



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 06:43 AM UTC

PDB ID : 6PPH / pdb_00006pph
EMDB ID : EMD-20436
Title : Kaposi's sarcoma-associated herpesvirus (KSHV), C1 penton vertex register, CATC-binding 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 : 3.80 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:

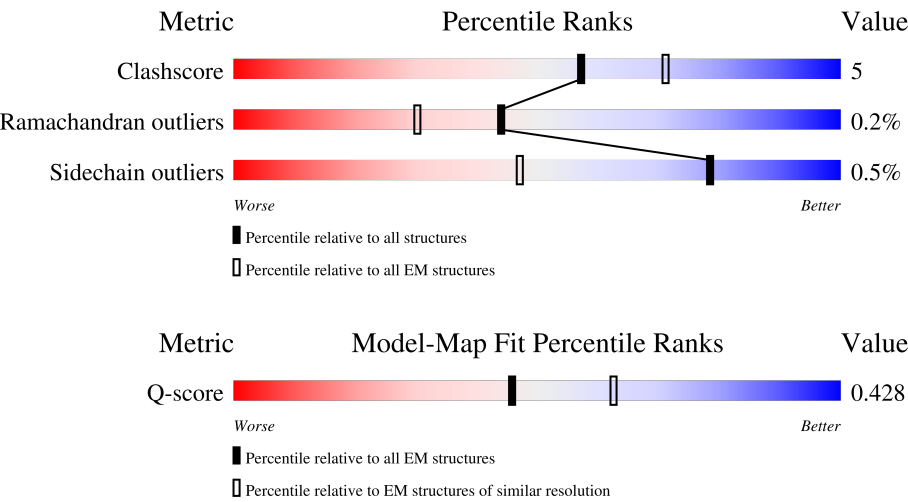
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh &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

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.80 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.



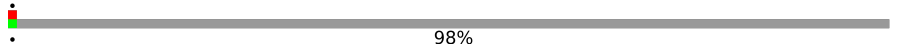
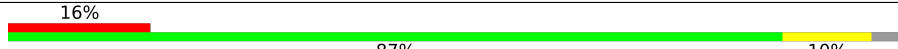
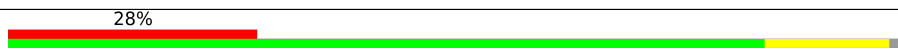
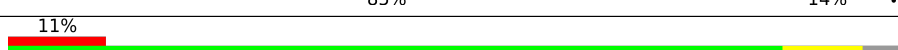
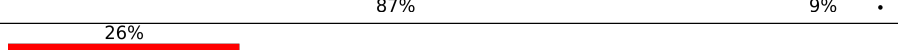
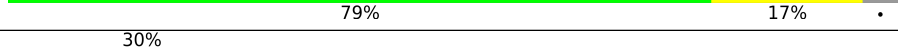
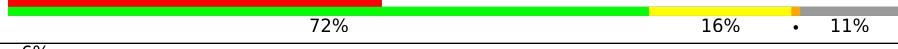
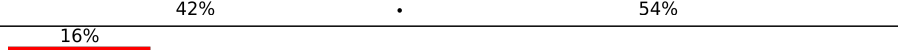
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10198 (3.30 - 4.30)

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	k	454	10% 65% 11% 24%
2	l	549	13% 85%
2	m	549	5% 13% 85%
3	n	2635	98%

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Mol	Chain	Length	Quality of chain
3	o	2635	
4	5	331	
4	b	331	
5	6	305	
5	7	305	
5	c	305	
5	d	305	
6	4	1376	
6	S	1376	
6	T	1376	
6	W	1376	
6	X	1376	
7	0	170	
7	1	170	
7	2	170	
7	3	170	
7	A	170	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 73502 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
1	k	344	Total	C	N	O	S	0	0
			2680	1722	467	477	14		

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
2	l	83	Total	C	N	O	S	0	0
			686	429	135	119	3		
2	m	80	Total	C	N	O	S	0	0
			645	406	121	115	3		

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

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

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 Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	314	Total	C	N	O	S	0	0
			2428	1557	416	442	13		
4	b	321	Total	C	N	O	S	0	0
			2478	1586	424	453	15		

- Molecule 5 is a protein called Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	302	Total	C	N	O	S	0	0
			2382	1514	406	447	15		
5	7	294	Total	C	N	O	S	0	0
			2315	1478	391	431	15		
5	c	294	Total	C	N	O	S	0	0
			2330	1485	397	434	14		
5	d	300	Total	C	N	O	S	0	0
			2365	1505	401	444	15		

- Molecule 6 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	4	1222	Total	C	N	O	S	0	0
			9634	6133	1673	1757	71		
6	S	1281	Total	C	N	O	S	0	0
			10061	6401	1739	1852	69		
6	T	1360	Total	C	N	O	S	0	0
			10667	6776	1851	1967	73		
6	X	1341	Total	C	N	O	S	0	0
			10519	6685	1824	1939	71		
6	W	1354	Total	C	N	O	S	0	0
			10622	6748	1842	1960	72		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	A	44	Total	C	N	O	S	0	0
			380	244	72	62	2		
7	2	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	3	78	Total	C	N	O	S	0	0
			666	418	130	115	3		
7	1	78	Total	C	N	O	S	0	0
			666	418	130	115	3		

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

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

Chain k:

10% 65% 11% 24%

Y117 L118 A126 GLY ARG ASN ASN ALA ARG ARG PRO THR THR VAL ASP GLY VAL SER PRO PRO PRO GLY GLY ALA VAL ALA HIS PRO LEU GLY GLU LEU GLN ARG GLN LEU LEU ALA ARG ALA THR PRO ASP PRO ALA PRO THR ARG ARG PRO N91 P94 V99 I102 P105 G106 S107 H108 L111 R114 F115 Y116 D262 D263 W264 I267 P268 L269 S270 F271 P272 E273 E274 P275 V276 P277 P278 L282 V283 F284 M285 D286 R306 R315 V316 R322 E325 H333 R342 E347 P358 PRO LEU GLY ARG HIS A364 D368 R376 T379 L384 R385 G386 V387 N388 C389 G390 G391 E398 I399 L400 K401 Q402 V409 S412 L413 T420 P430 R440 E444 G454

Chain 1: 13% 85%

MET	LEU	THR	SER	GLU	ARG	SER	THR	LEU	ARG	PRO	THR	VAL	GLN	LYS	ASN	ARG	THR	GLU	ALA	GLY	R22	R43	R44	L47	R50	SS1	Q52	R59	K60	T61	D71	R72	R80	V81	R82	D87	I88	K92	Q93	M94	I95	G96	N97	M98	T99	M100	S101	D102	N103	I104	ASP					
MET	PRO	GLN	SER	ARG	SER	HIS	GLU	PRO	PRO	LEU	THR	VAL	GLN	ALA	SER	HIS	ARG	ASN	PHE	THR	VAL	ALA	ILE	VAL	ASN	PRO	GLY	ASP	PRO	PHE	SER	VAL	ASP	THR	ARG	LEU	LEU	GLY	GLU	LEU	MET	THR	THR	LEU	TYR	MET	ASN	GLN	ASN	GLN	TRP	LEU	PRO	ASP	PHE	GLY
PRO	TRP	PHE	ILE	LEU	LEU	THR	ASP	ALA	ASN	MET	GLN	ARG	PRO	LYS	GLU	LEU	GLY	THR	VAL	ASN	PHE	GLN	ALA	ASN	SER	THR	LEU	LYS	ILE	SER	HIS	THR	LEU	THR	VAL	ALA	SER	THR	THR	ASP	PHE	THR	ALA	ASP	ARG	HIS	LEU	THR	ASP	THR	GLN					
ALA	ALA	LEU	CYS	LEU	VAL	ASN	ALA	TYR	CYS	GLN	LYS	THR	THR	ALA	THR	THR	THR	GLN	ASP	LEU	LEU	ALA	ALA	ASP	LEU	PRO	GLN	LEU	LEU	LEU	ILE	THR	GLN	LEU	LYS	GLN	GLU	GLY	GLY	GLY	THR	THR	THR	ASP	ASP	THR	PRO	PRO	GLN	GLY	ARG	ALA				

- Molecule 2: Capsid vertex component 2

[illegible]

- Molecule 3: Large tegument protein deneddylase



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

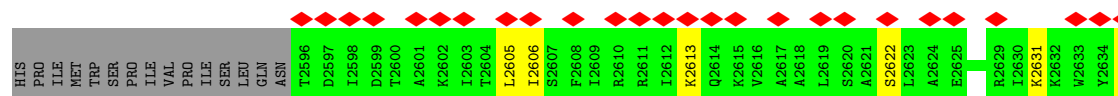




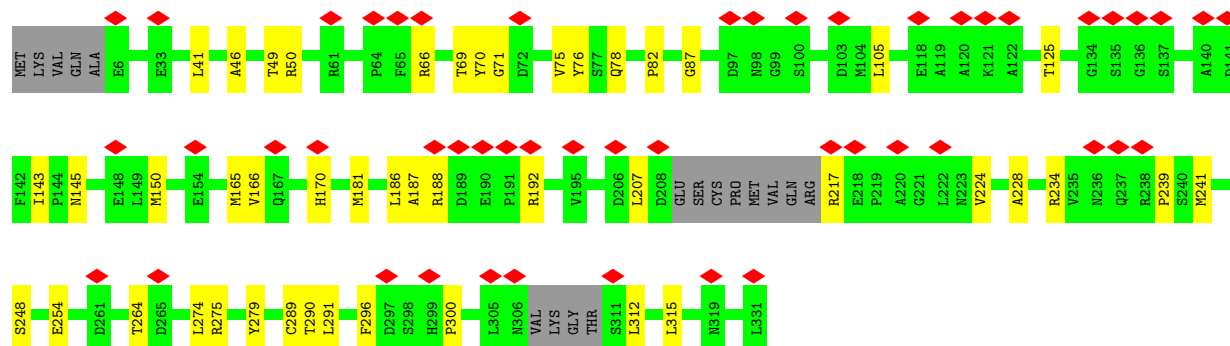
- Molecule 3: Large tegument protein deneddylase

[illegible]

