



Full wwPDB EM Validation Report ⓘ

Mar 9, 2026 – 01:44 PM UTC

PDB ID : 8Y6V / pdb_00008y6v
EMDB ID : EMD-39002
Title : Near-atomic structure of icosahedrally averaged jumbo bacteriophage PhiKZ capsid
Authors : Yang, Y.; Shao, Q.; Guo, M.; Han, L.; Zhao, X.; Wang, A.; Li, X.; Wang, B.; 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 ⓘ symbol.

The types of validation reports are described at

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

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

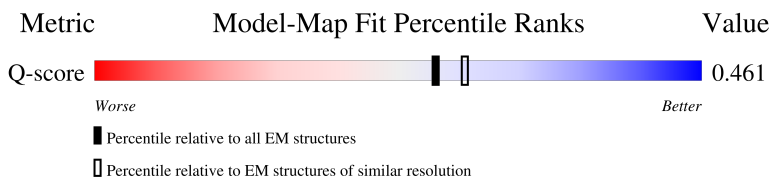
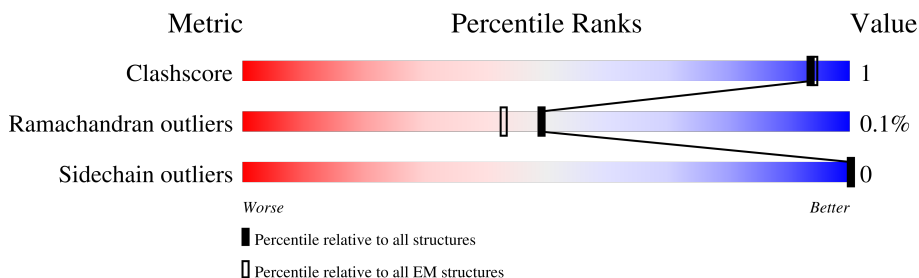
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance

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

The reported resolution of this entry is 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 (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13950 (3.00 - 4.00)

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	D	320	
2	B	271	
3	E	149	
3	F	149	

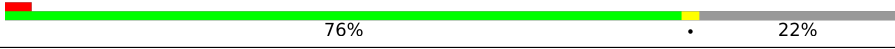
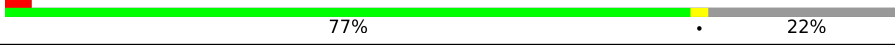
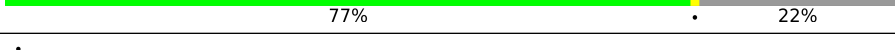
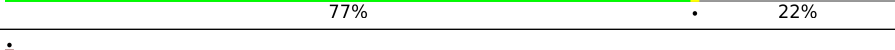
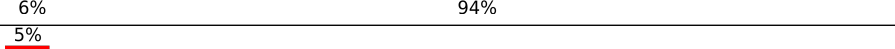
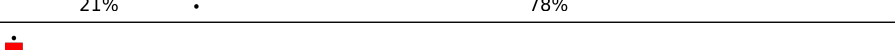
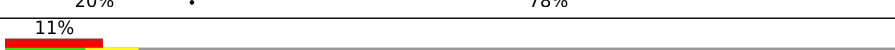
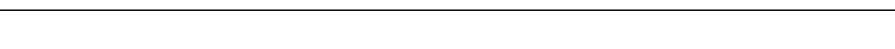
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	G	428	
5	H	181	
6	K	435	
6	L	435	
6	M	435	
7	J	177	
8	A	747	
8	a	747	
8	b	747	
8	c	747	
8	d	747	
8	e	747	
8	f	747	
8	g	747	
8	h	747	
8	i	747	
8	j	747	
8	k	747	
8	l	747	
8	m	747	
8	n	747	
8	o	747	
8	p	747	
8	q	747	
8	r	747	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
8	s	747	
8	t	747	
8	u	747	
8	v	747	
8	w	747	
8	x	747	
8	y	747	
8	z	747	
9	N	522	
9	O	522	
9	P	522	
10	I	230	
11	C	118	

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	Atoms					AltConf	Trace
1	D	319	Total	C	N	O	S	0	0
			2563	1647	432	475	9		

- Molecule 2 is a protein called gp35.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			862	568	135	155	4		

- Molecule 3 is a protein called gp85.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	142	Total	C	N	O	S	0	0
			1102	698	190	211	3		
3	F	141	Total	C	N	O	S	0	0
			1085	684	187	211	3		

- Molecule 4 is a protein called gp86.

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

- Molecule 5 is a protein called gp91.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	163	Total	C	N	O	S	0	0
			1333	857	226	245	5		

- Molecule 6 is a protein called gp93.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	K	51	Total	C	N	O	0	0
			380	227	59	94		
6	L	71	Total	C	N	O	0	0
			528	320	80	128		
6	M	71	Total	C	N	O	0	0
			528	320	80	128		

- Molecule 7 is a protein called gp119.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	J	176	Total	C	N	O	S	0	0
			1416	903	236	272	5		

- Molecule 8 is a protein called gp120.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	b	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	c	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	d	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	e	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	f	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	g	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	h	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	i	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	j	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	k	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	l	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	m	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	n	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf	Trace
8	o	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	p	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	q	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	r	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	s	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	t	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	u	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	v	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	w	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	x	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	y	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	z	584	Total	C	N	O	S	0	0
			4566	2887	788	874	17		
8	A	582	Total	C	N	O	S	0	0
			4550	2876	785	872	17		

- Molecule 9 is a protein called gp162.

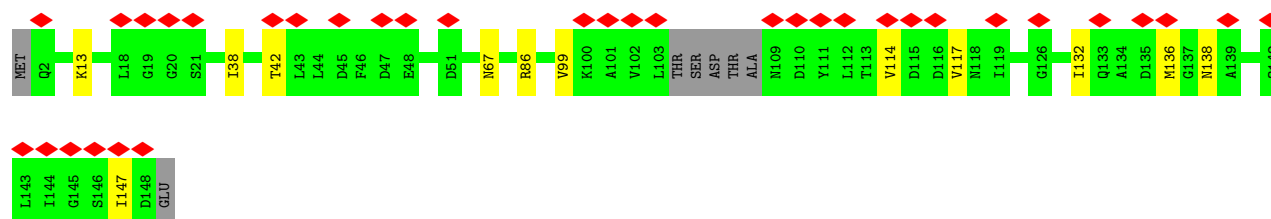
Mol	Chain	Residues	Atoms					AltConf	Trace
9	N	32	Total	C	N	O		0	0
			246	151	36	59			
9	O	116	Total	C	N	O	S	0	0
			885	538	149	195	3		
9	P	116	Total	C	N	O	S	0	0
			885	538	149	195	3		

- Molecule 10 is a protein called gp184.

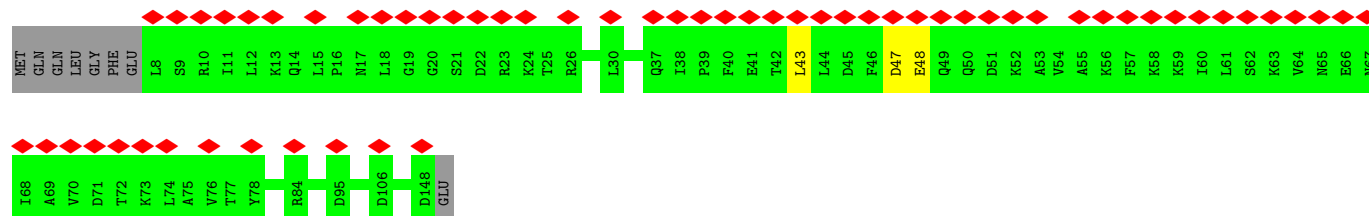
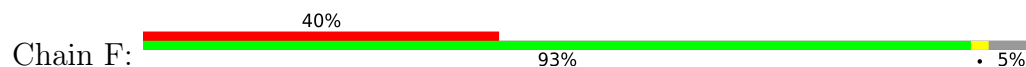
Mol	Chain	Residues	Atoms					AltConf	Trace
10	I	34	Total	C	N	O	S	0	0
			272	171	42	58	1		

- Molecule 11 is a protein called gp244.

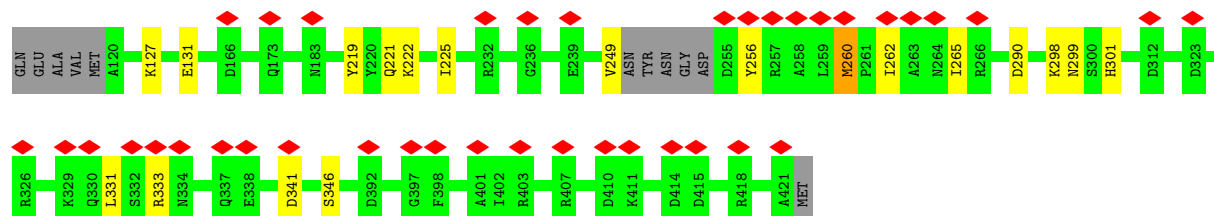
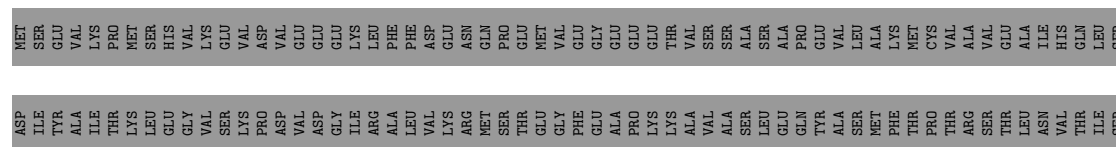
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	C	114	909	571	149	184	5	0	0



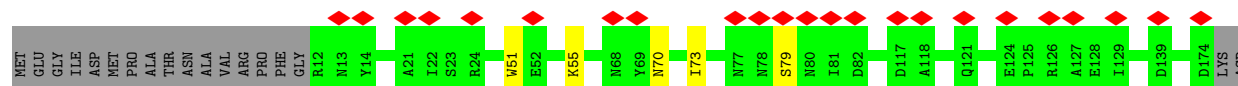
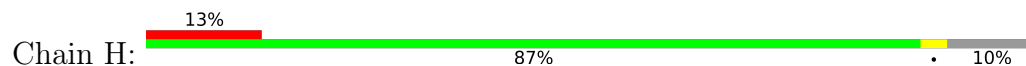
• Molecule 3: gp85



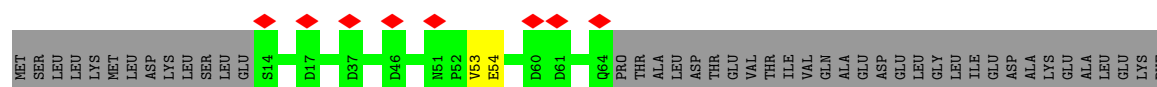
• Molecule 4: gp86



• Molecule 5: gp91



• Molecule 6: gp93



[illegible]

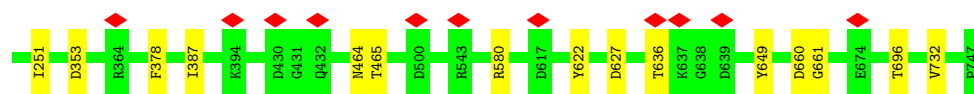
- Molecule 6: gp93

[illegible]

- Molecule 6: gp93

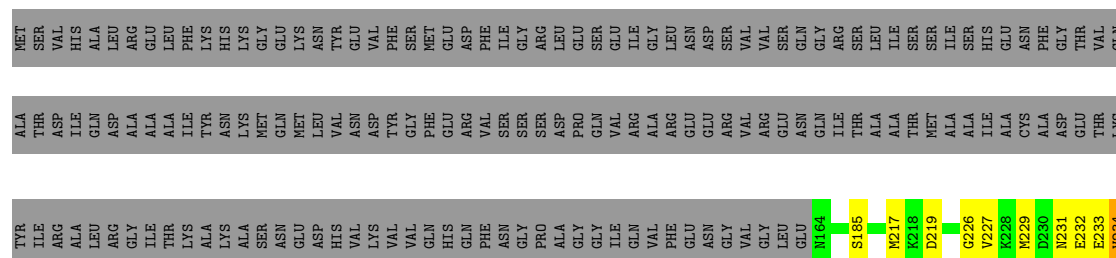


MET	SER	LEU	LEU	LYS	MET	LEU	ASP	LEU	LEU	GLU	\$14	E31	D46	E53	E54	D58	A59	V63	Q64	D69	D79	E80	L81	T84	GLU	ASP	ALA	LYS	GLU	ALA	LEU	GLU	LYS	PHE	GLN	GLY	GLY	LEU	LEU	GLN	ALA	GLY	GLU	ASP	GLY	ILE	SER	ARG	CYS											
ALA	ALA	ALA	PHE	MET	HIS	VAL	GLY	MET	GLU	SER	ILE	ASP	ARG	ILE	GLY	ILE	GLU	LYS	SER	GLY	LEU	THR	ALA	ALA	ASP	TYR	ASN	GLU	GLY	ASP	PRO	ARG	ASN	GLU	GLY	ASP	PRO	ARG	SER	ALA	ILE	LYS	SER	ILE	GLN	LYS	LYS	LEU	LEU	LYS	GLY	GLU	LYS	VAL	GLY	ASP	MET	LEU	SER	SER



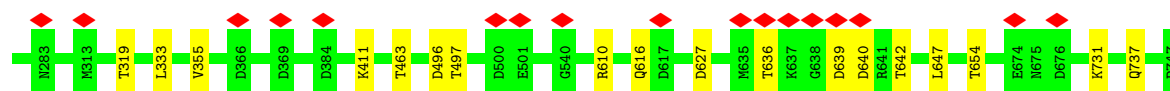
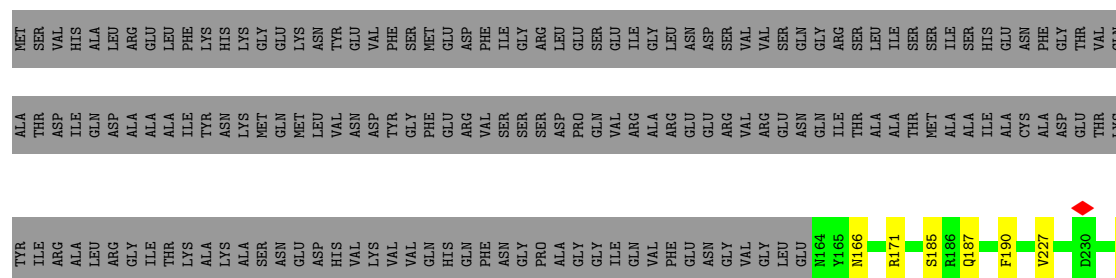
• Molecule 8: gp120

