



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 08:08 am BST

PDB ID : 9TIM / pdb_00009tim
EMDB ID : EMD-55961
Title : Phage 812 baseplate in the pre-contraction state - upper arm
Authors : Binovsky, J.; Plevka, P.
Deposited on : 2025-12-05
Resolution : 5.10 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:

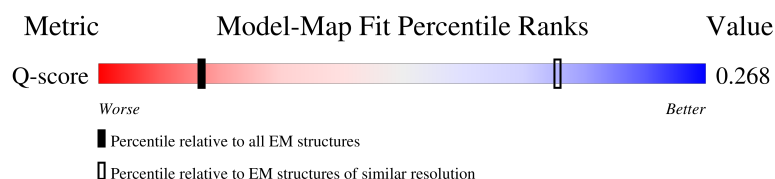
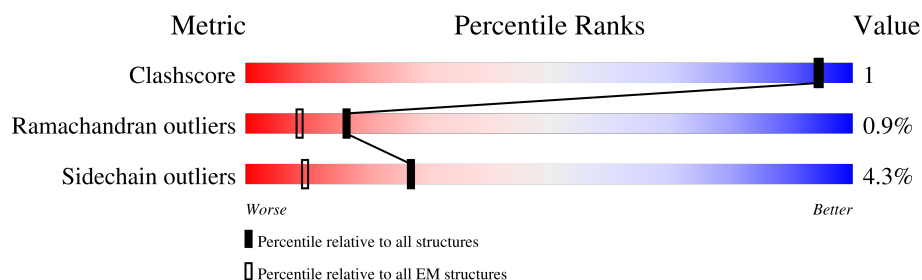
EMDB validation analysis : 0.0.1.dev133
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

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 5.10 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.



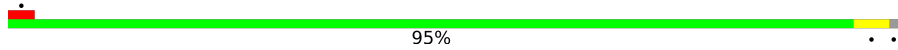
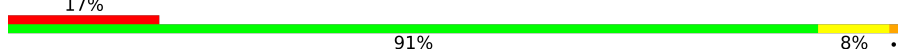
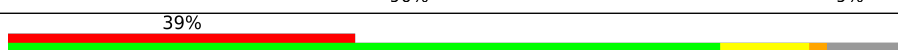
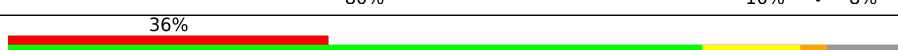
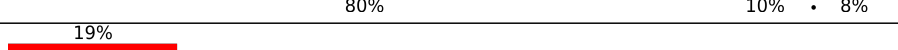
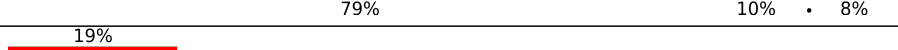
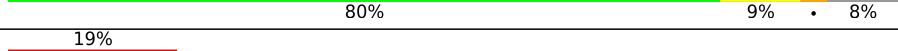
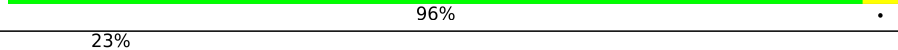
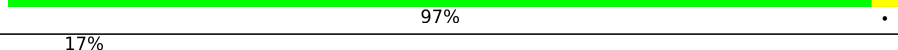
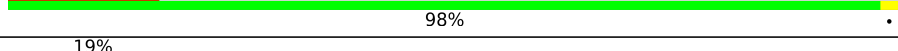
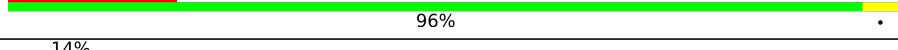
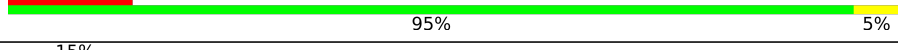
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	844 (4.60 - 5.60)

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	A	1019	20% 59% 38%
2	B	173	90% 5% 6%
2	C	173	89% 6%
2	D	173	94% 6%

Continued on next page...

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Mol	Chain	Length	Quality of chain
2	E	173	
2	F	173	
2	G	173	
2	H	173	
2	I	173	
2	J	173	
2	K	173	
2	L	173	
2	M	173	
3	N	1152	
3	O	1152	
3	P	1152	
3	Q	1152	
3	R	1152	
3	S	1152	
4	T	458	
4	U	458	
4	V	458	
5	W	640	
5	X	640	
5	Y	640	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 97106 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 ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	628	Total	C	N	O	S	0	0
			5070	3240	807	1013	10		

- Molecule 2 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	163	Total	C	N	O	S	0	0
			1280	818	209	252	1		
2	C	162	Total	C	N	O	S	0	0
			1270	811	207	251	1		
2	D	163	Total	C	N	O	S	0	0
			1278	817	208	252	1		
2	E	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	F	152	Total	C	N	O	S	0	0
			1199	769	196	233	1		
2	G	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	H	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	I	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	J	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	K	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	L	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		
2	M	172	Total	C	N	O	S	0	0
			1350	858	221	270	1		

- Molecule 3 is a protein called ORF65.

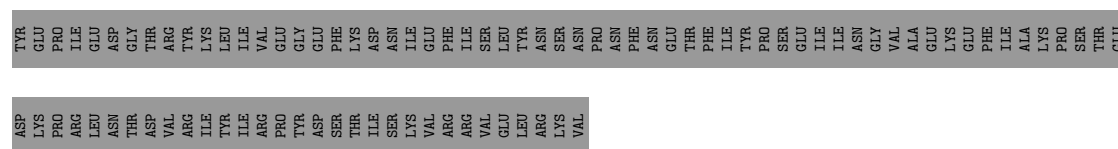
Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	O	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	P	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	Q	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	R	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		
3	S	1062	Total	C	N	O	S	0	0
			8364	5260	1398	1682	24		

- Molecule 4 is a protein called ORF68.

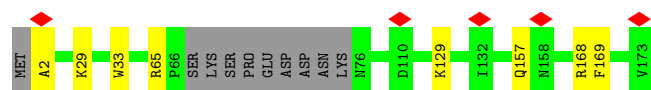
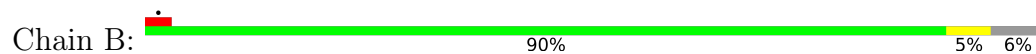
Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
4	U	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
4	V	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		

- Molecule 5 is a protein called CBM-cenC domain-containing protein.

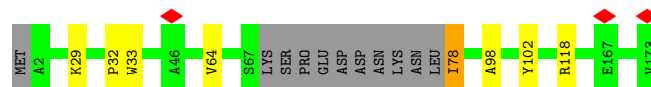
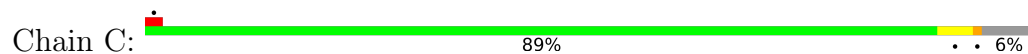
Mol	Chain	Residues	Atoms					AltConf	Trace
5	W	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	X	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		
5	Y	640	Total	C	N	O	S	0	0
			5127	3258	840	1016	13		



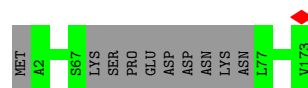
• Molecule 2: ORF64



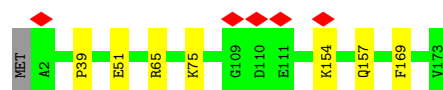
• Molecule 2: ORF64



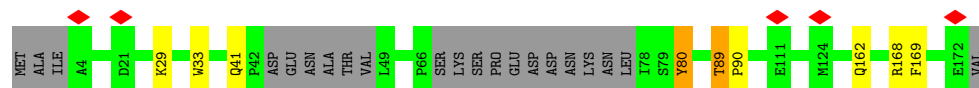
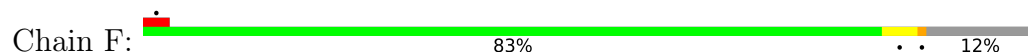
• Molecule 2: ORF64



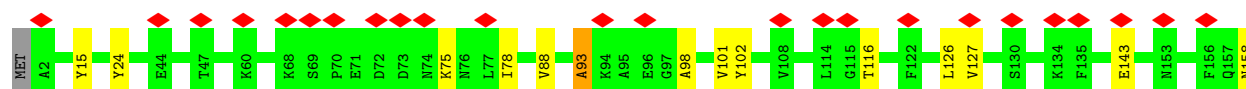
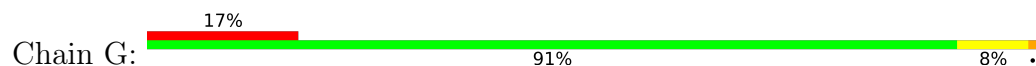
• Molecule 2: ORF64

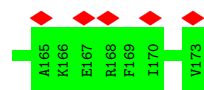


• Molecule 2: ORF64

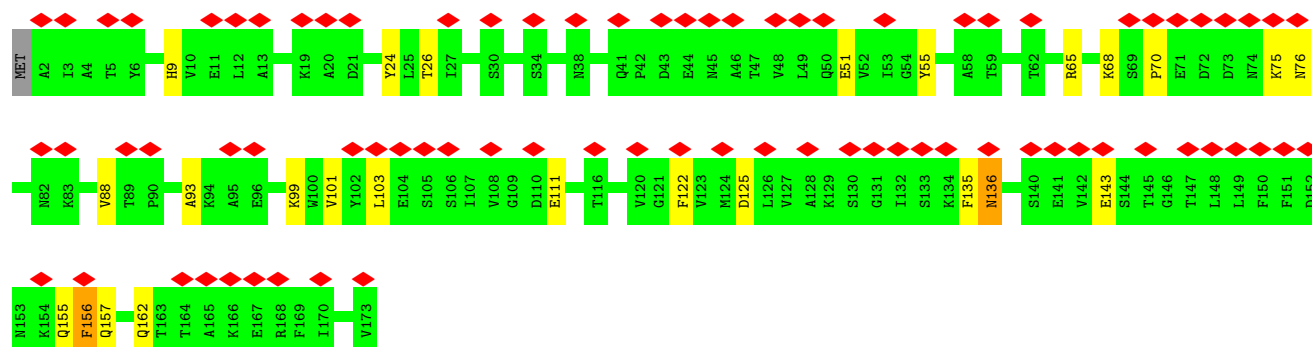
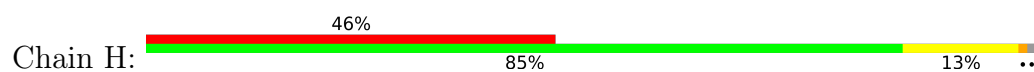


• Molecule 2: ORF64

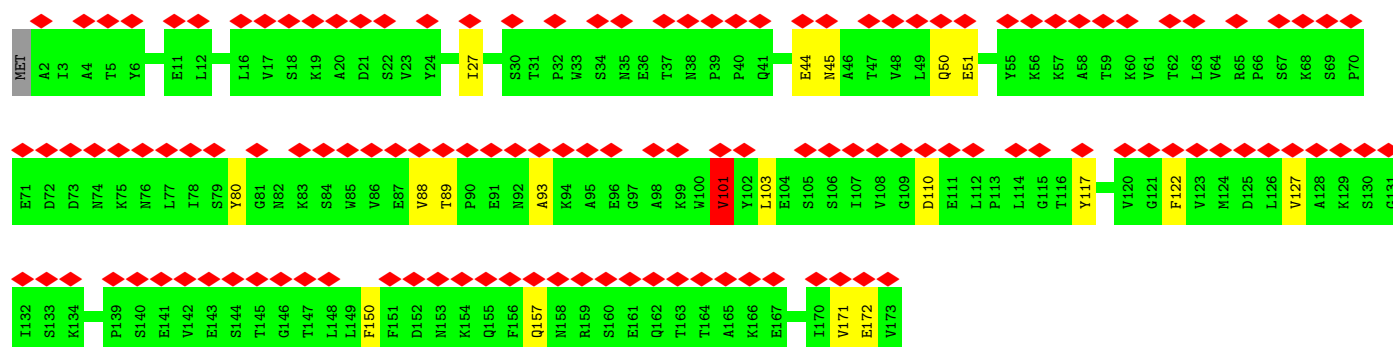
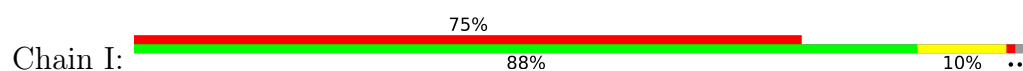




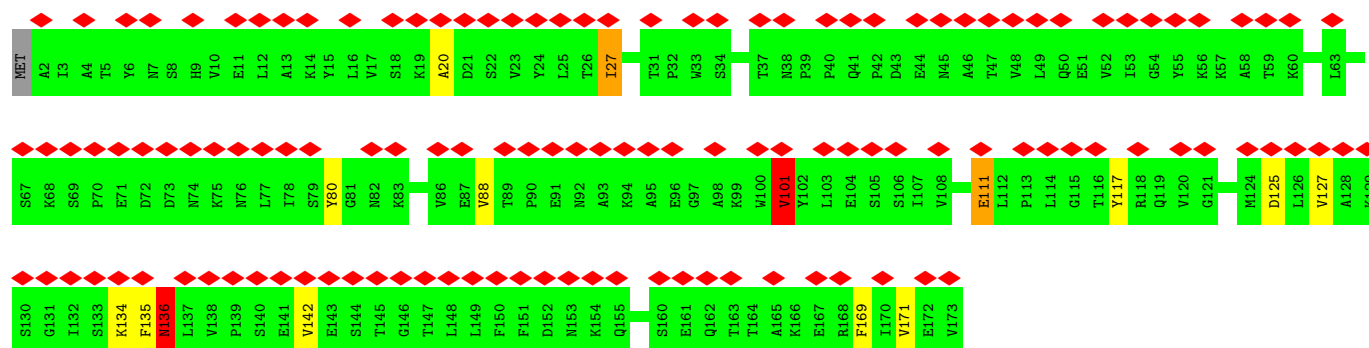
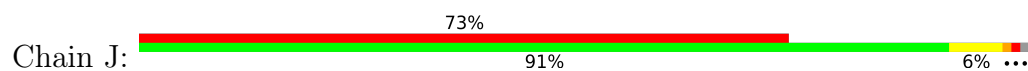
- Molecule 2: ORF64



- Molecule 2: ORF64

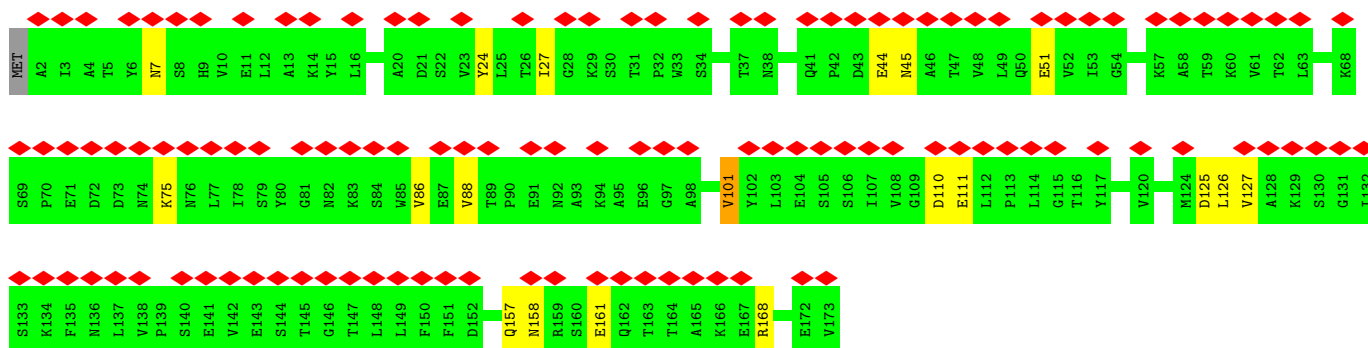


- Molecule 2: ORF64



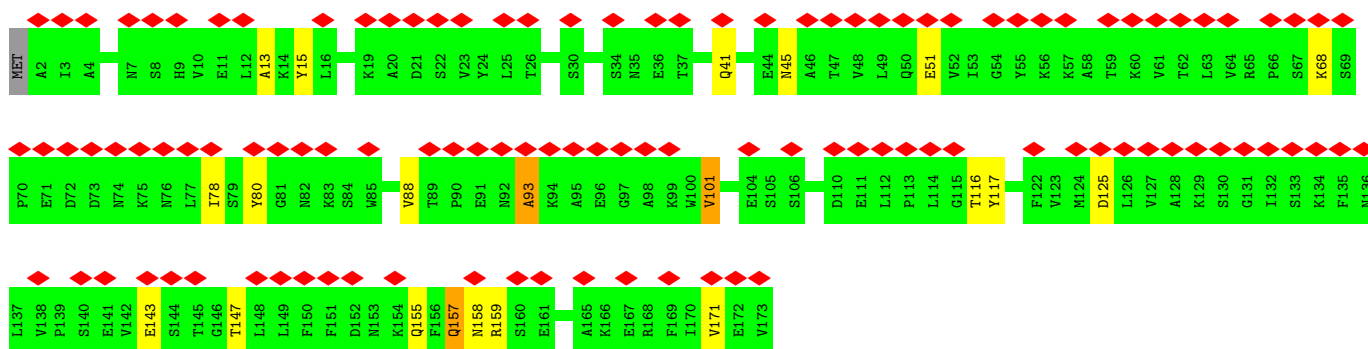
- Molecule 2: ORF64

Chain K: 

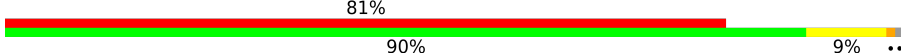


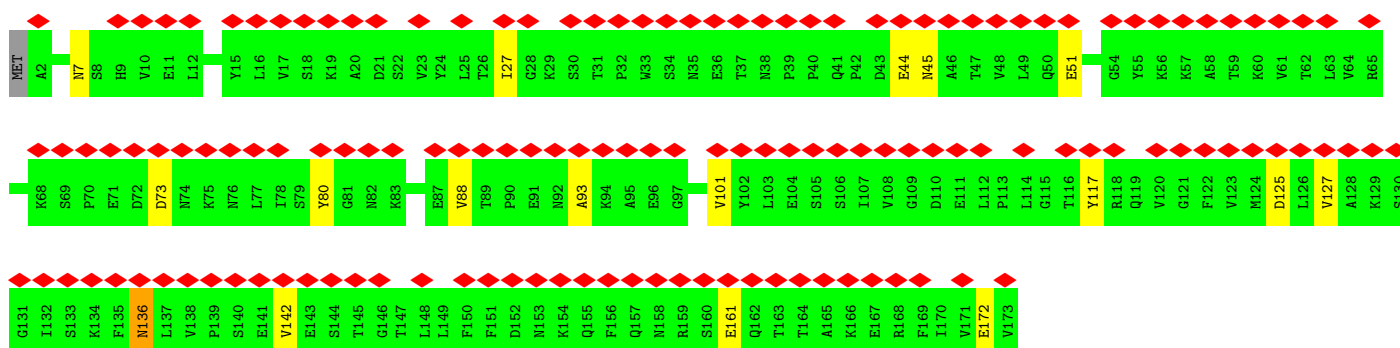
• Molecule 2: ORF64

Chain L: 



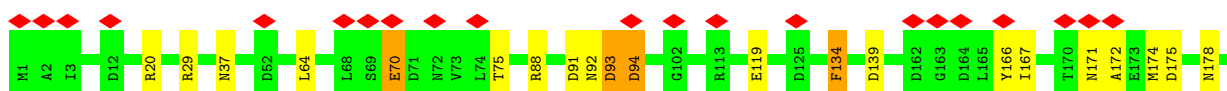
• Molecule 2: ORF64

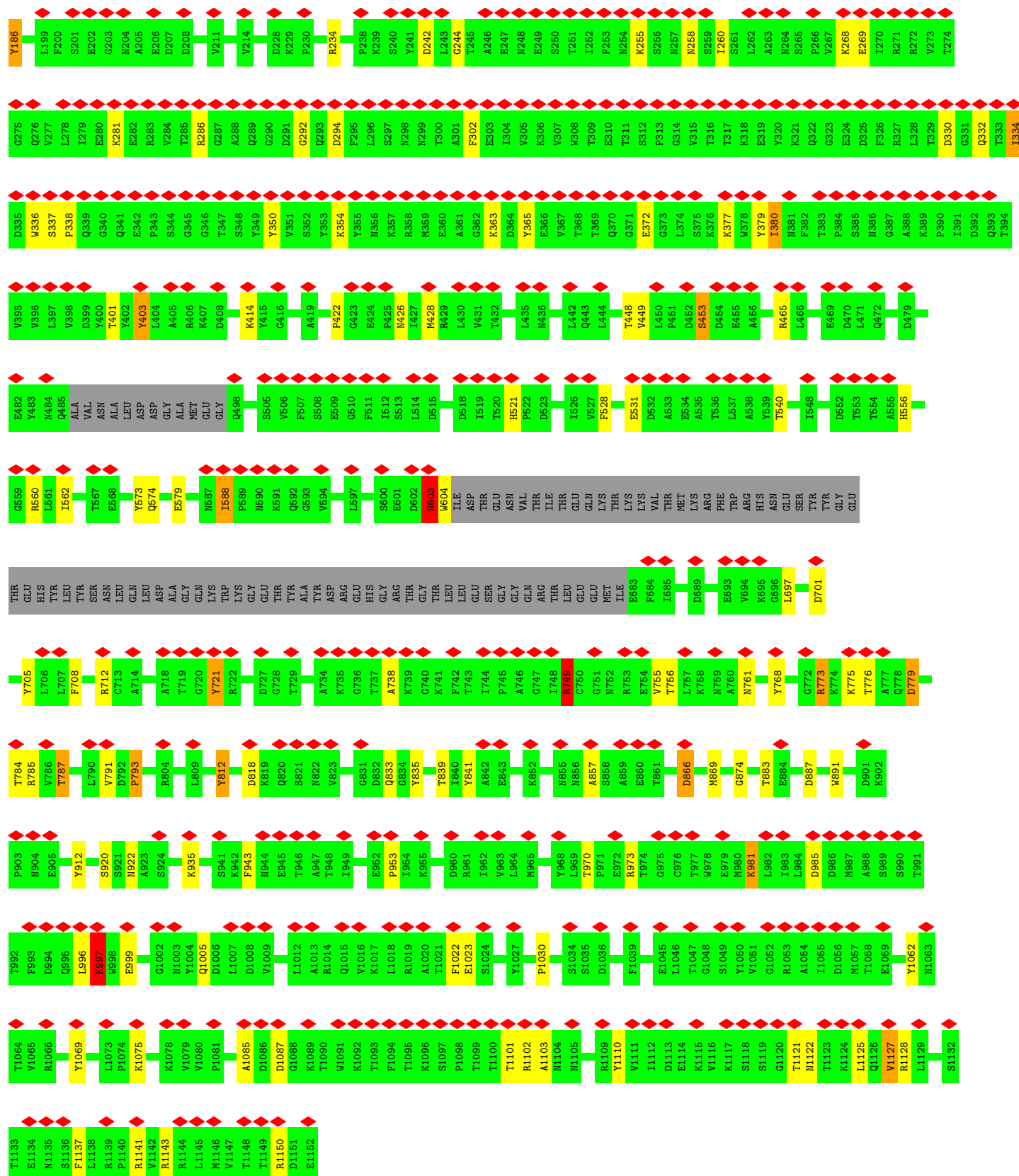
Chain M: 



