



## Full wwPDB EM Validation Report ⓘ

Mar 27, 2026 – 05:59 AM UTC

PDB ID : 6PPB / pdb\_00006ppb  
EMDB ID : EMD-20432  
Title : Kaposi's sarcoma-associated herpesvirus (KSHV), C5 portal vertex structure  
Authors : Gong, D.; Dai, X.; Jih, J.; Liu, Y.T.; Bi, G.Q.; Sun, R.; Zhou, Z.H.  
Deposited on : 2019-07-06  
Resolution : 4.30 Å (reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

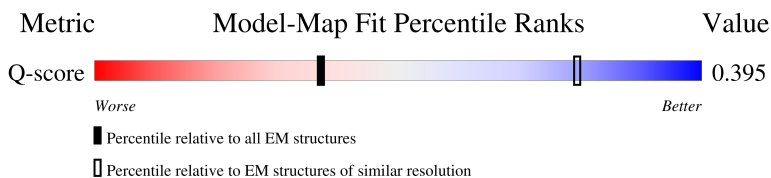
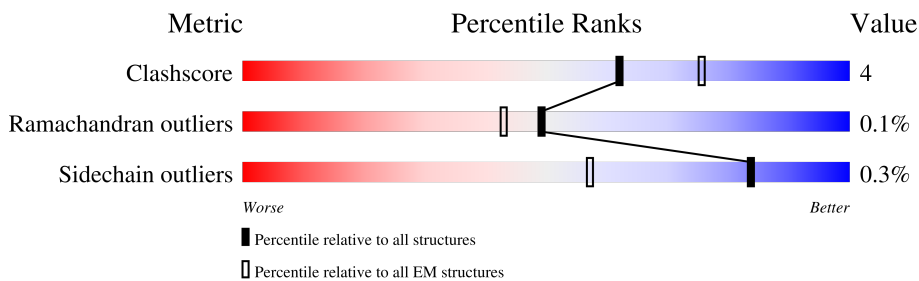
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 4.30 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.





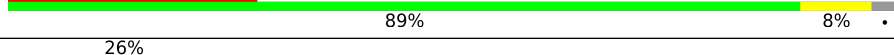




Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	4585 ( 3.80 - 4.80 )

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

Mol	Chain	Length	Quality of chain
1	k	454	<p>19% (red), 66% (green), 10% (yellow), 24% (grey)</p>
2	l	549	<p>8% (red), 14% (green), 85% (grey)</p>
2	m	549	<p>9% (red), 12% (green), 85% (grey)</p>
3	n	2635	<p>98% (grey)</p>

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Mol	Chain	Length	Quality of chain
3	o	2635	 98%
4	S	1376	 16% 82% 11% 7%
4	T	1376	 22% 85% 14%
4	W	1376	 29% 83% 15%
4	X	1376	 15% 81% 12% 6%
5	5	331	 29% 70% 11% 19%
5	b	331	 28% 89% 8%
6	6	305	 26% 87% 10%
6	7	305	 28% 90% 7%
6	c	305	 42% 81% 15%
6	d	305	 47% 90% 9%
7	0	170	 40% 41% 5% 54%
7	1	170	 34% 43% 0% 54%
7	2	170	 32% 42% 0% 54%
7	3	170	 30% 42% 0% 54%

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 62671 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 Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	k	344	2680	1722	467	477	14	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
k	165	PRO	LEU	conflict	UNP Q76RH8
k	281	SER	GLY	conflict	UNP Q76RH8

- Molecule 2 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	l	83	686	429	135	119	3	0	0
2	m	80	645	406	121	115	3	0	0

- Molecule 3 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
3	n	40	323	209	56	58	0	0
3	o	40	323	209	56	58	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
n	2220	THR	PRO	conflict	UNP Q2HR64
o	2220	THR	PRO	conflict	UNP Q2HR64

- Molecule 4 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	S	1281	10061	6401	1739	1852	69	0	0
4	T	1360	10667	6776	1851	1967	73	0	0
4	W	1354	10622	6748	1842	1960	72	0	0
4	X	1288	10108	6421	1755	1861	71	0	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
S	1146	PRO	SER	conflict	UNP Q2HRA7
S	1157	ALA	THR	conflict	UNP Q2HRA7
T	1146	PRO	SER	conflict	UNP Q2HRA7
T	1157	ALA	THR	conflict	UNP Q2HRA7
W	1146	PRO	SER	conflict	UNP Q2HRA7
W	1157	ALA	THR	conflict	UNP Q2HRA7
X	1146	PRO	SER	conflict	UNP Q2HRA7
X	1157	ALA	THR	conflict	UNP Q2HRA7

- Molecule 5 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	b	321	2478	1586	424	453	15	0	0
5	5	268	2074	1336	344	381	13	0	0

- Molecule 6 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	c	294	2330	1485	397	434	14	0	0
6	d	300	2365	1505	401	444	15	0	0
6	6	294	2330	1485	397	434	14	0	0
6	7	294	2315	1478	391	431	15	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	11	LEU	PHE	conflict	UNP Q98832
c	117	LEU	PHE	conflict	UNP Q98832
c	134	ILE	PRO	conflict	UNP Q98832
c	167	GLY	ASP	conflict	UNP Q98832
d	11	LEU	PHE	conflict	UNP Q98832
d	117	LEU	PHE	conflict	UNP Q98832
d	134	ILE	PRO	conflict	UNP Q98832
d	167	GLY	ASP	conflict	UNP Q98832
6	11	LEU	PHE	conflict	UNP Q98832
6	117	LEU	PHE	conflict	UNP Q98832
6	134	ILE	PRO	conflict	UNP Q98832
6	167	GLY	ASP	conflict	UNP Q98832
7	11	LEU	PHE	conflict	UNP Q98832
7	117	LEU	PHE	conflict	UNP Q98832
7	134	ILE	PRO	conflict	UNP Q98832
7	167	GLY	ASP	conflict	UNP Q98832

- Molecule 7 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	0	78	666	418	130	115	3	0	0
7	1	78	666	418	130	115	3	0	0
7	2	78	666	418	130	115	3	0	0
7	3	78	666	418	130	115	3	0	0





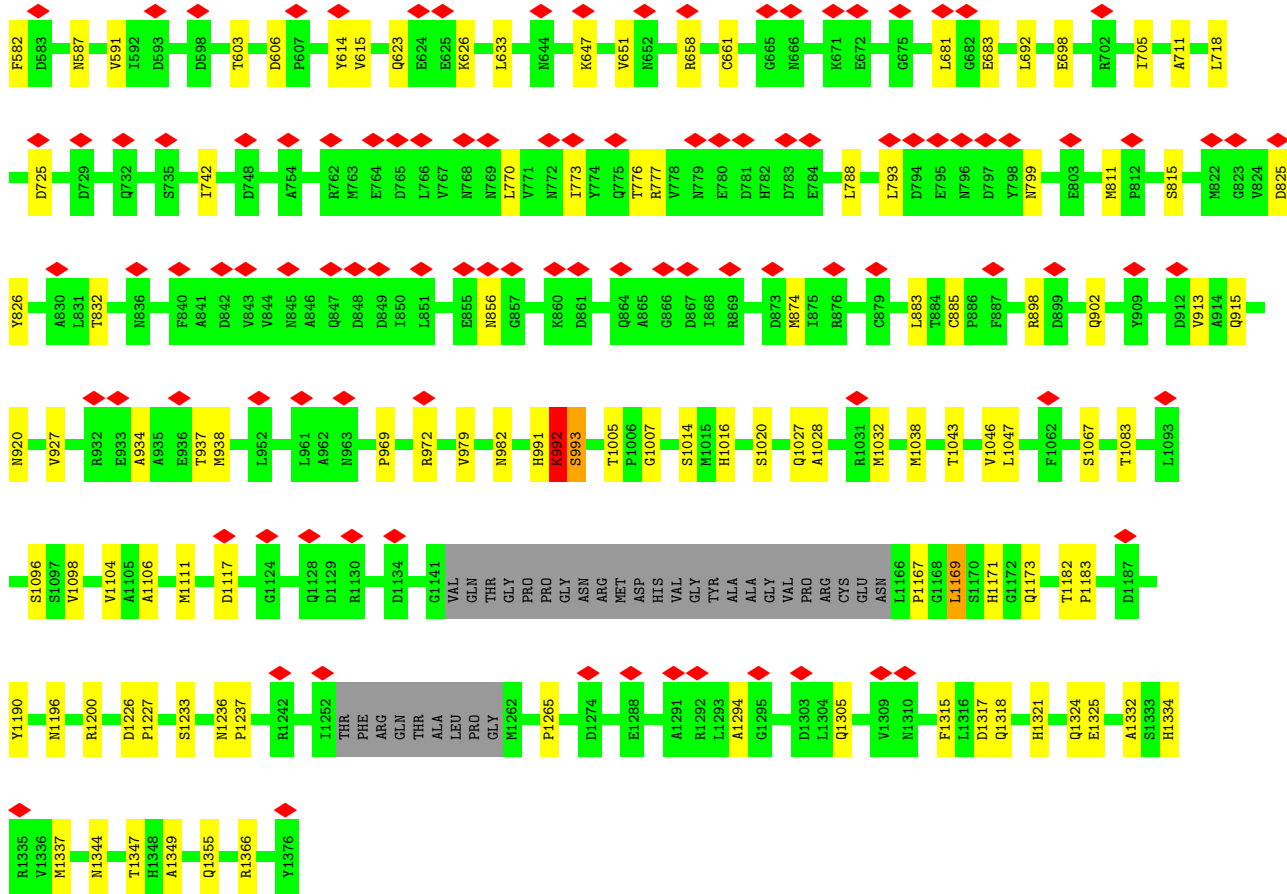




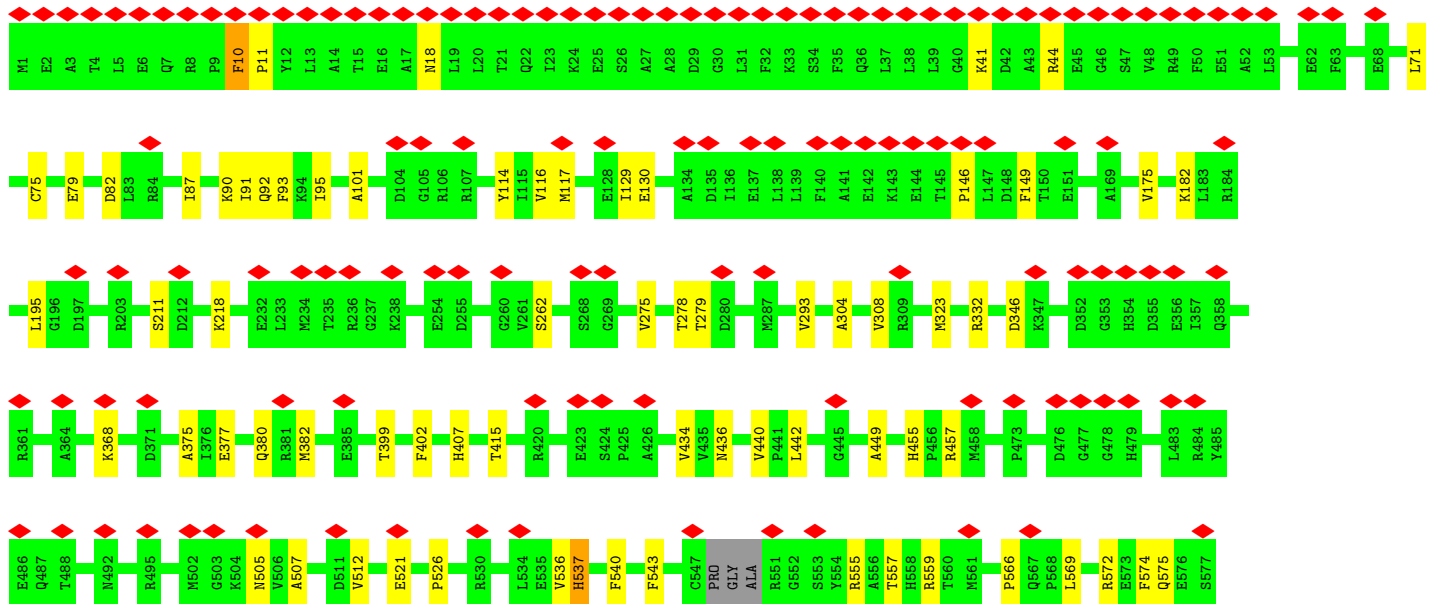
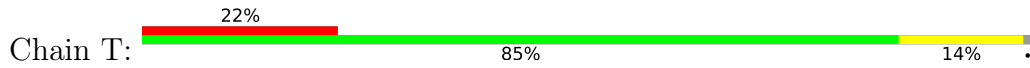


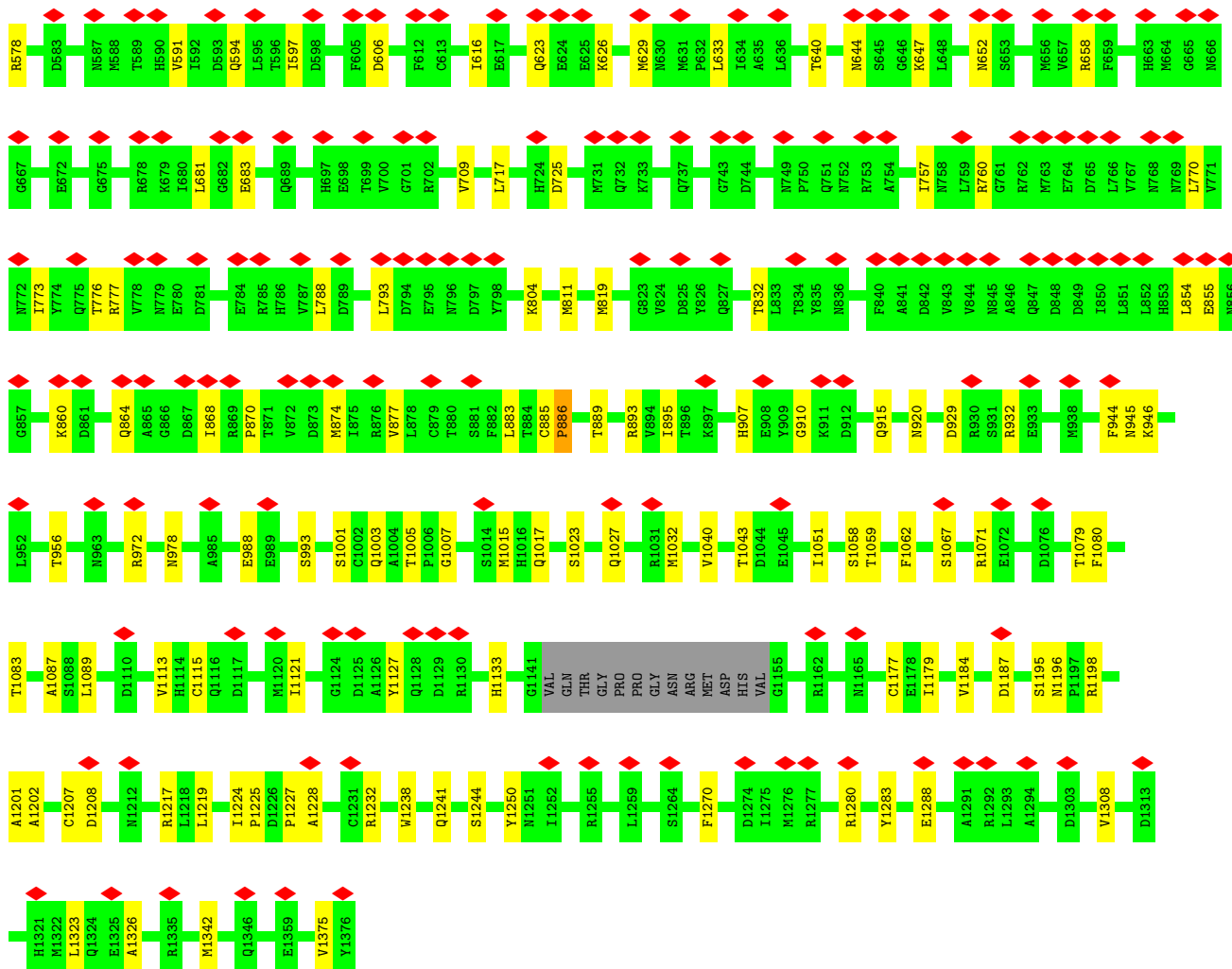




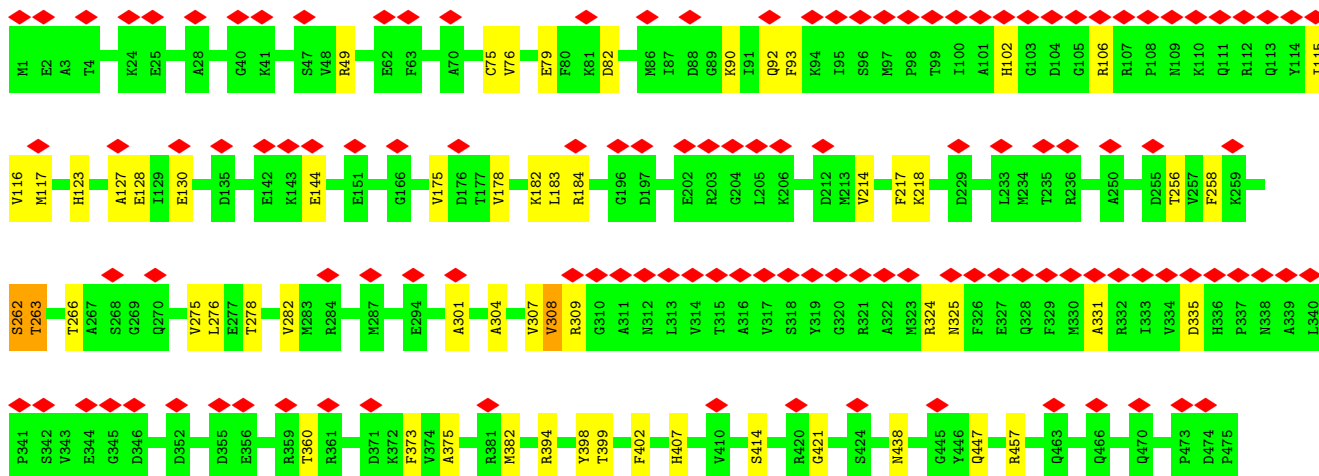
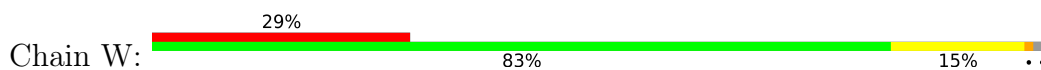