Chain c: 75% 22%



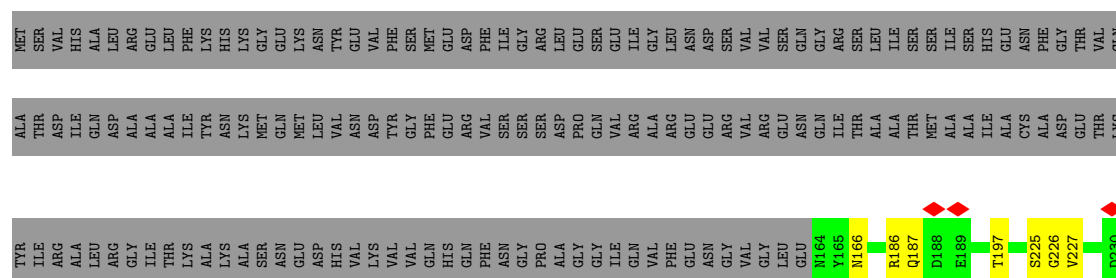
• Molecule 8: gp120

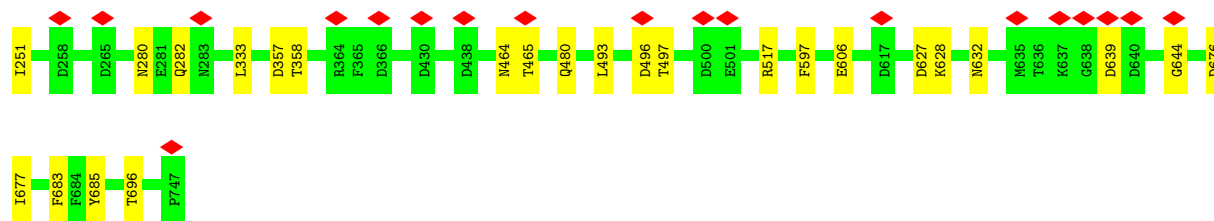
Chain d: 75% 22%



• Molecule 8: gp120

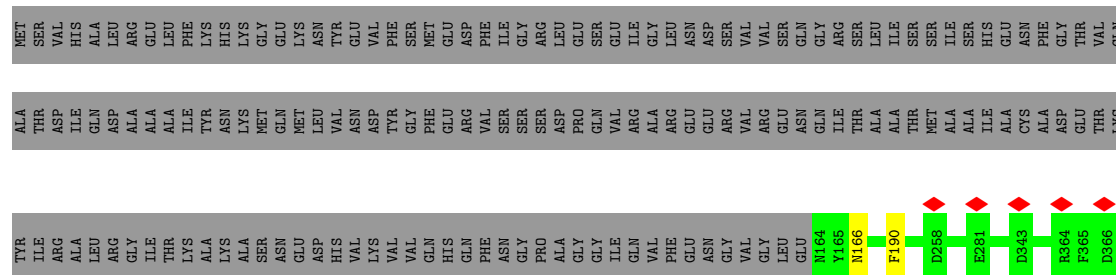
Chain e: 74% 22%





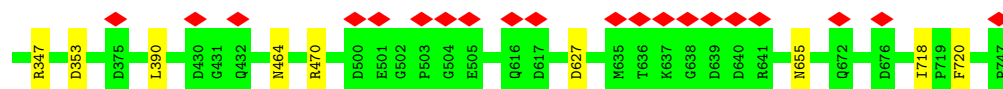
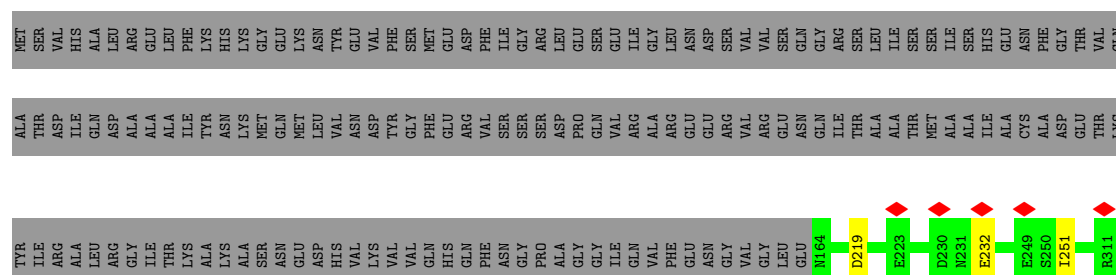
• Molecule 8: gp120

Chain f: 76% 22%



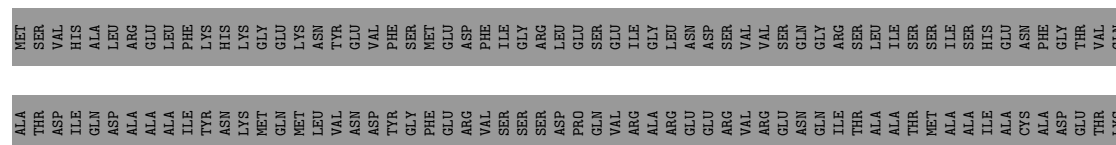
• Molecule 8: gp120

Chain g: 77% 22%

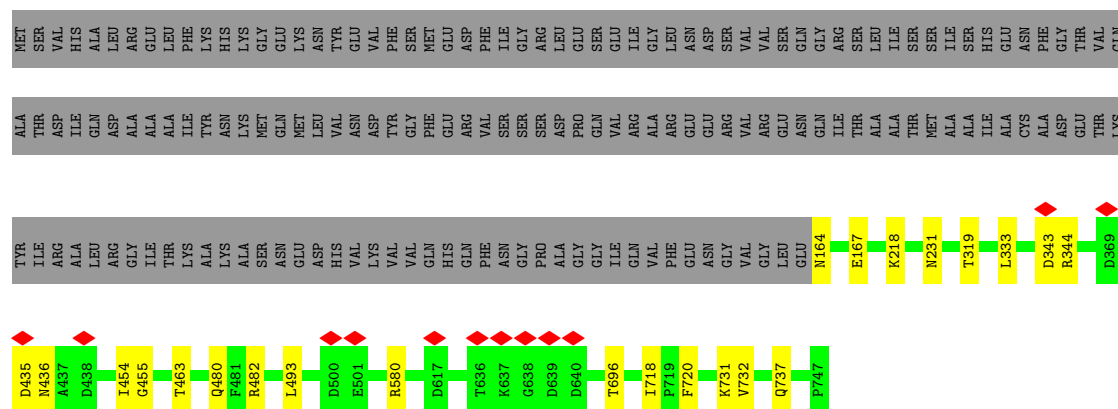


• Molecule 8: gp120

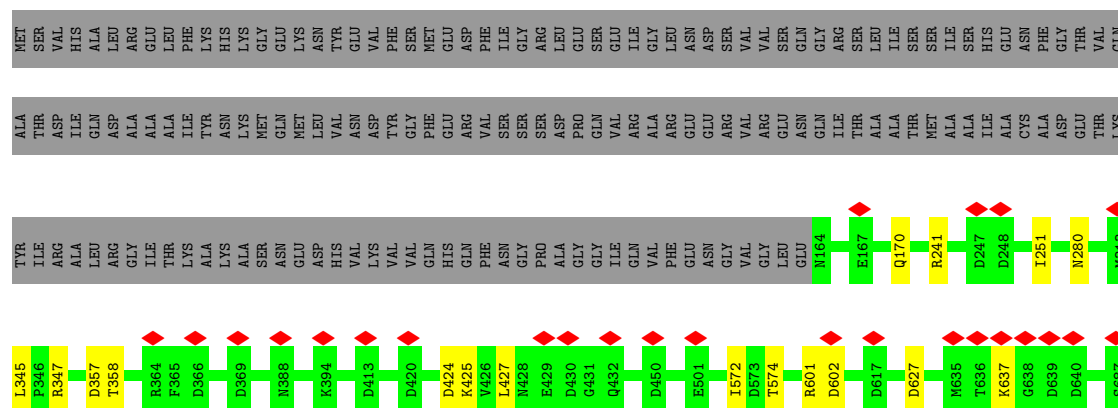
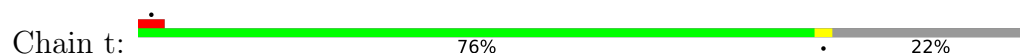
Chain h: 76% 22%



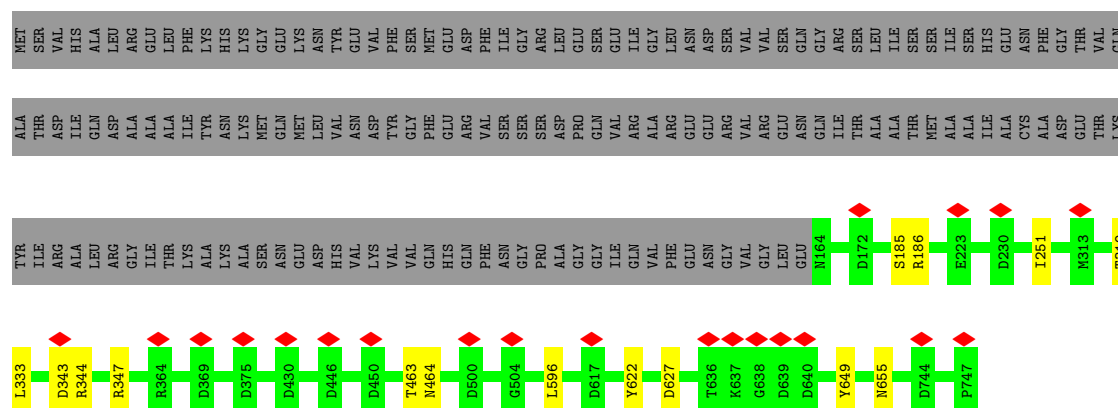
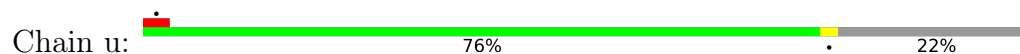




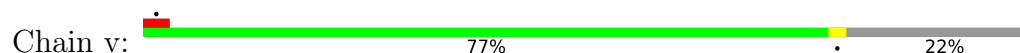
• Molecule 8: gp120

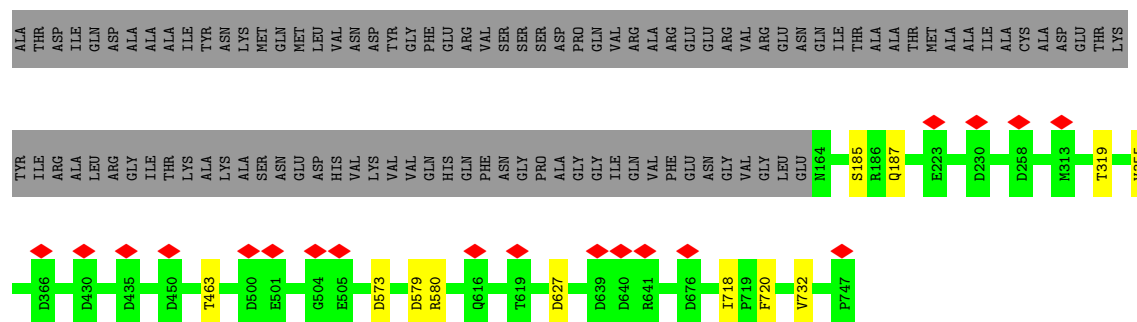


• Molecule 8: gp120

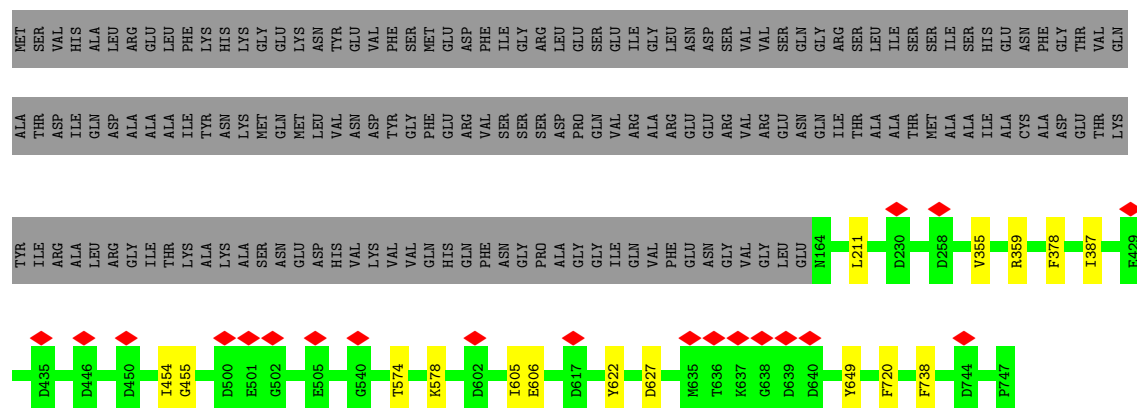
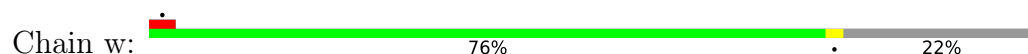