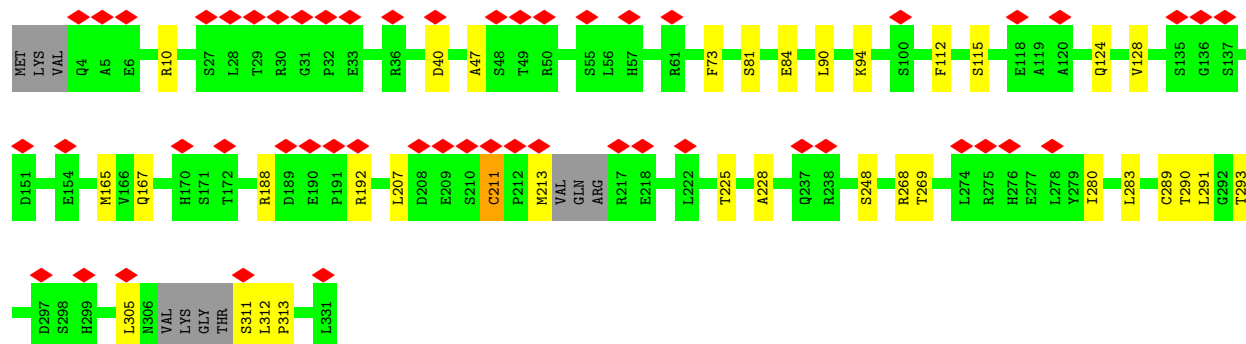




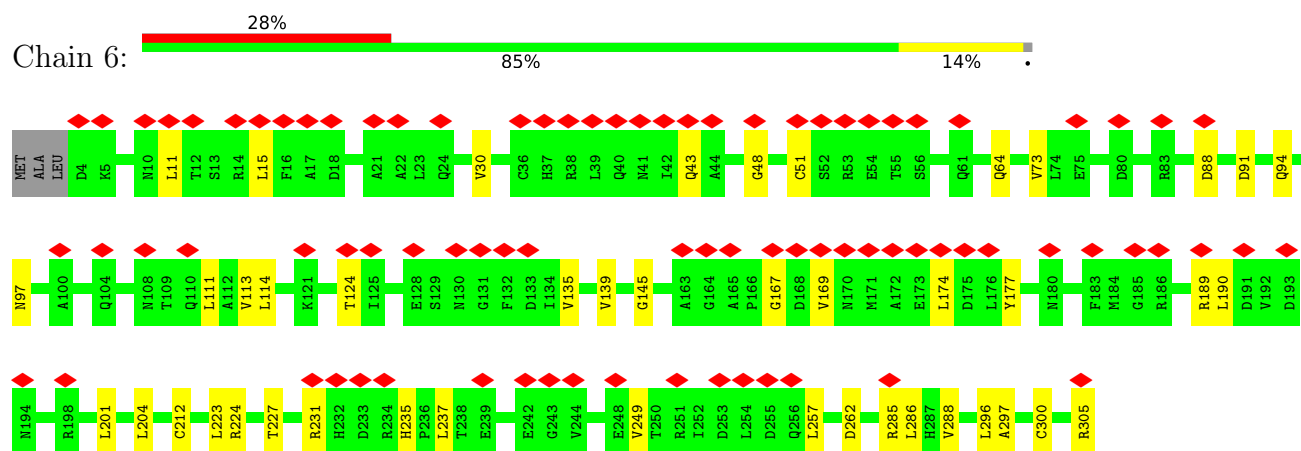
Chain 5: 15% 81% 14% 5%



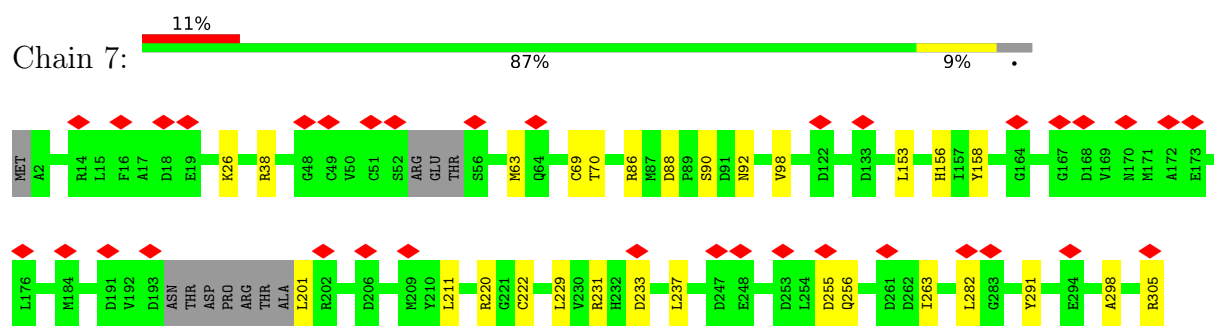
Chain b: 16% 87% 10%



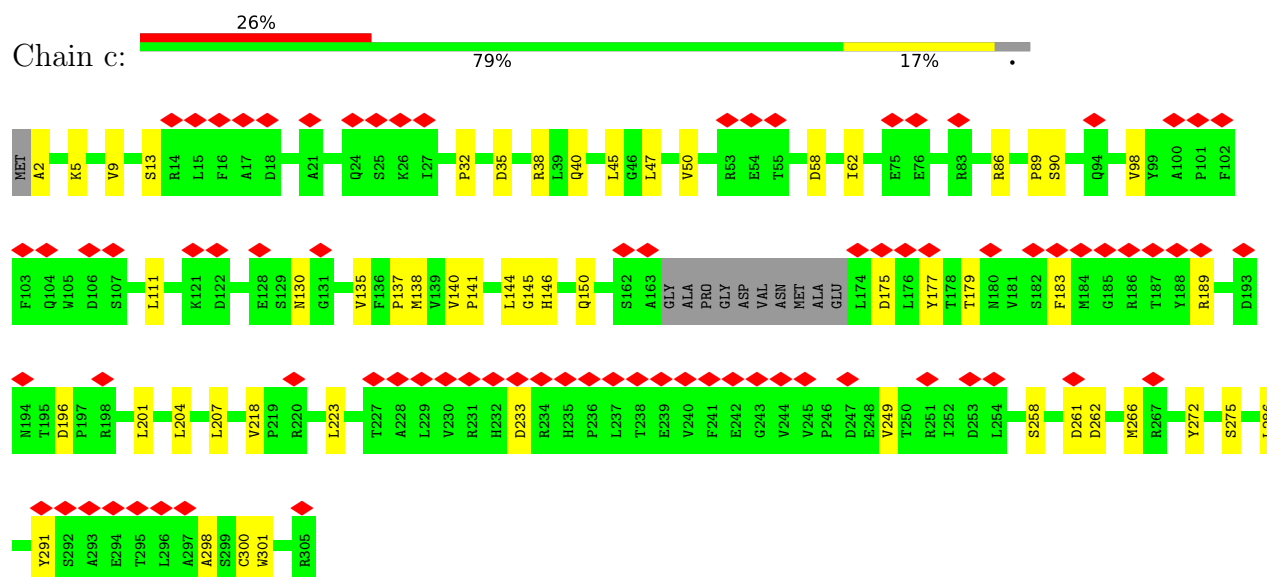
- Molecule 5: Triplex capsid protein 2



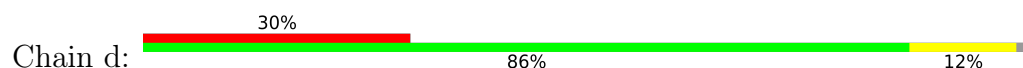
- Molecule 5: Triplex capsid protein 2

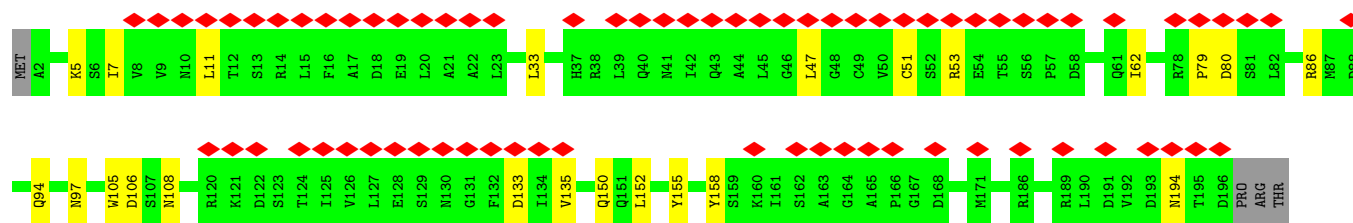


- Molecule 5: Triplex capsid protein 2

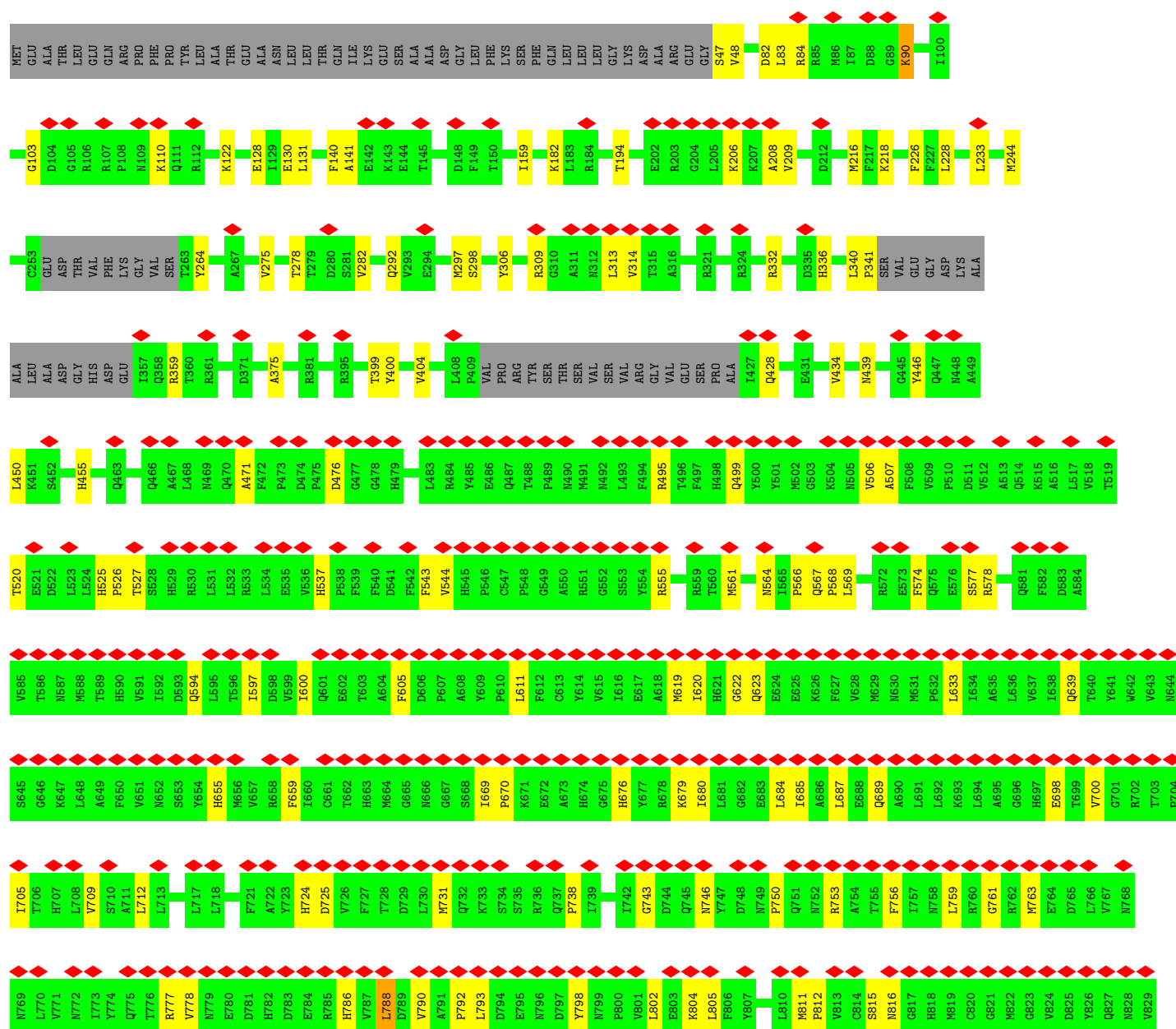


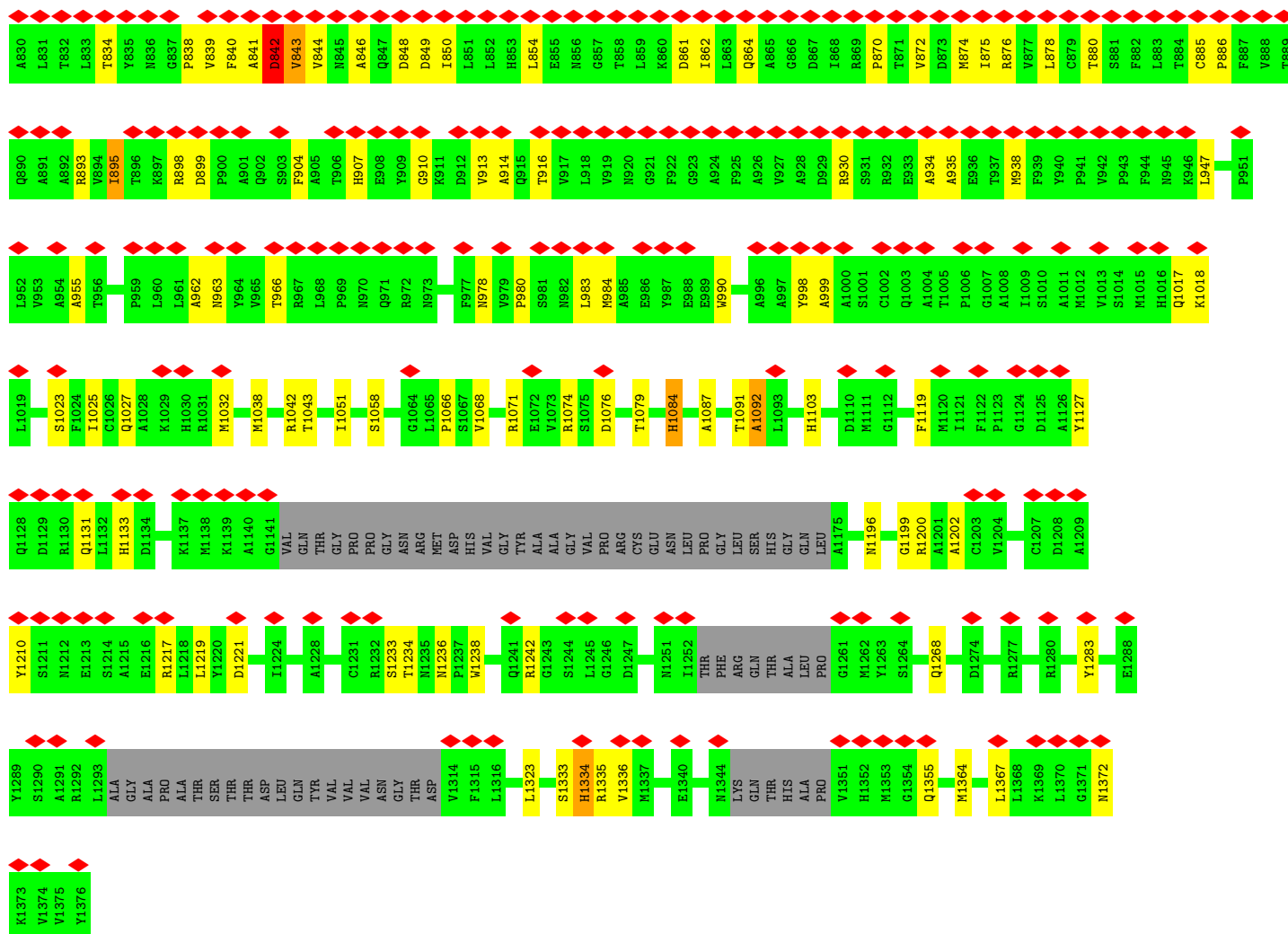
- Molecule 5: Triplex capsid protein 2

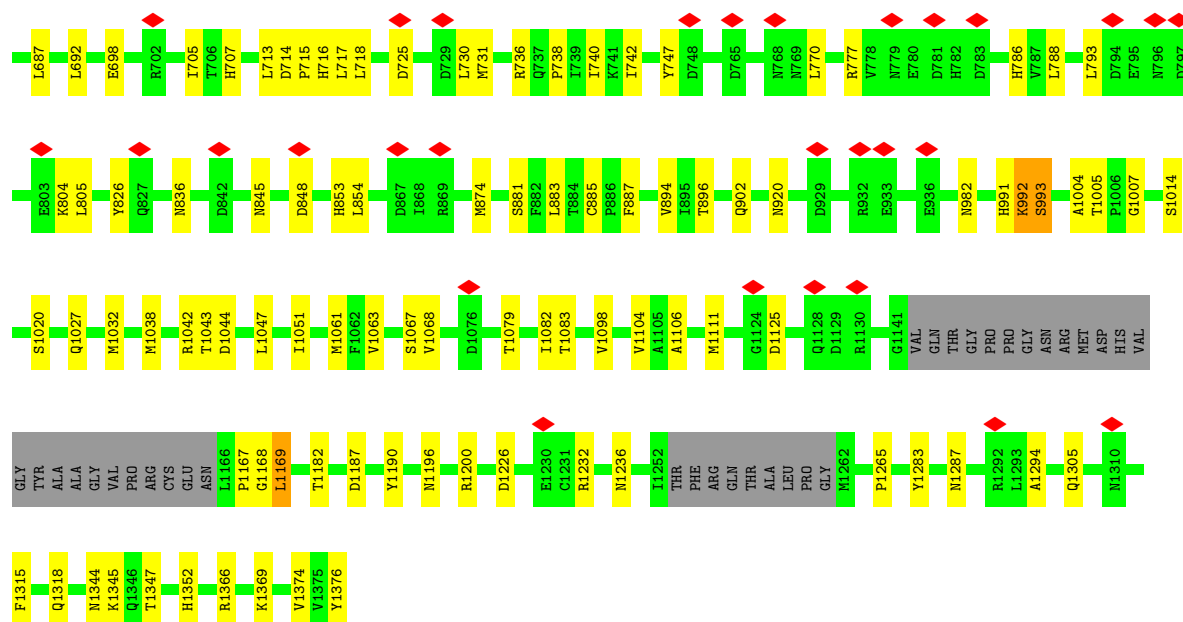




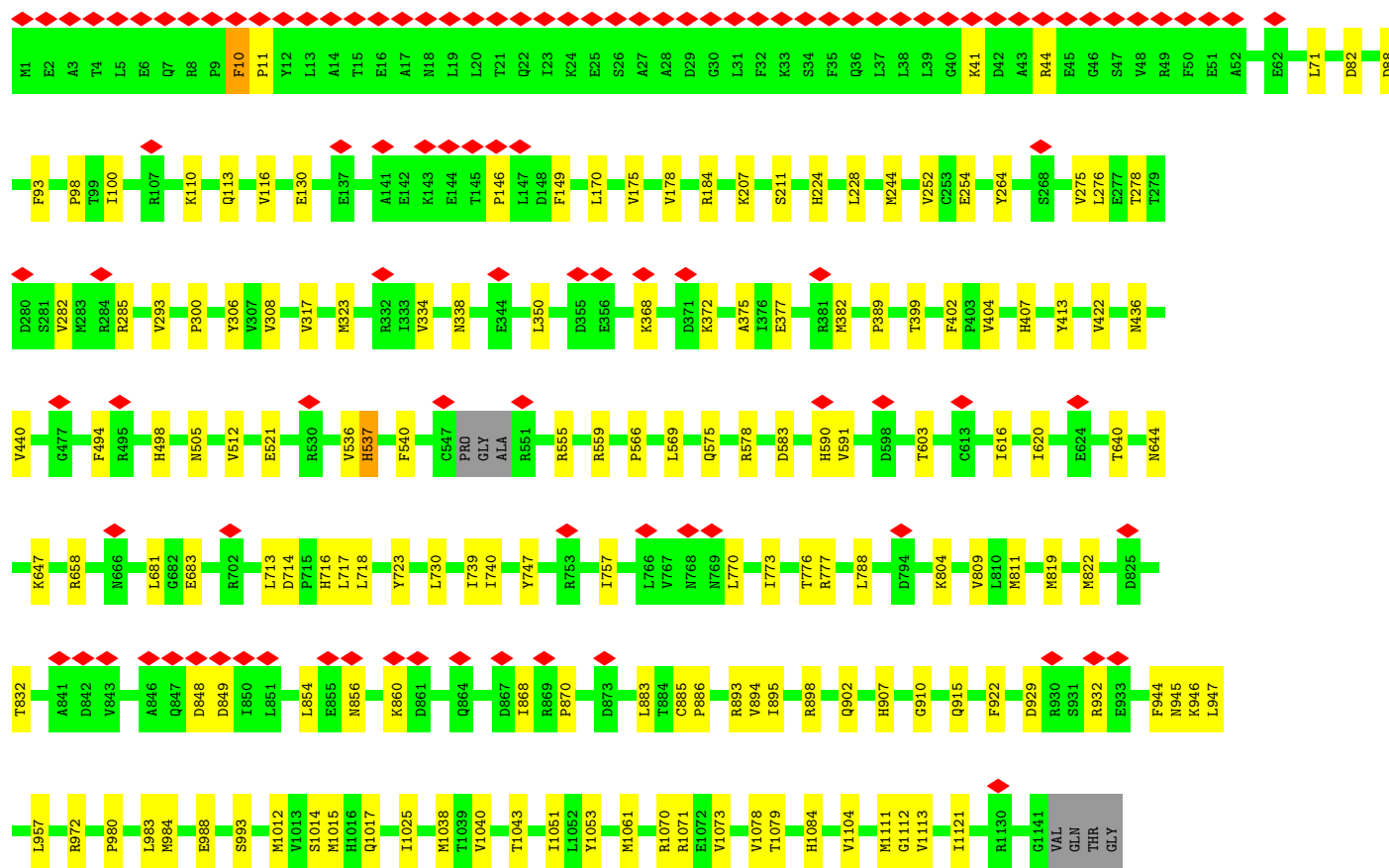
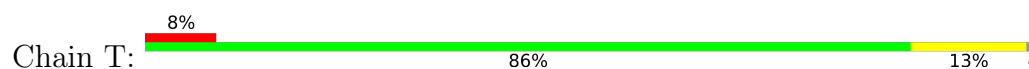
• Molecule 6: Major capsid protein

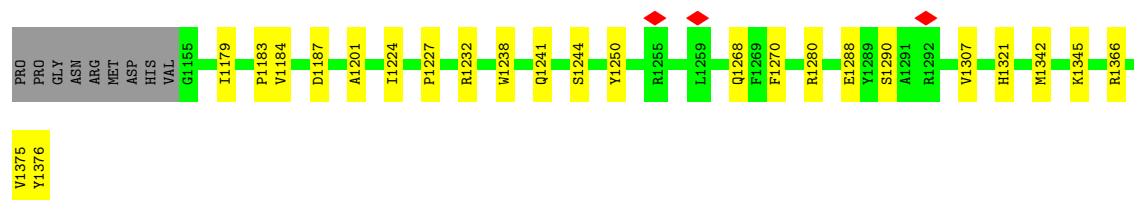






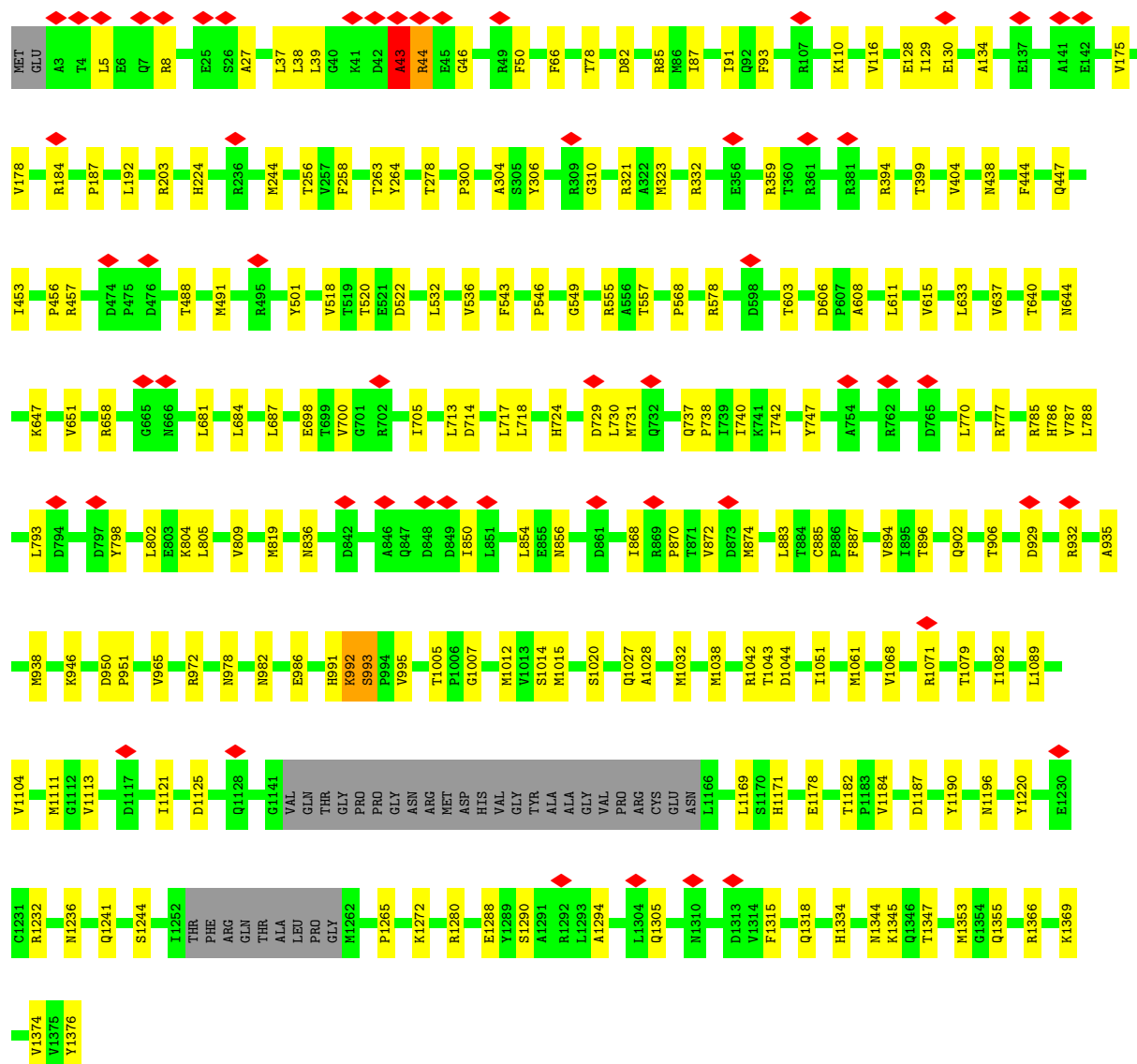
• Molecule 6: Major capsid protein





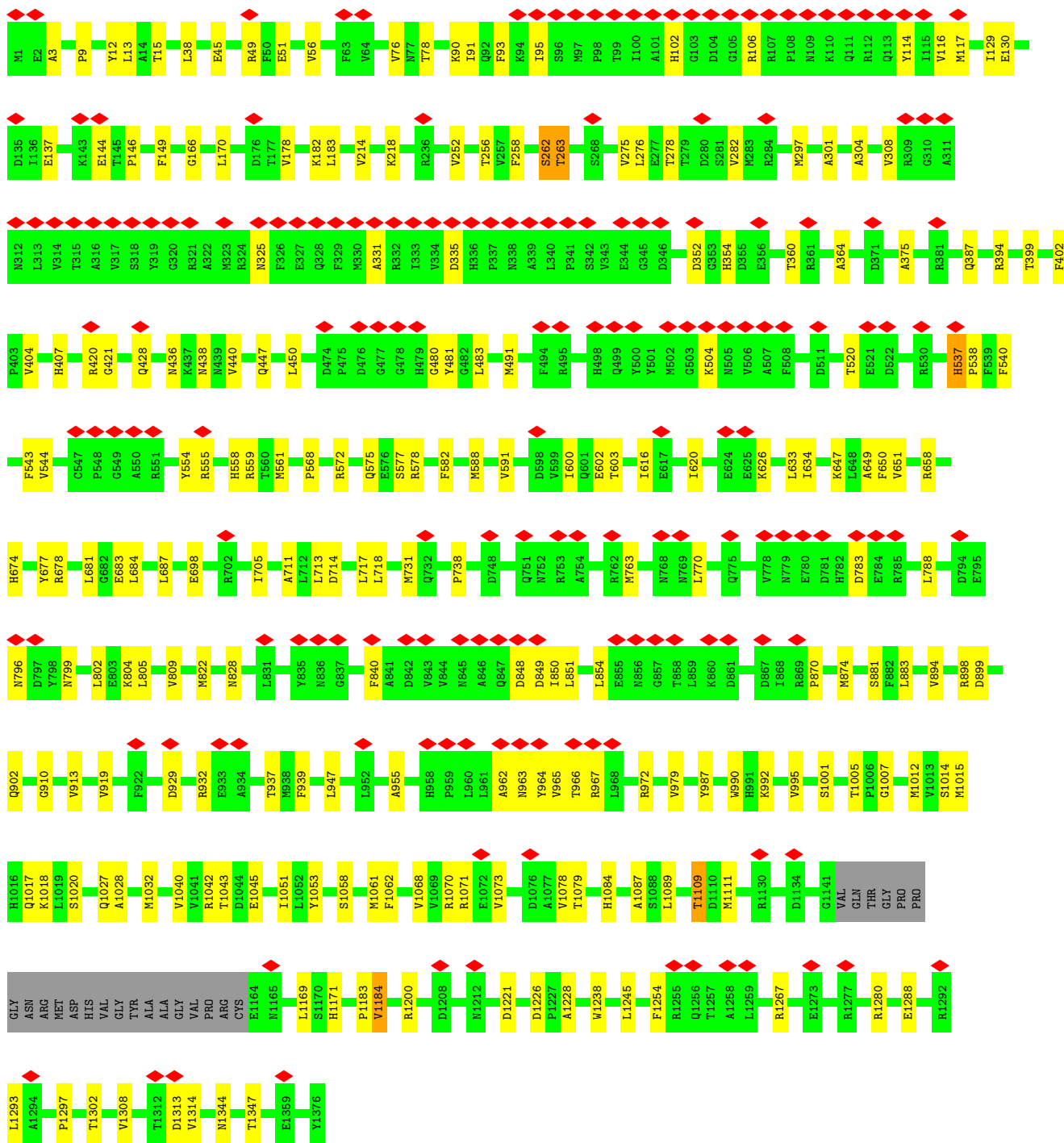
• Molecule 6: Major capsid protein

Chain X: 83% 14%



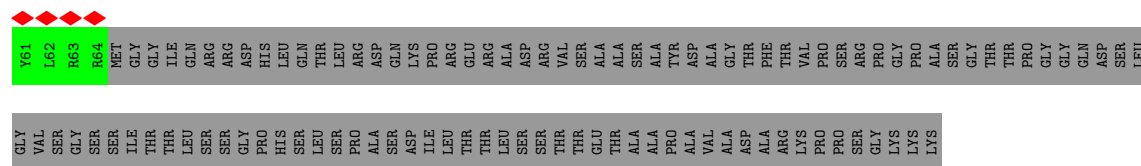
• Molecule 6: Major capsid protein

Chain W: 13% 82% 16%

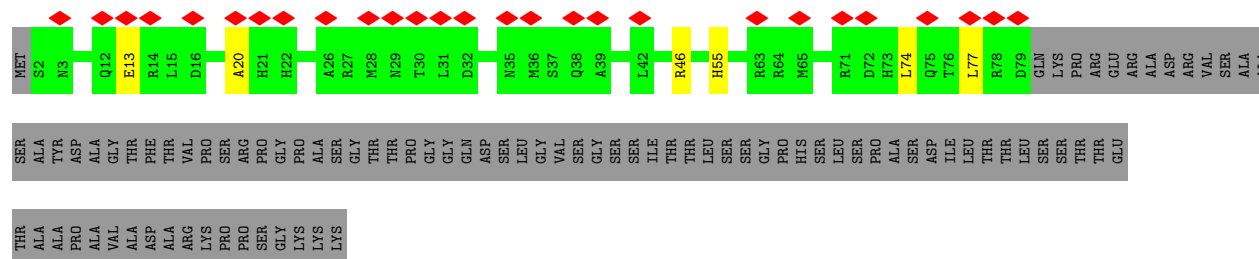
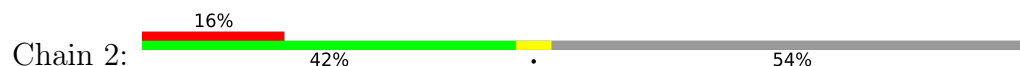