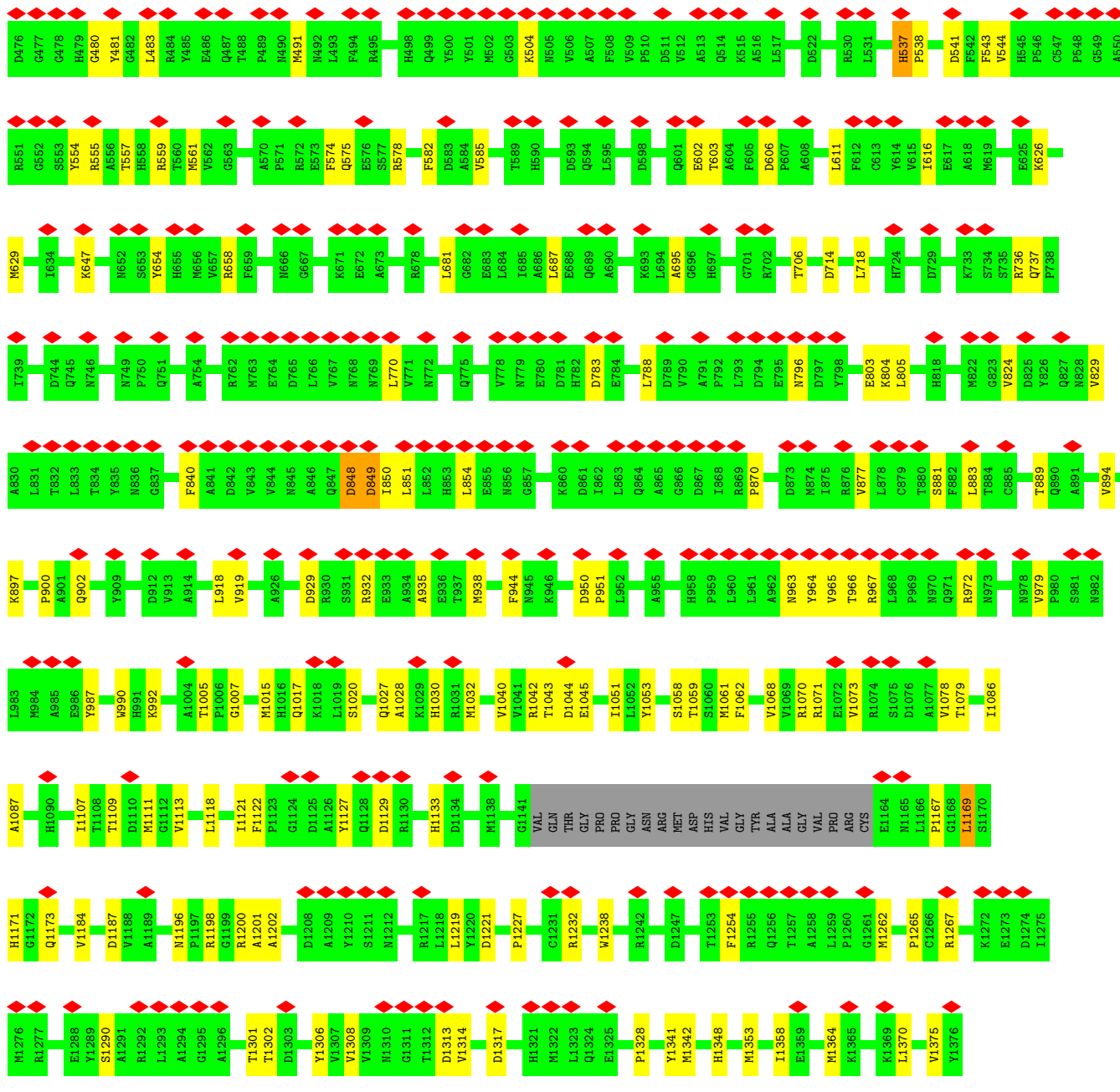
• Molecule 4: Major capsid protein



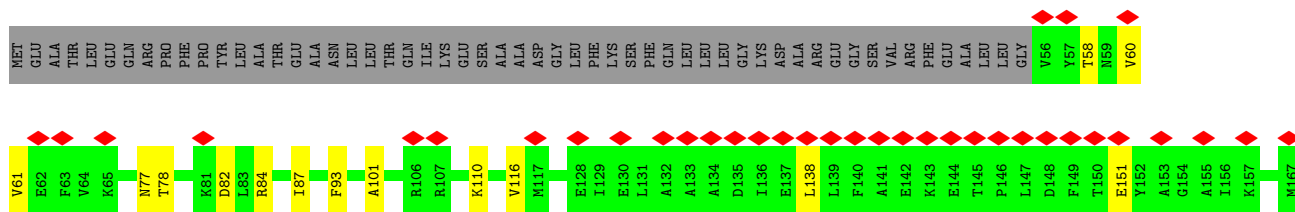
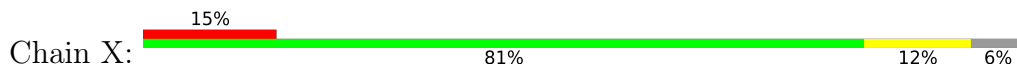


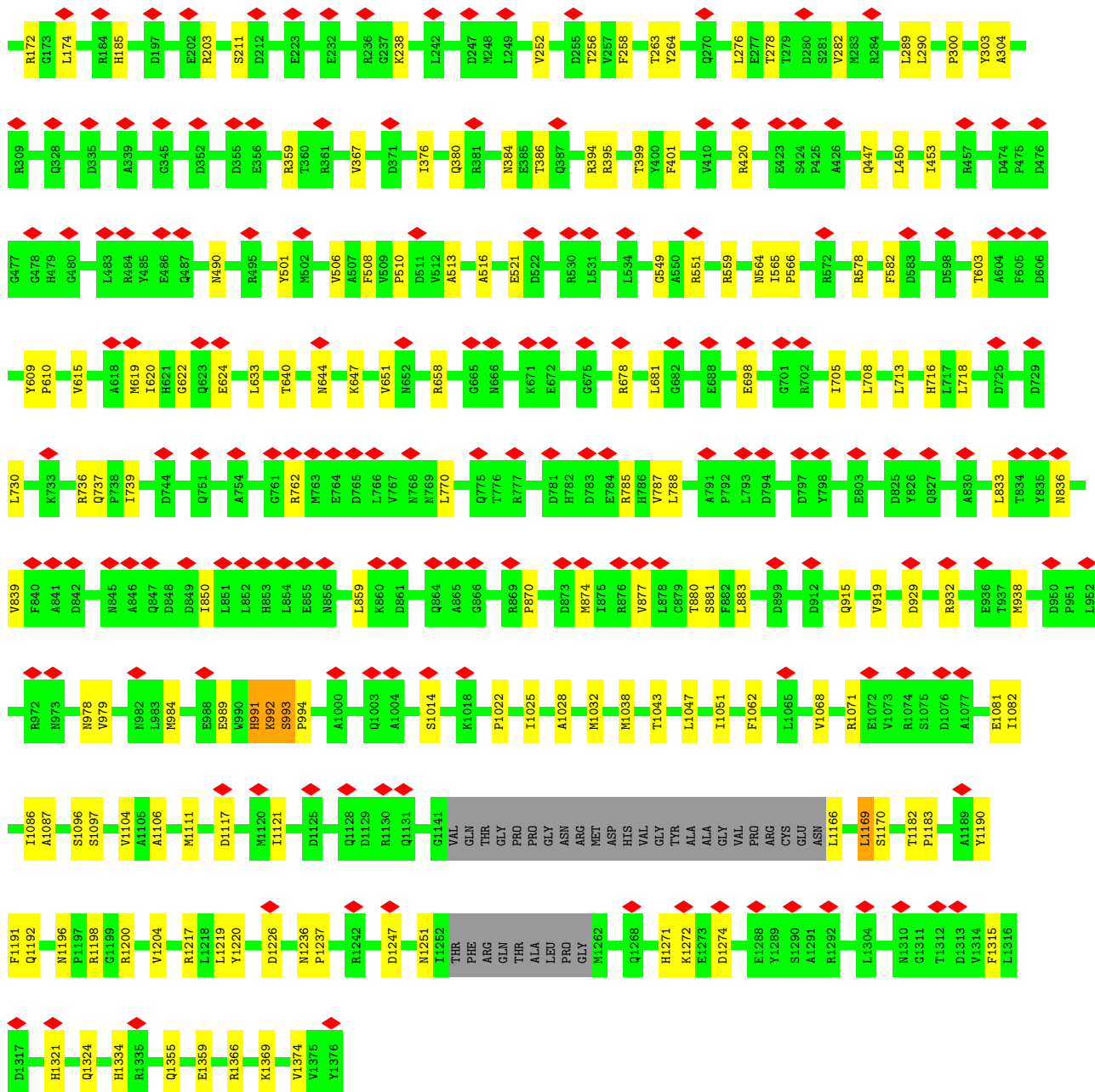
• Molecule 4: Major capsid protein



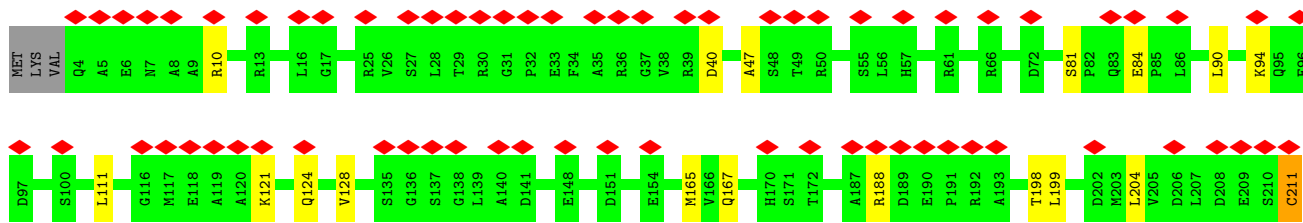
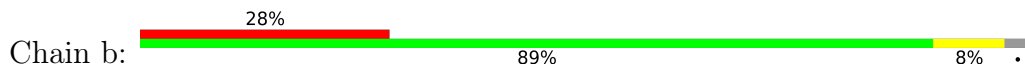


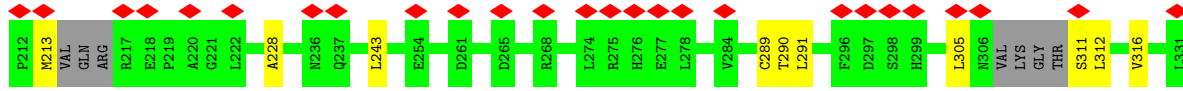
● Molecule 4: Major capsid protein



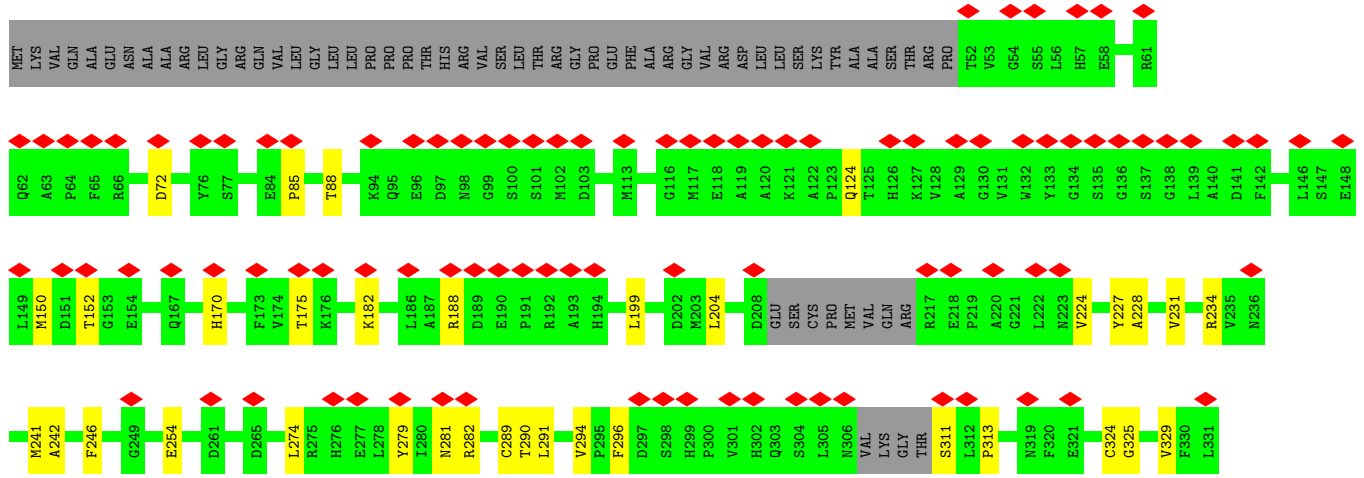


• Molecule 5: Triplex capsid protein 1

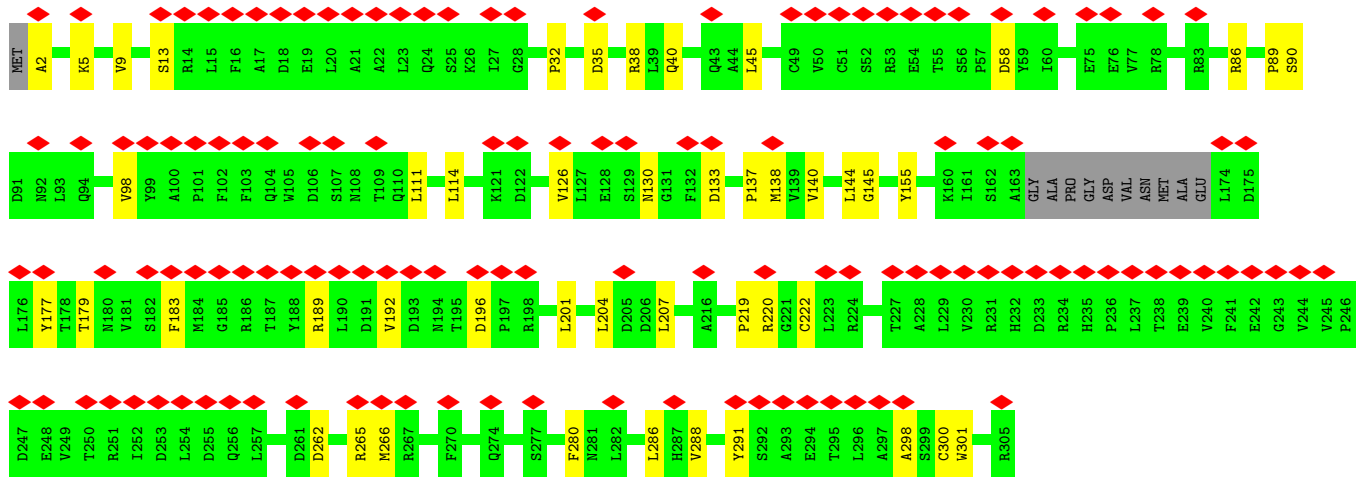
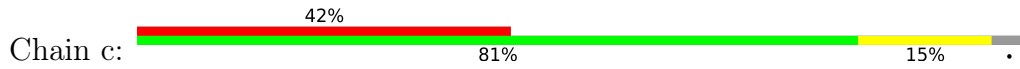




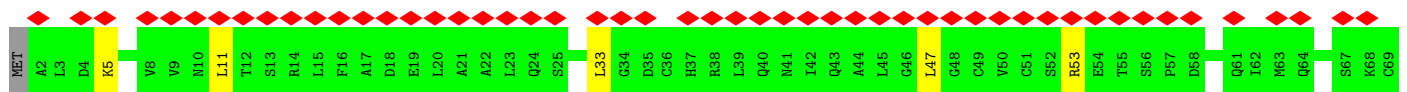
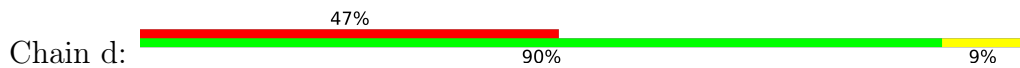
• Molecule 5: Triplex capsid protein 1