• Molecule 8: gp120

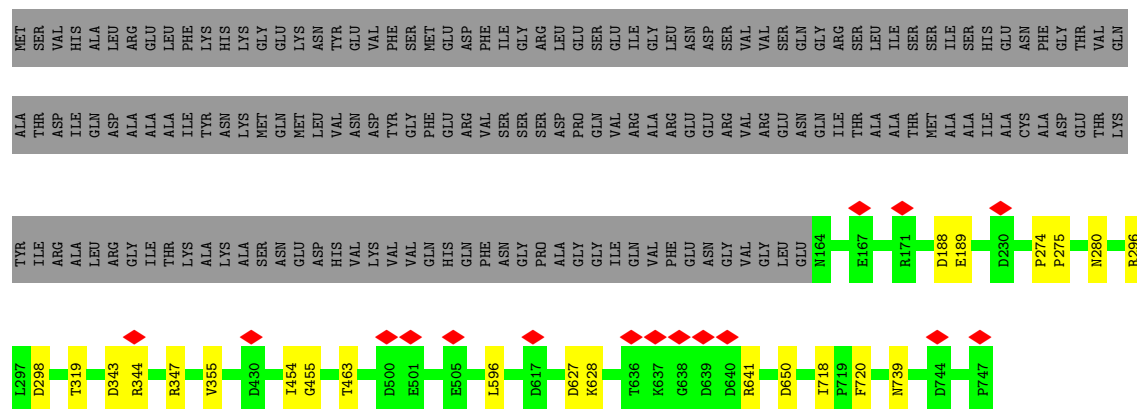




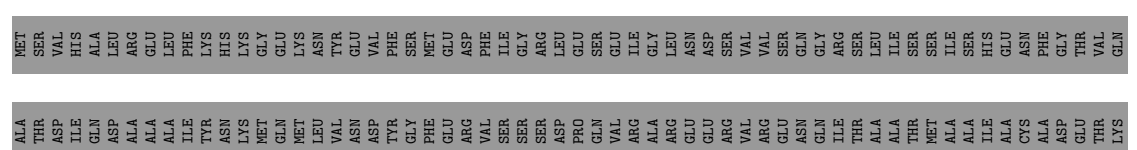
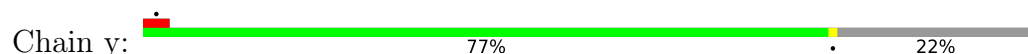
• Molecule 8: gp120

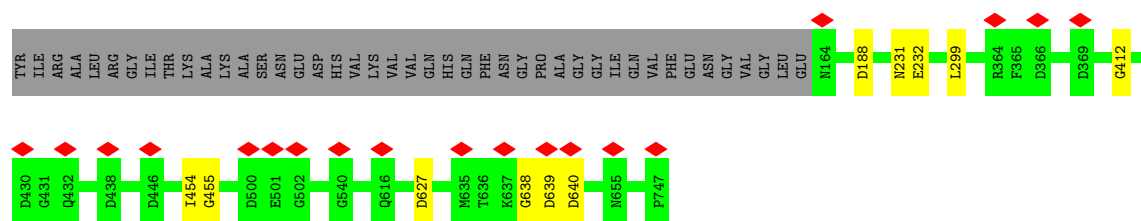


• Molecule 8: gp120



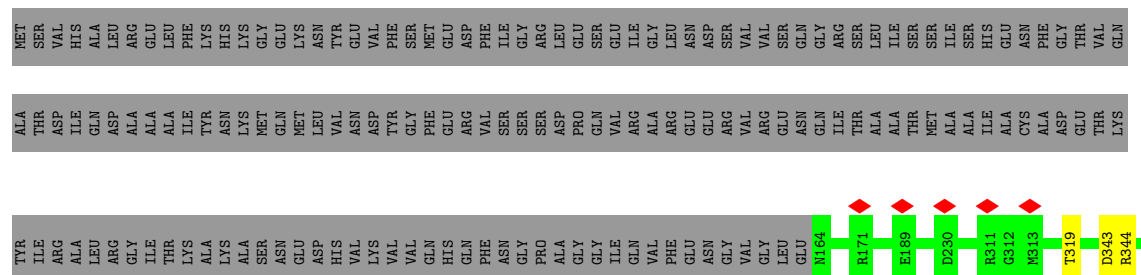
• Molecule 8: gp120





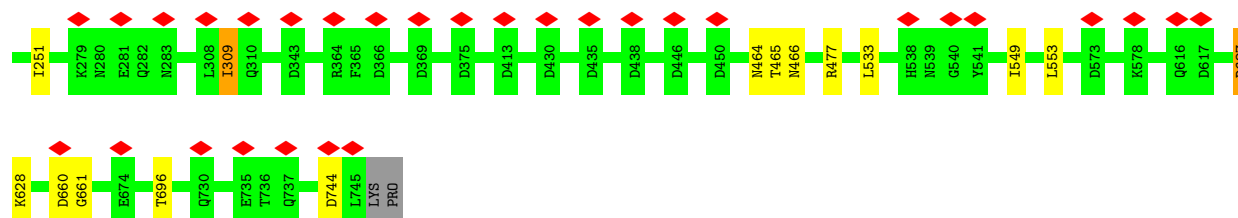
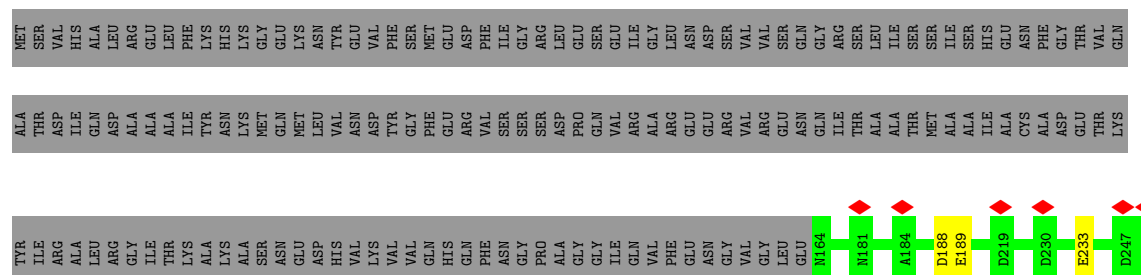
• Molecule 8: gp120

Chain z: 77% 22%



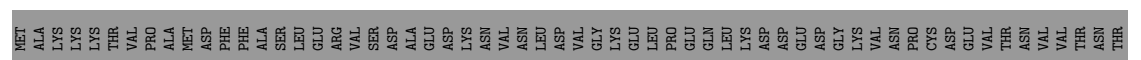
• Molecule 8: gp120

Chain A: 5% 76% 22%

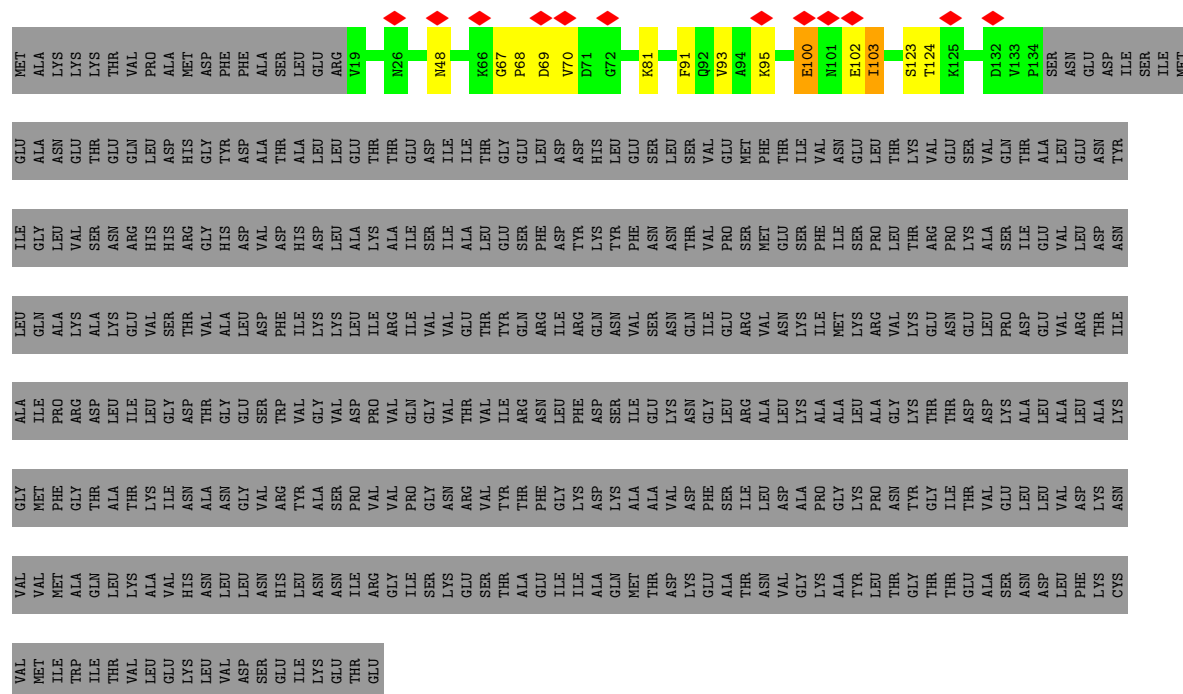


• Molecule 9: gp162

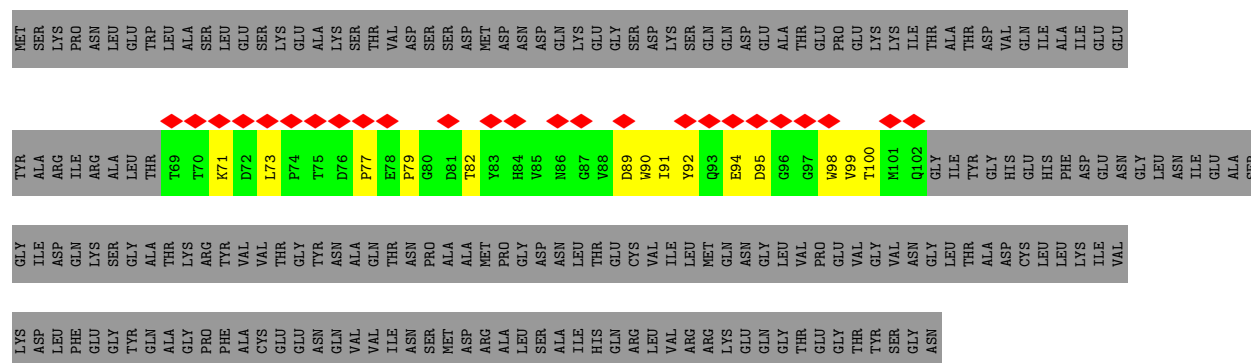
Chain N: 6% 94%







- Molecule 10: gp184



- Molecule 11: gp244



4 Experimental information

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 CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	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 ⓘ

5.1 Standard geometry ⓘ

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	D	0.49	0/2621	0.45	1/3561 (0.0%)
2	B	0.47	0/887	0.55	4/1207 (0.3%)
3	E	0.55	0/1112	0.63	2/1505 (0.1%)
3	F	0.51	0/1095	0.55	1/1486 (0.1%)
4	G	0.50	0/2467	0.44	0/3325
5	H	0.50	0/1367	0.51	1/1859 (0.1%)
6	K	0.71	0/381	0.59	0/522
6	L	0.76	0/530	0.82	0/728
6	M	0.75	0/530	0.77	2/728 (0.3%)
7	J	0.53	0/1445	0.54	1/1964 (0.1%)
8	A	0.55	0/4631	0.54	5/6288 (0.1%)
8	a	0.55	2/4648 (0.0%)	0.54	6/6311 (0.1%)
8	b	0.52	0/4648	0.43	1/6311 (0.0%)
8	c	0.53	1/4648 (0.0%)	0.49	1/6311 (0.0%)
8	d	0.51	0/4648	0.44	1/6311 (0.0%)
8	e	0.51	0/4648	0.43	1/6311 (0.0%)
8	f	0.53	0/4648	0.45	2/6311 (0.0%)
8	g	0.53	0/4648	0.48	0/6311
8	h	0.53	0/4648	0.50	0/6311
8	i	0.53	0/4648	0.49	0/6311
8	j	0.54	0/4648	0.52	0/6311
8	k	0.52	0/4648	0.47	0/6311
8	l	0.52	0/4648	0.47	0/6311
8	m	0.53	0/4648	0.50	0/6311
8	n	0.53	0/4648	0.49	1/6311 (0.0%)
8	o	0.54	0/4648	0.50	3/6311 (0.0%)
8	p	0.54	0/4648	0.54	0/6311
8	q	0.53	0/4648	0.47	0/6311
8	r	0.54	0/4648	0.48	0/6311
8	s	0.53	0/4648	0.48	0/6311
8	t	0.53	0/4648	0.53	1/6311 (0.0%)
8	u	0.52	0/4648	0.47	0/6311
8	v	0.53	0/4648	0.47	0/6311
8	w	0.53	0/4648	0.48	0/6311

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	x	0.53	0/4648	0.47	0/6311
8	y	0.54	0/4648	0.51	1/6311 (0.0%)
8	z	0.53	0/4648	0.49	0/6311
9	N	0.69	0/248	0.52	0/338
9	O	0.66	0/893	0.79	2/1210 (0.2%)
9	P	0.81	0/893	1.03	8/1210 (0.7%)
10	I	0.25	0/281	0.46	0/387
11	C	0.55	0/924	0.53	2/1249 (0.2%)
All	All	0.53	3/141153 (0.0%)	0.50	47/191653 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	c	234	VAL	C-O	-6.74	1.17	1.24
8	a	641	ARG	C-O	-5.50	1.16	1.24
8	a	640	ASP	CA-C	-5.42	1.46	1.53