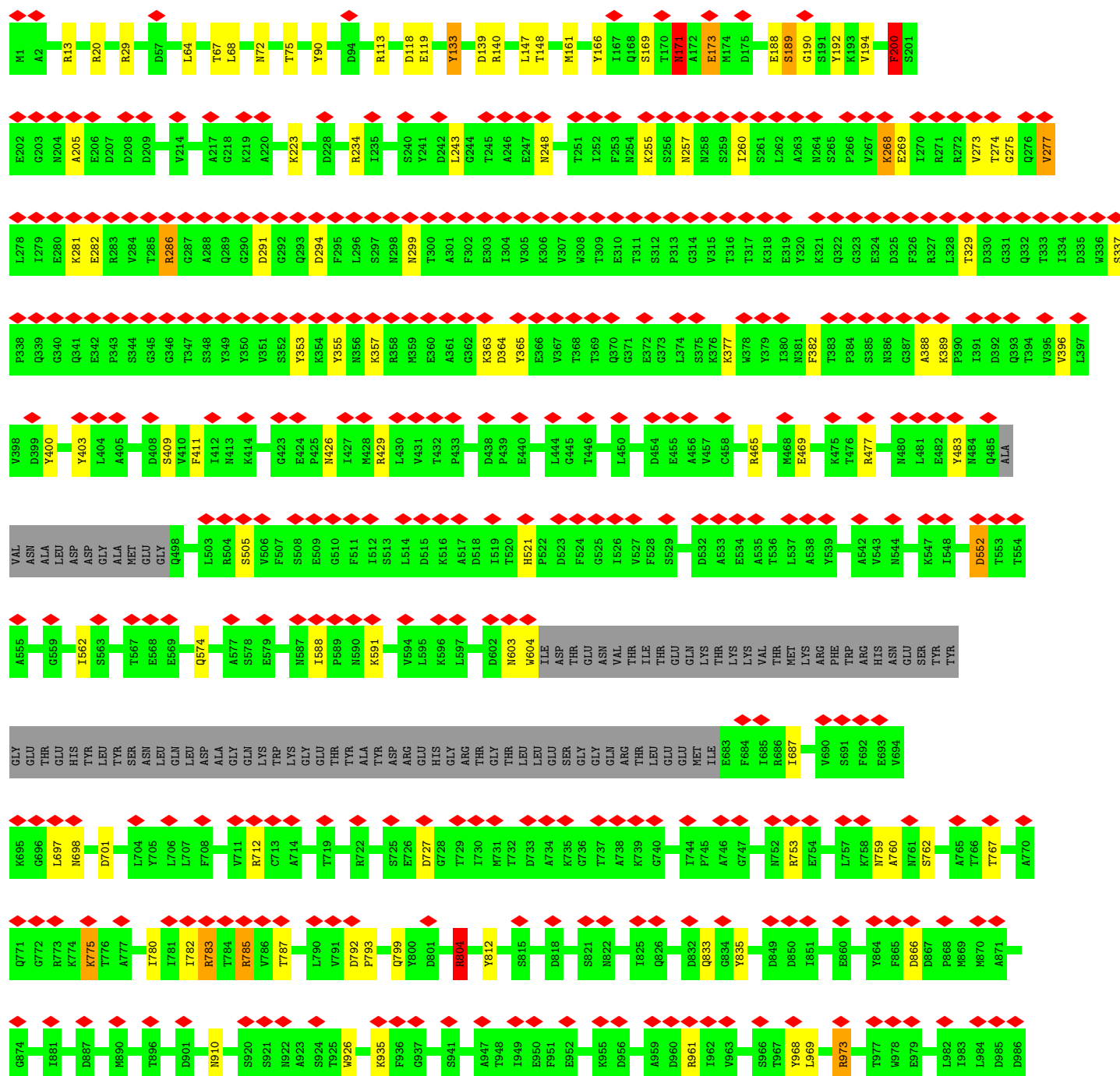
• Molecule 3: ORF65

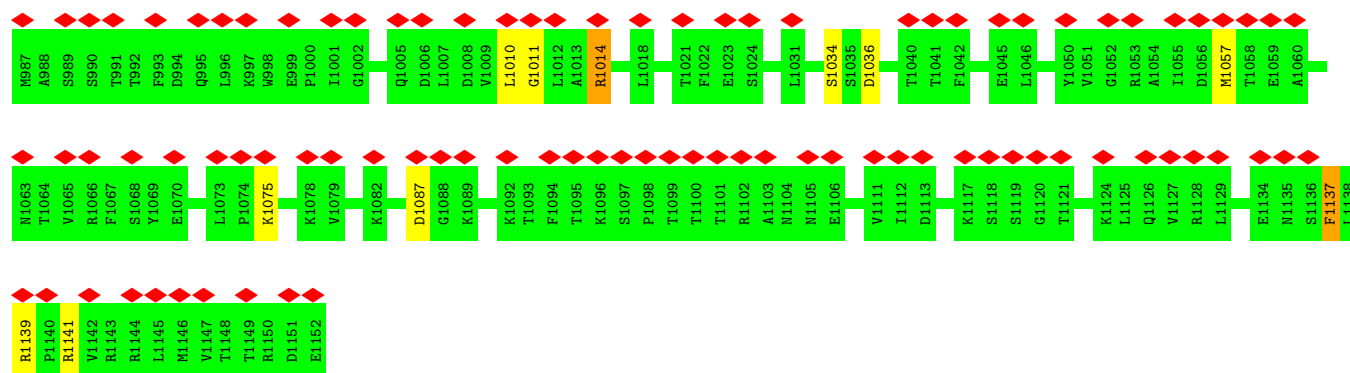
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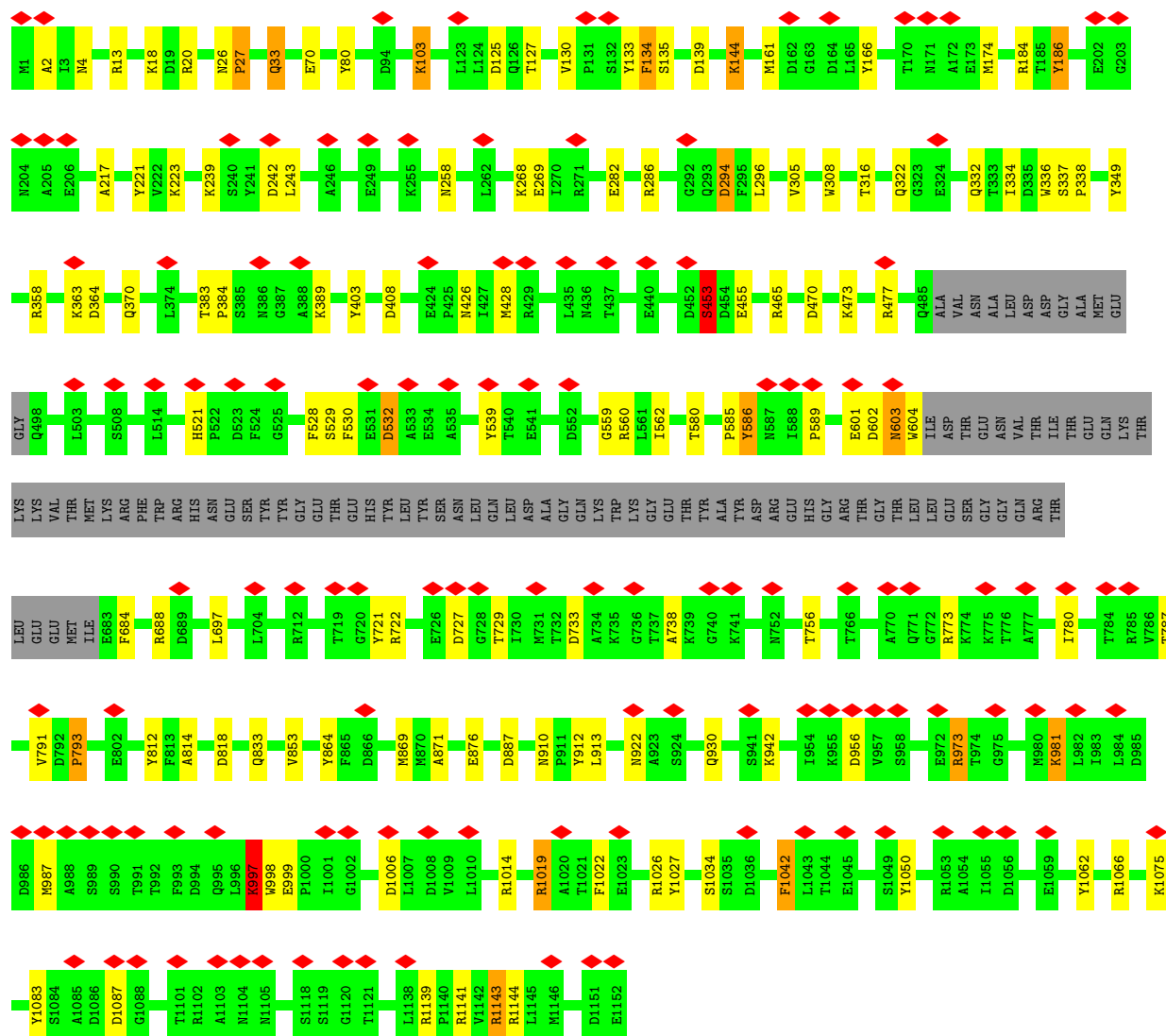
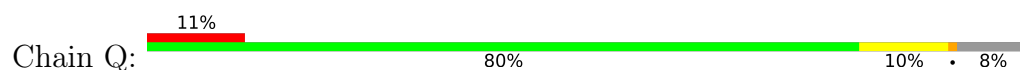