• Molecule 7: Small capsomere-interacting protein

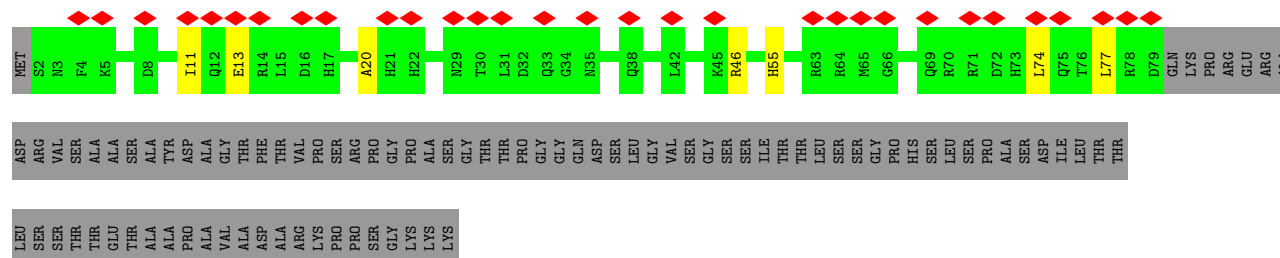
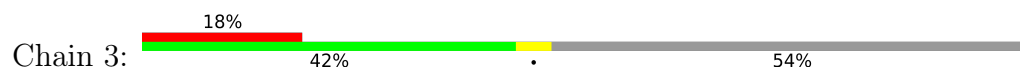




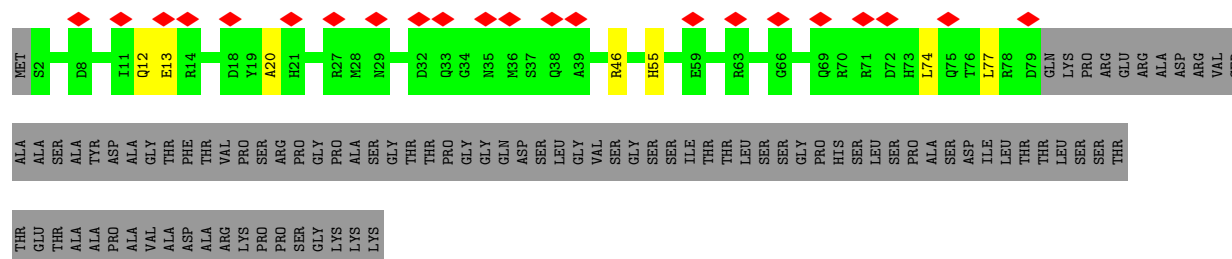
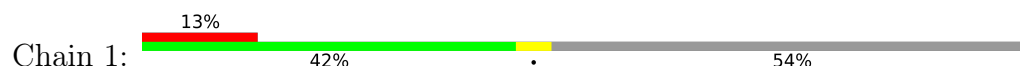
• Molecule 7: Small capsomere-interacting protein



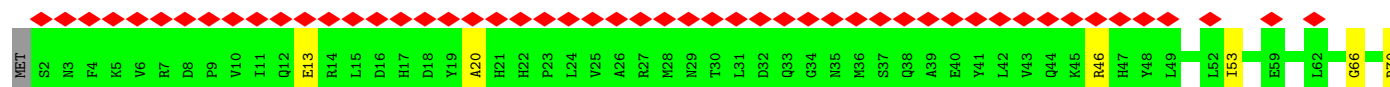
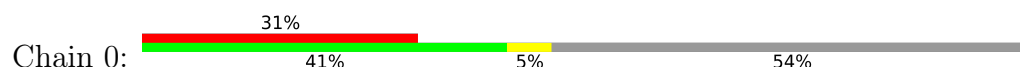
• Molecule 7: Small capsomere-interacting protein



• Molecule 7: Small capsomere-interacting protein



• Molecule 7: Small capsomere-interacting protein





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	928740	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	0.135	Depositor
Minimum map value	-0.085	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.022	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 ⓘ

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	k	0.24	0/2753	0.49	0/3755
2	l	0.21	0/698	0.46	0/942
2	m	0.21	0/656	0.50	0/887
3	n	0.25	0/326	0.45	0/437
3	o	0.25	0/326	0.45	0/437
4	5	0.23	0/2489	0.51	2/3383 (0.1%)
4	b	0.29	0/2540	0.62	2/3452 (0.1%)
5	6	0.24	0/2430	0.56	0/3309
5	7	0.26	0/2360	0.55	0/3210
5	c	0.27	0/2376	0.62	2/3234 (0.1%)
5	d	0.26	0/2411	0.57	0/3281
6	4	0.28	0/9861	0.70	8/13391 (0.1%)
6	S	0.29	0/10300	0.57	3/13998 (0.0%)
6	T	0.33	0/10919	0.68	6/14839 (0.0%)
6	W	0.32	0/10874	0.68	7/14780 (0.0%)
6	X	0.30	0/10768	0.58	5/14635 (0.0%)
7	0	0.22	0/682	0.56	2/919 (0.2%)
7	1	0.22	0/682	0.56	2/919 (0.2%)
7	2	0.22	0/682	0.56	2/919 (0.2%)
7	3	0.22	0/682	0.56	2/919 (0.2%)
7	A	0.17	0/391	0.44	0/528
All	All	0.29	0/75206	0.62	43/102174 (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
6	4	0	13
6	S	0	1
6	T	0	6
6	W	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
6	X	0	2
All	All	0	28

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	4	798	TYR	CA-C-N	7.24	134.74	121.70
6	4	798	TYR	C-N-CA	7.24	134.74	121.70
6	W	421	GLY	N-CA-C	6.78	120.69	112.49
6	T	1113	VAL	N-CA-CB	-6.56	104.53	112.33
7	1	20	ALA	CA-C-N	6.40	133.22	121.70
7	1	20	ALA	C-N-CA	6.40	133.22	121.70
7	0	20	ALA	CA-C-N	6.40	133.22	121.70
7	0	20	ALA	C-N-CA	6.40	133.22	121.70
7	2	20	ALA	CA-C-N	6.39	133.19	121.70
7	2	20	ALA	C-N-CA	6.39	133.19	121.70
7	3	20	ALA	CA-C-N	6.39	133.20	121.70
7	3	20	ALA	C-N-CA	6.39	133.20	121.70
6	4	848	ASP	CA-C-N	6.33	133.63	121.54
6	4	848	ASP	C-N-CA	6.33	133.63	121.54
6	W	262	SER	CA-C-N	6.29	133.56	121.54
6	W	262	SER	C-N-CA	6.29	133.56	121.54
6	W	308	VAL	N-CA-C	-6.14	106.44	111.91
6	X	993	SER	N-CA-C	6.09	123.28	109.81
6	4	103	GLY	CA-C-N	6.07	131.44	122.82
6	4	103	GLY	C-N-CA	6.07	131.44	122.82
6	T	389	PRO	CA-C-N	5.94	128.64	120.39
6	T	389	PRO	C-N-CA	5.94	128.64	120.39
6	T	1113	VAL	CB-CA-C	5.82	116.90	110.62
6	S	993	SER	N-CA-C	5.74	122.50	109.81
6	T	848	ASP	CA-C-N	5.62	132.28	121.54
6	T	848	ASP	C-N-CA	5.62	132.28	121.54
6	W	1302	THR	CA-C-N	5.61	128.11	120.54
6	W	1302	THR	C-N-CA	5.61	128.11	120.54
5	c	233	ASP	CA-C-N	5.58	130.27	121.56
5	c	233	ASP	C-N-CA	5.58	130.27	121.56
4	5	296	PHE	CA-C-N	5.26	135.47	126.32
4	5	296	PHE	C-N-CA	5.26	135.47	126.32
4	b	211	CYS	CA-C-N	5.20	139.48	127.00
4	b	211	CYS	C-N-CA	5.20	139.48	127.00
6	X	43	ALA	CA-C-N	5.14	131.37	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	X	43	ALA	C-N-CA	5.14	131.37	121.54
6	S	1004	ALA	CA-C-N	5.14	141.18	121.95
6	S	1004	ALA	C-N-CA	5.14	141.18	121.95
6	W	262	SER	N-CA-C	5.10	118.60	112.38
6	4	594	GLN	CA-C-N	5.07	128.43	120.82
6	4	594	GLN	C-N-CA	5.07	128.43	120.82
6	X	992	LYS	CA-C-N	5.02	134.05	121.80
6	X	992	LYS	C-N-CA	5.02	134.05	121.80

There are no chirality outliers.

All (28) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	4	1084	HIS	Peptide
6	4	1091	THR	Peptide
6	4	1092	ALA	Peptide
6	4	110	LYS	Peptide
6	4	1334	HIS	Peptide
6	4	292	GLN	Peptide
6	4	313	LEU	Peptide
6	4	506	VAL	Peptide
6	4	842	ASP	Peptide
6	4	843	VAL	Peptide
6	4	886	PRO	Peptide
6	4	899	ASP	Peptide
6	4	90	LYS	Peptide
6	S	991	HIS	Peptide
6	T	10	PHE	Peptide
6	T	1112	GLY	Peptide
6	T	505	ASN	Peptide
6	T	537	HIS	Peptide
6	T	886	PRO	Peptide
6	T	944	PHE	Peptide
6	W	262	SER	Peptide
6	W	263	THR	Mainchain
6	W	354	HIS	Peptide
6	W	537	HIS	Peptide
6	W	848	ASP	Peptide
6	W	849	ASP	Peptide
6	X	43	ALA	Peptide
6	X	991	HIS	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	k	2680	0	2675	32	0
2	l	686	0	704	12	0
2	m	645	0	653	6	0
3	n	323	0	353	4	0
3	o	323	0	353	5	0
4	5	2428	0	2421	29	0
4	b	2478	0	2466	22	0
5	6	2382	0	2396	27	0
5	7	2315	0	2335	21	0
5	c	2330	0	2354	32	0
5	d	2365	0	2379	26	0
6	4	9634	0	9527	130	0
6	S	10061	0	9956	90	0
6	T	10667	0	10543	101	0
6	W	10622	0	10500	131	0
6	X	10519	0	10399	114	0
7	0	666	0	647	5	0
7	1	666	0	647	4	0
7	2	666	0	647	3	0
7	3	666	0	647	4	0
7	A	380	0	369	9	0
All	All	73502	0	72971	706	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 5.

