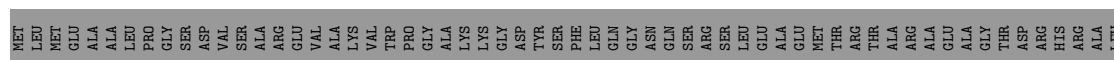
- Molecule 1: HK97 gp5-like major capsid protein

Chain JE: 73% 25%



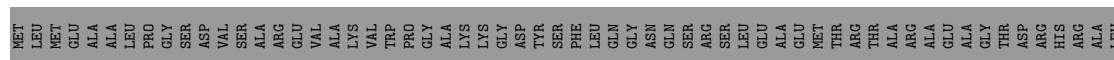
- Molecule 1: HK97 gp5-like major capsid protein

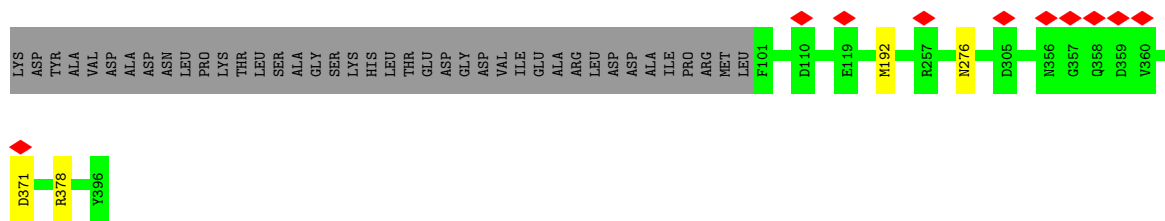
Chain JF: 70% 29%



- Molecule 1: HK97 gp5-like major capsid protein

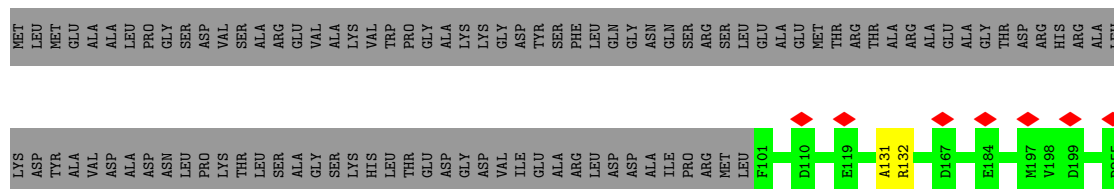
Chain KA: 74% 25%





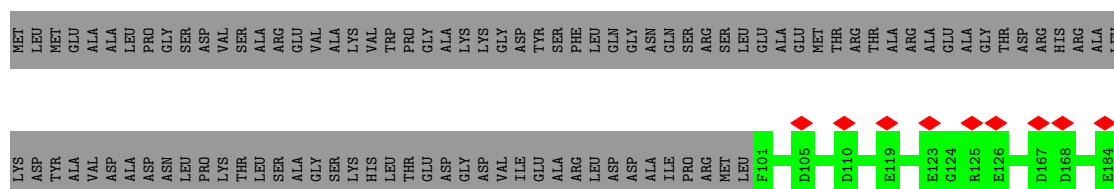
- Molecule 1: HK97 gp5-like major capsid protein

Chain KB: 73% 25%



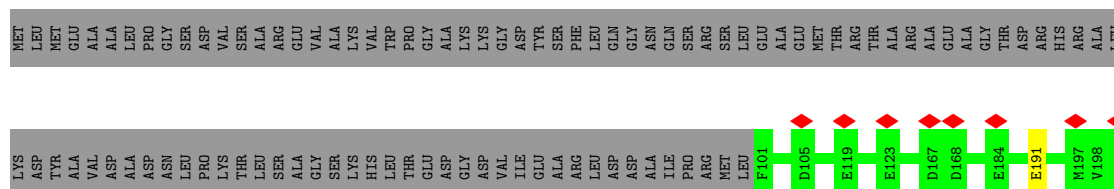
- Molecule 1: HK97 gp5-like major capsid protein

Chain KC: 74% 25% 6%




- Molecule 1: HK97 gp5-like major capsid protein

Chain KD: 73% 25%



- Molecule 1: HK97 gp5-like major capsid protein

Chain KE:  74% 25%

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

LYS ASP TYR ALA VAL ASP ALA ASP ASN PRO LYS THR LEU ALA ARG GLY VAL SER ALA LYS HIS THR PRO GLY ASP GLY VAL ILE ASP TYR GLU ARG LEU ASP ASP ALA ALA ILE PRO ARG MET LEU F101 D110 E119 E123 D152 D167 D168 E184 N245 R257 D294

D305 S311 E328 Q358 D359 D371 R378 Y396

- Molecule 1: HK97 gp5-like major capsid protein


Chain KF:  70% 29%

MET LEU MET TYR ALA VAL ASP ALA ASP ASN PRO LYS THR LEU ALA ARG GLY VAL SER ALA LYS HIS THR PRO GLY ASP GLY VAL ILE ASP TYR GLU ARG LEU ASP ASP ALA ALA ILE PRO ARG MET LEU PHE GLU ALA ALA SER ASP PRO GLU TYR VAL ASP THR ARG E115 Q116 L117 L118 E119

LYS ASP TYR ALA VAL ASP ALA ASP ASN PRO LYS THR LEU ALA ARG GLY VAL SER ALA LYS HIS THR PRO GLY ASP GLY VAL ILE ASP TYR GLU ARG LEU ASP ASP ALA ALA ILE PRO ARG MET LEU PHE GLU ALA ALA SER ASP PRO GLU TYR VAL ASP THR ARG E115 Q116 L117 L118 E119

H136 E170 D190 D194 D305 H349 D364 R378 Y396

- Molecule 1: HK97 gp5-like major capsid protein


Chain LA:  73% 25%

MET LEU MET TYR ALA VAL ASP ALA ASP ASN PRO LYS THR LEU ALA ARG GLY VAL SER ALA LYS HIS THR PRO GLY ASP GLY VAL ILE ASP TYR GLU ARG LEU ASP ASP ALA ALA ILE PRO ARG MET LEU PHE GLU ALA ALA SER ASP PRO GLU TYR VAL ASP THR ARG E115 Q116 L117 L118 E119

LYS ASP TYR ALA VAL ASP ALA ASP ASN PRO LYS THR LEU ALA ARG GLY VAL SER ALA LYS HIS THR PRO GLY ASP GLY VAL ILE ASP TYR GLU ARG LEU ASP ASP ALA ALA ILE PRO ARG MET LEU F101 D110 E119 E126 E164 D167 D168 V188 R257 N276 E328

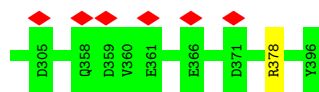
N356 G357 Q358 D359 R370 D371 R378 Y396

- Molecule 1: HK97 gp5-like major capsid protein

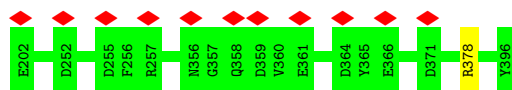
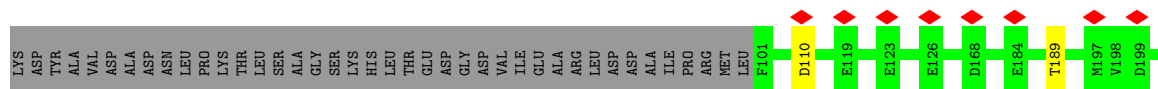
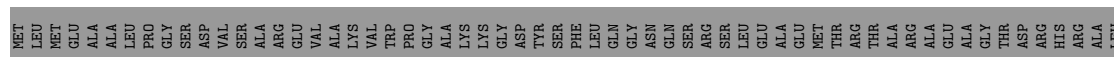
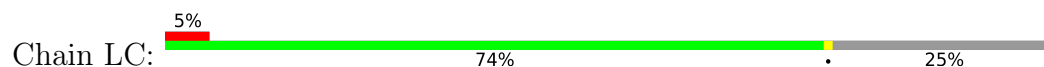
Chain LB:  74% 25%

MET LEU MET TYR ALA VAL ASP ALA ASP ASN PRO LYS THR LEU ALA ARG GLY VAL SER ALA LYS HIS THR PRO GLY ASP GLY VAL ILE ASP TYR GLU ARG LEU ASP ASP ALA ALA ILE PRO ARG MET LEU PHE GLU ALA ALA SER ASP PRO ARG MET LEU F101 S104 D105 D110 L117 L118 E119 D167 D199 E202 R257 D284

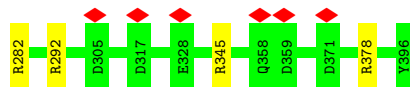
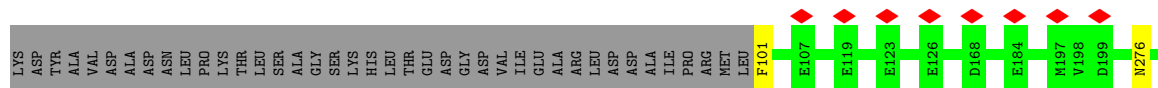
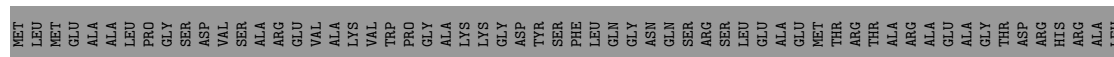
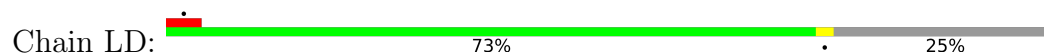
LYS ASP TYR ALA VAL ASP ALA ASP ASN PRO LYS THR LEU ALA ARG GLY VAL SER ALA LYS HIS THR PRO GLY ASP GLY VAL ILE ASP TYR GLU ARG LEU ASP ASP ALA ALA ILE PRO ARG MET LEU F101 S104 D105 D110 L117 L118 E119 D167 D199 E202 R257 D284



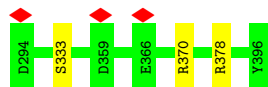
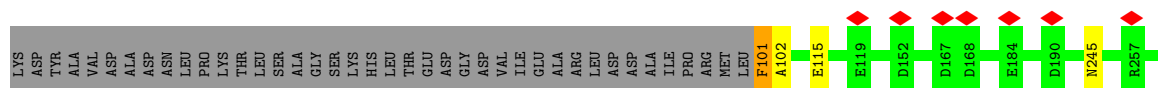
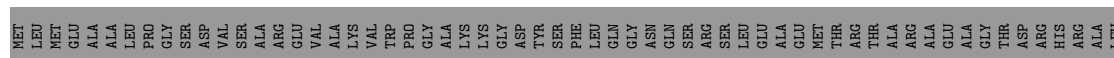
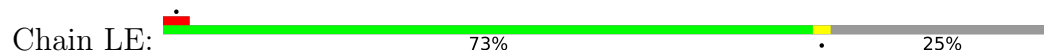
- Molecule 1: HK97 gp5-like major capsid protein



- Molecule 1: HK97 gp5-like major capsid protein

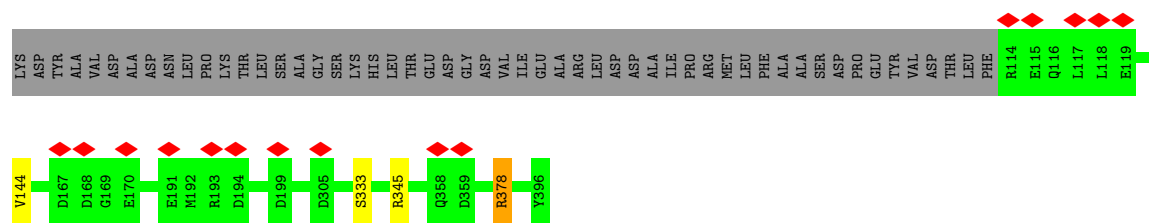


- Molecule 1: HK97 gp5-like major capsid protein



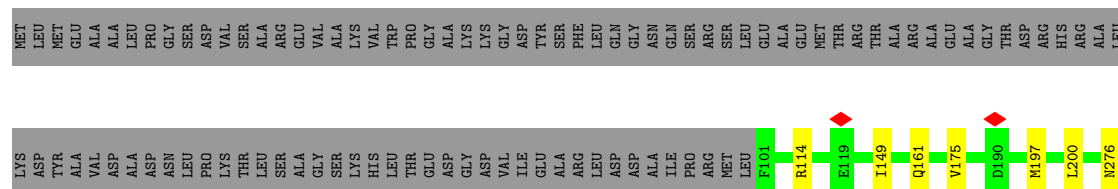
- Molecule 1: HK97 gp5-like major capsid protein





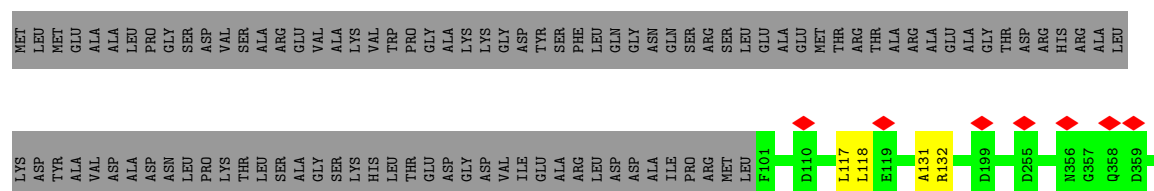
- Molecule 1: HK97 gp5-like major capsid protein

Chain MA: 73% 25%



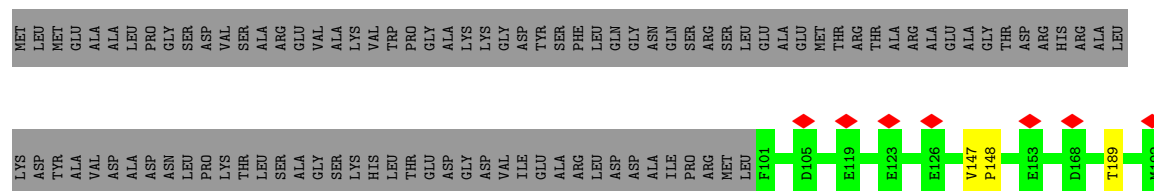
- Molecule 1: HK97 gp5-like major capsid protein

Chain MB: 73% 25%




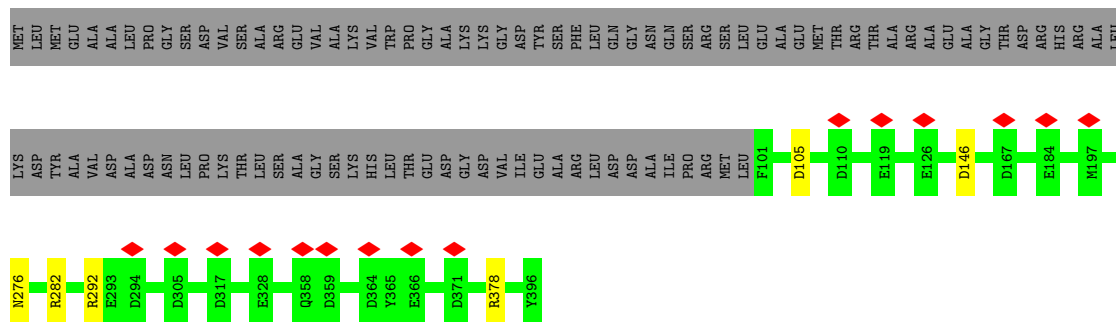
- Molecule 1: HK97 gp5-like major capsid protein

Chain MC: 73% 25%




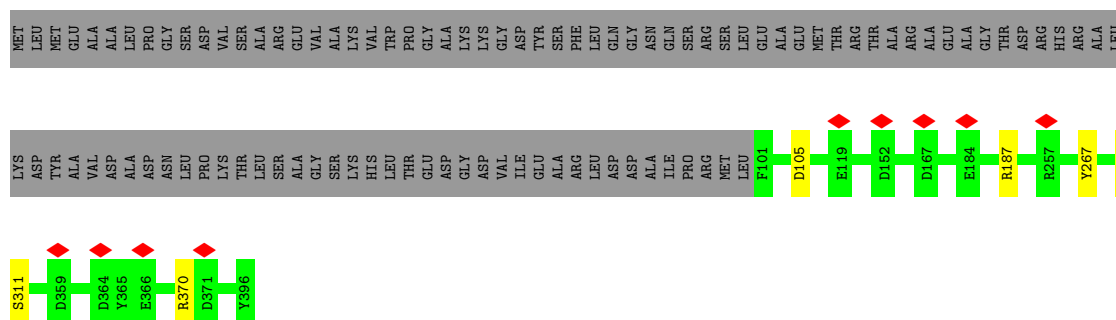
- Molecule 1: HK97 gp5-like major capsid protein