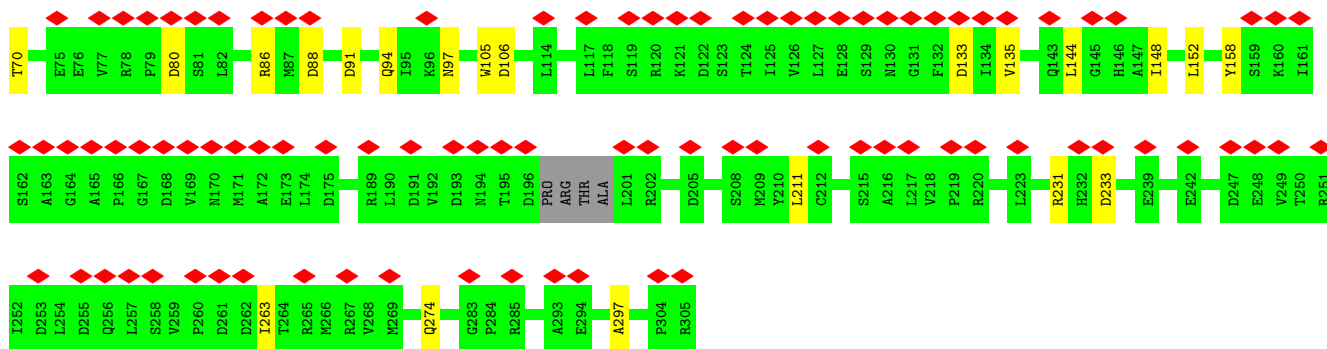


• Molecule 6: Triplex capsid protein 2

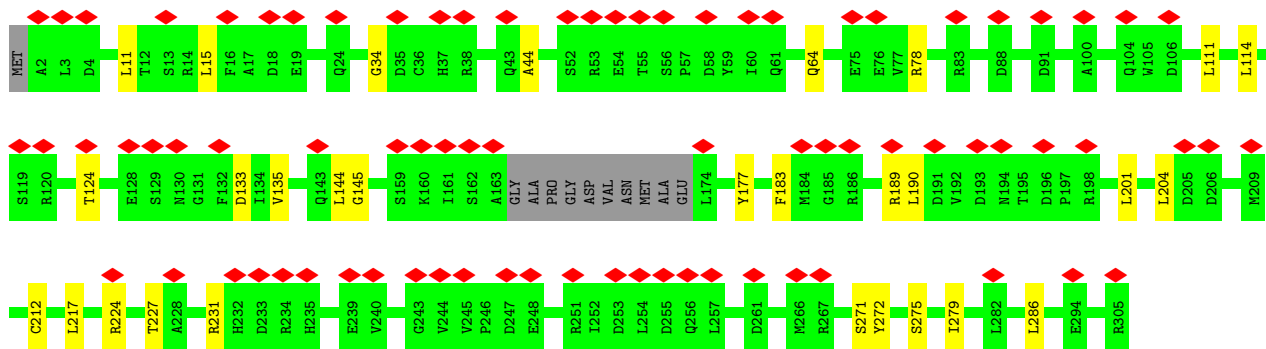
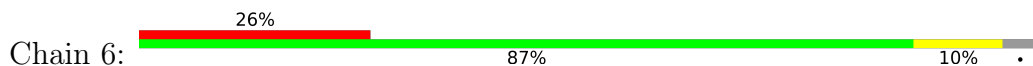


• Molecule 6: Triplex capsid protein 2

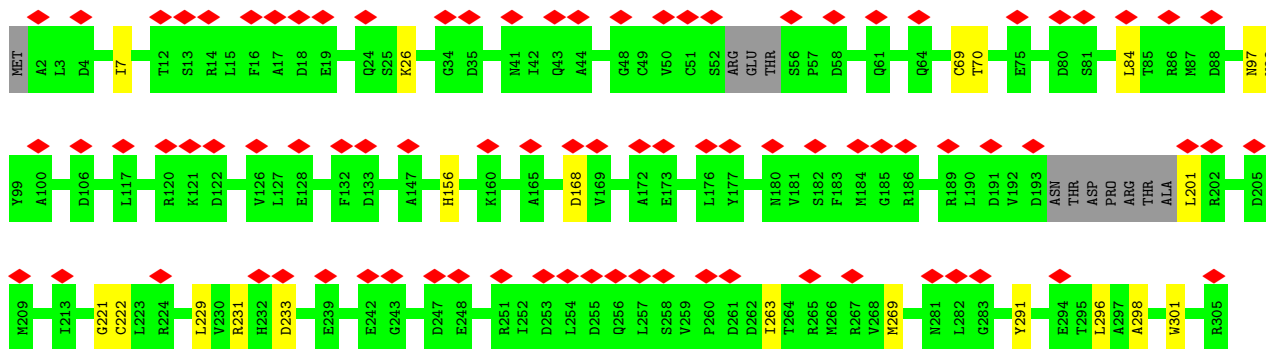
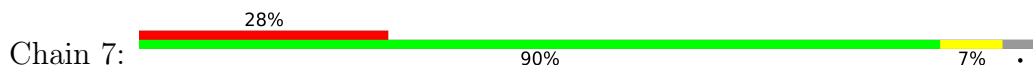




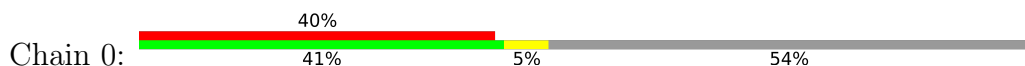
• Molecule 6: Triplex capsid protein 2



• Molecule 6: Triplex capsid protein 2



• Molecule 7: Small capsomere-interacting protein





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C5	Depositor
Number of particles used	39773	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 ( $e^-/\text{\AA}^2$ )	25	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	24271	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.052	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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 angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	k	0.23	0/2753	0.49	2/3755 (0.1%)
2	l	0.21	0/698	0.47	0/942
2	m	0.19	0/656	0.48	0/887
3	n	0.22	0/326	0.43	0/437
3	o	0.22	0/326	0.42	0/437
4	S	0.25	0/10300	0.53	3/13998 (0.0%)
4	T	0.28	0/10919	0.62	5/14839 (0.0%)
4	W	0.26	0/10874	0.63	7/14780 (0.0%)
4	X	0.25	0/10350	0.53	4/14071 (0.0%)
5	5	0.21	0/2127	0.48	2/2891 (0.1%)
5	b	0.25	0/2540	0.57	2/3452 (0.1%)
6	6	0.24	0/2376	0.54	1/3234 (0.0%)
6	7	0.22	0/2360	0.51	0/3210
6	c	0.24	0/2376	0.56	0/3234
6	d	0.23	0/2411	0.54	0/3281
7	0	0.21	0/682	0.55	2/919 (0.2%)
7	1	0.21	0/682	0.55	2/919 (0.2%)
7	2	0.21	0/682	0.55	2/919 (0.2%)
7	3	0.21	0/682	0.55	2/919 (0.2%)
All	All	0.25	0/64120	0.56	34/87124 (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
4	S	0	2
4	T	0	5
4	W	0	5
4	X	0	1
All	All	0	13

There are no bond length outliers.

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	W	262	SER	CA-C-N	6.90	134.73	121.54
4	W	262	SER	C-N-CA	6.90	134.73	121.54
7	3	20	ALA	CA-C-N	6.71	133.78	121.70
7	3	20	ALA	C-N-CA	6.71	133.78	121.70
7	2	20	ALA	CA-C-N	6.71	133.77	121.70
7	2	20	ALA	C-N-CA	6.71	133.77	121.70
7	1	20	ALA	CA-C-N	6.71	133.77	121.70
7	1	20	ALA	C-N-CA	6.71	133.77	121.70
7	0	20	ALA	CA-C-N	6.70	133.77	121.70
7	0	20	ALA	C-N-CA	6.70	133.77	121.70
4	T	262	SER	CA-C-N	6.05	129.21	120.79
4	T	262	SER	C-N-CA	6.05	129.21	120.79
4	X	1204	VAL	N-CA-C	-6.05	106.60	112.29
4	W	421	GLY	N-CA-C	5.95	119.69	112.49
6	6	279	ILE	N-CA-C	-5.83	108.17	113.71
4	W	308	VAL	N-CA-C	-5.55	106.97	111.91
5	5	296	PHE	CA-C-N	5.52	135.87	125.66
5	5	296	PHE	C-N-CA	5.52	135.87	125.66
4	X	993	SER	N-CA-C	5.50	121.98	109.81
4	T	415	THR	N-CA-C	-5.45	107.88	114.75
4	S	993	SER	N-CA-C	5.45	121.86	109.81
4	T	1113	VAL	N-CA-CB	-5.41	104.88	112.35
4	W	848	ASP	CA-C-N	5.38	131.81	121.54
4	W	848	ASP	C-N-CA	5.38	131.81	121.54
4	S	992	LYS	CA-C-N	5.32	134.78	121.80
4	S	992	LYS	C-N-CA	5.32	134.78	121.80
5	b	211	CYS	CA-C-N	5.25	139.60	127.00
5	b	211	CYS	C-N-CA	5.25	139.60	127.00
4	W	262	SER	N-CA-C	5.23	119.41	113.19
1	k	88	HIS	CA-C-N	5.23	131.52	121.54
1	k	88	HIS	C-N-CA	5.23	131.52	121.54
4	X	992	LYS	CA-C-N	5.08	134.20	121.80
4	X	992	LYS	C-N-CA	5.08	134.20	121.80
4	T	652	ASN	N-CA-C	5.04	116.59	111.14

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	S	991	HIS	Peptide

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Mol	Chain	Res	Type	Group
4	S	992	LYS	Peptide
4	T	10	PHE	Peptide
4	T	505	ASN	Peptide
4	T	537	HIS	Peptide
4	T	886	PRO	Peptide
4	T	944	PHE	Peptide
4	W	262	SER	Peptide
4	W	263	THR	Mainchain
4	W	537	HIS	Peptide
4	W	848	ASP	Peptide
4	W	849	ASP	Peptide
4	X	991	HIS	Peptide

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	k	2680	0	2675	28	0
2	l	686	0	704	7	0
2	m	645	0	653	11	0
3	n	323	0	353	3	0
3	o	323	0	353	2	0
4	S	10061	0	9954	99	0
4	T	10667	0	10542	103	0
4	W	10622	0	10500	121	0
4	X	10108	0	9980	106	0
5	5	2074	0	2050	19	0
5	b	2478	0	2466	18	0
6	6	2330	0	2354	19	0
6	7	2315	0	2335	14	0
6	c	2330	0	2354	30	0
6	d	2365	0	2379	19	0
7	0	666	0	647	5	0
7	1	666	0	647	3	0
7	2	666	0	647	5	0
7	3	666	0	647	4	0
All	All	62671	0	62240	537	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 4.