All (706) 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)
5:c:5:LYS:HB2	5:c:86:ARG:HB3	1.71	0.72
6:4:864:GLN:HB2	6:4:930:ARG:HH22	1.58	0.68
6:4:698:GLU:HG3	6:4:705:ILE:HD12	1.76	0.67
5:7:220:ARG:HH22	5:7:256:GLN:HE21	1.42	0.66
6:4:916:THR:HG23	6:4:984:MET:HG2	1.77	0.66
6:X:178:VAL:HG22	6:X:1061:MET:HE2	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:536:VAL:HG13	6:T:1244:SER:HA	1.78	0.66
6:4:777:ARG:NH2	6:4:885:CYS:O	2.30	0.65
6:4:875:ILE:HG23	6:4:878:LEU:HD12	1.79	0.64
6:S:187:PRO:HG2	6:S:192:LEU:HD12	1.78	0.64
7:1:55:HIS:HD2	6:X:770:LEU:HD22	1.61	0.64
6:4:566:PRO:HB2	6:4:568:PRO:HD2	1.79	0.64
6:S:845:ASN:HB3	6:S:848:ASP:HB2	1.78	0.64
6:W:278:THR:HG22	6:W:1051:ILE:HG12	1.80	0.64
6:T:113:GLN:HB3	6:W:38:LEU:HB2	1.80	0.64
6:4:893:ARG:NH2	6:4:984:MET:SD	2.71	0.64
6:4:611:LEU:HD22	6:4:862:ILE:HD13	1.80	0.63
5:d:97:ASN:HD22	5:d:105:TRP:HD1	1.45	0.63
7:2:55:HIS:HD2	6:S:770:LEU:HD22	1.63	0.63
6:S:1068:VAL:HG22	6:S:1082:ILE:HG12	1.78	0.63
6:W:658:ARG:HA	6:W:681:LEU:HD11	1.80	0.63
6:W:1073:VAL:HG13	6:W:1078:VAL:HG22	1.81	0.63
6:W:1200:ARG:NH1	6:W:1221:ASP:O	2.32	0.62
6:X:603:THR:HG22	6:X:647:LYS:HB3	1.81	0.62
5:6:114:LEU:HD11	5:6:145:GLY:HA2	1.80	0.62
6:T:1280:ARG:NH2	6:T:1288:GLU:OE1	2.33	0.62
6:W:561:MET:HE3	6:W:990:TRP:HB3	1.81	0.61
6:4:861:ASP:O	6:4:930:ARG:NH2	2.33	0.61
6:T:254:GLU:OE2	6:T:372:LYS:NZ	2.32	0.61
6:W:929:ASP:OD1	6:W:932:ARG:NH2	2.33	0.61
4:5:41:LEU:HD21	6:4:1068:VAL:HG11	1.82	0.61
6:T:407:HIS:HB2	6:T:1184:VAL:HG12	1.83	0.61
6:T:929:ASP:OD1	6:T:932:ARG:NH2	2.34	0.61
4:b:128:VAL:HG11	4:b:312:LEU:HD22	1.83	0.60
6:T:717:LEU:HA	6:T:915:GLN:HE22	1.65	0.60
6:X:37:LEU:HB2	6:X:50:PHE:HB2	1.81	0.60
6:T:566:PRO:HG2	6:T:569:LEU:HD12	1.82	0.60
6:T:868:ILE:HG22	6:T:870:PRO:HD3	1.83	0.60
6:4:525:HIS:HD2	6:4:527:THR:HG22	1.66	0.60
7:3:11:ILE:HD11	6:T:832:THR:HG22	1.84	0.60
6:S:692:LEU:HD13	6:T:972:ARG:HG2	1.82	0.60
1:k:114:ARG:NH1	1:k:286:ASP:OD2	2.34	0.60
2:m:95:ILE:HD13	3:n:2605:LEU:HB3	1.82	0.60
6:T:275:VAL:HG22	6:T:375:ALA:HB3	1.84	0.60
6:T:1241:GLN:HB3	6:T:1244:SER:HB3	1.83	0.60
6:W:130:GLU:HG2	6:W:1079:THR:HG22	1.83	0.60
5:d:7:ILE:HG21	5:d:33:LEU:HD21	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:608:ALA:HB3	6:W:678:ARG:HH22	1.67	0.59
6:S:1182:THR:HG23	6:S:1236:ASN:HB3	1.83	0.59
5:7:38:ARG:HH22	6:S:1083:THR:HG22	1.67	0.59
5:c:179:THR:OG1	5:c:189:ARG:NH1	2.35	0.59
6:T:1201:ALA:HB3	6:T:1227:PRO:HG2	1.83	0.59
1:k:409:VAL:HA	1:k:430:PRO:HA	1.83	0.59
6:4:838:PRO:HD2	6:4:854:LEU:HA	1.83	0.59
6:X:698:GLU:HG3	6:X:705:ILE:HD12	1.84	0.59
6:T:1187:ASP:OD2	6:T:1232:ARG:NH2	2.36	0.59
5:6:113:VAL:HG22	5:6:139:VAL:HG12	1.85	0.59
6:T:811:MET:HB3	6:T:819:MET:HE1	1.84	0.59
6:W:1293:LEU:HD21	6:W:1297:PRO:HG3	1.84	0.59
5:d:97:ASN:HD22	5:d:105:TRP:CD1	2.21	0.59
6:4:684:LEU:HD11	6:4:805:LEU:HB2	1.85	0.59
6:X:1187:ASP:OD2	6:X:1232:ARG:NH2	2.36	0.59
6:T:578:ARG:NH2	6:T:1017:GLN:OE1	2.35	0.58
6:W:256:THR:HG22	6:W:258:PHE:H	1.67	0.58
6:T:640:THR:O	6:T:644:ASN:ND2	2.36	0.58
6:X:203:ARG:NH1	6:W:1313:ASP:OD2	2.35	0.58
6:S:633:LEU:HA	6:S:874:MET:HE3	1.86	0.58
4:b:289:CYS:SG	4:b:290:THR:N	2.77	0.58
6:X:39:LEU:HB3	6:X:43:ALA:HB1	1.86	0.58
4:b:207:LEU:HB3	4:b:248:SER:HB3	1.85	0.58
6:S:1111:MET:SD	6:S:1366:ARG:NH2	2.70	0.58
6:4:399:THR:HG21	6:4:1268:GLN:HE22	1.69	0.58
6:4:439:ASN:ND2	6:4:1372:ASN:O	2.36	0.58
6:4:838:PRO:HA	6:4:841:ALA:HB3	1.84	0.58
6:W:1045:GLU:N	6:W:1109:THR:OG1	2.35	0.58
5:7:86:ARG:NH1	5:7:88:ASP:OD1	2.36	0.58
6:4:731:MET:HG2	6:4:738:PRO:HG2	1.86	0.58
6:S:578:ARG:NH1	6:S:1014:SER:O	2.37	0.58
6:W:214:VAL:HG12	6:W:218:LYS:HE2	1.86	0.58
1:k:46:ARG:NH2	1:k:347:GLU:OE2	2.37	0.57
1:k:116:LEU:HD23	1:k:118:LEU:H	1.68	0.57
5:6:111:LEU:HB2	5:6:286:LEU:HB2	1.86	0.57
6:X:1344:ASN:ND2	6:X:1347:THR:OG1	2.37	0.57
6:W:78:THR:HG22	6:W:304:ALA:HB3	1.86	0.57
6:W:543:PHE:HZ	6:W:555:ARG:HH11	1.52	0.57
6:W:537:HIS:HA	6:W:1238:TRP:CD1	2.39	0.57
6:W:850:ILE:HD12	6:W:870:PRO:HG2	1.86	0.57
4:5:150:MET:HE2	4:5:241:MET:HE3	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:7:GLN:NE2	6:S:36:GLN:OE1	2.38	0.57
6:X:606:ASP:OD1	6:W:678:ARG:NH1	2.37	0.57
6:W:538:PRO:O	6:W:559:ARG:NH1	2.37	0.57
6:4:623:GLN:NE2	6:4:761:GLY:O	2.37	0.57
6:S:698:GLU:HG3	6:S:705:ILE:HD12	1.85	0.57
6:X:128:GLU:OE2	6:X:1071:ARG:NH2	2.37	0.57
6:4:1066:PRO:HB3	6:4:1084:HIS:HA	1.86	0.57
6:X:777:ARG:NH2	6:X:885:CYS:O	2.38	0.57
6:4:1199:GLY:HA3	6:4:1236:ASN:H	1.70	0.57
6:W:578:ARG:NH2	6:W:1017:GLN:OE1	2.38	0.57
6:4:128:GLU:OE2	6:4:1071:ARG:NH2	2.37	0.57
5:c:177:TYR:HB3	5:d:263:ILE:HG21	1.86	0.57
6:4:724:HIS:HB3	6:4:793:LEU:HB2	1.87	0.57
6:S:1344:ASN:ND2	6:S:1347:THR:OG1	2.38	0.57
1:k:91:ASN:ND2	1:k:270:SER:OG	2.38	0.56
6:S:488:THR:OG1	6:S:982:ASN:ND2	2.39	0.56
6:4:639:GLN:HA	6:4:670:PRO:HG3	1.87	0.56
6:S:178:VAL:HG22	6:S:1061:MET:HE2	1.86	0.56
6:S:770:LEU:HD21	6:S:883:LEU:HD22	1.87	0.56
6:W:965:VAL:HG13	6:W:972:ARG:HG2	1.87	0.56
6:W:1071:ARG:O	6:W:1079:THR:OG1	2.24	0.56
6:W:799:ASN:HD21	6:W:802:LEU:HD12	1.69	0.56
6:4:507:ALA:HB1	6:4:978:ASN:HD21	1.71	0.56
6:X:1294:ALA:HB3	6:X:1318:GLN:HE21	1.69	0.56
6:W:481:TYR:OH	6:W:979:VAL:O	2.23	0.56
6:S:1294:ALA:HB3	6:S:1318:GLN:HE21	1.69	0.56
6:T:93:PHE:HB2	6:T:116:VAL:HB	1.88	0.56
1:k:315:ARG:NH2	1:k:391:GLY:O	2.39	0.56
5:c:9:VAL:HG21	5:c:45:LEU:HD21	1.88	0.56
7:2:13:GLU:OE1	7:2:46:ARG:NH2	2.37	0.56
6:T:1250:TYR:HB2	6:T:1270:PHE:HD2	1.70	0.56
6:W:91:ILE:HD12	6:W:1089:LEU:HD22	1.87	0.56
6:W:275:VAL:HG22	6:W:375:ALA:HB3	1.88	0.56
5:6:11:LEU:HG	5:6:15:LEU:HD23	1.87	0.56
6:S:640:THR:O	6:S:644:ASN:ND2	2.39	0.56
6:X:453:ILE:HD11	6:X:1038:MET:HE1	1.88	0.56
6:X:856:ASN:ND2	7:0:66:GLY:O	2.39	0.56
5:6:189:ARG:NH1	5:6:190:LEU:O	2.39	0.55
5:c:111:LEU:HB2	5:c:286:LEU:HB2	1.88	0.55
6:4:763:MET:HE1	7:A:54:ALA:HB1	1.88	0.55
1:k:25:ARG:NH2	6:X:737:GLN:O	2.38	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:143:ILE:HG22	4:5:145:ASN:H	1.71	0.55
6:T:178:VAL:HG22	6:T:1061:MET:HE2	1.89	0.55
6:T:537:HIS:HA	6:T:1238:TRP:CD1	2.42	0.55
6:T:717:LEU:HD23	6:T:804:LYS:HD3	1.88	0.55
6:T:1070:ARG:HH21	6:T:1073:VAL:HG21	1.70	0.55
6:T:1111:MET:SD	6:T:1366:ARG:NH2	2.79	0.55
6:X:640:THR:O	6:X:644:ASN:ND2	2.40	0.55
2:l:99:THR:O	2:l:103:ASN:ND2	2.39	0.55
4:b:94:LYS:NZ	5:d:106:ASP:OD2	2.38	0.55
6:W:182:LYS:NZ	6:W:1058:SER:OG	2.39	0.55
5:6:177:TYR:HB3	5:7:263:ILE:HG21	1.87	0.55
5:6:94:GLN:HE21	5:6:297:ALA:HB1	1.70	0.55
6:S:658:ARG:HA	6:S:681:LEU:HD11	1.87	0.55
6:T:399:THR:HG22	6:T:1043:THR:HG22	1.88	0.55
6:X:399:THR:HG22	6:X:1043:THR:HG22	1.88	0.55
6:W:1027:GLN:HB3	6:W:1032:MET:HB2	1.89	0.55
6:4:428:GLN:NE2	6:4:577:SER:OG	2.34	0.55
6:T:306:TYR:OH	6:T:323:MET:O	2.24	0.55
5:d:94:GLN:HE21	5:d:297:ALA:HB1	1.70	0.55
6:4:1333:SER:HB2	6:4:1355:GLN:HB2	1.88	0.55
6:X:777:ARG:HG2	6:X:887:PHE:HE1	1.71	0.55
6:S:902:GLN:NE2	6:S:1020:SER:OG	2.40	0.55
6:T:334:VAL:HG21	6:X:310:GLY:HA2	1.89	0.55
6:W:1280:ARG:NH2	6:W:1288:GLU:OE1	2.40	0.55
7:3:13:GLU:OE1	7:3:46:ARG:NH2	2.37	0.54
6:X:1043:THR:OG1	6:X:1305:GLN:NE2	2.39	0.54
1:k:277:PRO:HG2	1:k:282:LEU:HD12	1.89	0.54
4:5:50:ARG:NH2	6:4:140:PHE:O	2.40	0.54
4:5:254:GLU:HG2	5:6:64:GLN:HE21	1.72	0.54
6:S:603:THR:HG22	6:S:647:LYS:HB3	1.89	0.54
6:T:777:ARG:NH2	6:T:885:CYS:O	2.40	0.54
7:1:13:GLU:OE1	7:1:46:ARG:NH2	2.37	0.54
4:b:124:GLN:NE2	4:b:311:SER:O	2.41	0.54
4:5:66:ARG:NH1	5:7:90:SER:O	2.41	0.54
6:S:447:GLN:NE2	6:T:521:GLU:OE1	2.41	0.54
6:T:578:ARG:NH1	6:T:1014:SER:O	2.40	0.54
4:5:289:CYS:SG	4:5:290:THR:N	2.80	0.54
6:S:1167:PRO:HD3	6:T:1224:ILE:HD13	1.89	0.54
6:T:146:PRO:HA	6:T:149:PHE:HD2	1.72	0.54
5:c:38:ARG:H	6:W:1071:ARG:HH22	1.55	0.54
6:4:309:ARG:HD3	6:X:38:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:130:GLU:HG2	6:X:1079:THR:HG22	1.90	0.54
6:X:729:ASP:OD2	6:X:798:TYR:OH	2.25	0.54
5:d:155:TYR:OH	5:d:194:ASN:ND2	2.40	0.54
6:4:846:ALA:HA	6:4:872:VAL:HB	1.88	0.54
6:S:1283:TYR:O	6:S:1287:ASN:ND2	2.41	0.54
6:4:834:THR:HG22	7:A:53:ILE:HD12	1.90	0.54
6:T:658:ARG:HA	6:T:681:LEU:HD11	1.89	0.54
6:X:1280:ARG:NH2	6:X:1288:GLU:OE1	2.40	0.53
6:W:90:LYS:HE2	6:W:117:MET:HE1	1.89	0.53
4:b:40:ASP:O	5:c:2:ALA:N	2.41	0.53
6:4:567:GLN:HE21	6:4:998:TYR:HA	1.73	0.53
6:T:224:HIS:HD2	6:T:244:MET:HE1	1.73	0.53
6:X:770:LEU:HD21	6:X:883:LEU:HD22	1.90	0.53
6:X:1068:VAL:HG22	6:X:1082:ILE:HG12	1.90	0.53
6:W:1308:VAL:HG21	6:W:1314:VAL:HG21	1.91	0.53
4:b:280:ILE:HA	4:b:283:LEU:HD13	1.90	0.53
6:S:130:GLU:HG2	6:S:1079:THR:HG22	1.90	0.53
6:4:700:VAL:O	6:4:1131:GLN:NE2	2.41	0.53
6:S:157:LYS:HD2	6:T:338:ASN:HA	1.90	0.53
5:6:201:LEU:HD13	5:7:231:ARG:HH12	1.72	0.53
6:S:707:HIS:HD2	6:S:715:PRO:HD3	1.72	0.53
5:c:291:TYR:HD1	5:c:298:ALA:HB2	1.72	0.53
6:4:47:SER:OG	6:4:48:VAL:N	2.41	0.53
2:l:80:ARG:NH2	3:n:2622:SER:OG	2.41	0.53
6:S:399:THR:HG22	6:S:1043:THR:HG22	1.90	0.53
7:0:13:GLU:OE1	7:0:46:ARG:NH2	2.37	0.53
5:7:291:TYR:HD1	5:7:298:ALA:HB2	1.73	0.53
5:d:47:LEU:HB2	5:d:135:VAL:HB	1.91	0.53
6:4:1071:ARG:O	6:4:1079:THR:OG1	2.25	0.53
6:T:1071:ARG:O	6:T:1079:THR:OG1	2.24	0.53
6:X:278:THR:HG22	6:X:1051:ILE:HG12	1.90	0.53
6:4:495:ARG:O	6:4:499:GLN:N	2.41	0.53
6:T:591:VAL:HB	6:T:683:GLU:HB2	1.90	0.53
6:X:785:ARG:NH1	6:X:787:VAL:O	2.41	0.53
4:5:186:LEU:HD23	4:5:192:ARG:HB3	1.91	0.53
6:X:91:ILE:HD11	6:X:1089:LEU:HD22	1.89	0.53
4:5:264:THR:HA	5:7:237:LEU:HD21	1.91	0.52
5:6:285:ARG:HD2	5:7:305:ARG:HE	1.73	0.52
4:b:10:ARG:NH1	6:W:144:GLU:OE1	2.42	0.52
6:4:206:LYS:HG3	6:4:208:ALA:H	1.73	0.52
6:X:687:LEU:HD23	6:X:805:LEU:HD22	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:963:ASN:HA	6:W:966:THR:HG22	1.91	0.52
6:W:399:THR:HG22	6:W:1043:THR:HG22	1.91	0.52
6:4:684:LEU:HA	6:4:687:LEU:HB2	1.91	0.52
6:S:11:PRO:HB2	6:X:332:ARG:HD2	1.91	0.52
6:S:421:GLY:HA3	6:T:413:TYR:HA	1.91	0.52
6:T:854:LEU:HD13	6:T:860:LYS:HG2	1.91	0.52
1:k:19:ALA:HB3	1:k:83:LEU:HB2	1.91	0.52
4:5:217:ARG:NH2	5:6:43:GLN:O	2.43	0.52
6:S:491:MET:HE3	6:S:786:HIS:HA	1.90	0.52
6:T:946:LYS:HE2	6:T:993:SER:HA	1.91	0.52
4:5:234:ARG:HD3	4:5:274:LEU:HD11	1.91	0.52
6:4:84:ARG:HH21	6:X:134:ALA:HB2	1.74	0.52
6:X:578:ARG:NH1	6:X:1014:SER:O	2.43	0.52
6:4:913:VAL:HG12	6:4:990:TRP:HD1	1.75	0.52
6:4:963:ASN:HA	6:4:966:THR:HG22	1.92	0.52
6:W:588:MET:HE1	6:W:687:LEU:HD12	1.91	0.52
6:W:603:THR:HG22	6:W:647:LYS:HB3	1.92	0.52
6:W:851:LEU:HD23	6:W:854:LEU:HD12	1.92	0.52
6:4:275:VAL:HG22	6:4:375:ALA:HB3	1.92	0.52
6:X:488:THR:OG1	6:X:982:ASN:ND2	2.43	0.52
6:4:130:GLU:HG2	6:4:1079:THR:HG22	1.90	0.52
6:S:731:MET:HG2	6:S:738:PRO:HG2	1.91	0.52
6:X:66:PHE:HD1	6:X:175:VAL:HG22	1.75	0.52
6:W:902:GLN:NE2	6:W:1020:SER:OG	2.42	0.52
1:k:412:SER:HB3	2:m:34:ILE:HG12	1.92	0.51
6:4:399:THR:HG22	6:4:1043:THR:HG22	1.91	0.51
6:4:935:ALA:HA	6:4:938:MET:HB2	1.91	0.51
6:S:1042:ARG:NH1	6:S:1044:ASP:OD2	2.43	0.51
6:X:306:TYR:OH	6:X:323:MET:O	2.28	0.51
6:T:512:VAL:HG12	6:T:993:SER:HB3	1.92	0.51
6:X:394:ARG:HD3	6:X:1315:PHE:HB3	1.91	0.51
6:4:182:LYS:NZ	6:4:1058:SER:OG	2.44	0.51
6:W:183:LEU:HD13	6:W:394:ARG:HH21	1.74	0.51
5:c:2:ALA:O	6:W:1070:ARG:NH1	2.43	0.51
5:d:5:LYS:HB2	5:d:86:ARG:HB3	1.92	0.51
6:4:759:LEU:HD22	6:4:792:PRO:HB3	1.93	0.51
6:S:777:ARG:NH2	6:S:885:CYS:O	2.43	0.51
6:T:350:LEU:HD12	6:W:13:LEU:HD23	1.92	0.51
6:W:602:GLU:HB3	6:W:647:LYS:HE2	1.92	0.51
4:b:47:ALA:HB2	6:W:1068:VAL:HG23	1.92	0.51
6:T:1342:MET:HA	6:T:1375:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:1005:THR:HG22	6:W:1007:GLY:H	1.74	0.51
5:6:97:ASN:HB3	5:6:296:LEU:HB3	1.93	0.51
5:c:266:MET:HE1	5:d:211:LEU:HD13	1.91	0.51
7:A:28:MET:HE3	7:A:45:LYS:HE2	1.91	0.51
6:W:407:HIS:HB2	6:W:1184:VAL:HG12	1.93	0.51
4:5:207:LEU:HB2	4:5:248:SER:HB3	1.91	0.51
5:d:53:ARG:NH2	5:d:133:ASP:OD2	2.43	0.51
6:S:687:LEU:HD23	6:S:805:LEU:HD22	1.93	0.51
6:T:603:THR:HG22	6:T:647:LYS:HB3	1.92	0.51
6:4:676:HIS:HA	6:4:679:LYS:HB2	1.93	0.50
4:5:300:PRO:HB2	4:5:315:LEU:HD22	1.92	0.50
5:6:124:THR:HG22	5:6:135:VAL:HG22	1.93	0.50
4:b:305:LEU:O	4:b:312:LEU:N	2.41	0.50
1:k:47:PHE:HB2	1:k:52:GLY:HA2	1.94	0.50
6:X:87:ILE:HD11	6:W:49:ARG:HD3	1.93	0.50
6:X:1345:LYS:NZ	6:X:1376:TYR:OXT	2.37	0.50
6:W:963:ASN:O	6:W:967:ARG:N	2.43	0.50
6:4:778:VAL:HG13	7:A:44:GLN:HE22	1.76	0.50
6:S:192:LEU:HD13	6:S:1098:VAL:HG22	1.92	0.50
4:5:70:TYR:HB2	4:5:188:ARG:HH11	1.75	0.50
5:c:138:MET:HE2	5:c:140:VAL:HG22	1.92	0.50
5:d:285:ARG:HH21	5:d:305:ARG:HD2	1.76	0.50
6:S:716:HIS:HD2	6:S:736:ARG:HH21	1.59	0.50
6:T:278:THR:HG22	6:T:1051:ILE:HG12	1.93	0.50
6:W:93:PHE:HB2	6:W:116:VAL:HB	1.91	0.50
6:W:537:HIS:HB2	6:W:1245:LEU:HB2	1.94	0.50
6:T:436:ASN:HD22	6:T:440:VAL:HB	1.77	0.50
6:T:1073:VAL:HG22	6:T:1078:VAL:HG13	1.92	0.50
6:X:1353:MET:HE1	6:W:420:ARG:HD3	1.93	0.50
6:W:447:GLN:HB3	6:W:1028:ALA:HB1	1.93	0.50
6:4:1200:ARG:HG3	6:4:1234:THR:HG23	1.93	0.50
6:X:93:PHE:HB2	6:X:116:VAL:HB	1.93	0.50
6:W:633:LEU:HD12	6:W:874:MET:HB3	1.94	0.50
6:4:471:ALA:HB1	6:4:1242:ARG:HG3	1.94	0.49
6:4:743:GLY:O	6:4:746:ASN:ND2	2.45	0.49
2:m:71:ASP:OD1	3:n:2631:LYS:NZ	2.34	0.49
4:5:234:ARG:HG2	4:5:239:PRO:HA	1.93	0.49
5:6:48:GLY:HA2	5:6:51:CYS:HB3	1.93	0.49
6:4:537:HIS:HA	6:4:1238:TRP:HD1	1.75	0.49
6:X:611:LEU:HD11	6:X:935:ALA:HB2	1.94	0.49
4:5:228:ALA:HB2	4:5:291:LEU:HD11	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:12:TYR:HA	6:W:56:VAL:HG12	1.93	0.49
6:S:453:ILE:HD11	6:S:1038:MET:HE1	1.94	0.49
6:W:828:ASN:ND2	6:W:937:THR:O	2.45	0.49
5:c:175:ASP:HB3	5:c:189:ARG:HH12	1.77	0.49
2:l:95:ILE:HD13	3:o:2605:LEU:HB3	1.94	0.49
6:T:1268:GLN:HG2	6:T:1321:HIS:CD2	2.46	0.49
5:6:30:VAL:HG22	5:6:73:VAL:HG22	1.94	0.49
6:4:1217:ARG:HG3	6:4:1221:ASP:HB2	1.94	0.49
6:X:740:ILE:HB	6:X:747:TYR:HB3	1.95	0.49
5:d:11:LEU:HD12	5:d:80:ASP:HB2	1.93	0.49
6:4:725:ASP:HB2	6:4:790:VAL:HG11	1.95	0.49
6:4:898:ARG:NH1	6:4:904:PHE:O	2.45	0.49
5:6:169:VAL:HG11	5:6:174:LEU:HD13	1.95	0.49
6:S:66:PHE:HD1	6:S:175:VAL:HG22	1.78	0.49
6:S:495:ARG:HE	6:S:499:GLN:HE21	1.59	0.49
5:c:201:LEU:HD22	5:d:231:ARG:HH21	1.76	0.49
6:4:340:LEU:HD12	6:4:341:PRO:HD2	1.94	0.49
6:X:658:ARG:HA	6:X:681:LEU:HD11	1.94	0.49
6:W:1344:ASN:ND2	6:W:1347:THR:OG1	2.45	0.49
1:k:94:PRO:HG3	1:k:271:PHE:HD1	1.78	0.48
5:6:262:ASP:OD2	5:7:158:TYR:OH	2.31	0.48
6:X:1369:LYS:HG2	6:X:1374:VAL:HG22	1.95	0.48
5:c:58:ASP:OD1	5:c:58:ASP:N	2.43	0.48
6:W:1073:VAL:HG22	6:W:1078:VAL:HG13	1.95	0.48
6:W:578:ARG:NH1	6:W:1014:SER:O	2.42	0.48
6:W:591:VAL:HB	6:W:683:GLU:HB2	1.95	0.48
6:W:600:ILE:HG23	6:W:651:VAL:HG11	1.94	0.48
6:S:23:ILE:HB	6:W:387:GLN:HE22	1.78	0.48
1:k:316:VAL:HG13	1:k:400:LEU:HD11	1.95	0.48
6:X:615:VAL:HG22	6:X:938:MET:HE1	1.96	0.48
6:4:633:LEU:HD11	6:4:874:MET:HA	1.94	0.48
6:S:725:ASP:HB3	6:S:793:LEU:HD22	1.94	0.48
6:T:740:ILE:HB	6:T:747:TYR:HB3	1.94	0.48
6:X:256:THR:HG22	6:X:258:PHE:H	1.79	0.48
6:X:929:ASP:HA	6:X:932:ARG:HG3	1.96	0.48
6:W:731:MET:HG2	6:W:738:PRO:HG2	1.96	0.48
4:5:87:GLY:H	4:5:165:MET:HB2	1.78	0.48
6:4:228:LEU:HD22	6:4:1103:HIS:HB2	1.95	0.48
6:S:740:ILE:HB	6:S:747:TYR:HB3	1.96	0.48
6:T:739:ILE:HB	6:T:895:ILE:HB	1.95	0.48
6:W:276:LEU:HB3	6:W:1053:TYR:HD1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:206:LYS:HB3	6:4:209:VAL:HG23	1.96	0.48
6:4:756:PHE:O	6:4:788:LEU:N	2.47	0.48
6:S:619:MET:SD	6:S:881:SER:OG	2.69	0.48
6:S:1369:LYS:HG2	6:S:1374:VAL:HG22	1.95	0.48
6:X:932:ARG:HH12	6:W:796:ASN:HB3	1.79	0.48
5:7:69:CYS:SG	5:7:70:THR:N	2.86	0.48
6:4:520:THR:HG22	6:4:568:PRO:HA	1.96	0.48
6:4:578:ARG:NH2	6:4:1017:GLN:OE1	2.46	0.48
6:4:895:ILE:HG13	6:4:914:ALA:HB2	1.96	0.48
6:S:826:TYR:OH	6:S:920:ASN:O	2.31	0.48
6:S:1169:LEU:O	6:T:211:SER:OG	2.26	0.48
6:X:742:ILE:HG12	6:X:788:LEU:HD22	1.94	0.48
6:W:95:ILE:HB	6:W:114:TYR:HB2	1.96	0.48
5:6:212:CYS:N	5:7:222:CYS:SG	2.87	0.47
5:c:266:MET:HB3	5:d:150:GLN:HE21	1.80	0.47
6:X:518:VAL:HG13	6:X:522:ASP:HB3	1.94	0.47
6:X:718:LEU:HD12	6:X:894:VAL:HG21	1.96	0.47
5:d:79:PRO:HA	5:d:80:ASP:HA	1.60	0.47
6:4:685:ILE:O	6:4:689:GLN:N	2.46	0.47
6:W:9:PRO:HB3	6:W:45:GLU:HB3	1.97	0.47
6:S:1187:ASP:OD2	6:S:1232:ARG:NH2	2.47	0.47
6:X:532:LEU:O	6:X:1241:GLN:NE2	2.40	0.47
5:c:262:ASP:OD2	5:d:158:TYR:OH	2.32	0.47
6:S:714:ASP:OD1	6:S:736:ARG:NH2	2.48	0.47
6:S:1047:LEU:HD12	6:S:1106:ALA:HB3	1.97	0.47
6:X:1353:MET:HE1	6:W:420:ARG:HH11	1.79	0.47
6:X:836:ASN:HD21	6:X:854:LEU:HD12	1.79	0.47
6:X:1027:GLN:HB3	6:X:1032:MET:HB2	1.96	0.47
2:l:52:GLN:HG3	2:m:54:VAL:HG22	1.96	0.47
4:5:76:TYR:HB3	4:5:78:GLN:HG2	1.97	0.47
6:S:514:GLN:HG3	6:S:531:LEU:HD21	1.97	0.47
6:S:558:HIS:O	6:S:992:LYS:NZ	2.46	0.47
6:S:1043:THR:OG1	6:S:1305:GLN:NE2	2.47	0.47
6:T:228:LEU:HD21	6:T:285:ARG:HG3	1.97	0.47
6:T:494:PHE:HB3	6:T:498:HIS:HD2	1.80	0.47
6:X:902:GLN:NE2	6:X:1020:SER:OG	2.43	0.47
6:W:276:LEU:HA	6:W:1053:TYR:HA	1.97	0.47
6:W:438:ASN:HD22	6:W:1171:HIS:CD2	2.32	0.47
1:k:55:ARG:NH1	5:7:255:ASP:OD2	2.48	0.47
1:k:221:PRO:HB2	4:5:279:TYR:HB3	1.96	0.47
4:b:167:GLN:HB2	4:b:188:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:218:LYS:NZ	6:4:1323:LEU:O	2.47	0.47
5:d:51:CYS:HB2	5:d:62:ILE:HD11	1.97	0.47
6:4:750:PRO:HA	6:4:753:ARG:HB3	1.96	0.47
6:S:742:ILE:HG12	6:S:788:LEU:HD22	1.96	0.47
6:X:110:LYS:HD2	6:W:130:GLU:HG3	1.96	0.47
6:W:278:THR:HB	6:W:282:VAL:HB	1.97	0.47
6:W:325:ASN:ND2	6:W:352:ASP:OD2	2.47	0.47
5:6:305:ARG:O	5:7:305:ARG:NH2	2.48	0.47
6:4:1210:TYR:HB3	6:4:1283:TYR:HE2	1.79	0.47
6:S:423:GLU:HG2	6:S:1352:HIS:HE1	1.80	0.47
6:T:41:LYS:O	6:T:44:ARG:NH1	2.47	0.47
6:T:276:LEU:HB3	6:T:1053:TYR:HD1	1.80	0.47
6:T:856:ASN:OD1	6:T:860:LYS:NZ	2.43	0.47
6:W:626:LYS:NZ	6:W:881:SER:O	2.44	0.47
6:W:711:ALA:HB2	6:W:1018:LYS:HD3	1.97	0.47
6:W:718:LEU:HD12	6:W:894:VAL:HG21	1.96	0.47
6:T:770:LEU:HD21	6:T:883:LEU:HD22	1.97	0.46
6:X:491:MET:HE3	6:X:786:HIS:HA	1.96	0.46
6:W:955:ALA:HB1	6:W:962:ALA:HA	1.97	0.46
6:X:543:PHE:HE1	6:X:557:THR:HG23	1.80	0.46
6:W:575:GLN:NE2	6:W:1015:MET:SD	2.88	0.46
1:k:322:ARG:HH11	2:l:22:ARG:HD2	1.80	0.46
4:b:90:LEU:HD11	4:b:165:MET:HG3	1.96	0.46
5:c:58:ASP:HB3	5:c:196:ASP:HB3	1.97	0.46
5:c:218:VAL:HG13	5:d:215:SER:HB2	1.98	0.46
6:T:718:LEU:HD12	6:T:894:VAL:HG21	1.98	0.46
6:T:898:ARG:HD3	6:T:902:GLN:HG3	1.96	0.46
6:X:995:VAL:HG22	6:X:1015:MET:HE3	1.96	0.46
6:W:438:ASN:HB2	6:W:1171:HIS:HD2	1.80	0.46
1:k:56:ARG:HD2	5:6:167:GLY:HA3	1.97	0.46
6:4:278:THR:HG22	6:4:1051:ILE:HG12	1.98	0.46
6:X:717:LEU:HD23	6:X:804:LYS:HD3	1.98	0.46
6:W:591:VAL:N	6:W:683:GLU:OE1	2.37	0.46
5:6:204:LEU:HB3	5:7:229:LEU:HD11	1.97	0.46
6:4:1196:ASN:HD22	6:4:1202:ALA:H	1.63	0.46
6:S:718:LEU:HD12	6:S:894:VAL:HG21	1.97	0.46
6:W:297:MET:HE3	6:W:364:ALA:HB3	1.98	0.46
4:5:125:THR:HG22	4:5:312:LEU:HD11	1.98	0.46
4:b:211:CYS:HB2	4:b:213:MET:HB2	1.97	0.46
6:T:224:HIS:CD2	6:T:244:MET:HE1	2.49	0.46
6:T:350:LEU:HD21	6:W:15:THR:HG22	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:1005:THR:HG22	6:X:1007:GLY:H	1.80	0.46
6:T:82:ASP:OD1	6:T:82:ASP:N	2.48	0.46
6:X:444:PHE:HB2	6:X:1113:VAL:HG11	1.98	0.46
6:W:402:PHE:HD2	6:W:1040:VAL:HB	1.80	0.46
6:W:763:MET:HE3	6:W:883:LEU:HB2	1.97	0.46
6:W:770:LEU:HD21	6:W:883:LEU:HD22	1.97	0.46
6:4:655:HIS:O	6:4:659:PHE:N	2.46	0.45
6:S:836:ASN:HD21	6:S:854:LEU:HD12	1.82	0.45
6:W:331:ALA:HA	6:W:335:ASP:HB2	1.98	0.45
6:W:913:VAL:HG21	6:W:990:TRP:HE1	1.80	0.45
6:S:718:LEU:HD21	6:S:730:LEU:HD12	1.99	0.45
6:X:78:THR:HG22	6:X:304:ALA:HB3	1.97	0.45
2:l:97:ASN:O	2:l:101:SER:N	2.45	0.45
5:d:285:ARG:HH12	5:d:287:HIS:CE1	2.34	0.45
6:4:839:VAL:HG11	6:4:875:ILE:HB	1.98	0.45
6:X:456:PRO:HG2	6:X:1125:ASP:HB3	1.98	0.45
6:W:684:LEU:HD23	6:W:802:LEU:HD22	1.99	0.45
6:W:822:MET:SD	6:W:939:PHE:HB3	2.57	0.45
4:b:228:ALA:HB2	4:b:291:LEU:HD11	1.98	0.45
6:S:9:PRO:HG2	6:T:317:VAL:HG13	1.98	0.45
6:S:1169:LEU:H	6:S:1169:LEU:HG	1.63	0.45
6:X:224:HIS:CD2	6:X:244:MET:HE1	2.52	0.45
6:X:714:ASP:O	6:X:804:LYS:NZ	2.48	0.45
6:W:717:LEU:HD23	6:W:804:LYS:HD3	1.97	0.45
4:b:268:ARG:HG2	5:d:240:VAL:HG21	1.99	0.45
6:4:122:LYS:HD2	6:4:1087:ALA:HB2	1.98	0.45
6:S:457:ARG:NE	6:S:1125:ASP:OD2	2.50	0.45
7:3:55:HIS:HD2	6:T:770:LEU:HD22	1.81	0.45
6:X:520:THR:HG22	6:X:568:PRO:HA	1.99	0.45
6:X:700:VAL:HG23	6:X:705:ILE:HG12	1.99	0.45
6:X:1220:TYR:HE2	6:X:1272:LYS:HD3	1.81	0.45
4:b:124:GLN:HG2	4:b:313:PRO:HD2	1.98	0.45
6:4:264:TYR:HD2	6:4:297:MET:HE2	1.81	0.45
6:4:574:PHE:O	6:4:578:ARG:N	2.49	0.45
6:S:386:THR:HG21	6:T:100:ILE:HG13	1.98	0.45
6:S:717:LEU:HD23	6:S:804:LYS:HD3	1.98	0.45
6:W:987:TYR:O	6:W:992:LYS:NZ	2.50	0.45
3:n:2631:LYS:HA	3:n:2635:LEU:HB3	1.99	0.45
6:S:56:VAL:HG12	6:W:12:TYR:HA	1.98	0.45
6:S:79:GLU:HG2	6:S:1063:VAL:HB	1.98	0.45
6:S:100:ILE:O	6:S:109:ASN:ND2	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:555:ARG:HE	6:T:907:HIS:CD2	2.35	0.45
6:T:1345:LYS:NZ	6:T:1376:TYR:OXT	2.50	0.45
5:7:156:HIS:HD2	5:7:201:LEU:HB2	1.82	0.45
6:4:90:LYS:HE2	6:X:27:ALA:HB3	1.99	0.45
6:S:151:GLU:HG2	6:X:85:ARG:HH22	1.82	0.45
6:T:293:VAL:HG21	6:T:368:LYS:HE3	1.98	0.45
6:T:757:ILE:HG12	6:T:788:LEU:HD22	1.98	0.45
6:T:907:HIS:HB2	6:T:910:GLY:N	2.31	0.45
1:k:342:ARG:HH12	2:l:43:ARG:HG3	1.82	0.45
2:l:92:LYS:HE3	3:o:2606:ILE:HG23	1.98	0.45
6:T:264:TYR:HE1	6:T:300:PRO:HD2	1.82	0.45
6:W:447:GLN:HA	6:W:450:LEU:HB2	1.98	0.45
6:W:572:ARG:NH2	6:W:1001:SER:O	2.50	0.45
1:k:384:LEU:HD22	1:k:402:GLN:HG3	1.99	0.45
3:o:2631:LYS:HA	3:o:2635:LEU:HB3	1.99	0.45
6:S:394:ARG:HD3	6:S:1315:PHE:HB3	1.99	0.45
6:X:1111:MET:SD	6:X:1366:ARG:NH2	2.81	0.45
6:W:1062:PHE:HB2	6:W:1087:ALA:HB3	1.99	0.45
1:k:387:VAL:HG22	1:k:398:GLU:HB3	1.99	0.44
6:4:842:ASP:O	6:4:844:VAL:N	2.49	0.44
6:W:178:VAL:HG22	6:W:1061:MET:HE2	1.99	0.44
6:W:504:LYS:HG2	6:W:964:TYR:HE1	1.82	0.44
6:4:82:ASP:N	6:4:82:ASP:OD1	2.46	0.44
6:4:404:VAL:HG13	6:4:1038:MET:HG3	1.98	0.44
6:S:1345:LYS:NZ	6:S:1376:TYR:OXT	2.41	0.44
6:W:491:MET:HB2	6:W:783:ASP:HA	1.99	0.44
6:W:520:THR:HG22	6:W:568:PRO:HA	1.99	0.44
4:b:112:PHE:O	4:b:115:SER:OG	2.29	0.44
6:4:278:THR:HB	6:4:282:VAL:HB	1.99	0.44
6:T:170:LEU:HD11	6:T:1084:HIS:HB2	1.98	0.44
6:T:494:PHE:O	6:T:498:HIS:N	2.35	0.44
6:X:633:LEU:HA	6:X:874:MET:HE3	1.99	0.44
5:c:223:LEU:HD22	5:c:249:VAL:HG13	1.99	0.44
6:4:298:SER:HB3	6:4:359:ARG:HD2	1.98	0.44
6:4:306:TYR:HE1	6:X:39:LEU:HD23	1.82	0.44
6:4:455:HIS:HD2	6:4:1119:PHE:HD1	1.65	0.44
6:X:447:GLN:HB3	6:X:1028:ALA:HB1	2.00	0.44
6:W:898:ARG:NH1	6:W:910:GLY:O	2.51	0.44
5:c:50:VAL:HG13	5:c:62:ILE:HG12	2.00	0.44
6:S:1043:THR:HG23	6:S:1265:PRO:HB3	1.99	0.44
5:6:223:LEU:HD22	5:6:249:VAL:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:4:684:LEU:HD22	6:4:802:LEU:HA	1.98	0.44
6:X:724:HIS:HB3	6:X:793:LEU:HB3	1.99	0.44
6:W:102:HIS:HE1	6:W:106:ARG:HD2	1.83	0.44
6:4:476:ASP:H	6:4:544:VAL:HG11	1.82	0.44
6:T:130:GLU:HG2	6:T:1079:THR:HG22	1.99	0.44
6:W:540:PHE:HD1	6:W:558:HIS:HA	1.82	0.44
6:W:788:LEU:HD11	6:W:919:VAL:HG21	2.00	0.44
5:c:272:TYR:O	5:c:275:SER:OG	2.34	0.44
6:4:812:PRO:HB2	6:4:999:ALA:HB1	1.99	0.44
6:4:980:PRO:HD2	6:4:983:LEU:HD12	1.99	0.44
6:X:718:LEU:HD21	6:X:730:LEU:HD12	2.00	0.44
6:X:965:VAL:HG13	6:X:972:ARG:HG2	1.99	0.44
6:4:332:ARG:O	6:4:336:HIS:N	2.50	0.44
6:S:777:ARG:HG2	6:S:887:PHE:HE1	1.83	0.44
6:T:175:VAL:HG21	6:T:382:MET:HE1	1.99	0.44
6:W:252:VAL:HG21	6:W:1053:TYR:HD2	1.83	0.44
6:4:777:ARG:HH22	6:4:885:CYS:H	1.66	0.43
6:4:1017:GLN:NE2	6:4:1023:SER:O	2.48	0.43
6:X:738:PRO:HB3	6:X:896:THR:HG22	1.99	0.43
5:7:231:ARG:HG2	5:7:233:ASP:H	1.83	0.43
4:b:225:THR:HG22	4:b:293:THR:HG22	1.99	0.43
5:c:13:SER:OG	5:c:130:ASN:ND2	2.51	0.43
6:4:620:ILE:HG22	6:4:622:GLY:H	1.83	0.43
6:4:1127:TYR:HB2	6:4:1133:HIS:HB2	1.99	0.43
6:S:256:THR:HG22	6:S:258:PHE:H	1.82	0.43
6:X:5:LEU:HD13	6:X:8:ARG:HH22	1.83	0.43
6:W:428:GLN:NE2	6:W:577:SER:OG	2.43	0.43
6:W:1254:PHE:HB2	6:W:1267:ARG:HH22	1.83	0.43
6:4:712:LEU:HD23	6:4:804:LYS:HD2	1.99	0.43
6:4:743:GLY:HA3	6:4:786:HIS:CE1	2.54	0.43
6:X:184:ARG:O	6:X:1290:SER:OG	2.33	0.43
6:W:129:ILE:HD11	6:W:166:GLY:HA3	2.01	0.43
5:c:258:SER:OG	5:c:261:ASP:OD2	2.36	0.43
6:S:130:GLU:HG3	6:T:110:LYS:HD2	2.01	0.43
6:S:520:THR:HG22	6:S:568:PRO:HA	1.99	0.43
6:T:402:PHE:HD2	6:T:1040:VAL:HB	1.83	0.43
6:T:714:ASP:O	6:T:804:LYS:NZ	2.51	0.43
6:X:187:PRO:HG2	6:X:192:LEU:HD12	2.00	0.43
6:X:731:MET:HG2	6:X:738:PRO:HG2	1.98	0.43
6:X:1182:THR:HG23	6:X:1236:ASN:HB3	2.00	0.43
6:4:680:ILE:O	6:4:684:LEU:HB2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:1190:TYR:OH	6:X:1196:ASN:O	2.35	0.43
6:W:301:ALA:HB2	6:W:360:THR:HB	2.00	0.43
6:W:947:LEU:HD21	6:W:995:VAL:HG12	2.00	0.43
6:4:619:MET:HE2	6:4:878:LEU:HA	1.99	0.43
6:T:984:MET:HE2	6:T:984:MET:HB3	1.85	0.43
6:X:950:ASP:HA	6:X:951:PRO:HD3	1.90	0.43
7:0:53:ILE:HD13	6:W:840:PHE:CE1	2.54	0.43
6:W:714:ASP:O	6:W:804:LYS:NZ	2.51	0.43
6:4:811:MET:O	6:4:815:SER:N	2.50	0.43
6:X:536:VAL:HG13	6:X:1244:SER:HA	2.00	0.43
6:X:809:VAL:HG13	6:X:1012:MET:HB2	2.01	0.43
6:W:674:HIS:CE1	6:W:678:ARG:HH21	2.37	0.43
1:k:269:LEU:HD12	2:l:72:ARG:HE	1.83	0.43
5:7:63:MET:HG3	5:7:282:LEU:HD12	2.00	0.43
6:T:893:ARG:NH2	6:T:988:GLU:OE1	2.51	0.43
1:k:35:LEU:HD12	1:k:63:ARG:HH11	1.84	0.43
5:7:26:LYS:HA	5:7:98:VAL:HG21	2.01	0.43
6:4:605:PHE:HZ	6:4:816:ASN:HB2	1.84	0.43
6:4:1074:ARG:HG2	6:4:1076:ASP:H	1.84	0.43
6:T:88:ASP:HB3	6:W:3:ALA:HB2	2.01	0.42
6:X:946:LYS:NZ	6:X:986:GLU:OE2	2.39	0.42
6:W:809:VAL:HG13	6:W:1012:MET:HB2	2.01	0.42
6:W:1183:PRO:HB3	6:W:1238:TRP:HZ3	1.84	0.42
1:k:267:ILE:HA	1:k:268:PRO:HD3	1.92	0.42
1:k:376:ARG:NH1	6:X:546:PRO:O	2.52	0.42
4:5:82:PRO:HB3	4:5:170:HIS:CD2	2.54	0.42
5:c:35:ASP:HB2	5:c:40:GLN:HE22	1.84	0.42
6:4:934:ALA:O	6:4:938:MET:N	2.40	0.42
6:4:1027:GLN:HB3	6:4:1032:MET:HB2	2.01	0.42
6:4:1334:HIS:O	6:4:1336:VAL:N	2.51	0.42
6:S:224:HIS:CD2	6:S:244:MET:HE1	2.54	0.42
6:S:278:THR:HG22	6:S:1051:ILE:HG12	2.01	0.42
6:X:264:TYR:CE1	6:X:300:PRO:HD2	2.54	0.42
6:W:170:LEU:HD11	6:W:1084:HIS:HB2	2.02	0.42
1:k:379:THR:HG21	6:X:549:GLY:H	1.84	0.42
6:4:226:PHE:HD2	6:4:1364:MET:HB3	1.84	0.42
6:S:525:HIS:HD2	6:S:527:THR:HG22	1.84	0.42
6:S:1027:GLN:HB3	6:S:1032:MET:HB2	2.01	0.42
6:4:1196:ASN:ND2	6:4:1202:ALA:H	2.17	0.42
6:S:707:HIS:CD2	6:S:715:PRO:HD3	2.54	0.42
6:T:71:LEU:N	6:T:377:GLU:OE2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:777:ARG:HG2	6:X:887:PHE:CE1	2.53	0.42
7:0:74:LEU:HD23	7:0:77:LEU:HD12	2.02	0.42
6:W:698:GLU:HG3	6:W:705:ILE:HD12	2.01	0.42
6:W:1226:ASP:O	6:W:1228:ALA:N	2.47	0.42
1:k:102:ILE:HB	1:k:111:LEU:HB2	2.00	0.42
5:c:146:HIS:O	5:c:150:GLN:HG2	2.20	0.42
6:4:709:VAL:O	6:4:1018:LYS:HB2	2.20	0.42
6:4:955:ALA:HB1	6:4:962:ALA:HA	2.01	0.42
6:T:893:ARG:HG3	6:T:915:GLN:O	2.20	0.42
5:6:288:VAL:HG22	5:6:300:CYS:HB3	2.01	0.42
4:b:81:SER:OG	4:b:84:GLU:OE2	2.38	0.42
6:4:1127:TYR:H	6:4:1133:HIS:CD2	2.37	0.42
6:X:501:TYR:OH	6:X:978:ASN:O	2.32	0.42
6:W:480:GLY:HA3	6:W:483:LEU:HD11	2.01	0.42
5:6:88:ASP:HB2	5:6:91:ASP:HB2	2.01	0.42
6:4:561:MET:H	6:4:564:ASN:ND2	2.18	0.42
6:4:834:THR:HB	7:A:49:LEU:HB3	2.02	0.42
6:4:1200:ARG:NE	6:4:1219:LEU:O	2.52	0.42
6:X:819:MET:N	6:X:950:ASP:OD2	2.44	0.42
1:k:389:CYS:HB2	1:k:420:THR:HG22	2.02	0.42
5:c:300:CYS:SG	5:c:301:TRP:N	2.92	0.42
6:4:446:TYR:O	6:4:450:LEU:N	2.52	0.42
6:4:898:ARG:NE	6:4:910:GLY:O	2.52	0.42
6:S:738:PRO:HB3	6:S:896:THR:HG22	2.00	0.42
6:T:723:TYR:OH	6:T:922:PHE:HB3	2.20	0.42
6:W:634:ILE:HB	6:W:650:PHE:HE2	1.85	0.42
5:c:32:PRO:HD3	5:c:137:PRO:HG3	2.02	0.42
5:d:261:ASP:O	5:d:264:THR:OG1	2.35	0.42
6:4:525:HIS:CD2	6:4:527:THR:HG22	2.50	0.42
6:4:880:THR:HG22	7:A:54:ALA:HA	2.01	0.42
6:S:1190:TYR:OH	6:S:1196:ASN:O	2.31	0.42
6:4:543:PHE:CZ	6:4:555:ARG:HD3	2.55	0.41
6:4:839:VAL:HG13	6:4:872:VAL:HG13	2.02	0.41
6:W:1042:ARG:NH2	6:W:1111:MET:O	2.53	0.41
5:6:224:ARG:HD3	5:6:257:LEU:HD21	2.02	0.41
5:c:144:LEU:HD21	5:c:183:PHE:HB2	2.02	0.41
6:4:526:PRO:HB3	6:4:1233:SER:HB2	2.02	0.41
6:T:278:THR:HB	6:T:282:VAL:HB	2.01	0.41
6:T:540:PHE:O	6:T:559:ARG:NH1	2.53	0.41
6:X:321:ARG:NH1	6:W:51:GLU:OE2	2.53	0.41
6:X:1042:ARG:NH1	6:X:1044:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:W:146:PRO:HA	6:W:149:PHE:HD2	1.85	0.41
6:W:544:VAL:HG22	6:W:554:TYR:HE1	1.86	0.41
6:W:899:ASP:OD1	6:W:899:ASP:N	2.53	0.41
4:5:69:THR:HG21	5:7:92:ASN:HD21	1.85	0.41
6:4:131:LEU:HD22	6:4:159:ILE:HG13	2.02	0.41
6:T:809:VAL:HG13	6:T:1012:MET:HB2	2.01	0.41
6:T:980:PRO:HD2	6:T:983:LEU:HD12	2.02	0.41
1:k:226:PHE:HD2	4:5:275:ARG:HG3	1.85	0.41
7:2:74:LEU:HD23	7:2:77:LEU:HD12	2.02	0.41
6:X:1178:GLU:CD	6:X:1265:PRO:HD2	2.44	0.41
1:k:99:VAL:HG22	1:k:114:ARG:HG2	2.02	0.41
2:m:80:ARG:NH1	3:o:2622:SER:OG	2.53	0.41
4:5:75:VAL:HG21	4:5:105:LEU:HD22	2.03	0.41
5:c:47:LEU:HB3	5:c:135:VAL:HB	2.02	0.41
5:c:89:PRO:HA	5:c:90:SER:HA	1.59	0.41
5:c:204:LEU:HD23	5:c:207:LEU:HD12	2.01	0.41
6:4:566:PRO:HD2	6:4:569:LEU:HD12	2.03	0.41
6:4:876:ARG:HG2	7:A:57:TYR:CG	2.55	0.41
6:X:850:ILE:HD11	6:X:872:VAL:HA	2.01	0.41
1:k:284:PHE:HE2	2:l:61:THR:HG21	1.86	0.41
6:T:822:MET:HE1	6:T:957:LEU:HD13	2.02	0.41
6:T:1038:MET:HB2	6:T:1179:ILE:HG23	2.03	0.41
6:X:263:THR:O	6:X:359:ARG:NH1	2.48	0.41
6:X:438:ASN:HD22	6:X:1171:HIS:CD2	2.38	0.41
6:X:457:ARG:NE	6:X:1125:ASP:OD2	2.54	0.41
6:W:649:ALA:O	6:W:677:TYR:OH	2.29	0.41
2:l:88:ILE:HG21	3:o:2613:LYS:HB2	2.02	0.41
4:5:46:ALA:O	4:5:50:ARG:NH1	2.53	0.41
4:b:192:ARG:NE	6:W:137:GLU:OE1	2.54	0.41
5:d:152:LEU:HD23	5:d:152:LEU:HA	1.85	0.41
6:4:555:ARG:HG3	6:4:907:HIS:ND1	2.36	0.41
6:X:850:ILE:HG13	6:X:870:PRO:HG2	2.02	0.41
7:A:22:HIS:NE2	7:A:24:LEU:HB2	2.36	0.41
7:3:74:LEU:HD23	7:3:77:LEU:HD12	2.02	0.41
2:m:24:TRP:H	4:b:269:THR:HG22	1.86	0.41
4:5:49:THR:HG22	6:S:1067:SER:HB2	2.02	0.41
5:6:227:THR:HB	5:6:231:ARG:HH12	1.86	0.41
5:6:235:HIS:CD2	5:6:237:LEU:HG	2.56	0.41
6:4:400:TYR:N	6:4:1042:ARG:O	2.38	0.41
6:S:61:VAL:HG11	6:T:98:PRO:HG3	2.01	0.41
6:S:633:LEU:HD12	6:S:874:MET:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:T:184:ARG:O	6:T:1290:SER:OG	2.39	0.41
7:1:74:LEU:HD23	7:1:77:LEU:HD12	2.02	0.41
6:X:1334:HIS:HB2	6:X:1355:GLN:HG2	2.03	0.41
4:5:71:GLY:HA3	4:5:181:MET:HE3	2.02	0.41
6:4:233:LEU:HD11	6:4:1367:LEU:HD21	2.02	0.41
7:1:12:GLN:O	7:0:70:ARG:NH1	2.54	0.41
6:X:684:LEU:HB3	6:X:802:LEU:HD22	2.03	0.41
5:d:220:ARG:HH21	5:d:257:LEU:HB2	1.86	0.40
6:4:597:ILE:HA	6:4:600:ILE:HB	2.02	0.40
6:4:840:PHE:CG	7:A:53:ILE:HG12	2.56	0.40
6:S:1005:THR:HG22	6:S:1007:GLY:H	1.86	0.40
6:S:1200:ARG:HG2	6:S:1226:ASP:HB3	2.02	0.40
6:T:773:ILE:O	6:T:776:THR:OG1	2.37	0.40
5:d:269:MET:HE3	5:d:269:MET:HB3	1.92	0.40
6:4:194:THR:HG21	6:4:216:MET:HB3	2.03	0.40
6:S:183:LEU:HD13	6:S:394:ARG:HH21	1.86	0.40
6:S:848:ASP:OD2	6:S:853:HIS:NE2	2.43	0.40
6:X:637:VAL:HG22	6:X:868:ILE:HD13	2.02	0.40
6:W:582:PHE:HA	6:W:1032:MET:HE1	2.02	0.40
2:l:95:ILE:HA	2:l:98:MET:HB2	2.02	0.40
4:5:50:ARG:HH21	6:4:141:ALA:HA	1.86	0.40
4:b:73:PHE:HE1	5:d:108:ASN:HD21	1.69	0.40
6:4:669:ILE:H	6:4:669:ILE:HG13	1.82	0.40
6:T:575:GLN:HE21	6:T:1015:MET:HG3	1.86	0.40
6:T:947:LEU:H	6:T:947:LEU:HG	1.74	0.40
6:X:902:GLN:HE21	6:X:1020:SER:HG	1.62	0.40
6:W:687:LEU:HD23	6:W:805:LEU:HD22	2.03	0.40
1:k:368:ASP:OD1	1:k:368:ASP:N	2.52	0.40
4:5:166:VAL:HG13	4:5:187:ALA:HA	2.04	0.40
5:7:153:LEU:HD21	5:7:211:LEU:HD13	2.02	0.40
5:c:141:PRO:O	5:c:145:GLY:N	2.52	0.40
6:S:1168:GLY:HA2	6:T:207:LYS:HD3	2.04	0.40
6:T:252:VAL:HG21	6:T:1053:TYR:HD2	1.86	0.40
6:X:82:ASP:OD1	6:X:82:ASP:N	2.52	0.40
6:W:436:ASN:HB2	6:W:440:VAL:O	2.21	0.40
1:k:333:HIS:CE1	1:k:413:LEU:H	2.40	0.40
6:4:244:MET:HE2	6:4:244:MET:HB2	1.97	0.40
6:4:850:ILE:HD12	6:4:870:PRO:HG2	2.04	0.40
6:T:583:ASP:OD1	6:T:590:HIS:NE2	2.54	0.40
6:T:716:HIS:HA	6:T:730:LEU:HD11	2.03	0.40
6:T:1183:PRO:HD3	6:T:1238:TRP:CE3	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:X:44:ARG:HB3	6:X:46:GLY:H	1.87	0.40
6:X:555:ARG:HA	6:X:906:THR:HG21	2.04	0.40
6:W:76:VAL:HG21	6:W:258:PHE:HD2	1.87	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%)	321 (96%)	13 (4%)	0	100	100
2	l	81/549 (15%)	81 (100%)	0	0	100	100
2	m	76/549 (14%)	76 (100%)	0	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	5	308/331 (93%)	297 (96%)	11 (4%)	0	100	100
4	b	315/331 (95%)	309 (98%)	6 (2%)	0	100	100
5	6	300/305 (98%)	289 (96%)	11 (4%)	0	100	100
5	7	288/305 (94%)	273 (95%)	15 (5%)	0	100	100
5	c	290/305 (95%)	283 (98%)	7 (2%)	0	100	100
5	d	296/305 (97%)	290 (98%)	6 (2%)	0	100	100
6	4	1206/1376 (88%)	1120 (93%)	80 (7%)	6 (0%)	24	57
6	S	1273/1376 (92%)	1196 (94%)	75 (6%)	2 (0%)	43	73
6	T	1354/1376 (98%)	1274 (94%)	76 (6%)	4 (0%)	36	67
6	W	1350/1376 (98%)	1276 (94%)	73 (5%)	1 (0%)	48	79
6	X	1335/1376 (97%)	1261 (94%)	71 (5%)	3 (0%)	43	73
7	0	76/170 (45%)	75 (99%)	1 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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
7	A	42/170 (25%)	42 (100%)	0	0	100	100
All	All	9228/16434 (56%)	8764 (95%)	448 (5%)	16 (0%)	44	73