Chain MD:  73% 25%




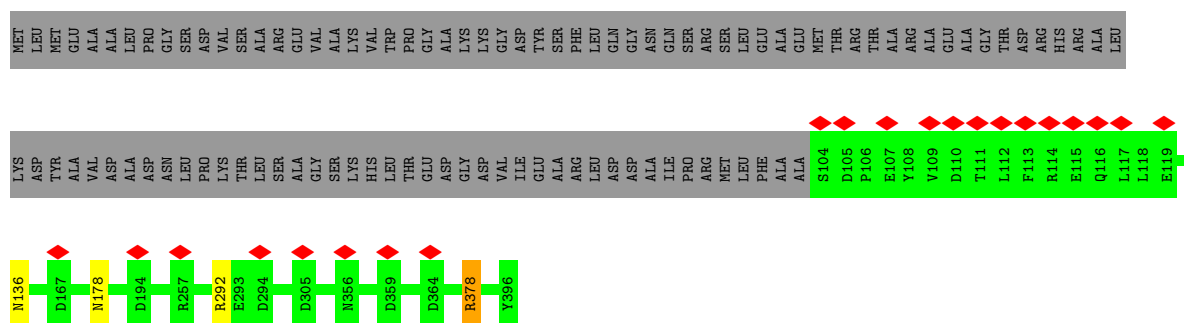
- Molecule 1: HK97 gp5-like major capsid protein

Chain ME:  73% 25%




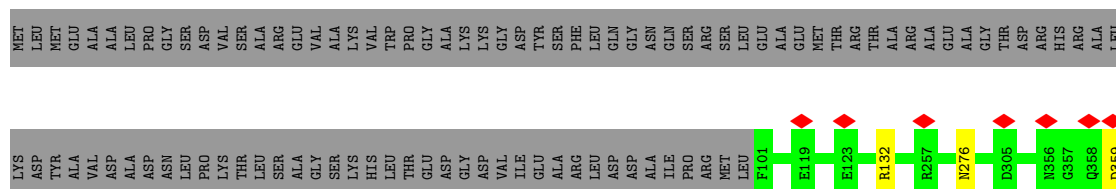
- Molecule 1: HK97 gp5-like major capsid protein

Chain MF:  5% 73% 26%



- Molecule 1: HK97 gp5-like major capsid protein

Chain NA:  74% 25%



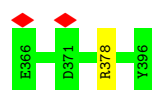


- Molecule 1: HK97 gp5-like major capsid protein

Chain NB: 74% 25%

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

LYS ASP TYR VAL ASP ALA ASP ASN PRO SER THR LEU SER ALA VAL SER LYS HIS LEU THR PRO GLY ASP LYS ASP VAL ILE ASP GLU ARG ALA LEU ASP ASP ASP ILE PRO ARG MET LEU F101 D105 D110 E119 E126 D167 D199 R257 N356 D359

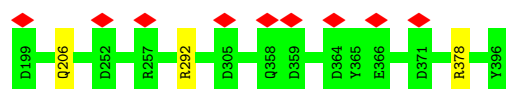


- Molecule 1: HK97 gp5-like major capsid protein

Chain NC: 5% 74% 25%

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LYS ASP TYR VAL ASP ALA ASP ASN PRO SER THR LEU SER ALA VAL SER LYS HIS LEU THR PRO GLY ASP LYS ASP VAL ILE ASP GLU ARG ALA LEU ASP ASP ASP ILE PRO ARG MET LEU F101 D105 D110 E115 E119 E123 E126 E153 D168 E184

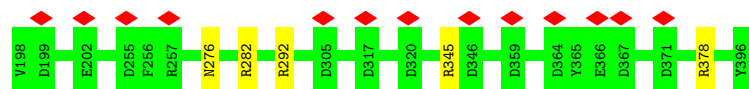


- Molecule 1: HK97 gp5-like major capsid protein

Chain ND: 6% 73% 25%

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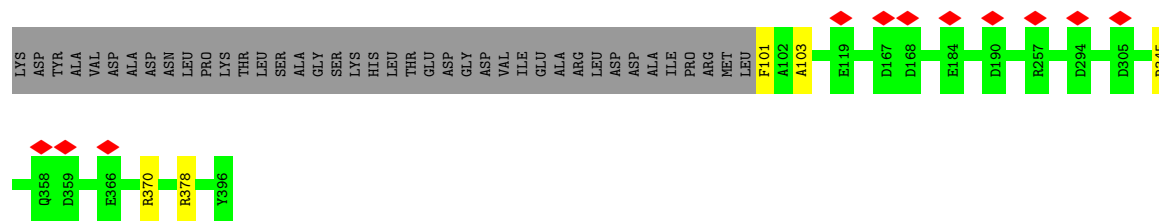
LYS ASP TYR VAL ASP ALA ASP ASN PRO SER THR LEU SER ALA VAL SER LYS HIS LEU THR PRO GLY ASP LYS ASP VAL ILE ASP GLU ARG ALA LEU ASP ASP ASP ILE PRO ARG MET LEU F101 D105 D110 E119 E123 E126 R143 D167 D168 E184 M197



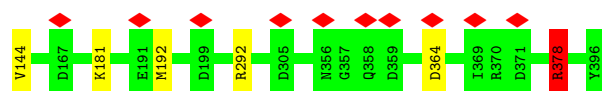
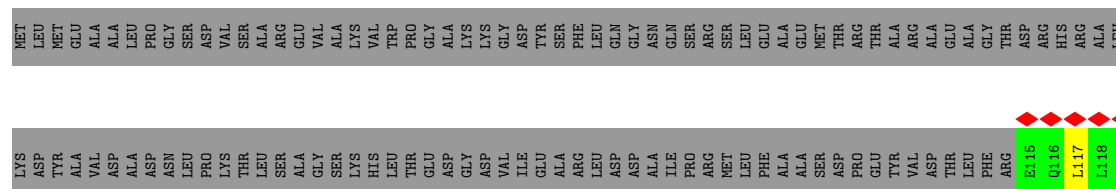
- Molecule 1: HK97 gp5-like major capsid protein

Chain NE: 73% 25%

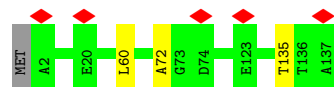
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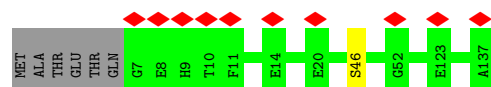
- Molecule 1: HK97 gp5-like major capsid protein



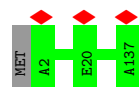
- Molecule 2: Capsid stabilization protein



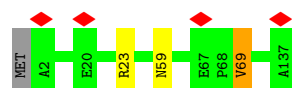
- Molecule 2: Capsid stabilization protein



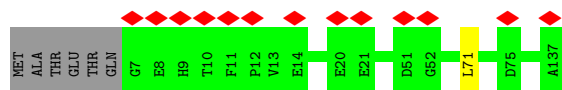
- Molecule 2: Capsid stabilization protein



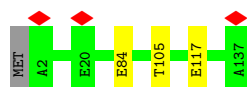
- Molecule 2: Capsid stabilization protein



• Molecule 2: Capsid stabilization protein



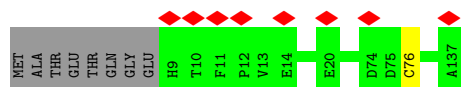
• Molecule 2: Capsid stabilization protein



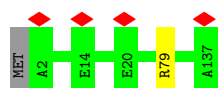
• Molecule 2: Capsid stabilization protein



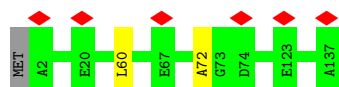
• Molecule 2: Capsid stabilization protein



• Molecule 2: Capsid stabilization protein

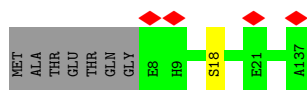


• Molecule 2: Capsid stabilization protein

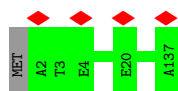


• Molecule 2: Capsid stabilization protein

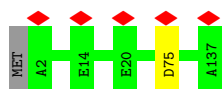




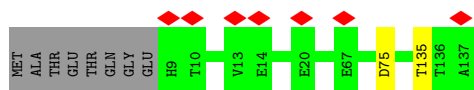
- Molecule 2: Capsid stabilization protein



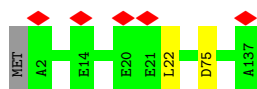
- Molecule 2: Capsid stabilization protein



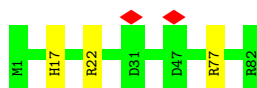
- Molecule 2: Capsid stabilization protein



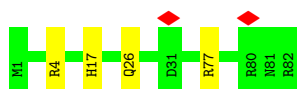
- Molecule 2: Capsid stabilization protein



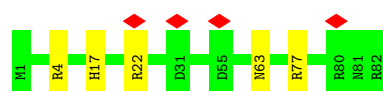
- Molecule 3: Hypothetical protein gp21



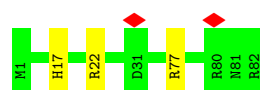
- Molecule 3: Hypothetical protein gp21



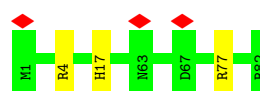
- Molecule 3: Hypothetical protein gp21



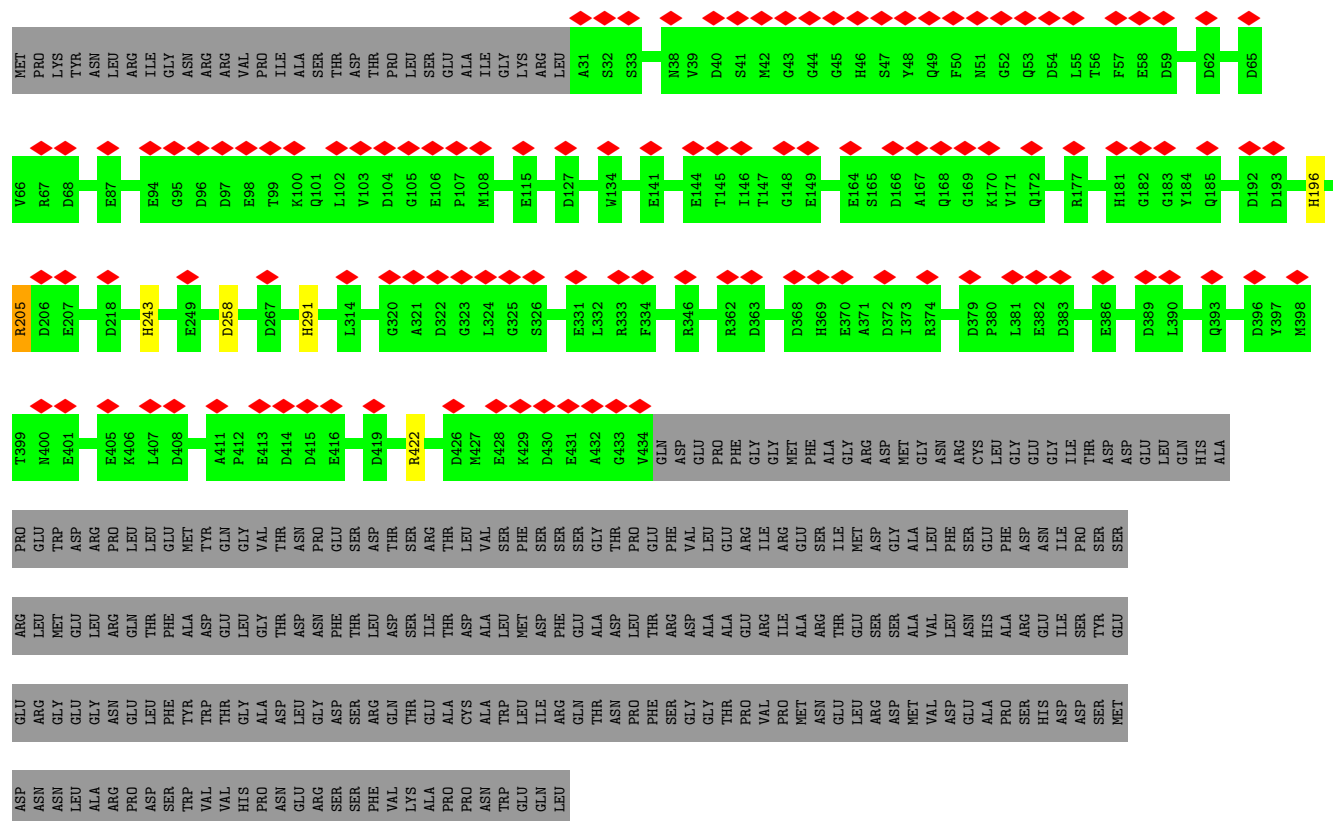
- Chain P8:  96%



- Chain P9: 96%



- Chain PA: 



- 
- WORLDWIDE
PDB
PROTEIN DATA BANK



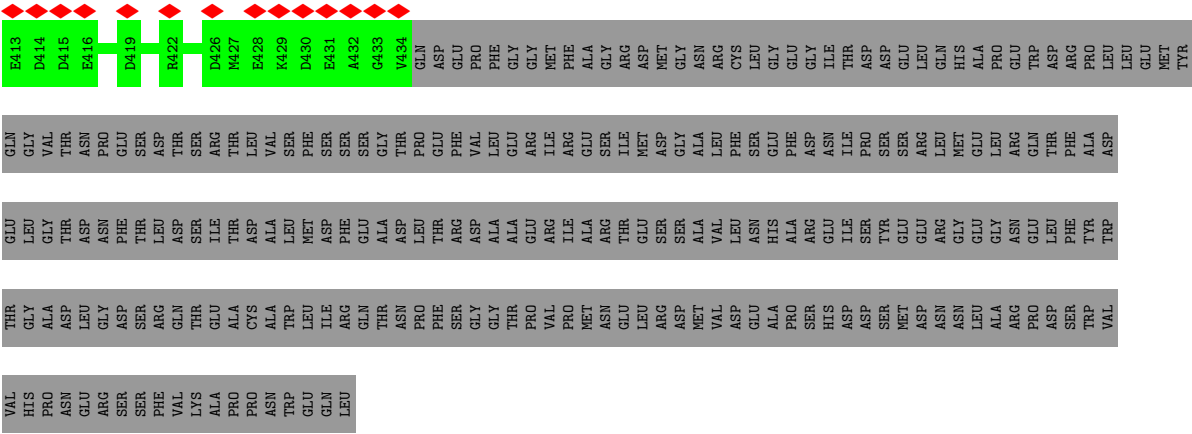
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GLU	GLY	ASN	GLU	LEU	PHE	THR	THR	THR	GLY	ALA	ASP	LEU	GLY	ASP	SER	ARG	GLN	ARG	GLN	THR	GLU	ALA	CYS	TRP	TRP	LEU	ILE	ARG	GLN	THR	ASN	PRO	PHE	THR	VAL	PRO	THR	GLY	GLY	THR	PRO	VAL	PRO	PRO	PRO	ASP	ASP	VAL	MET	ASN	GLU	LEU	ARG	GLU	ASP	HIS	ASP	ASP	SER	ASP	ASP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

- Molecule 4: Portal protein

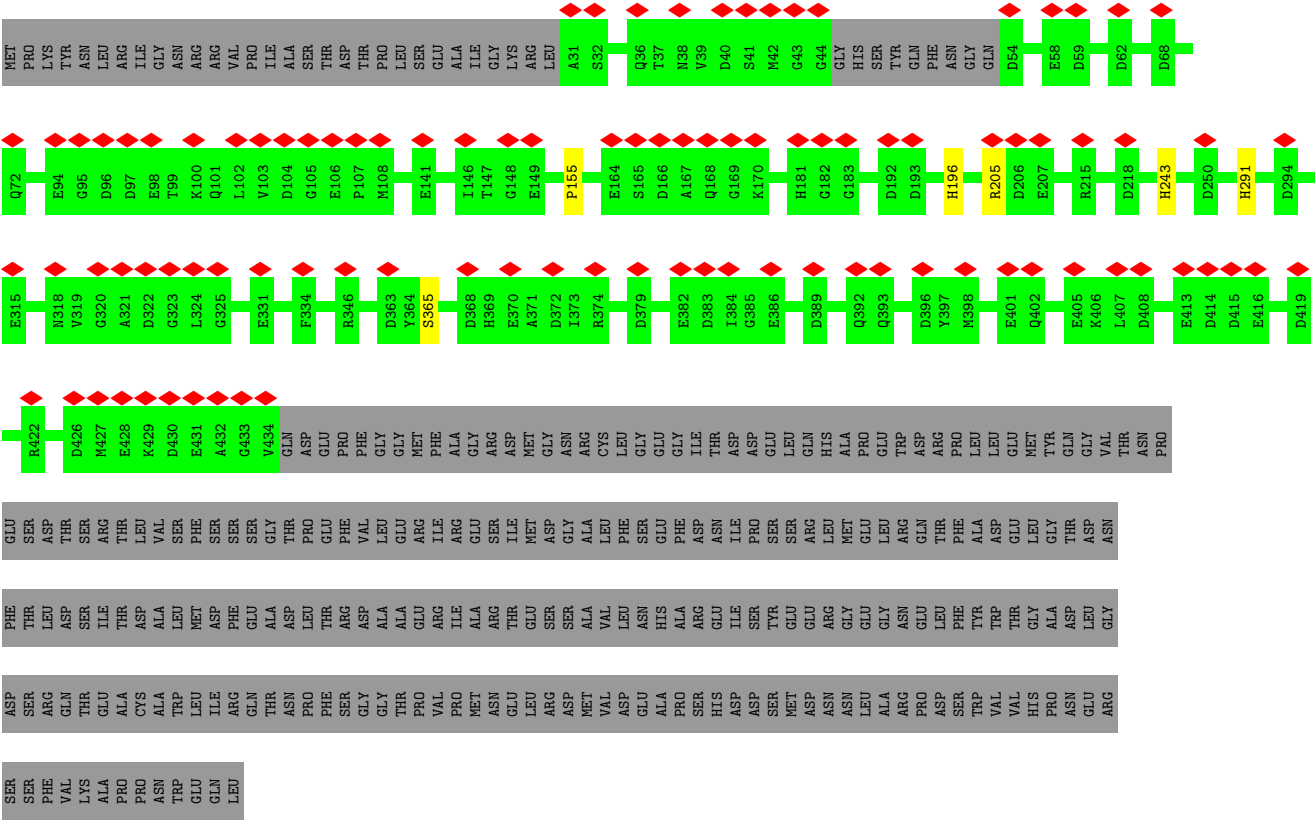
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- Molecule 4: Portal protein

