

Full wwPDB EM Validation Report (i)

Aug 6, 2024 – 07:22 PM JST

PDB ID : 8Y6V

EMDB ID : EMD-39002

Title: Near-atomic structure of icosahedrally averaged jumbo bacteriophage PhiKZ

capsid

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Pan, J.; Chen, Z.; Fokine, A.; Sun, L.; Fang, Q.

Deposited on : 2024-02-03

Resolution : 3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) 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 (1)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev92

MolProbity : 4.02b-467

Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)

 $MapQ \quad : \quad 1.9.13$

Ideal geometry (proteins) : Engh & Huber (2001) Ideal geometry (DNA, RNA) : Parkinson et al. (1996)

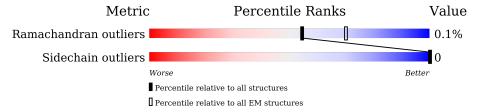
Validation Pipeline (wwPDB-VP) : 2.37.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.50 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 $(\# \mathrm{Entries})$	${ m EM\ structures} \ (\#{ m Entries})$
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain	
1	D	320	36%	
2	В	271	39% 61%	
3	Е	149	23% 95%	5%
3	F	149	40% 95%	5%
4	G	428	9%	31%
5	Н	181	13%	10%
6	K	435	12% 88%	
6	L	435	16% 84%	
6	M	435	16% 84%	



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Mol	Chain	Length	Quality of chain	
7	J	177	99%	
8	A	747	78%	22%
			-	
8	a	747	78%	22%
8	b	747	78%	22%
8	c	747	78%	22%
8	d	747	78%	22%
8	е	747	78%	22%
8	f	747	78%	22%
8	g	747	78%	22%
8	h	747	78%	22%
8	i	747	78%	22%
8	j	747	78%	22%
8	k	747	•	
			78%	22%
8	1	747	78%	22%
8	m	747	78%	22%
8	n	747	78%	22%
8	О	747	78%	22%
8	p	747	78%	22%
8	q	747	7%	22%
8	r	747	78%	22%
8	s	747	78%	22%
8	t	747	78%	22%
			-	
8	u	747	78%	22%
8	V	747	78%	22%
8	W	747	78%	22%



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Mol	Chain	Length		Quality of chain	
8	X	747	<u>•</u>	78%	22%
8	У	747	•	78%	22%
8	Z	747	-	78%	22%
9	N	522	6%	94%	
9	О	522	22%	78%	
9	Р	522	22%	78%	
10	I	230	11%	85%	
11	С	118	7%	97%	•



2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 138685 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 gp28.

Mol	Chain	Residues		Ato	oms			AltConf	Trace
1	D	319	Total 2563	C 1647	N 432	O 475	S 9	0	0

• Molecule 2 is a protein called gp35.

Mol	Chain	Residues		At	oms			AltConf	Trace
2	D	107	Total	С	N	О	S	0	0
2	Б	107	862	568	135	155	4	0	U

• Molecule 3 is a protein called gp85.

Mol	Chain	Residues		At	oms		AltConf	Trace	
2	E	1.49	Total	С	N	О	S	0	0
3	12	142	1102	698	190	211	3	0	
2	Г	141	Total	С	N	О	S	0	0
3	Г	141	1085	684	187	211	3	0	U

• Molecule 4 is a protein called gp86.

Mol	Chain	Residues		Ato	oms			AltConf	Trace
4	G	297	Total 2425	C 1547	N 423	O 447	S 8	0	0

• Molecule 5 is a protein called gp91.

Mol	Chain	Residues		At	oms			AltConf	Trace
5	П	163	Total	С	N	О	S	0	0
	11	105	1333	857	226	245	5	0	U

• Molecule 6 is a protein called gp93.



Mol	Chain	Residues		Aton	ns		AltConf	Trace
6	K	51	Total			О	0	0
	11	91	380	227	59	94	Ü	U
6	Т	71	Total	С	N	Ο	0	0
0	ш	/ 1	528	320	80	128	0	0
6	M	71	Total	С	N	О	0	0
	1V1	11	528	320	80	128	U	U

• Molecule 7 is a protein called gp119.

Mol	Chain	Residues		At	oms			AltConf	Trace
7	Ţ	176	Total	С	N	О	S	0	0
'	J	176	1416	903	236	272	5	0	U

 \bullet Molecule 8 is a protein called gp120.

Mol	Chain	Residues		At	oms			AltConf	Trace
0	_	F04	Total	С	N	О	S	0	0
8	a	584	4566	2887	788	874	17	0	0
0	1_	F04	Total	С	N	О	S	0	0
8	b	584	4566	2887	788	874	17	0	0
8		E01	Total	С	N	О	S	0	0
0	С	584	4566	2887	788	874	17	0	0
8	d	584	Total	С	N	О	S	0	0
0	a	304	4566	2887	788	874	17	U	0
8	e	584	Total	С	N	О	S	0	0
O	е	304	4566	2887	788	874	17	U	0
8	f	584	Total	С	N	О	S	0	0
O	1	304	4566	2887	788	874	17	0	
8	ď	584	Total	С	N	О	S	0	0
O	g	304	4566	2887	788	874	17	U	0
8	h	584	Total	С	N	Ο	S	0	0
O	11	304	4566	2887	788	874	17	U	0
8	i	584	Total	С	N	Ο	S	0	0
O	1	304	4566	2887	788	874	17	U	0
8	j	584	Total	С	N	Ο	S	0	0
O	J	304	4566	2887	788	874	17	U	U
8	k	584	Total	С	N	Ο	S	0	0
O	K	304	4566	2887	788	874	17	U	
8	1	584	Total	С	N	Ο	S	0	0
O	1	304	4566	2887	788	874	17	0	
8	m	584	Total	С	N	О	S	0	0
O	m	304	4566	2887	788	874	17	U	
8	n	584	Total	С	N	О	S	0	0
O	n	304	4566	2887	788	874	17	U	
							Contin	nued on nex	t nage



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Mol	Chain	Residues		At	oms			AltConf	Trace
0	_	F04	Total	С	N	О	S	0	0
8	О	584	4566	2887	788	874	17	0	0
0		E01	Total	С	N	О	S	0	0
8	p	584	4566	2887	788	874	17	U	0
8	a	584	Total	С	N	О	S	0	0
0	q	304	4566	2887	788	874	17	0	U
8	r	584	Total	С	N	О	S	0	0
0	r	304	4566	2887	788	874	17	U	U
8	S	584	Total	С	N	О	S	0	0
0	5	304	4566	2887	788	874	17	0	0
8	t	584	Total	С	N	О	S	0	0
	8	901	4566	2887	788	874	17	U	U
8	u	584	Total	С	N	Ο	S	0	0
	u	304	4566	2887	788	874	17		
8	V	584	Total	С	N	О	S	0	0
	v	904	4566	2887	788	874	17	0	U
8	W	584	Total	С	N	Ο	S	0	0
	VV	904	4566	2887	788	874	17	0	U
8	X	584	Total	\mathbf{C}	N	Ο	S	0	0
0	Λ	904	4566	2887	788	874	17	U	U
8	37	584	Total	С	N	Ο	\mathbf{S}	0	0
6	У	904	4566	2887	788	874	17	U	U
8	7	584	Total	С	N	О	S	0	0
	L	z 584	4566	2887	788	874	17	0	
8	Δ	582	Total	С	N	О	S	0	0
	8 A	A 582	4550	2876	785	872	17		U

• Molecule 9 is a protein called gp162.