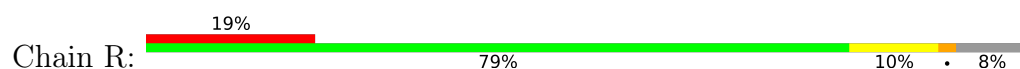


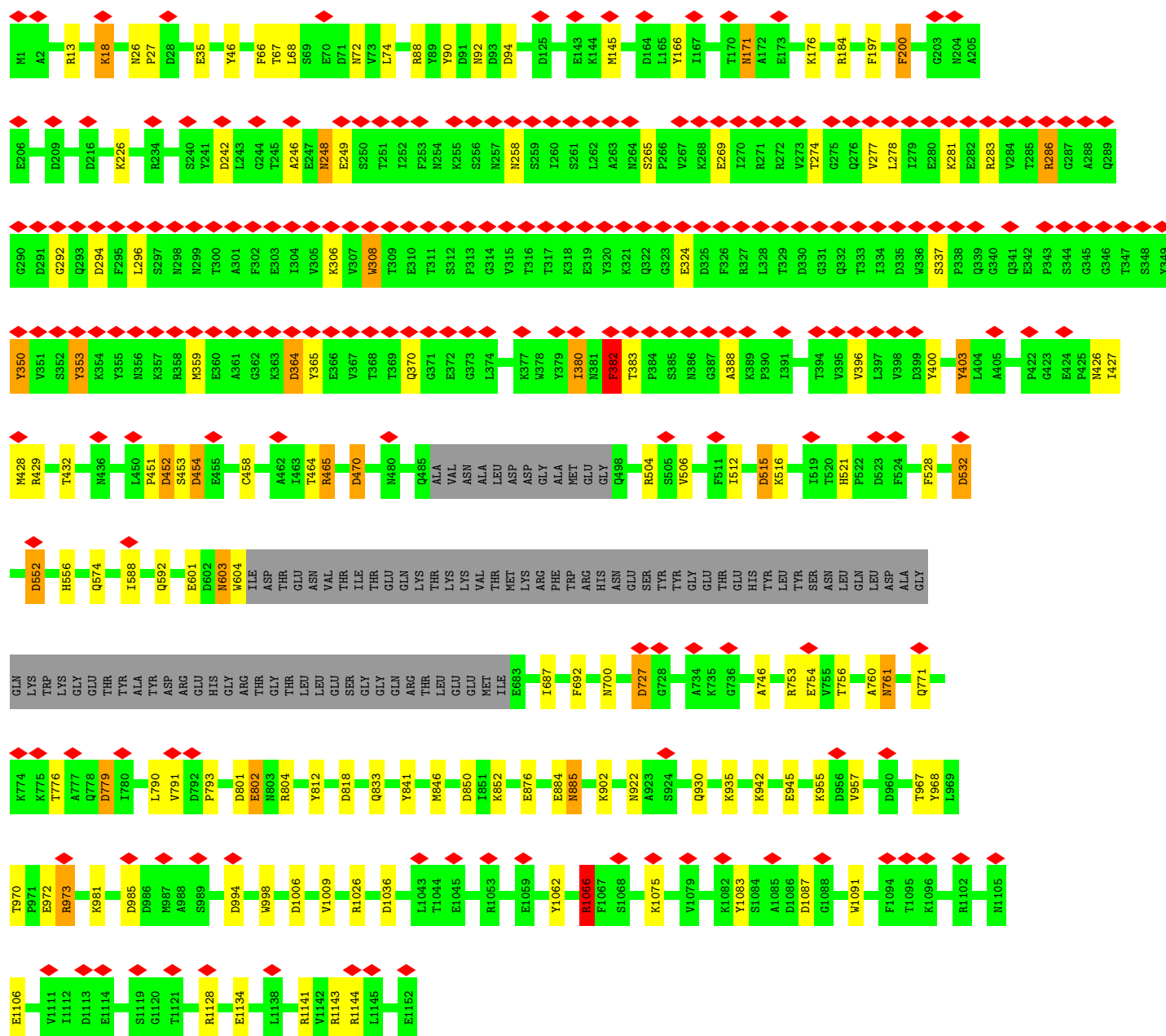


• Molecule 3: ORF65

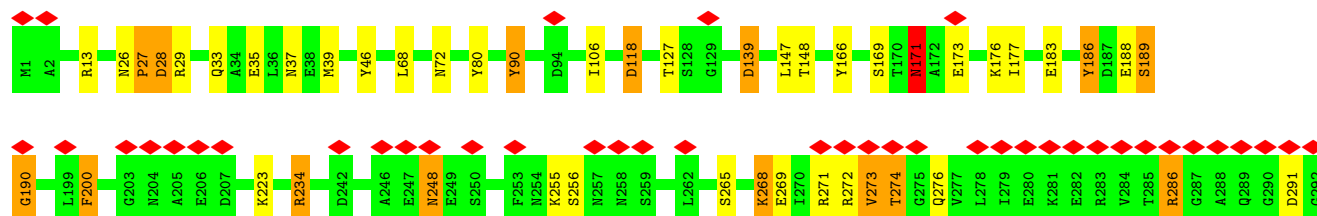


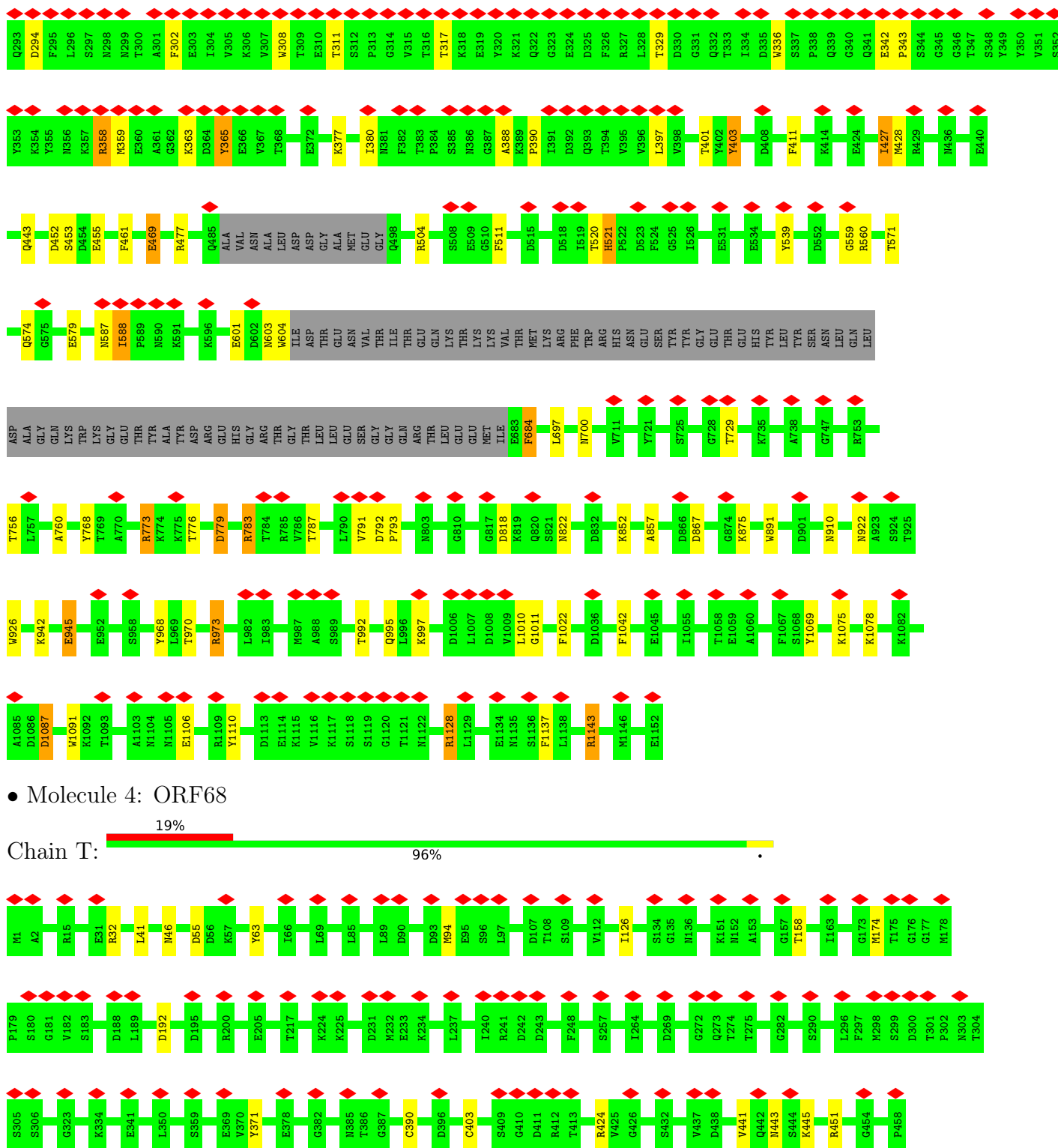
• Molecule 3: ORF65





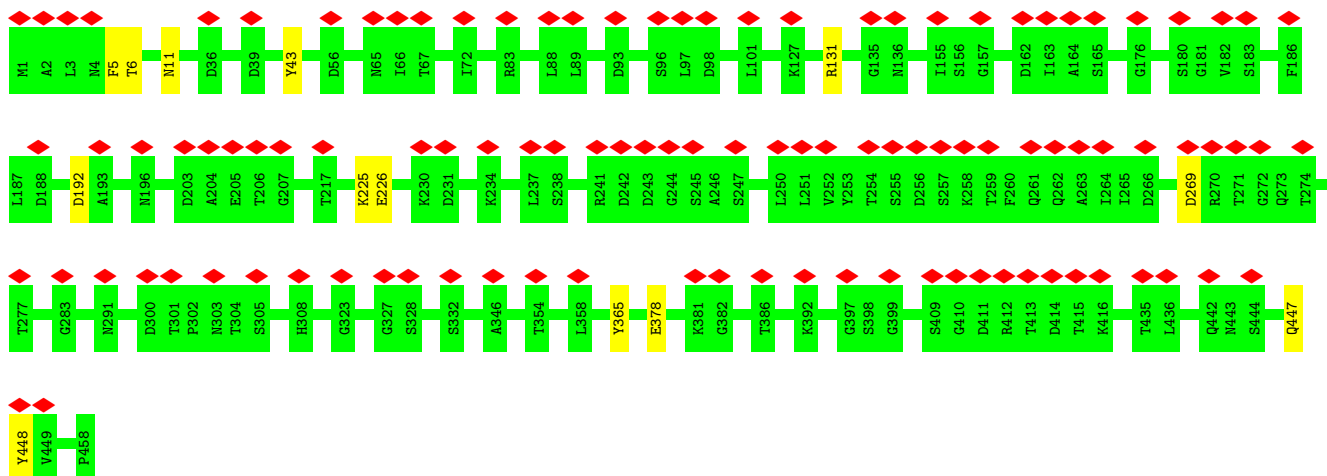
• Molecule 3: ORF65



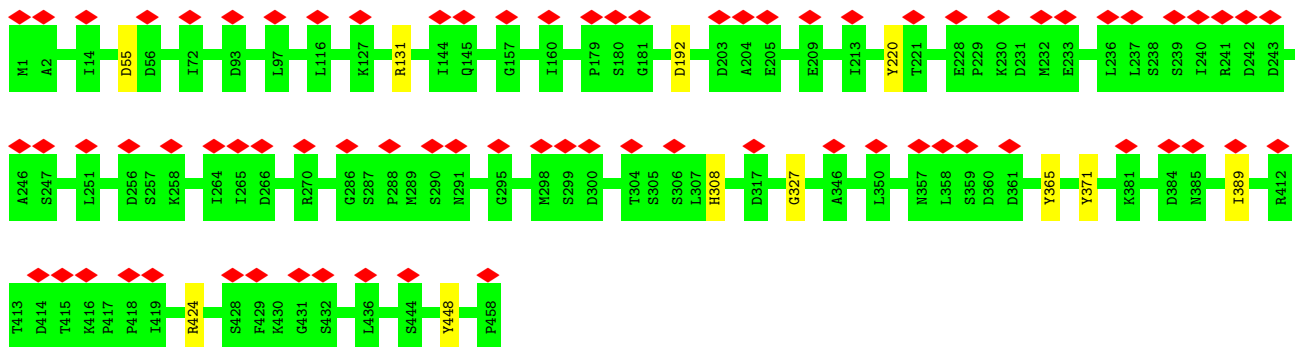


• Molecule 4: ORF68

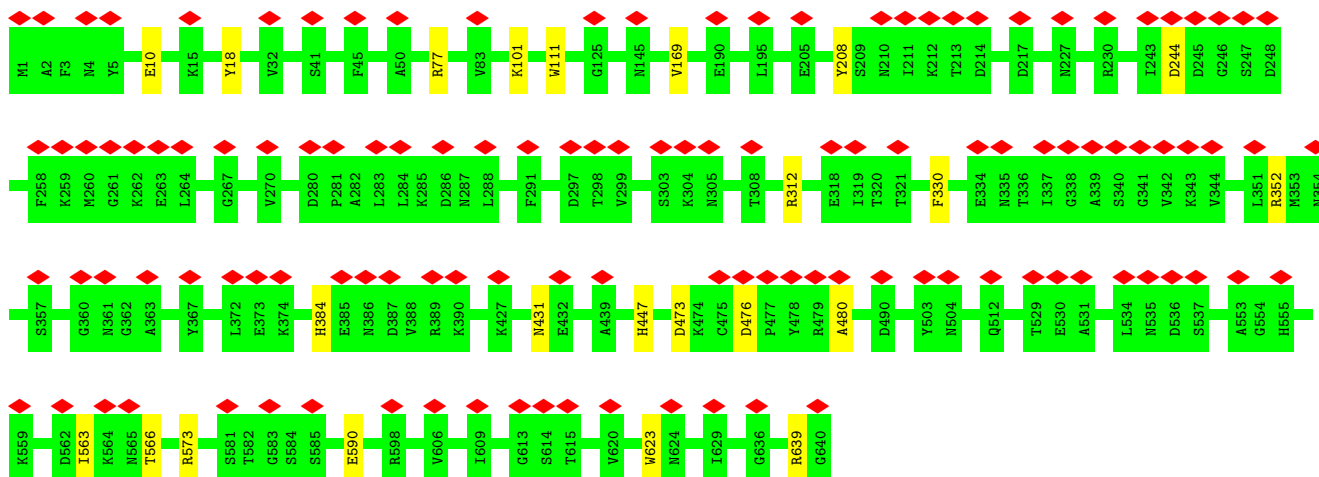




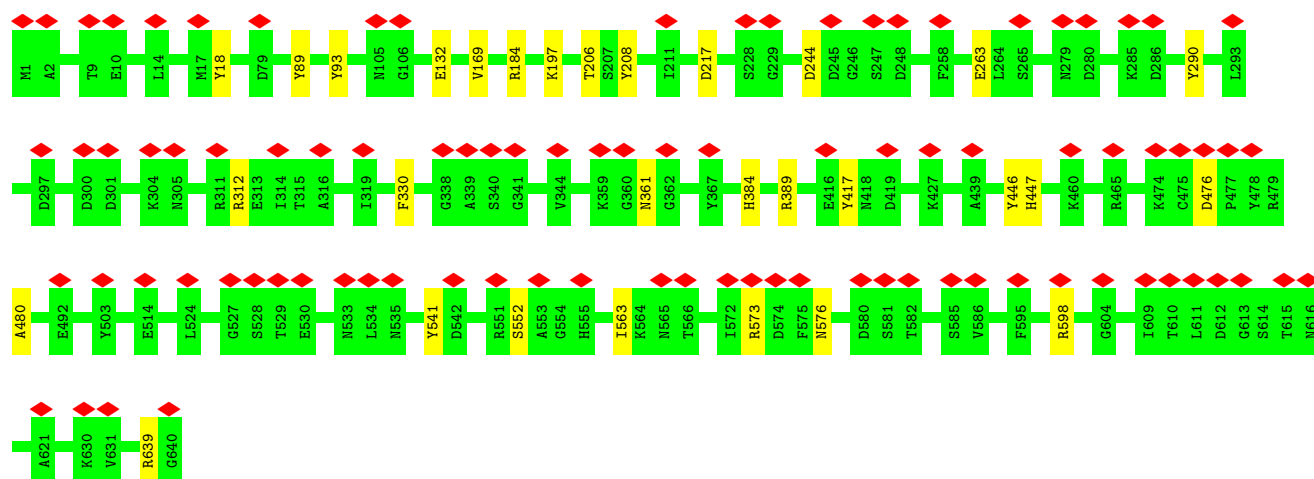
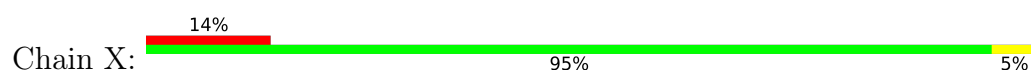
- Molecule 4: ORF68



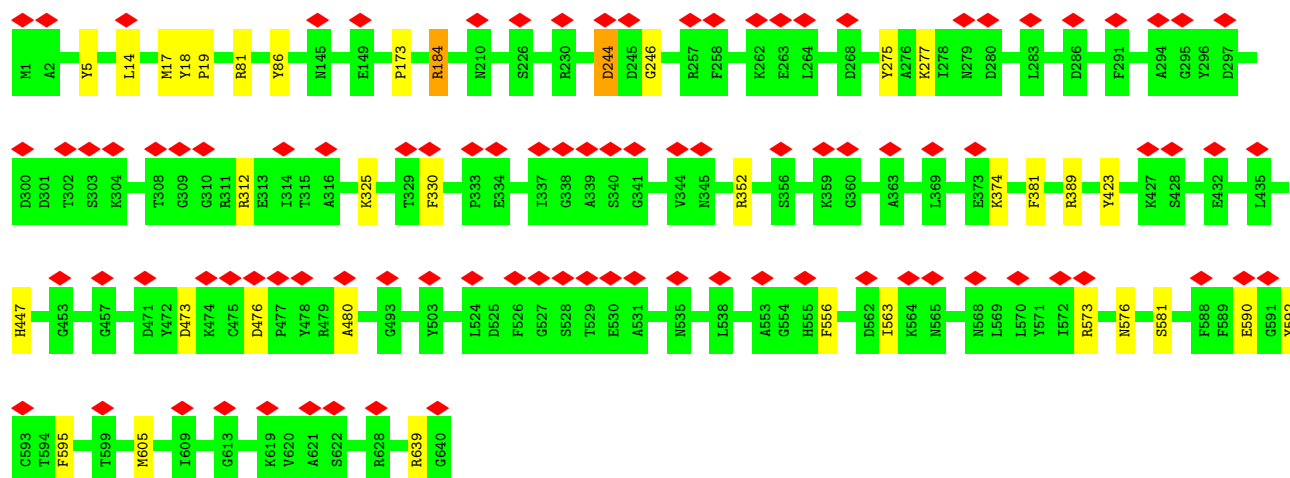
- Molecule 5: CBM-cenC domain-containing protein



- Molecule 5: CBM-cenC domain-containing protein



• Molecule 5: CBM-cenC domain-containing protein



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	19727	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40.8	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.112	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	600.192, 600.192, 600.192	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.6672001, 1.6672001, 1.6672001	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	A	0.72	0/5179	1.19	7/7040 (0.1%)
2	B	0.67	0/1306	1.14	2/1774 (0.1%)
2	C	0.66	0/1296	1.17	0/1760
2	D	0.65	0/1304	1.12	0/1771
2	E	0.66	0/1378	1.18	3/1872 (0.2%)
2	F	0.68	0/1224	1.27	4/1660 (0.2%)
2	G	0.73	0/1378	1.33	2/1872 (0.1%)
2	H	0.74	0/1378	1.38	6/1872 (0.3%)
2	I	0.77	0/1378	1.39	6/1872 (0.3%)
2	J	0.77	0/1378	1.37	5/1872 (0.3%)
2	K	0.76	0/1378	1.39	3/1872 (0.2%)
2	L	0.78	0/1378	1.36	4/1872 (0.2%)
2	M	0.79	0/1378	1.35	3/1872 (0.2%)
3	N	0.78	0/8526	1.40	42/11565 (0.4%)
3	O	0.79	0/8526	1.42	54/11565 (0.5%)
3	P	0.79	0/8526	1.33	31/11565 (0.3%)
3	Q	0.75	0/8526	1.38	42/11565 (0.4%)
3	R	0.76	0/8526	1.36	36/11565 (0.3%)
3	S	0.76	0/8526	1.37	45/11565 (0.4%)
4	T	0.75	0/3619	1.25	4/4913 (0.1%)
4	U	0.72	0/3619	1.22	3/4913 (0.1%)
4	V	0.72	0/3619	1.19	4/4913 (0.1%)
5	W	0.73	0/5253	1.22	6/7135 (0.1%)
5	X	0.72	0/5253	1.23	6/7135 (0.1%)
5	Y	0.72	0/5253	1.23	11/7135 (0.2%)
All	All	0.75	0/99105	1.32	329/134515 (0.2%)

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.

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	6
2	B	0	1
2	F	0	1
2	G	0	2
2	H	0	1
2	I	0	2
2	J	0	1
2	L	0	4
2	M	0	2
3	N	0	19
3	O	0	17
3	P	0	17
3	Q	0	21
3	R	0	16
3	S	0	16
4	T	0	2
4	U	0	3
4	V	0	5
5	W	0	2
5	X	0	5
5	Y	0	4
All	All	0	147

There are no bond length outliers.