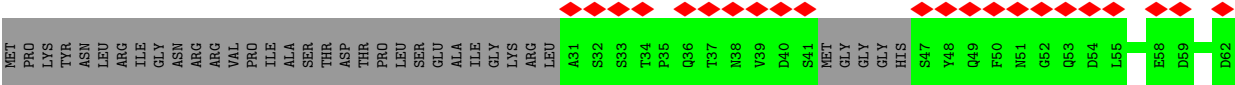
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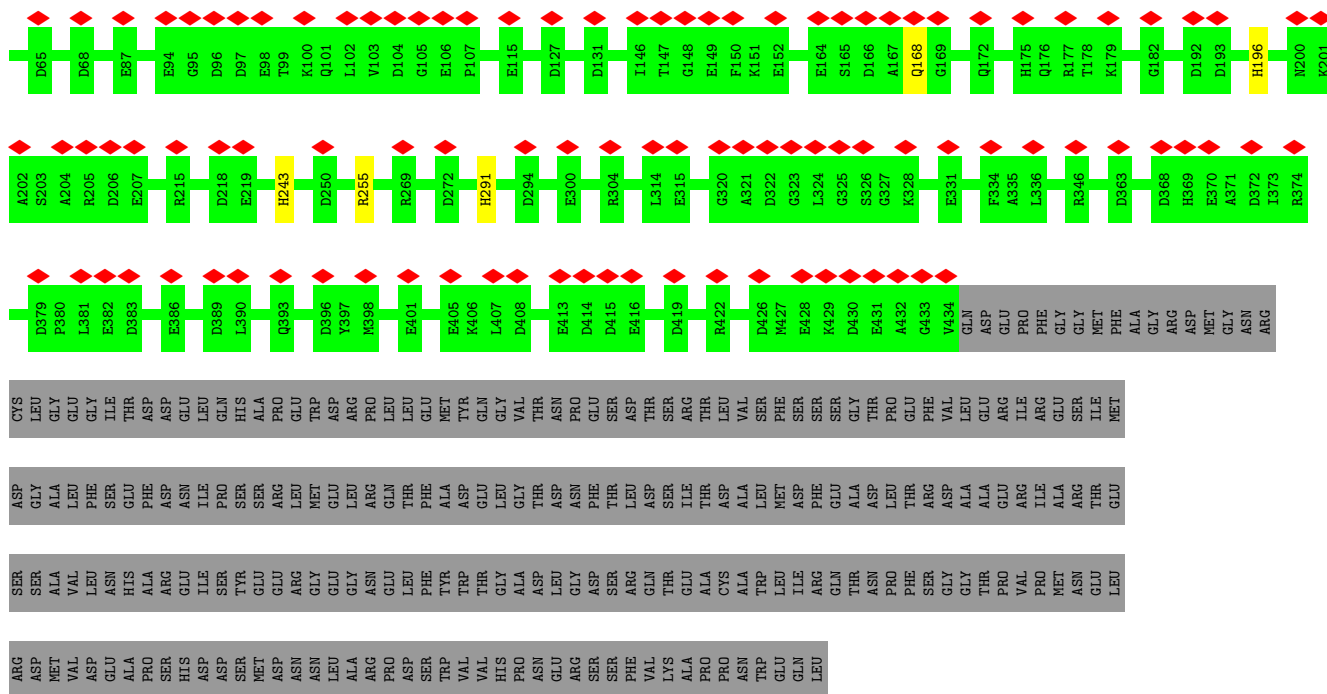


● Molecule 4: Portal protein

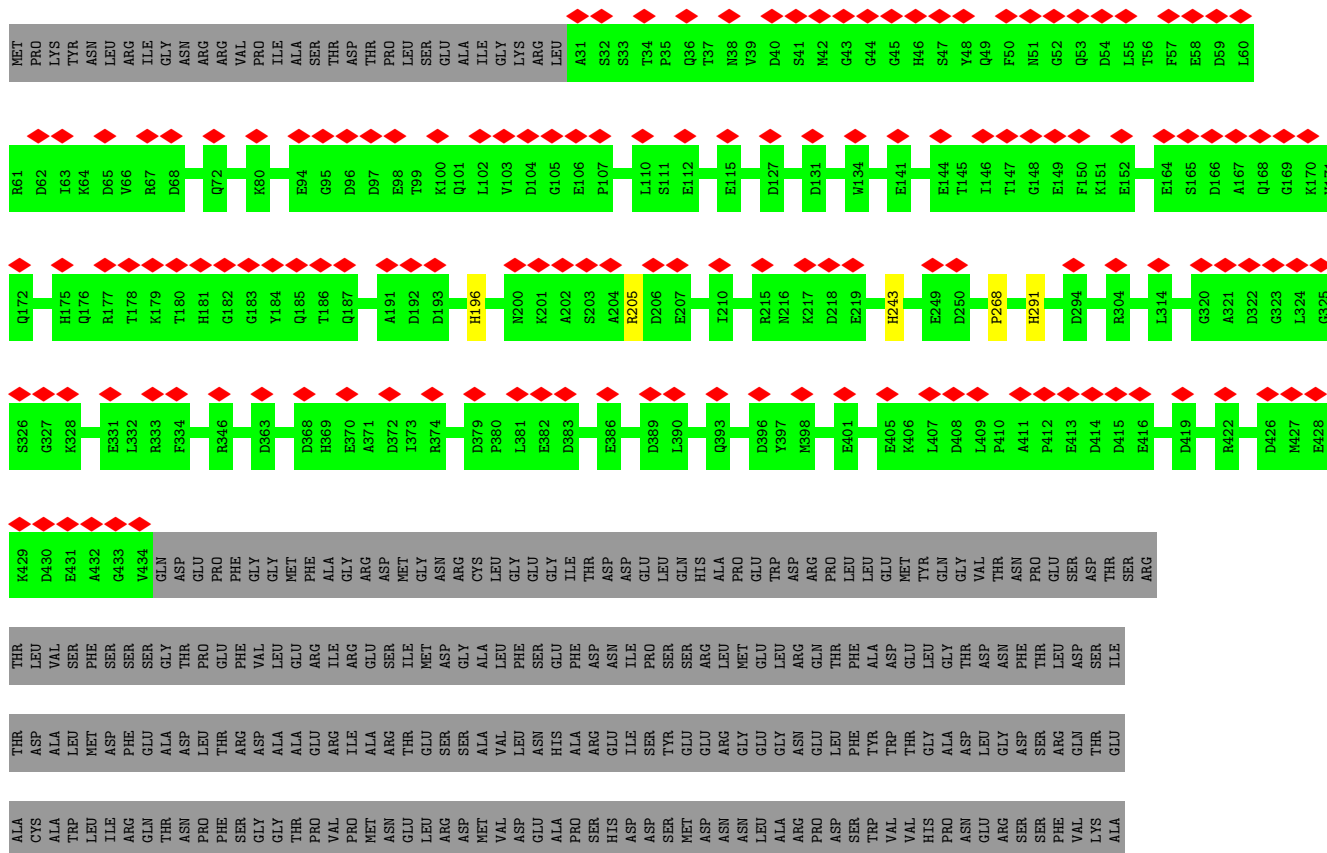


● Molecule 4: Portal protein





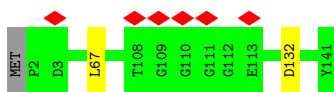
- Molecule 4: Portal protein



ARG	ASP	SER	ASP	GLY	ASP	CYS
ASP	MET	VAL	VAL	LEU	GLY	LEU
VAL	ASP	GLU	GLU	PHE	GLY	GLU
GLU	GLU	ASN	ASN	SER	ILE	ILE
ALA	GLU	HIS	ALA	GLU	THR	THR
PRO	PRO	ALA	PHE	PHE	ASP	ASP
SER	SER	ARG	ASP	ASP	ASP	GLU
HIS	HIS	GLU	ASN	ASN	GLU	ASP
ASP	ASP	ILE	ILE	ILE	LEU	LEU
ASP	ASP	SER	PRO	SER	GLN	HIS
SER	SER	TYR	GLU	SER	ALA	ALA
MET	MET	GLU	GLU	SER	PRO	PRO
ASP	ASN	ARG	LEU	LEU	GLU	GLU
ASN	ASN	GLY	GLY	MET	TRP	ASP
LEU	LEU	GLU	GLU	GLU	ASP	ASP
ALA	ALA	GLY	GLY	LEU	ARG	ARG
ARG	ARG	ASN	ASN	ARG	PRO	PRO
PRO	PRO	GLU	GLN	LEU	LEU	LEU
ASP	ASP	LEU	THR	PHE	GLU	GLU
SER	SER	PHE	THR	ALA	MET	MET
TRP	TRP	TVR	ALA	ALA	GLU	GLU
VAL	VAL	TRP	ASP	ASP	TYR	TYR
VAL	VAL	THR	GLU	GLU	GLN	GLN
HIS	HIS	GLY	LEU	LEU	VAL	VAL
PRO	PRO	ALA	ASP	GLY	THR	THR
ASN	ASN	LEU	ASP	ASN	ASN	ASN
GLU	GLU	GLY	ASP	ASN	PRO	PRO
ARG	ARG	GLY	ASP	PHE	GLU	GLU
SER	SER	SER	THR	THR	SER	SER
PHE	PHE	ARG	LEU	LEU	ASP	ASP
VAL	VAL	GLN	ASP	THR	THR	THR
LYS	LYS	THR	SER	SER	SER	SER
ALA	ALA	GLU	ILE	ARG	ARG	ARG
PRO	PRO	ALA	THR	THR	LEU	LEU
PRO	PRO	CYS	ASP	ASP	VAL	VAL
ASN	ASN	ALA	ALA	ALA	ALA	ALA
TRP	TRP	ALA	LEU	LEU	SER	SER
GLU	GLU	LEU	MET	MET	THR	THR
GLN	GLN	ILE	ASP	ASP	GLY	GLY
LEU	LEU	ARG	PHE	PHE	THR	THR
		ASN	ASN	ASP	PRO	PRO
		PHE	PHE	LEU	GLU	GLU
		SER	SER	THR	PHE	PHE
		GLY	GLY	ASP	ARG	ARG
		GLY	ALA	ALA	VAL	VAL
		THR	ALA	LEU	LEU	LEU
		PRO	GLU	GLU	ARG	ARG
		VAL	ARG	THR	ILE	ILE
		PRO	ILE	ARG	GLU	GLU
		MET	ALA	ALA	SER	SER
		GLU	THR	THR	THR	THR
		LEU	GLU	GLU	ILE	ILE
		LEU	LEU	LEU	GLU	GLU

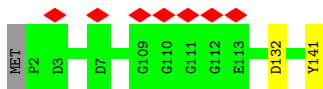
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PM:  98%



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

Chain PN: 



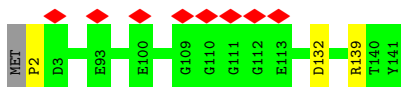
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PO: 



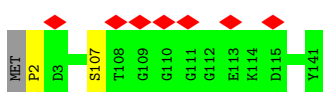
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector

Chain PP:  97% 6% ..

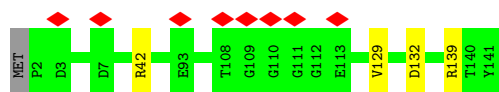


- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector

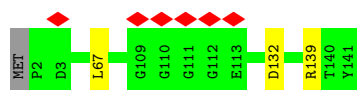
Chain PQ:  5% 98%



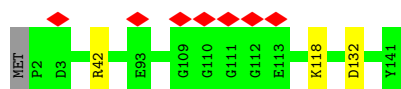
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



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



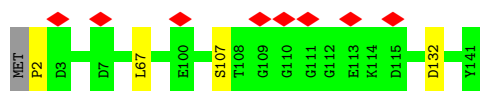
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



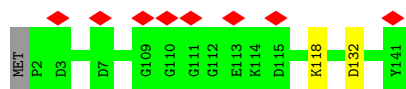
- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



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

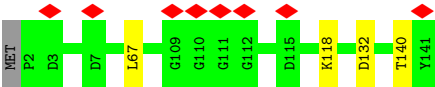


- Molecule 5: HK97 gp6-like/SPP1 gp15-like head-tail connector



- 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 (\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 (\AA)	1.171, 1.171, 1.171	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.34	0/2335	0.79	3/3172 (0.1%)
1	JB	0.33	0/2335	0.77	1/3172 (0.0%)
1	JC	0.33	0/2335	0.77	2/3172 (0.1%)
1	JD	0.33	0/2335	0.75	1/3172 (0.0%)
1	JE	0.33	0/2335	0.76	1/3172 (0.0%)
1	JF	0.34	0/2216	0.79	4/3009 (0.1%)
1	KA	0.33	0/2335	0.76	0/3172
1	KB	0.34	0/2335	0.77	0/3172
1	KC	0.33	0/2335	0.76	0/3172
1	KD	0.34	0/2335	0.76	1/3172 (0.0%)
1	KE	0.33	0/2335	0.77	0/3172
1	KF	0.33	0/2216	0.77	2/3009 (0.1%)
1	LA	0.34	0/2335	0.79	3/3172 (0.1%)
1	LB	0.34	0/2335	0.77	0/3172
1	LC	0.33	0/2335	0.77	0/3172
1	LD	0.33	0/2335	0.74	1/3172 (0.0%)
1	LE	0.33	0/2335	0.75	1/3172 (0.0%)
1	LF	0.33	0/2227	0.77	3/3023 (0.1%)
1	MA	0.34	0/2335	0.80	2/3172 (0.1%)
1	MB	0.34	0/2335	0.78	1/3172 (0.0%)
1	MC	0.33	0/2335	0.78	2/3172 (0.1%)
1	MD	0.33	0/2335	0.77	1/3172 (0.0%)
1	ME	0.33	0/2335	0.75	1/3172 (0.0%)
1	MF	0.33	0/2313	0.76	0/3142
1	NA	0.33	0/2335	0.78	2/3172 (0.1%)
1	NB	0.34	0/2335	0.76	0/3172
1	NC	0.34	0/2335	0.78	0/3172
1	ND	0.33	0/2335	0.75	2/3172 (0.1%)
1	NE	0.33	0/2335	0.78	3/3172 (0.1%)
1	NF	0.33	0/2216	0.78	2/3009 (0.1%)
2	JI	0.37	0/980	0.71	0/1337
2	JJ	0.38	0/943	0.71	0/1286

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	JK	0.37	0/980	0.70	0/1337
2	KI	0.37	0/980	0.75	2/1337 (0.1%)
2	KJ	0.39	0/943	0.71	0/1286
2	KK	0.37	0/980	0.69	0/1337
2	LI	0.36	0/980	0.69	0/1337
2	LJ	0.38	0/930	0.69	0/1269
2	LK	0.38	0/980	0.71	1/1337 (0.1%)
2	MI	0.38	0/980	0.68	0/1337
2	MJ	0.39	0/939	0.70	0/1281
2	MK	0.37	0/980	0.70	0/1337
2	NI	0.37	0/980	0.69	0/1337
2	NJ	0.39	0/930	0.71	0/1269
2	NK	0.37	0/980	0.69	0/1337
3	P5	0.35	0/685	0.88	2/918 (0.2%)
3	P6	0.35	0/685	0.85	1/918 (0.1%)
3	P7	0.35	0/685	0.87	2/918 (0.2%)
3	P8	0.36	0/685	0.85	1/918 (0.1%)
3	P9	0.35	0/685	0.87	1/918 (0.1%)
4	PA	0.33	0/3190	0.69	4/4326 (0.1%)
4	PB	0.33	0/3190	0.68	0/4326
4	PC	0.33	0/3130	0.66	0/4243
4	PD	0.33	0/3119	0.70	4/4228 (0.1%)
4	PE	0.33	0/3190	0.69	2/4326 (0.0%)
4	PF	0.32	0/3190	0.66	0/4326
4	PG	0.33	0/3190	0.69	2/4326 (0.0%)
4	PH	0.33	0/3113	0.67	2/4221 (0.0%)
4	PI	0.33	0/3158	0.68	0/4283
4	PJ	0.33	0/3190	0.68	0/4326
4	PK	0.33	0/3159	0.67	0/4282
4	PL	0.33	0/3130	0.65	0/4243
5	PM	0.38	0/1105	0.78	0/1492
5	PN	0.38	0/1105	0.75	0/1492
5	PO	0.38	0/1105	0.77	0/1492
5	PP	0.38	0/1105	0.78	0/1492
5	PQ	0.38	0/1105	0.77	0/1492
5	PR	0.38	0/1105	0.77	1/1492 (0.1%)
5	PS	0.37	0/1105	0.78	0/1492
5	PT	0.38	0/1105	0.77	1/1492 (0.1%)
5	PU	0.37	0/1105	0.77	0/1492
5	PV	0.37	0/1105	0.73	0/1492
5	PW	0.37	0/1105	0.77	0/1492
5	PX	0.38	0/1105	0.73	0/1492
All	All	0.34	0/138682	0.74	65/188203 (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	LE	0	1
1	ME	0	1
1	NE	0	1
All	All	0	3

There are no bond length outliers.