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	4	843	VAL
6	W	263	THR
6	S	992	LYS
6	T	10	PHE
6	X	992	LYS
6	4	842	ASP
6	T	945	ASN
6	X	44	ARG
6	4	849	ASP
6	4	1092	ALA
6	S	993	SER
6	X	993	SER
6	T	849	ASP
6	4	1335	ARG
6	4	314	VAL
6	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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	n	35/2239 (2%)	35 (100%)	0	100	100
3	o	35/2239 (2%)	35 (100%)	0	100	100
4	5	266/281 (95%)	265 (100%)	1 (0%)	84	83
4	b	272/281 (97%)	272 (100%)	0	100	100
5	6	272/274 (99%)	272 (100%)	0	100	100
5	7	264/274 (96%)	264 (100%)	0	100	100
5	c	267/274 (97%)	266 (100%)	1 (0%)	84	83
5	d	270/274 (98%)	270 (100%)	0	100	100
6	4	1044/1166 (90%)	1038 (99%)	6 (1%)	78	79
6	S	1094/1166 (94%)	1088 (100%)	6 (0%)	81	81
6	T	1154/1166 (99%)	1144 (99%)	10 (1%)	70	74
6	W	1150/1166 (99%)	1143 (99%)	7 (1%)	78	79
6	X	1139/1166 (98%)	1131 (99%)	8 (1%)	76	77
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
7	A	39/141 (28%)	39 (100%)	0	100	100
All	All	8021/13994 (57%)	7982 (100%)	39 (0%)	78	81