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	465	THR	N-CA-C	-10.07	100.38	111.36
8	A	627	ASP	N-CA-C	9.76	123.85	112.72
8	a	642	THR	N-CA-C	9.33	123.79	108.96
8	a	645	ALA	N-CA-C	9.32	123.92	112.54
7	J	107	ASN	N-CA-C	8.45	122.83	109.39
8	y	640	ASP	N-CA-C	-8.22	103.24	113.18
6	M	63	VAL	N-CA-C	7.97	119.74	112.17
8	f	649	TYR	N-CA-C	7.77	120.72	109.14
9	P	81	LYS	N-CA-C	-7.62	97.83	109.95
8	d	636	THR	N-CA-C	7.45	121.95	111.30
9	O	46	LYS	N-CA-C	7.44	121.29	110.42
9	P	70	VAL	N-CA-C	7.33	120.22	111.05
8	a	641	ARG	N-CA-C	-7.29	103.95	112.92
9	P	69	ASP	N-CA-C	-7.24	102.71	112.26
8	t	637	LYS	N-CA-C	7.07	122.33	112.72
9	O	100	GLU	N-CA-C	-6.96	105.32	113.88
8	e	227	VAL	N-CA-C	-6.68	106.28	112.96
6	M	64	GLN	N-CA-C	6.62	124.44	109.81
8	a	506	VAL	N-CA-C	-6.56	104.37	110.53
9	P	48	ASN	CA-C-N	-6.47	112.96	119.56
9	P	48	ASN	C-N-CA	-6.47	112.96	119.56
2	B	193	PRO	CA-C-N	-6.42	113.33	120.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	193	PRO	C-N-CA	-6.42	113.33	120.45
2	B	264	ASP	CA-C-N	-6.32	113.44	120.45
2	B	264	ASP	C-N-CA	-6.32	113.44	120.45
11	C	15	THR	CA-C-N	-5.98	114.11	120.03
11	C	15	THR	C-N-CA	-5.98	114.11	120.03
8	o	643	LEU	N-CA-C	5.94	120.71	112.45
3	E	99	VAL	N-CA-C	-5.88	105.00	110.53
8	c	185	SER	N-CA-C	5.83	118.36	109.62
8	a	504	GLY	CA-C-N	5.81	131.30	121.14
8	a	504	GLY	C-N-CA	5.81	131.30	121.14
3	F	43	LEU	N-CA-C	5.64	118.97	111.75
9	P	67	GLY	N-CA-C	-5.63	100.85	112.34
8	f	635	MET	N-CA-C	5.60	118.30	109.39
8	A	466	ASN	N-CA-C	-5.59	100.01	108.67
5	H	79	SER	N-CA-C	-5.58	106.36	114.12
9	P	68	PRO	CA-C-O	-5.57	115.21	122.12
8	A	309	ILE	N-CA-C	5.53	120.83	109.34
8	b	636	THR	N-CA-C	5.43	117.40	110.61
9	P	100	GLU	N-CA-C	-5.40	105.56	111.82
8	A	553	LEU	N-CA-C	5.25	119.17	112.87
8	o	636	THR	N-CA-C	-5.21	102.60	110.06
1	D	298	SER	N-CA-C	5.17	117.16	109.25
8	n	638	GLY	N-CA-C	5.14	116.40	111.67
8	o	532	GLN	N-CA-C	-5.11	105.35	112.45
3	E	42	THR	N-CA-C	5.09	117.56	111.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2563	0	2584	9	0
2	B	862	0	869	0	0
3	E	1102	0	1141	8	0
3	F	1085	0	1125	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	2425	0	2456	21	0
5	H	1333	0	1295	6	0
6	K	380	0	345	1	0
6	L	528	0	493	0	0
6	M	528	0	493	2	0
7	J	1416	0	1402	3	0
8	A	4550	0	4554	8	0
8	a	4566	0	4574	23	0
8	b	4566	0	4574	14	0
8	c	4566	0	4574	17	0
8	d	4566	0	4574	17	0
8	e	4566	0	4574	23	0
8	f	4566	0	4574	11	0
8	g	4566	0	4574	10	0
8	h	4566	0	4574	12	0
8	i	4566	0	4574	5	0
8	j	4566	0	4574	14	0
8	k	4566	0	4574	11	0
8	l	4566	0	4574	13	0
8	m	4566	0	4574	13	0
8	n	4566	0	4574	10	0
8	o	4566	0	4574	6	0
8	p	4566	0	4574	14	0
8	q	4566	0	4574	11	0
8	r	4566	0	4574	16	0
8	s	4566	0	4574	15	0
8	t	4566	0	4574	15	0
8	u	4566	0	4574	11	0
8	v	4566	0	4574	8	0
8	w	4566	0	4574	12	0
8	x	4566	0	4574	16	0
8	y	4566	0	4574	6	0
8	z	4566	0	4574	6	0
9	N	246	0	223	1	0
9	O	885	0	868	4	0
9	P	885	0	868	8	0
10	I	272	0	237	23	0
11	C	909	0	891	3	0
All	All	138685	0	138768	361	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 1.