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	PD	205	ARG	CG-CD-NE	7.67	127.92	111.80
1	LA	378	ARG	NE-CZ-NH2	7.37	123.99	120.30
4	PE	205	ARG	CG-CD-NE	7.31	127.15	111.80
2	KI	23	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	NF	378	ARG	NE-CZ-NH2	6.92	123.76	120.30
3	P7	77	ARG	NE-CZ-NH1	-6.76	116.92	120.30
4	PD	205	ARG	NE-CZ-NH1	-6.75	116.92	120.30
3	P9	77	ARG	NE-CZ-NH1	-6.73	116.94	120.30
1	NA	132	ARG	NE-CZ-NH1	-6.71	116.95	120.30
3	P5	77	ARG	NE-CZ-NH1	-6.70	116.95	120.30
4	PH	205	ARG	CG-CD-NE	6.69	125.84	111.80
1	JA	378	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	LA	378	ARG	NE-CZ-NH1	-6.64	116.98	120.30
4	PE	205	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	LF	378	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	NE	345	ARG	NE-CZ-NH1	-6.54	117.03	120.30
4	PG	205	ARG	CG-CD-NE	6.52	125.48	111.80
4	PA	205	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	MD	282	ARG	CG-CD-NE	6.42	125.29	111.80
1	KF	378	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	LF	378	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	JA	370	ARG	NE-CZ-NH1	-6.22	117.19	120.30
1	JC	389	ARG	NE-CZ-NH1	-6.20	117.20	120.30
1	JE	370	ARG	NE-CZ-NH1	-6.20	117.20	120.30
3	P5	22	ARG	NE-CZ-NH2	6.19	123.39	120.30
2	LK	79	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	JA	378	ARG	NE-CZ-NH1	-6.05	117.28	120.30
4	PD	205	ARG	NE-CZ-NH2	6.03	123.31	120.30
1	NA	132	ARG	NE-CZ-NH2	6.02	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	KI	23	ARG	NE-CZ-NH2	5.99	123.30	120.30
1	JF	292	ARG	NE-CZ-NH1	-5.96	117.32	120.30
3	P8	77	ARG	NE-CZ-NH1	-5.90	117.35	120.30
5	PR	42	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	KF	378	ARG	NE-CZ-NH1	-5.76	117.42	120.30
4	PG	205	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	LA	370	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	NE	370	ARG	NE-CZ-NH1	-5.66	117.47	120.30
4	PA	205	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	NF	378	ARG	NE-CZ-NH1	-5.65	117.48	120.30
1	LF	345	ARG	NE-CZ-NH2	5.62	123.11	120.30
3	P7	22	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	JF	378	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	JD	282	ARG	CG-CD-NE	5.53	123.42	111.80
1	JF	345	ARG	NE-CZ-NH2	5.53	123.07	120.30
1	ME	370	ARG	NE-CZ-NH1	-5.52	117.54	120.30
4	PA	205	ARG	CG-CD-NE	5.52	123.39	111.80
1	KD	345	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	MA	114	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	MA	114	ARG	CG-CD-NE	5.49	123.33	111.80
1	LD	345	ARG	NE-CZ-NH2	5.49	123.05	120.30
1	JF	378	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	ND	143	ARG	NE-CZ-NH1	-5.46	117.57	120.30
3	P6	77	ARG	NE-CZ-NH1	-5.41	117.59	120.30
4	PD	177	ARG	CG-CD-NE	5.40	123.14	111.80
1	LE	370	ARG	NE-CZ-NH1	-5.39	117.61	120.30
1	JC	389	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	NE	345	ARG	NE-CZ-NH2	5.29	122.95	120.30
5	PT	42	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	ND	345	ARG	NE-CZ-NH2	5.15	122.87	120.30
1	MC	290	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	JB	370	ARG	NE-CZ-NH1	-5.09	117.75	120.30
4	PA	422	ARG	NE-CZ-NH2	5.07	122.84	120.30
1	MC	378	ARG	NE-CZ-NH2	5.05	122.83	120.30
4	PH	205	ARG	NE-CZ-NH1	-5.05	117.77	120.30
1	MB	370	ARG	NE-CZ-NH1	-5.04	117.78	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	LE	101	PHE	Peptide

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

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	JA	2298	0	2139	0	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	1	0
1	KA	2298	0	2138	4	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	1	0
1	KF	2183	0	2036	1	0
1	LA	2298	0	2139	2	0
1	LB	2298	0	2139	0	0
1	LC	2298	0	2139	0	0
1	LD	2298	0	2139	1	0
1	LE	2298	0	2139	3	0
1	LF	2194	0	2049	1	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	2	0
1	MF	2277	0	2120	1	0
1	NA	2298	0	2139	1	0
1	NB	2298	0	2139	0	0
1	NC	2298	0	2139	0	0
1	ND	2298	0	2139	0	0
1	NE	2298	0	2139	2	0
1	NF	2183	0	2036	2	0
2	JI	967	0	894	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	1	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	0	0
2	NI	967	0	894	0	0
2	NJ	917	0	852	0	0
2	NK	967	0	894	0	0
3	P5	689	0	651	0	0
3	P6	689	0	651	0	0
3	P7	689	0	651	0	0
3	P8	689	0	651	1	0
3	P9	689	0	651	0	0
4	PA	3175	0	2999	1	0
4	PB	3175	0	2998	1	0
4	PC	3119	0	2953	0	0
4	PD	3108	0	2941	0	0
4	PE	3175	0	2998	1	0
4	PF	3175	0	2998	1	0
4	PG	3175	0	2999	2	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	2976	2	0
4	PL	3119	0	2953	2	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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	128173	39	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 (39) 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:KA:192:MET:HE1	1:NE:103:ALA:HB1	1.92	0.51
4:PG:263:ARG:HH21	4:PG:263:ARG:HG2	1.76	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:LD:292:ARG:NH2	1:LE:245:ASN:OD1	2.49	0.45
1:KD:292:ARG:NH2	1:KE:245:ASN:OD1	2.51	0.44
4:PL:237:HIS:HD1	4:PL:291:HIP:P	2.40	0.44
1:MF:378:ARG:NH2	1:NA:371:ASP:OD1	2.52	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
4:PA:258:ASP:HA	5:PV:67:LEU:HD21	2.01	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
4:PJ:268:PRO:HD2	5:PX:140:THR:HG21	2.03	0.40
1:KA:371:ASP:CG	1:NF:378:ARG:HE	2.25	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
2:KK:84:GLU:CD	2:KK:105:THR:HG1	2.24	0.40
4:PK:237:HIS:HD1	4:PK:291:HIP:P	2.45	0.40
1:JF:378:ARG:HE	1:LA:371:ASP:CG	2.24	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	JA	294/396 (74%)	277 (94%)	17 (6%)	0	100	100
1	JB	294/396 (74%)	280 (95%)	14 (5%)	0	100	100
1	JC	294/396 (74%)	280 (95%)	14 (5%)	0	100	100
1	JD	294/396 (74%)	282 (96%)	12 (4%)	0	100	100
1	JE	294/396 (74%)	283 (96%)	11 (4%)	0	100	100
1	JF	280/396 (71%)	266 (95%)	14 (5%)	0	100	100
1	KA	294/396 (74%)	282 (96%)	12 (4%)	0	100	100
1	KB	294/396 (74%)	279 (95%)	15 (5%)	0	100	100
1	KC	294/396 (74%)	279 (95%)	15 (5%)	0	100	100
1	KD	294/396 (74%)	277 (94%)	17 (6%)	0	100	100
1	KE	294/396 (74%)	280 (95%)	14 (5%)	0	100	100
1	KF	280/396 (71%)	267 (95%)	13 (5%)	0	100	100
1	LA	294/396 (74%)	279 (95%)	15 (5%)	0	100	100
1	LB	294/396 (74%)	279 (95%)	15 (5%)	0	100	100
1	LC	294/396 (74%)	277 (94%)	17 (6%)	0	100	100
1	LD	294/396 (74%)	283 (96%)	11 (4%)	0	100	100
1	LE	294/396 (74%)	282 (96%)	12 (4%)	0	100	100
1	LF	281/396 (71%)	269 (96%)	12 (4%)	0	100	100
1	MA	294/396 (74%)	281 (96%)	13 (4%)	0	100	100
1	MB	294/396 (74%)	278 (95%)	16 (5%)	0	100	100
1	MC	294/396 (74%)	278 (95%)	16 (5%)	0	100	100
1	MD	294/396 (74%)	279 (95%)	15 (5%)	0	100	100
1	ME	294/396 (74%)	282 (96%)	12 (4%)	0	100	100
1	MF	291/396 (74%)	276 (95%)	15 (5%)	0	100	100
1	NA	294/396 (74%)	281 (96%)	13 (4%)	0	100	100
1	NB	294/396 (74%)	282 (96%)	12 (4%)	0	100	100
1	NC	294/396 (74%)	281 (96%)	13 (4%)	0	100	100
1	ND	294/396 (74%)	283 (96%)	11 (4%)	0	100	100
1	NE	294/396 (74%)	281 (96%)	13 (4%)	0	100	100
1	NF	280/396 (71%)	267 (95%)	13 (5%)	0	100	100
2	JI	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
2	JJ	129/137 (94%)	124 (96%)	5 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	JK	134/137 (98%)	132 (98%)	2 (2%)	0	100	100
2	KI	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
2	KJ	129/137 (94%)	123 (95%)	6 (5%)	0	100	100
2	KK	134/137 (98%)	129 (96%)	5 (4%)	0	100	100
2	LI	134/137 (98%)	130 (97%)	4 (3%)	0	100	100
2	LJ	127/137 (93%)	125 (98%)	2 (2%)	0	100	100
2	LK	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
2	MI	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
2	MJ	128/137 (93%)	124 (97%)	4 (3%)	0	100	100
2	MK	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
2	NI	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
2	NJ	127/137 (93%)	123 (97%)	4 (3%)	0	100	100
2	NK	134/137 (98%)	131 (98%)	3 (2%)	0	100	100
3	P5	79/82 (96%)	75 (95%)	4 (5%)	0	100	100
3	P6	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
3	P7	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
3	P8	79/82 (96%)	76 (96%)	3 (4%)	0	100	100
3	P9	79/82 (96%)	77 (98%)	2 (2%)	0	100	100
4	PA	399/675 (59%)	386 (97%)	13 (3%)	0	100	100
4	PB	399/675 (59%)	389 (98%)	10 (2%)	0	100	100
4	PC	391/675 (58%)	385 (98%)	6 (2%)	0	100	100
4	PD	389/675 (58%)	385 (99%)	4 (1%)	0	100	100
4	PE	399/675 (59%)	388 (97%)	11 (3%)	0	100	100
4	PF	399/675 (59%)	385 (96%)	14 (4%)	0	100	100
4	PG	399/675 (59%)	386 (97%)	13 (3%)	0	100	100
4	PH	388/675 (58%)	380 (98%)	8 (2%)	0	100	100
4	PI	392/675 (58%)	382 (97%)	10 (3%)	0	100	100
4	PJ	399/675 (59%)	385 (96%)	14 (4%)	0	100	100
4	PK	394/675 (58%)	384 (98%)	10 (2%)	0	100	100
4	PL	391/675 (58%)	381 (97%)	10 (3%)	0	100	100
5	PM	138/141 (98%)	129 (94%)	9 (6%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	PN	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
5	PO	138/141 (98%)	129 (94%)	9 (6%)	0	100	100
5	PP	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
5	PQ	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
5	PR	138/141 (98%)	129 (94%)	9 (6%)	0	100	100
5	PS	138/141 (98%)	130 (94%)	8 (6%)	0	100	100
5	PT	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
5	PU	138/141 (98%)	131 (95%)	7 (5%)	0	100	100
5	PV	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
5	PW	138/141 (98%)	133 (96%)	5 (4%)	0	100	100
5	PX	138/141 (98%)	132 (96%)	6 (4%)	0	100	100
All	All	17532/24137 (73%)	16844 (96%)	688 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	JA	244/322 (76%)	241 (99%)	3 (1%)	67	85
1	JB	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	JC	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	JD	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	JE	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	JF	232/322 (72%)	229 (99%)	3 (1%)	65	84
1	KA	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	KB	244/322 (76%)	241 (99%)	3 (1%)	67	85
1	KC	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	KD	244/322 (76%)	240 (98%)	4 (2%)	58	80

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	KE	244/322 (76%)	241 (99%)	3 (1%)	67	85
1	KF	232/322 (72%)	230 (99%)	2 (1%)	75	89
1	LA	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	LB	244/322 (76%)	240 (98%)	4 (2%)	58	80
1	LC	244/322 (76%)	241 (99%)	3 (1%)	67	85
1	LD	244/322 (76%)	240 (98%)	4 (2%)	58	80
1	LE	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	LF	233/322 (72%)	231 (99%)	2 (1%)	75	89
1	MA	244/322 (76%)	240 (98%)	4 (2%)	58	80
1	MB	244/322 (76%)	241 (99%)	3 (1%)	67	85
1	MC	244/322 (76%)	240 (98%)	4 (2%)	58	80
1	MD	244/322 (76%)	239 (98%)	5 (2%)	50	76
1	ME	244/322 (76%)	241 (99%)	3 (1%)	67	85
1	MF	243/322 (76%)	239 (98%)	4 (2%)	58	80
1	NA	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	NB	244/322 (76%)	242 (99%)	2 (1%)	79	91
1	NC	244/322 (76%)	240 (98%)	4 (2%)	58	80
1	ND	244/322 (76%)	240 (98%)	4 (2%)	58	80
1	NE	244/322 (76%)	243 (100%)	1 (0%)	89	96
1	NF	232/322 (72%)	226 (97%)	6 (3%)	41	68
2	JI	99/100 (99%)	98 (99%)	1 (1%)	73	88
2	JJ	95/100 (95%)	94 (99%)	1 (1%)	70	86
2	JK	99/100 (99%)	99 (100%)	0	100	100
2	KI	99/100 (99%)	98 (99%)	1 (1%)	73	88
2	KJ	95/100 (95%)	94 (99%)	1 (1%)	70	86
2	KK	99/100 (99%)	98 (99%)	1 (1%)	73	88
2	LI	99/100 (99%)	98 (99%)	1 (1%)	73	88
2	LJ	94/100 (94%)	93 (99%)	1 (1%)	70	86
2	LK	99/100 (99%)	99 (100%)	0	100	100
2	MI	99/100 (99%)	99 (100%)	0	100	100
2	MJ	95/100 (95%)	94 (99%)	1 (1%)	70	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	MK	99/100 (99%)	99 (100%)	0	100	100
2	NI	99/100 (99%)	98 (99%)	1 (1%)	73	88
2	NJ	94/100 (94%)	92 (98%)	2 (2%)	48	74
2	NK	99/100 (99%)	97 (98%)	2 (2%)	50	76
3	P5	73/73 (100%)	73 (100%)	0	100	100
3	P6	73/73 (100%)	71 (97%)	2 (3%)	40	67
3	P7	73/73 (100%)	71 (97%)	2 (3%)	40	67
3	P8	73/73 (100%)	73 (100%)	0	100	100
3	P9	73/73 (100%)	72 (99%)	1 (1%)	62	82
4	PA	334/568 (59%)	333 (100%)	1 (0%)	91	97
4	PB	334/568 (59%)	329 (98%)	5 (2%)	60	82
4	PC	328/568 (58%)	324 (99%)	4 (1%)	67	85
4	PD	327/568 (58%)	323 (99%)	4 (1%)	67	85
4	PE	334/568 (59%)	333 (100%)	1 (0%)	91	97
4	PF	334/568 (59%)	332 (99%)	2 (1%)	84	93
4	PG	334/568 (59%)	332 (99%)	2 (1%)	84	93
4	PH	327/568 (58%)	326 (100%)	1 (0%)	91	97
4	PI	332/568 (58%)	330 (99%)	2 (1%)	84	93
4	PJ	334/568 (59%)	333 (100%)	1 (0%)	91	97
4	PK	331/568 (58%)	330 (100%)	1 (0%)	91	97
4	PL	328/568 (58%)	325 (99%)	3 (1%)	75	89
5	PM	116/117 (99%)	115 (99%)	1 (1%)	75	89
5	PN	116/117 (99%)	115 (99%)	1 (1%)	75	89
5	PO	116/117 (99%)	115 (99%)	1 (1%)	75	89
5	PP	116/117 (99%)	113 (97%)	3 (3%)	41	68
5	PQ	116/117 (99%)	114 (98%)	2 (2%)	56	79
5	PR	116/117 (99%)	114 (98%)	2 (2%)	56	79
5	PS	116/117 (99%)	114 (98%)	2 (2%)	56	79
5	PT	116/117 (99%)	114 (98%)	2 (2%)	56	79
5	PU	116/117 (99%)	115 (99%)	1 (1%)	75	89
5	PV	116/117 (99%)	113 (97%)	3 (3%)	41	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	PW	116/117 (99%)	114 (98%)	2 (2%)	56	79
5	PX	116/117 (99%)	114 (98%)	2 (2%)	56	79
All	All	14469/19745 (73%)	14313 (99%)	156 (1%)	69	86