All (329) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	171	ASN	CA-CB-CG	10.40	123.00	112.60
3	S	26	ASN	CA-C-N	8.94	129.84	119.47
3	S	26	ASN	C-N-CA	8.94	129.84	119.47
3	R	779	ASP	CA-CB-CG	8.89	121.50	112.60
3	S	28	ASP	CA-CB-CG	8.59	121.19	112.60
2	M	136	ASN	CA-CB-CG	8.42	121.02	112.60
3	O	779	ASP	CA-CB-CG	8.38	120.98	112.60
3	R	470	ASP	CA-CB-CG	8.04	120.64	112.60
3	R	171	ASN	CA-CB-CG	8.03	120.63	112.60
3	R	603	ASN	CA-CB-CG	7.91	120.51	112.60
3	Q	1042	PHE	CA-CB-CG	7.89	121.69	113.80
3	N	94	ASP	CA-CB-CG	7.83	120.44	112.60
3	R	1066	ARG	NE-CZ-NH2	7.76	126.19	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	801	ASP	CA-CB-CG	7.74	120.34	112.60
3	O	26	ASN	CA-C-N	7.73	129.50	119.84
3	O	26	ASN	C-N-CA	7.73	129.50	119.84
3	O	1137	PHE	CA-CB-CG	7.63	121.44	113.80
3	Q	294	ASP	CA-CB-CG	7.62	120.22	112.60
3	S	461	PHE	CA-CB-CG	7.54	121.34	113.80
3	S	272	ARG	CA-C-N	7.53	132.37	122.51
3	S	272	ARG	C-N-CA	7.53	132.37	122.51
3	N	866	ASP	CA-CB-CG	7.51	120.11	112.60
3	R	286	ARG	NE-CZ-NH2	7.47	125.93	119.20
3	S	27	PRO	N-CA-C	7.45	124.61	113.81
3	N	603	ASN	CA-CB-CG	7.34	119.94	112.60
3	Q	603	ASN	CA-CB-CG	7.25	119.85	112.60
3	S	200	PHE	CA-CB-CG	7.18	120.98	113.80
3	O	470	ASP	CA-CB-CG	7.16	119.76	112.60
3	O	248	ASN	CA-CB-CG	7.10	119.70	112.60
3	P	866	ASP	CA-CB-CG	7.05	119.65	112.60
3	S	29	ARG	N-CA-C	7.03	118.21	110.13
3	S	428	MET	N-CA-C	7.02	120.74	111.75
3	Q	26	ASN	CA-C-N	7.02	128.62	119.84
3	Q	26	ASN	C-N-CA	7.02	128.62	119.84
3	Q	1144	ARG	NE-CZ-NH2	6.98	125.48	119.20
3	S	118	ASP	CA-CB-CG	6.96	119.56	112.60
3	N	93	ASP	CA-CB-CG	6.93	119.53	112.60
3	O	1066	ARG	CD-NE-CZ	6.92	134.09	124.40
5	Y	244	ASP	CA-CB-CG	6.91	119.51	112.60
3	P	785	ARG	CA-C-N	6.76	129.63	120.63
3	P	785	ARG	C-N-CA	6.76	129.63	120.63
3	Q	530	PHE	CA-CB-CG	6.76	120.56	113.80
2	J	169	PHE	CA-CB-CG	6.74	120.54	113.80
3	Q	135	SER	N-CA-C	6.67	120.75	110.20
3	O	1036	ASP	CA-CB-CG	-6.66	105.94	112.60
3	Q	956	ASP	CA-C-N	6.63	129.36	122.27
3	Q	956	ASP	C-N-CA	6.63	129.36	122.27
3	O	1128	ARG	NE-CZ-NH2	6.62	125.16	119.20
3	S	302	PHE	CA-CB-CG	6.55	120.35	113.80
3	R	552	ASP	CA-CB-CG	6.52	119.12	112.60
3	O	364	ASP	CA-CB-CG	6.51	119.11	112.60
3	S	477	ARG	NE-CZ-NH2	6.51	125.06	119.20
3	Q	1022	PHE	CA-CB-CG	6.50	120.30	113.80
3	N	37	ASN	CA-C-N	6.49	129.51	120.29
3	N	37	ASN	C-N-CA	6.49	129.51	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	P	286	ARG	NE-CZ-NH2	6.49	125.04	119.20
3	N	380	ILE	CB-CA-C	6.48	117.77	111.23
3	O	1066	ARG	NE-CZ-NH2	6.46	125.02	119.20
5	W	77	ARG	NE-CZ-NH2	6.43	124.99	119.20
5	W	312	ARG	NE-CZ-NH2	6.41	124.96	119.20
3	R	364	ASP	CA-CB-CG	6.37	118.97	112.60
3	N	255	LYS	CA-C-N	6.37	130.44	120.89
3	N	255	LYS	C-N-CA	6.37	130.44	120.89
3	S	286	ARG	NE-CZ-NH2	6.36	124.93	119.20
3	S	783	ARG	NE-CZ-NH2	6.34	124.91	119.20
5	Y	312	ARG	NE-CZ-NH2	6.32	124.89	119.20
3	N	178	ASN	CA-CB-CG	-6.32	106.28	112.60
3	O	792	ASP	CA-C-N	6.29	127.70	119.84
3	O	792	ASP	C-N-CA	6.29	127.70	119.84
3	N	749	ARG	NE-CZ-NH2	6.27	124.85	119.20
3	O	243	LEU	CA-C-N	6.26	126.43	121.61
3	O	243	LEU	C-N-CA	6.26	126.43	121.61
3	O	1143	ARG	NE-CZ-NH2	6.26	124.83	119.20
3	N	528	PHE	CA-CB-CG	6.25	120.05	113.80
3	P	477	ARG	NE-CZ-NH2	6.22	124.80	119.20
3	S	401	THR	CA-CB-CG2	6.22	121.08	110.50
3	N	521	HIS	CA-CB-CG	-6.22	107.58	113.80
3	R	265	SER	N-CA-C	6.22	113.81	108.22
3	P	200	PHE	CA-CB-CG	6.21	120.01	113.80
3	N	943	PHE	CA-CB-CG	-6.19	107.61	113.80
3	N	773	ARG	NE-CZ-NH2	6.18	124.77	119.20
3	R	532	ASP	CA-CB-CG	6.18	118.78	112.60
3	P	759	ASN	CA-CB-CG	6.16	118.75	112.60
3	O	1150	ARG	NE-CZ-NH2	6.15	124.74	119.20
3	Q	602	ASP	N-CA-C	6.15	118.47	108.76
4	V	389	ILE	CA-C-N	6.14	129.59	120.87
4	V	389	ILE	C-N-CA	6.14	129.59	120.87
3	O	504	ARG	NE-CZ-NH2	6.14	124.72	119.20
3	O	27	PRO	N-CA-C	6.13	125.10	112.47
3	Q	560	ARG	NE-CZ-NH2	6.12	124.71	119.20
3	S	1143	ARG	NE-CZ-NH2	6.12	124.70	119.20
2	I	110	ASP	N-CA-C	6.11	117.74	111.14
3	S	521	HIS	CB-CG-CD2	-6.09	123.28	131.20
2	B	169	PHE	CA-CB-CG	6.05	119.85	113.80
3	N	588	ILE	N-CA-C	6.04	114.64	109.02
3	O	139	ASP	CA-CB-CG	6.03	118.63	112.60
3	Q	477	ARG	NE-CZ-NH2	5.98	124.58	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Y	595	PHE	CA-CB-CG	5.97	119.77	113.80
2	F	169	PHE	CA-CB-CG	5.97	119.77	113.80
3	R	761	ASN	CA-CB-CG	5.97	118.57	112.60
3	R	382	PHE	CA-C-N	5.96	127.15	120.06
3	R	382	PHE	C-N-CA	5.96	127.15	120.06
3	N	380	ILE	N-CA-CB	-5.96	106.69	112.65
3	N	175	ASP	CA-C-N	5.95	129.07	120.38
3	N	175	ASP	C-N-CA	5.95	129.07	120.38
2	K	110	ASP	N-CA-C	5.93	117.83	111.36
3	P	1036	ASP	CA-CB-CG	-5.93	106.67	112.60
3	R	727	ASP	CA-CB-CG	-5.93	106.67	112.60
1	A	344	ARG	NE-CZ-NH2	5.89	124.50	119.20
5	X	312	ARG	NE-CZ-NH2	5.89	124.50	119.20
3	R	26	ASN	N-CA-C	5.89	115.09	108.25
3	Q	1006	ASP	CA-CB-CG	5.89	118.49	112.60
3	R	248	ASN	CA-CB-CG	5.87	118.47	112.60
3	R	885	ASN	CA-CB-CG	5.86	118.46	112.60
3	O	461	PHE	CA-CB-CG	5.85	119.65	113.80
3	N	422	PRO	CA-C-N	5.85	126.73	121.82
3	N	422	PRO	C-N-CA	5.85	126.73	121.82
3	Q	1019	ARG	NE-CZ-NH2	5.85	124.46	119.20
3	Q	243	LEU	CA-C-N	5.84	127.64	121.45
3	Q	243	LEU	C-N-CA	5.84	127.64	121.45
2	H	156	PHE	CA-CB-CG	5.82	119.62	113.80
2	J	101	VAL	CA-CB-CG1	5.82	120.29	110.40
3	P	382	PHE	CB-CA-C	5.81	120.08	111.88
3	P	140	ARG	NE-CZ-NH2	5.80	124.42	119.20
3	N	372	GLU	N-CA-C	5.80	118.22	109.23
3	Q	603	ASN	OD1-CG-ND2	-5.79	116.81	122.60
3	N	603	ASN	OD1-CG-ND2	-5.79	116.81	122.60
3	S	29	ARG	CA-C-N	5.79	126.11	119.92
3	S	29	ARG	C-N-CA	5.79	126.11	119.92
2	I	101	VAL	CA-CB-CG1	5.78	120.23	110.40
3	P	1014	ARG	NE-CZ-NH2	5.77	124.39	119.20
3	Q	33	GLN	OE1-CD-NE2	-5.76	116.83	122.60
3	Q	1143	ARG	NE-CZ-NH1	-5.75	115.75	121.50
3	N	20	ARG	NE-CZ-NH2	5.75	124.37	119.20
3	S	521	HIS	CA-CB-CG	-5.74	108.06	113.80
3	N	996	LEU	CA-C-N	5.73	132.49	121.54
3	N	996	LEU	C-N-CA	5.73	132.49	121.54
2	J	136	ASN	CA-CB-CG	5.73	118.33	112.60
3	S	189	SER	CA-C-N	5.72	132.63	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	189	SER	C-N-CA	5.72	132.63	121.41
3	S	1087	ASP	CA-C-N	5.71	130.80	122.46
3	S	1087	ASP	C-N-CA	5.71	130.80	122.46
3	N	1005	GLN	OE1-CD-NE2	-5.70	116.90	122.60
5	W	639	ARG	NE-CZ-NH2	5.69	124.32	119.20
4	U	131	ARG	NE-CZ-NH2	5.68	124.32	119.20
3	N	1141	ARG	NE-CZ-NH2	5.68	124.31	119.20
3	O	1022	PHE	CA-CB-CG	5.68	119.48	113.80
3	R	556	HIS	CB-CG-CD2	-5.68	123.82	131.20
3	S	427	ILE	CA-C-N	5.67	128.66	120.38
3	S	427	ILE	C-N-CA	5.67	128.66	120.38
3	S	779	ASP	CA-CB-CG	5.67	118.27	112.60
3	Q	1143	ARG	NE-CZ-NH2	5.66	124.30	119.20
3	P	552	ASP	CA-CB-CG	5.66	118.26	112.60
3	O	785	ARG	NE-CZ-NH2	5.66	124.29	119.20
3	Q	1066	ARG	NE-CZ-NH2	5.66	124.29	119.20
2	H	135	PHE	CA-CB-CG	5.64	119.44	113.80
3	N	428	MET	N-CA-C	5.64	116.89	108.31
3	N	521	HIS	CB-CG-CD2	-5.62	123.89	131.20
3	S	139	ASP	CA-CB-CG	5.62	118.22	112.60
2	H	136	ASN	CA-CB-CG	5.61	118.21	112.60
3	P	969	LEU	CA-C-N	5.60	127.99	122.28
3	P	969	LEU	C-N-CA	5.60	127.99	122.28
2	K	111	GLU	N-CA-C	5.59	119.36	112.54
3	P	785	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	I	89	THR	CA-C-N	5.58	125.25	119.05
2	I	89	THR	C-N-CA	5.58	125.25	119.05
3	O	286	ARG	NE-CZ-NH2	5.58	124.23	119.20
3	O	1141	ARG	NE-CZ-NH2	5.58	124.22	119.20
2	B	65	ARG	NE-CZ-NH2	5.58	124.22	119.20
2	G	93	ALA	CA-C-N	5.58	128.07	120.54
2	G	93	ALA	C-N-CA	5.58	128.07	120.54
3	N	401	THR	CA-C-N	5.58	129.90	120.81
3	N	401	THR	C-N-CA	5.58	129.90	120.81
5	X	184	ARG	NE-CZ-NH2	5.58	124.22	119.20
3	O	773	ARG	NE-CZ-NH2	5.57	124.21	119.20
3	O	443	GLN	OE1-CD-NE2	-5.57	117.03	122.60
3	O	356	ASN	CB-CA-C	5.56	120.96	112.00
3	R	973	ARG	CD-NE-CZ	5.56	132.19	124.40
1	A	154	PHE	CA-C-N	5.56	125.53	120.03
1	A	154	PHE	C-N-CA	5.56	125.53	120.03
2	E	65	ARG	NE-CZ-NH2	5.56	124.20	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	556	HIS	CB-CG-CD2	-5.55	123.98	131.20
3	O	367	VAL	CA-CB-CG2	5.55	119.83	110.40
3	S	13	ARG	NE-CZ-NH1	-5.55	115.95	121.50
3	S	248	ASN	CA-CB-CG	5.55	118.15	112.60
3	S	255	LYS	CA-C-N	5.54	127.97	120.38
3	S	255	LYS	C-N-CA	5.54	127.97	120.38
2	I	172	GLU	CA-C-N	5.52	131.64	121.70
2	I	172	GLU	C-N-CA	5.52	131.64	121.70
2	H	65	ARG	NE-CZ-NH2	5.52	124.17	119.20
3	Q	684	PHE	N-CA-C	5.51	117.77	109.23
3	P	1141	ARG	NE-CZ-NH2	5.50	124.15	119.20
3	S	684	PHE	CA-CB-CG	5.49	119.29	113.80
3	Q	1141	ARG	NE-CZ-NH2	5.49	124.14	119.20
3	S	773	ARG	NE-CZ-NH2	5.47	124.12	119.20
4	V	131	ARG	NE-CZ-NH2	5.46	124.12	119.20
4	T	46	ASN	CA-CB-CG	-5.46	107.14	112.60
5	Y	184	ARG	NE-CZ-NH2	5.46	124.12	119.20
5	Y	389	ARG	NE-CZ-NH2	5.44	124.09	119.20
3	N	985	ASP	CA-CB-CG	5.43	118.03	112.60
3	Q	727	ASP	CA-CB-CG	-5.42	107.18	112.60
3	R	1143	ARG	NE-CZ-NH2	5.42	124.08	119.20
3	P	277	VAL	CB-CA-C	-5.41	105.39	111.45
3	R	171	ASN	OD1-CG-ND2	-5.41	117.19	122.60
2	J	20	ALA	N-CA-C	5.40	118.66	111.75
3	S	1143	ARG	NE-CZ-NH1	-5.39	116.11	121.50
3	Q	364	ASP	CA-CB-CG	5.39	117.99	112.60
3	S	1022	PHE	CA-CB-CG	5.38	119.18	113.80
3	R	1066	ARG	CD-NE-CZ	5.37	131.91	124.40
2	E	39	PRO	N-CA-CB	5.37	106.20	103.19
3	P	429	ARG	NE-CZ-NH2	5.36	124.03	119.20
4	U	269	ASP	CA-CB-CG	5.36	117.96	112.60
3	Q	134	PHE	N-CA-C	5.36	122.20	110.80
5	Y	14	LEU	CA-C-N	5.35	128.19	120.38
5	Y	14	LEU	C-N-CA	5.35	128.19	120.38
3	O	264	ASN	CA-CB-CG	5.35	117.95	112.60
1	A	285	ARG	NE-CZ-NH2	5.35	124.01	119.20
3	P	257	ASN	CA-CB-CG	5.34	117.94	112.60
3	O	688	ARG	NE-CZ-NH2	5.34	124.01	119.20
5	W	384	HIS	CB-CG-CD2	-5.34	124.26	131.20
3	R	380	ILE	CB-CA-C	5.32	116.61	111.23
3	Q	560	ARG	CD-NE-CZ	5.32	131.84	124.40
3	R	504	ARG	NE-CZ-NH2	5.32	123.99	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	O	276	GLN	OE1-CD-NE2	-5.30	117.30	122.60
3	O	887	ASP	CA-CB-CG	5.30	117.90	112.60
3	P	785	ARG	N-CA-C	5.28	118.06	109.24
3	N	779	ASP	CA-CB-CG	5.28	117.88	112.60
2	J	111	GLU	CB-CG-CD	5.28	121.58	112.60
3	O	765	ALA	N-CA-C	5.28	116.87	108.79
4	T	32	ARG	NE-CZ-NH2	5.28	123.95	119.20
2	H	76	ASN	CA-CB-CG	5.27	117.87	112.60
3	N	712	ARG	NE-CZ-NH2	5.27	123.94	119.20
3	P	189	SER	CA-C-N	5.27	131.73	121.41
3	P	189	SER	C-N-CA	5.27	131.73	121.41
3	O	560	ARG	NE-CZ-NH2	5.26	123.93	119.20
3	Q	521	HIS	CB-CG-CD2	-5.26	124.36	131.20
3	R	1141	ARG	NE-CZ-NH2	5.25	123.93	119.20
3	O	570	ARG	NE-CZ-NH2	5.25	123.92	119.20
3	P	133	TYR	CA-CB-CG	5.25	123.34	113.90
3	P	521	HIS	CB-CG-CD2	-5.24	124.38	131.20
3	S	1087	ASP	CA-CB-CG	5.24	117.84	112.60
3	P	20	ARG	NE-CZ-NH2	5.24	123.92	119.20
2	M	172	GLU	CA-C-N	5.24	131.12	121.70
2	M	172	GLU	C-N-CA	5.24	131.12	121.70
3	N	920	SER	N-CA-C	5.24	116.76	108.96
3	R	1006	ASP	CA-CB-CG	5.23	117.83	112.60
3	R	973	ARG	NE-CZ-NH2	5.22	123.90	119.20
3	S	504	ARG	NE-CZ-NH2	5.22	123.90	119.20
5	X	389	ARG	NE-CZ-NH2	5.22	123.90	119.20
3	S	358	ARG	NE-CZ-NH2	5.22	123.89	119.20
3	P	255	LYS	CA-C-N	5.21	128.04	120.79
3	P	255	LYS	C-N-CA	5.21	128.04	120.79
3	R	283	ARG	NE-CZ-NH2	5.21	123.89	119.20
5	Y	81	ARG	NE-CZ-NH2	5.21	123.89	119.20
1	A	662	PRO	N-CA-CB	5.21	106.11	103.19
2	E	157	GLN	OE1-CD-NE2	-5.20	117.40	122.60
5	X	217	ASP	CA-CB-CG	5.20	117.80	112.60
3	O	168	GLN	OE1-CD-NE2	-5.20	117.40	122.60
3	P	1139	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	R	13	ARG	NE-CZ-NH2	5.20	123.88	119.20
5	X	573	ARG	NE-CZ-NH2	5.20	123.88	119.20
5	Y	352	ARG	NE-CZ-NH2	5.20	123.88	119.20
3	Q	20	ARG	NE-CZ-NH2	5.19	123.87	119.20
3	O	809	LEU	CA-C-N	5.19	126.12	122.33
3	O	809	LEU	C-N-CA	5.19	126.12	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	S	342	GLU	N-CA-C	5.19	114.27	108.25
3	R	380	ILE	N-CA-CB	-5.19	107.46	112.65
3	S	37	ASN	OD1-CG-ND2	-5.18	117.42	122.60
5	Y	447	HIS	CB-CG-CD2	-5.18	124.46	131.20
3	P	113	ARG	NE-CZ-NH2	5.18	123.86	119.20
5	W	447	HIS	CB-CG-CD2	-5.18	124.47	131.20
3	R	427	ILE	CA-C-N	5.17	131.41	121.54
3	R	427	ILE	C-N-CA	5.17	131.41	121.54
3	R	200	PHE	CA-CB-CG	5.16	118.96	113.80
3	P	286	ARG	NE-CZ-NH1	-5.16	116.34	121.50
3	Q	1139	ARG	NE-CZ-NH2	5.16	123.84	119.20
3	O	451	PRO	CA-C-O	-5.15	115.72	121.23
4	T	55	ASP	CA-CB-CG	5.15	117.75	112.60
2	L	93	ALA	CA-C-N	5.15	127.49	120.54
2	L	93	ALA	C-N-CA	5.15	127.49	120.54
3	O	536	THR	CA-C-N	5.15	129.59	121.56
3	O	536	THR	C-N-CA	5.15	129.59	121.56
3	Q	453	SER	N-CA-C	5.14	121.75	110.80
1	A	364	PRO	N-CA-CB	5.14	106.07	103.19
3	R	94	ASP	CA-CB-CG	5.13	117.73	112.60
5	X	447	HIS	CB-CG-CD2	-5.13	124.53	131.20
3	Q	322	GLN	OE1-CD-NE2	-5.13	117.47	122.60
3	O	560	ARG	NE-CZ-NH1	-5.12	116.38	121.50
3	O	477	ARG	NE-CZ-NH2	5.12	123.81	119.20
2	F	80	TYR	CA-C-N	5.12	125.76	120.03
2	F	80	TYR	C-N-CA	5.12	125.76	120.03
3	N	761	ASN	CA-CB-CG	5.10	117.70	112.60
4	U	447	GLN	OE1-CD-NE2	-5.10	117.50	122.60
3	Q	529	SER	CA-C-N	5.09	129.29	120.58
3	Q	529	SER	C-N-CA	5.09	129.29	120.58
3	R	454	ASP	CA-CB-CG	5.09	117.69	112.60
3	O	776	THR	CA-CB-CG2	5.09	119.16	110.50
2	F	168	ARG	NE-CZ-NH2	5.09	123.78	119.20
3	O	423	GLY	N-CA-C	5.09	119.54	112.57
3	O	373	GLY	N-CA-C	5.08	120.58	110.77
3	Q	125	ASP	CA-CB-CG	-5.08	107.52	112.60
3	S	603	ASN	CA-CB-CG	5.08	117.68	112.60
3	Q	532	ASP	CA-CB-CG	5.07	117.67	112.60
3	Q	688	ARG	NE-CZ-NH2	5.07	123.76	119.20
3	O	725	SER	CA-C-N	5.07	130.42	122.21
3	O	725	SER	C-N-CA	5.07	130.42	122.21
5	W	352	ARG	NE-CZ-NH2	5.06	123.75	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	Q	408	ASP	CA-CB-CG	5.05	117.66	112.60
2	L	13	ALA	CA-C-N	5.05	127.55	120.28
2	L	13	ALA	C-N-CA	5.05	127.55	120.28
3	N	1128	ARG	NE-CZ-NH2	5.05	123.74	119.20
3	N	1143	ARG	NE-CZ-NH2	5.05	123.74	119.20
3	P	961	ARG	NE-CZ-NH2	5.04	123.74	119.20
4	V	55	ASP	CA-CB-CG	5.04	117.64	112.60
3	S	276	GLN	OE1-CD-NE2	-5.04	117.56	122.60
3	S	234	ARG	NE-CZ-NH2	5.03	123.73	119.20
3	Q	133	TYR	CA-C-N	5.03	131.15	121.54
3	Q	133	TYR	C-N-CA	5.03	131.15	121.54
1	A	533	ASN	CA-CB-CG	5.02	117.62	112.60
3	R	521	HIS	CA-CB-CG	-5.02	108.78	113.80
4	T	451	ARG	NE-CZ-NH2	5.02	123.72	119.20
3	N	560	ARG	CD-NE-CZ	5.01	131.42	124.40
2	H	9	HIS	CB-CG-CD2	-5.01	124.69	131.20
5	Y	173	PRO	N-CA-CB	5.01	108.00	103.34
3	N	1103	ALA	CA-C-N	5.01	128.97	120.81
3	N	1103	ALA	C-N-CA	5.01	128.97	120.81
2	K	101	VAL	CA-CB-CG1	5.00	118.91	110.40
3	O	547	LYS	CA-C-N	5.00	127.21	120.50
3	O	547	LYS	C-N-CA	5.00	127.21	120.50

There are no chirality outliers.

All (147) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	205	ARG	Sidechain
1	A	293	TYR	Sidechain
1	A	453	TYR	Sidechain
1	A	468	TYR	Sidechain
1	A	599	TYR	Sidechain
1	A	608	TYR	Sidechain
2	B	168	ARG	Sidechain
2	F	80	TYR	Sidechain
2	G	102	TYR	Sidechain
2	G	15	TYR	Sidechain
2	H	24	TYR	Sidechain
2	I	117	TYR	Sidechain
2	I	80	TYR	Sidechain
2	J	80	TYR	Sidechain
2	L	117	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	L	15	TYR	Sidechain
2	L	159	ARG	Sidechain
2	L	80	TYR	Sidechain
2	M	117	TYR	Sidechain
2	M	80	TYR	Sidechain
3	N	1062	TYR	Sidechain
3	N	1150	ARG	Sidechain
3	N	134	PHE	Sidechain
3	N	166	TYR	Sidechain
3	N	186	TYR	Sidechain
3	N	234	ARG	Sidechain
3	N	29	ARG	Sidechain
3	N	379	TYR	Sidechain
3	N	403	TYR	Sidechain
3	N	556	HIS	Sidechain
3	N	573	TYR	Sidechain
3	N	705	TYR	Sidechain
3	N	721	TYR	Sidechain
3	N	749	ARG	Sidechain
3	N	768	TYR	Sidechain
3	N	785	ARG	Sidechain
3	N	812	TYR	Sidechain
3	N	835	TYR	Sidechain
3	N	912	TYR	Sidechain
3	O	1004	TYR	Sidechain
3	O	1062	TYR	Sidechain
3	O	1066	ARG	Sidechain
3	O	1150	ARG	Sidechain
3	O	166	TYR	Sidechain
3	O	184	ARG	Sidechain
3	O	286	ARG	Sidechain
3	O	349	TYR	Sidechain
3	O	403	TYR	Sidechain
3	O	566	PHE	Sidechain
3	O	705	TYR	Sidechain
3	O	749	ARG	Sidechain
3	O	753	ARG	Sidechain
3	O	80	TYR	Sidechain
3	O	804	ARG	Sidechain
3	O	841	TYR	Sidechain
3	O	968	TYR	Sidechain
3	P	1014	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	P	13	ARG	Sidechain
3	P	166	TYR	Sidechain
3	P	192	TYR	Sidechain
3	P	286	ARG	Sidechain
3	P	29	ARG	Sidechain
3	P	353	TYR	Sidechain
3	P	355	TYR	Sidechain
3	P	365	TYR	Sidechain
3	P	400	TYR	Sidechain
3	P	483	TYR	Sidechain
3	P	712	ARG	Sidechain
3	P	783	ARG	Sidechain
3	P	804	ARG	Sidechain
3	P	835	TYR	Sidechain
3	P	90	TYR	Sidechain
3	P	968	TYR	Sidechain
3	Q	1062	TYR	Sidechain
3	Q	1083	TYR	Sidechain
3	Q	1143	ARG	Sidechain
3	Q	13	ARG	Sidechain
3	Q	134	PHE	Peptide
3	Q	166	TYR	Sidechain
3	Q	184	ARG	Sidechain
3	Q	186	TYR	Sidechain
3	Q	221	TYR	Sidechain
3	Q	286	ARG	Sidechain
3	Q	349	TYR	Sidechain
3	Q	403	TYR	Sidechain
3	Q	465	ARG	Sidechain
3	Q	528	PHE	Sidechain
3	Q	539	TYR	Sidechain
3	Q	586	TYR	Sidechain
3	Q	722	ARG	Sidechain
3	Q	80	TYR	Sidechain
3	Q	812	TYR	Sidechain
3	Q	864	TYR	Sidechain
3	Q	912	TYR	Sidechain
3	R	1062	TYR	Sidechain
3	R	1066	ARG	Sidechain
3	R	1083	TYR	Sidechain
3	R	1144	ARG	Sidechain
3	R	166	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	R	197	PHE	Sidechain
3	R	350	TYR	Sidechain
3	R	353	TYR	Sidechain
3	R	403	TYR	Sidechain
3	R	429	ARG	Sidechain
3	R	46	TYR	Sidechain
3	R	465	ARG	Sidechain
3	R	528	PHE	Sidechain
3	R	753	ARG	Sidechain
3	R	841	TYR	Sidechain
3	R	968	TYR	Sidechain
3	S	1128	ARG	Sidechain
3	S	166	TYR	Sidechain
3	S	171	ASN	Peptide
3	S	186	TYR	Sidechain
3	S	286	ARG	Sidechain
3	S	358	ARG	Sidechain
3	S	365	TYR	Sidechain
3	S	403	TYR	Sidechain
3	S	411	PHE	Sidechain
3	S	46	TYR	Sidechain
3	S	521	HIS	Sidechain
3	S	539	TYR	Sidechain
3	S	768	TYR	Sidechain
3	S	80	TYR	Sidechain
3	S	90	TYR	Sidechain
3	S	968	TYR	Sidechain
4	T	424	ARG	Sidechain
4	T	63	TYR	Sidechain
4	U	365	TYR	Sidechain
4	U	43	TYR	Sidechain
4	U	448	TYR	Sidechain
4	V	220	TYR	Sidechain
4	V	365	TYR	Sidechain
4	V	371	TYR	Sidechain
4	V	424	ARG	Sidechain
4	V	448	TYR	Sidechain
5	W	18	TYR	Sidechain
5	W	208	TYR	Sidechain
5	X	417	TYR	Sidechain
5	X	446	TYR	Sidechain
5	X	541	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	X	639	ARG	Sidechain
5	X	89	TYR	Sidechain
5	Y	184	ARG	Sidechain
5	Y	423	TYR	Sidechain
5	Y	5	TYR	Sidechain
5	Y	86	TYR	Sidechain

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	A	5070	0	4932	12	0
2	B	1280	0	1275	2	0
2	C	1270	0	1263	4	0
2	D	1278	0	1274	0	0
2	E	1350	0	1339	2	0
2	F	1199	0	1195	4	0
2	G	1350	0	1339	2	0
2	H	1350	0	1339	2	0
2	I	1350	0	1339	3	0
2	J	1350	0	1339	4	0
2	K	1350	0	1339	5	0
2	L	1350	0	1339	6	0
2	M	1350	0	1339	1	0
3	N	8364	0	8206	28	0
3	O	8364	0	8206	40	0
3	P	8364	0	8206	23	0
3	Q	8364	0	8206	20	0
3	R	8364	0	8206	28	0
3	S	8364	0	8206	27	0
4	T	3548	0	3468	3	0
4	U	3548	0	3468	3	0
4	V	3548	0	3468	1	0
5	W	5127	0	4969	7	0
5	X	5127	0	4969	6	0
5	Y	5127	0	4969	9	0
All	All	97106	0	95198	222	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 1.