All (537) 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)
4:S:777:ARG:NH2	4:S:885:CYS:O	2.27	0.67
4:T:536:VAL:HG13	4:T:1244:SER:HA	1.77	0.66
4:S:770:LEU:HD21	4:S:883:LEU:HD22	1.76	0.66
4:W:770:LEU:HD21	4:W:883:LEU:HD22	1.76	0.66
4:W:929:ASP:OD1	4:W:932:ARG:NH2	2.29	0.66
4:S:1182:THR:HG23	4:S:1236:ASN:HB3	1.78	0.65
4:T:1201:ALA:HB3	4:T:1227:PRO:HG2	1.79	0.65
4:W:602:GLU:HB3	4:W:647:LYS:HE2	1.78	0.64
4:W:658:ARG:HA	4:W:681:LEU:HD11	1.78	0.64
4:W:1200:ARG:NH1	4:W:1221:ASP:O	2.30	0.64
4:T:1187:ASP:OD2	4:T:1232:ARG:NH2	2.32	0.63
4:T:1241:GLN:HB3	4:T:1244:SER:HB3	1.82	0.62
4:X:658:ARG:HA	4:X:681:LEU:HD11	1.81	0.62
4:S:1111:MET:SD	4:S:1366:ARG:NH2	2.72	0.62
4:W:144:GLU:OE1	5:b:10:ARG:NH1	2.32	0.62
4:T:929:ASP:OD1	4:T:932:ARG:NH2	2.33	0.61
2:m:80:ARG:NH1	3:o:2622:SER:OG	2.34	0.61
6:7:69:CYS:SG	6:7:70:THR:N	2.74	0.61
4:W:796:ASN:OD1	4:X:932:ARG:NH1	2.33	0.61
4:W:278:THR:HG22	4:W:1051:ILE:HG12	1.83	0.61
4:T:1280:ARG:NH2	4:T:1288:GLU:OE1	2.34	0.60
4:S:658:ARG:HA	4:S:681:LEU:HD11	1.83	0.60
6:6:201:LEU:HD13	6:7:231:ARG:HH22	1.66	0.60
5:5:150:MET:HE2	5:5:241:MET:HE3	1.82	0.60
5:5:234:ARG:HD3	5:5:274:LEU:HD11	1.82	0.60
4:T:540:PHE:O	4:T:559:ARG:NH1	2.35	0.59
4:S:416:SER:HB3	4:S:1349:ALA:HB2	1.82	0.59
6:c:111:LEU:HB2	6:c:286:LEU:HB2	1.84	0.59
4:T:129:ILE:HB	4:T:1080:PHE:HB2	1.84	0.59
4:T:717:LEU:HA	4:T:915:GLN:HE22	1.66	0.59
1:k:46:ARG:NH2	1:k:347:GLU:OE2	2.35	0.59
4:X:633:LEU:HD12	4:X:874:MET:HB3	1.85	0.59
4:X:1182:THR:HG23	4:X:1236:ASN:HB3	1.85	0.59
6:c:58:ASP:HB3	6:c:196:ASP:HB3	1.84	0.59
4:T:591:VAL:HB	4:T:683:GLU:HB2	1.85	0.59
1:k:277:PRO:HG2	1:k:282:LEU:HD12	1.83	0.59
6:c:5:LYS:HB2	6:c:86:ARG:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:259:LYS:HE2	4:X:60:VAL:HB	1.84	0.58
4:S:1047:LEU:HD12	4:S:1106:ALA:HB3	1.85	0.58
4:W:481:TYR:OH	4:W:979:VAL:O	2.20	0.58
4:W:578:ARG:NH2	4:W:1017:GLN:OE1	2.37	0.58
4:S:742:ILE:HG12	4:S:788:LEU:HD22	1.85	0.58
4:T:275:VAL:HG22	4:T:375:ALA:HB3	1.84	0.58
4:S:587:ASN:HB2	4:T:572:ARG:HH22	1.68	0.58
2:m:95:ILE:HD13	3:n:2605:LEU:HB3	1.85	0.58
4:W:850:ILE:HD12	4:W:870:PRO:HG2	1.86	0.58
2:m:37:PRO:HB3	4:X:506:VAL:HG21	1.86	0.57
4:S:692:LEU:HD13	4:T:972:ARG:HG2	1.86	0.57
4:X:718:LEU:O	4:X:915:GLN:NE2	2.37	0.57
5:b:90:LEU:HD11	5:b:165:MET:HG3	1.85	0.57
4:X:1192:GLN:NE2	4:X:1359:GLU:O	2.36	0.57
4:S:603:THR:HG22	4:S:647:LYS:HB3	1.87	0.57
4:W:447:GLN:HB3	4:W:1028:ALA:HB1	1.87	0.57
4:W:182:LYS:NZ	4:W:1058:SER:OG	2.38	0.57
4:W:1313:ASP:OD2	4:X:203:ARG:NH1	2.38	0.56
4:S:447:GLN:NE2	4:T:521:GLU:OE1	2.38	0.56
4:T:946:LYS:HE2	4:T:993:SER:HA	1.86	0.56
5:5:289:CYS:SG	5:5:290:THR:N	2.78	0.56
6:6:189:ARG:NH1	6:6:190:LEU:O	2.38	0.56
4:S:718:LEU:O	4:S:915:GLN:NE2	2.35	0.56
1:k:412:SER:HB3	2:m:34:ILE:HG12	1.87	0.56
4:W:965:VAL:HG13	4:W:972:ARG:HG2	1.88	0.56
4:X:698:GLU:HG3	4:X:705:ILE:HD12	1.88	0.56
6:6:111:LEU:HB2	6:6:286:LEU:HB2	1.88	0.56
6:7:156:HIS:HD2	6:7:201:LEU:HB2	1.71	0.56
4:T:658:ARG:HA	4:T:681:LEU:HD11	1.88	0.56
4:T:293:VAL:HG21	4:T:368:LYS:HE3	1.88	0.55
5:b:289:CYS:SG	5:b:290:THR:N	2.79	0.55
6:6:227:THR:O	6:6:231:ARG:NH1	2.39	0.55
4:S:94:LYS:HB2	4:X:58:THR:HG22	1.89	0.55
4:X:785:ARG:NH1	4:X:787:VAL:O	2.39	0.55
6:c:300:CYS:SG	6:c:301:TRP:N	2.79	0.55
6:7:231:ARG:HG2	6:7:233:ASP:H	1.71	0.55
6:7:7:ILE:HB	6:7:84:LEU:HB2	1.89	0.55
4:W:399:THR:HG22	4:W:1043:THR:HG22	1.87	0.55
4:X:516:ALA:HB2	4:X:994:PRO:HG3	1.89	0.55
4:X:559:ARG:HH11	4:X:565:ILE:HG12	1.72	0.55
6:c:35:ASP:HB2	6:c:40:GLN:HE22	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:b:40:ASP:O	6:c:2:ALA:N	2.40	0.55
4:T:640:THR:O	4:T:644:ASN:ND2	2.39	0.55
4:X:278:THR:HG22	4:X:1051:ILE:HG12	1.89	0.55
6:c:9:VAL:HG21	6:c:45:LEU:HD21	1.89	0.55
5:b:128:VAL:HG11	5:b:312:LEU:HD22	1.88	0.55
4:X:833:LEU:HA	4:X:859:LEU:HD11	1.88	0.54
4:X:559:ARG:O	4:X:564:ASN:ND2	2.35	0.54
4:S:127:ALA:HB2	4:T:101:ALA:HB2	1.89	0.54
6:c:179:THR:OG1	6:c:189:ARG:NH1	2.41	0.54
4:S:218:LYS:NZ	4:S:1325:GLU:OE1	2.36	0.54
4:T:832:THR:HG22	7:3:11:ILE:HD11	1.88	0.54
1:k:91:ASN:ND2	1:k:270:SER:OG	2.41	0.54
4:W:1044:ASP:HA	4:W:1109:THR:HG21	1.87	0.54
4:X:708:LEU:HD21	4:X:1022:PRO:HG2	1.90	0.54
4:T:572:ARG:NH1	4:T:1001:SER:O	2.41	0.54
4:S:633:LEU:HA	4:S:874:MET:HE3	1.87	0.54
4:W:93:PHE:HB2	4:W:116:VAL:HB	1.90	0.54
6:c:201:LEU:HD22	6:d:231:ARG:HH21	1.73	0.54
4:T:182:LYS:NZ	4:T:1058:SER:OG	2.41	0.53
4:W:1198:ARG:NH2	4:W:1219:LEU:O	2.40	0.53
5:5:72:ASP:OD1	5:5:188:ARG:NH1	2.40	0.53
1:k:116:LEU:HD23	1:k:118:LEU:H	1.73	0.53
4:S:7:GLN:NE2	4:S:36:GLN:OE1	2.41	0.53
4:T:537:HIS:HA	4:T:1238:TRP:CD1	2.42	0.53
4:W:736:ARG:HH21	4:W:900:PRO:HB3	1.74	0.53
4:W:1107:ILE:HD11	4:W:1364:MET:HE1	1.90	0.53
4:X:619:MET:SD	4:X:881:SER:OG	2.67	0.53
4:W:537:HIS:HA	4:W:1238:TRP:CD1	2.44	0.53
6:7:97:ASN:HB3	6:7:296:LEU:HD22	1.90	0.53
1:k:404:ASP:OD1	4:X:551:ARG:NH1	2.41	0.53
4:W:1027:GLN:HB3	4:W:1032:MET:HB2	1.90	0.53
4:W:1045:GLU:N	4:W:1109:THR:OG1	2.40	0.53
4:X:1111:MET:SD	4:X:1366:ARG:NH2	2.79	0.53
6:d:88:ASP:HB2	6:d:91:ASP:HB2	1.91	0.53
4:S:183:LEU:HD13	4:S:394:ARG:HH21	1.72	0.53
6:c:126:VAL:HG23	6:c:133:ASP:HB3	1.90	0.53
4:W:214:VAL:HA	4:W:217:PHE:HD2	1.74	0.53
6:6:224:ARG:NH2	6:7:168:ASP:OD2	2.41	0.53
4:W:561:MET:HE3	4:W:990:TRP:HB3	1.90	0.53
5:5:254:GLU:HG2	6:6:64:GLN:HE21	1.74	0.53
4:T:93:PHE:HB2	4:T:116:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:183:LEU:HD13	4:W:394:ARG:HH21	1.73	0.53
4:W:447:GLN:NE2	4:X:521:GLU:OE1	2.42	0.53
4:X:1183:PRO:HG2	4:X:1237:PRO:HD2	1.91	0.53
5:b:94:LYS:NZ	6:d:106:ASP:OD2	2.38	0.53
5:5:324:CYS:SG	5:5:325:GLY:N	2.81	0.53
4:W:543:PHE:HZ	4:W:555:ARG:HH11	1.57	0.52
4:S:770:LEU:HD22	7:2:55:HIS:HD2	1.75	0.52
4:S:1167:PRO:HD3	4:T:1224:ILE:HD13	1.91	0.52
6:c:177:TYR:HB3	6:d:263:ILE:HG21	1.90	0.52
1:k:19:ALA:HB3	1:k:83:LEU:HB2	1.89	0.52
4:T:1071:ARG:O	4:T:1079:THR:OG1	2.25	0.52
4:W:582:PHE:HA	4:W:1032:MET:HE1	1.91	0.52
6:c:262:ASP:OD2	6:d:158:TYR:OH	2.27	0.52
4:S:1027:GLN:HB3	4:S:1032:MET:HB2	1.91	0.52
4:W:275:VAL:HG22	4:W:375:ALA:HB3	1.90	0.52
4:S:451:LYS:HB3	4:S:1117:ASP:HB3	1.90	0.52
4:W:1073:VAL:HG13	4:W:1078:VAL:HG22	1.92	0.52
7:0:78:ARG:NH2	7:1:19:TYR:O	2.43	0.52
4:T:770:LEU:HD21	4:T:883:LEU:HD22	1.92	0.52
5:5:228:ALA:HB2	5:5:291:LEU:HD11	1.91	0.52
4:S:49:ARG:HD3	4:T:87:ILE:HD11	1.91	0.52
4:W:90:LYS:HE2	4:W:117:MET:HE1	1.90	0.52
4:S:623:GLN:HG3	4:S:626:LYS:HD3	1.91	0.52
4:S:725:ASP:HB3	4:S:793:LEU:HD22	1.91	0.52
4:S:1169:LEU:O	4:T:211:SER:OG	2.22	0.52
6:6:212:CYS:N	6:7:222:CYS:SG	2.83	0.52
2:l:80:ARG:NH2	3:n:2622:SER:OG	2.43	0.52
4:T:1005:THR:HG22	4:T:1007:GLY:H	1.76	0.51
4:W:75:CYS:SG	4:W:1059:THR:OG1	2.68	0.51
4:S:698:GLU:HG3	4:S:705:ILE:HD12	1.92	0.51
4:T:526:PRO:HG3	4:T:1225:PRO:HB3	1.92	0.51
4:X:256:THR:HG22	4:X:258:PHE:H	1.75	0.51
6:d:97:ASN:HD22	6:d:105:TRP:CD1	2.29	0.51
4:W:1070:ARG:NH1	6:c:2:ALA:O	2.42	0.51
4:S:1344:ASN:ND2	4:S:1347:THR:OG1	2.43	0.51
4:T:854:LEU:HD13	4:T:860:LYS:HG2	1.92	0.51
4:X:624:GLU:HB3	4:X:762:ARG:HH12	1.74	0.51
4:S:1332:ALA:HB1	4:S:1337:MET:HB2	1.92	0.51
4:W:92:GLN:HE22	4:W:115:ILE:HG23	1.76	0.51
6:c:58:ASP:OD1	6:c:58:ASP:N	2.43	0.51
4:S:1117:ASP:OD1	4:S:1117:ASP:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:k:409:VAL:HA	1:k:430:PRO:HA	1.92	0.51
4:T:278:THR:HG22	4:T:1051:ILE:HG12	1.93	0.51
4:X:264:TYR:HE1	4:X:300:PRO:HD2	1.76	0.51
4:S:9:PRO:HB3	4:S:45:GLU:HB3	1.93	0.50
4:T:889:THR:HA	4:T:920:ASN:HB3	1.91	0.50
4:W:480:GLY:HA3	4:W:483:LEU:HD11	1.93	0.50
6:d:97:ASN:HD22	6:d:105:TRP:HD1	1.59	0.50
4:T:578:ARG:NH2	4:T:1017:GLN:OE1	2.44	0.50
4:W:851:LEU:HD23	4:W:854:LEU:HD12	1.92	0.50
6:d:47:LEU:HB2	6:d:135:VAL:HB	1.94	0.50
4:S:1294:ALA:HB3	4:S:1318:GLN:HE21	1.77	0.50
4:T:146:PRO:HA	4:T:149:PHE:HD2	1.77	0.50
1:k:94:PRO:HG3	1:k:271:PHE:HD1	1.76	0.50
4:S:100:ILE:HG12	4:X:172:ARG:HB3	1.93	0.50
4:W:398:TYR:O	4:W:1044:ASP:N	2.44	0.50
1:k:315:ARG:NH2	1:k:391:GLY:O	2.45	0.50
4:S:295:SER:HA	4:S:365:SER:HA	1.93	0.50
6:6:11:LEU:HG	6:6:15:LEU:HD23	1.93	0.50
4:S:826:TYR:OH	4:S:920:ASN:O	2.30	0.50
4:W:438:ASN:HD22	4:W:1171:HIS:HD2	1.59	0.50
1:k:25:ARG:NH2	4:X:737:GLN:O	2.45	0.50
4:S:211:SER:OG	4:X:1169:LEU:O	2.22	0.50
4:T:332:ARG:NH2	4:T:346:ASP:OD1	2.44	0.50
4:T:777:ARG:NH2	4:T:885:CYS:O	2.45	0.50
6:d:53:ARG:NH2	6:d:133:ASP:OD2	2.45	0.50
4:S:773:ILE:O	4:S:776:THR:OG1	2.30	0.49
4:S:1337:MET:HE1	4:S:1349:ALA:HB3	1.94	0.49
4:W:695:ALA:HB1	4:W:706:THR:HG22	1.94	0.49
4:W:603:THR:HG22	4:W:647:LYS:HB3	1.94	0.49
4:W:963:ASN:O	4:W:967:ARG:N	2.44	0.49
4:T:717:LEU:HD23	4:T:804:LYS:HD3	1.95	0.49
6:c:266:MET:HE1	6:d:211:LEU:HD13	1.94	0.49
6:6:114:LEU:HD11	6:6:145:GLY:HA2	1.92	0.49
4:T:868:ILE:HG22	4:T:870:PRO:HD3	1.95	0.49
4:T:757:ILE:HG12	4:T:788:LEU:HD22	1.94	0.49
4:X:1247:ASP:OD1	4:X:1251:ASN:ND2	2.39	0.49
1:k:114:ARG:NH1	1:k:286:ASP:OD2	2.46	0.49
4:T:543:PHE:HE1	4:T:557:THR:HG23	1.76	0.49
4:W:963:ASN:HA	4:W:966:THR:HG22	1.94	0.49
4:S:559:ARG:O	4:S:564:ASN:ND2	2.37	0.49
4:T:811:MET:HB3	4:T:819:MET:HE1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:824:VAL:H	4:W:889:THR:HG21	1.78	0.49
4:T:218:LYS:HZ3	4:T:1323:LEU:HB3	1.78	0.49
5:b:211:CYS:HB2	5:b:213:MET:HB2	1.94	0.49
4:T:1198:ARG:NH2	4:T:1219:LEU:O	2.43	0.49
4:X:394:ARG:HD3	4:X:1315:PHE:HB3	1.95	0.49
4:X:1220:TYR:HE2	4:X:1272:LYS:HD3	1.78	0.48
1:k:379:THR:HG21	4:X:549:GLY:H	1.76	0.48
4:W:714:ASP:O	4:W:804:LYS:NZ	2.46	0.48
4:X:380:GLN:HG2	4:X:384:ASN:HD21	1.77	0.48
4:X:447:GLN:HB3	4:X:1028:ALA:HB1	1.95	0.48
4:X:1071:ARG:HH12	4:X:1081:GLU:HB3	1.77	0.48
5:b:167:GLN:HB2	5:b:188:ARG:HG3	1.93	0.48
6:7:26:LYS:HA	6:7:98:VAL:HG21	1.95	0.48
4:X:1190:TYR:OH	4:X:1196:ASN:O	2.25	0.48
2:m:92:LYS:HA	2:m:95:ILE:HD12	1.95	0.48
4:W:402:PHE:HD2	4:W:1040:VAL:HB	1.78	0.48
4:W:1071:ARG:O	4:W:1079:THR:OG1	2.29	0.48
4:X:578:ARG:NH1	4:X:1014:SER:O	2.43	0.48
1:k:269:LEU:HD12	2:l:72:ARG:HE	1.79	0.48
4:W:266:THR:HG21	4:W:373:PHE:HD2	1.78	0.48
4:W:606:ASP:OD1	4:W:647:LYS:NZ	2.37	0.48
5:b:124:GLN:NE2	5:b:311:SER:O	2.47	0.48
5:b:198:THR:HG22	5:b:316:VAL:HG23	1.96	0.48
4:W:1042:ARG:NH2	4:W:1111:MET:O	2.47	0.48
4:X:510:PRO:HD2	4:X:513:ALA:HB3	1.96	0.48
4:X:1047:LEU:HD12	4:X:1106:ALA:HB3	1.95	0.48
5:5:152:THR:HA	5:5:281:ASN:HB3	1.95	0.48
1:k:25:ARG:HH22	4:X:739:ILE:HG12	1.78	0.48
4:T:770:LEU:HD11	4:T:883:LEU:HD13	1.96	0.48
4:W:394:ARG:NH1	4:W:1317:ASP:OD2	2.46	0.48
4:W:575:GLN:NE2	4:W:1015:MET:SD	2.87	0.48
4:X:238:LYS:HG2	4:X:289:LEU:HD22	1.96	0.48
4:X:1068:VAL:HG22	4:X:1082:ILE:HG12	1.95	0.48
4:T:402:PHE:HD2	4:T:1040:VAL:HB	1.79	0.47
4:T:575:GLN:NE2	4:T:1015:MET:SD	2.87	0.47
4:W:1062:PHE:HB2	4:W:1087:ALA:HB3	1.96	0.47
4:X:450:LEU:HD11	4:X:1025:ILE:HG13	1.94	0.47
6:c:138:MET:HE2	6:c:140:VAL:HG22	1.96	0.47
6:d:94:GLN:HE21	6:d:297:ALA:HB1	1.79	0.47
5:5:124:GLN:NE2	5:5:311:SER:O	2.47	0.47
4:T:90:LYS:HE2	4:T:117:MET:HE1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:1118:LEU:HD23	4:W:1121:ILE:HD13	1.96	0.47
4:W:1341:TYR:HA	4:W:1348:HIS:HD2	1.77	0.47
4:T:41:LYS:O	4:T:44:ARG:NH1	2.47	0.47
4:W:256:THR:HG22	4:W:258:PHE:H	1.79	0.47
6:c:291:TYR:HD1	6:c:298:ALA:HB2	1.79	0.47
2:l:91:VAL:HG22	3:n:2608:PHE:HB3	1.97	0.47
4:S:53:LEU:HD22	4:T:323:MET:HE1	1.97	0.47
4:S:1043:THR:HG23	4:S:1265:PRO:HB3	1.96	0.47
4:T:399:THR:HG22	4:T:1043:THR:HG22	1.96	0.47
4:X:640:THR:O	4:X:644:ASN:ND2	2.47	0.47
4:X:1062:PHE:HB2	4:X:1087:ALA:HB3	1.96	0.47
5:5:329:VAL:HG21	6:6:271:SER:HB2	1.97	0.47
2:m:21:GLY:H	5:b:121:LYS:HZ1	1.61	0.47
4:T:1250:TYR:HB2	4:T:1270:PHE:HD2	1.79	0.47
4:W:324:ARG:NH1	4:W:325:ASN:OD1	2.48	0.47
5:b:81:SER:OG	5:b:84:GLU:OE2	2.32	0.47
1:k:368:ASP:N	1:k:368:ASP:OD1	2.47	0.47
4:S:1334:HIS:HB2	4:S:1355:GLN:HG2	1.95	0.47
4:T:1342:MET:HA	4:T:1375:VAL:HG21	1.97	0.47
4:X:252:VAL:HG13	4:X:1096:SER:HA	1.96	0.47
4:X:929:ASP:OD1	4:X:932:ARG:NH2	2.47	0.47
6:6:133:ASP:OD1	6:6:133:ASP:N	2.47	0.47
4:T:770:LEU:HD22	7:3:55:HIS:HD2	1.80	0.47
4:T:1207:CYS:SG	4:T:1208:ASP:N	2.87	0.47
4:W:214:VAL:HG12	4:W:218:LYS:HE2	1.95	0.47
4:W:407:HIS:HB2	4:W:1184:VAL:HG12	1.96	0.47
4:X:716:HIS:HD2	4:X:736:ARG:HH21	1.61	0.47
4:X:1198:ARG:NH2	4:X:1219:LEU:O	2.42	0.47
4:S:1200:ARG:HG2	4:S:1226:ASP:HB3	1.96	0.47
4:T:82:ASP:OD1	4:T:82:ASP:N	2.46	0.47
4:T:1067:SER:OG	4:T:1083:THR:OG1	2.33	0.47
4:X:77:ASN:HB3	4:X:303:TYR:HD1	1.78	0.47
4:X:1271:HIS:ND1	4:X:1274:ASP:OD2	2.47	0.47
4:W:276:LEU:HA	4:W:1053:TYR:HA	1.97	0.47
4:X:620:ILE:HG22	4:X:622:GLY:H	1.80	0.47
4:W:491:MET:HB2	4:W:783:ASP:HA	1.96	0.47
4:S:488:THR:OG1	4:S:982:ASN:ND2	2.34	0.46
4:S:526:PRO:HB3	4:S:1233:SER:HB2	1.97	0.46