All (156) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	JA	199	ASP
1	JA	276	ASN
1	JA	378	ARG
1	JB	114	ARG
1	JB	378	ARG
1	JC	189	THR
1	JC	378	ARG
1	JD	276	ASN
1	JD	378	ARG
1	JE	333	SER
1	JE	378	ARG
1	JF	144	VAL
1	JF	178	ASN
1	JF	378	ARG
2	JI	135	THR
2	JJ	46	SER
1	KA	276	ASN
1	KA	378	ARG
1	KB	257	ARG
1	KB	349	HIS
1	KB	378	ARG
1	KC	333	SER
1	KC	378	ARG
1	KD	191	GLU
1	KD	276	ASN
1	KD	289	LEU
1	KD	378	ARG
1	KE	110	ASP
1	KE	311	SER
1	KE	378	ARG
1	KF	117	LEU
1	KF	378	ARG
2	KI	69	VAL
2	KJ	71	LEU

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Mol	Chain	Res	Type
2	KK	117	GLU
1	LA	276	ASN
1	LA	378	ARG
1	LB	104	SER
1	LB	117	LEU
1	LB	257	ARG
1	LB	378	ARG
1	LC	110	ASP
1	LC	189	THR
1	LC	378	ARG
1	LD	101	PHE
1	LD	276	ASN
1	LD	282	ARG
1	LD	378	ARG
1	LE	333	SER
1	LE	378	ARG
1	LF	333	SER
1	LF	378	ARG
2	LI	32	SER
2	LJ	76	CYS
1	MA	197	MET
1	MA	200	LEU
1	MA	276	ASN
1	MA	378	ARG
1	MB	117	LEU
1	MB	118	LEU
1	MB	378	ARG
1	MC	189	THR
1	MC	244	LEU
1	MC	292	ARG
1	MC	378	ARG
1	MD	105	ASP
1	MD	146	ASP
1	MD	276	ASN
1	MD	292	ARG
1	MD	378	ARG
1	ME	187	ARG
1	ME	289	LEU
1	ME	311	SER
1	MF	136	ASN
1	MF	178	ASN
1	MF	292	ARG

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Mol	Chain	Res	Type
1	MF	378	ARG
2	MJ	18	SER
1	NA	276	ASN
1	NA	359	ASP
1	NB	110	ASP
1	NB	378	ARG
1	NC	105	ASP
1	NC	206	GLN
1	NC	292	ARG
1	NC	378	ARG
1	ND	276	ASN
1	ND	282	ARG
1	ND	292	ARG
1	ND	378	ARG
1	NE	378	ARG
1	NF	117	LEU
1	NF	144	VAL
1	NF	192	MET
1	NF	292	ARG
1	NF	364	ASP
1	NF	378	ARG
2	NI	75	ASP
2	NJ	75	ASP
2	NJ	135	THR
2	NK	22	LEU
2	NK	75	ASP
3	P6	4	ARG
3	P6	26	GLN
3	P7	4	ARG
3	P7	63	ASN
3	P9	4	ARG
4	PA	205	ARG
4	PB	55	LEU
4	PB	205	ARG
4	PB	255	ARG
4	PB	269	ARG
4	PB	423	SER
4	PC	42	MET
4	PC	255	ARG
4	PC	365	SER
4	PC	423	SER
4	PD	100	LYS

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Mol	Chain	Res	Type
4	PD	185	GLN
4	PD	255	ARG
4	PD	365	SER
4	PE	423	SER
4	PF	365	SER
4	PF	423	SER
4	PG	168	GLN
4	PG	255	ARG
4	PH	365	SER
4	PI	168	GLN
4	PI	255	ARG
4	PJ	205	ARG
4	PK	274	ASN
4	PL	168	GLN
4	PL	255	ARG
4	PL	423	SER
5	PM	132	ASP
5	PN	132	ASP
5	PO	118	LYS
5	PP	2	PRO
5	PP	132	ASP
5	PP	139	ARG
5	PQ	2	PRO
5	PQ	107	SER
5	PR	132	ASP
5	PR	139	ARG
5	PS	132	ASP
5	PS	139	ARG
5	PT	118	LYS
5	PT	132	ASP
5	PU	132	ASP
5	PV	2	PRO
5	PV	107	SER
5	PV	132	ASP
5	PW	118	LYS
5	PW	132	ASP
5	PX	118	LYS
5	PX	132	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	JB	178	ASN
2	JK	116	GLN
1	KA	380	HIS
1	KB	161	GLN
1	KC	161	GLN
1	KE	347	ASN
2	KK	116	GLN
1	MA	161	GLN
1	MA	380	HIS
1	MB	161	GLN
1	MF	136	ASN
1	NA	380	HIS
1	NB	161	GLN
1	NC	281	ASN
2	NK	116	GLN
3	P6	18	GLN
3	P7	2	GLN
4	PA	181	HIS
4	PA	392	GLN
4	PA	393	GLN
4	PE	392	GLN
4	PF	392	GLN
4	PG	232	GLN
4	PH	392	GLN
4	PI	392	GLN
4	PK	392	GLN
4	PL	392	GLN

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	2.06	3 (30%)	6,20,22	1.09	0
4	HIP	PI	196	4	10,14,15	2.19	4 (40%)	6,20,22	1.27	0
4	HIP	PI	291	4	10,14,15	1.97	3 (30%)	6,20,22	1.48	1 (16%)
4	HIP	PG	196	4	10,14,15	2.18	3 (30%)	6,20,22	1.09	0
4	HIP	PC	196	4	10,14,15	2.15	3 (30%)	6,20,22	1.14	0
4	HIP	PA	196	4	10,14,15	2.21	3 (30%)	6,20,22	1.16	0
4	HIP	PL	243	4	10,14,15	2.17	4 (40%)	6,20,22	1.28	0
4	HIP	PB	243	4	10,14,15	2.13	4 (40%)	6,20,22	1.30	0
4	HIP	PA	291	4	10,14,15	1.75	2 (20%)	6,20,22	2.08	3 (50%)
4	HIP	PH	243	4	10,14,15	2.15	4 (40%)	6,20,22	1.35	1 (16%)
4	HIP	PH	196	4	10,14,15	2.14	3 (30%)	6,20,22	1.24	0
4	HIP	PJ	291	4	10,14,15	1.88	3 (30%)	6,20,22	1.64	1 (16%)
3	HIP	P8	17	3	10,14,15	1.87	3 (30%)	6,20,22	1.06	0
3	HIP	P9	17	3	10,14,15	1.96	3 (30%)	6,20,22	0.88	0
4	HIP	PG	243	4	10,14,15	2.04	4 (40%)	6,20,22	1.33	1 (16%)
4	HIP	PD	291	4	10,14,15	2.91	4 (40%)	6,20,22	1.89	1 (16%)
4	HIP	PF	243	4	10,14,15	1.90	3 (30%)	6,20,22	1.35	1 (16%)
4	HIP	PH	291	4	10,14,15	1.79	3 (30%)	6,20,22	2.01	2 (33%)
4	HIP	PF	196	4	10,14,15	2.09	3 (30%)	6,20,22	1.17	0
3	HIP	P5	17	3	10,14,15	1.93	3 (30%)	6,20,22	0.88	0
4	HIP	PK	196	4	10,14,15	2.25	3 (30%)	6,20,22	1.18	0
4	HIP	PJ	196	4	10,14,15	2.21	3 (30%)	6,20,22	1.06	0
4	HIP	PJ	243	4	10,14,15	2.09	4 (40%)	6,20,22	1.33	0
4	HIP	PB	291	4	10,14,15	1.93	3 (30%)	6,20,22	1.62	1 (16%)
4	HIP	PL	196	4	10,14,15	2.20	3 (30%)	6,20,22	1.14	0
4	HIP	PG	291	4	10,14,15	1.85	3 (30%)	6,20,22	1.50	1 (16%)
4	HIP	PA	243	4	10,14,15	2.19	4 (40%)	6,20,22	1.31	0
3	HIP	P7	17	3	10,14,15	1.83	3 (30%)	6,20,22	0.99	0
4	HIP	PF	291	4	10,14,15	1.93	3 (30%)	6,20,22	1.73	1 (16%)
4	HIP	PD	196	4	10,14,15	2.00	2 (20%)	6,20,22	1.16	0
4	HIP	PD	243	4	10,14,15	2.12	4 (40%)	6,20,22	1.30	0
4	HIP	PE	196	4	10,14,15	2.11	3 (30%)	6,20,22	1.25	0
4	HIP	PL	291	4	10,14,15	1.86	3 (30%)	6,20,22	1.66	1 (16%)
4	HIP	PC	243	4	10,14,15	2.00	4 (40%)	6,20,22	1.25	0
4	HIP	PK	243	4	10,14,15	2.12	4 (40%)	6,20,22	1.35	0

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	1.95	3 (30%)	6,20,22	1.77	1 (16%)
4	HIP	PC	291	4	10,14,15	1.89	3 (30%)	6,20,22	1.66	1 (16%)
4	HIP	PE	291	4	10,14,15	1.93	3 (30%)	6,20,22	1.63	1 (16%)
4	HIP	PI	243	4	10,14,15	2.21	4 (40%)	6,20,22	1.31	1 (16%)
3	HIP	P6	17	3	10,14,15	2.03	3 (30%)	6,20,22	1.05	0
4	HIP	PE	243	4	10,14,15	2.06	4 (40%)	6,20,22	1.27	0

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
4	HIP	PI	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PI	291	4	-	1/5/12/14	0/1/1/1
4	HIP	PG	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PC	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PA	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PL	243	4	-	3/5/12/14	0/1/1/1
4	HIP	PB	243	4	-	3/5/12/14	0/1/1/1
4	HIP	PA	291	4	-	0/5/12/14	0/1/1/1
4	HIP	PH	243	4	-	2/5/12/14	0/1/1/1
4	HIP	PH	196	4	-	2/5/12/14	0/1/1/1
4	HIP	PJ	291	4	-	0/5/12/14	0/1/1/1
3	HIP	P8	17	3	-	0/5/12/14	0/1/1/1
3	HIP	P9	17	3	-	1/5/12/14	0/1/1/1
4	HIP	PG	243	4	-	3/5/12/14	0/1/1/1
4	HIP	PD	291	4	-	1/5/12/14	0/1/1/1
4	HIP	PF	243	4	-	3/5/12/14	0/1/1/1
4	HIP	PH	291	4	-	0/5/12/14	0/1/1/1
4	HIP	PF	196	4	-	2/5/12/14	0/1/1/1
3	HIP	P5	17	3	-	1/5/12/14	0/1/1/1
4	HIP	PK	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	PJ	243	4	-	3/5/12/14	0/1/1/1
4	HIP	PB	291	4	-	1/5/12/14	0/1/1/1
4	HIP	PL	196	4	-	2/5/12/14	0/1/1/1