Mol	Chain	Residues	Atoms	AltConf	Trace
9	N	32	Total C N O 246 151 36 59	0	0
9	О	116	Total C N O S 885 538 149 195 3	0	0
9	Р	116	Total C N O S 885 538 149 195 3	0	0

 \bullet Molecule 10 is a protein called gp184.

Mol	Chain	Residues	Atoms				AltConf	Trace	
10	Ţ	34	Total	С	N	О	S	0	0
10	1	04	272	171	42	58	1		O



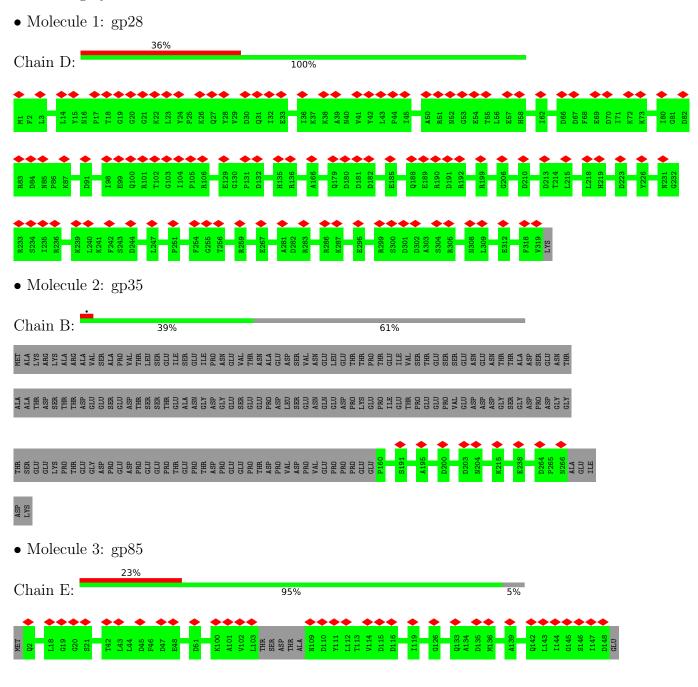
 $\bullet\,$ Molecule 11 is a protein called gp244.

Mol	Chain	Residues	Atoms				AltConf	Trace	
11	С	114	Total	C	N 140	0	S	0	0
			909	571	149	184	Э		

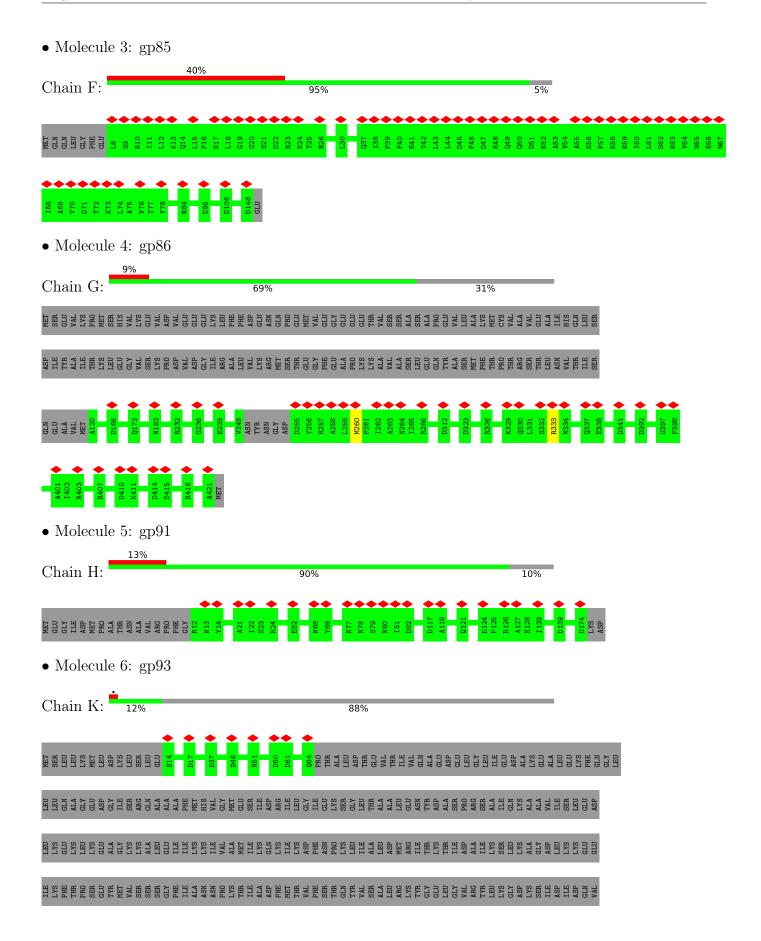


3 Residue-property plots (i)

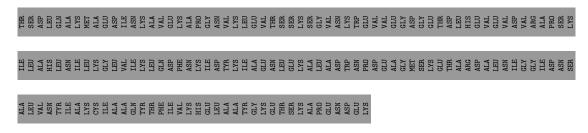
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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