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	5	224	VAL
5	c	98	VAL
6	4	83	LEU
6	4	434	VAL
6	4	788	LEU
6	4	895	ILE
6	4	947	LEU
6	4	1025	ILE
6	S	404	VAL
6	S	419	VAL
6	S	651	VAL
6	S	713	LEU
6	S	1104	VAL

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Mol	Chain	Res	Type
6	S	1169	LEU
6	T	308	VAL
6	T	404	VAL
6	T	422	VAL
6	T	616	ILE
6	T	620	ILE
6	T	713	LEU
6	T	1025	ILE
6	T	1104	VAL
6	T	1121	ILE
6	T	1307	VAL
6	X	129	ILE
6	X	404	VAL
6	X	651	VAL
6	X	713	LEU
6	X	1104	VAL
6	X	1121	ILE
6	X	1169	LEU
6	X	1184	VAL
6	W	404	VAL
6	W	616	ILE
6	W	620	ILE
6	W	713	LEU
6	W	1109	THR
6	W	1169	LEU
6	W	1184	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (175) such sidechains are listed below:

Mol	Chain	Res	Type
1	k	7	ASN
1	k	88	HIS
1	k	91	ASN
1	k	333	HIS
2	l	77	HIS
2	l	103	ASN
2	m	52	GLN
4	5	24	HIS
4	5	95	GLN
4	5	303	GLN
5	6	40	GLN
5	6	64	GLN

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Mol	Chain	Res	Type
5	6	94	GLN
5	6	150	GLN
5	6	151	GLN
5	6	232	HIS
5	7	92	ASN
5	7	97	ASN
5	7	156	HIS
5	7	256	GLN
5	7	274	GLN
5	7	281	ASN
4	b	124	GLN
4	b	126	HIS
4	b	262	HIS
5	c	40	GLN
5	c	61	GLN
5	c	130	ASN
5	c	146	HIS
5	c	150	GLN
5	d	24	GLN
5	d	94	GLN
5	d	108	ASN
5	d	150	GLN
5	d	156	HIS
5	d	180	ASN
5	d	194	ASN
5	d	274	GLN
6	4	77	ASN
6	4	271	GLN
6	4	407	HIS
6	4	459	HIS
6	4	498	HIS
6	4	525	HIS
6	4	537	HIS
6	4	564	ASN
6	4	567	GLN
6	4	590	HIS
6	4	652	ASN
6	4	655	HIS
6	4	689	GLN
6	4	978	ASN
6	4	1090	HIS
6	4	1131	GLN

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Mol	Chain	Res	Type
6	4	1133	HIS
6	4	1196	ASN
6	4	1222	HIS
6	4	1268	GLN
6	4	1355	GLN
7	A	38	GLN
7	A	44	GLN
7	2	17	HIS
7	2	38	GLN
7	2	55	HIS
7	2	73	HIS
7	2	75	GLN
6	S	109	ASN
6	S	123	HIS
6	S	224	HIS
6	S	292	GLN
6	S	407	HIS
6	S	428	GLN
6	S	438	ASN
6	S	439	ASN
6	S	499	GLN
6	S	525	HIS
6	S	575	GLN
6	S	590	HIS
6	S	623	GLN
6	S	630	ASN
6	S	652	ASN
6	S	707	HIS
6	S	716	HIS
6	S	746	ASN
6	S	786	HIS
6	S	902	GLN
6	S	978	ASN
6	S	1017	GLN
6	S	1084	HIS
6	S	1090	HIS
6	S	1114	HIS
6	S	1171	HIS
6	S	1235	ASN
6	S	1318	GLN
6	S	1324	GLN
6	S	1344	ASN

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Mol	Chain	Res	Type
7	3	17	HIS
7	3	38	GLN
7	3	55	HIS
6	T	36	GLN
6	T	113	GLN
6	T	224	HIS
6	T	288	ASN
6	T	312	ASN
6	T	436	ASN
6	T	623	GLN
6	T	663	HIS
6	T	689	GLN
6	T	697	HIS
6	T	724	HIS
6	T	746	ASN
6	T	786	HIS
6	T	827	GLN
6	T	907	HIS
6	T	915	GLN
6	T	1116	GLN
6	T	1133	HIS
6	T	1171	HIS
6	T	1241	GLN
6	T	1321	HIS
6	T	1324	GLN
6	T	1344	ASN
7	1	17	HIS
7	1	38	GLN
7	1	55	HIS
6	X	123	HIS
6	X	224	HIS
6	X	312	ASN
6	X	325	ASN
6	X	328	GLN
6	X	336	HIS
6	X	387	GLN
6	X	407	HIS
6	X	428	GLN
6	X	438	ASN
6	X	575	GLN
6	X	652	ASN
6	X	666	ASN

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Mol	Chain	Res	Type
6	X	716	HIS
6	X	746	ASN
6	X	786	HIS
6	X	982	ASN
6	X	1017	GLN
6	X	1084	HIS
6	X	1114	HIS
6	X	1235	ASN
6	X	1318	GLN
6	X	1344	ASN
7	0	17	HIS
7	0	38	GLN
7	0	73	HIS
6	W	92	GLN
6	W	102	HIS
6	W	113	GLN
6	W	123	HIS
6	W	224	HIS
6	W	312	ASN
6	W	380	GLN
6	W	387	GLN
6	W	537	HIS
6	W	545	HIS
6	W	623	GLN
6	W	674	HIS
6	W	689	GLN
6	W	746	ASN
6	W	799	ASN
6	W	902	GLN
6	W	907	HIS
6	W	920	ASN
6	W	1030	HIS
6	W	1103	HIS
6	W	1133	HIS
6	W	1171	HIS
6	W	1334	HIS
6	W	1344	ASN

5.3.3 RNA ⓘ

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.

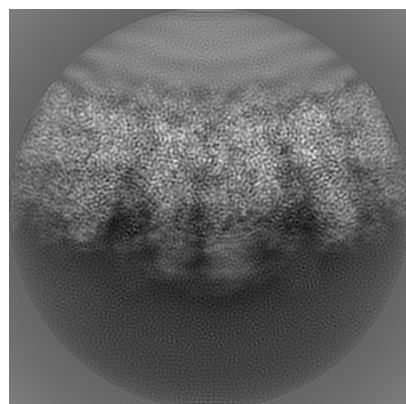
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-20436. These allow visual inspection of the internal detail of the map and identification of artifacts.