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

All (134) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	PD	291	HIP	P-O1P	6.45	1.52	1.47
4	PE	196	HIP	CG-ND1	5.39	1.44	1.37
4	PI	196	HIP	CG-ND1	5.34	1.44	1.37
4	PK	196	HIP	CG-ND1	5.25	1.44	1.37
4	PJ	196	HIP	CG-ND1	5.21	1.44	1.37
4	PH	196	HIP	CG-ND1	5.14	1.44	1.37
4	PF	196	HIP	CG-ND1	5.08	1.44	1.37
4	PG	196	HIP	CG-ND1	5.02	1.44	1.37
4	PD	291	HIP	CG-ND1	5.01	1.44	1.37
4	PD	196	HIP	CG-ND1	4.98	1.44	1.37
4	PC	196	HIP	CG-ND1	4.95	1.44	1.37
4	PL	196	HIP	CG-ND1	4.95	1.44	1.37
4	PA	196	HIP	CG-ND1	4.94	1.44	1.37
4	PB	196	HIP	CG-ND1	4.78	1.43	1.37
4	PK	243	HIP	CG-ND1	4.60	1.43	1.37
4	PH	243	HIP	CG-ND1	4.60	1.43	1.37
4	PI	291	HIP	CG-ND1	4.52	1.43	1.37
4	PL	243	HIP	CG-ND1	4.50	1.43	1.37
4	PG	243	HIP	CG-ND1	4.49	1.43	1.37
4	PJ	243	HIP	CG-ND1	4.48	1.43	1.37
4	PI	243	HIP	CG-ND1	4.46	1.43	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	PF	291	HIP	CG-ND1	4.43	1.43	1.37
4	PB	243	HIP	CG-ND1	4.39	1.43	1.37
4	PD	243	HIP	CG-ND1	4.31	1.43	1.37
4	PA	243	HIP	CG-ND1	4.30	1.43	1.37
4	PC	291	HIP	CG-ND1	4.29	1.43	1.37
4	PC	243	HIP	CG-ND1	4.29	1.43	1.37
4	PK	291	HIP	CG-ND1	4.25	1.43	1.37
4	PJ	291	HIP	CG-ND1	4.19	1.43	1.37
4	PE	291	HIP	CG-ND1	4.17	1.43	1.37
3	P5	17	HIP	CG-ND1	4.14	1.43	1.37
4	PH	291	HIP	CG-ND1	4.12	1.43	1.37
4	PF	243	HIP	CG-ND1	4.06	1.42	1.37
4	PG	291	HIP	CG-ND1	4.04	1.42	1.37
4	PL	291	HIP	CG-ND1	4.02	1.42	1.37
4	PB	291	HIP	CG-ND1	3.99	1.42	1.37
4	PE	243	HIP	CG-ND1	3.97	1.42	1.37
3	P6	17	HIP	P-O1P	3.96	1.50	1.47
4	PA	291	HIP	CG-ND1	3.91	1.42	1.37
3	P9	17	HIP	CG-ND1	3.82	1.42	1.37
4	PA	196	HIP	P-O1P	3.65	1.50	1.47
3	P6	17	HIP	CG-ND1	3.61	1.42	1.37
4	PL	196	HIP	P-O1P	3.56	1.50	1.47
4	PE	243	HIP	P-O1P	3.55	1.50	1.47
4	PA	243	HIP	P-O1P	3.51	1.50	1.47
4	PI	243	HIP	P-O1P	3.49	1.50	1.47
3	P7	17	HIP	P-O1P	3.45	1.50	1.47
3	P9	17	HIP	P-O1P	3.44	1.50	1.47
4	PK	196	HIP	P-O1P	3.44	1.50	1.47
3	P8	17	HIP	CG-ND1	3.41	1.42	1.37
4	PL	243	HIP	P-O1P	3.36	1.50	1.47
4	PK	291	HIP	P-O3P	-3.33	1.48	1.54
4	PB	291	HIP	P-O3P	-3.31	1.48	1.54
4	PD	243	HIP	P-O1P	3.27	1.50	1.47
4	PE	291	HIP	P-O3P	-3.26	1.48	1.54
3	P8	17	HIP	P-O1P	3.25	1.50	1.47
4	PG	196	HIP	P-O1P	3.23	1.50	1.47
4	PC	196	HIP	P-O1P	3.23	1.50	1.47
4	PJ	196	HIP	P-O1P	3.17	1.50	1.47
4	PF	291	HIP	P-O3P	-3.16	1.48	1.54
4	PI	291	HIP	P-O3P	-3.16	1.48	1.54
4	PG	291	HIP	P-O3P	-3.14	1.48	1.54
3	P7	17	HIP	CG-ND1	3.10	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	PJ	291	HIP	P-O3P	-3.06	1.48	1.54
4	PC	291	HIP	P-O3P	-3.05	1.48	1.54
4	PL	291	HIP	P-O3P	-3.05	1.48	1.54
3	P5	17	HIP	P-O1P	3.03	1.49	1.47
4	PK	243	HIP	P-O1P	3.02	1.49	1.47
4	PB	243	HIP	P-O1P	3.02	1.49	1.47
4	PB	243	HIP	P-O3P	-3.00	1.48	1.54
4	PD	291	HIP	P-O3P	-2.99	1.48	1.54
4	PA	243	HIP	P-O3P	-2.96	1.48	1.54
4	PG	243	HIP	P-O1P	2.95	1.49	1.47
4	PH	196	HIP	P-O1P	2.95	1.49	1.47
4	PH	243	HIP	P-O1P	2.93	1.49	1.47
4	PI	243	HIP	P-O3P	-2.90	1.48	1.54
4	PI	196	HIP	P-O1P	2.86	1.49	1.47
4	PB	196	HIP	P-O1P	2.82	1.49	1.47
4	PH	243	HIP	P-O3P	-2.79	1.49	1.54
4	PL	243	HIP	P-O3P	-2.78	1.49	1.54
4	PF	243	HIP	P-O3P	-2.75	1.49	1.54
4	PJ	243	HIP	P-O3P	-2.74	1.49	1.54
4	PC	243	HIP	P-O1P	2.74	1.49	1.47
4	PA	291	HIP	P-O3P	-2.70	1.49	1.54
4	PJ	243	HIP	P-O1P	2.68	1.49	1.47
4	PD	291	HIP	P-O2P	-2.67	1.49	1.54
4	PC	243	HIP	P-O3P	-2.66	1.49	1.54
4	PE	243	HIP	P-O3P	-2.63	1.49	1.54
4	PD	243	HIP	P-O3P	-2.62	1.49	1.54
4	PK	243	HIP	P-O3P	-2.59	1.49	1.54
4	PD	243	HIP	P-O2P	-2.56	1.49	1.54
4	PG	243	HIP	P-O3P	-2.56	1.49	1.54
4	PF	196	HIP	P-O1P	2.55	1.49	1.47
4	PH	243	HIP	P-O2P	-2.53	1.49	1.54
4	PA	196	HIP	P-O2P	-2.52	1.49	1.54
4	PJ	243	HIP	P-O2P	-2.51	1.49	1.54
3	P6	17	HIP	P-O3P	-2.51	1.49	1.54
4	PA	243	HIP	P-O2P	-2.50	1.49	1.54
4	PG	196	HIP	P-O2P	-2.49	1.49	1.54
4	PB	291	HIP	P-O1P	2.49	1.49	1.47
4	PC	196	HIP	P-O2P	-2.49	1.49	1.54
4	PD	196	HIP	P-O2P	-2.49	1.49	1.54
4	PL	196	HIP	P-O2P	-2.49	1.49	1.54
3	P9	17	HIP	P-O3P	-2.48	1.49	1.54
4	PB	196	HIP	P-O2P	-2.48	1.49	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	PJ	196	HIP	P-O2P	-2.47	1.49	1.54
4	PH	196	HIP	P-O2P	-2.46	1.49	1.54
4	PI	243	HIP	P-O2P	-2.45	1.49	1.54
4	PB	243	HIP	P-O2P	-2.44	1.49	1.54
4	PF	243	HIP	P-O1P	2.43	1.49	1.47
4	PE	196	HIP	P-O2P	-2.43	1.49	1.54
3	P7	17	HIP	P-O3P	-2.42	1.49	1.54
4	PE	291	HIP	P-O1P	2.41	1.49	1.47
4	PL	243	HIP	P-O2P	-2.40	1.49	1.54
4	PF	196	HIP	P-O2P	-2.40	1.49	1.54
4	PK	243	HIP	P-O2P	-2.40	1.49	1.54
4	PH	291	HIP	P-O3P	-2.39	1.49	1.54
3	P8	17	HIP	P-O3P	-2.34	1.50	1.54
4	PK	196	HIP	P-O2P	-2.30	1.50	1.54
4	PI	196	HIP	P-O2P	-2.27	1.50	1.54
4	PL	291	HIP	P-O1P	2.26	1.49	1.47
4	PK	291	HIP	P-O1P	2.26	1.49	1.47
4	PE	243	HIP	P-O2P	-2.23	1.50	1.54
4	PI	291	HIP	P-O1P	2.23	1.49	1.47
4	PH	291	HIP	P-O1P	2.23	1.49	1.47
3	P5	17	HIP	P-O3P	-2.21	1.50	1.54
4	PC	243	HIP	P-O2P	-2.20	1.50	1.54
4	PE	196	HIP	P-O1P	2.20	1.49	1.47
4	PF	291	HIP	P-O1P	2.18	1.49	1.47
4	PJ	291	HIP	P-O1P	2.18	1.49	1.47
4	PC	291	HIP	P-O1P	2.16	1.49	1.47
4	PG	291	HIP	P-O1P	2.09	1.49	1.47
4	PI	196	HIP	P-O3P	-2.05	1.50	1.54
4	PG	243	HIP	P-O2P	-2.01	1.50	1.54

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	PH	291	HIP	O3P-P-O1P	3.40	120.81	113.44
4	PD	291	HIP	O2P-P-O3P	3.38	119.85	106.57
4	PF	291	HIP	CB-CA-C	3.31	117.67	111.47
4	PK	291	HIP	CB-CA-C	3.26	117.58	111.47
4	PA	291	HIP	O3P-P-O1P	3.16	120.27	113.44
4	PJ	291	HIP	CB-CA-C	3.15	117.37	111.47
4	PC	291	HIP	CB-CA-C	2.83	116.77	111.47
4	PL	291	HIP	CB-CA-C	2.76	116.64	111.47
4	PB	291	HIP	CB-CA-C	2.62	116.38	111.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	PG	291	HIP	CB-CA-C	2.57	116.29	111.47
4	PA	291	HIP	CB-CA-C	2.56	116.27	111.47
4	PE	291	HIP	CB-CA-C	2.50	116.15	111.47
4	PI	291	HIP	CB-CA-C	2.47	116.10	111.47
4	PA	291	HIP	O2P-P-O3P	2.38	115.93	106.57
4	PG	243	HIP	O2P-P-O3P	2.24	115.39	106.57
4	PF	243	HIP	O2P-P-O3P	2.20	115.20	106.57
4	PH	291	HIP	O2P-P-O3P	2.06	114.68	106.57
4	PI	243	HIP	O2P-P-O3P	2.05	114.63	106.57
4	PH	243	HIP	O2P-P-O3P	2.02	114.51	106.57

There are no chirality outliers.

All (65) 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	PC	243	HIP	O-C-CA-CB
4	PD	243	HIP	O-C-CA-CB
4	PE	243	HIP	O-C-CA-CB
4	PE	291	HIP	O-C-CA-CB
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
4	PK	243	HIP	O-C-CA-CB
4	PK	291	HIP	O-C-CA-CB
4	PL	243	HIP	O-C-CA-CB
4	PL	291	HIP	O-C-CA-CB
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

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Mol	Chain	Res	Type	Atoms
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	PJ	243	HIP	CA-CB-CG-CD2
4	PA	243	HIP	CA-CB-CG-ND1
4	PB	243	HIP	CA-CB-CG-ND1
4	PC	243	HIP	CA-CB-CG-ND1
4	PE	243	HIP	CA-CB-CG-ND1
4	PF	243	HIP	CA-CB-CG-ND1
4	PG	243	HIP	CA-CB-CG-ND1
4	PH	243	HIP	CA-CB-CG-ND1
4	PI	243	HIP	CA-CB-CG-ND1
4	PJ	243	HIP	CA-CB-CG-ND1
4	PK	243	HIP	CA-CB-CG-ND1
4	PL	243	HIP	CA-CB-CG-ND1
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	PJ	196	HIP	C-CA-CB-CG
4	PK	196	HIP	C-CA-CB-CG
4	PL	196	HIP	C-CA-CB-CG
3	P5	17	HIP	C-CA-CB-CG
3	P9	17	HIP	C-CA-CB-CG
4	PB	243	HIP	CA-CB-CG-CD2
4	PC	243	HIP	CA-CB-CG-CD2
4	PE	243	HIP	CA-CB-CG-CD2
4	PF	243	HIP	CA-CB-CG-CD2
4	PG	243	HIP	CA-CB-CG-CD2
4	PI	243	HIP	CA-CB-CG-CD2
4	PK	243	HIP	CA-CB-CG-CD2
4	PL	243	HIP	CA-CB-CG-CD2
4	PD	291	HIP	CA-CB-CG-ND1
4	PI	196	HIP	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	PL	291	HIP	1	0
4	PK	291	HIP	1	0

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 [i](#)

There are no chain breaks in this entry.

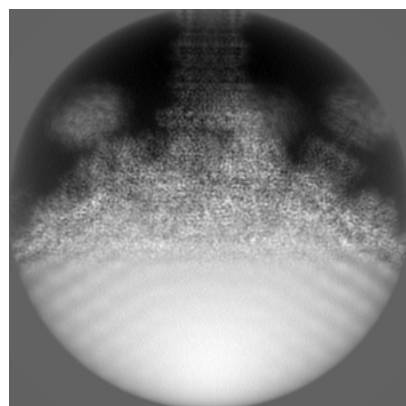
6 Map visualisation [i](#)

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.

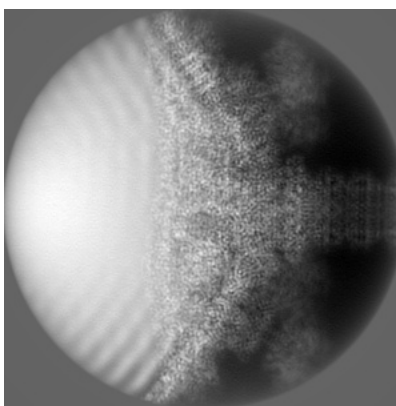
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

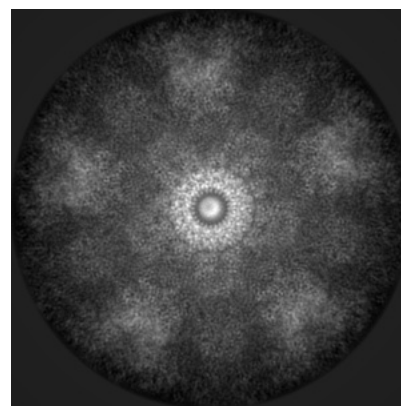
6.1.1 Primary map



X

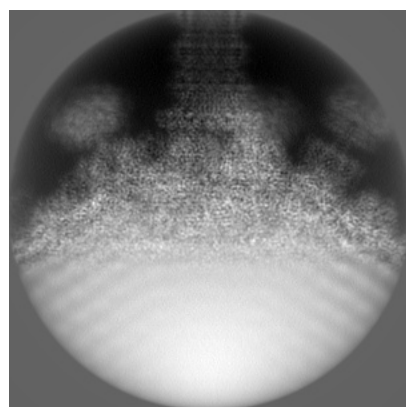


Y

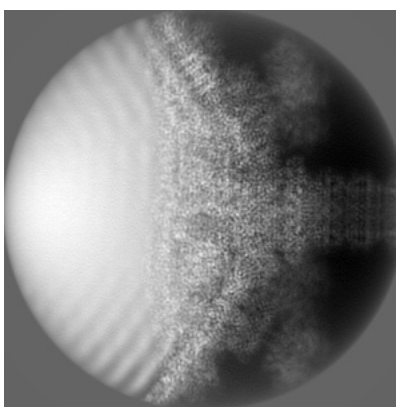


Z

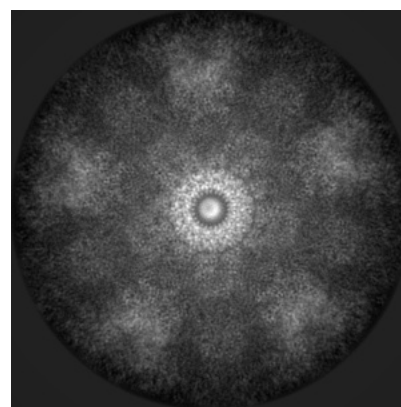
6.1.2 Raw map



X



Y

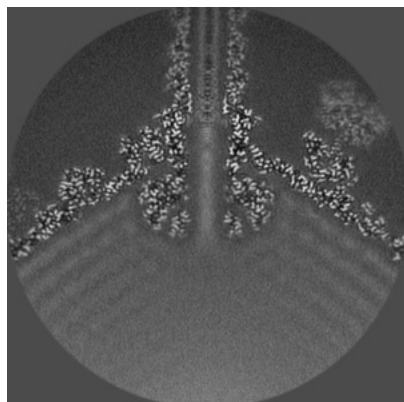


Z

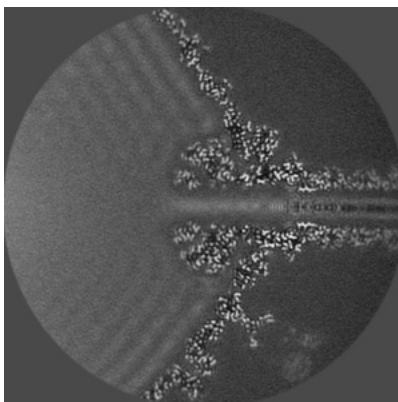
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

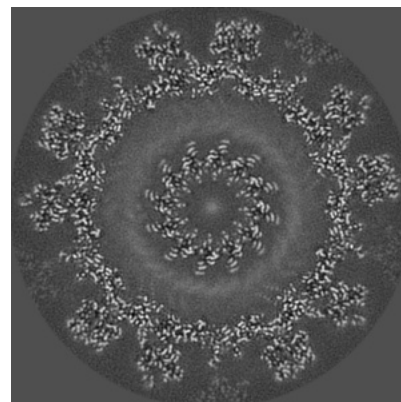
6.2.1 Primary map



X Index: 176

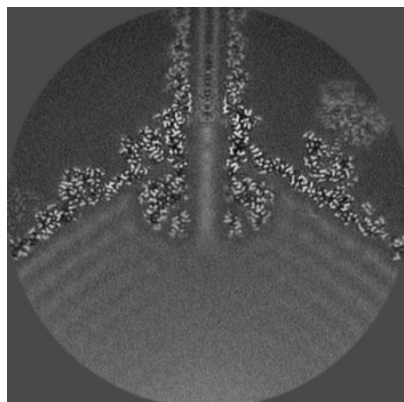


Y Index: 176

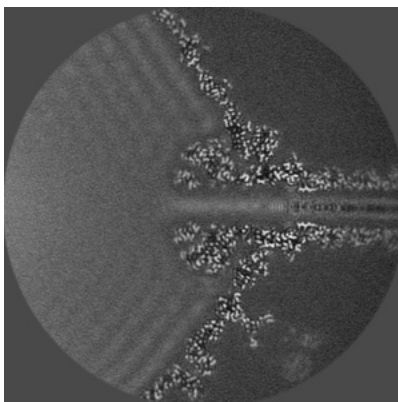


Z Index: 176

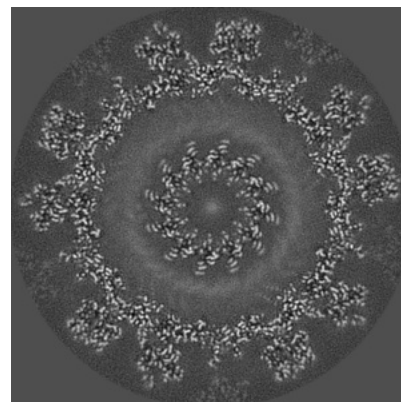
6.2.2 Raw map



X Index: 176



Y Index: 176

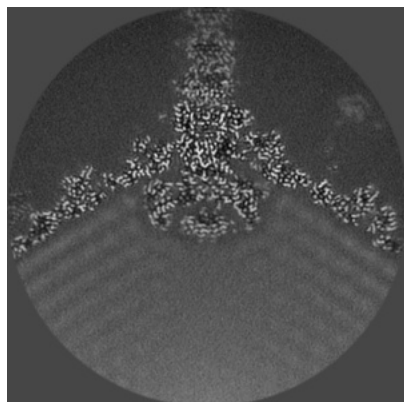


Z Index: 176

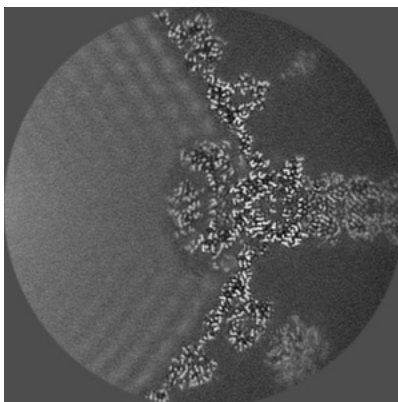
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