All (222) 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)
3:Q:981:LYS:HA	3:Q:981:LYS:HE2	1.73	0.69
3:O:268:LYS:HB2	3:O:403:TYR:CZ	2.35	0.62
1:A:197:ILE:HD11	2:B:2:ALA:HA	1.81	0.61
3:S:147:LEU:HD23	3:S:148:THR:N	2.16	0.61
3:O:582:ASN:HA	3:O:889:THR:HG22	1.83	0.61
2:K:157:GLN:OE1	2:L:157:GLN:CG	2.50	0.59
3:N:981:LYS:HE3	3:N:997:LYS:C	2.28	0.58
2:K:157:GLN:OE1	2:L:157:GLN:HG2	2.03	0.58
3:R:981:LYS:HE3	3:R:998:TRP:CE2	2.39	0.58
1:A:460:TYR:CE1	2:F:162:GLN:HA	2.38	0.57
3:S:311:THR:HG23	3:S:317:THR:HG21	1.86	0.56
3:Q:103:LYS:HE3	3:Q:161:MET:SD	2.45	0.56
3:O:186:TYR:CD1	3:O:223:LYS:HE3	2.41	0.56
3:N:334:ILE:HD12	3:N:334:ILE:H	1.70	0.56
3:O:299:ASN:HA	3:O:332:GLN:HB3	1.88	0.56
3:O:981:LYS:HE3	3:O:998:TRP:CE2	2.41	0.55
2:B:29:LYS:HE3	2:B:33:TRP:CZ3	2.42	0.55
3:N:812:TYR:CZ	3:N:935:LYS:HE2	2.41	0.55
3:P:147:LEU:HD23	3:P:148:THR:N	2.22	0.54
3:S:1091:TRP:CD1	3:S:1128:ARG:HH21	2.24	0.54
5:W:476:ASP:O	5:W:480:ALA:HB3	2.08	0.54
2:I:101:VAL:HB	2:I:171:VAL:CG2	2.38	0.54
5:X:197:LYS:HE2	5:X:384:HIS:CE1	2.44	0.53
3:Q:470:ASP:HA	3:Q:473:LYS:HE2	1.91	0.53
3:Q:585:PRO:HG2	3:Q:586:TYR:CE2	2.44	0.53
2:L:116:THR:HG22	2:L:158:ASN:HA	1.91	0.53
5:X:476:ASP:O	5:X:480:ALA:HB3	2.09	0.52
3:Q:998:TRP:CD1	3:Q:1019:ARG:HH12	2.28	0.52
2:K:158:ASN:ND2	2:L:155:GLN:HB3	2.23	0.52
2:C:64:VAL:HG21	2:C:102:TYR:CD1	2.45	0.52
3:O:275:GLY:C	3:O:356:ASN:HA	2.35	0.52
3:S:273:VAL:HG22	3:S:365:TYR:CE2	2.45	0.52
3:N:465:ARG:HA	3:O:468:MET:SD	2.50	0.52
3:N:857:ALA:HB2	3:N:891:TRP:CD2	2.45	0.52
1:A:425:LYS:HG3	5:X:132:GLU:OE1	2.10	0.52
3:P:804:ARG:CG	3:P:804:ARG:HH21	2.23	0.51
3:R:365:TYR:CD1	3:R:380:ILE:HG23	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:O:355:TYR:CE2	3:O:357:LYS:HA	2.45	0.51
5:Y:573:ARG:HE	5:Y:590:GLU:CD	2.19	0.51
3:O:912:TYR:CZ	3:O:914:GLN:HB2	2.45	0.50
3:P:697:LEU:HD22	3:P:762:SER:HB3	1.94	0.50
3:O:857:ALA:HB2	3:O:891:TRP:CD2	2.47	0.50
4:V:308:HIS:CE1	4:V:327:GLY:H	2.30	0.50
3:R:603:ASN:CG	3:R:771:GLN:H	2.20	0.49
2:G:116:THR:HG22	2:G:158:ASN:HA	1.94	0.49
2:H:103:LEU:HD11	2:H:122:PHE:CD2	2.47	0.49
3:N:365:TYR:CG	3:N:380:ILE:HG23	2.48	0.49
3:Q:981:LYS:HE3	3:Q:998:TRP:HA	1.94	0.48
5:Y:476:ASP:O	5:Y:480:ALA:HB3	2.13	0.48
3:P:194:VAL:HG13	3:P:465:ARG:CZ	2.43	0.48
3:S:106:ILE:HG23	3:S:147:LEU:HD21	1.94	0.48
2:F:89:THR:HG22	2:F:90:PRO:HD2	1.95	0.48
2:L:147:THR:HG23	2:M:7:ASN:HB3	1.96	0.48
3:S:469:GLU:H	3:S:469:GLU:CD	2.20	0.48
2:C:29:LYS:HE3	2:C:33:TRP:CE3	2.49	0.48
3:Q:144:LYS:HE3	3:Q:144:LYS:HA	1.95	0.48
3:S:147:LEU:HD23	3:S:148:THR:H	1.79	0.47
3:R:306:LYS:HE3	3:R:308:TRP:CD2	2.49	0.47
1:A:470:GLU:CD	4:U:11:ASN:HD22	2.22	0.47
3:N:281:LYS:HE3	3:N:350:TYR:CD1	2.49	0.47
3:O:403:TYR:CG	3:O:452:ASP:HB2	2.50	0.47
5:W:573:ARG:HE	5:W:590:GLU:CD	2.22	0.47
1:A:508:ILE:HD12	1:A:696:ILE:HD13	1.96	0.47
2:J:101:VAL:HB	2:J:171:VAL:CG2	2.44	0.47
2:J:134:LYS:HE2	2:J:136:ASN:O	2.13	0.47
3:R:68:LEU:HD11	3:R:72:ASN:HA	1.95	0.47
4:T:158:THR:O	4:T:174:MET:HE3	2.15	0.47
3:N:981:LYS:HA	3:N:981:LYS:CE	2.44	0.47
3:P:377:LYS:HA	3:P:377:LYS:HE2	1.97	0.47
3:Q:33:GLN:NE2	3:S:27:PRO:HA	2.30	0.47
3:Q:580:THR:HG21	3:Q:814:ALA:CB	2.45	0.47
3:Q:580:THR:HG21	3:Q:814:ALA:HB3	1.97	0.47
3:N:603:ASN:HB2	3:N:775:LYS:HE2	1.95	0.46
3:N:981:LYS:HE3	3:N:997:LYS:O	2.16	0.46
1:A:136:LEU:HD22	3:O:33:GLN:HE21	1.80	0.46
3:O:273:VAL:HG11	3:O:365:TYR:CZ	2.50	0.46
1:A:460:TYR:CZ	2:F:162:GLN:C	2.93	0.46
3:O:70:GLU:H	3:O:70:GLU:CD	2.23	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:S:1069:TYR:CE2	3:S:1110:TYR:CD2	3.03	0.46
5:Y:18:TYR:CD1	5:Y:19:PRO:HD3	2.50	0.46
2:I:103:LEU:HD11	2:I:122:PHE:CD2	2.51	0.46
5:W:101:LYS:HB2	5:W:111:TRP:CE3	2.51	0.46
3:R:274:THR:O	3:R:396:VAL:HG13	2.16	0.46
3:S:857:ALA:HB2	3:S:891:TRP:CG	2.51	0.46
2:J:27:ILE:HD11	2:J:117:TYR:CE2	2.50	0.46
3:Q:336:TRP:C	3:Q:338:PRO:HD2	2.41	0.46
5:Y:473:ASP:HB3	5:Y:480:ALA:HB1	1.97	0.46
3:N:1085:ALA:HB1	3:N:1122:ASN:HD21	1.82	0.45
3:O:90:TYR:CD1	3:O:90:TYR:C	2.95	0.45
3:S:186:TYR:HA	3:S:190:GLY:HA3	1.97	0.45
3:S:791:VAL:C	3:S:793:PRO:HD3	2.42	0.45
3:S:511:PHE:CD2	3:S:1143:ARG:HA	2.51	0.45
3:S:992:THR:H	3:S:995:GLN:NE2	2.14	0.45
3:O:376:LYS:HE2	3:O:378:TRP:CH2	2.52	0.45
3:P:243:LEU:HG	3:P:403:TYR:CE2	2.52	0.45
3:O:186:TYR:CG	3:O:223:LYS:HE3	2.52	0.45
2:I:150:PHE:CZ	2:I:171:VAL:HG11	2.52	0.45
3:N:244:GLY:H	3:N:403:TYR:HA	1.81	0.45
3:S:588:ILE:HG13	3:S:792:ASP:H	1.81	0.45
4:U:225:LYS:HE3	4:U:226:GLU:O	2.17	0.45
3:Q:1026:ARG:HD2	3:Q:1027:TYR:CE2	2.52	0.45
5:X:552:SER:HB3	5:X:576:ASN:CG	2.42	0.45
3:N:787:THR:HG23	3:N:839:THR:HA	1.98	0.44
3:Q:981:LYS:HE3	3:Q:997:LYS:O	2.17	0.44
3:R:812:TYR:CE2	3:R:935:LYS:HE2	2.51	0.44
5:Y:275:TYR:CE2	5:Y:325:LYS:HE3	2.53	0.44
3:O:301:ALA:HA	3:O:355:TYR:HA	1.99	0.44
3:S:268:LYS:HE3	3:S:268:LYS:HA	2.00	0.44
3:N:336:TRP:C	3:N:338:PRO:HD2	2.42	0.44
3:O:697:LEU:HD22	3:O:762:SER:HB3	2.00	0.44
3:S:365:TYR:CE2	3:S:380:ILE:HG21	2.52	0.44
3:N:812:TYR:CE1	3:N:935:LYS:HE2	2.51	0.44
3:O:103:LYS:HE3	3:O:161:MET:SD	2.58	0.44
3:O:833:GLN:CD	3:O:833:GLN:N	2.76	0.44
3:R:281:LYS:HE2	3:R:350:TYR:CE1	2.52	0.44
4:U:5:PHE:CG	4:U:6:THR:N	2.86	0.44
3:O:791:VAL:H	3:O:923:ALA:HB3	1.82	0.44
3:N:1101:THR:HG22	3:N:1102:ARG:O	2.18	0.43
3:R:200:PHE:HA	3:R:458:CYS:SG	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:W:431:ASN:CG	5:X:206:THR:HA	2.43	0.43
3:O:266:PRO:HG3	3:O:451:PRO:O	2.19	0.43
1:A:459:ASN:HB2	2:E:169:PHE:CE2	2.53	0.43
3:N:171:ASN:HA	3:O:833:GLN:HA	2.00	0.43
3:O:833:GLN:CD	3:O:833:GLN:H	2.26	0.43
3:P:171:ASN:C	3:P:173:GLU:H	2.26	0.43
3:P:1011:GLY:HA2	3:P:1137:PHE:CE2	2.52	0.43
3:Q:869:MET:HE1	3:Q:871:ALA:HB2	2.00	0.43
3:R:18:LYS:HE3	3:R:18:LYS:HA	2.00	0.43
3:R:692:PHE:CD1	3:R:692:PHE:C	2.96	0.43
3:R:833:GLN:CD	3:R:833:GLN:H	2.27	0.43
3:O:281:LYS:HE2	3:O:350:TYR:CD1	2.53	0.43
3:O:403:TYR:CZ	3:O:452:ASP:CG	2.96	0.43
3:R:281:LYS:HE2	3:R:350:TYR:CD1	2.53	0.43
3:N:70:GLU:N	3:N:70:GLU:CD	2.77	0.43
3:S:336:TRP:CH2	3:S:343:PRO:HD3	2.54	0.43
5:W:473:ASP:HB3	5:W:480:ALA:HB1	2.01	0.43
5:X:263:GLU:H	5:X:263:GLU:CD	2.26	0.43
3:P:268:LYS:HE3	3:P:268:LYS:HA	2.00	0.43
3:O:793:PRO:HG2	3:O:926:TRP:CZ3	2.53	0.43
3:P:1137:PHE:CD1	3:P:1137:PHE:N	2.85	0.43
3:R:88:ARG:HG2	3:R:88:ARG:HH21	1.82	0.43
3:P:812:TYR:CE2	3:P:935:LYS:HE2	2.54	0.43
1:A:459:ASN:OD1	2:E:154:LYS:HE2	2.19	0.43
3:P:409:SER:HB3	3:P:411:PHE:CZ	2.54	0.43
3:Q:562:ILE:HD11	3:Q:1034:SER:HB3	2.00	0.43
3:R:90:TYR:HA	3:R:145:MET:HE1	2.00	0.43
3:R:687:ILE:HD11	3:R:746:ALA:HA	2.01	0.42
1:A:495:LYS:HB2	1:A:734:TRP:CH2	2.54	0.42
2:K:24:TYR:HB2	2:K:126:LEU:HD21	2.01	0.42
3:N:1069:TYR:CE1	3:N:1110:TYR:HB2	2.55	0.42
3:O:793:PRO:CG	3:O:926:TRP:CH2	3.02	0.42
3:S:945:GLU:N	3:S:945:GLU:CD	2.77	0.42
3:N:302:PHE:CZ	3:N:354:LYS:HB3	2.54	0.42
3:O:945:GLU:N	3:O:945:GLU:CD	2.77	0.42
3:O:987:MET:SD	3:O:991:THR:HG21	2.59	0.42
3:R:403:TYR:HB2	3:R:451:PRO:HB3	2.01	0.42
3:S:90:TYR:CD2	3:S:90:TYR:C	2.97	0.42
1:A:265:TYR:CE2	1:A:285:ARG:HD3	2.55	0.42
2:G:24:TYR:CE1	2:G:126:LEU:HD11	2.54	0.42
2:H:26:THR:HB	2:H:55:TYR:CD2	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:749:ARG:NH1	3:P:200:PHE:CG	2.87	0.42
5:W:623:TRP:CE2	5:Y:581:SER:HB3	2.54	0.42
2:C:32:PRO:HA	2:C:118:ARG:NE	2.34	0.42
3:P:833:GLN:CD	3:P:833:GLN:H	2.28	0.42
3:Q:721:TYR:CE1	3:Q:738:ALA:HA	2.54	0.42
3:Q:239:LYS:HE2	3:Q:453:SER:O	2.20	0.42
4:T:441:VAL:HG12	4:T:443:ASN:H	1.85	0.42
2:K:75:LYS:HE3	2:K:86:VAL:HG21	2.02	0.42
3:R:246:ALA:HB3	3:R:400:TYR:CD1	2.55	0.42
3:R:296:LEU:HD22	3:R:353:TYR:CE1	2.54	0.42
3:S:271:ARG:O	3:S:359:MET:HE3	2.20	0.42
3:N:970:THR:HG22	3:N:1030:PRO:HB3	2.02	0.42
3:P:505:SER:HB3	3:P:1057:MET:HE1	2.02	0.42
3:R:380:ILE:HG22	3:R:382:PHE:CZ	2.55	0.42
3:P:68:LEU:HD11	3:P:72:ASN:HA	2.01	0.42
3:P:171:ASN:C	3:P:173:GLU:N	2.78	0.41
3:Q:296:LEU:HG	3:Q:334:ILE:HD11	2.02	0.41
2:J:101:VAL:HB	2:J:171:VAL:HG22	2.03	0.41
3:O:832:ASP:CG	3:O:833:GLN:HE22	2.28	0.41
3:R:27:PRO:HA	3:S:33:GLN:NE2	2.35	0.41
3:R:277:VAL:HG12	3:R:278:LEU:H	1.85	0.41
3:R:1066:ARG:HH21	3:R:1066:ARG:HG2	1.85	0.41
1:A:150:ILE:HG21	1:A:154:PHE:HB3	2.02	0.41
2:F:29:LYS:HE3	2:F:33:TRP:CE3	2.55	0.41
3:P:260:ILE:HG21	3:P:396:VAL:HG21	2.02	0.41
3:R:66:PHE:CD1	3:R:74:LEU:HD11	2.56	0.41
4:T:371:TYR:CE2	4:T:390:CYS:HB2	2.55	0.41
3:N:708:PHE:CD2	3:N:755:VAL:HG22	2.55	0.41
3:O:808:SER:HB3	3:O:864:TYR:CE2	2.56	0.41
3:O:945:GLU:CD	3:O:945:GLU:H	2.28	0.41
3:P:793:PRO:CG	3:P:926:TRP:CH2	3.03	0.41
5:W:566:THR:HA	5:Y:556:PHE:CD2	2.56	0.41
3:N:721:TYR:CE1	3:N:738:ALA:HA	2.56	0.41
3:P:687:ILE:HD12	3:P:687:ILE:H	1.86	0.41
3:S:403:TYR:CD1	3:S:452:ASP:HB2	2.55	0.41
3:O:88:ARG:HG2	3:O:88:ARG:HH21	1.85	0.41
3:O:273:VAL:HG11	3:O:365:TYR:CE2	2.56	0.41
3:P:562:ILE:HD11	3:P:1034:SER:HB3	2.01	0.41
3:P:591:LYS:HE3	3:P:698:ASN:OD1	2.20	0.41
2:C:78:ILE:HD12	2:C:78:ILE:N	2.35	0.41
3:N:286:ARG:HH22	3:N:292:GLY:C	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:N:588:ILE:HD12	3:N:883:THR:O	2.20	0.41
3:O:266:PRO:HA	3:O:378:TRP:CZ3	2.56	0.41
3:O:354:LYS:HE2	3:O:391:ILE:HD12	2.02	0.41
3:O:403:TYR:CD1	3:O:452:ASP:HB2	2.56	0.41
3:Q:308:TRP:CD1	3:Q:316:THR:HG1	2.38	0.41
3:S:274:THR:HB	3:S:397:LEU:H	1.86	0.41
3:R:1091:TRP:CD1	3:R:1128:ARG:HH21	2.38	0.41
5:Y:381:PHE:CD1	5:Y:381:PHE:C	2.99	0.41
3:P:603:ASN:O	3:P:775:LYS:HE2	2.20	0.40
3:Q:1050:TYR:CD1	3:Q:1050:TYR:C	2.99	0.40
3:S:1011:GLY:HA2	3:S:1137:PHE:CZ	2.56	0.40
5:Y:592:TYR:CE2	5:Y:605:MET:HB3	2.56	0.40
3:O:983:ILE:HA	3:O:987:MET:SD	2.61	0.40
3:N:841:TYR:HB3	3:N:869:MET:SD	2.61	0.40
3:N:1125:LEU:HD11	3:N:1127:VAL:HG13	2.03	0.40
3:R:286:ARG:HH12	3:R:292:GLY:N	2.19	0.40
3:R:802:GLU:CD	3:R:804:ARG:HH22	2.30	0.40
3:S:68:LEU:HD11	3:S:72:ASN:HA	2.04	0.40
2:L:101:VAL:HB	2:L:171:VAL:HG22	2.02	0.40
3:R:603:ASN:ND2	3:R:771:GLN:H	2.20	0.40
3:S:793:PRO:HG2	3:S:926:TRP:CH2	2.57	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	A	620/1019 (61%)	590 (95%)	28 (4%)	2 (0%)	36	72
2	B	159/173 (92%)	155 (98%)	4 (2%)	0	100	100
2	C	158/173 (91%)	153 (97%)	4 (2%)	1 (1%)	21	58
2	D	159/173 (92%)	152 (96%)	7 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	E	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
2	F	146/173 (84%)	138 (94%)	8 (6%)	0	100	100
2	G	170/173 (98%)	157 (92%)	11 (6%)	2 (1%)	10	42
2	H	170/173 (98%)	152 (89%)	16 (9%)	2 (1%)	10	42
2	I	170/173 (98%)	161 (95%)	8 (5%)	1 (1%)	21	58
2	J	170/173 (98%)	161 (95%)	9 (5%)	0	100	100
2	K	170/173 (98%)	162 (95%)	8 (5%)	0	100	100
2	L	170/173 (98%)	159 (94%)	10 (6%)	1 (1%)	21	58
2	M	170/173 (98%)	161 (95%)	7 (4%)	2 (1%)	10	42
3	N	1056/1152 (92%)	927 (88%)	112 (11%)	17 (2%)	7	36
3	O	1056/1152 (92%)	943 (89%)	96 (9%)	17 (2%)	7	36
3	P	1056/1152 (92%)	962 (91%)	80 (8%)	14 (1%)	9	40
3	Q	1056/1152 (92%)	943 (89%)	88 (8%)	25 (2%)	4	26
3	R	1056/1152 (92%)	941 (89%)	100 (10%)	15 (1%)	9	38
3	S	1056/1152 (92%)	945 (90%)	99 (9%)	12 (1%)	11	45
4	T	456/458 (100%)	429 (94%)	25 (6%)	2 (0%)	30	67
4	U	456/458 (100%)	439 (96%)	17 (4%)	0	100	100
4	V	456/458 (100%)	438 (96%)	18 (4%)	0	100	100
5	W	638/640 (100%)	611 (96%)	27 (4%)	0	100	100
5	X	638/640 (100%)	601 (94%)	36 (6%)	1 (0%)	43	78
5	Y	638/640 (100%)	598 (94%)	38 (6%)	2 (0%)	36	72
All	All	12220/13301 (92%)	11240 (92%)	864 (7%)	116 (1%)	16	50