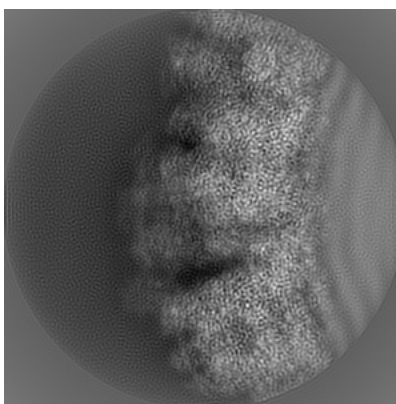
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

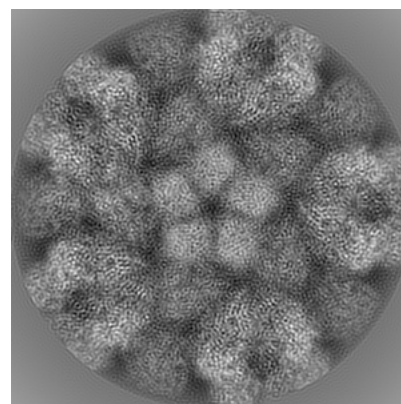
6.1.1 Primary map



X

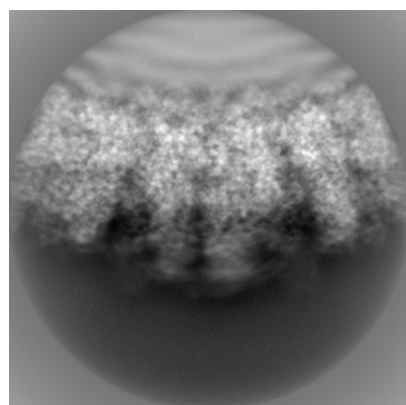


Y

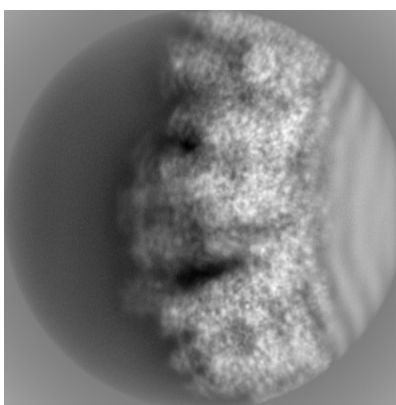


Z

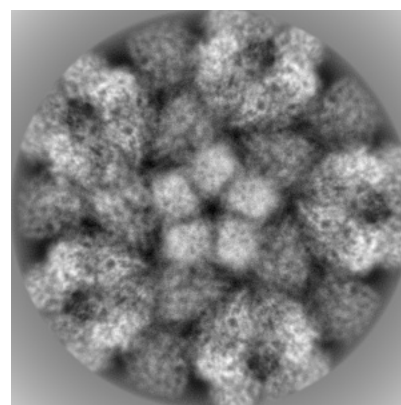
6.1.2 Raw map



X



Y

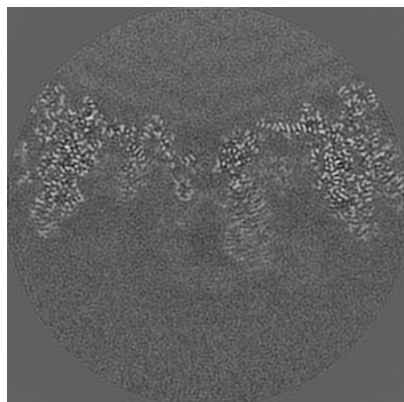


Z

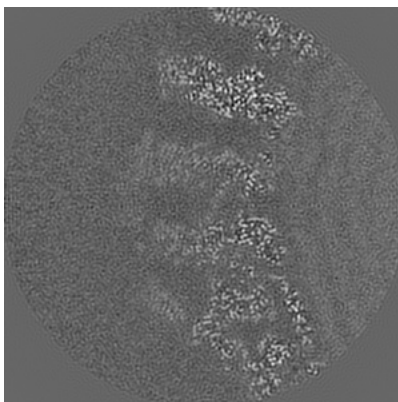
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

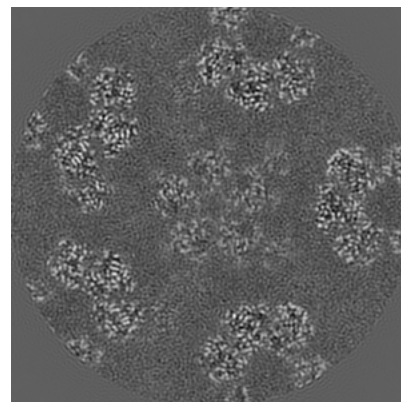
6.2.1 Primary map



X Index: 192

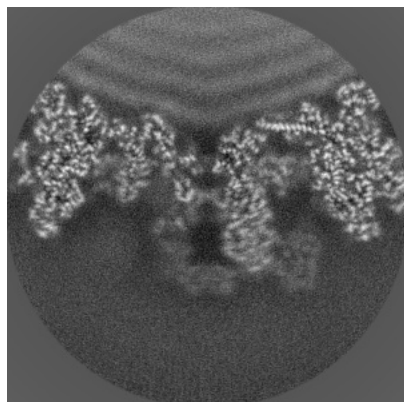


Y Index: 192

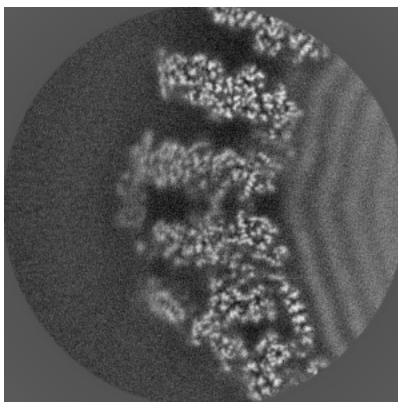


Z Index: 192

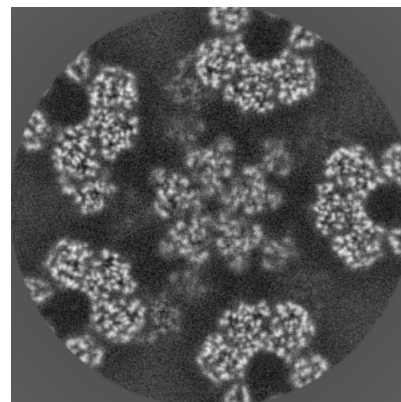
6.2.2 Raw map



X Index: 192



Y Index: 192

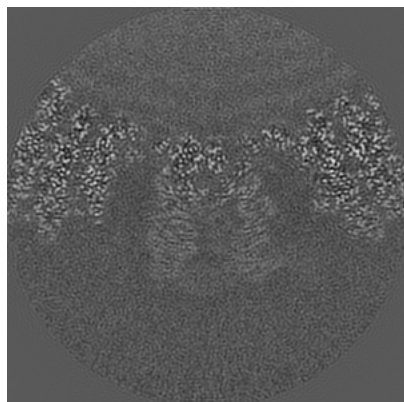


Z Index: 192

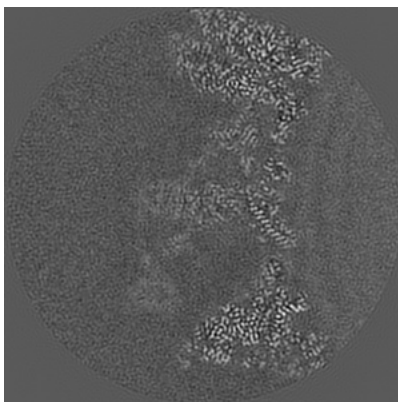
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

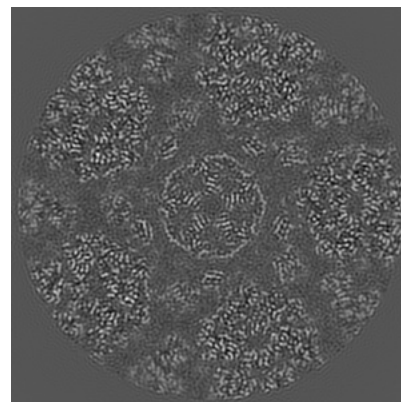
6.3.1 Primary map



X Index: 207

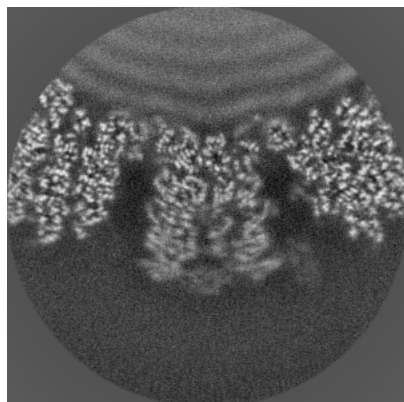


Y Index: 229

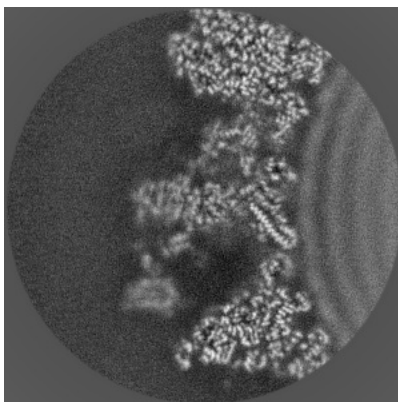


Z Index: 246

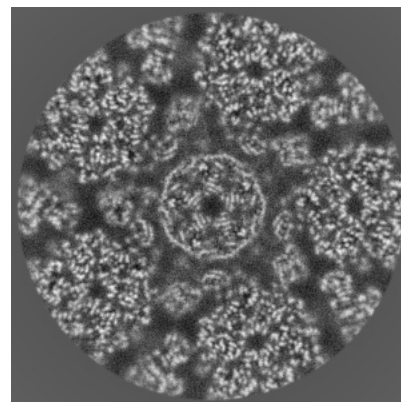
6.3.2 Raw map



X Index: 210



Y Index: 230

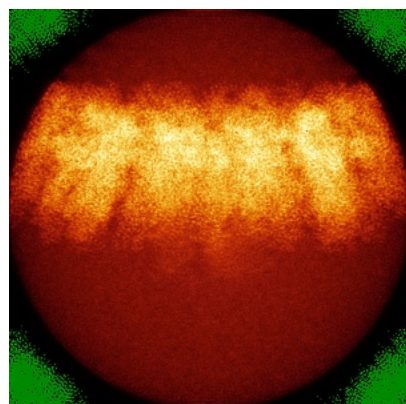


Z Index: 246

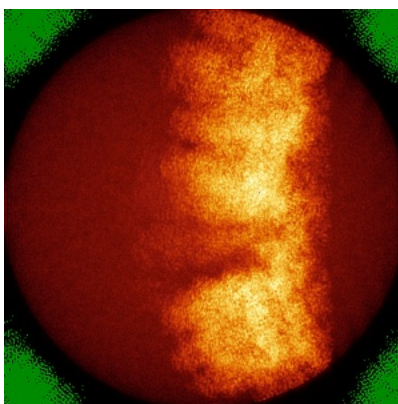
The images above show the largest variance slices of the map in three orthogonal directions.

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

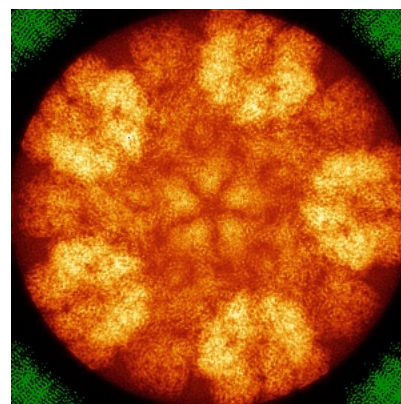
6.4.1 Primary map



X

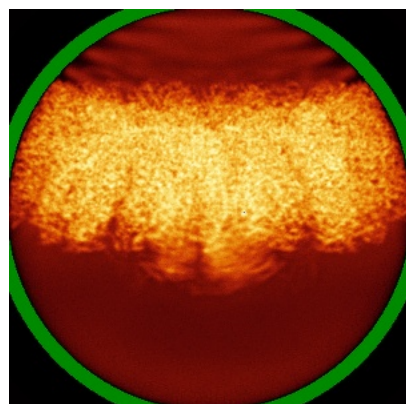


Y

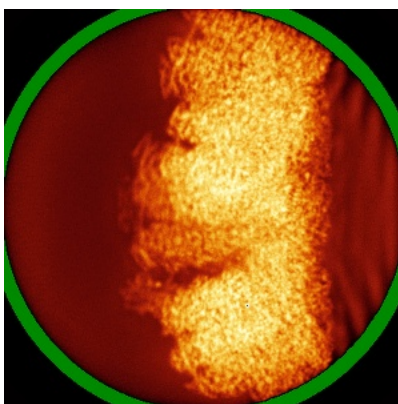


Z

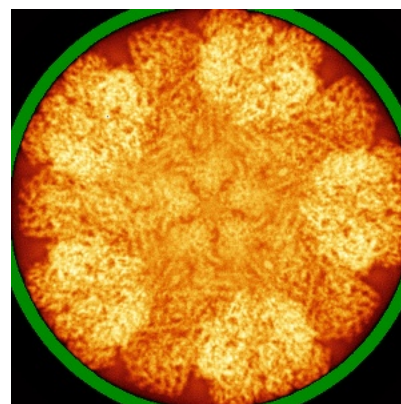
6.4.2 Raw map



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.

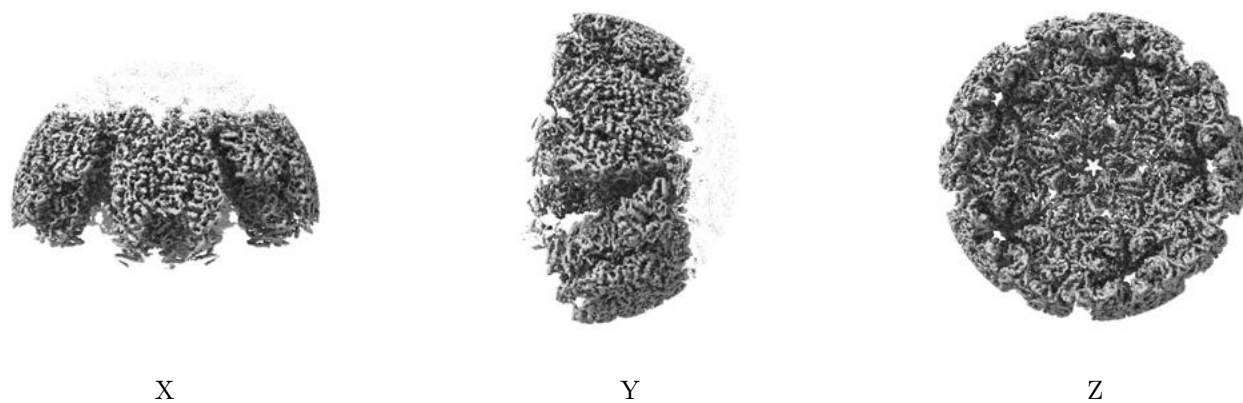
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.022. 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.

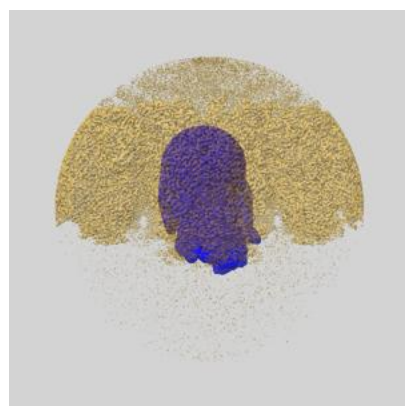
6.6 Mask visualisation [i](#)

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

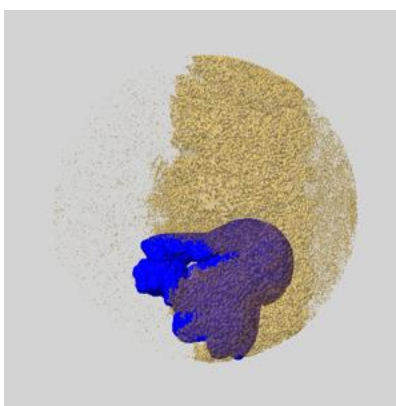
A mask typically either:

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

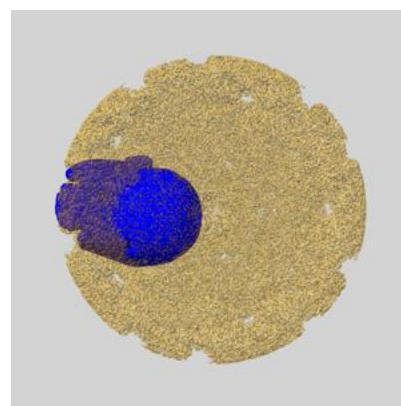
6.6.1 emd_20436_msk_1.map [i](#)



X



Y

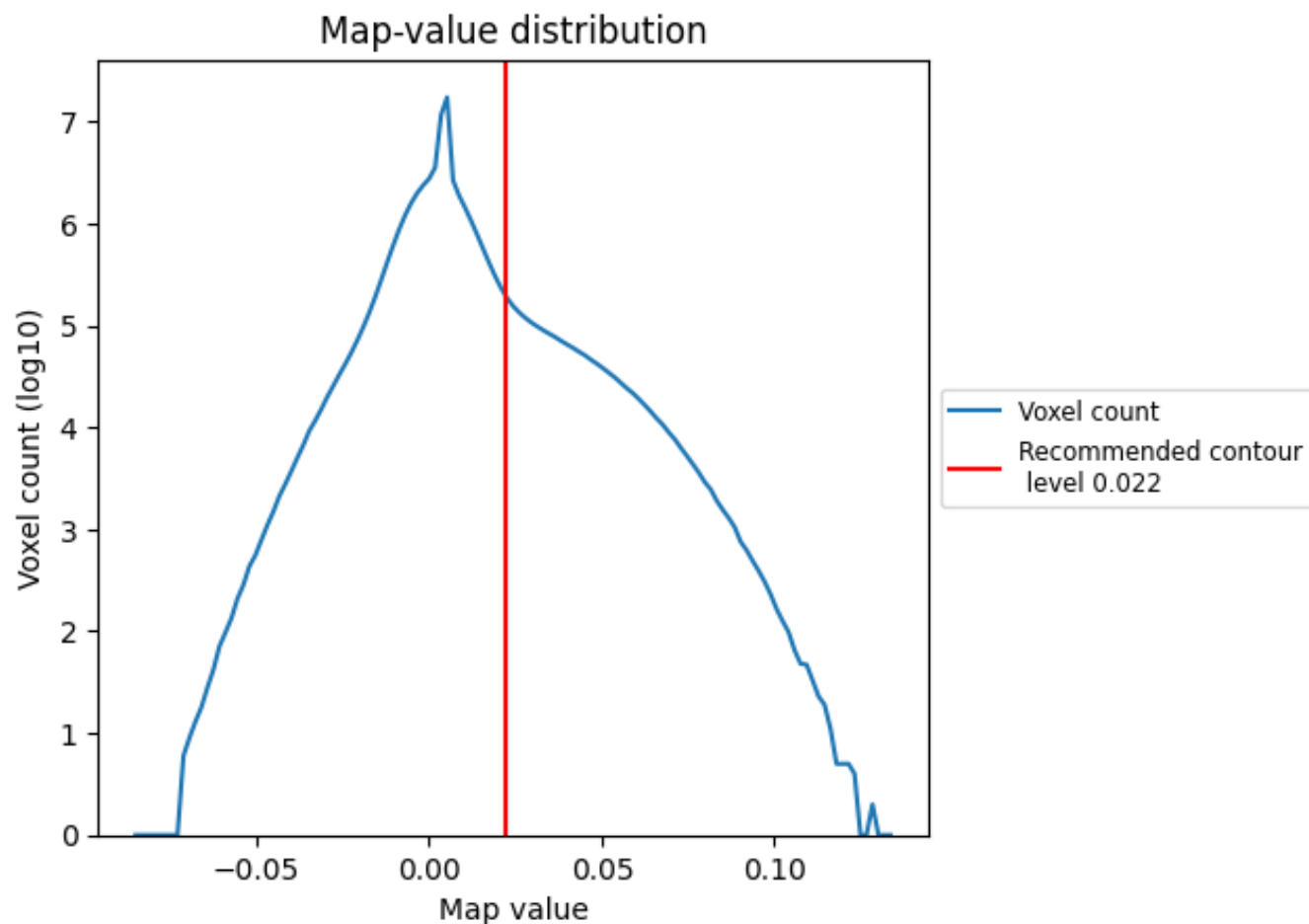


Z

7 Map analysis [i](#)

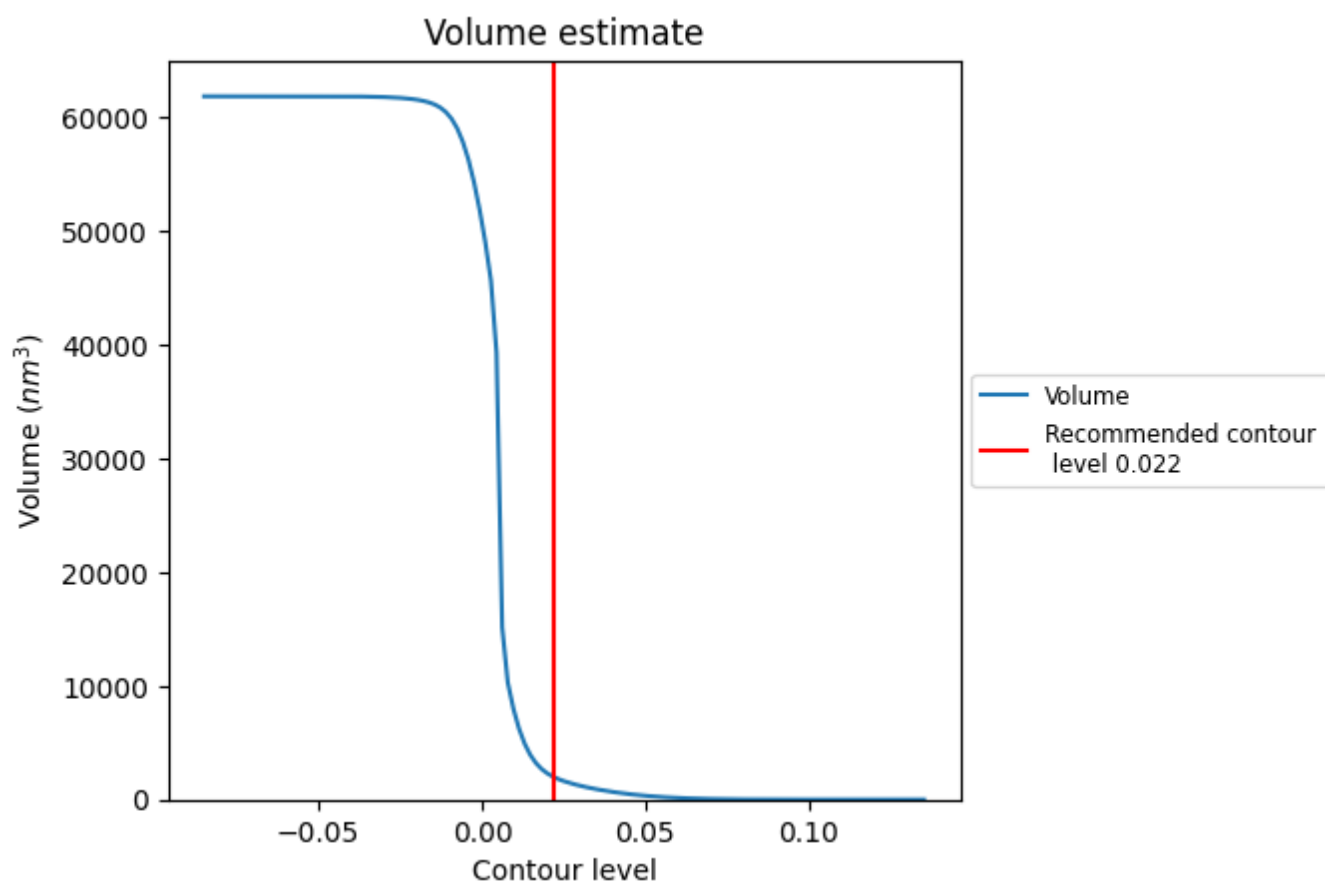
This section contains the results of statistical analysis of the map.