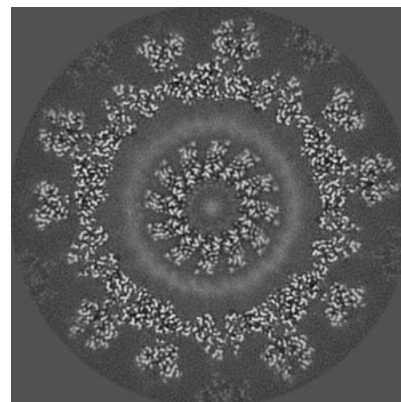
6.3.1 Primary map



X Index: 199

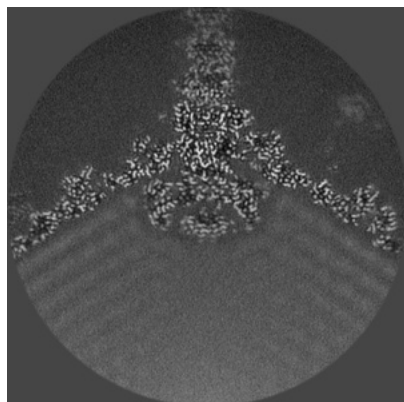


Y Index: 194

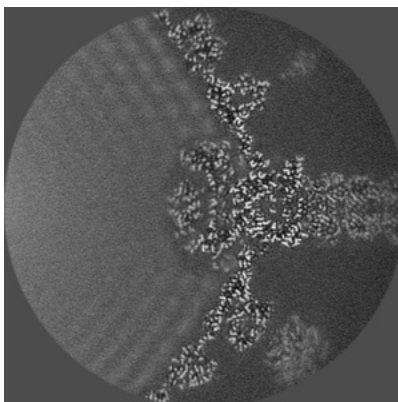


Z Index: 180

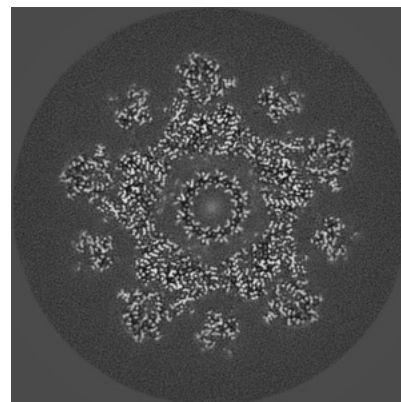
6.3.2 Raw map



X Index: 199



Y Index: 194

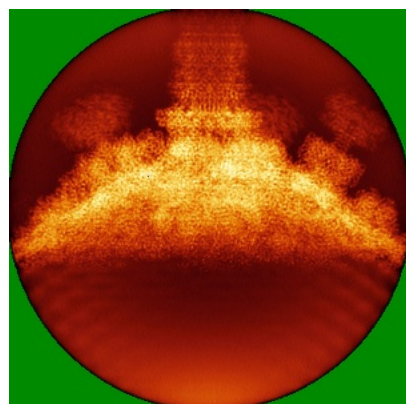


Z Index: 206

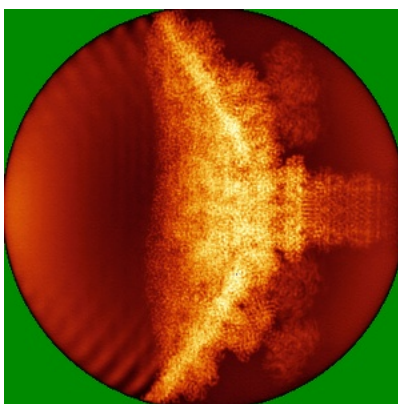
The images above show the largest variance slices of the map in three orthogonal directions.

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

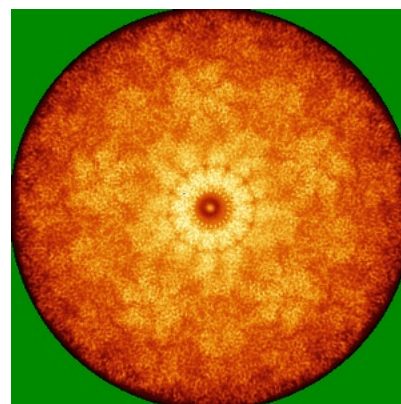
6.4.1 Primary map



X

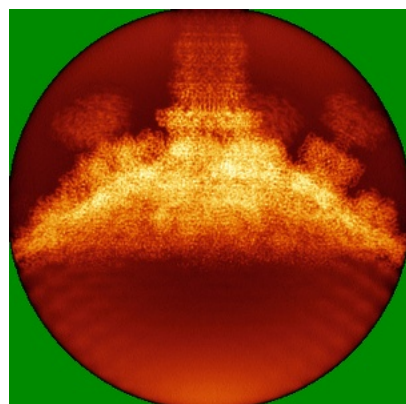


Y

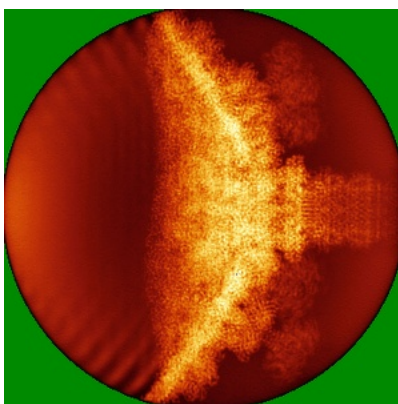


Z

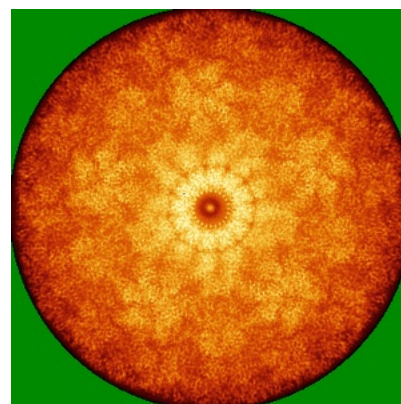
6.4.2 Raw map



X



Y

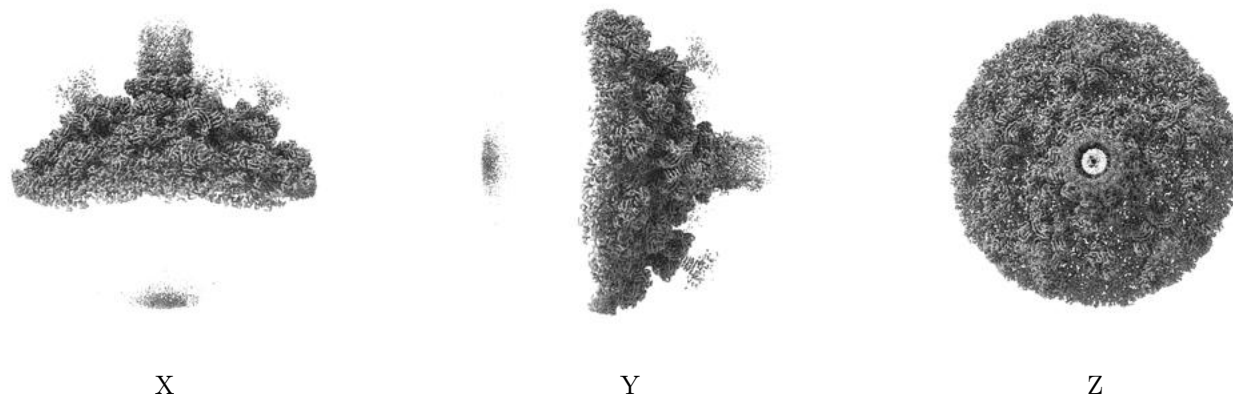


Z

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.

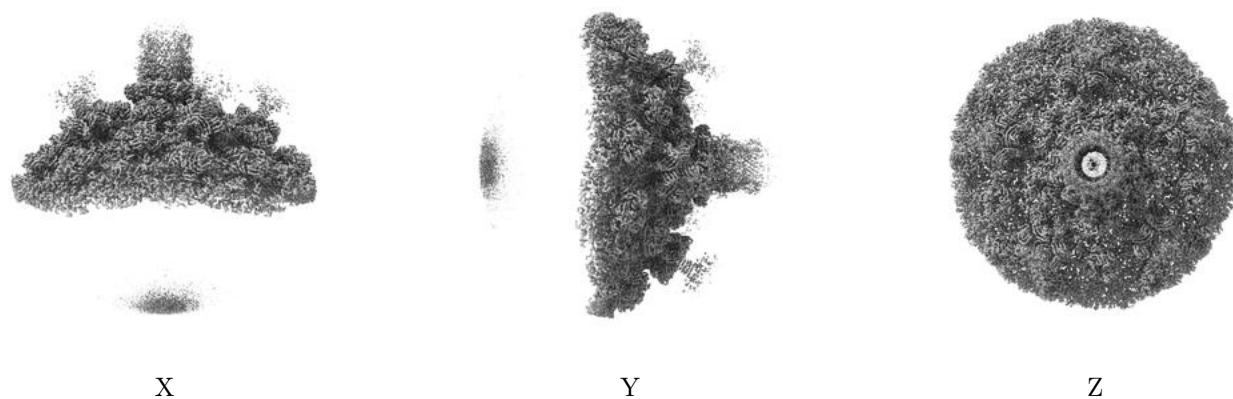
6.5 Orthogonal surface views [i](#)

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.

6.5.2 Raw map



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

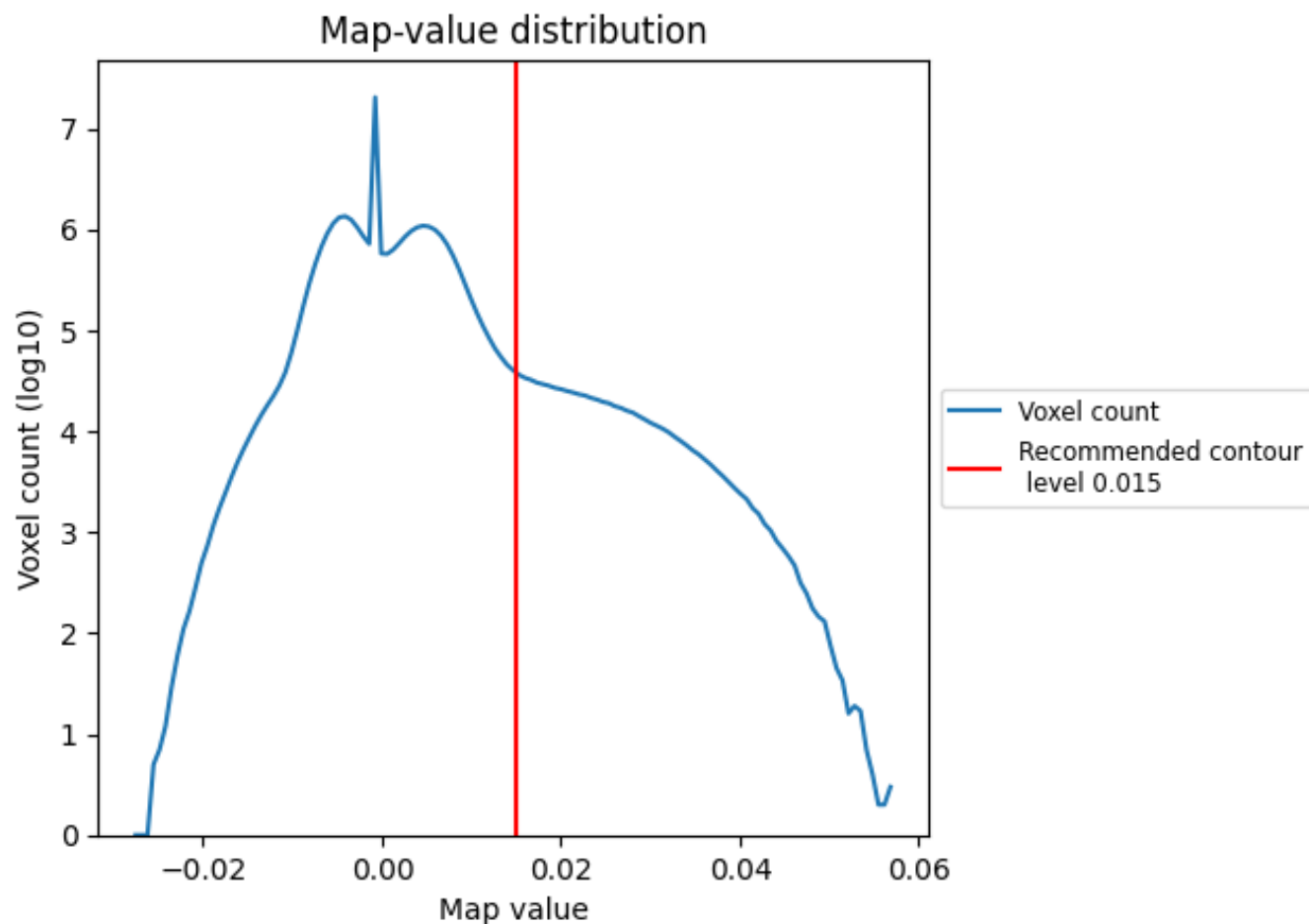
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

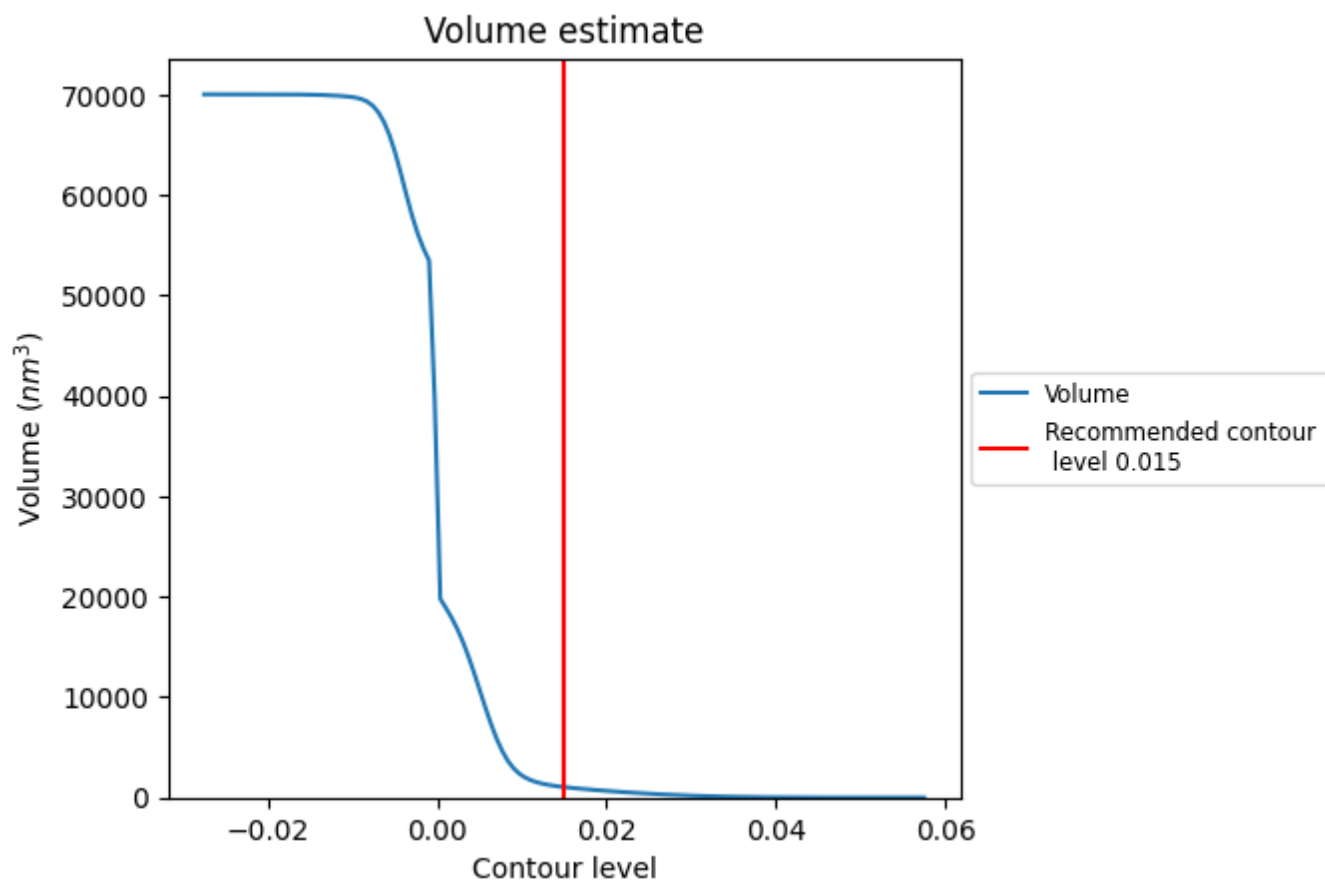
This section contains the results of statistical analysis of the map.

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.