All (361) 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)
8:e:639:ASP:HB2	10:I:89:ASP:OD2	1.47	1.11
3:E:138:ASN:OD1	7:J:100:LEU:HD11	1.54	1.07
4:G:225:ILE:CD1	10:I:71:LYS:HE3	1.84	1.05
4:G:225:ILE:HD12	10:I:71:LYS:HE3	1.43	0.99
5:H:70:ASN:O	5:H:73:ILE:HG22	1.69	0.92
8:a:634:LEU:HD13	8:a:651:ILE:HD12	1.59	0.85
4:G:222:LYS:HE2	10:I:71:LYS:O	1.78	0.84
8:a:632:ASN:ND2	8:f:597:PHE:CD1	2.50	0.80
8:e:639:ASP:CB	10:I:89:ASP:OD2	2.31	0.77
8:c:229:MET:HE3	8:c:231:ASN:HB2	1.66	0.75
9:P:91:PHE:HB3	9:P:93:VAL:HG23	1.71	0.72
8:e:683:PHE:CE2	8:e:685:TYR:HB2	2.27	0.69
4:G:301:HIS:CE1	10:I:100:THR:HG21	2.29	0.68
8:k:696:THR:HG23	8:k:701:GLN:O	1.95	0.67
8:k:428:ASN:CG	8:k:429:GLU:H	2.03	0.67
4:G:221:GLN:OE1	10:I:71:LYS:HD3	1.95	0.65
8:c:232:GLU:O	8:c:234:VAL:HG23	1.96	0.65
4:G:290:ASP:HA	10:I:95:ASP:O	1.96	0.65
8:e:597:PHE:HZ	8:e:644:GLY:HA3	1.61	0.65
3:E:138:ASN:OD1	7:J:100:LEU:CD1	2.40	0.65
8:t:241:ARG:HG2	8:u:655:ASN:ND2	2.12	0.64
8:m:166:ASN:ND2	8:q:463:THR:OG1	2.32	0.62
8:k:496:ASP:OD1	8:k:497:THR:N	2.33	0.61
5:H:70:ASN:O	5:H:73:ILE:CG2	2.46	0.61
3:E:132:ILE:O	3:E:136:MET:HG2	2.02	0.60
8:n:509:ALA:HA	8:n:512:VAL:HG12	1.84	0.60
8:d:411:LYS:NZ	8:h:233:GLU:OE1	2.35	0.60
11:C:50:LYS:NZ	11:C:52:HIS:NE2	2.50	0.60
8:c:610:ARG:NH1	8:c:616:GLN:O	2.35	0.60
8:d:463:THR:OG1	8:f:166:ASN:ND2	2.34	0.60
9:P:91:PHE:CB	9:P:93:VAL:HG23	2.31	0.60
3:E:13:LYS:NZ	8:b:192:GLU:OE2	2.29	0.59
8:i:476:THR:HG1	8:s:164:ASN:N	2.00	0.59
8:j:231:ASN:O	8:j:232:GLU:C	2.44	0.59
4:G:301:HIS:CE1	10:I:100:THR:CG2	2.86	0.59
4:G:219:TYR:OH	10:I:77:PRO:HD3	2.02	0.59
8:m:496:ASP:OD1	8:m:497:THR:N	2.36	0.59
4:G:301:HIS:HE1	10:I:100:THR:CG2	2.16	0.59
8:j:496:ASP:OD1	8:j:497:THR:N	2.36	0.58
8:e:683:PHE:HE2	8:e:685:TYR:HB2	1.67	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:t:241:ARG:HH21	8:t:601:ARG:HG2	1.68	0.58
8:w:606:GLU:OE1	8:x:628:LYS:NZ	2.36	0.58
4:G:127:LYS:NZ	4:G:131:GLU:OE2	2.36	0.58
8:e:496:ASP:OD1	8:e:497:THR:N	2.37	0.58
5:H:70:ASN:HB3	5:H:73:ILE:HG22	1.85	0.57
8:n:496:ASP:OD1	8:n:497:THR:N	2.37	0.57
8:d:496:ASP:OD1	8:d:497:THR:N	2.38	0.57
5:H:70:ASN:HB3	5:H:73:ILE:CG2	2.34	0.57
10:I:82:THR:HG22	10:I:91:ILE:HG12	1.87	0.57
8:k:696:THR:O	8:k:696:THR:HG22	2.06	0.56
8:b:465:THR:OG1	8:d:166:ASN:ND2	2.39	0.56
4:G:260:MET:HE1	4:G:346:SER:HB2	1.88	0.56
8:t:241:ARG:NH2	8:t:602:ASP:HA	2.20	0.56
4:G:222:LYS:HE2	10:I:71:LYS:HB3	1.88	0.56
8:d:610:ARG:NH1	8:d:616:GLN:O	2.40	0.55
8:s:435:ASP:OD1	8:s:436:ASN:N	2.39	0.55
8:a:634:LEU:O	8:a:636:THR:HG23	2.07	0.54
8:s:482:ARG:NH2	8:t:170:GLN:O	2.41	0.54
8:a:166:ASN:ND2	8:e:465:THR:OG1	2.41	0.54
8:a:639:ASP:O	8:a:641:ARG:NH1	2.41	0.53
8:v:319:THR:OG1	8:v:463:THR:OG1	2.26	0.53
8:e:676:ASP:OD1	8:e:677:ILE:N	2.41	0.53
4:G:341:ASP:OD1	8:c:508:LYS:NZ	2.42	0.53
7:J:59:ASP:OD1	7:J:61:LYS:NZ	2.41	0.53
8:a:435:ASP:OD1	8:a:436:ASN:N	2.41	0.53
8:m:319:THR:OG1	8:m:463:THR:OG1	2.26	0.52
9:O:19:VAL:O	9:O:19:VAL:HG22	2.09	0.52
10:I:79:PRO:HB3	10:I:94:GLU:HG2	1.92	0.52
8:x:718:ILE:HG22	8:x:720:PHE:H	1.74	0.52
8:t:357:ASP:OD1	8:t:358:THR:N	2.43	0.52
8:c:217:MET:HB2	8:c:231:ASN:CG	2.35	0.52
8:g:718:ILE:HG22	8:g:720:PHE:H	1.75	0.52
4:G:222:LYS:HE2	10:I:71:LYS:C	2.35	0.52
8:a:218:LYS:O	8:a:231:ASN:ND2	2.41	0.52
8:x:188:ASP:OD1	8:x:189:GLU:N	2.43	0.52
8:A:627:ASP:O	8:A:628:LYS:HB2	2.09	0.52
8:e:696:THR:OG1	8:s:696:THR:OG1	2.28	0.51
8:k:185:SER:O	8:k:186:ARG:C	2.53	0.51
8:a:639:ASP:O	8:a:640:ASP:C	2.53	0.51
8:r:319:THR:OG1	8:r:463:THR:OG1	2.26	0.51
8:r:718:ILE:HG22	8:r:720:PHE:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:I:77:PRO:HG3	10:I:98:TRP:CZ2	2.46	0.51
8:l:357:ASP:OD1	8:l:358:THR:N	2.44	0.51
8:n:509:ALA:O	8:n:512:VAL:HG12	2.11	0.51
1:D:50:ALA:N	1:D:54:GLU:O	2.45	0.50
8:o:319:THR:OG1	8:o:463:THR:OG1	2.29	0.50
8:y:638:GLY:O	8:y:639:ASP:HB2	2.11	0.50
8:n:424:ASP:OD2	8:n:425:LYS:NZ	2.40	0.50
8:d:355:VAL:O	8:g:347:ARG:NH1	2.44	0.50
8:m:718:ILE:HG22	8:m:720:PHE:H	1.76	0.50
8:n:319:THR:OG1	8:n:463:THR:OG1	2.29	0.50
8:c:347:ARG:NH1	8:x:355:VAL:O	2.44	0.50
8:e:357:ASP:OD1	8:e:358:THR:N	2.44	0.50
6:M:58:ASP:OD1	6:M:59:ALA:N	2.45	0.50
8:g:232:GLU:OE1	8:g:232:GLU:N	2.44	0.50
8:a:616:GLN:NE2	8:b:183:ALA:O	2.45	0.49
1:D:156:LYS:NZ	9:N:152:HIS:O	2.38	0.49
1:D:282:ASP:OD1	1:D:283:ARG:N	2.45	0.49
8:x:319:THR:OG1	8:x:463:THR:OG1	2.31	0.49
8:r:576:LYS:NZ	8:r:579:ASP:OD2	2.37	0.49
8:t:241:ARG:CG	8:u:655:ASN:ND2	2.75	0.49
8:e:597:PHE:CZ	8:e:644:GLY:HA3	2.45	0.49
8:p:231:ASN:O	8:p:232:GLU:C	2.54	0.49
8:g:251:ILE:CG2	8:g:464:ASN:HD21	2.25	0.49
8:m:347:ARG:NH1	8:v:355:VAL:O	2.47	0.48
8:v:185:SER:OG	8:v:187:GLN:O	2.30	0.48
3:F:47:ASP:CG	3:F:48:GLU:H	2.21	0.48
8:a:188:ASP:OD1	8:a:189:GLU:N	2.47	0.48
8:q:273:VAL:HG23	8:q:273:VAL:O	2.13	0.48
8:c:463:THR:OG1	8:e:166:ASN:ND2	2.46	0.48
8:l:241:ARG:NE	8:l:601:ARG:O	2.47	0.48
8:q:241:ARG:NH1	8:q:602:ASP:O	2.46	0.48
8:c:231:ASN:O	8:c:233:GLU:N	2.42	0.48
9:P:102:GLU:O	9:P:103:ILE:C	2.56	0.48
8:d:639:ASP:OD1	8:d:640:ASP:N	2.47	0.48
8:a:225:SER:OG	8:a:226:GLY:N	2.47	0.47
8:r:231:ASN:O	8:r:232:GLU:C	2.56	0.47
6:M:53:VAL:O	6:M:54:GLU:C	2.56	0.47
8:b:660:ASP:OD1	8:b:661:GLY:N	2.48	0.47
8:g:655:ASN:O	8:l:241:ARG:NH1	2.47	0.47
8:u:347:ARG:NH1	8:z:355:VAL:O	2.47	0.47
8:d:731:LYS:O	8:d:737:GLN:NE2	2.48	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:343:ASP:OD1	8:j:344:ARG:N	2.47	0.47
5:H:70:ASN:C	5:H:73:ILE:HG22	2.38	0.47
8:a:636:THR:O	8:a:637:LYS:C	2.58	0.47
8:b:580:ARG:NH1	8:b:732:VAL:O	2.48	0.47
8:s:718:ILE:HG22	8:s:720:PHE:H	1.79	0.47
9:O:19:VAL:O	9:O:19:VAL:HG13	2.13	0.47
8:h:488:HIS:HB2	8:h:710:PRO:HB2	1.96	0.47
8:p:579:ASP:OD1	8:q:578:LYS:NZ	2.46	0.47
8:a:627:ASP:OD1	8:a:627:ASP:C	2.57	0.47
8:a:632:ASN:ND2	8:f:597:PHE:CE1	2.83	0.47
8:b:627:ASP:C	8:b:627:ASP:OD1	2.57	0.47
8:h:319:THR:OG1	8:h:463:THR:OG1	2.31	0.47
8:p:641:ARG:HD2	8:p:649:TYR:CZ	2.50	0.47
3:E:147:ILE:HD12	3:E:147:ILE:C	2.40	0.47
8:a:633:TYR:O	8:a:634:LEU:C	2.57	0.46
8:a:596:LEU:C	8:a:596:LEU:HD23	2.40	0.46
8:e:480:GLN:NE2	8:g:353:ASP:O	2.48	0.46
8:i:355:VAL:O	8:r:347:ARG:NH1	2.47	0.46
4:G:249:VAL:HG11	4:G:331:LEU:CD2	2.46	0.46
8:A:233:GLU:OE2	8:A:477:ARG:NH1	2.48	0.46
8:A:188:ASP:OD1	8:A:189:GLU:N	2.45	0.46
8:e:187:GLN:NE2	8:e:197:THR:OG1	2.47	0.46
8:t:358:THR:HG23	9:P:93:VAL:HG22	1.98	0.46
8:y:299:LEU:N	8:y:412:GLY:O	2.47	0.46
8:e:628:LYS:O	8:e:632:ASN:ND2	2.48	0.46
8:s:580:ARG:NH1	8:s:732:VAL:O	2.49	0.46
8:b:622:TYR:O	8:b:649:TYR:HA	2.15	0.46
8:k:228:LYS:NZ	8:k:230:ASP:OD1	2.49	0.46
8:l:628:LYS:O	8:l:632:ASN:ND2	2.47	0.46
8:s:333:LEU:C	8:s:333:LEU:HD23	2.41	0.46
8:e:627:ASP:OD1	8:e:627:ASP:C	2.58	0.46
8:f:677:ILE:HG22	8:f:677:ILE:O	2.15	0.46
8:f:692:ASP:OD1	8:f:693:LEU:N	2.49	0.46
8:u:319:THR:OG1	8:u:463:THR:OG1	2.34	0.46
8:i:319:THR:OG1	8:i:463:THR:OG1	2.32	0.45
8:a:580:ARG:NH1	8:a:732:VAL:O	2.49	0.45
8:c:596:LEU:C	8:c:596:LEU:HD23	2.41	0.45
8:w:211:LEU:HD23	8:w:211:LEU:C	2.42	0.45
8:m:596:LEU:C	8:m:596:LEU:HD23	2.42	0.45
8:p:637:LYS:CE	8:p:640:ASP:HB2	2.46	0.45
8:p:637:LYS:HE3	8:p:640:ASP:HB2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:p:639:ASP:O	8:p:641:ARG:HG2	2.16	0.45
8:u:627:ASP:C	8:u:627:ASP:OD1	2.59	0.45
8:e:333:LEU:HD23	8:e:333:LEU:C	2.42	0.45
8:m:607:ALA:O	8:m:611:VAL:HG22	2.17	0.45
8:u:596:LEU:HD23	8:u:596:LEU:C	2.41	0.45
8:v:718:ILE:HG22	8:v:720:PHE:H	1.80	0.45
8:d:319:THR:OG1	8:d:463:THR:OG1	2.32	0.45
8:e:251:ILE:CG2	8:e:464:ASN:HD21	2.30	0.45
8:j:188:ASP:OD1	8:j:189:GLU:N	2.48	0.45
1:D:254:PHE:CD1	1:D:254:PHE:C	2.95	0.45
3:E:67:ASN:C	8:b:185:SER:OG	2.59	0.45
8:t:572:ILE:HG22	8:t:574:THR:H	1.81	0.45
8:a:237:VAL:HG11	8:a:556:VAL:O	2.17	0.45
8:y:231:ASN:O	8:y:232:GLU:C	2.59	0.45
8:y:454:ILE:HG13	8:y:455:GLY:N	2.32	0.45
8:r:241:ARG:NE	8:r:601:ARG:O	2.50	0.45
8:r:426:VAL:O	8:r:426:VAL:HG23	2.17	0.45
8:m:627:ASP:OD1	8:m:627:ASP:C	2.59	0.44
8:v:573:ASP:OD1	8:w:738:PHE:N	2.50	0.44
8:z:343:ASP:OD1	8:z:344:ARG:N	2.50	0.44
8:p:580:ARG:NH1	8:p:732:VAL:O	2.50	0.44
4:G:298:LYS:O	10:I:100:THR:OG1	2.29	0.44
8:l:622:TYR:O	8:l:649:TYR:HA	2.17	0.44
8:r:536:VAL:HG13	8:r:537:VAL:N	2.32	0.44
8:u:251:ILE:CG2	8:u:464:ASN:HD21	2.30	0.44
4:G:256:TYR:CG	4:G:256:TYR:O	2.70	0.44
8:l:219:ASP:OD1	8:l:470:ARG:NH2	2.51	0.44
8:l:525:ARG:NH1	8:l:550:GLU:OE2	2.51	0.44
8:d:333:LEU:C	8:d:333:LEU:HD23	2.43	0.44
8:q:343:ASP:OD1	8:q:344:ARG:N	2.50	0.44
8:c:217:MET:HB2	8:c:231:ASN:OD1	2.17	0.44
8:u:185:SER:O	8:u:186:ARG:C	2.61	0.44
8:q:627:ASP:OD1	8:q:627:ASP:C	2.60	0.44
8:A:660:ASP:OD1	8:A:661:GLY:N	2.50	0.44
8:c:354:LEU:O	8:s:480:GLN:NE2	2.51	0.44
8:w:574:THR:H	8:x:739:ASN:ND2	2.15	0.44
8:A:533:LEU:HD23	8:A:549:ILE:CD1	2.48	0.44
10:I:77:PRO:HG2	10:I:92:TYR:CG	2.53	0.44
8:t:251:ILE:HG13	8:t:251:ILE:O	2.16	0.43
8:x:627:ASP:C	8:x:627:ASP:OD1	2.61	0.43
4:G:301:HIS:HE1	10:I:100:THR:HG23	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:f:627:ASP:OD1	8:f:627:ASP:C	2.58	0.43
8:h:596:LEU:C	8:h:596:LEU:HD23	2.43	0.43
8:s:319:THR:OG1	8:s:463:THR:OG1	2.36	0.43
8:u:333:LEU:C	8:u:333:LEU:HD23	2.43	0.43
8:g:627:ASP:C	8:g:627:ASP:OD1	2.59	0.43
8:j:280:ASN:OD1	8:j:280:ASN:C	2.61	0.43
8:n:509:ALA:CA	8:n:512:VAL:HG12	2.48	0.43
8:s:218:LYS:O	8:s:231:ASN:ND2	2.51	0.43
8:v:580:ARG:NH1	8:v:732:VAL:O	2.51	0.43
3:F:47:ASP:CG	3:F:48:GLU:N	2.77	0.43
8:a:637:LYS:O	8:a:638:GLY:C	2.61	0.43
8:c:248:ASP:OD1	8:c:249:GLU:N	2.51	0.43
8:h:627:ASP:OD1	8:h:627:ASP:C	2.59	0.43
8:n:627:ASP:C	8:n:627:ASP:OD1	2.62	0.43
8:p:241:ARG:HH12	8:q:657:GLN:HA	1.83	0.43
8:s:493:LEU:HD23	8:s:493:LEU:C	2.44	0.43
8:x:596:LEU:C	8:x:596:LEU:HD23	2.43	0.43
8:A:744:ASP:OD2	11:C:115:LYS:NZ	2.48	0.43
4:G:262:ILE:O	4:G:265:ILE:HB	2.18	0.43
8:e:280:ASN:OD1	8:e:282:GLN:N	2.51	0.43
8:h:347:ARG:NH1	8:w:355:VAL:O	2.52	0.43
8:k:428:ASN:CG	8:k:429:GLU:N	2.71	0.43
8:w:627:ASP:OD1	8:w:627:ASP:C	2.60	0.43
4:G:301:HIS:HE2	10:I:90:TRP:HZ2	1.61	0.43
8:q:333:LEU:C	8:q:333:LEU:HD23	2.43	0.43
8:r:627:ASP:OD1	8:r:627:ASP:C	2.62	0.43
8:k:357:ASP:OD1	8:k:358:THR:N	2.50	0.43
8:d:627:ASP:C	8:d:627:ASP:OD1	2.59	0.43
8:i:218:LYS:O	8:i:231:ASN:ND2	2.51	0.43
8:l:333:LEU:C	8:l:333:LEU:HD23	2.43	0.43
8:a:663:LEU:C	8:a:663:LEU:HD23	2.44	0.43
8:l:718:ILE:HG22	8:l:720:PHE:H	1.83	0.42
8:s:343:ASP:OD1	8:s:344:ARG:N	2.52	0.42
8:z:319:THR:OG1	8:z:463:THR:OG1	2.37	0.42
4:G:299:ASN:HD21	10:I:99:VAL:HA	1.85	0.42
8:g:251:ILE:HG22	8:g:464:ASN:HD21	1.84	0.42
8:o:326:LEU:C	8:o:326:LEU:HD23	2.44	0.42
8:q:454:ILE:HG13	8:q:455:GLY:N	2.34	0.42
8:r:280:ASN:HD21	8:r:308:LEU:HD11	1.84	0.42
8:w:454:ILE:HG13	8:w:455:GLY:N	2.34	0.42
1:D:150:SER:OG	1:D:168:TRP:NE1	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:b:185:SER:O	8:b:186:ARG:C	2.62	0.42
8:f:190:PHE:CG	8:f:654:THR:HB	2.53	0.42
8:f:580:ARG:NH1	8:f:732:VAL:O	2.47	0.42
8:j:622:TYR:O	8:j:649:TYR:HA	2.20	0.42
8:o:228:LYS:NZ	8:o:230:ASP:OD1	2.51	0.42
8:q:185:SER:O	8:q:186:ARG:C	2.62	0.42
9:O:89:LYS:C	9:O:91:PHE:H	2.28	0.42
8:b:251:ILE:CG2	8:b:464:ASN:HD21	2.33	0.42
8:r:596:LEU:C	8:r:596:LEU:HD23	2.43	0.42
8:j:319:THR:OG1	8:j:463:THR:OG1	2.38	0.42
8:j:343:ASP:OD1	8:k:532:GLN:NE2	2.50	0.42
8:m:607:ALA:O	8:m:611:VAL:HG13	2.19	0.42
8:o:627:ASP:OD1	8:o:627:ASP:C	2.61	0.42
8:p:241:ARG:NE	8:p:601:ARG:O	2.53	0.42
8:x:454:ILE:HG13	8:x:455:GLY:N	2.33	0.42
8:y:627:ASP:OD1	8:y:627:ASP:C	2.61	0.42
9:P:95:LYS:HG3	9:P:100:GLU:CD	2.45	0.42
8:d:185:SER:OG	8:d:187:GLN:O	2.37	0.42
8:n:731:LYS:O	8:n:737:GLN:NE2	2.52	0.42
10:I:73:LEU:HD21	10:I:90:TRP:CG	2.54	0.42
5:H:51:TRP:CE2	5:H:55:LYS:HB3	2.55	0.42
8:f:444:ILE:HG13	8:f:445:LEU:N	2.33	0.42
8:j:627:ASP:OD1	8:j:627:ASP:C	2.62	0.42
8:b:696:THR:OG1	8:A:696:THR:OG1	2.26	0.42
8:d:227:VAL:HG23	8:x:296:ARG:O	2.20	0.42
8:g:219:ASP:OD2	8:g:470:ARG:HD3	2.19	0.42
8:k:428:ASN:OD1	8:k:429:GLU:N	2.52	0.42
8:m:639:ASP:CG	8:m:640:ASP:N	2.78	0.42
8:p:627:ASP:C	8:p:627:ASP:OD1	2.61	0.42
8:t:424:ASP:OD2	8:t:425:LYS:NZ	2.42	0.42
8:n:639:ASP:OD1	8:n:640:ASP:N	2.51	0.42
9:P:91:PHE:C	9:P:93:VAL:N	2.77	0.42
8:a:633:TYR:O	8:a:635:MET:N	2.52	0.42
9:P:123:SER:O	9:P:124:THR:C	2.62	0.42
8:d:642:THR:HG23	8:d:647:LEU:O	2.20	0.41
8:g:390:LEU:HD23	8:g:390:LEU:C	2.45	0.41
8:a:336:LYS:HB2	8:a:378:PHE:CE1	2.55	0.41
8:c:622:TYR:O	8:c:649:TYR:HA	2.20	0.41
8:e:225:SER:OG	8:e:226:GLY:N	2.52	0.41
8:j:580:ARG:NH1	8:j:732:VAL:O	2.54	0.41
8:s:731:LYS:O	8:s:737:GLN:NE2	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:t:427:LEU:C	8:t:427:LEU:HD23	2.45	0.41
1:D:99:GLU:HG2	1:D:101:ARG:H	1.85	0.41
8:h:185:SER:O	8:h:186:ARG:C	2.63	0.41
8:t:627:ASP:OD1	8:t:627:ASP:C	2.62	0.41
8:w:622:TYR:O	8:w:649:TYR:HA	2.20	0.41
8:d:246:LEU:O	8:e:517:ARG:HG2	2.20	0.41
8:e:493:LEU:C	8:e:493:LEU:HD23	2.45	0.41
8:h:171:ARG:NH2	8:l:353:ASP:O	2.53	0.41
8:l:663:LEU:C	8:l:663:LEU:HD23	2.45	0.41
8:p:621:MET:O	8:p:668:THR:N	2.48	0.41
8:w:378:PHE:CE2	8:w:387:ILE:HD12	2.55	0.41
8:x:274:PRO:HA	8:x:275:PRO:HD3	1.98	0.41
8:A:251:ILE:HG22	8:A:464:ASN:HD21	1.85	0.41
8:b:353:ASP:O	8:d:171:ARG:NH2	2.54	0.41
8:h:667:PRO:HD3	8:h:720:PHE:CD1	2.55	0.41
8:j:306:ASN:O	8:j:310:GLN:O	2.39	0.41
8:m:343:ASP:OD1	8:m:344:ARG:N	2.54	0.41
8:n:185:SER:O	8:n:186:ARG:C	2.61	0.41
8:r:299:LEU:N	8:r:412:GLY:O	2.51	0.41
8:h:454:ILE:HG13	8:h:455:GLY:N	2.35	0.41
8:o:680:TRP:CD1	8:o:718:ILE:CG2	3.03	0.41
8:v:579:ASP:OD1	8:w:578:LYS:NZ	2.53	0.41
3:E:38:ILE:O	3:E:86:ARG:NH1	2.50	0.41
8:a:276:TYR:CD1	8:a:276:TYR:C	2.99	0.41
8:b:378:PHE:CE2	8:b:387:ILE:HD12	2.56	0.41
8:c:355:VAL:O	8:x:347:ARG:NH1	2.53	0.41
8:h:560:THR:CG2	8:h:720:PHE:CD2	3.03	0.41
8:i:627:ASP:OD1	8:i:627:ASP:C	2.63	0.41
8:j:171:ARG:NH1	9:O:38:GLN:O	2.50	0.41
8:p:736:THR:HG22	8:p:740:GLY:H	1.86	0.41
8:s:167:GLU:O	8:w:359:ARG:NH1	2.49	0.41
8:x:280:ASN:OD1	8:x:280:ASN:C	2.64	0.41
1:D:194:ILE:HB	1:D:195:PRO:HD3	2.03	0.41
8:d:190:PHE:CG	8:d:654:THR:HB	2.56	0.41
8:v:627:ASP:OD1	8:v:627:ASP:C	2.62	0.41
8:x:343:ASP:OD1	8:x:344:ARG:N	2.54	0.41
8:z:449:THR:O	8:z:449:THR:HG22	2.20	0.41
3:E:114:VAL:O	3:E:117:VAL:HG12	2.21	0.41
8:b:187:GLN:NE2	8:b:195:TYR:O	2.53	0.41
8:c:219:ASP:OD1	8:c:470:ARG:NH2	2.54	0.41
8:e:606:GLU:OE1	8:f:628:LYS:NZ	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:j:605:ILE:CD1	8:j:667:PRO:HG3	2.51	0.41
8:q:535:GLU:O	8:q:539:ASN:ND2	2.54	0.41
8:u:622:TYR:O	8:u:649:TYR:HA	2.21	0.41
8:z:627:ASP:C	8:z:627:ASP:OD1	2.64	0.41
8:c:692:ASP:OD1	8:c:693:LEU:N	2.54	0.41
8:s:454:ILE:HG13	8:s:455:GLY:N	2.35	0.41
8:t:280:ASN:OD1	8:t:280:ASN:C	2.64	0.41
8:m:639:ASP:CG	8:m:640:ASP:H	2.29	0.40
8:r:235:ASN:OD1	8:r:236:MET:N	2.54	0.40
8:r:575:ILE:HG13	8:r:576:LYS:N	2.36	0.40
8:t:704:ARG:O	8:t:704:ARG:HG3	2.20	0.40
8:x:641:ARG:NH1	8:x:650:ASP:OD1	2.54	0.40
11:C:19:ASP:OD1	11:C:61:LYS:NZ	2.54	0.40
8:f:441:VAL:O	8:f:444:ILE:HG12	2.21	0.40
8:m:639:ASP:OD1	8:m:640:ASP:N	2.50	0.40
8:r:597:PHE:HB2	8:r:598:PRO:HD3	2.02	0.40
10:I:82:THR:HA	10:I:90:TRP:O	2.21	0.40
1:D:82:ASP:OD1	1:D:82:ASP:C	2.65	0.40
8:k:398:ARG:NE	8:l:541:TYR:OH	2.55	0.40
8:o:336:LYS:HB2	8:o:378:PHE:CE1	2.56	0.40
8:t:345:LEU:C	8:t:347:ARG:H	2.29	0.40
8:u:343:ASP:OD1	8:u:344:ARG:N	2.54	0.40
8:c:500:ASP:OD1	8:c:500:ASP:N	2.54	0.40
8:h:424:ASP:OD2	8:h:425:LYS:NZ	2.41	0.40
8:l:280:ASN:OD1	8:l:281:GLU:N	2.46	0.40
8:p:165:TYR:CZ	8:z:475:GLN:HG2	2.57	0.40
8:w:605:ILE:HD11	8:w:720:PHE:CD2	2.56	0.40
8:x:298:ASP:OD1	8:x:298:ASP:C	2.64	0.40
9:P:95:LYS:HE3	9:P:100:GLU:OE1	2.21	0.40
1:D:46:PRO:O	1:D:60:GLY:HA2	2.21	0.40
6:K:53:VAL:O	6:K:54:GLU:C	2.64	0.40
8:j:546:PHE:CZ	8:r:356:GLY:HA2	2.56	0.40
8:p:622:TYR:O	8:p:649:TYR:HA	2.22	0.40
8:y:188:ASP:OD1	8:y:188:ASP:C	2.65	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	D	317/320 (99%)	313 (99%)	4 (1%)	0	100	100
2	B	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%)	18	51
5	H	161/181 (89%)	154 (96%)	7 (4%)	0	100	100
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%)	21	54
8	A	580/747 (78%)	562 (97%)	17 (3%)	1 (0%)	43	74
8	a	582/747 (78%)	564 (97%)	17 (3%)	1 (0%)	43	74
8	b	582/747 (78%)	569 (98%)	13 (2%)	0	100	100
8	c	582/747 (78%)	555 (95%)	24 (4%)	3 (0%)	24	57
8	d	582/747 (78%)	564 (97%)	18 (3%)	0	100	100
8	e	582/747 (78%)	561 (96%)	20 (3%)	1 (0%)	43	74
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	l	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	m	582/747 (78%)	563 (97%)	18 (3%)	1 (0%)	43	74
8	n	582/747 (78%)	573 (98%)	9 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	o	582/747 (78%)	570 (98%)	12 (2%)	0	100	100
8	p	582/747 (78%)	568 (98%)	13 (2%)	1 (0%)	43	74
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	y	582/747 (78%)	571 (98%)	11 (2%)	0	100	100
8	z	582/747 (78%)	574 (99%)	8 (1%)	0	100	100
9	N	30/522 (6%)	30 (100%)	0	0	100	100
9	O	114/522 (22%)	104 (91%)	9 (8%)	1 (1%)	14	47
9	P	114/522 (22%)	102 (90%)	11 (10%)	1 (1%)	14	47
10	I	32/230 (14%)	29 (91%)	3 (9%)	0	100	100
11	C	112/118 (95%)	112 (100%)	0	0	100	100
All	All	17628/25063 (70%)	17148 (97%)	467 (3%)	13 (0%)	49	79