4:T:893:ARG:NH2	4:T:988:GLU:OE1	2.47	0.46
4:W:184:ARG:O	4:W:1290:SER:OG	2.33	0.46
4:X:716:HIS:CD2	4:X:736:ARG:HE	2.33	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:c:204:LEU:HD23	6:c:207:LEU:HD12	1.97	0.46
4:S:100:ILE:HG13	4:X:386:THR:HG21	1.97	0.46
4:S:394:ARG:NH1	4:S:1317:ASP:OD2	2.49	0.46
4:W:175:VAL:HG21	4:W:382:MET:HE1	1.97	0.46
4:S:1173:GLN:HE21	4:S:1305:GLN:HA	1.80	0.46
4:T:1062:PHE:HB2	4:T:1087:ALA:HB3	1.97	0.46
6:c:280:PHE:O	6:d:274:GLN:NE2	2.49	0.46
4:T:773:ILE:O	4:T:776:THR:OG1	2.33	0.46
4:W:1254:PHE:HB2	4:W:1267:ARG:HH22	1.79	0.46
4:X:401:PHE:HE2	4:X:1191:PHE:HD1	1.62	0.46
5:5:224:VAL:HG13	5:5:294:VAL:HB	1.97	0.46
4:W:79:GLU:N	4:W:304:ALA:O	2.49	0.46
4:S:481:TYR:HH	4:S:979:VAL:H	1.59	0.46
4:X:138:LEU:HD13	4:X:151:GLU:HG3	1.97	0.46
4:X:718:LEU:HD21	4:X:730:LEU:HD12	1.97	0.46
1:k:356:THR:HG22	1:k:450:ARG:HG2	1.98	0.46
4:S:811:MET:O	4:S:815:SER:OG	2.26	0.46
4:S:1067:SER:OG	4:S:1083:THR:OG1	2.33	0.46
4:T:91:ILE:HD12	4:T:1089:LEU:HD21	1.97	0.46
4:T:175:VAL:HG21	4:T:382:MET:HE1	1.97	0.46
4:T:860:LYS:O	4:T:864:GLN:N	2.47	0.46
4:T:1195:SER:O	4:T:1326:ALA:N	2.47	0.46
4:W:1005:THR:HG22	4:W:1007:GLY:H	1.79	0.46
4:X:453:ILE:HD11	4:X:1038:MET:HE1	1.97	0.46
1:k:371:GLY:H	1:k:378:HIS:CE1	2.34	0.46
4:S:98:PRO:HG3	4:X:61:VAL:HG11	1.97	0.46
4:W:918:LEU:HD22	4:W:944:PHE:HZ	1.80	0.46
4:X:1321:HIS:O	4:X:1324:GLN:NE2	2.46	0.46
4:S:1190:TYR:OH	4:S:1196:ASN:O	2.30	0.46
4:T:95:ILE:HB	4:T:114:TYR:HB2	1.98	0.46
4:X:84:ARG:O	6:6:78:ARG:NH2	2.48	0.46
4:W:718:LEU:HD12	4:W:894:VAL:HG21	1.98	0.45
4:W:1308:VAL:HG21	4:W:1314:VAL:HG21	1.97	0.45
4:X:399:THR:HG22	4:X:1043:THR:HG22	1.97	0.45
4:X:1369:LYS:HG2	4:X:1374:VAL:HG22	1.98	0.45
4:W:1342:MET:HE1	4:W:1370:LEU:HB3	1.98	0.45
4:X:276:LEU:HB3	4:X:376:ILE:HG12	1.97	0.45
4:X:633:LEU:HA	4:X:874:MET:HE3	1.98	0.45
4:S:582:PHE:HA	4:S:1032:MET:HE1	1.98	0.45
4:S:615:VAL:HG22	4:S:938:MET:HE1	1.97	0.45
4:T:1115:CYS:HA	4:T:1177:CYS:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:X:82:ASP:OD1	4:X:82:ASP:N	2.48	0.45
4:S:898:ARG:HE	4:S:913:VAL:HB	1.81	0.45
4:W:1201:ALA:HB3	4:W:1227:PRO:HG2	1.99	0.45
4:S:1227:PRO:O	4:X:1170:SER:OG	2.31	0.45
4:X:1200:ARG:HG2	4:X:1226:ASP:HB3	1.99	0.45
2:m:52:GLN:HE22	4:X:490:ASN:HD21	1.64	0.45
4:S:71:LEU:N	4:S:377:GLU:OE2	2.48	0.45
4:X:603:THR:HG22	4:X:647:LYS:HB3	1.99	0.45
4:S:1236:ASN:OD1	4:S:1236:ASN:N	2.49	0.45
4:T:623:GLN:HB2	4:T:626:LYS:HB2	1.99	0.45
4:W:1173:GLN:NE2	4:W:1302:THR:O	2.50	0.45
4:W:130:GLU:HG3	4:X:110:LYS:HD2	1.98	0.45
4:T:725:ASP:HB3	4:T:793:LEU:HG	1.99	0.45
4:W:276:LEU:HB3	4:W:1053:TYR:HD1	1.82	0.45
4:X:788:LEU:HD12	4:X:919:VAL:HG11	1.99	0.45
4:S:1183:PRO:HG2	4:S:1237:PRO:HD2	1.98	0.45
4:T:130:GLU:HG2	4:T:1079:THR:HG22	1.98	0.45
6:d:144:LEU:O	6:d:148:ILE:N	2.38	0.45
4:S:245:LEU:HD22	4:S:369:ILE:HD13	1.99	0.44
4:S:1005:THR:HG22	4:S:1007:GLY:H	1.82	0.44
4:T:555:ARG:HE	4:T:907:HIS:CD2	2.34	0.44
4:W:611:LEU:HD13	4:W:935:ALA:HB1	1.98	0.44
4:W:902:GLN:NE2	4:W:1020:SER:OG	2.43	0.44
4:W:987:TYR:O	4:W:992:LYS:NZ	2.50	0.44
1:k:3:ALA:O	1:k:7:ASN:ND2	2.51	0.44
4:S:521:GLU:CD	4:X:447:GLN:HE22	2.24	0.44
4:W:504:LYS:HG2	4:W:964:TYR:HE1	1.82	0.44
4:X:501:TYR:OH	4:X:978:ASN:O	2.31	0.44
6:7:291:TYR:HD1	6:7:298:ALA:HB2	1.82	0.44
4:S:423:GLU:OE2	4:X:420:ARG:NH2	2.51	0.44
4:W:278:THR:HB	4:W:282:VAL:HB	2.00	0.44
5:b:199:LEU:HD12	5:b:204:LEU:HD12	1.99	0.44
5:5:85:PRO:O	5:5:88:THR:OG1	2.27	0.44
4:S:453:ILE:HD11	4:S:1038:MET:HE1	1.99	0.44
4:W:788:LEU:HD11	4:W:919:VAL:HG21	1.99	0.44
1:k:342:ARG:HH12	2:l:43:ARG:HG3	1.83	0.44
4:T:566:PRO:HG2	4:T:569:LEU:HD12	2.00	0.44
4:W:128:GLU:OE1	4:X:110:LYS:NZ	2.37	0.44
6:c:32:PRO:HD3	6:c:137:PRO:HG3	2.00	0.44
6:7:221:GLY:HA3	6:7:269:MET:HE1	1.99	0.44
4:X:185:HIS:O	4:X:1097:SER:OG	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:S:591:VAL:N	4:S:683:GLU:OE1	2.50	0.44
4:S:1169:LEU:H	4:S:1169:LEU:HG	1.47	0.44
5:5:227:TYR:HB2	5:5:246:PHE:HB2	1.99	0.44
4:S:56:VAL:HG22	4:T:92:GLN:HB3	2.00	0.44
4:S:93:PHE:HE1	4:S:257:VAL:HG21	1.82	0.44
4:S:578:ARG:NH1	4:S:1014:SER:OG	2.50	0.44
4:X:582:PHE:HA	4:X:1032:MET:HE1	1.98	0.44
6:d:231:ARG:HB3	6:d:233:ASP:H	1.82	0.44
4:W:585:VAL:HG11	4:W:1030:HIS:HB3	1.99	0.43
4:S:711:ALA:HB3	4:S:1016:HIS:HB3	2.00	0.43
4:T:407:HIS:HB2	4:T:1184:VAL:HG12	1.99	0.43
4:T:436:ASN:HD21	4:T:442:LEU:HG	1.82	0.43
4:W:626:LYS:NZ	4:W:881:SER:O	2.44	0.43
4:T:75:CYS:SG	4:T:1059:THR:OG1	2.74	0.43
6:6:272:TYR:O	6:6:275:SER:OG	2.30	0.43
1:k:47:PHE:HB2	1:k:52:GLY:HA2	1.99	0.43
4:T:79:GLU:N	4:T:304:ALA:O	2.51	0.43
4:W:770:LEU:HD22	7:0:55:HIS:HD2	1.82	0.43
4:X:850:ILE:HG13	4:X:870:PRO:HG2	2.01	0.43
4:W:737:GLN:HE21	4:W:897:LYS:HD2	1.84	0.43
4:X:174:LEU:HD23	4:X:1086:ILE:HD11	2.00	0.43
4:X:290:LEU:HB3	4:X:367:VAL:HG21	2.01	0.43
4:X:979:VAL:HG11	4:X:984:MET:HE2	1.99	0.43
6:d:11:LEU:HD12	6:d:80:ASP:HB2	1.99	0.43
4:T:760:ARG:HH22	4:T:886:PRO:HA	1.83	0.43
4:W:1342:MET:HA	4:W:1375:VAL:HG21	2.00	0.43
4:X:1334:HIS:HB2	4:X:1355:GLN:HG2	2.01	0.43
5:b:228:ALA:HB2	5:b:291:LEU:HD11	2.01	0.43
6:6:124:THR:HG22	6:6:135:VAL:HG13	2.00	0.43
4:S:969:PRO:HB2	4:S:972:ARG:NH2	2.33	0.43
4:W:414:SER:HB2	4:W:1353:MET:HG3	2.00	0.43
4:X:263:THR:O	4:X:359:ARG:NH1	2.43	0.43
4:X:1166:LEU:HD11	4:X:1169:LEU:HD23	1.99	0.43
6:c:89:PRO:HA	6:c:90:SER:HA	1.58	0.43
4:S:825:ASP:HB2	7:2:6:VAL:HG21	2.00	0.43
4:T:633:LEU:HD12	4:T:874:MET:HB3	2.00	0.43
4:W:407:HIS:CE1	4:W:574:PHE:HB2	2.54	0.43
4:X:836:ASN:HD22	4:X:839:VAL:HG23	1.84	0.43
4:X:1169:LEU:H	4:X:1169:LEU:HG	1.56	0.43
6:c:114:LEU:HD12	6:c:140:VAL:HG21	2.01	0.43
4:S:661:CYS:HB2	4:S:681:LEU:HD12	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:T:1027:GLN:HB3	4:T:1032:MET:HB2	2.00	0.43
4:W:49:ARG:HD3	4:X:87:ILE:HD11	2.00	0.43
4:W:1043:THR:HG23	4:W:1265:PRO:HB3	2.01	0.43
4:W:1196:ASN:ND2	4:W:1202:ALA:H	2.17	0.43
4:W:1262:MET:HA	4:W:1306:TYR:HA	2.00	0.43
5:5:279:TYR:HB2	5:5:282:ARG:HG2	2.01	0.43
6:6:144:LEU:HD11	6:6:183:PHE:HB2	2.01	0.43
2:m:39:MET:HE2	2:m:43:ARG:HH21	1.84	0.42
4:W:127:ALA:HB2	4:X:101:ALA:HB2	2.01	0.42
5:b:111:LEU:HD23	5:b:243:LEU:HD13	2.01	0.42
1:k:316:VAL:HG13	1:k:400:LEU:HD11	2.01	0.42
4:T:455:HIS:ND1	4:T:457:ARG:HG2	2.34	0.42
4:W:123:HIS:HB2	4:W:1086:ILE:HB	2.00	0.42
4:X:93:PHE:HB2	4:X:116:VAL:HB	2.00	0.42
4:T:512:VAL:HG12	4:T:993:SER:HB3	2.02	0.42
5:5:182:LYS:HD2	6:7:301:TRP:CG	2.55	0.42
4:S:82:ASP:OD1	4:S:82:ASP:N	2.52	0.42
4:T:606:ASP:OD1	4:T:647:LYS:NZ	2.39	0.42
4:W:1328:PRO:HB2	4:W:1358:ILE:HG21	2.02	0.42
4:S:587:ASN:OD1	4:T:1003:GLN:NE2	2.53	0.42
6:d:152:LEU:HD23	6:d:152:LEU:HA	1.91	0.42
4:S:623:GLN:HB2	4:S:626:LYS:HB2	2.01	0.42
4:W:950:ASP:HA	4:W:951:PRO:HD3	1.86	0.42
4:W:1068:VAL:HG23	5:b:47:ALA:HB2	2.00	0.42
4:W:1127:TYR:H	4:W:1133:HIS:CD2	2.38	0.42
4:W:1187:ASP:OD2	4:W:1232:ARG:NH1	2.52	0.42
4:S:1321:HIS:O	4:S:1324:GLN:NE2	2.52	0.42
4:T:932:ARG:HH21	4:T:956:THR:HG23	1.83	0.42
4:T:1196:ASN:ND2	4:T:1202:ALA:H	2.18	0.42
4:W:82:ASP:OD1	4:W:82:ASP:N	2.46	0.42
4:W:438:ASN:HD22	4:W:1171:HIS:CD2	2.36	0.42
4:W:829:VAL:HA	4:W:938:MET:HE1	2.02	0.42
6:6:204:LEU:HB3	6:7:229:LEU:HD11	2.00	0.42
1:k:16:HIS:CD2	1:k:87:SER:H	2.37	0.42
4:S:1046:VAL:HG13	4:S:1104:VAL:HG23	2.01	0.42
4:T:629:MET:HE3	4:T:877:VAL:HG13	2.01	0.42
4:T:855:GLU:HG2	7:2:70:ARG:HE	1.84	0.42
4:W:102:HIS:HE1	4:W:106:ARG:HD2	1.85	0.42
4:X:78:THR:HG22	4:X:304:ALA:HB3	2.02	0.42
6:6:201:LEU:HD23	6:6:204:LEU:HD12	2.01	0.42
4:T:407:HIS:CE1	4:T:574:PHE:HB2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:W:541:ASP:N	4:W:557:THR:O	2.52	0.42
4:S:529:HIS:O	4:S:533:ARG:N	2.48	0.42
4:T:279:THR:HB	4:T:380:GLN:HE21	1.84	0.42
4:S:394:ARG:HD3	4:S:1315:PHE:HB3	2.01	0.41
4:S:520:THR:HG22	4:S:568:PRO:HA	2.02	0.41
4:S:902:GLN:NE2	4:S:1020:SER:OG	2.47	0.41
4:X:770:LEU:HD21	4:X:883:LEU:HD22	2.01	0.41
6:c:13:SER:OG	6:c:130:ASN:ND2	2.53	0.41
4:S:832:THR:HG22	7:2:11:ILE:HD11	2.02	0.41
4:T:195:LEU:HD23	4:T:1283:TYR:HE1	1.86	0.41
4:W:331:ALA:HA	4:W:335:ASP:HB2	2.02	0.41
4:W:538:PRO:O	4:W:559:ARG:NH1	2.53	0.41
1:k:399:ILE:HG22	1:k:405:VAL:HG11	2.02	0.41
4:S:399:THR:HG22	4:S:1043:THR:HG22	2.01	0.41
4:T:709:VAL:HG22	4:T:1023:SER:HA	2.02	0.41
4:X:565:ILE:HA	4:X:566:PRO:HD3	1.94	0.41
4:X:877:VAL:O	4:X:880:THR:OG1	2.27	0.41
5:b:305:LEU:O	5:b:312:LEU:N	2.45	0.41
6:c:114:LEU:HD11	6:c:145:GLY:HA2	2.01	0.41
6:c:220:ARG:HG2	6:c:265:ARG:HH12	1.84	0.41
5:5:124:GLN:HG2	5:5:313:PRO:HD2	2.01	0.41
4:T:1127:TYR:H	4:T:1133:HIS:CD2	2.39	0.41
6:6:34:GLY:H	6:6:44:ALA:HB1	1.84	0.41
4:S:192:LEU:HD13	4:S:1098:VAL:HG22	2.01	0.41
4:W:76:VAL:HG21	4:W:258:PHE:HD2	1.86	0.41
4:W:457:ARG:HG3	4:W:1122:PHE:HD2	1.86	0.41
4:W:629:MET:HE3	4:W:877:VAL:HG13	2.03	0.41
4:X:278:THR:HB	4:X:282:VAL:HB	2.02	0.41
4:X:1071:ARG:NH1	4:X:1081:GLU:HB3	2.36	0.41
6:c:219:PRO:HG2	6:c:222:CYS:HB3	2.02	0.41
5:5:199:LEU:HD12	5:5:204:LEU:HD12	2.01	0.41
5:5:231:VAL:O	5:5:242:ALA:N	2.53	0.41
7:0:28:MET:HE2	7:0:45:LYS:HG2	2.02	0.41
7:2:28:MET:HE2	7:2:45:LYS:HG2	2.02	0.41
2:m:38:THR:HG22	4:X:508:PHE:HE1	1.85	0.41
4:S:447:GLN:HB3	4:S:1028:ALA:HB1	2.02	0.41
6:6:177:TYR:HB3	6:7:263:ILE:HG21	2.02	0.41
7:1:28:MET:HE2	7:1:45:LYS:HG2	2.02	0.41
4:W:1167:PRO:HG3	4:X:1217:ARG:HB2	2.03	0.41
6:d:5:LYS:HB2	6:d:86:ARG:HB3	2.02	0.41
1:k:98:SER:HB3	1:k:117:TYR:HE1	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:l:95:ILE:HD13	3:o:2605:LEU:HB3	2.01	0.41
4:S:192:LEU:O	4:S:196:GLY:N	2.50	0.41
4:S:1043:THR:OG1	4:S:1305:GLN:NE2	2.53	0.41
4:T:436:ASN:ND2	4:T:440:VAL:O	2.54	0.41
4:T:449:ALA:HB1	4:T:1179:ILE:HG12	2.03	0.41
4:T:907:HIS:HB2	4:T:910:GLY:N	2.36	0.41
4:W:687:LEU:HD23	4:W:805:LEU:HD22	2.02	0.41
4:X:989:GLU:HG2	4:X:991:HIS:H	1.86	0.41
4:X:1117:ASP:N	4:X:1117:ASP:OD1	2.44	0.41
6:c:144:LEU:HD21	6:c:183:PHE:HB2	2.03	0.41
1:k:339:LEU:HD23	2:l:46:ALA:HB2	2.03	0.41
1:k:389:CYS:HB2	1:k:420:THR:HG22	2.02	0.41
2:m:96:GLY:O	2:m:99:THR:OG1	2.37	0.41
4:S:1171:HIS:HE1	4:T:1228:ALA:HA	1.86	0.41
4:W:1071:ARG:HH22	6:c:38:ARG:H	1.69	0.41
6:c:288:VAL:HG22	6:c:300:CYS:HB2	2.02	0.41
6:d:33:LEU:N	6:d:70:THR:O	2.54	0.41
1:k:284:PHE:HE2	2:l:61:THR:HG21	1.87	0.40
4:S:606:ASP:OD1	4:X:678:ARG:NH1	2.53	0.40
4:S:614:TYR:HE2	4:S:927:VAL:HG22	1.85	0.40
4:S:934:ALA:O	4:S:937:THR:OG1	2.37	0.40
4:T:71:LEU:N	4:T:377:GLU:OE2	2.54	0.40
4:X:615:VAL:HG22	4:X:938:MET:HE1	2.02	0.40
5:5:170:HIS:HA	5:5:175:THR:HG23	2.03	0.40
7:3:27:ARG:O	7:3:30:THR:OG1	2.31	0.40
4:T:946:LYS:HD2	4:T:946:LYS:HA	1.92	0.40
4:W:178:VAL:HG22	4:W:1061:MET:HE2	2.03	0.40
4:W:301:ALA:HB2	4:W:360:THR:HB	2.03	0.40
4:S:252:VAL:HG13	4:S:1096:SER:HA	2.02	0.40
4:T:507:ALA:HB1	4:T:978:ASN:ND2	2.37	0.40
4:X:609:TYR:HA	4:X:610:PRO:HD3	1.97	0.40
6:c:155:TYR:CE2	6:c:192:VAL:HG11	2.57	0.40
6:d:5:LYS:HD2	6:d:86:ARG:HB3	2.04	0.40
7:0:27:ARG:O	7:0:30:THR:OG1	2.31	0.40
4:S:297:MET:HE2	4:S:366:LEU:HD11	2.02	0.40
4:S:799:ASN:OD1	4:S:799:ASN:N	2.55	0.40
4:T:594:GLN:HA	4:T:597:ILE:HD12	2.03	0.40
4:T:1217:ARG:HH21	4:T:1224:ILE:HD11	1.85	0.40
4:W:307:VAL:HB	4:W:309:ARG:HH11	1.86	0.40
4:W:736:ARG:NH2	4:W:1129:ASP:OD2	2.54	0.40
4:W:1169:LEU:O	4:X:211:SER:OG	2.29	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:m:21:GLY:H	5:b:121:LYS:NZ	2.20	0.40
4:S:856:ASN:ND2	7:1:66:GLY:O	2.55	0.40
4:T:18:ASN:OD1	4:T:18:ASN:N	2.54	0.40
4:W:544:VAL:HG22	4:W:554:TYR:HE1	1.85	0.40
4:W:654:TYR:CD2	4:W:803:GLU:HG2	2.57	0.40
4:W:840:PHE:CE1	7:0:53:ILE:HD13	2.56	0.40
4:X:395:ARG:HG2	4:X:1047:LEU:HD23	2.04	0.40
7:3:28:MET:HE2	7:3:45:LYS:HG2	2.02	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	k	334/454 (74%)	322 (96%)	12 (4%)	0	100	100
2	l	81/549 (15%)	81 (100%)	0	0	100	100
2	m	76/549 (14%)	75 (99%)	1 (1%)	0	100	100
3	n	38/2635 (1%)	38 (100%)	0	0	100	100
3	o	38/2635 (1%)	38 (100%)	0	0	100	100
4	S	1273/1376 (92%)	1179 (93%)	92 (7%)	2 (0%)	43	77
4	T	1354/1376 (98%)	1273 (94%)	78 (6%)	3 (0%)	43	77
4	W	1350/1376 (98%)	1287 (95%)	61 (4%)	2 (0%)	48	83
4	X	1282/1376 (93%)	1201 (94%)	79 (6%)	2 (0%)	43	77
5	5	262/331 (79%)	250 (95%)	12 (5%)	0	100	100
5	b	315/331 (95%)	307 (98%)	8 (2%)	0	100	100
6	6	290/305 (95%)	275 (95%)	15 (5%)	0	100	100
6	7	288/305 (94%)	275 (96%)	13 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c	290/305 (95%)	282 (97%)	8 (3%)	0	100	100
6	d	296/305 (97%)	292 (99%)	4 (1%)	0	100	100
7	0	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	1	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	2	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
7	3	76/170 (45%)	75 (99%)	1 (1%)	0	100	100
All	All	7871/14888 (53%)	7475 (95%)	387 (5%)	9 (0%)	49	83