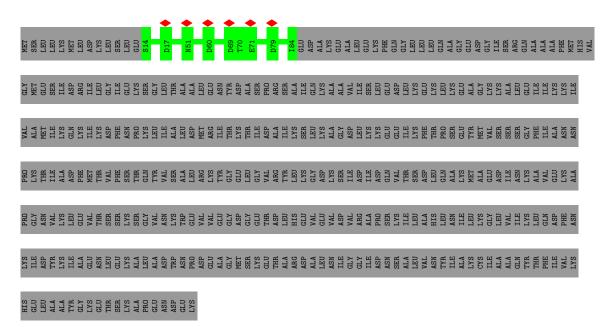






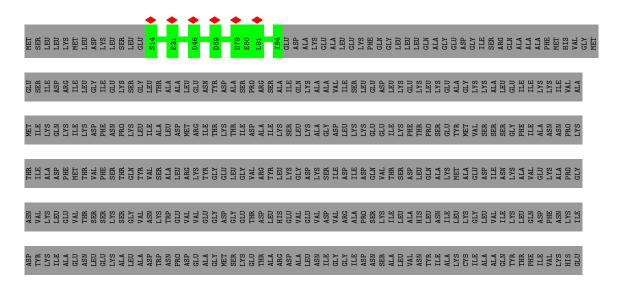
• Molecule 6: gp93

Chain L: 16% 84%

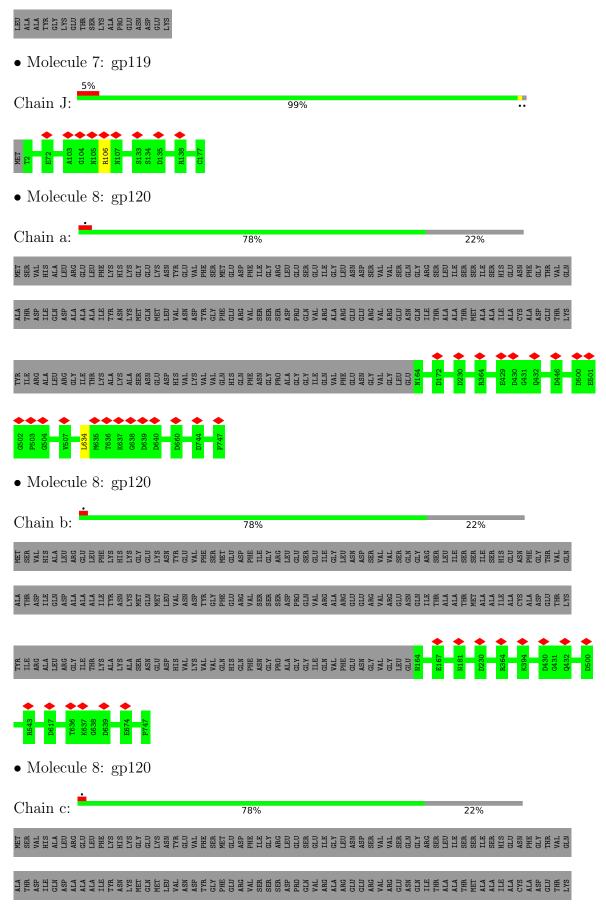


• Molecule 6: gp93

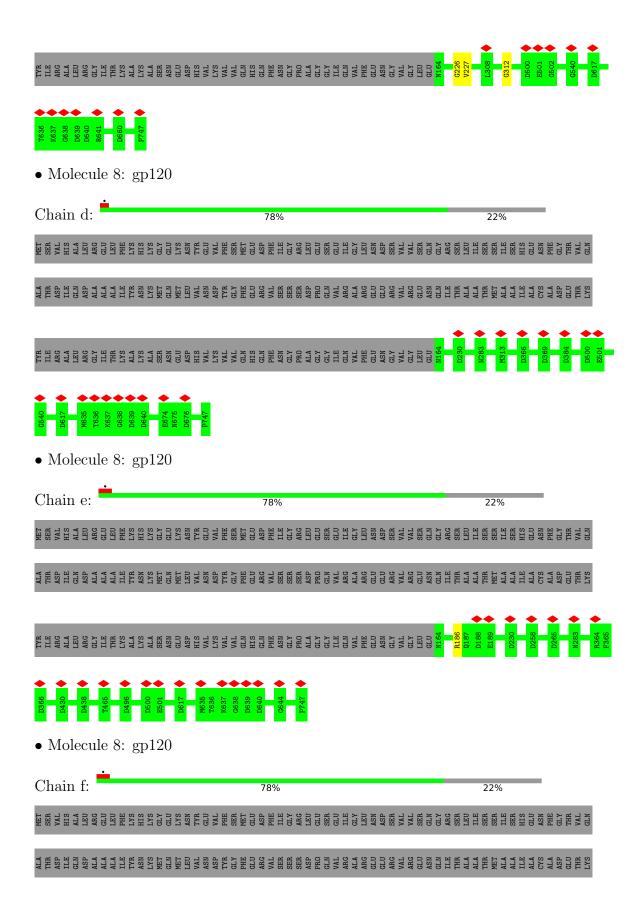
Chain M: 16% 84%



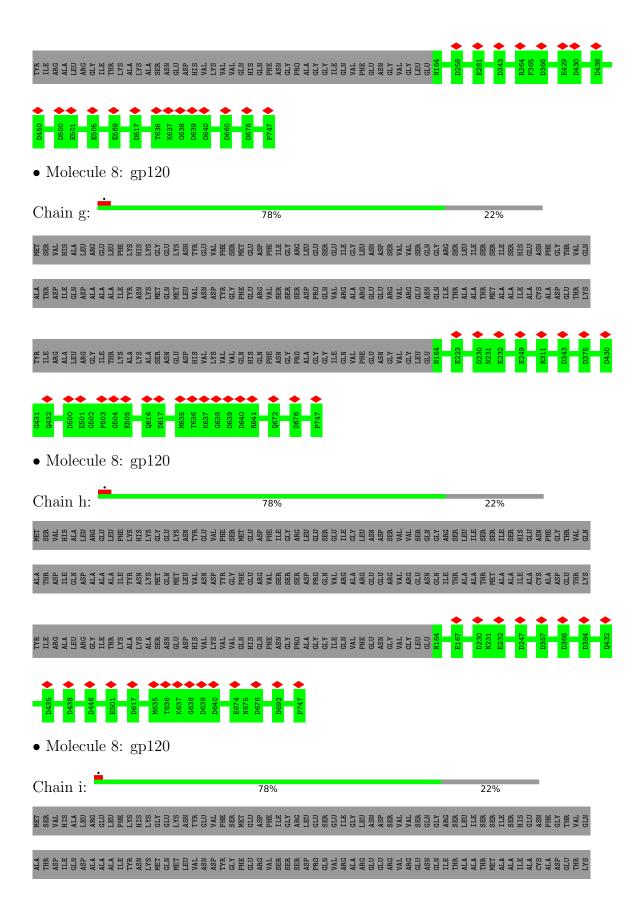




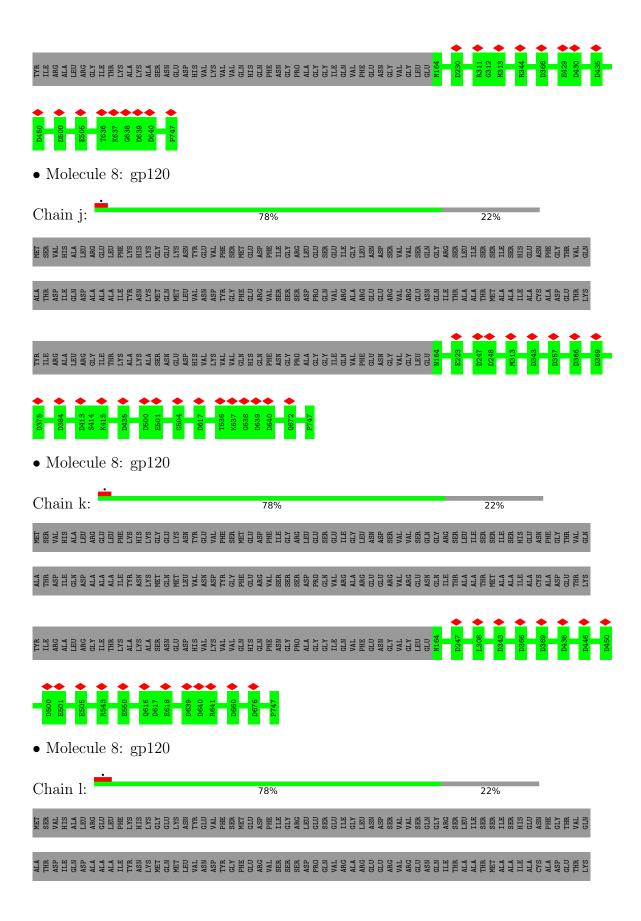




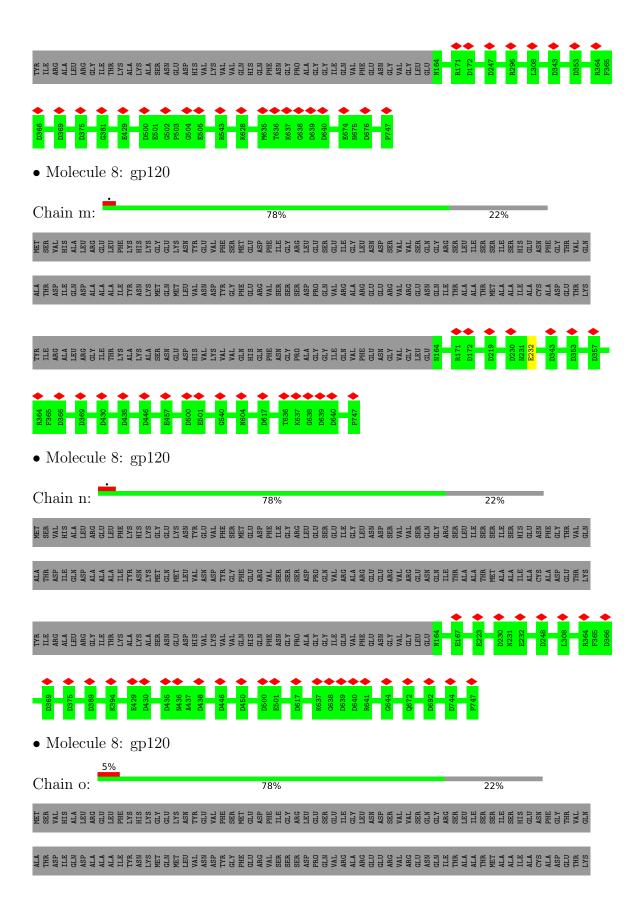