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	P	103	ILE
8	c	226	GLY
8	c	227	VAL
8	m	232	GLU
4	G	333	ARG
8	a	634	LEU
8	e	186	ARG
8	p	640	ASP
4	G	260	MET
8	A	309	ILE
7	J	106	ARG
9	O	99	VAL
8	c	312	GLY

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	D	283/284 (100%)	283 (100%)	0	100	100
2	B	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
4	G	260/374 (70%)	260 (100%)	0	100	100
5	H	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	l	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	o	503/638 (79%)	503 (100%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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
8	y	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	O	105/456 (23%)	105 (100%)	0	100	100
9	P	105/456 (23%)	105 (100%)	0	100	100
10	I	30/193 (16%)	30 (100%)	0	100	100
11	C	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 (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	58	HIS
1	D	110	GLN
1	D	231	ASN
2	B	253	GLN
3	E	125	ASN
3	F	14	GLN
4	G	167	GLN
4	G	369	GLN
5	H	54	HIS
5	H	78	ASN
5	H	164	HIS
7	J	45	GLN
7	J	98	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	a	166	ASN
8	a	464	ASN
8	a	515	ASN
8	a	672	GLN
8	b	464	ASN
8	b	480	GLN
8	b	657	GLN
8	c	166	ASN
8	c	328	ASN
8	d	181	ASN
8	d	682	GLN
8	e	187	GLN
8	e	282	GLN
8	e	464	ASN
8	f	166	ASN
8	f	616	GLN
8	g	464	ASN
8	h	170	GLN
8	h	328	ASN
8	h	672	GLN
8	h	737	GLN
8	i	447	GLN
8	i	475	GLN
8	j	166	ASN
8	j	328	ASN
8	j	480	GLN
8	j	700	HIS
8	j	737	GLN
8	j	739	ASN
8	k	222	HIS
8	k	447	GLN
8	k	464	ASN
8	k	700	HIS
8	k	737	GLN
8	l	306	ASN
8	l	483	HIS
8	l	739	ASN
8	m	447	GLN
8	m	480	GLN
8	m	655	ASN
8	n	187	GLN
8	n	632	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	n	716	ASN
8	n	737	GLN
8	o	166	ASN
8	o	700	HIS
8	p	282	GLN
8	p	283	ASN
8	p	447	GLN
8	q	164	ASN
8	q	328	ASN
8	q	464	ASN
8	q	737	GLN
8	r	187	GLN
8	r	436	ASN
8	r	483	HIS
8	r	539	ASN
8	r	737	GLN
8	s	682	GLN
8	s	737	GLN
8	t	222	HIS
8	t	282	GLN
8	t	351	GLN
8	t	447	GLN
8	t	464	ASN
8	t	672	GLN
8	u	464	ASN
8	u	716	ASN
8	u	737	GLN
8	v	263	ASN
8	v	310	GLN
8	v	616	GLN
8	v	716	ASN
8	w	475	GLN
8	w	480	GLN
8	x	737	GLN
8	y	282	GLN
8	y	682	GLN
8	y	716	ASN
8	y	737	GLN
8	A	328	ASN
8	A	464	ASN
9	O	92	GLN
11	C	28	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 oligosaccharides 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.

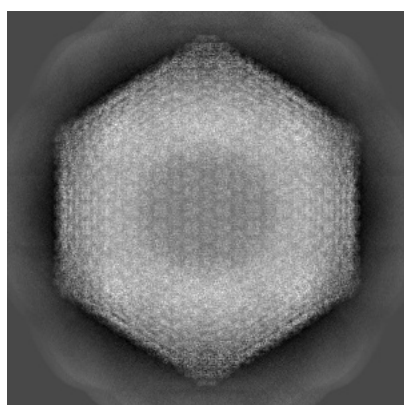
6 Map visualisation [i](#)

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.

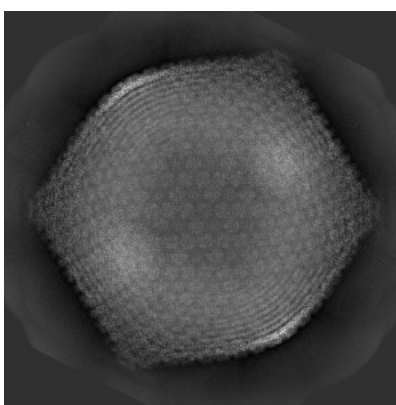
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

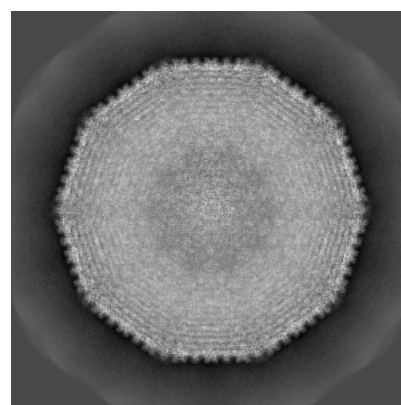
6.1.1 Primary map



X



Y

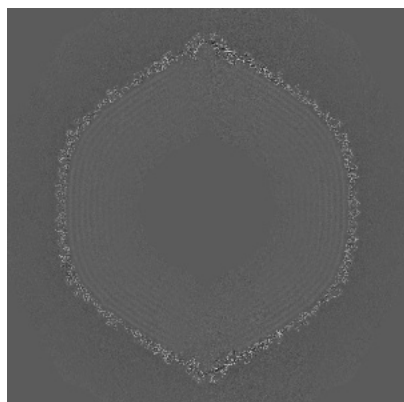


Z

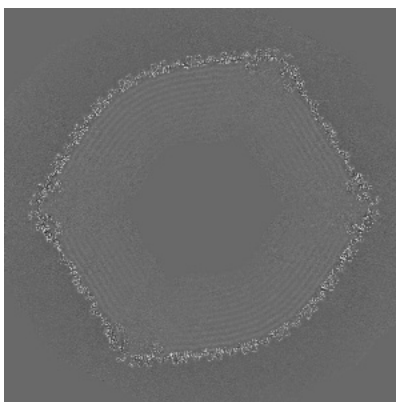
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

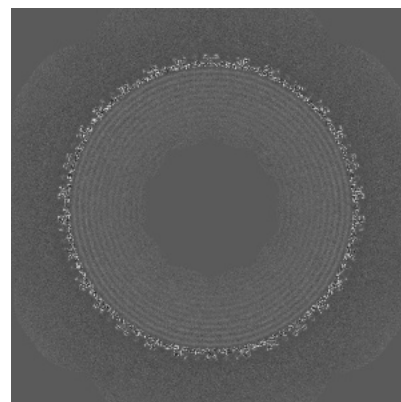
6.2.1 Primary map



X Index: 500



Y Index: 500

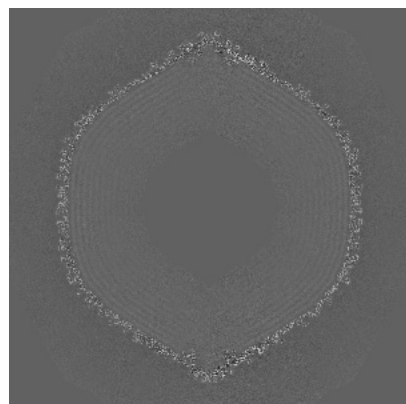


Z Index: 500

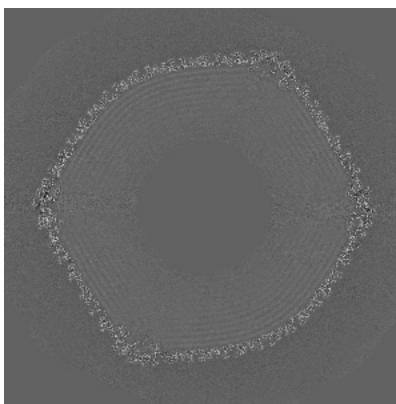
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

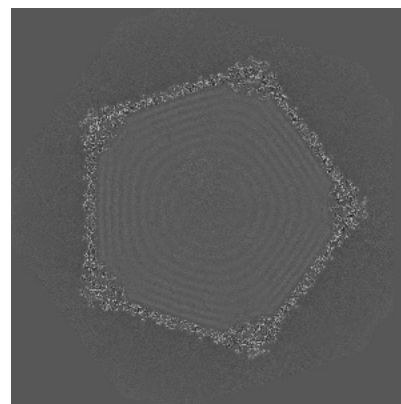
6.3.1 Primary map



X Index: 507



Y Index: 531

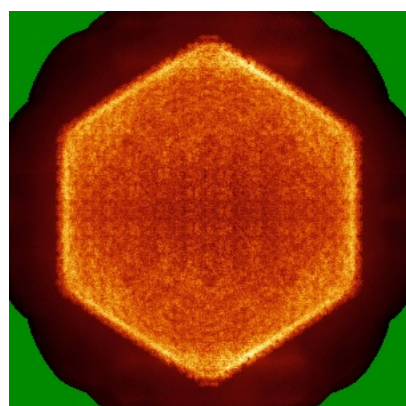


Z Index: 703

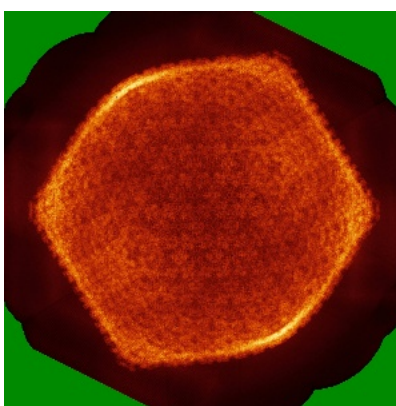
The images above show the largest variance slices of the map in three orthogonal directions.