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	W	263	THR
4	T	10	PHE
4	X	992	LYS
4	S	992	LYS
4	S	993	SER
4	T	945	ASN
4	X	993	SER
4	W	849	ASP
4	T	11	PRO

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

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	k	293/377 (78%)	293 (100%)	0	100	100
2	l	76/473 (16%)	76 (100%)	0	100	100
2	m	71/473 (15%)	71 (100%)	0	100	100
3	n	35/2239 (2%)	35 (100%)	0	100	100
3	o	35/2239 (2%)	35 (100%)	0	100	100
4	S	1094/1166 (94%)	1091 (100%)	3 (0%)	86	84

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	T	1154/1166 (99%)	1148 (100%)	6 (0%)	81	81
4	W	1150/1166 (99%)	1145 (100%)	5 (0%)	84	82
4	X	1097/1166 (94%)	1092 (100%)	5 (0%)	81	81
5	5	229/281 (82%)	229 (100%)	0	100	100
5	b	272/281 (97%)	272 (100%)	0	100	100
6	6	267/274 (97%)	266 (100%)	1 (0%)	84	82
6	7	264/274 (96%)	264 (100%)	0	100	100
6	c	267/274 (97%)	266 (100%)	1 (0%)	84	82
6	d	270/274 (98%)	270 (100%)	0	100	100
7	0	70/141 (50%)	70 (100%)	0	100	100
7	1	70/141 (50%)	70 (100%)	0	100	100
7	2	70/141 (50%)	70 (100%)	0	100	100
7	3	70/141 (50%)	70 (100%)	0	100	100
All	All	6854/12687 (54%)	6833 (100%)	21 (0%)	84	84

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	S	91	ILE
4	S	651	VAL
4	S	1169	LEU
4	T	308	VAL
4	T	434	VAL
4	T	616	ILE
4	T	895	ILE
4	T	1121	ILE
4	T	1308	VAL
4	W	308	VAL
4	W	616	ILE
4	W	1113	VAL
4	W	1169	LEU
4	W	1301	THR
4	X	651	VAL
4	X	713	LEU
4	X	1104	VAL
4	X	1121	ILE
4	X	1169	LEU

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Mol	Chain	Res	Type
6	c	98	VAL
6	6	217	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	16	HIS
1	k	91	ASN
1	k	333	HIS
2	m	52	GLN
4	S	123	HIS
4	S	224	HIS
4	S	479	HIS
4	S	630	ASN
4	S	746	ASN
4	S	890	GLN
4	S	1084	HIS
4	S	1114	HIS
4	S	1133	HIS
4	S	1171	HIS
4	S	1173	GLN
4	S	1318	GLN
4	S	1344	ASN
4	T	36	GLN
4	T	113	GLN
4	T	224	HIS
4	T	325	ASN
4	T	328	GLN
4	T	380	GLN
4	T	436	ASN
4	T	492	ASN
4	T	655	HIS
4	T	689	GLN
4	T	746	ASN
4	T	818	HIS
4	T	907	HIS
4	T	915	GLN
4	T	982	ASN
4	T	1003	GLN
4	T	1050	HIS
4	T	1116	GLN
4	T	1133	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	T	1196	ASN
4	T	1305	GLN
4	T	1321	HIS
4	T	1334	HIS
4	W	92	GLN
4	W	102	HIS
4	W	113	GLN
4	W	123	HIS
4	W	224	HIS
4	W	312	ASN
4	W	380	GLN
4	W	438	ASN
4	W	537	HIS
4	W	623	GLN
4	W	674	HIS
4	W	689	GLN
4	W	697	HIS
4	W	716	HIS
4	W	737	GLN
4	W	746	ASN
4	W	816	ASN
4	W	958	HIS
4	W	978	ASN
4	W	1030	HIS
4	W	1116	GLN
4	W	1133	HIS
4	W	1196	ASN
4	W	1334	HIS
4	W	1348	HIS
4	X	102	HIS
4	X	123	HIS
4	X	312	ASN
4	X	325	ASN
4	X	336	HIS
4	X	384	ASN
4	X	387	GLN
4	X	447	GLN
4	X	514	GLN
4	X	575	GLN
4	X	630	ASN
4	X	666	ASN
4	X	716	HIS

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
4	X	1084	HIS
4	X	1114	HIS
4	X	1171	HIS
4	X	1235	ASN
4	X	1344	ASN
5	b	124	GLN
5	b	194	HIS
5	b	302	HIS
6	c	37	HIS
6	c	40	GLN
6	c	130	ASN
6	c	146	HIS
6	c	151	GLN
6	d	24	GLN
6	d	94	GLN
6	d	146	HIS
6	d	150	GLN
6	d	156	HIS
6	d	194	ASN
6	d	274	GLN
5	5	126	HIS
5	5	145	ASN
5	5	303	GLN
6	6	40	GLN
6	6	64	GLN
6	6	151	GLN
6	6	232	HIS
6	7	97	ASN
6	7	143	GLN
7	0	33	GLN
7	0	44	GLN
7	0	55	HIS
7	0	75	GLN
7	1	33	GLN
7	1	44	GLN
7	1	55	HIS
7	1	75	GLN
7	2	33	GLN
7	2	44	GLN
7	2	55	HIS
7	2	75	GLN
7	3	33	GLN

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Mol	Chain	Res	Type
7	3	44	GLN
7	3	55	HIS
7	3	75	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.

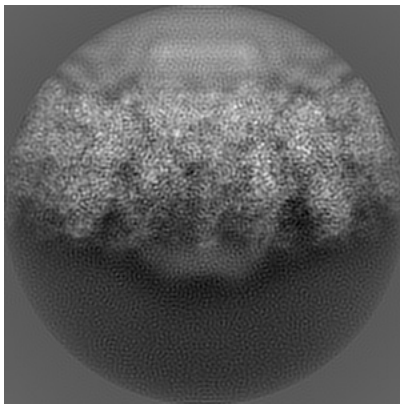
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20432. These allow visual inspection of the internal detail of the map and identification of artifacts.

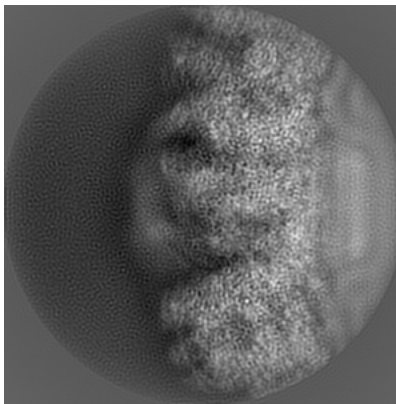
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

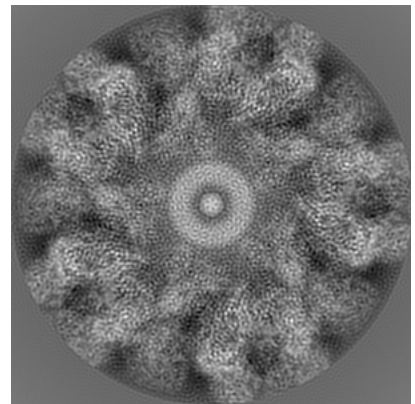
#### 6.1.1 Primary map



X

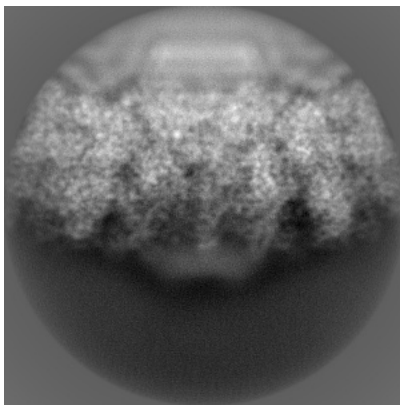


Y

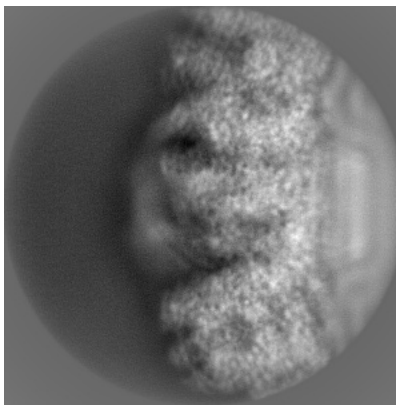


Z

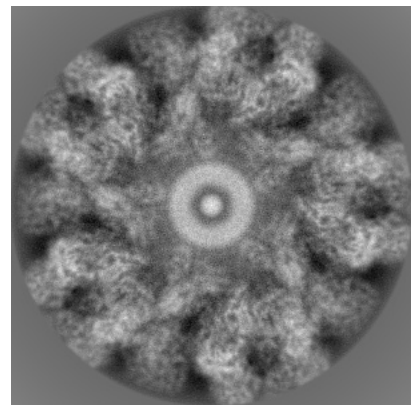
#### 6.1.2 Raw map



X



Y

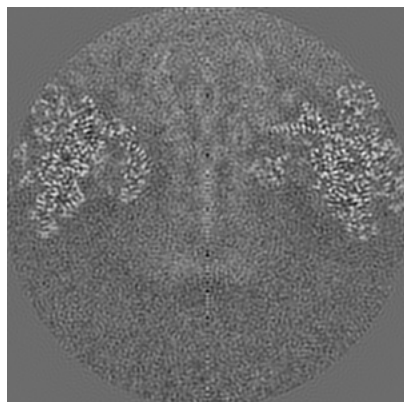


Z

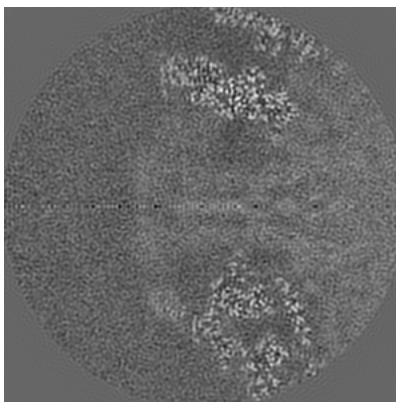
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

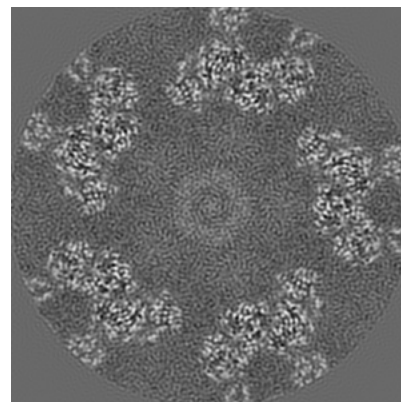
### 6.2.1 Primary map



X Index: 192

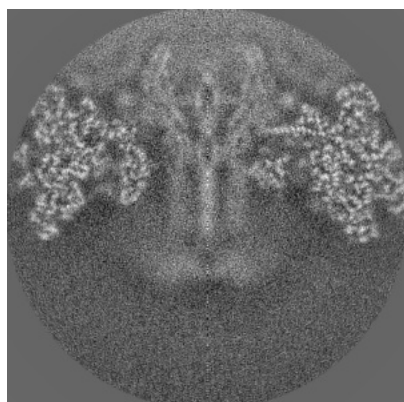


Y Index: 192

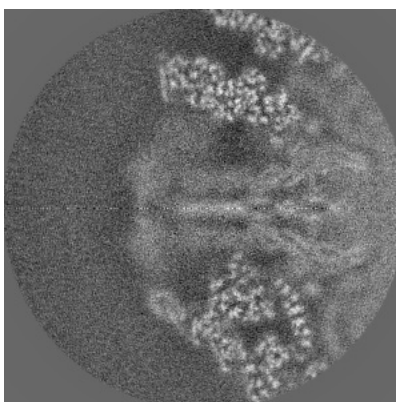


Z Index: 192

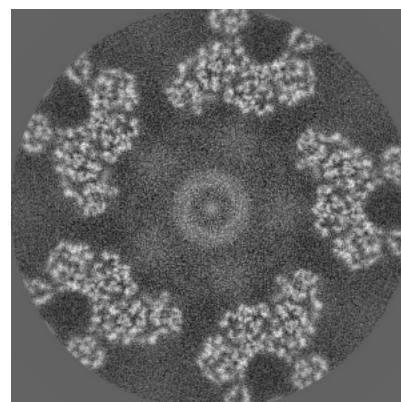
### 6.2.2 Raw map



X Index: 192



Y Index: 192

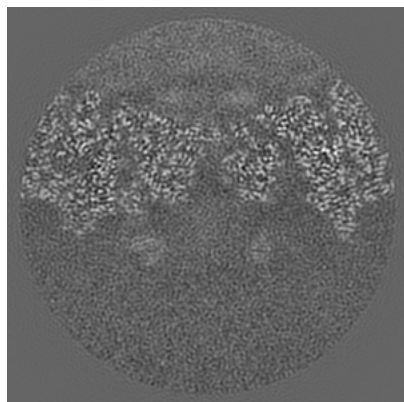


Z Index: 192

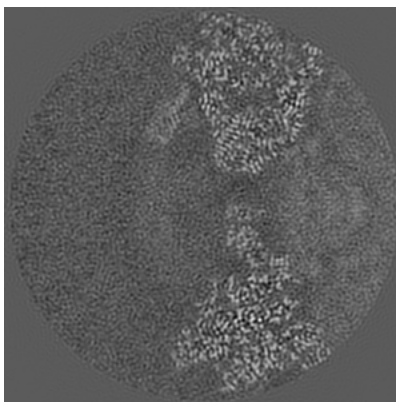
The images above show central slices of the map in three orthogonal directions.