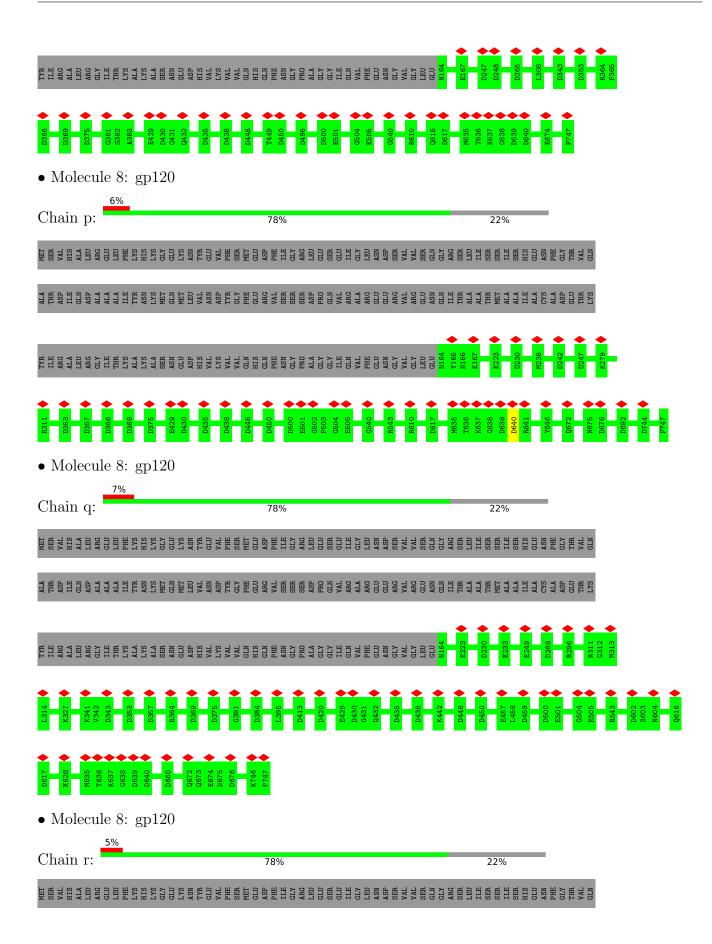




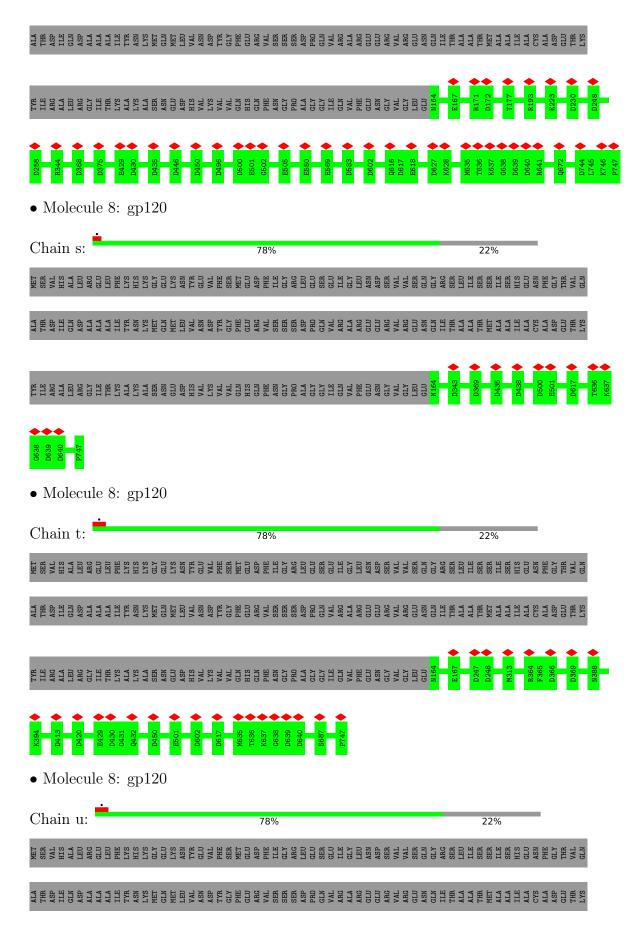




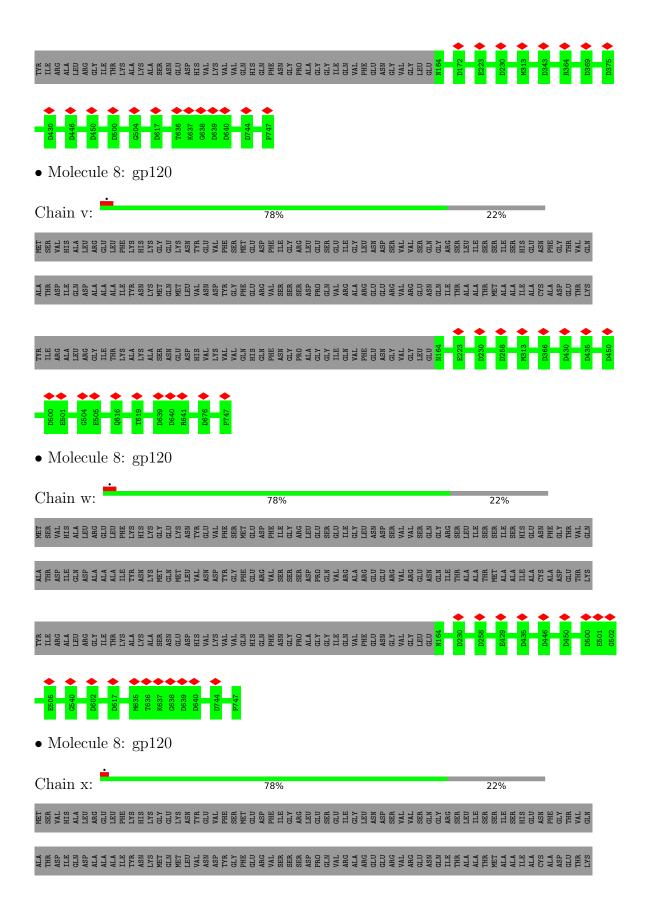




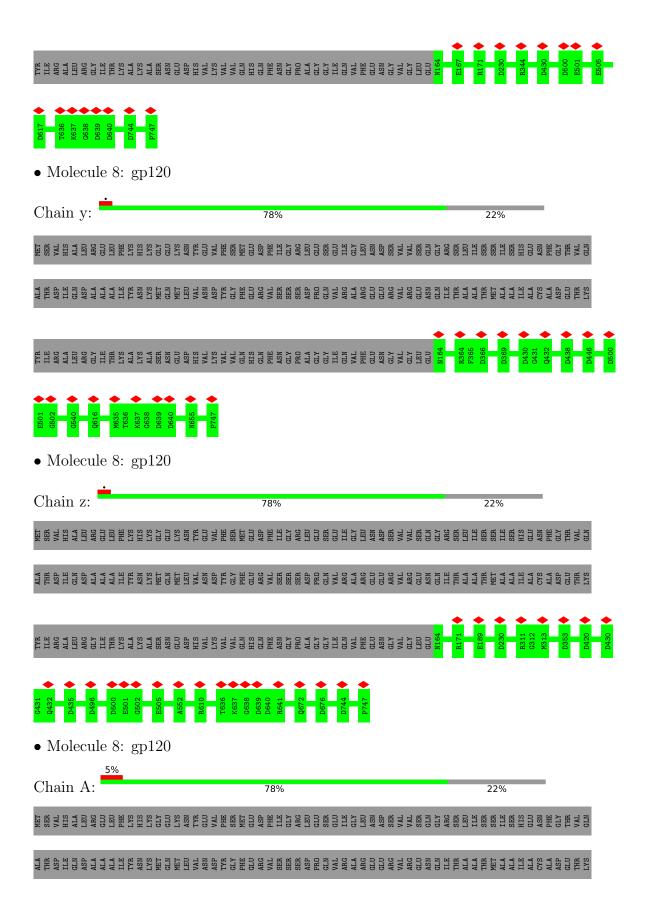




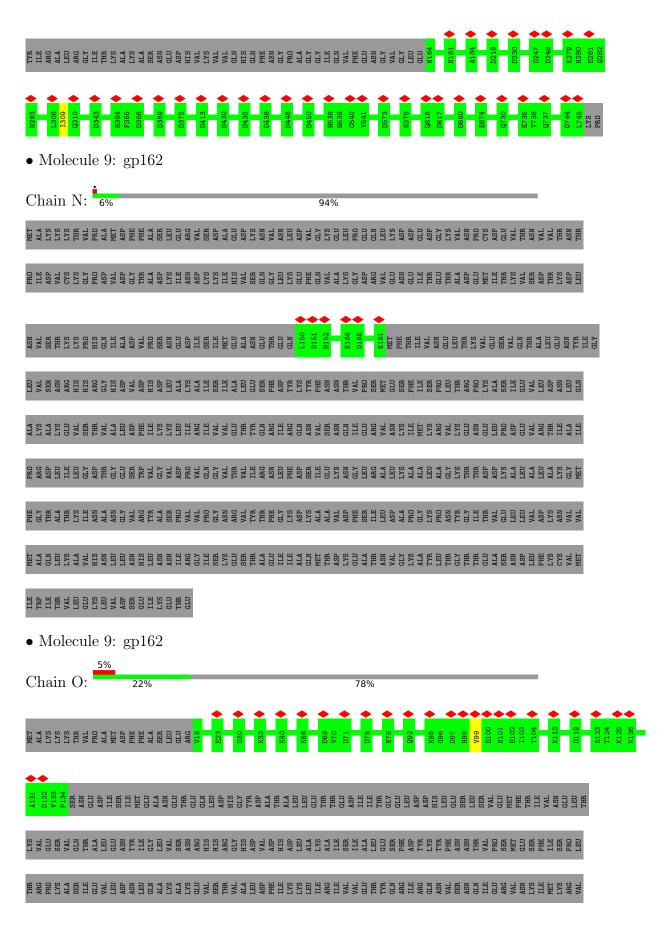




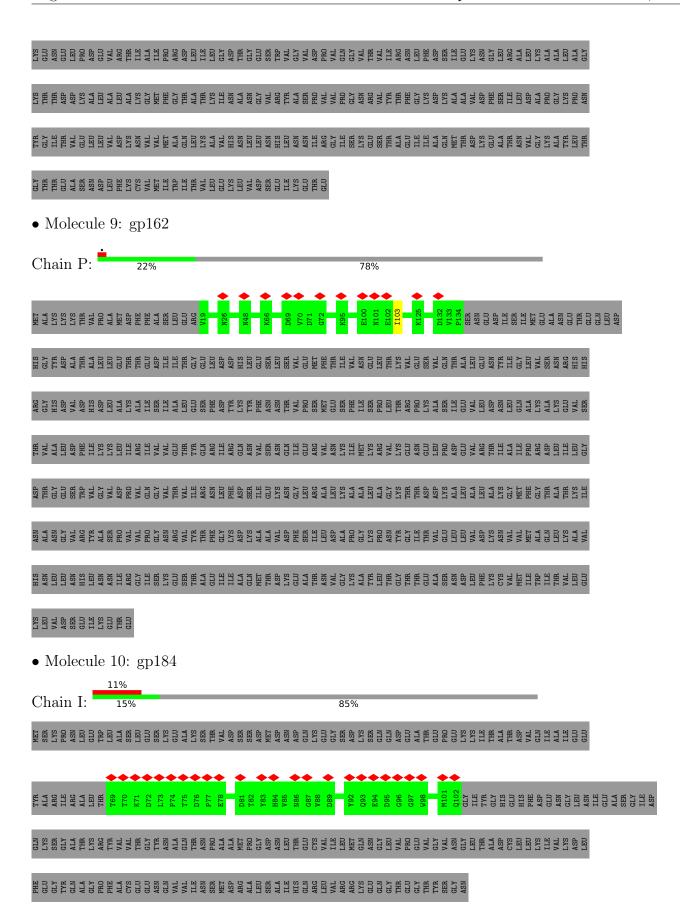






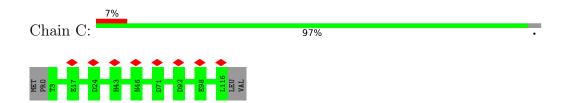






• Molecule 11: gp244







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	903900	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{Å}^2)$	30	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	64000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.082	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.0165	Depositor
Map size (Å)	1600.0, 1600.0, 1600.0	wwPDB
Map dimensions	1000, 1000, 1000	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.6, 1.6, 1.6	Depositor