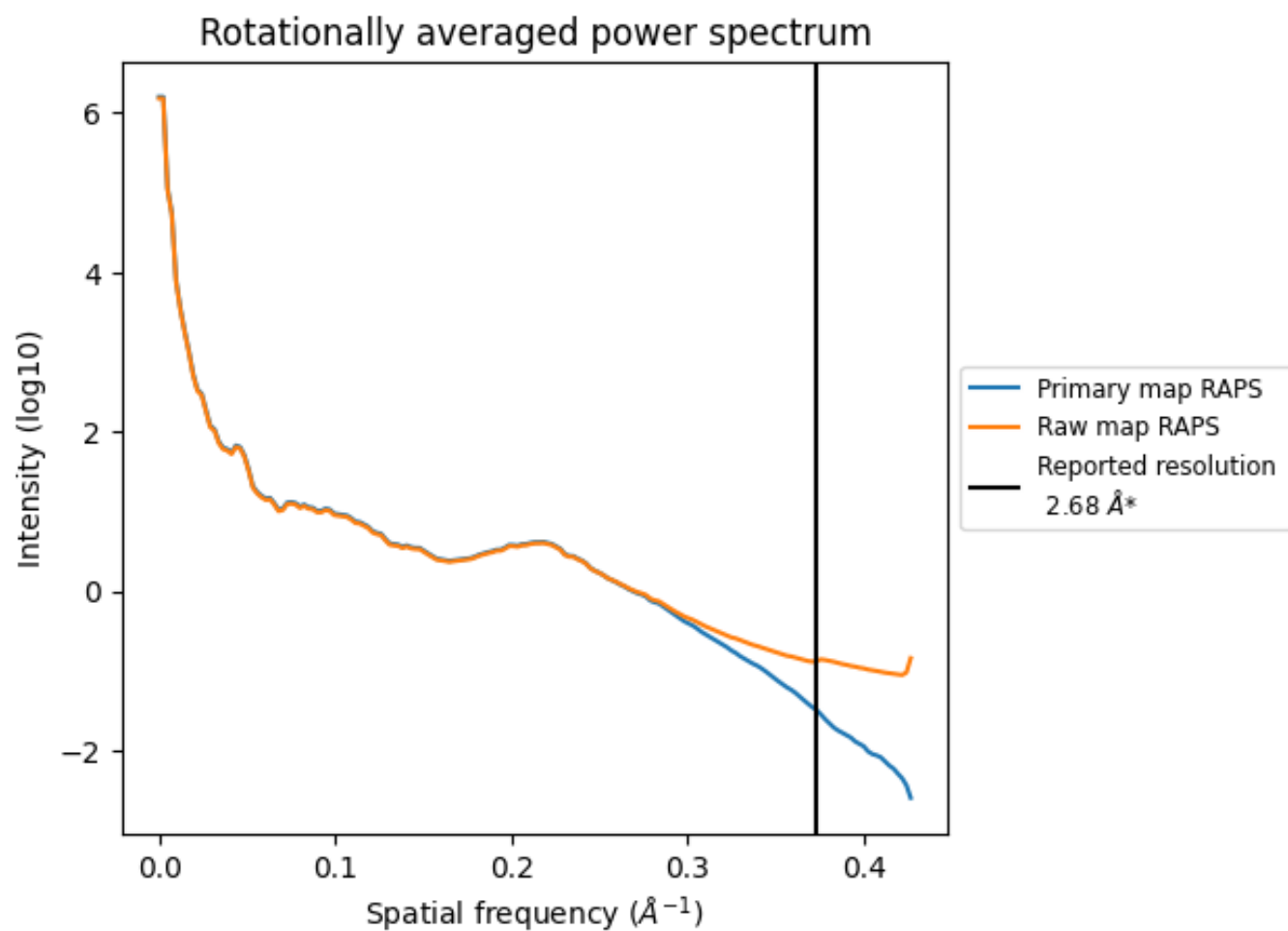
7.2 Volume estimate [i](#)



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 ⓘ

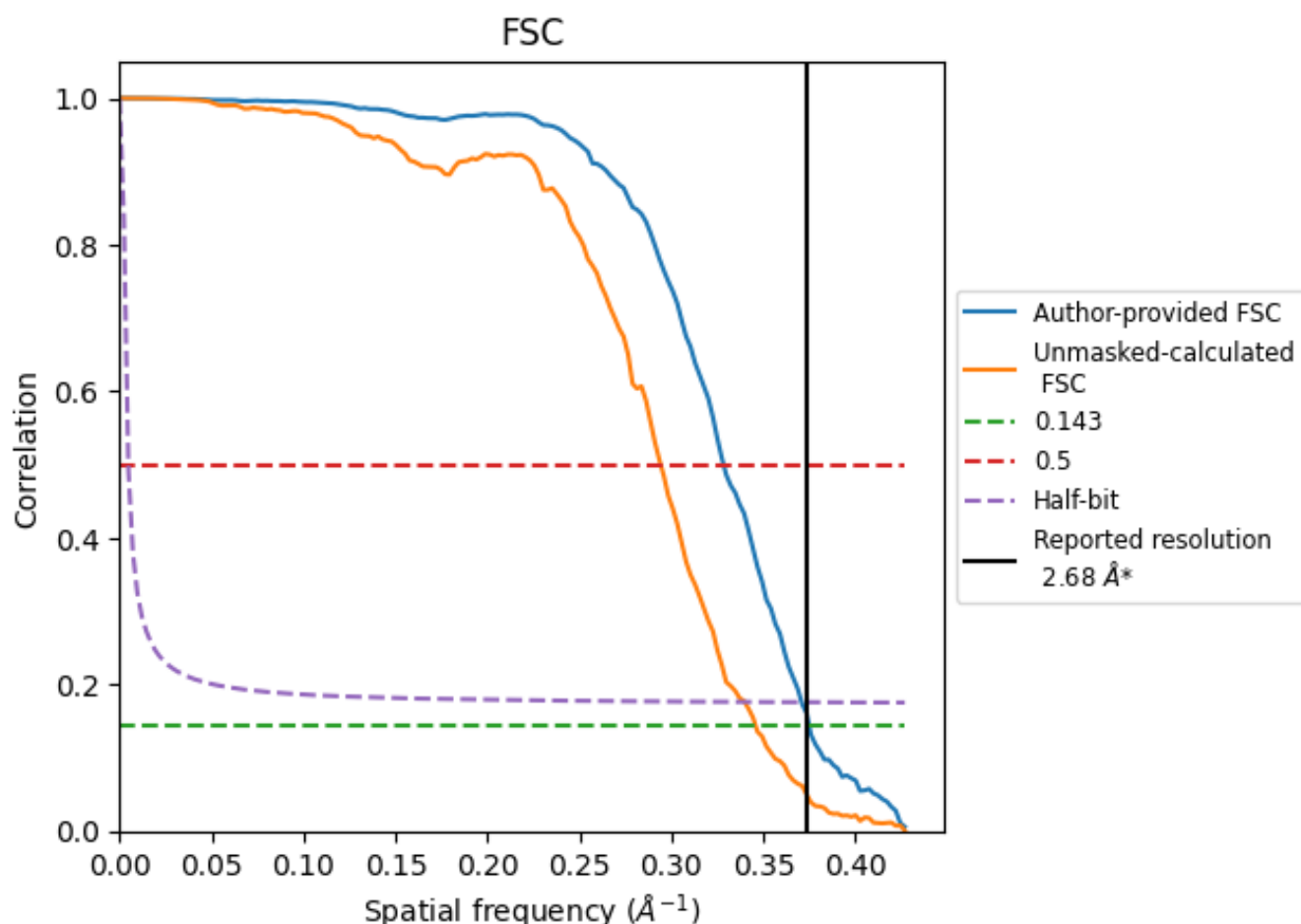


*Reported resolution corresponds to spatial frequency of 0.373 Å⁻¹

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 Å⁻¹

8.2 Resolution estimates [i](#)

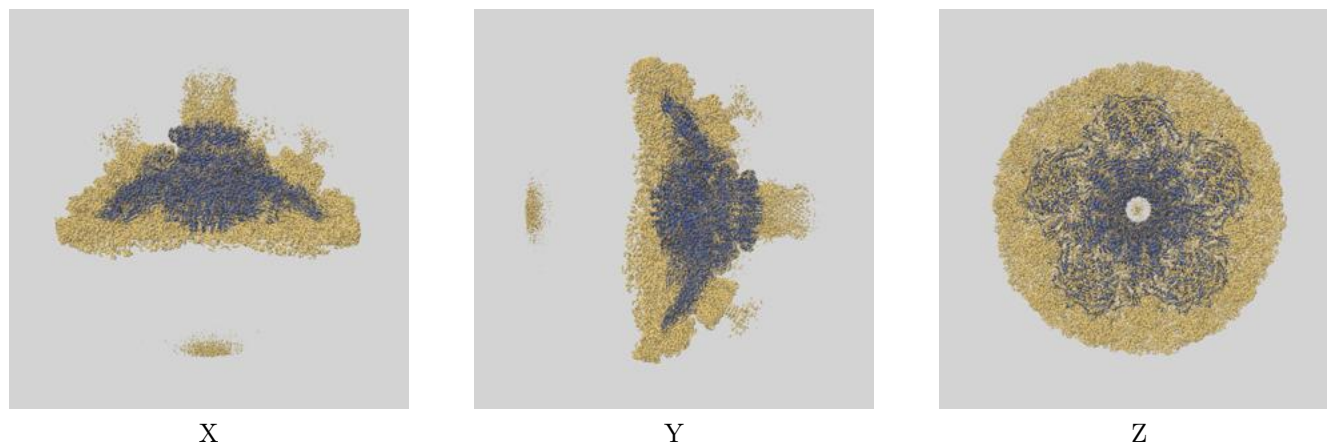
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.68	-	-
Author-provided FSC curve	2.67	3.04	2.70
Unmasked-calculated*	2.89	3.40	2.94

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

9 Map-model fit [i](#)

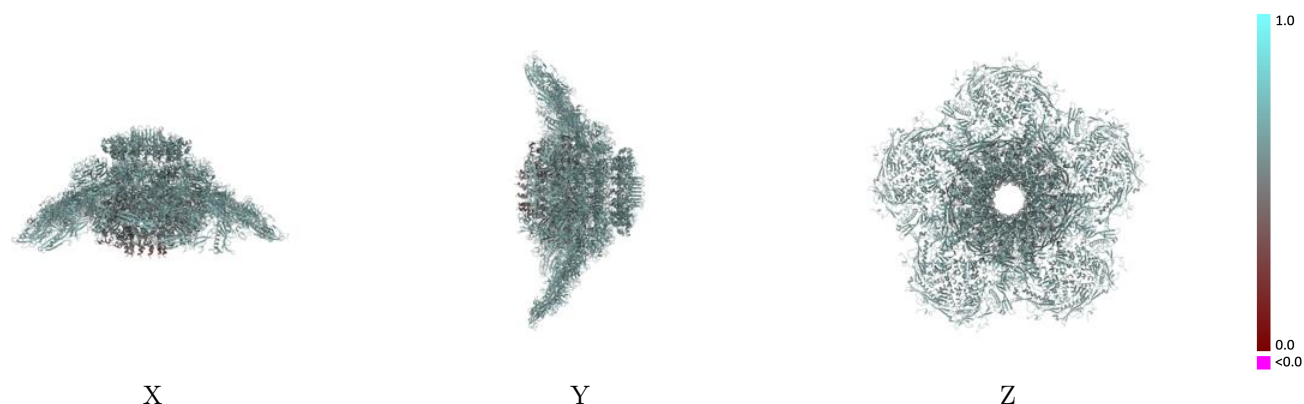
This section contains information regarding the fit between EMDB map EMD-18642 and PDB model 8QSY. Per-residue inclusion information can be found in section 3 on page 14.

9.1 Map-model overlay [i](#)



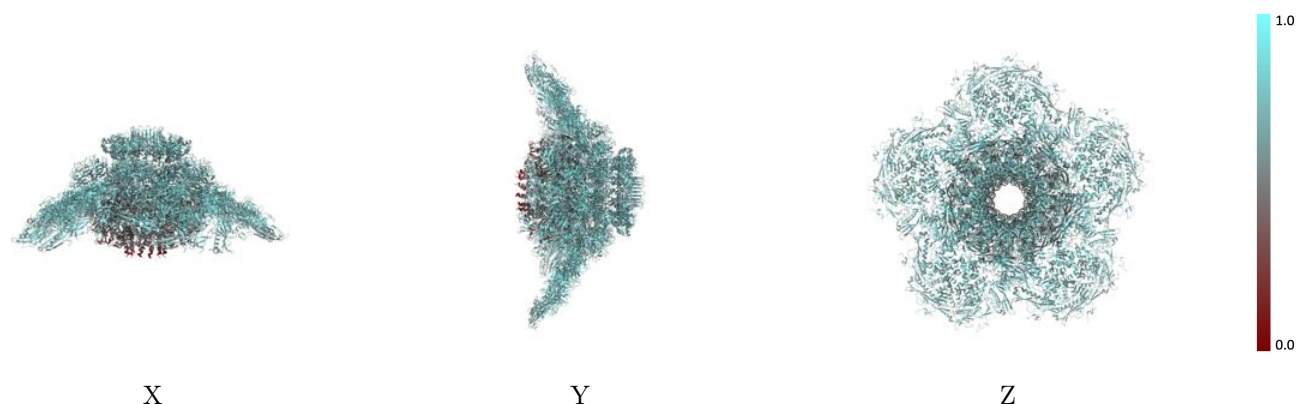
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



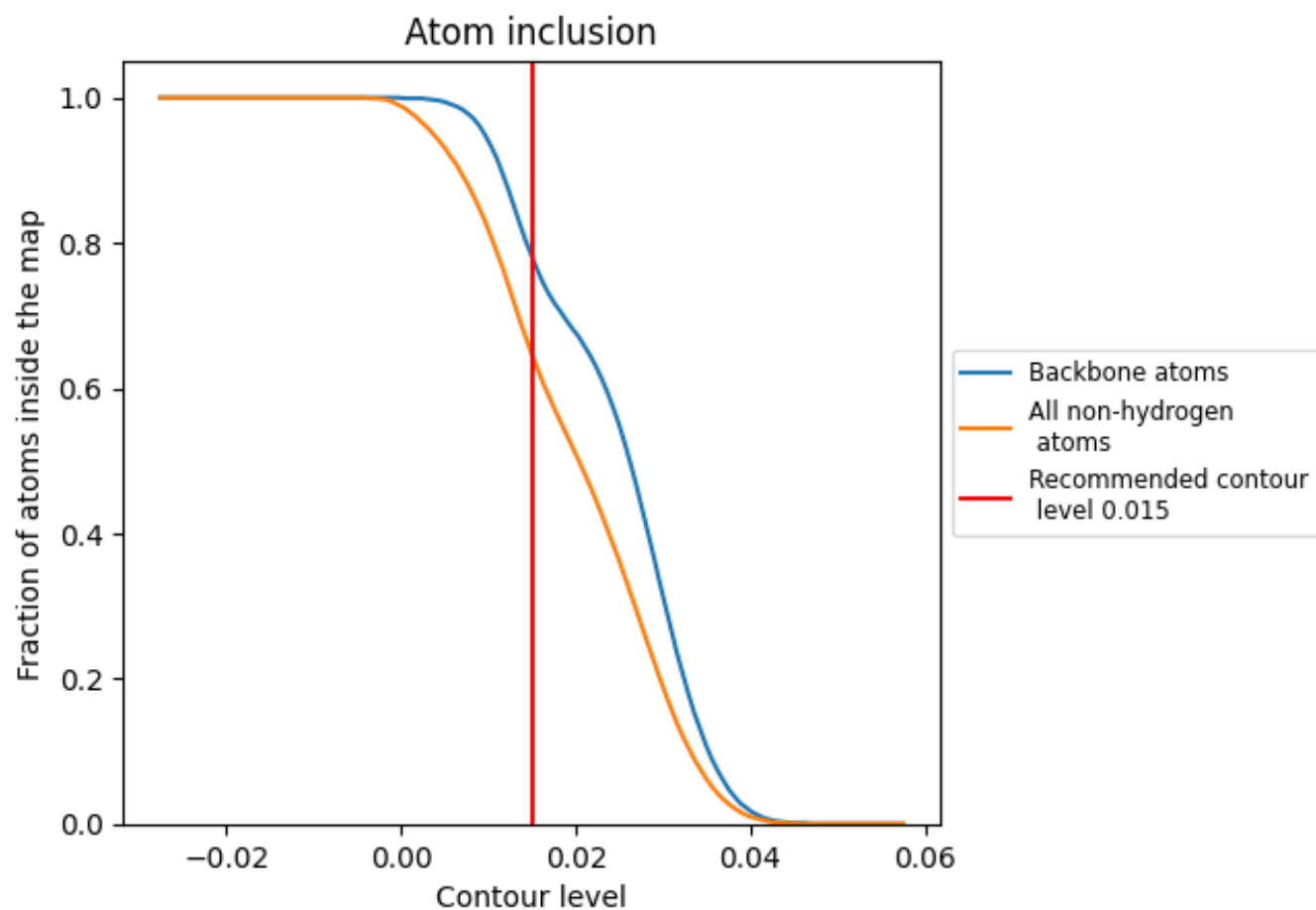
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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