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

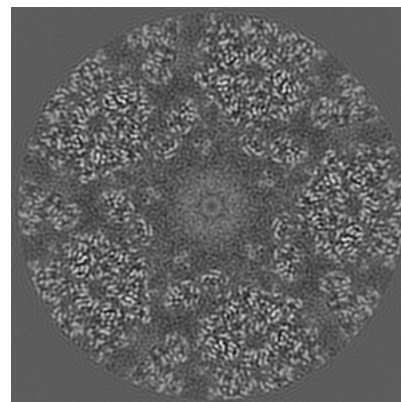
### 6.3.1 Primary map



X Index: 262

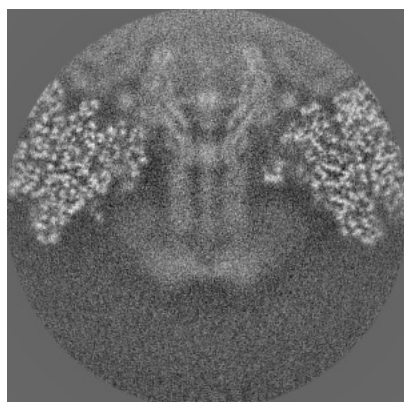


Y Index: 242

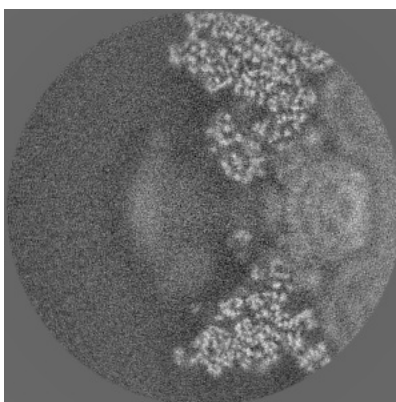


Z Index: 246

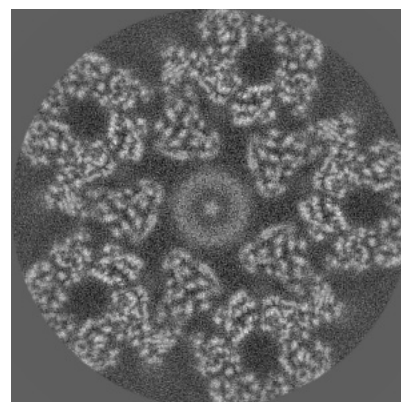
### 6.3.2 Raw map



X Index: 199



Y Index: 154

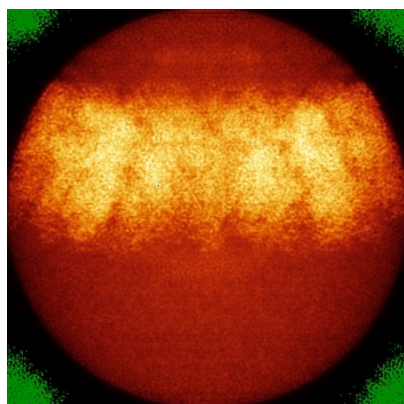


Z Index: 216

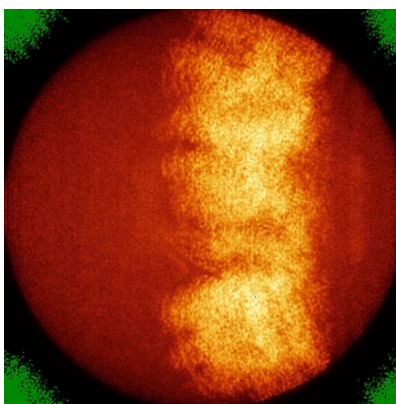
The images above show the largest variance slices of the map in three orthogonal directions.

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

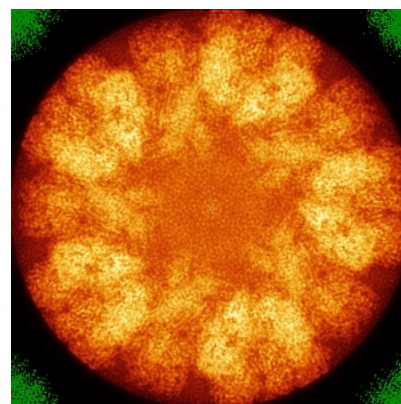
### 6.4.1 Primary map



X

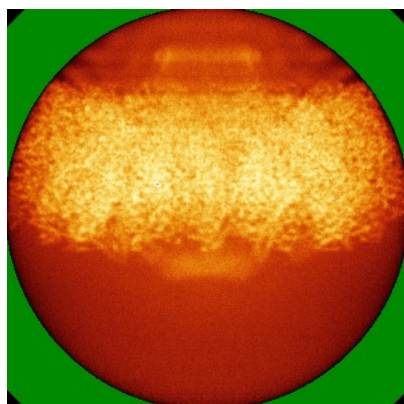


Y

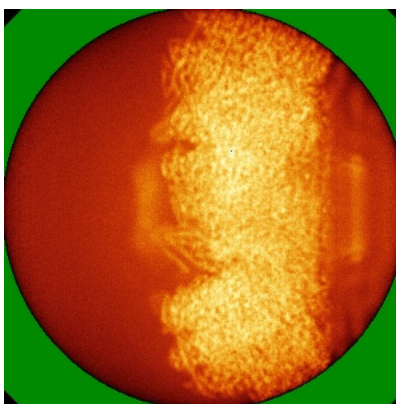


Z

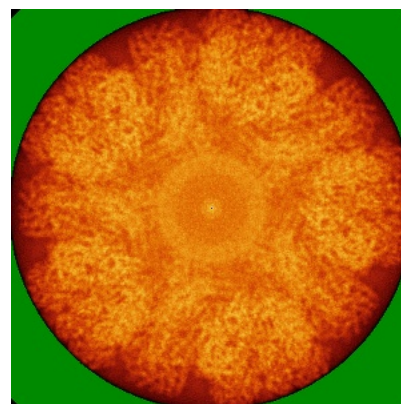
### 6.4.2 Raw map



X



Y

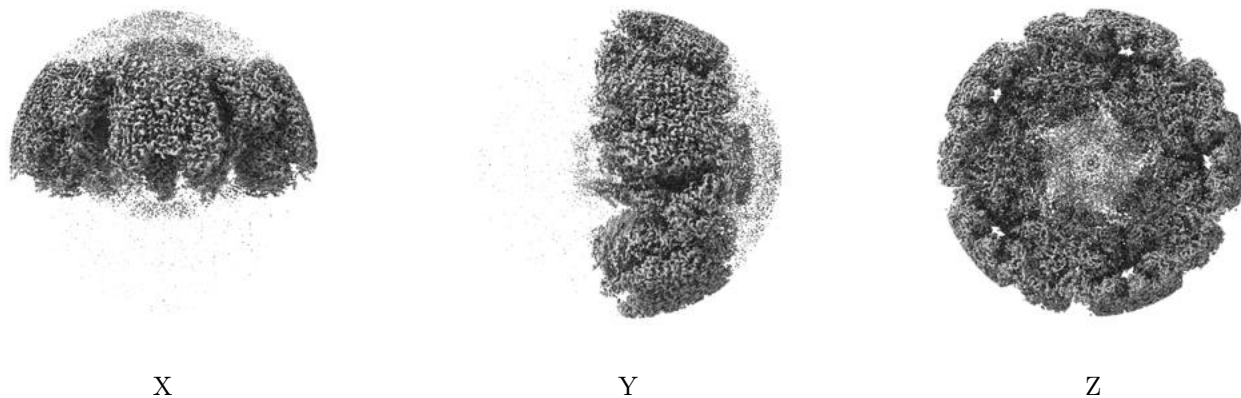


Z

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

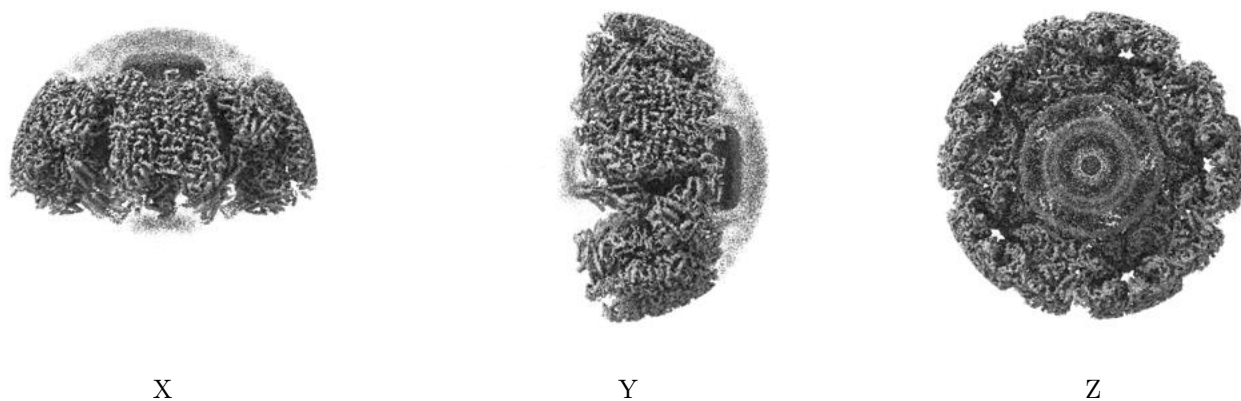
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. 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.

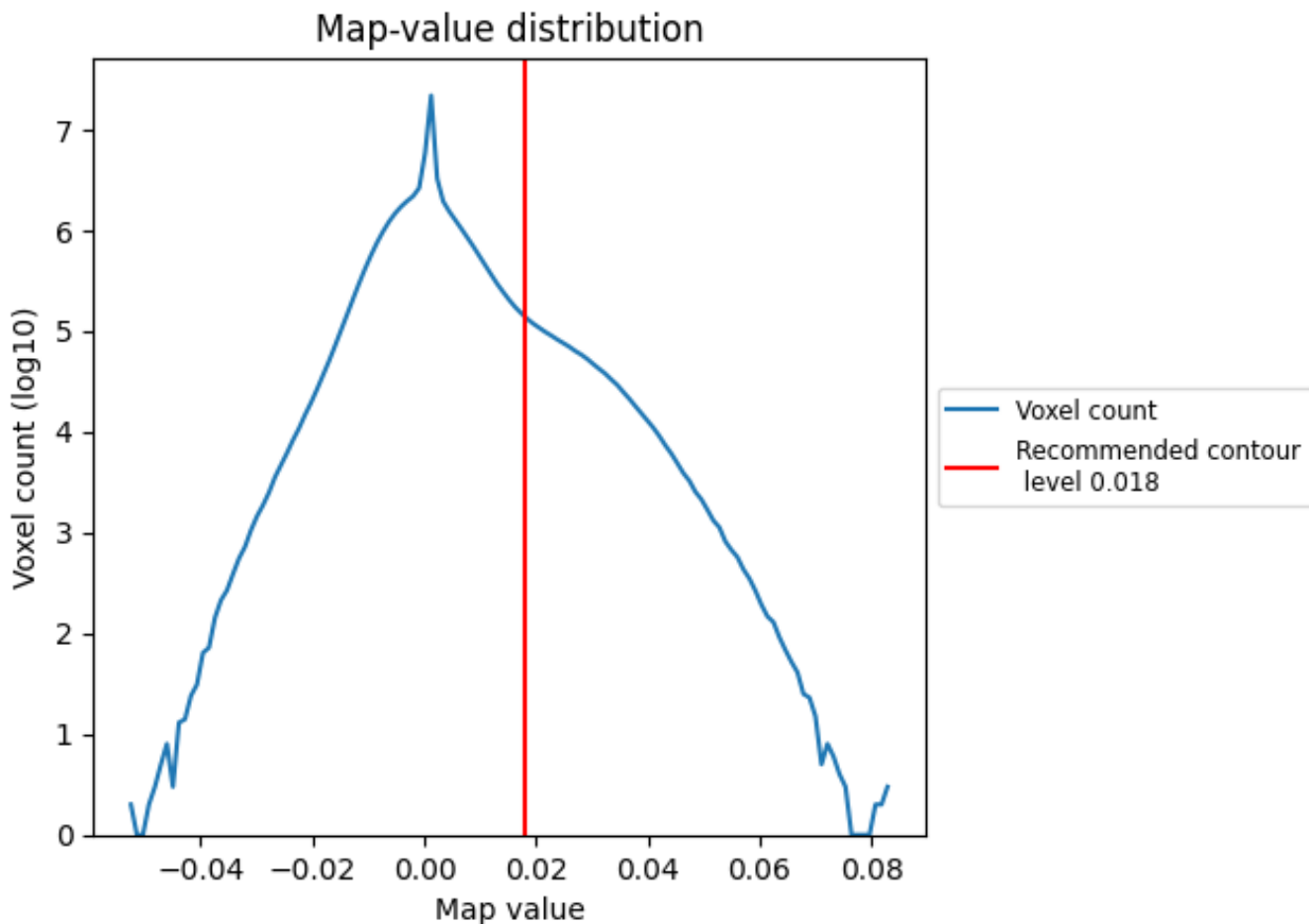
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

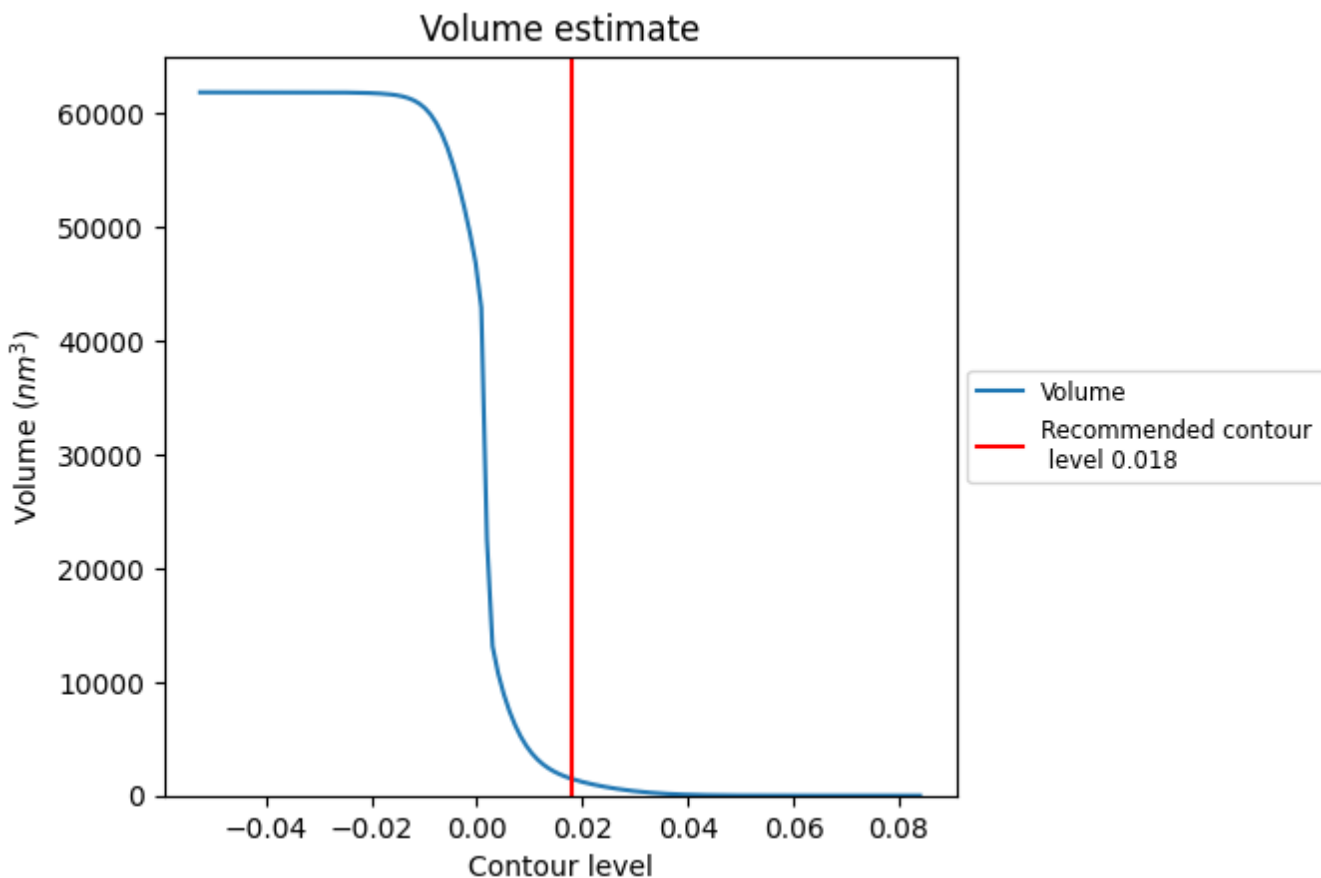
This section contains the results of statistical analysis of the map.