5 Model quality (i)

5.1 Standard geometry (i)

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	langles
MIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z >5
1	D	0.60	0/2621	0.49	0/3561
2	В	0.55	0/887	0.51	0/1207
3	Е	0.55	0/1112	0.50	0/1505
3	F	0.52	0/1095	0.50	0/1486
4	G	0.65	0/2467	0.50	0/3325
5	Н	0.61	0/1367	0.49	0/1859
6	K	0.94	0/381	0.44	0/522
6	L	0.94	0/530	0.47	0/728
6	M	0.95	0/530	0.55	0/728
7	J	0.68	0/1445	0.51	0/1964
8	A	0.62	0/4631	0.52	0/6288
8	a	0.62	0/4648	0.52	0/6311
8	b	0.62	0/4648	0.50	0/6311
8	С	0.62	0/4648	0.51	0/6311
8	d	0.61	0/4648	0.49	0/6311
8	е	0.62	0/4648	0.49	0/6311
8	f	0.62	0/4648	0.51	0/6311
8	g	0.62	0/4648	0.50	0/6311
8	h	0.62	0/4648	0.51	0/6311
8	i	0.61	0/4648	0.50	0/6311
8	j	0.62	0/4648	0.50	0/6311
8	k	0.62	0/4648	0.50	0/6311
8	1	0.61	0/4648	0.49	0/6311
8	m	0.60	0/4648	0.51	0/6311
8	n	0.62	0/4648	0.50	0/6311
8	О	0.62	0/4648	0.51	0/6311
8	р	0.62	0/4648	0.50	0/6311
8	q	0.62	0/4648	0.49	0/6311
8	r	0.62	0/4648	0.50	0/6311
8	s	0.63	0/4648	0.49	0/6311
8	t	0.62	0/4648	0.52	0/6311
8	u	0.62	0/4648	0.49	0/6311
8	V	0.63	0/4648	0.50	0/6311
8	W	0.62	0/4648	0.50	0/6311



Mol	Chain	Bond	lengths	Bond	langles
MIOI	Chain	RMSZ	# Z >5	RMSZ	# Z > 5
8	X	0.63	0/4648	0.49	0/6311
8	у	0.62	0/4648	0.50	0/6311
8	Z	0.62	0/4648	0.50	0/6311
9	N	0.93	0/248	0.51	0/338
9	О	0.74	0/893	0.54	0/1210
9	Р	0.79	0/893	0.60	0/1210
10	I	0.33	0/281	0.48	0/387
11	С	0.64	0/924	0.49	0/1249
All	All	0.63	0/141153	0.50	0/191653

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percei	ntiles
1	D	317/320~(99%)	313 (99%)	4 (1%)	0	100	100
2	В	$105/271\ (39\%)$	101 (96%)	4 (4%)	0	100	100
3	E	138/149~(93%)	133 (96%)	5 (4%)	0	100	100
3	F	$139/149\ (93\%)$	136 (98%)	3 (2%)	0	100	100
4	G	293/428~(68%)	285 (97%)	6 (2%)	2 (1%)	22	61
5	Н	161/181~(89%)	154 (96%)	7 (4%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
6	K	49/435 (11%)	48 (98%)	1 (2%)	0	100	100
6	L	69/435 (16%)	63 (91%)	6 (9%)	0	100	100
6	M	69/435 (16%)	66 (96%)	3 (4%)	0	100	100
7	J	174/177 (98%)	168 (97%)	5 (3%)	1 (1%)	25	64
8	A	580/747 (78%)	562 (97%)	17 (3%)	1 (0%)	47	81
8	a	582/747 (78%)	564 (97%)	17 (3%)	1 (0%)	47	81
8	b	582/747 (78%)	569 (98%)	13 (2%)	0	100	100
8	c	582/747 (78%)	555 (95%)	24 (4%)	3 (0%)	29	68
8	d	582/747 (78%)	564 (97%)	18 (3%)	0	100	100
8	e	582/747 (78%)	561 (96%)	20 (3%)	1 (0%)	47	81
8	f	582/747 (78%)	565 (97%)	17 (3%)	0	100	100
8	g	582/747 (78%)	568 (98%)	14 (2%)	0	100	100
8	h	582/747 (78%)	567 (97%)	15 (3%)	0	100	100
8	i	582/747 (78%)	563 (97%)	19 (3%)	0	100	100
8	j	582/747 (78%)	561 (96%)	21 (4%)	0	100	100
8	k	582/747 (78%)	566 (97%)	16 (3%)	0	100	100
8	1	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	m	582/747 (78%)	563 (97%)	18 (3%)	1 (0%)	47	81
8	n	582/747 (78%)	573 (98%)	9 (2%)	0	100	100
8	О	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	р	582/747 (78%)	568 (98%)	13 (2%)	1 (0%)	47	81
8	q	582/747 (78%)	572 (98%)	10 (2%)	0	100	100
8	r	582/747 (78%)	566 (97%)	16 (3%)	0	100	100
8	S	582/747 (78%)	572 (98%)	10 (2%)	0	100	100
8	t	582/747 (78%)	554 (95%)	28 (5%)	0	100	100
8	u	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	v	582/747 (78%)	574 (99%)	8 (1%)	0	100	100
8	w	582/747 (78%)	572 (98%)	10 (2%)	0	100	100
8	x	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	У	582/747 (78%)	571 (98%)	11 (2%)	0	100	100
8	Z	582/747 (78%)	574 (99%)	8 (1%)	0	100	100



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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	ntiles
9	N	30/522~(6%)	30 (100%)	0	0	100	100
9	О	114/522~(22%)	104 (91%)	9 (8%)	1 (1%)	17	56
9	Р	114/522~(22%)	102 (90%)	11 (10%)	1 (1%)	17	56
10	I	32/230 (14%)	29 (91%)	3 (9%)	0	100	100
11	С	112/118 (95%)	112 (100%)	0	0	100	100
All	All	17628/25063 (70%)	17148 (97%)	467 (3%)	13 (0%)	54	84

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	Р	103	ILE
8	С	226	GLY
8	c	227	VAL
8	m	232	GLU
4	G	333	ARG
8	a	634	LEU
8	е	186	ARG
8	р	640	ASP
4	G	260	MET
8	A	309	ILE
7	J	106	ARG
9	О	99	VAL
8	С	312	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percer	ntiles
1	D	$283/284\ (100\%)$	283 (100%)	0	100	100
2	В	$95/242\ (39\%)$	95 (100%)	0	100	100
3	E	123/129~(95%)	123 (100%)	0	100	100
3	F	122/129~(95%)	122 (100%)	0	100	100



 $Continued\ from\ previous\ page...$

Mol	Chain	Analysed	Rotameric	Outliers	Perce	ntiles
4	G	260/374 (70%)	260 (100%)	0	100	100
5	Н	143/157 (91%)	143 (100%)	0	100	100
6	K	45/365 (12%)	45 (100%)	0	100	100
6	L	$62/365\ (17\%)$	62 (100%)	0	100	100
6	M	$62/365\ (17\%)$	62 (100%)	0	100	100
7	J	$159/160\ (99\%)$	159 (100%)	0	100	100
8	A	501/638~(78%)	501 (100%)	0	100	100
8	a	503/638~(79%)	503 (100%)	0	100	100
8	b	503/638~(79%)	503 (100%)	0	100	100
8	c	503/638~(79%)	503 (100%)	0	100	100
8	d	503/638 (79%)	503 (100%)	0	100	100
8	e	503/638~(79%)	503 (100%)	0	100	100
8	f	503/638~(79%)	503 (100%)	0	100	100
8	g	503/638~(79%)	503 (100%)	0	100	100
8	h	503/638 (79%)	503 (100%)	0	100	100
8	i	503/638~(79%)	503 (100%)	0	100	100
8	j	503/638 (79%)	503 (100%)	0	100	100
8	k	503/638~(79%)	503 (100%)	0	100	100
8	1	503/638~(79%)	503 (100%)	0	100	100
8	m	503/638 (79%)	503 (100%)	0	100	100
8	n	503/638 (79%)	503 (100%)	0	100	100
8	О	503/638~(79%)	503 (100%)	0	100	100
8	p	503/638 (79%)	503 (100%)	0	100	100
8	q	503/638~(79%)	503 (100%)	0	100	100
8	r	503/638 (79%)	503 (100%)	0	100	100
8	S	503/638 (79%)	503 (100%)	0	100	100
8	t	503/638 (79%)	503 (100%)	0	100	100
8	u	503/638 (79%)	503 (100%)	0	100	100
8	v	503/638 (79%)	503 (100%)	0	100	100
8	W	503/638 (79%)	503 (100%)	0	100	100
8	X	503/638 (79%)	503 (100%)	0	100	100



Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
8	У	503/638 (79%)	503 (100%)	0	100 100
8	Z	503/638~(79%)	503 (100%)	0	100 100
9	N	28/456~(6%)	28 (100%)	0	100 100
9	О	105/456~(23%)	105 (100%)	0	100 100
9	Р	105/456~(23%)	105 (100%)	0	100 100
10	I	30/193 (16%)	30 (100%)	0	100 100
11	С	$105/109\ (96\%)$	105 (100%)	0	100 100
All	All	15306/21466 (71%)	15306 (100%)	0	100 100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
3	F	14	GLN
8	a	166	ASN
8	a	464	ASN
8	b	464	ASN
8	С	166	ASN
8	С	464	ASN
8	е	166	ASN
8	е	464	ASN
8	f	166	ASN
8	g h	464	ASN
8	h	166	ASN
8	h	170	GLN
8	h	672	GLN
8	h	737	GLN
8	k	222	HIS
8	k	464	ASN
8	n	632	ASN
8	n	737	GLN
8	q	164	ASN
8	s	737	GLN
8	t	464	ASN
8	u	464	ASN
8	W	739	ASN
8	у	682	GLN
8	A	464	ASN



Continued from previous page...

Mol	Chain	Res	Type
9	O	92	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

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.



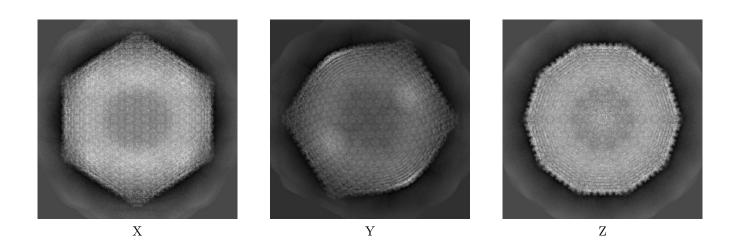
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-39002. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

Orthogonal projections (i) 6.1

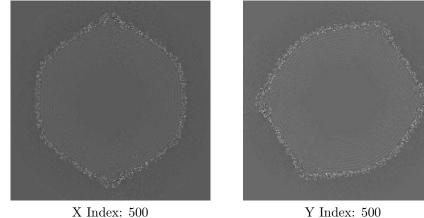
6.1.1 Primary map



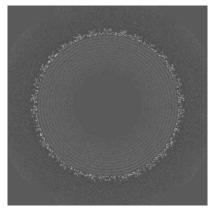
The images above show the map projected in three orthogonal directions.

Central slices (i) 6.2

6.2.1Primary map







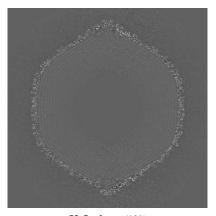
Z Index: 500

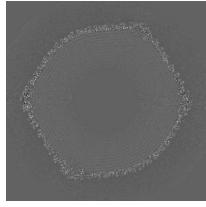


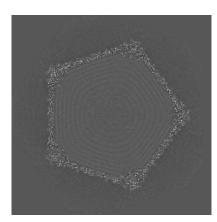
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map







X Index: 507

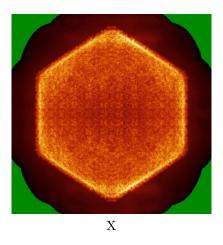
Y Index: 531

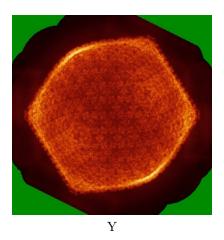
Z Index: 703

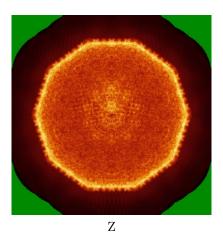
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map





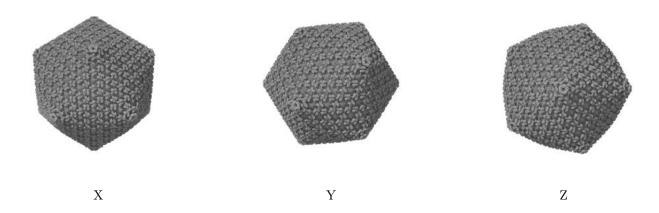


The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.



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 0.0165. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



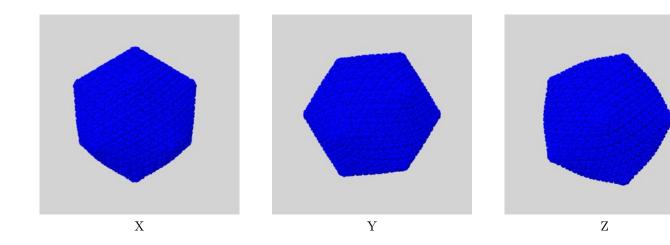
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

$6.6.1 \quad \mathrm{emd}_39002_\mathrm{msk}_1.\mathrm{map} \ \ \mathbf{\mathring{1}}$

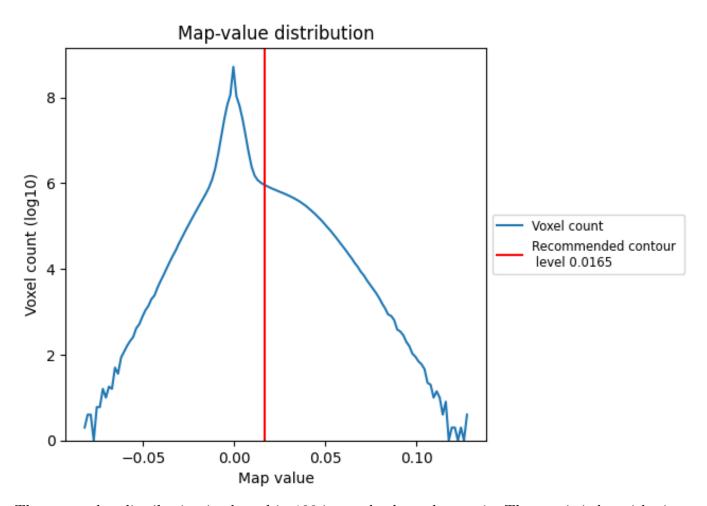




7 Map analysis (i)

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

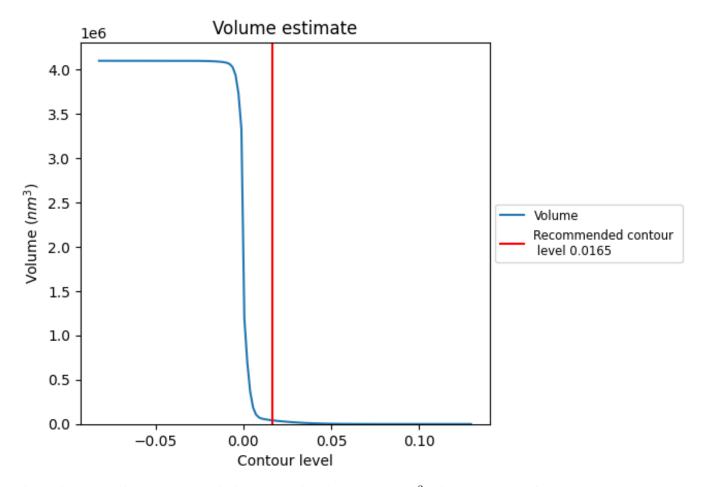
7.1 Map-value distribution (i)