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.

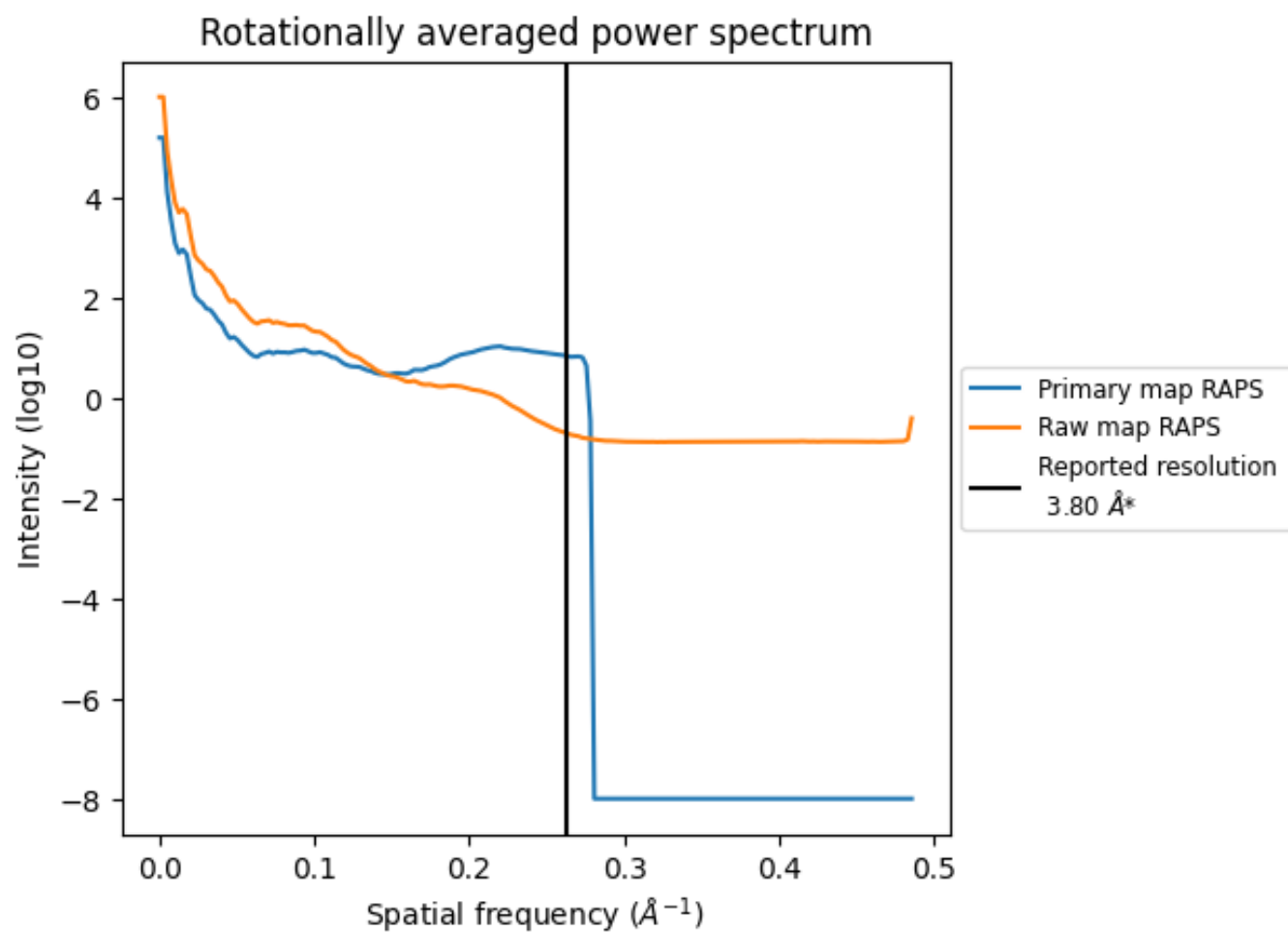
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1988 nm³; this corresponds to an approximate mass of 1796 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 ⓘ

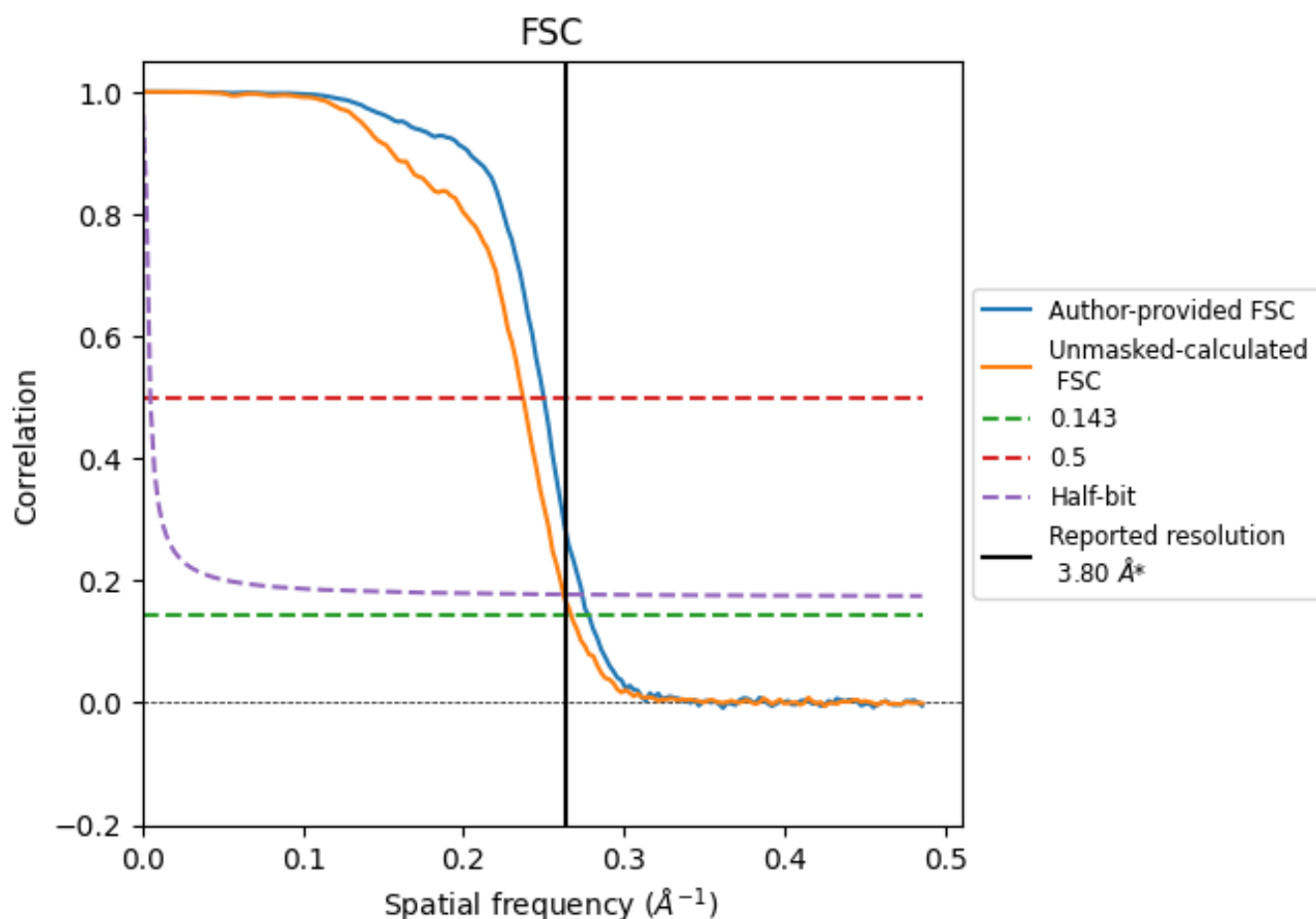


*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.263 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

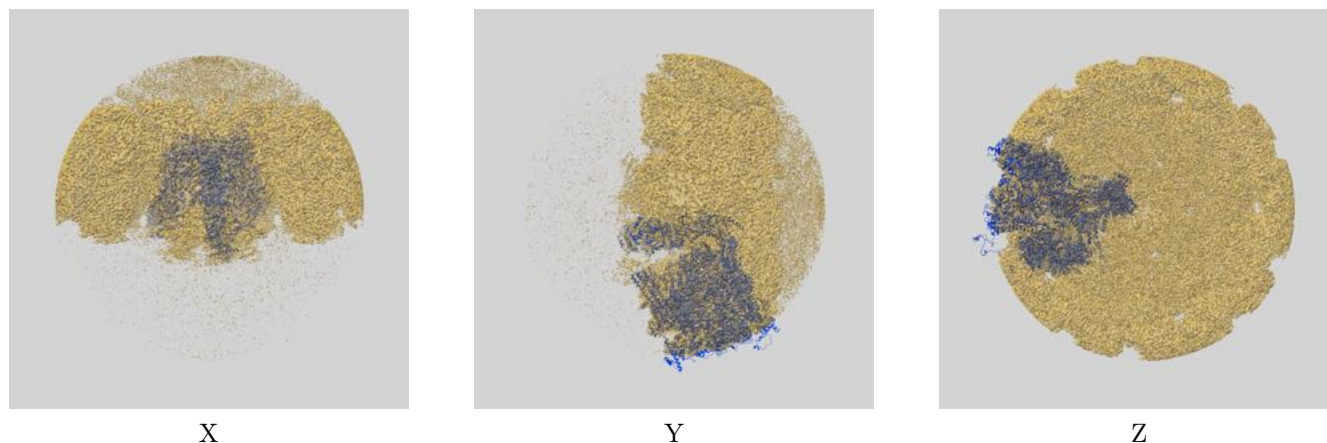
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.80	-	-
Author-provided FSC curve	3.60	4.00	3.65
Unmasked-calculated*	3.75	4.22	3.81

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

9 Map-model fit [i](#)

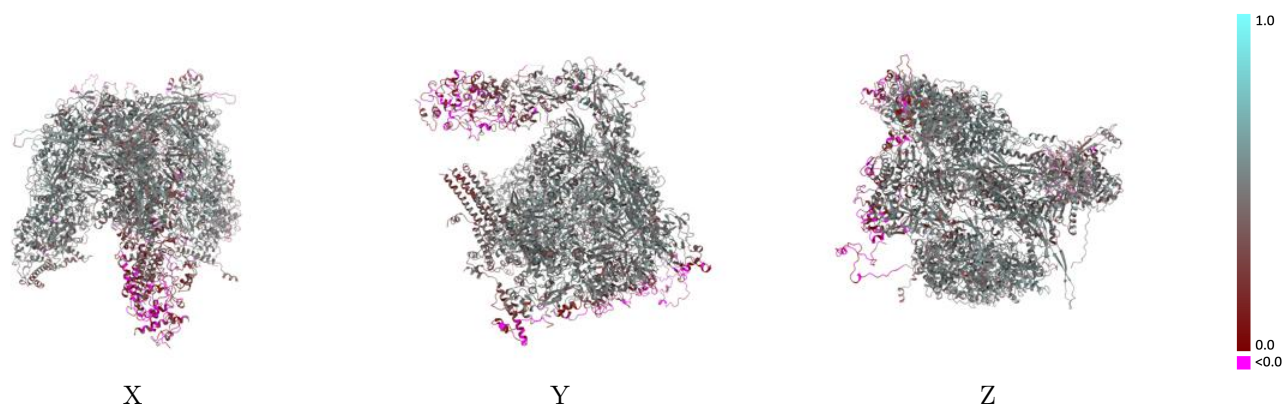
This section contains information regarding the fit between EMDB map EMD-20436 and PDB model 6PPH. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



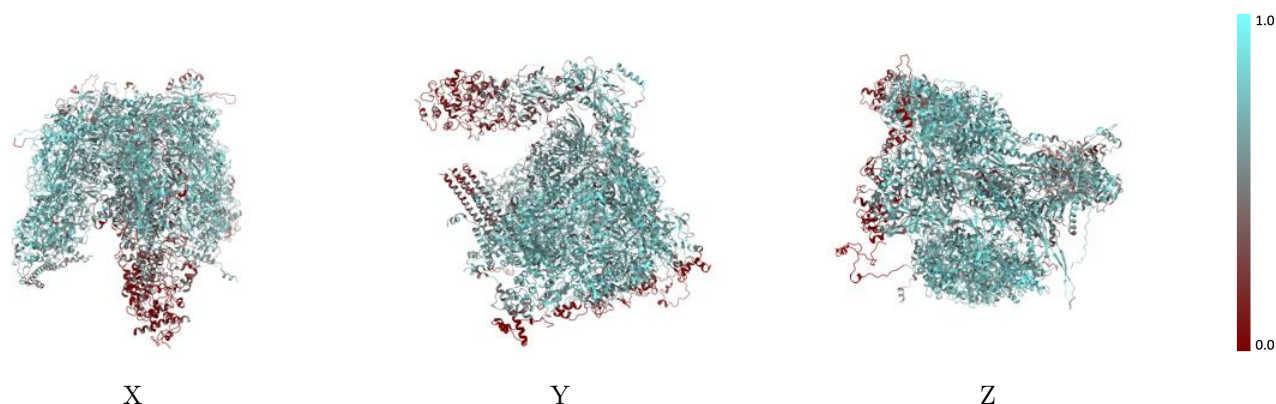
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



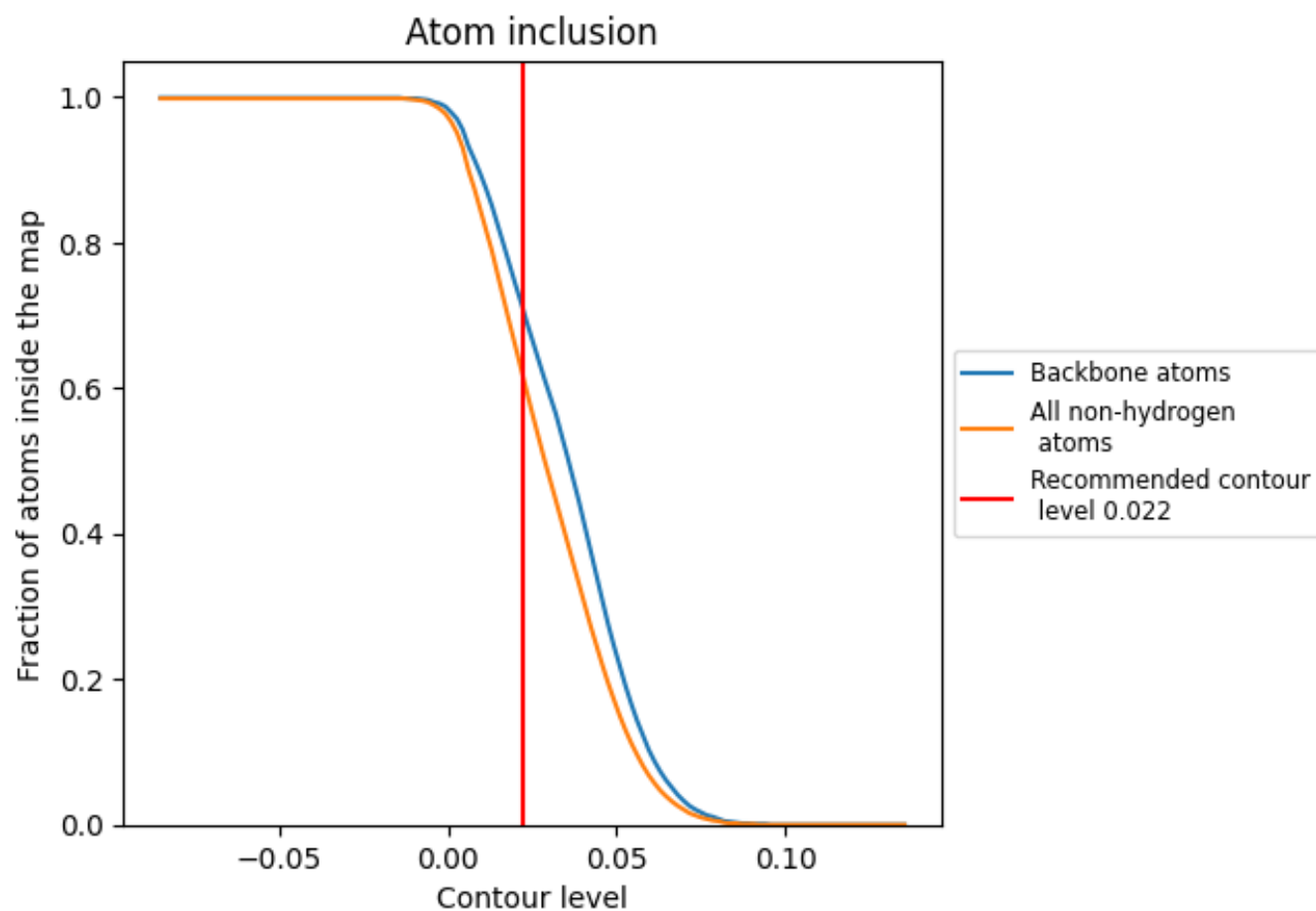
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 62% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6220	 0.4280
0	 0.2200	 0.1440
1	 0.5760	 0.3820
2	 0.5140	 0.3540
3	 0.5060	 0.3590
4	 0.4210	 0.2970
5	 0.6060	 0.4710
6	 0.5430	 0.4440
7	 0.6390	 0.4720
A	 0.1550	 0.1670
S	 0.7180	 0.4930
T	 0.6940	 0.4510
W	 0.6550	 0.4320
X	 0.7430	 0.5020
b	 0.6440	 0.4370
c	 0.5410	 0.3610
d	 0.5180	 0.3400
k	 0.6560	 0.4910
l	 0.5270	 0.4210
m	 0.4880	 0.4040
n	 0.4220	 0.3150
o	 0.3460	 0.3170