### 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.

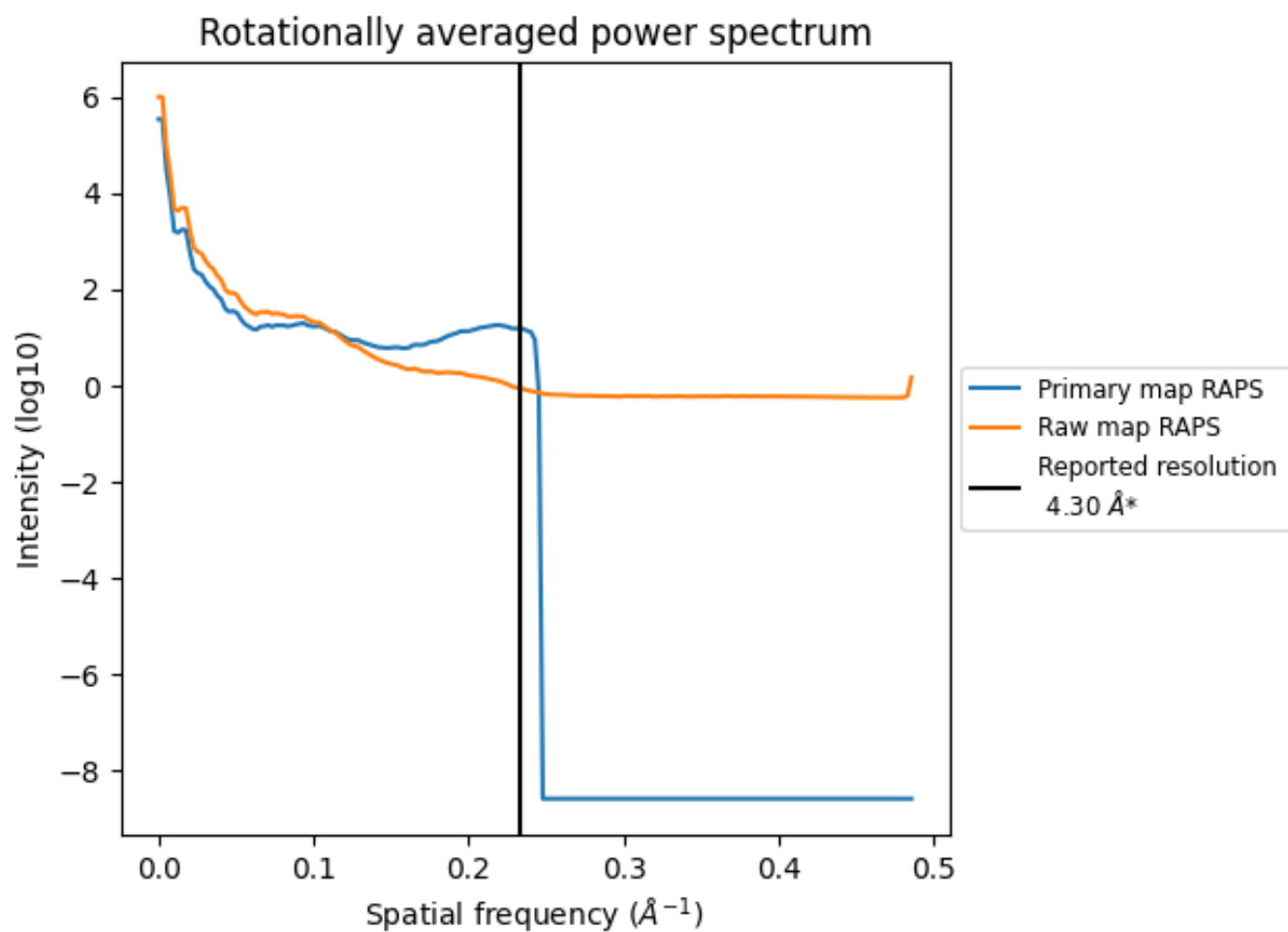
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1471 nm<sup>3</sup>; this corresponds to an approximate mass of 1329 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

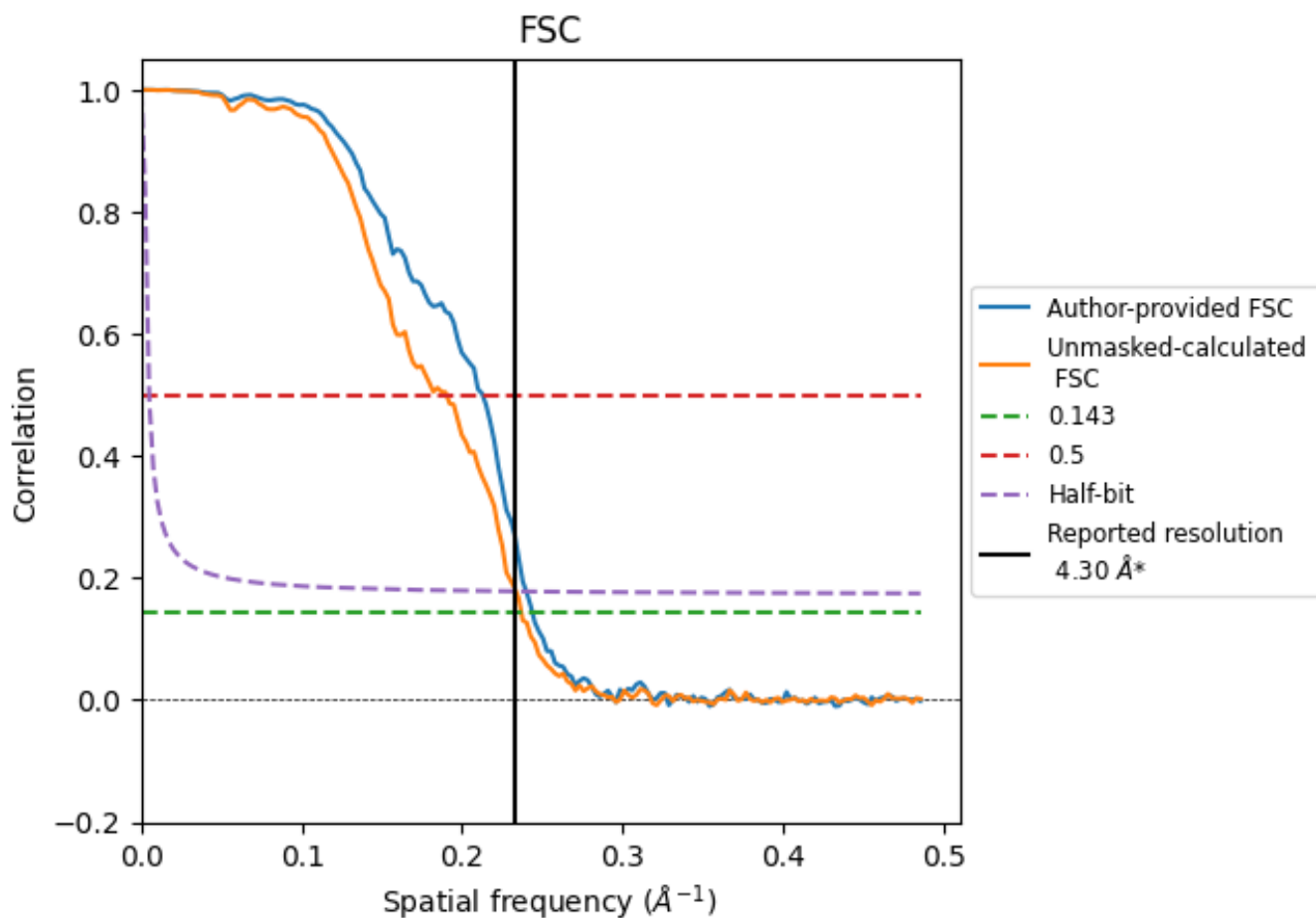


\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8 Fourier-Shell correlation [i](#)

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.233 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

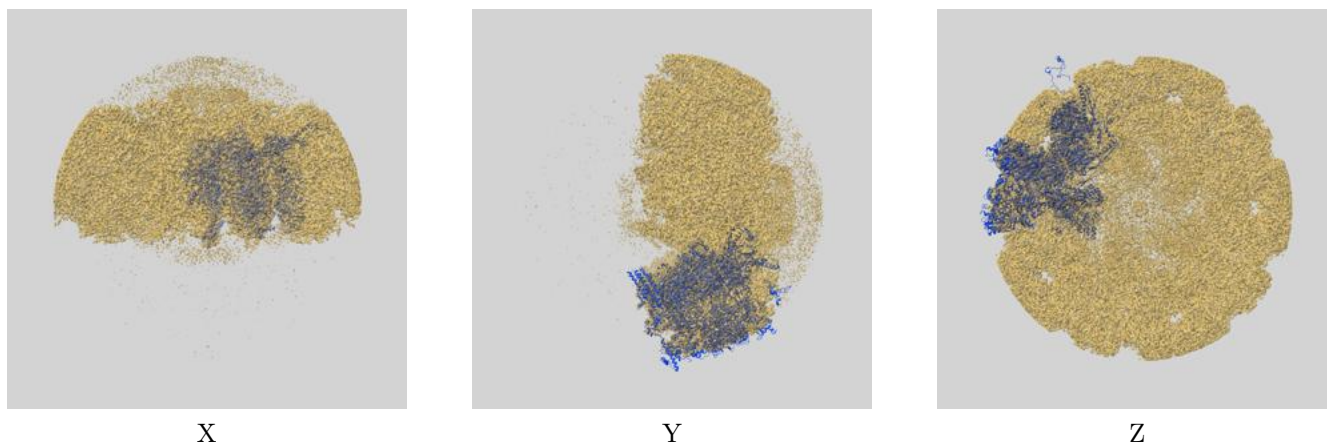
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.10	4.70	4.17
Unmasked-calculated*	4.22	5.26	4.28

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

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

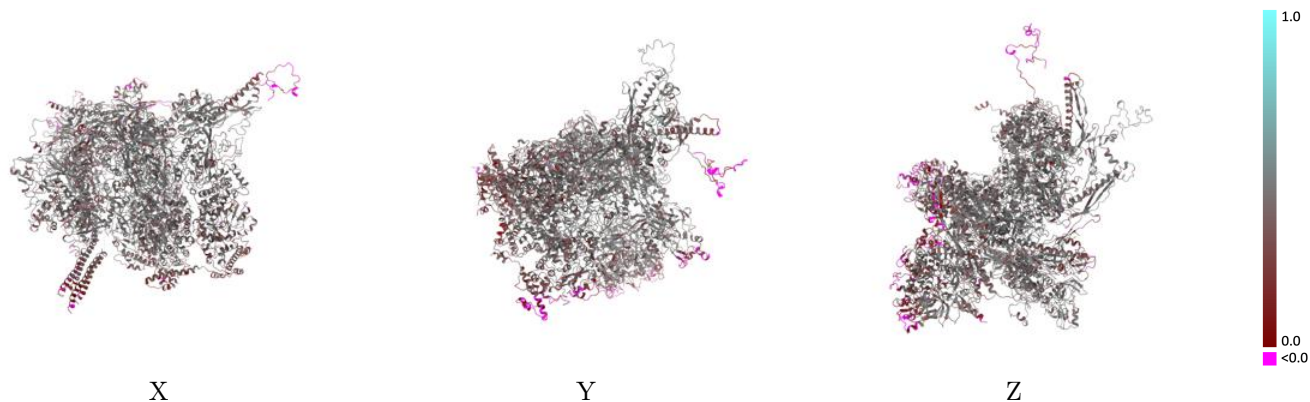
This section contains information regarding the fit between EMDB map EMD-20432 and PDB model 6PPB. Per-residue inclusion information can be found in section 3 on page 7.

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



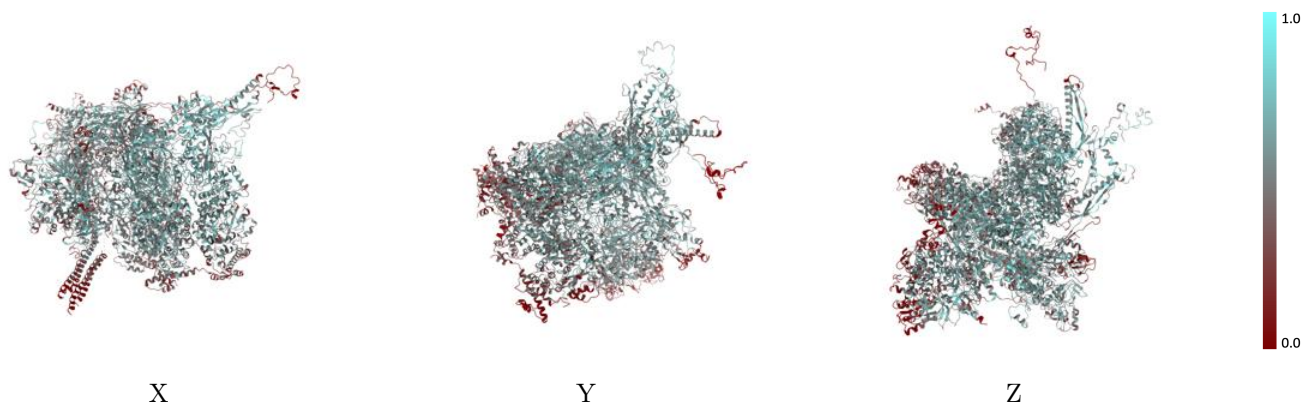
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



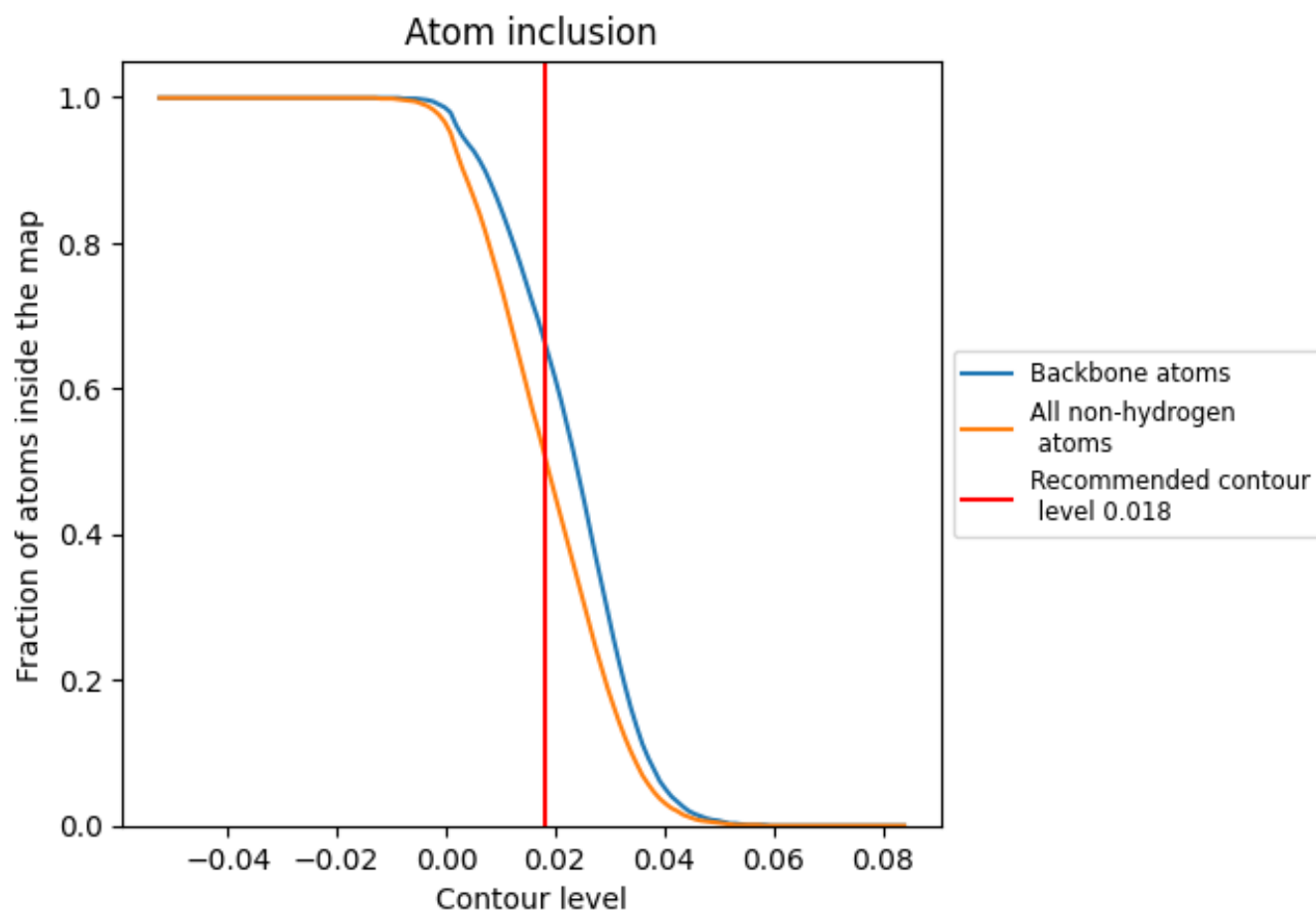
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).









































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 67% of all backbone atoms, 51% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5110	 0.3950
0	 0.1250	 0.1290
1	 0.3440	 0.3100
2	 0.3320	 0.3150
3	 0.3210	 0.3080
5	 0.4660	 0.4070
6	 0.5320	 0.4240
7	 0.5110	 0.4190
S	 0.5790	 0.4360
T	 0.5480	 0.3970
W	 0.4930	 0.3780
X	 0.5870	 0.4410
b	 0.5020	 0.3890
c	 0.3940	 0.3340
d	 0.3860	 0.3190
k	 0.5200	 0.4070
l	 0.3660	 0.3370
m	 0.2960	 0.3030
n	 0.2190	 0.2400
o	 0.1520	 0.2560