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)

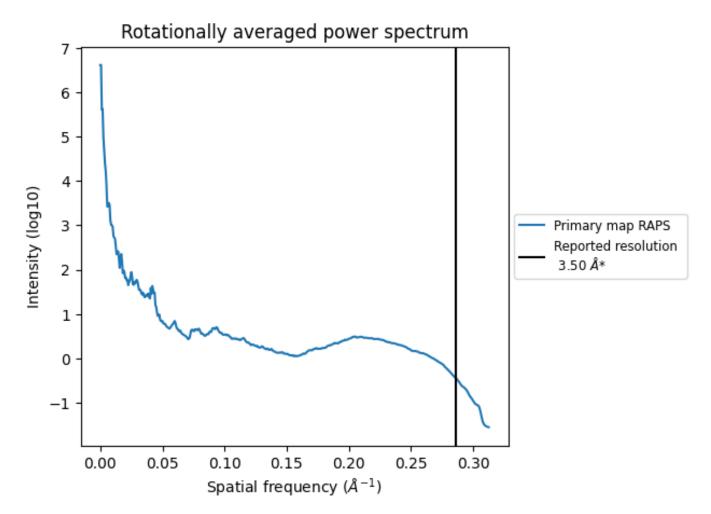


The volume at the recommended contour level is $41513~\mathrm{nm}^3$; this corresponds to an approximate mass of $37499~\mathrm{kDa}$.

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



7.3 Rotationally averaged power spectrum (i)



^{*}Reported resolution corresponds to spatial frequency of 0.286 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

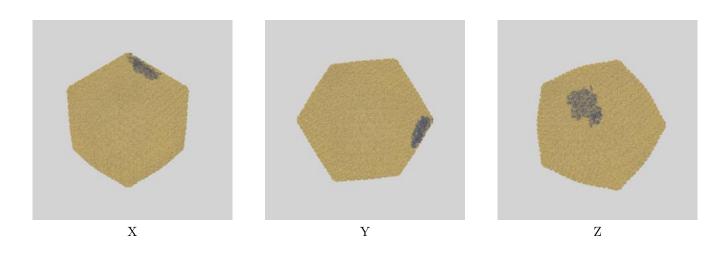


9 Map-model fit (i)

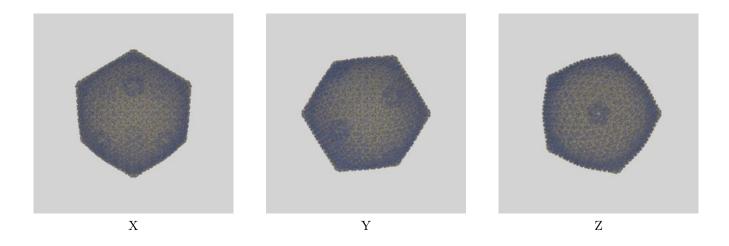
This section contains information regarding the fit between EMDB map EMD-39002 and PDB model 8Y6V. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay (i)



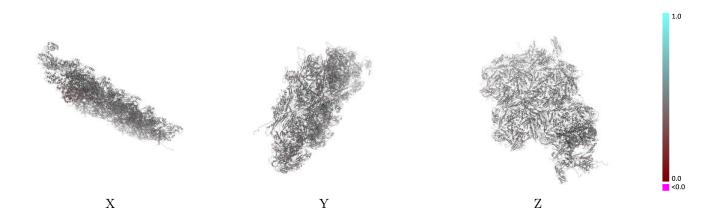
9.1.2 Map-model assembly overlay (i)



The images above show the 3D surface view of the map at the recommended contour level 0.0165 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.

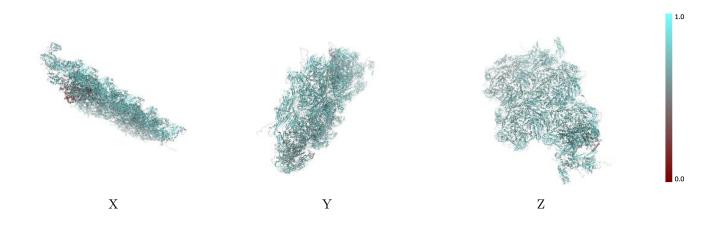


9.2 Q-score mapped to coordinate model (i)



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.

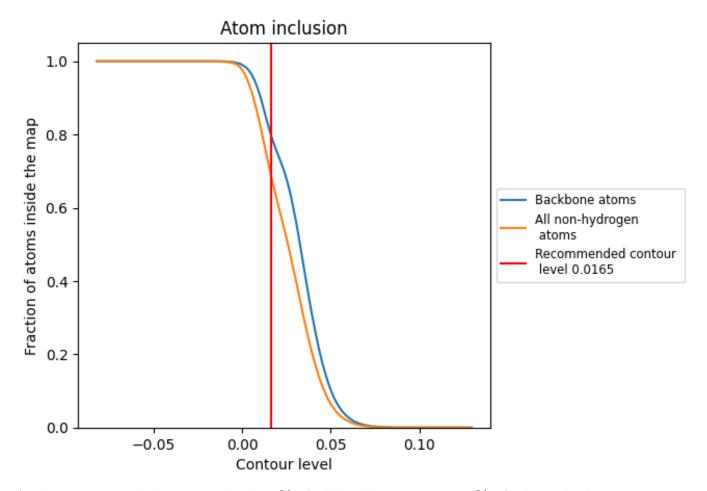
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0165).



9.4 Atom inclusion (i)



At the recommended contour level, 79% of all backbone atoms, 68% of all non-hydrogen atoms, are inside the map.



9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0165) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6830	0.4610
A	0.6840	0.4650
В	0.6710	0.4640
С	0.6490	0.4460
D	0.4730	0.4310
E	0.5480	0.4110
F	0.4090	0.3750
G	0.6050	0.4360
Н	0.6290	0.4550
I	0.2650	0.4210
J	0.6670	0.4620
K	0.5550	0.4110
L	0.6210	0.4290
M	0.6000	0.4280
N	0.5880	0.4230
О	0.5270	0.3970
Р	0.5610	0.4120
a	0.7260	0.4690
b	0.7310	0.4710
С	0.7390	0.4660
d	0.7380	0.4670
е	0.7290	0.4700
f	0.7340	0.4740
g	0.6980	0.4640
h	0.7080	0.4630
i	0.7060	0.4730
j	0.7000	0.4710
k	0.6900	0.4620
1	0.6870	0.4590
m	0.6820	0.4670
n	0.6920	0.4670
О	0.6500	0.4570
p	0.6190	0.4530
q	0.6110	0.4480
r	0.6360	0.4540





 $Continued\ from\ previous\ page...$

Chain	Atom inclusion	Q-score
S	0.7390	0.4680
t	0.7140	0.4630
u	0.7010	0.4760
V	0.7010	0.4700
W	0.7040	0.4640
X	0.7270	0.4700
У	0.7110	0.4670
Z	0.6820	0.4620