All (116) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	G	93	ALA
2	H	93	ALA
2	I	93	ALA
2	L	93	ALA
3	N	997	LYS
3	O	452	ASP
3	O	791	VAL
3	P	189	SER
3	P	190	GLY

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Mol	Chain	Res	Type
3	Q	337	SER
3	Q	589	PRO
3	Q	773	ARG
3	Q	791	VAL
3	Q	973	ARG
3	Q	997	LYS
3	R	452	ASP
3	S	171	ASN
3	S	190	GLY
1	A	694	ASN
2	M	93	ALA
3	N	172	ALA
3	N	332	GLN
3	N	337	SER
3	N	453	SER
3	N	784	THR
3	N	791	VAL
3	N	793	PRO
3	N	973	ARG
3	O	426	ASN
3	O	760	ALA
3	P	171	ASN
3	P	173	GLU
3	P	275	GLY
3	Q	4	ASN
3	Q	242	ASP
3	Q	426	ASN
3	Q	428	MET
3	Q	697	LEU
3	Q	793	PRO
3	Q	913	LEU
3	Q	922	ASN
3	Q	930	GLN
3	R	428	MET
3	R	453	SER
3	R	972	GLU
3	S	173	GLU
3	S	388	ALA
3	S	922	ASN
3	S	973	ARG
2	C	98	ALA
3	N	697	LEU

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Mol	Chain	Res	Type
3	O	276	GLN
3	P	205	ALA
3	P	388	ALA
3	P	389	LYS
3	P	973	ARG
3	Q	2	ALA
3	Q	733	ASP
3	R	242	ASP
3	R	388	ALA
3	R	426	ASN
3	R	760	ALA
3	R	791	VAL
3	R	793	PRO
3	R	930	GLN
3	S	189	SER
3	S	760	ALA
4	T	445	LYS
2	M	73	ASP
3	N	330	ASP
3	N	414	LYS
3	N	426	ASN
3	N	922	ASN
3	O	376	LYS
3	O	388	ALA
3	P	282	GLU
3	P	426	ASN
3	Q	27	PRO
3	Q	217	ALA
3	S	773	ARG
5	Y	246	GLY
2	G	98	ALA
2	H	70	PRO
3	O	223	LYS
3	O	332	GLN
3	O	435	LEU
3	O	453	SER
3	O	922	ASN
3	O	972	GLU
3	P	133	TYR
3	P	760	ALA
3	Q	332	GLN
3	Q	384	PRO

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Mol	Chain	Res	Type
3	Q	453	SER
3	R	337	SER
3	R	382	PHE
3	R	922	ASN
3	S	559	GLY
3	S	697	LEU
5	X	598	ARG
3	N	242	ASP
3	N	953	PRO
3	O	205	ALA
3	O	431	VAL
3	Q	389	LYS
3	R	515	ASP
5	Y	374	LYS
3	O	27	PRO
3	Q	1076	GLY
3	N	874	GLY
3	Q	559	GLY
4	T	126	ILE
1	A	550	ILE
3	O	425	PRO
3	S	390	PRO
3	P	337	SER

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	573/928 (62%)	568 (99%)	5 (1%)	70	77
2	B	143/153 (94%)	141 (99%)	2 (1%)	59	72
2	C	142/153 (93%)	141 (99%)	1 (1%)	76	80
2	D	143/153 (94%)	143 (100%)	0	100	100
2	E	152/153 (99%)	150 (99%)	2 (1%)	61	73
2	F	134/153 (88%)	132 (98%)	2 (2%)	57	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	152/153 (99%)	146 (96%)	6 (4%)	28	49
2	H	152/153 (99%)	138 (91%)	14 (9%)	8	27
2	I	152/153 (99%)	143 (94%)	9 (6%)	18	39
2	J	152/153 (99%)	143 (94%)	9 (6%)	18	39
2	K	152/153 (99%)	141 (93%)	11 (7%)	13	34
2	L	152/153 (99%)	142 (93%)	10 (7%)	15	37
2	M	152/153 (99%)	141 (93%)	11 (7%)	13	34
3	N	934/1010 (92%)	881 (94%)	53 (6%)	18	40
3	O	934/1010 (92%)	868 (93%)	66 (7%)	13	35
3	P	934/1010 (92%)	883 (94%)	51 (6%)	19	41
3	Q	934/1010 (92%)	887 (95%)	47 (5%)	22	43
3	R	934/1010 (92%)	863 (92%)	71 (8%)	12	32
3	S	934/1010 (92%)	867 (93%)	67 (7%)	13	34
4	T	405/405 (100%)	401 (99%)	4 (1%)	68	77
4	U	405/405 (100%)	403 (100%)	2 (0%)	81	82
4	V	405/405 (100%)	404 (100%)	1 (0%)	87	86
5	W	577/577 (100%)	572 (99%)	5 (1%)	70	77
5	X	577/577 (100%)	568 (98%)	9 (2%)	55	69
5	Y	577/577 (100%)	570 (99%)	7 (1%)	63	74
All	All	10901/11770 (93%)	10436 (96%)	465 (4%)	27	47

All (465) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	PHE
1	A	143	PHE
1	A	201	GLN
1	A	506	SER
1	A	718	THR
2	B	129	LYS
2	B	157	GLN
2	C	78	ILE
2	E	51	GLU
2	E	75	LYS
2	F	41	GLN

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Mol	Chain	Res	Type
2	F	89	THR
2	G	75	LYS
2	G	78	ILE
2	G	88	VAL
2	G	101	VAL
2	G	127	VAL
2	G	143	GLU
2	H	51	GLU
2	H	68	LYS
2	H	75	LYS
2	H	88	VAL
2	H	99	LYS
2	H	101	VAL
2	H	111	GLU
2	H	125	ASP
2	H	136	ASN
2	H	143	GLU
2	H	155	GLN
2	H	156	PHE
2	H	157	GLN
2	H	162	GLN
2	I	27	ILE
2	I	44	GLU
2	I	45	ASN
2	I	50	GLN
2	I	51	GLU
2	I	88	VAL
2	I	101	VAL
2	I	127	VAL
2	I	157	GLN
2	J	27	ILE
2	J	88	VAL
2	J	101	VAL
2	J	111	GLU
2	J	125	ASP
2	J	127	VAL
2	J	135	PHE
2	J	136	ASN
2	J	142	VAL
2	K	7	ASN
2	K	27	ILE
2	K	44	GLU

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Mol	Chain	Res	Type
2	K	45	ASN
2	K	51	GLU
2	K	88	VAL
2	K	101	VAL
2	K	125	ASP
2	K	127	VAL
2	K	161	GLU
2	K	168	ARG
2	L	41	GLN
2	L	45	ASN
2	L	51	GLU
2	L	68	LYS
2	L	78	ILE
2	L	88	VAL
2	L	101	VAL
2	L	125	ASP
2	L	143	GLU
2	L	157	GLN
2	M	27	ILE
2	M	44	GLU
2	M	45	ASN
2	M	51	GLU
2	M	88	VAL
2	M	101	VAL
2	M	125	ASP
2	M	127	VAL
2	M	136	ASN
2	M	142	VAL
2	M	161	GLU
3	N	64	LEU
3	N	70	GLU
3	N	75	THR
3	N	88	ARG
3	N	91	ASP
3	N	92	ASN
3	N	93	ASP
3	N	94	ASP
3	N	119	GLU
3	N	134	PHE
3	N	139	ASP
3	N	167	ILE
3	N	174	MET

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Mol	Chain	Res	Type
3	N	186	TYR
3	N	258	ASN
3	N	260	ILE
3	N	268	LYS
3	N	269	GLU
3	N	294	ASP
3	N	334	ILE
3	N	363	LYS
3	N	377	LYS
3	N	448	THR
3	N	449	VAL
3	N	453	SER
3	N	531	GLU
3	N	540	THR
3	N	562	ILE
3	N	574	GLN
3	N	579	GLU
3	N	603	ASN
3	N	604	TRP
3	N	701	ASP
3	N	756	THR
3	N	773	ARG
3	N	776	THR
3	N	779	ASP
3	N	787	THR
3	N	793	PRO
3	N	818	ASP
3	N	833	GLN
3	N	866	ASP
3	N	887	ASP
3	N	981	LYS
3	N	997	LYS
3	N	999	GLU
3	N	1022	PHE
3	N	1023	GLU
3	N	1075	LYS
3	N	1087	ASP
3	N	1121	THR
3	N	1127	VAL
3	N	1137	PHE
3	O	1	MET
3	O	27	PRO

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Mol	Chain	Res	Type
3	O	70	GLU
3	O	88	ARG
3	O	103	LYS
3	O	115	VAL
3	O	139	ASP
3	O	168	GLN
3	O	180	VAL
3	O	183	GLU
3	O	248	ASN
3	O	249	GLU
3	O	258	ASN
3	O	294	ASP
3	O	359	MET
3	O	367	VAL
3	O	383	THR
3	O	391	ILE
3	O	430	LEU
3	O	432	THR
3	O	454	ASP
3	O	465	ARG
3	O	470	ASP
3	O	472	GLN
3	O	498	GLN
3	O	519	ILE
3	O	541	GLU
3	O	547	LYS
3	O	560	ARG
3	O	574	GLN
3	O	579	GLU
3	O	582	ASN
3	O	601	GLU
3	O	723	LYS
3	O	729	THR
3	O	754	GLU
3	O	756	THR
3	O	776	THR
3	O	779	ASP
3	O	790	LEU
3	O	799	GLN
3	O	801	ASP
3	O	802	GLU
3	O	804	ARG

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Mol	Chain	Res	Type
3	O	839	THR
3	O	850	ASP
3	O	876	GLU
3	O	887	ASP
3	O	910	ASN
3	O	942	LYS
3	O	945	GLU
3	O	970	THR
3	O	973	ARG
3	O	986	ASP
3	O	994	ASP
3	O	1006	ASP
3	O	1026	ARG
3	O	1027	TYR
3	O	1041	THR
3	O	1045	GLU
3	O	1066	ARG
3	O	1075	LYS
3	O	1087	ASP
3	O	1101	THR
3	O	1134	GLU
3	O	1137	PHE
3	P	64	LEU
3	P	67	THR
3	P	75	THR
3	P	118	ASP
3	P	119	GLU
3	P	139	ASP
3	P	161	MET
3	P	169	SER
3	P	171	ASN
3	P	188	GLU
3	P	200	PHE
3	P	223	LYS
3	P	234	ARG
3	P	248	ASN
3	P	268	LYS
3	P	269	GLU
3	P	273	VAL
3	P	274	THR
3	P	277	VAL
3	P	281	LYS

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Mol	Chain	Res	Type
3	P	291	ASP
3	P	294	ASP
3	P	299	ASN
3	P	329	THR
3	P	357	LYS
3	P	363	LYS
3	P	364	ASP
3	P	469	GLU
3	P	552	ASP
3	P	574	GLN
3	P	588	ILE
3	P	604	TRP
3	P	701	ASP
3	P	727	ASP
3	P	753	ARG
3	P	767	THR
3	P	775	LYS
3	P	780	ILE
3	P	782	ILE
3	P	783	ARG
3	P	785	ARG
3	P	787	THR
3	P	792	ASP
3	P	799	GLN
3	P	804	ARG
3	P	910	ASN
3	P	973	ARG
3	P	1010	LEU
3	P	1075	LYS
3	P	1087	ASP
3	P	1137	PHE
3	Q	18	LYS
3	Q	27	PRO
3	Q	70	GLU
3	Q	103	LYS
3	Q	127	THR
3	Q	130	VAL
3	Q	139	ASP
3	Q	144	LYS
3	Q	174	MET
3	Q	186	TYR
3	Q	223	LYS

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Mol	Chain	Res	Type
3	Q	258	ASN
3	Q	268	LYS
3	Q	269	GLU
3	Q	282	GLU
3	Q	294	ASP
3	Q	305	VAL
3	Q	358	ARG
3	Q	363	LYS
3	Q	370	GLN
3	Q	383	THR
3	Q	455	GLU
3	Q	532	ASP
3	Q	601	GLU
3	Q	603	ASN
3	Q	604	TRP
3	Q	729	THR
3	Q	756	THR
3	Q	780	ILE
3	Q	787	THR
3	Q	793	PRO
3	Q	818	ASP
3	Q	833	GLN
3	Q	853	VAL
3	Q	876	GLU
3	Q	887	ASP
3	Q	910	ASN
3	Q	942	LYS
3	Q	973	ARG
3	Q	981	LYS
3	Q	987	MET
3	Q	997	LYS
3	Q	999	GLU
3	Q	1014	ARG
3	Q	1042	PHE
3	Q	1075	LYS
3	Q	1087	ASP
3	R	18	LYS
3	R	35	GLU
3	R	67	THR
3	R	92	ASN
3	R	171	ASN
3	R	176	LYS

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Mol	Chain	Res	Type
3	R	184	ARG
3	R	226	LYS
3	R	248	ASN
3	R	249	GLU
3	R	258	ASN
3	R	269	GLU
3	R	294	ASP
3	R	308	TRP
3	R	324	GLU
3	R	359	MET
3	R	364	ASP
3	R	370	GLN
3	R	383	THR
3	R	432	THR
3	R	452	ASP
3	R	454	ASP
3	R	464	THR
3	R	465	ARG
3	R	470	ASP
3	R	506	VAL
3	R	512	ILE
3	R	515	ASP
3	R	516	LYS
3	R	532	ASP
3	R	552	ASP
3	R	574	GLN
3	R	588	ILE
3	R	592	GLN
3	R	601	GLU
3	R	604	TRP
3	R	700	ASN
3	R	727	ASP
3	R	754	GLU
3	R	756	THR
3	R	761	ASN
3	R	776	THR
3	R	779	ASP
3	R	790	LEU
3	R	801	ASP
3	R	802	GLU
3	R	818	ASP
3	R	846	MET

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Mol	Chain	Res	Type
3	R	850	ASP
3	R	852	LYS
3	R	876	GLU
3	R	884	GLU
3	R	885	ASN
3	R	902	LYS
3	R	942	LYS
3	R	945	GLU
3	R	955	LYS
3	R	957	VAL
3	R	967	THR
3	R	970	THR
3	R	973	ARG
3	R	985	ASP
3	R	994	ASP
3	R	1009	VAL
3	R	1026	ARG
3	R	1036	ASP
3	R	1066	ARG
3	R	1075	LYS
3	R	1087	ASP
3	R	1106	GLU
3	R	1134	GLU
3	S	28	ASP
3	S	35	GLU
3	S	39	MET
3	S	118	ASP
3	S	127	THR
3	S	139	ASP
3	S	169	SER
3	S	171	ASN
3	S	176	LYS
3	S	177	ILE
3	S	183	GLU
3	S	188	GLU
3	S	200	PHE
3	S	223	LYS
3	S	234	ARG
3	S	248	ASN
3	S	256	SER
3	S	265	SER
3	S	268	LYS

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Mol	Chain	Res	Type
3	S	269	GLU
3	S	273	VAL
3	S	274	THR
3	S	291	ASP
3	S	294	ASP
3	S	308	TRP
3	S	329	THR
3	S	363	LYS
3	S	377	LYS
3	S	427	ILE
3	S	443	GLN
3	S	453	SER
3	S	455	GLU
3	S	469	GLU
3	S	520	THR
3	S	560	ARG
3	S	571	THR
3	S	574	GLN
3	S	579	GLU
3	S	587	ASN
3	S	588	ILE
3	S	601	GLU
3	S	604	TRP
3	S	684	PHE
3	S	700	ASN
3	S	729	THR
3	S	756	THR
3	S	776	THR
3	S	779	ASP
3	S	783	ARG
3	S	787	THR
3	S	818	ASP
3	S	822	ASN
3	S	852	LYS
3	S	867	ASP
3	S	875	LYS
3	S	910	ASN
3	S	942	LYS
3	S	945	GLU
3	S	970	THR
3	S	973	ARG
3	S	997	LYS

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Mol	Chain	Res	Type
3	S	1010	LEU
3	S	1042	PHE
3	S	1075	LYS
3	S	1078	LYS
3	S	1087	ASP
3	S	1106	GLU
4	T	41	LEU
4	T	94	MET
4	T	192	ASP
4	T	403	CYS
4	U	192	ASP
4	U	378	GLU
4	V	192	ASP
5	W	10	GLU
5	W	169	VAL
5	W	244	ASP
5	W	330	PHE
5	W	563	ILE
5	X	18	TYR
5	X	93	TYR
5	X	169	VAL
5	X	208	TYR
5	X	244	ASP
5	X	290	TYR
5	X	330	PHE
5	X	361	ASN
5	X	563	ILE
5	Y	17	MET
5	Y	244	ASP
5	Y	277	LYS
5	Y	330	PHE
5	Y	563	ILE
5	Y	576	ASN
5	Y	639	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (103) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	147	ASN
1	A	236	ASN
1	A	320	ASN

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Mol	Chain	Res	Type
1	A	414	ASN
2	B	9	HIS
2	B	157	GLN
2	C	7	ASN
2	D	7	ASN
2	E	82	ASN
2	F	41	GLN
2	G	7	ASN
2	G	119	GLN
2	G	153	ASN
2	G	158	ASN
2	H	7	ASN
2	H	153	ASN
2	I	9	HIS
2	I	119	GLN
2	I	153	ASN
2	J	9	HIS
2	J	119	GLN
2	J	153	ASN
2	J	158	ASN
2	L	7	ASN
2	L	119	GLN
2	L	153	ASN
2	M	7	ASN
2	M	92	ASN
2	M	162	GLN
3	N	49	ASN
3	N	168	GLN
3	N	257	ASN
3	N	393	GLN
3	N	480	ASN
3	N	484	ASN
3	N	576	GLN
3	N	771	GLN
3	N	778	GLN
3	N	833	GLN
3	N	914	GLN
3	O	37	ASN
3	O	61	GLN
3	O	258	ASN
3	O	381	ASN
3	O	582	ASN

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Mol	Chain	Res	Type
3	O	587	ASN
3	O	799	GLN
3	O	914	GLN
3	O	931	ASN
3	P	49	ASN
3	P	289	GLN
3	P	393	GLN
3	P	587	ASN
3	P	944	ASN
3	P	1126	GLN
3	Q	77	ASN
3	Q	257	ASN
3	Q	441	ASN
3	Q	484	ASN
3	Q	930	GLN
3	Q	944	ASN
3	R	171	ASN
3	R	257	ASN
3	R	381	ASN
3	R	441	ASN
3	R	485	GLN
3	R	778	GLN
3	R	799	GLN
3	R	910	ASN
3	R	930	GLN
3	S	332	GLN
3	S	386	ASN
3	S	443	GLN
3	S	576	GLN
3	S	820	GLN
3	S	995	GLN
3	S	1015	GLN
4	T	102	HIS
4	T	442	GLN
4	U	11	ASN
4	U	102	HIS
4	U	145	GLN
4	U	291	ASN
4	U	320	ASN
4	V	102	HIS
4	V	145	GLN
4	V	320	ASN

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Mol	Chain	Res	Type
4	V	391	HIS
5	W	189	GLN
5	W	579	ASN
5	W	602	GLN
5	X	57	ASN
5	X	145	ASN
5	X	189	GLN
5	X	335	ASN
5	X	431	ASN
5	X	444	GLN
5	X	568	ASN
5	Y	126	ASN
5	Y	139	GLN
5	Y	345	ASN
5	Y	624	ASN

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.

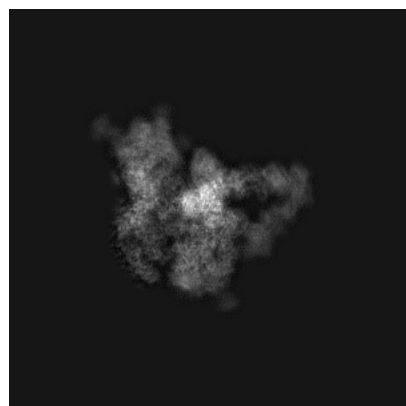
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55961. These allow visual inspection of the internal detail of the map and identification of artifacts.