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

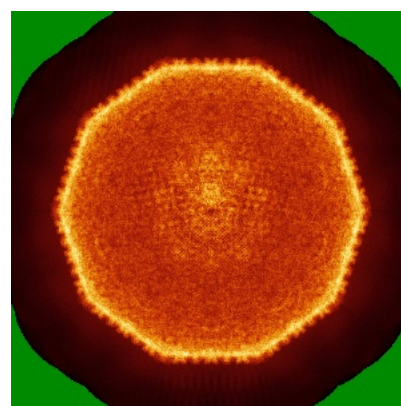
6.4.1 Primary map



X



Y

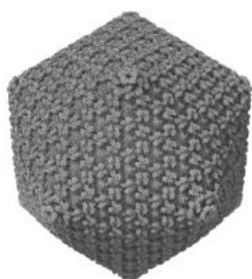


Z

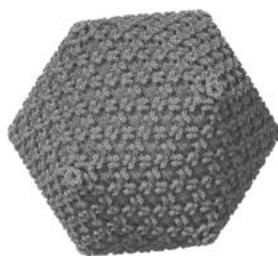
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

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.

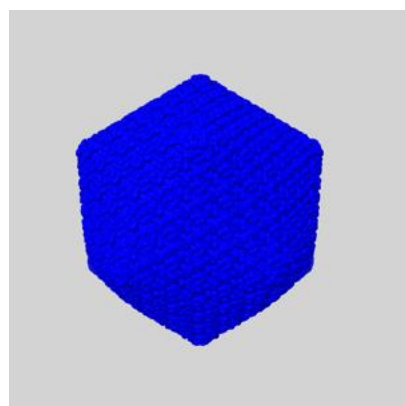
6.6 Mask visualisation [i](#)

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

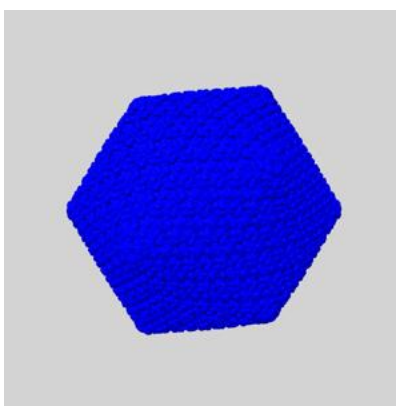
A mask typically either:

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

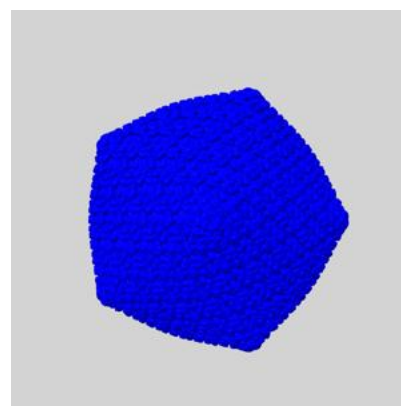
6.6.1 emd_39002_msk_1.map [i](#)



X



Y

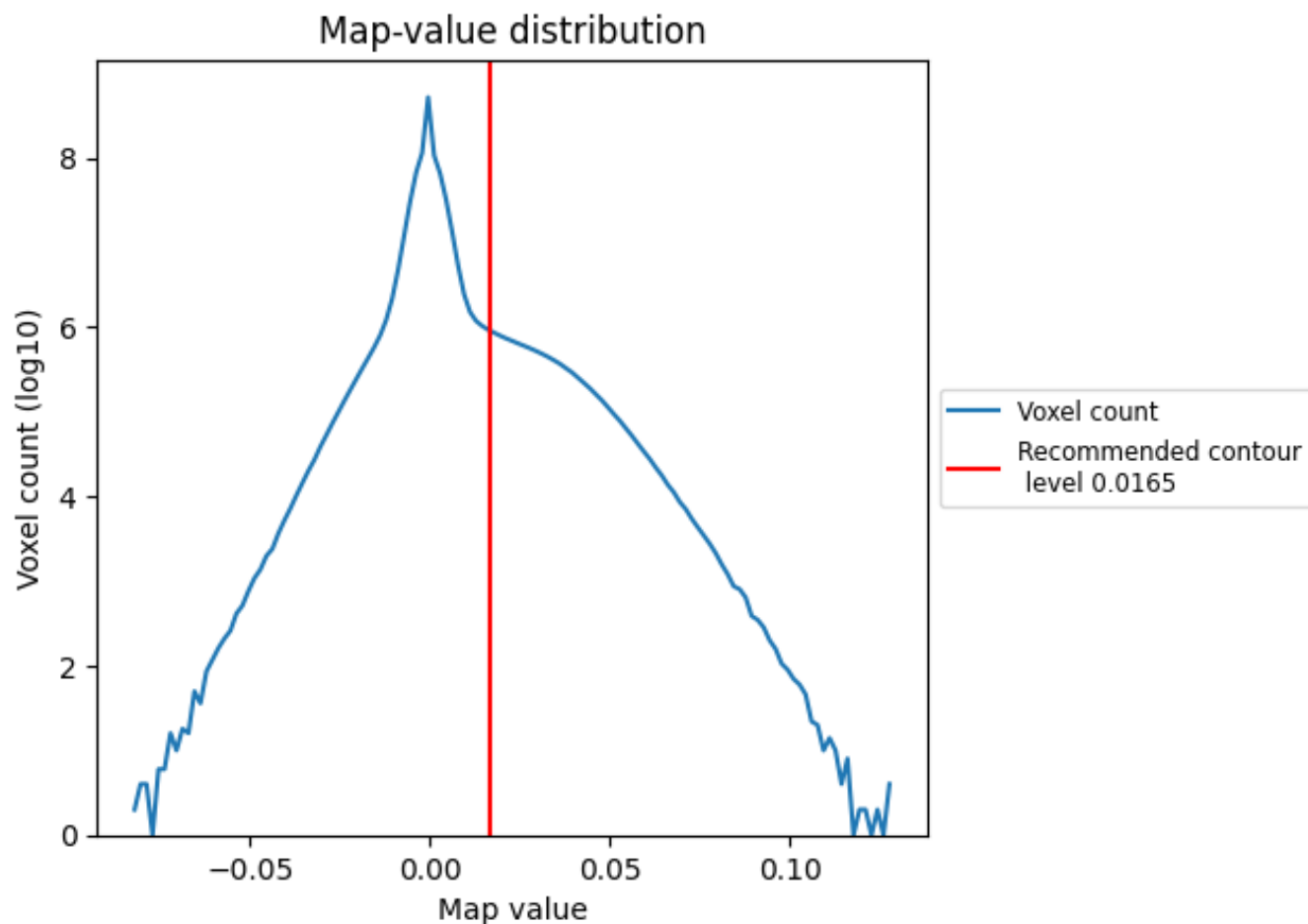


Z

7 Map analysis [i](#)

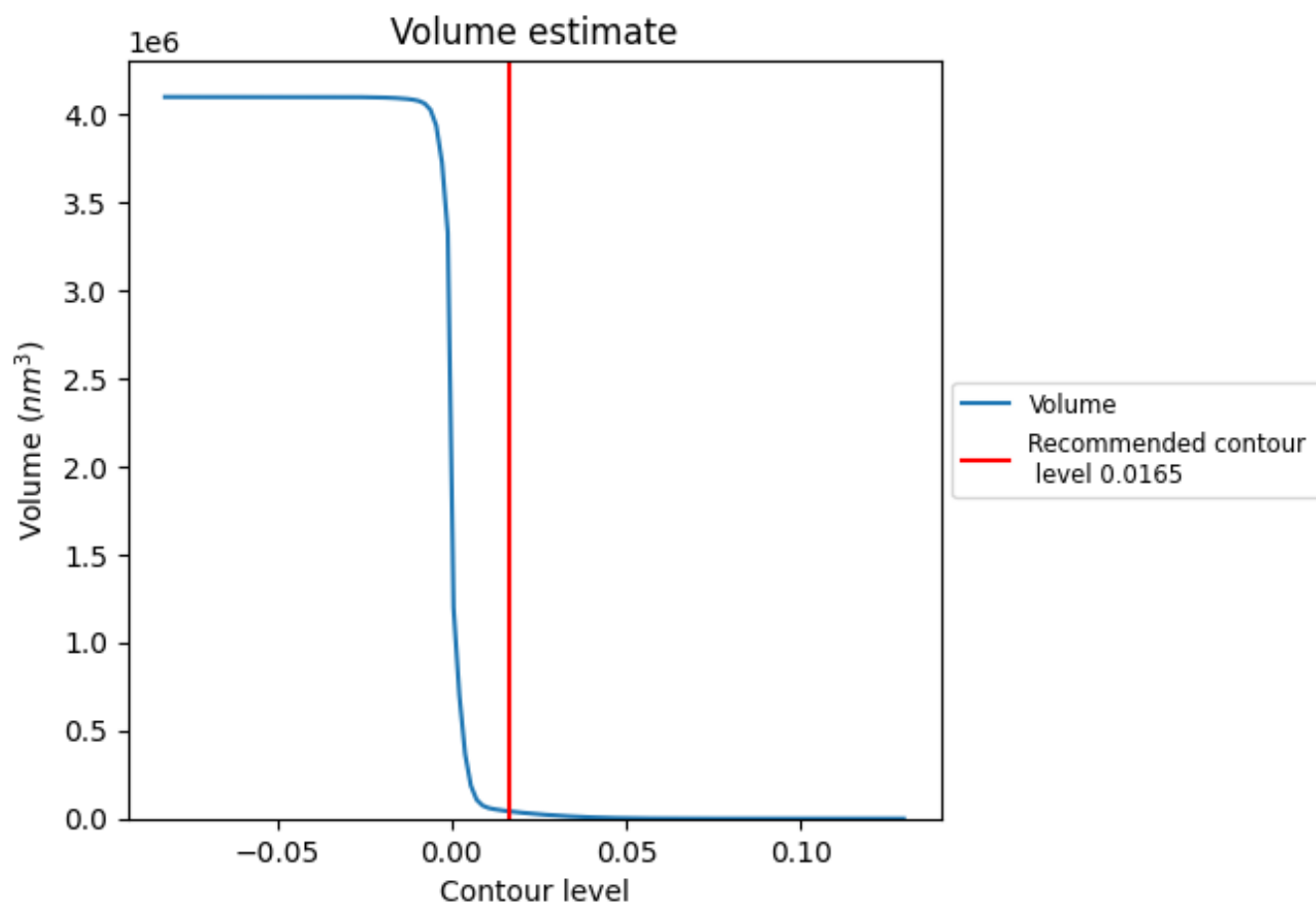
This section contains the results of statistical analysis of the map.

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.