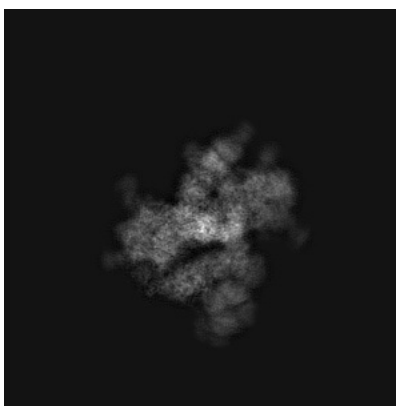
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

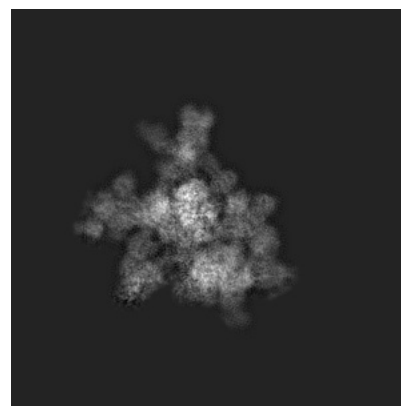
6.1.1 Primary map



X

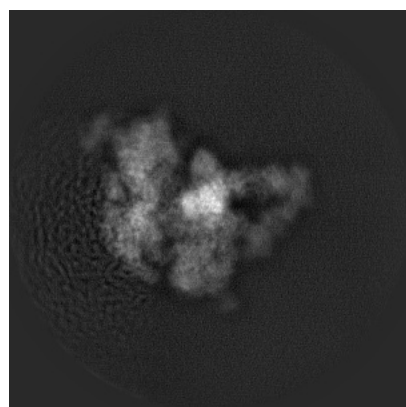


Y

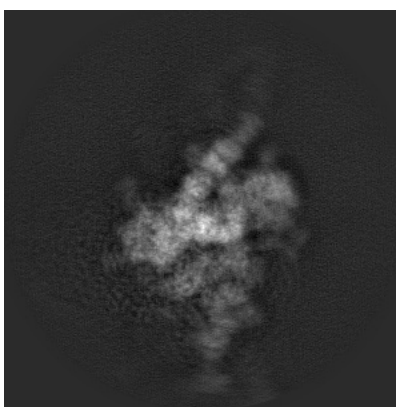


Z

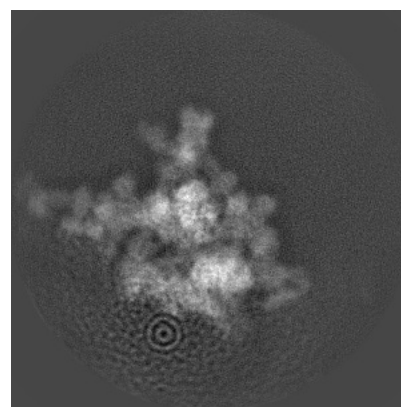
6.1.2 Raw map



X



Y



Z

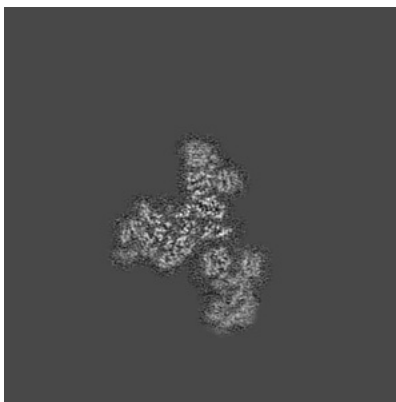
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

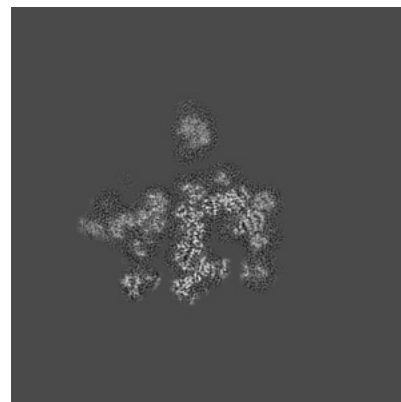
6.2.1 Primary map



X Index: 180

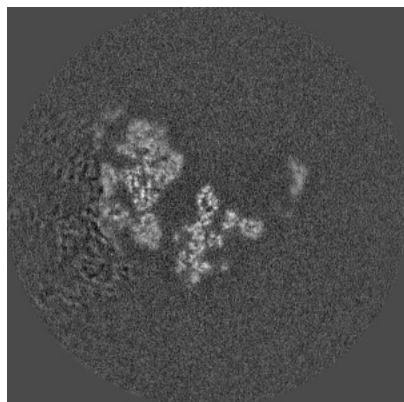


Y Index: 180

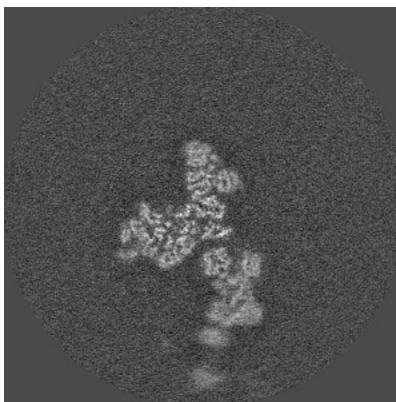


Z Index: 180

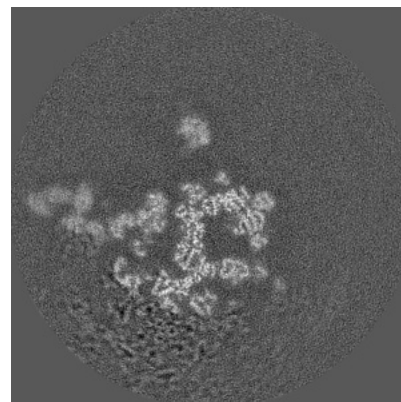
6.2.2 Raw map



X Index: 180



Y Index: 180

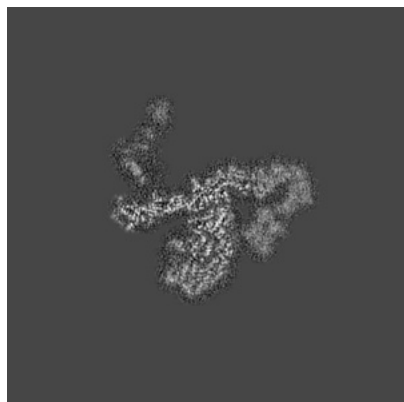


Z Index: 180

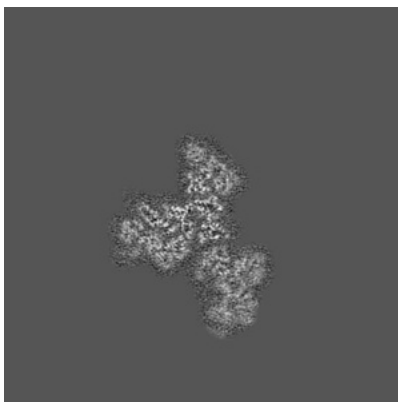
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

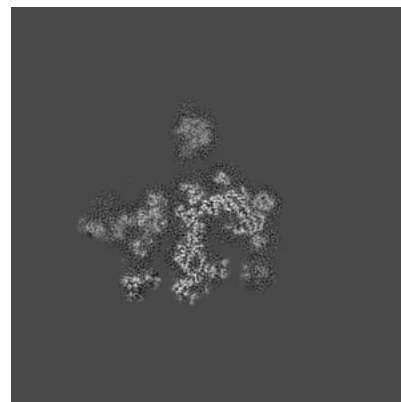
6.3.1 Primary map



X Index: 159

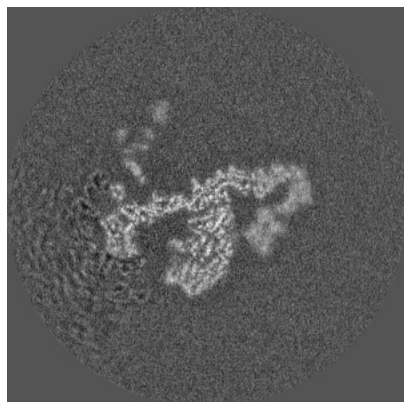


Y Index: 177

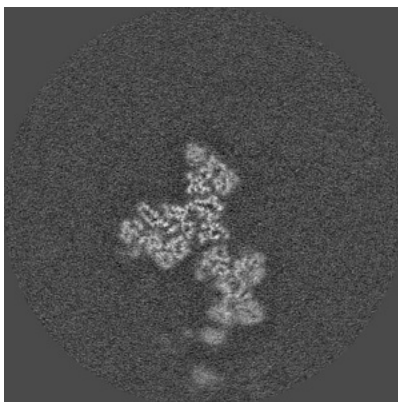


Z Index: 179

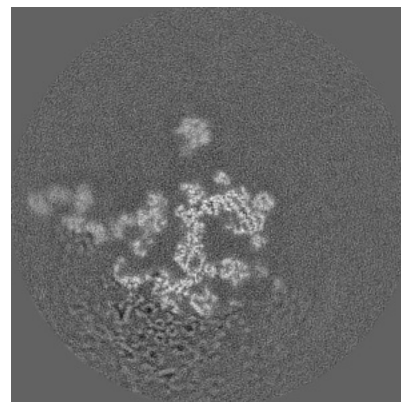
6.3.2 Raw map



X Index: 159



Y Index: 177

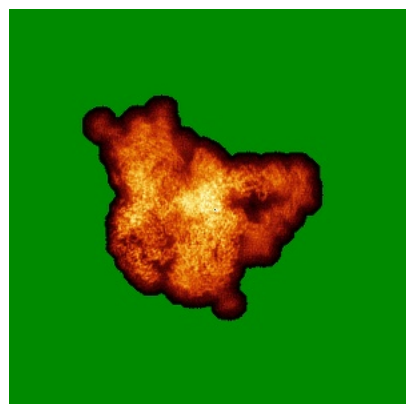


Z Index: 179

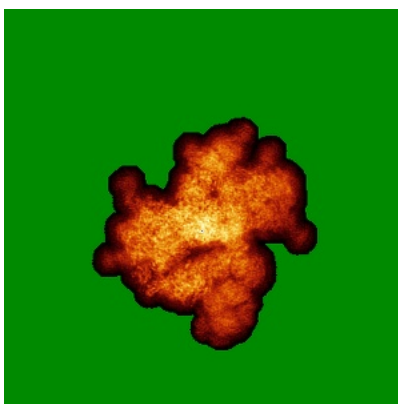
The images above show the largest variance slices of the map in three orthogonal directions.

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

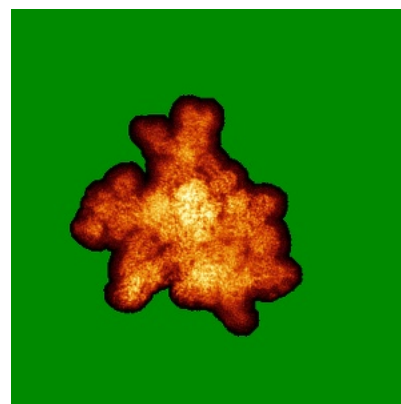
6.4.1 Primary map



X

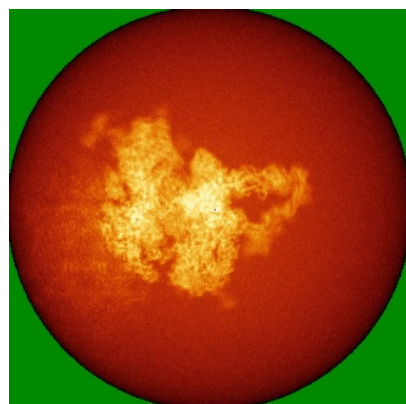


Y

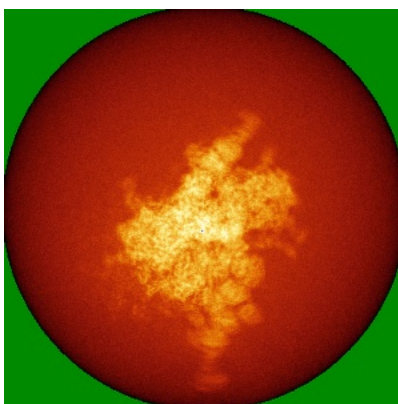


Z

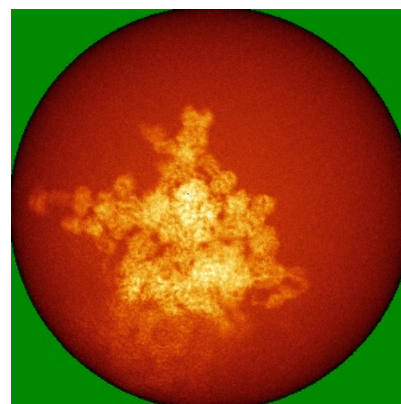
6.4.2 Raw map



X



Y

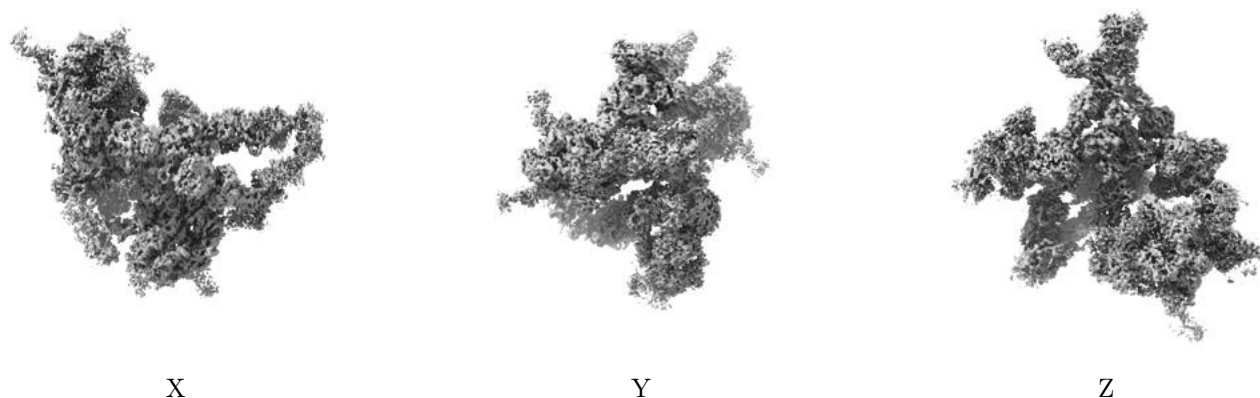


Z

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.

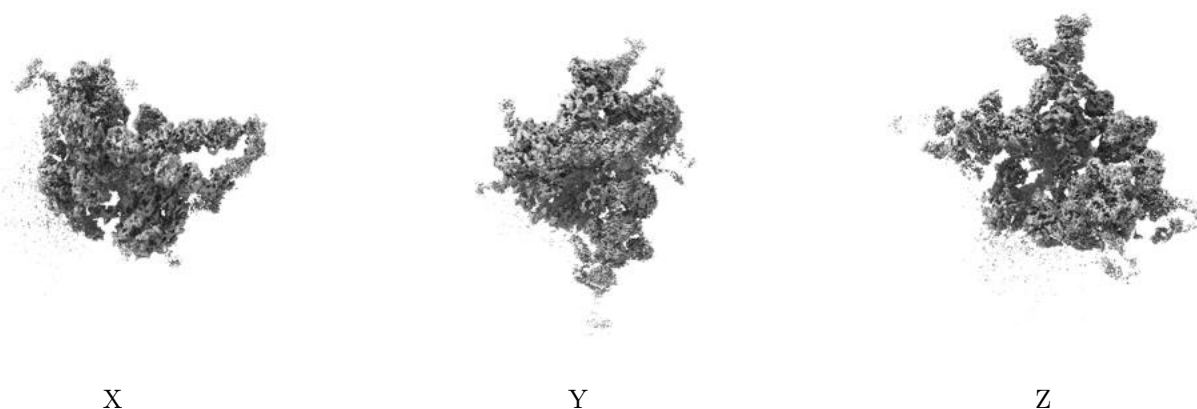
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.03. 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.

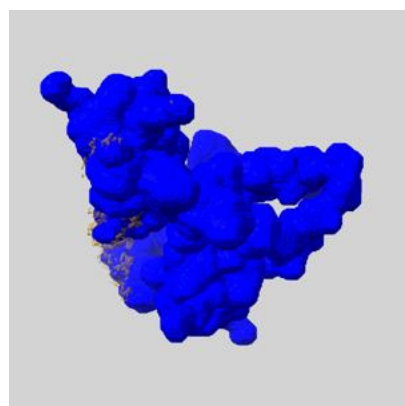
6.6 Mask visualisation [i](#)

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

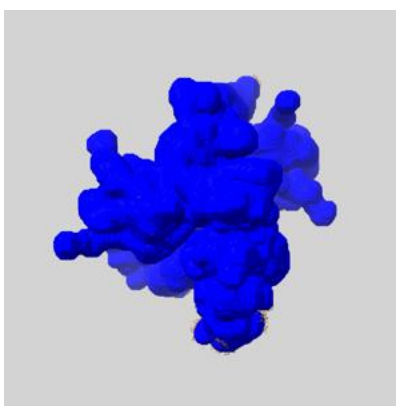
A mask typically either:

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

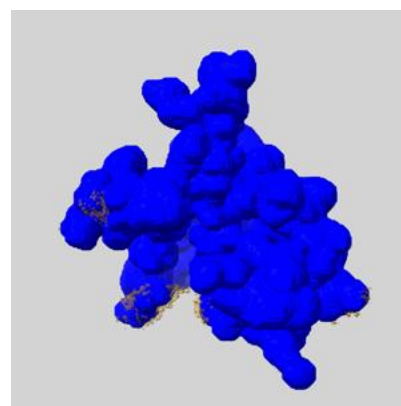
6.6.1 emd_55961_msk_1.map [i](#)