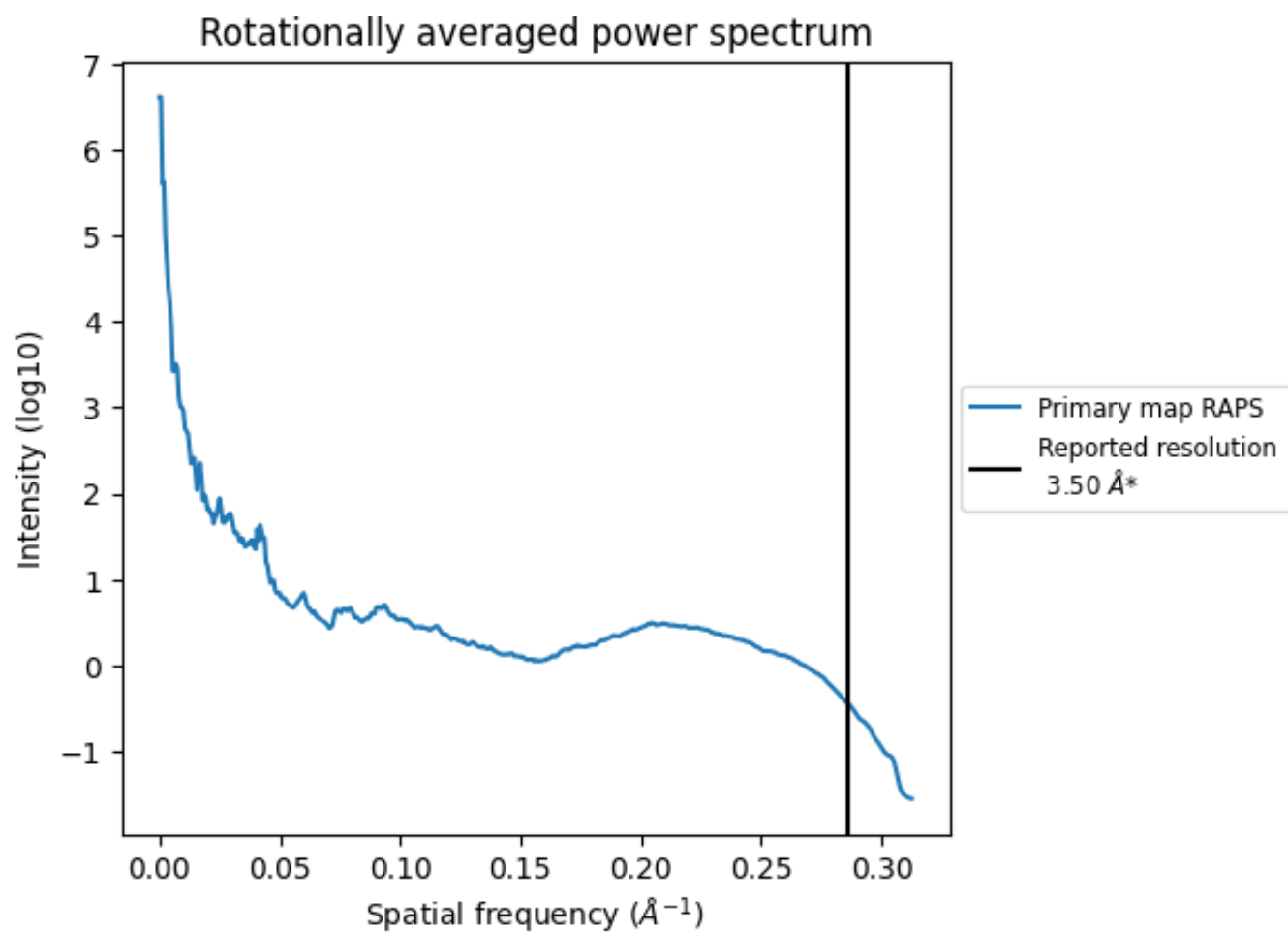
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 41513 nm³; this corresponds to an approximate mass of 37499 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 0.286 Å⁻¹

8 Fourier-Shell correlation ⓘ

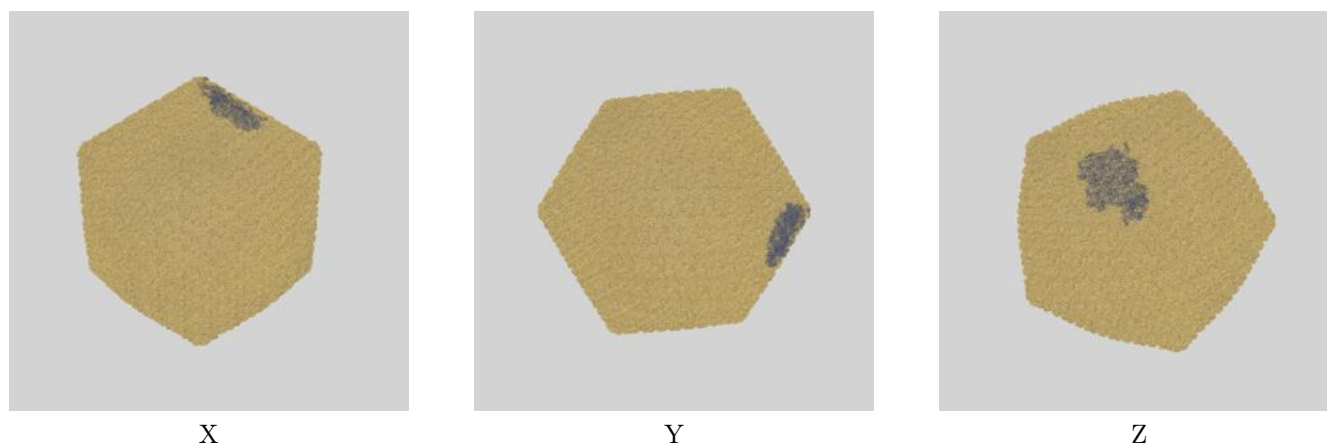
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

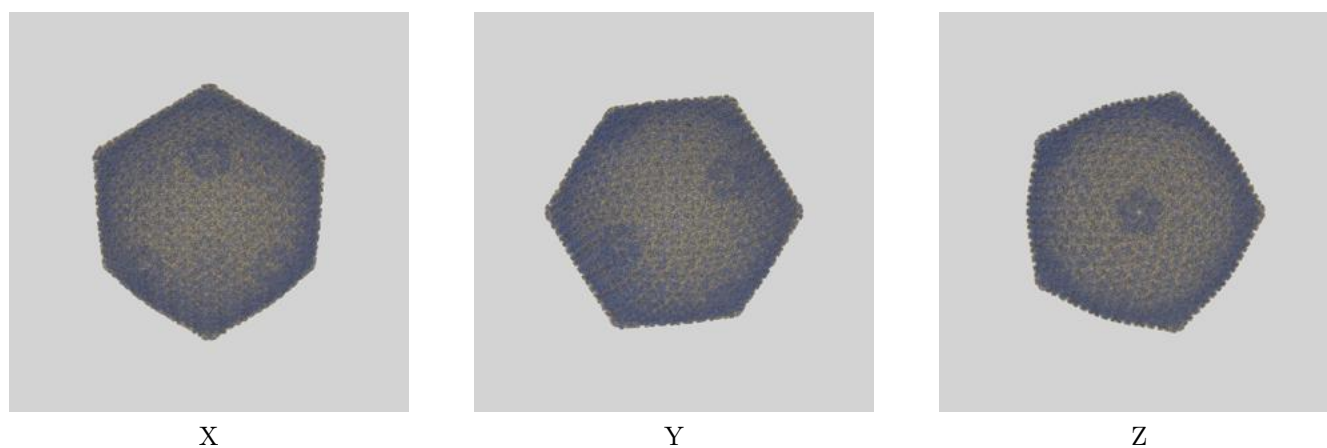
This section contains information regarding the fit between EMDB map EMD-39002 and PDB model 8Y6V. Per-residue inclusion information can be found in section 3 on page 9.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

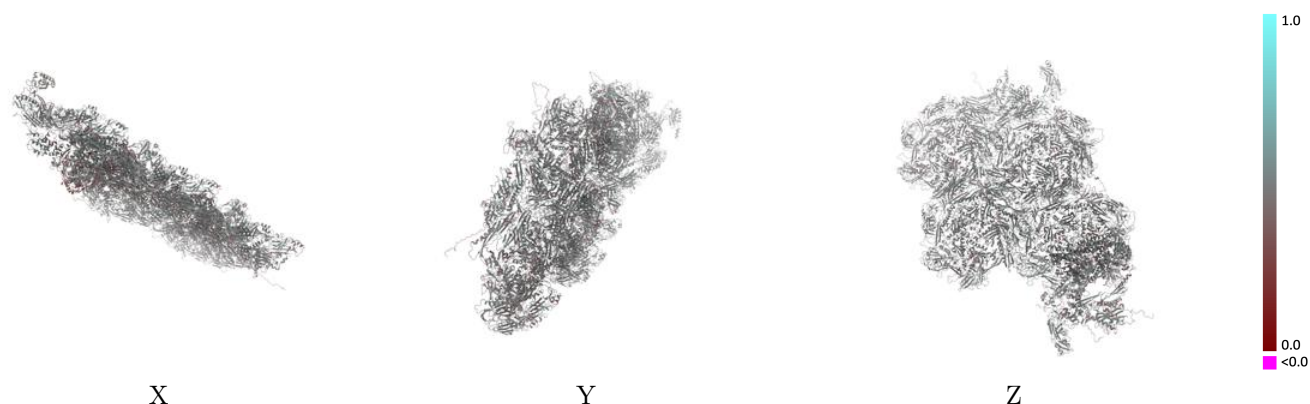


9.1.2 Map-model assembly overlay [i](#)



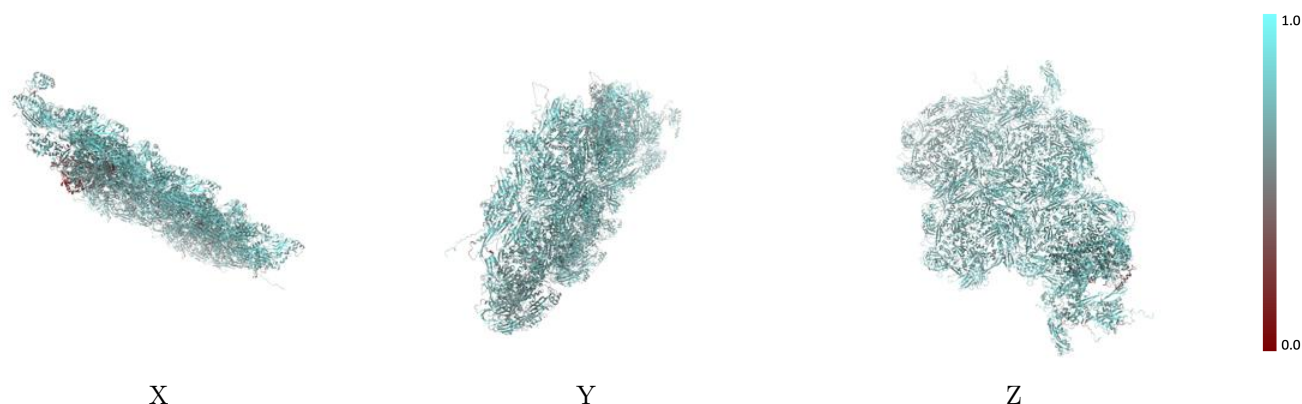
The images above show the 3D surface view of the map at the recommended contour level 0.0165 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



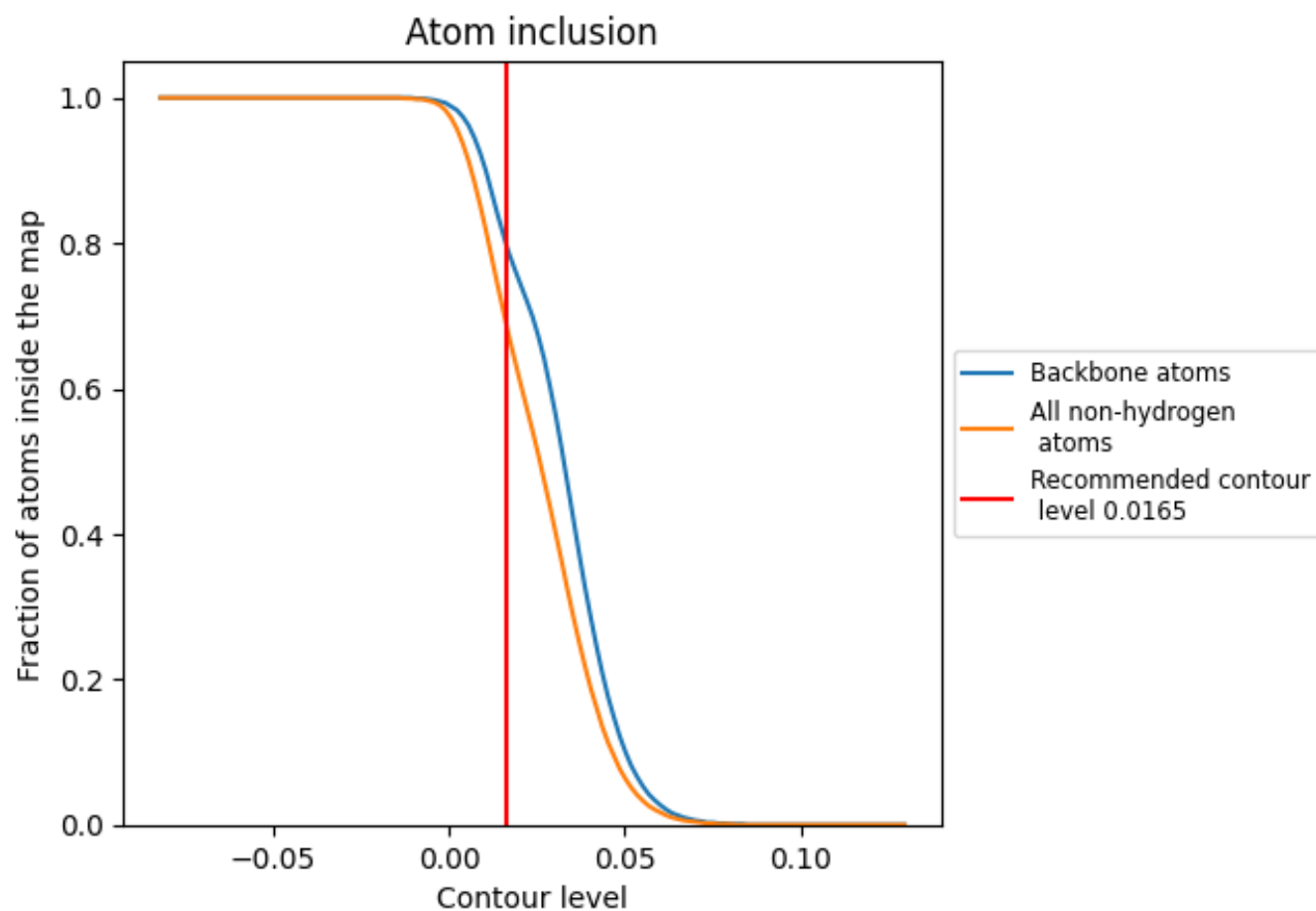
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0165).

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 ⓘ

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
B	 0.6710	 0.4640
C	 0.6490	 0.4460
D	 0.4730	 0.4310
E	 0.5480	 0.4110
F	 0.4090	 0.3750
G	 0.6050	 0.4360
H	 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
O	 0.5270	 0.3970
P	 0.5610	 0.4120
a	 0.7260	 0.4690
b	 0.7310	 0.4710
c	 0.7390	 0.4660
d	 0.7380	 0.4670
e	 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
l	 0.6870	 0.4590
m	 0.6820	 0.4670
n	 0.6920	 0.4670
o	 0.6500	 0.4570
p	 0.6190	 0.4530
q	 0.6110	 0.4480
r	 0.6360	 0.4540



Continued on next page...

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
y	 0.7110	 0.4670
z	 0.6820	 0.4620