X



Y

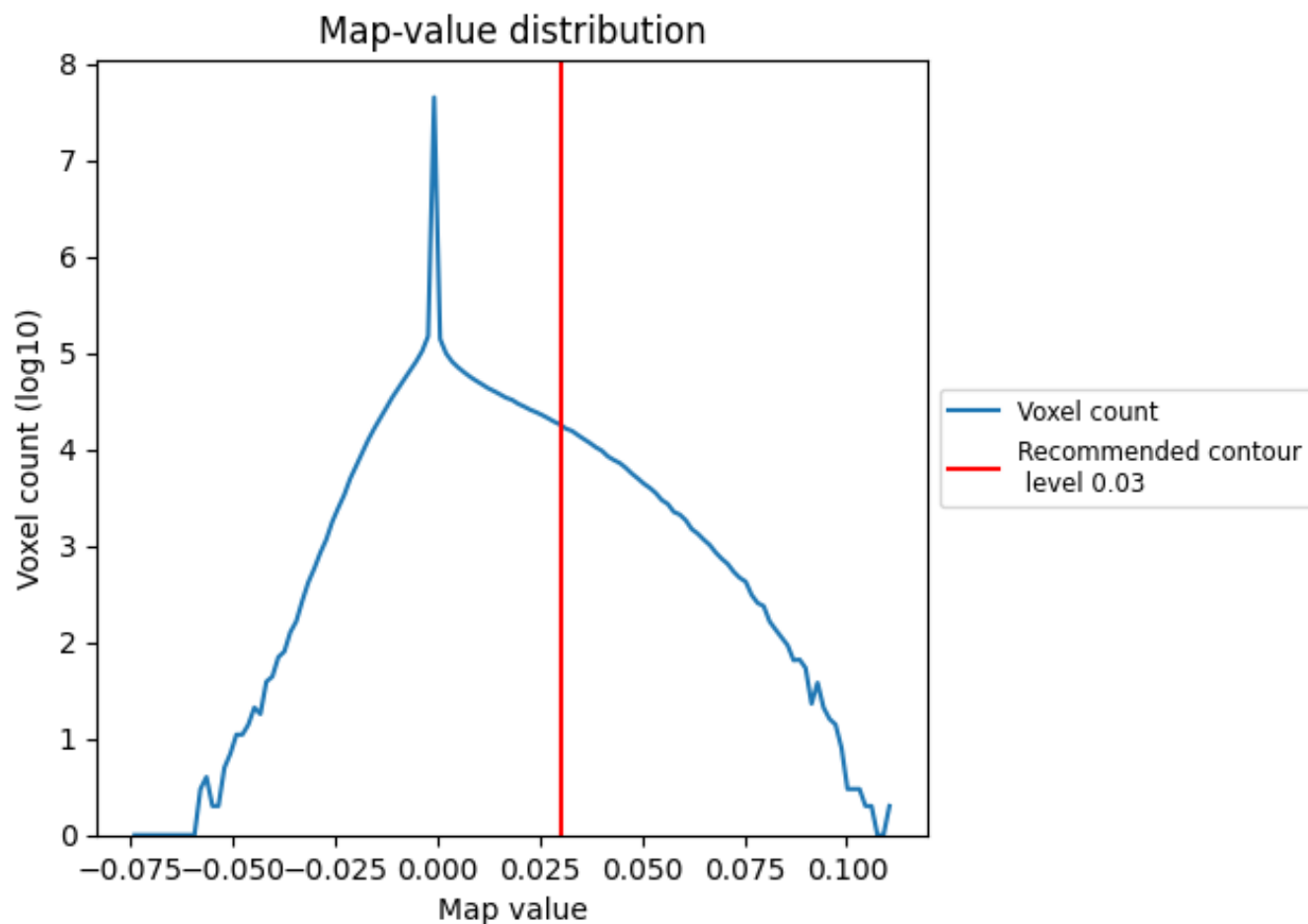


Z

7 Map analysis [i](#)

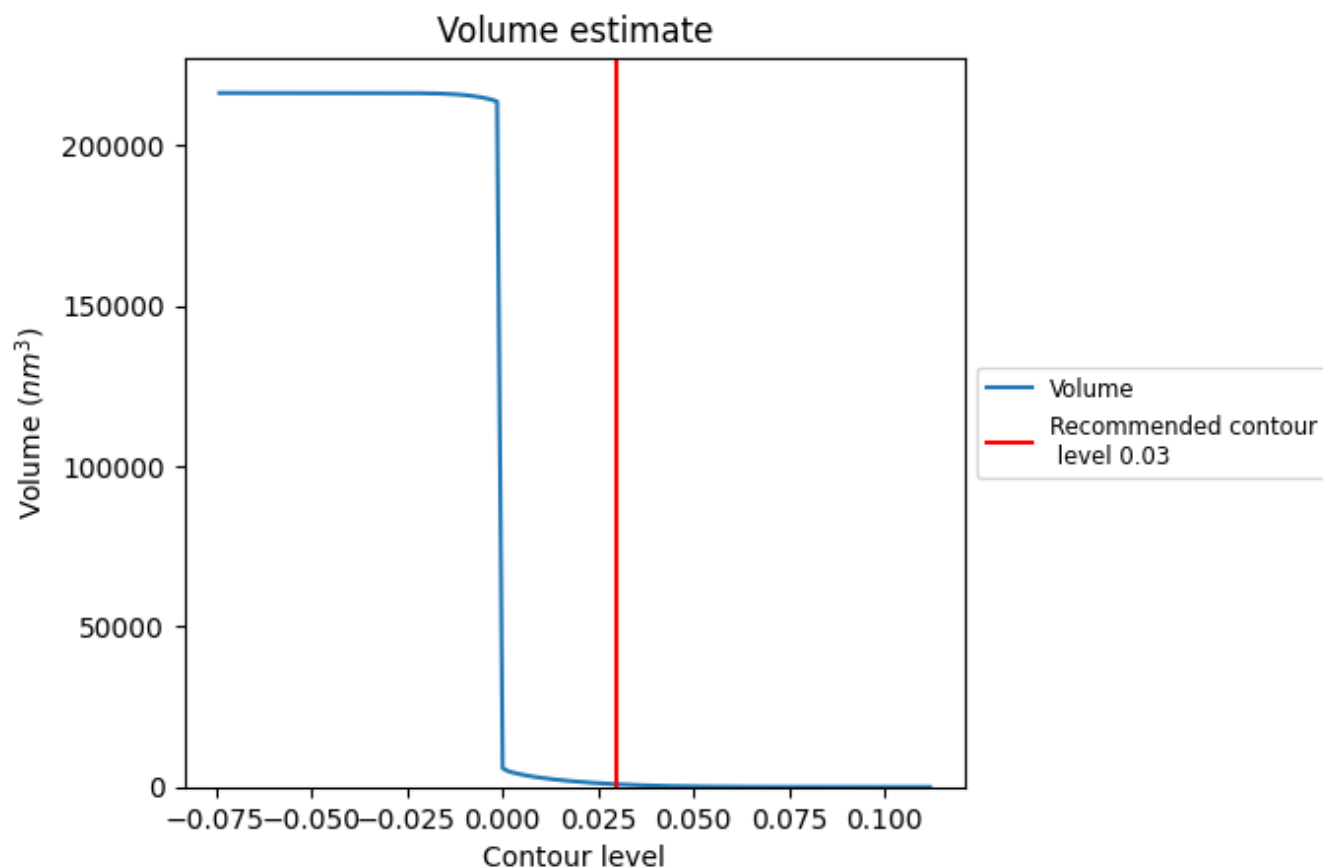
This section contains the results of statistical analysis of the map.

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.

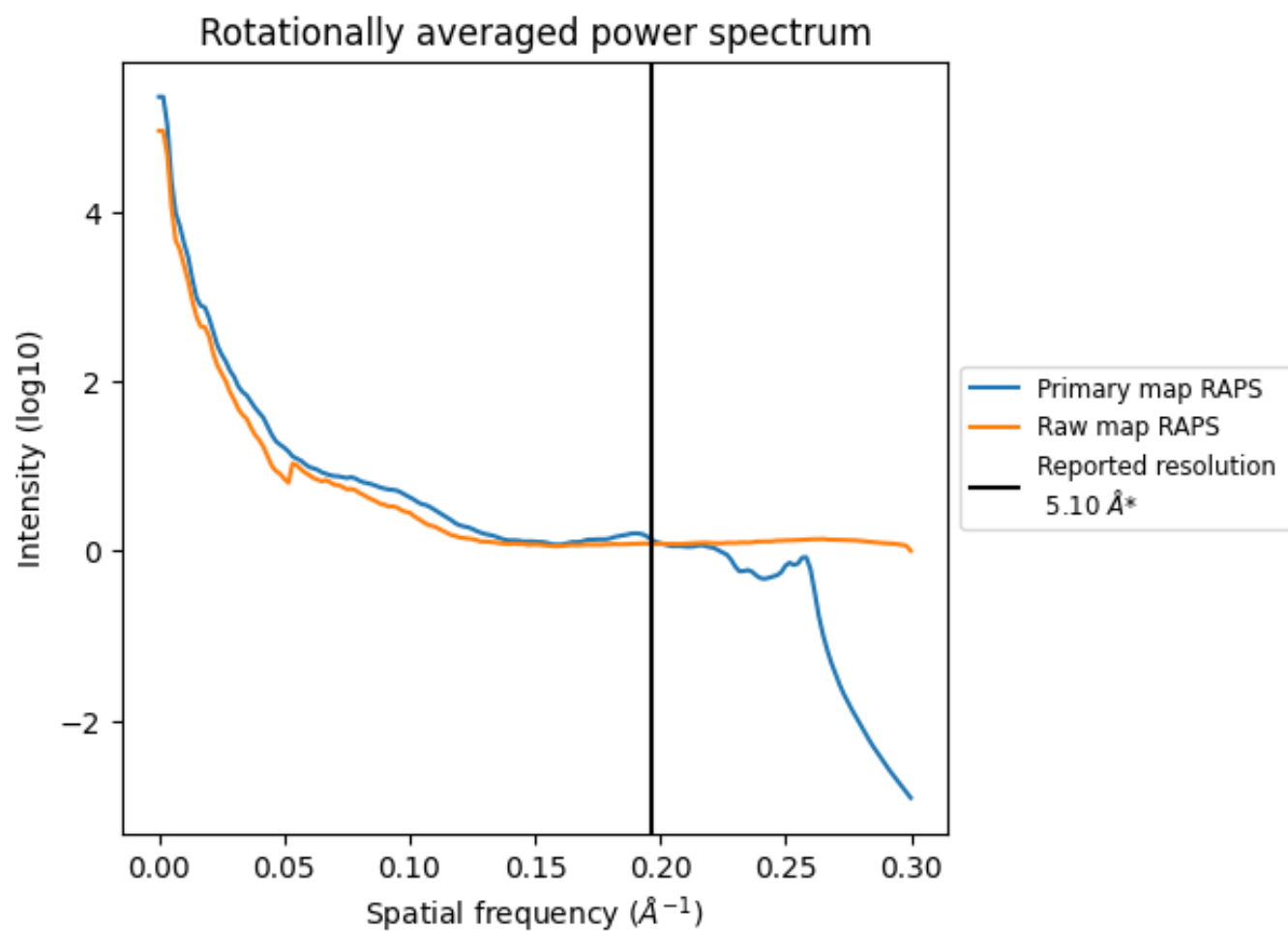
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 849 nm³; this corresponds to an approximate mass of 767 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 ⓘ

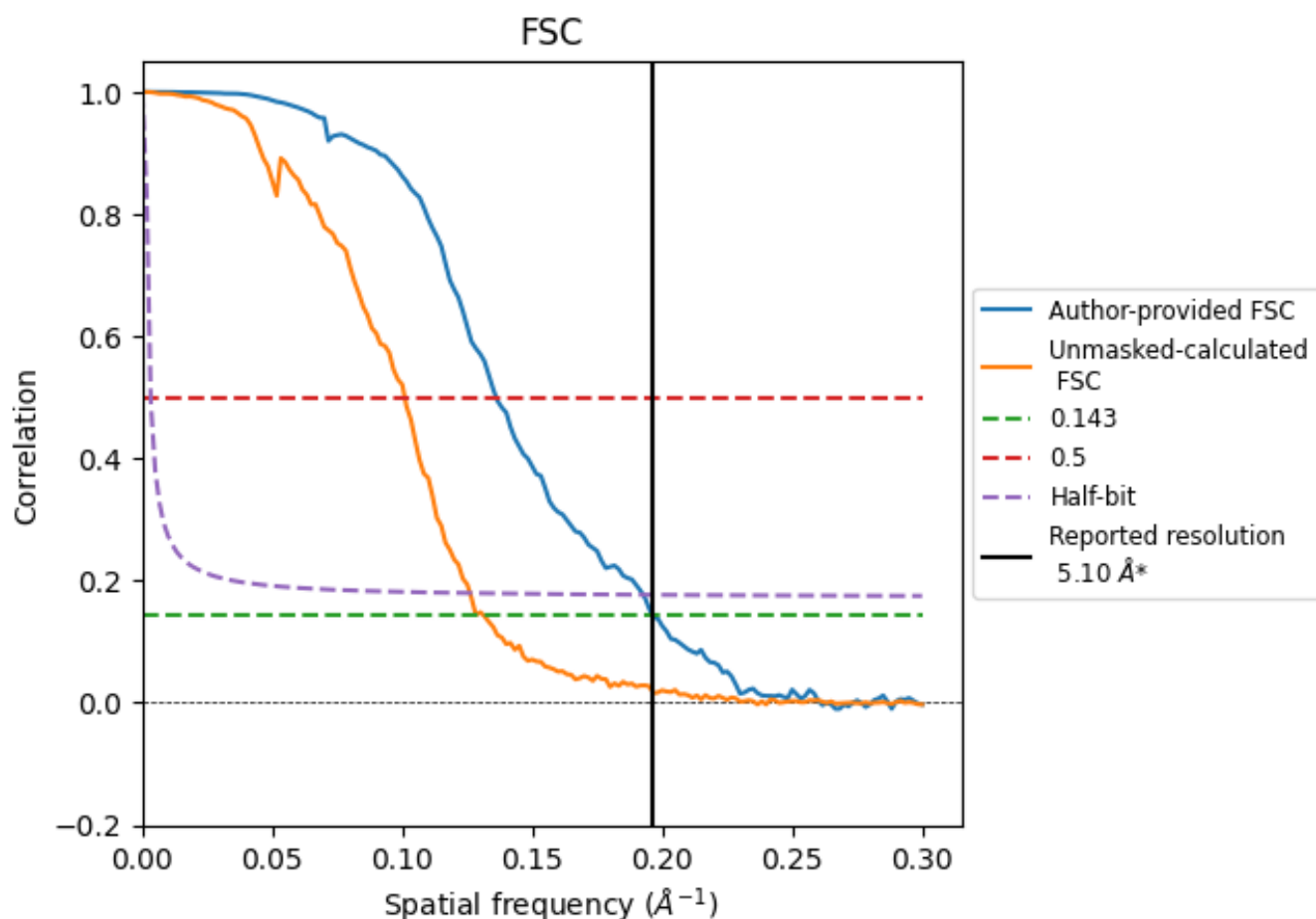


*Reported resolution corresponds to spatial frequency of 0.196 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.196 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

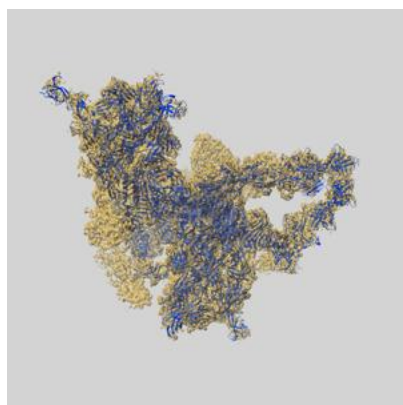
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.10	-	-
Author-provided FSC curve	5.10	7.35	5.19
Unmasked-calculated*	7.62	9.91	7.94

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.62 differs from the reported value 5.1 by more than 10 %

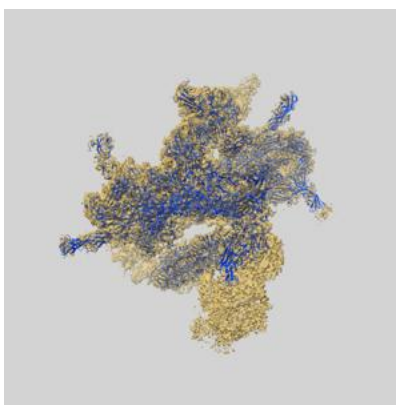
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-55961 and PDB model 9TIM. Per-residue inclusion information can be found in section [3](#) on page [6](#).

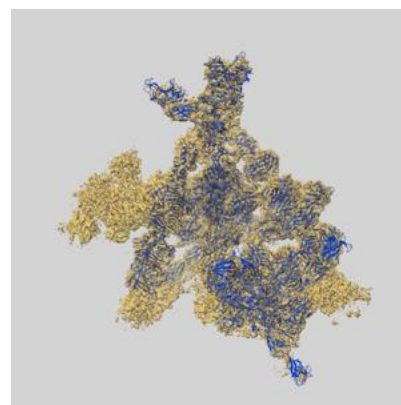
9.1 Map-model overlay [i](#)



X



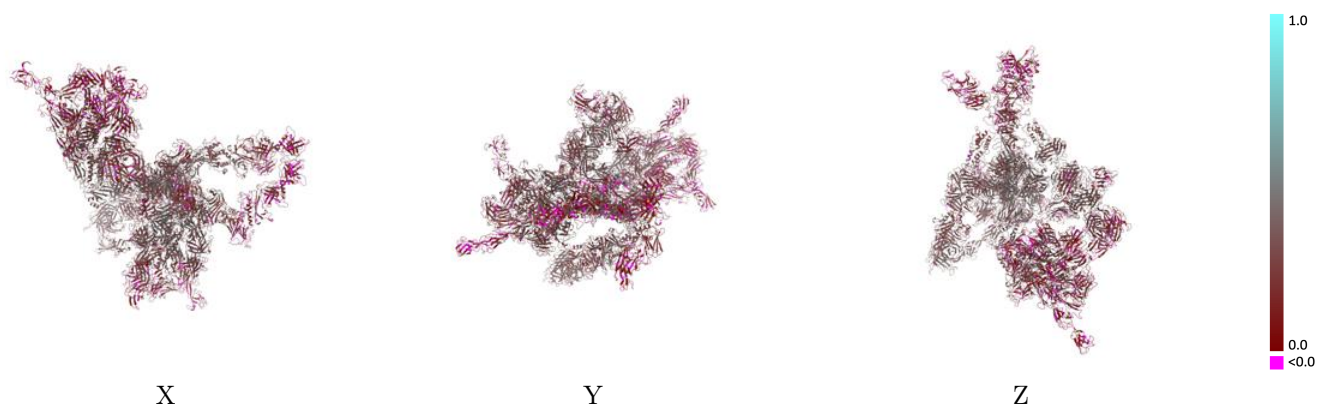
Y



Z

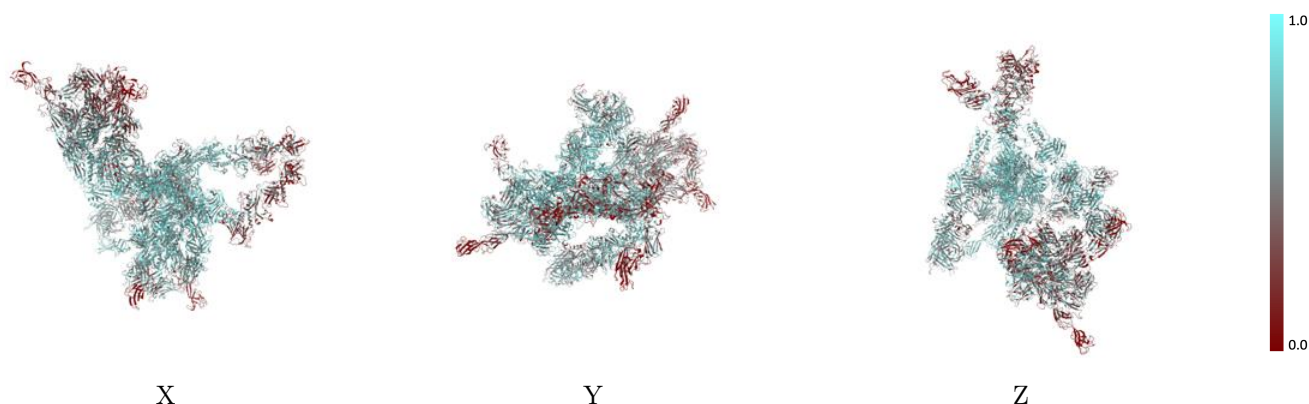
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



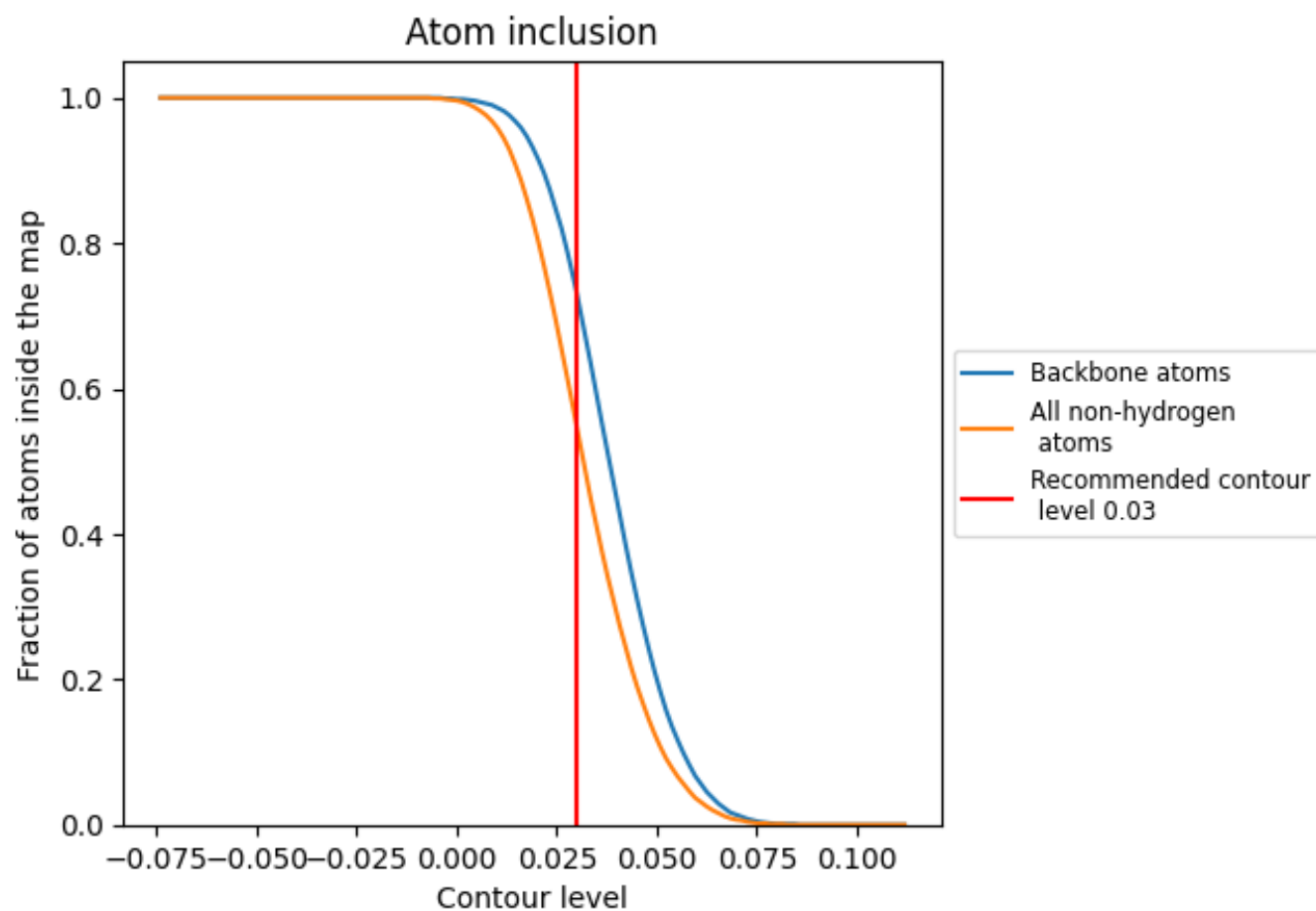
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 55% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5490	 0.2680
A	 0.5480	 0.2880
B	 0.7220	 0.3860
C	 0.7280	 0.3890
D	 0.7440	 0.3990
E	 0.7150	 0.3630
F	 0.6980	 0.3360
G	 0.6030	 0.2950
H	 0.4420	 0.2130
I	 0.2840	 0.1570
J	 0.2470	 0.1280
K	 0.2960	 0.1550
L	 0.3210	 0.1500
M	 0.2150	 0.1420
N	 0.4540	 0.2200
O	 0.4720	 0.2190
P	 0.4500	 0.2150
Q	 0.6550	 0.2980
R	 0.6000	 0.2840
S	 0.5960	 0.2850
T	 0.5970	 0.3080
U	 0.5640	 0.2950
V	 0.5960	 0.3200
W	 0.5960	 0.2790
X	 0.6330	 0.3120
Y	 0.6250	 0.2940

