



## Full wwPDB EM Validation Report ⓘ

May 11, 2026 – 10:35 pm BST

PDB ID : 9TIR / pdb\_00009tir  
EMDB ID : EMD-55967  
Title : Phage 812 baseplate in the post-contraction state (C6)  
Authors : Binovsky, J.; Plevka, P.  
Deposited on : 2025-12-05  
Resolution : 4.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

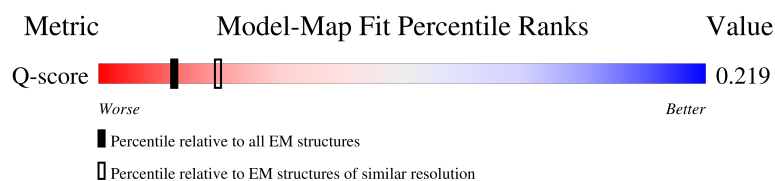
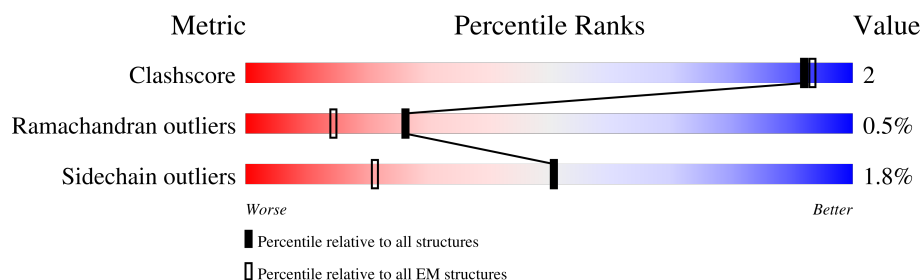
EMDB validation analysis : 0.0.1.dev132  
MolProbity : 4-5-2 with Phenix2.0  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)  
MapQ : 1.9.13  
Ideal geometry (proteins)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

# 1 Overall quality at a glance

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

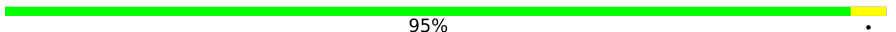
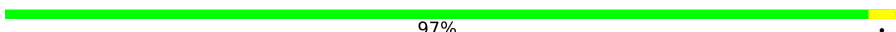
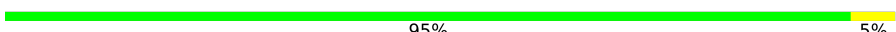

The reported resolution of this entry is 4.40 Å.

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.








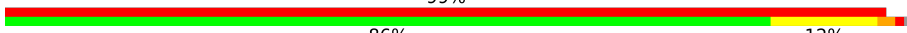















Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 ( 3.91 - 4.90 )

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

Mol	Chain	Length	Quality of chain
1	A	234	 95% .
2	B	348	 97% .
2	C	348	 95% 5%
3	D	1019	 39% 5% . 55%

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Mol	Chain	Length	Quality of chain
4	E	173	 87% 10% ...
4	F	173	 85% 11% ...
4	G	173	 7% 91% 6% ..
4	H	173	 25% 86% 9% ...
4	I	173	 96% 83% 12% ..
4	J	173	 99% 86% 12% ...
5	K	1152	 75% . 21%
5	L	1152	 75% . 21%
5	M	1152	 75% . 21%
5	N	1152	 73% 5% . 21%
5	O	1152	 10% 73% 5% . 21%
5	P	1152	 7% 74% . . 21%
6	Q	458	 100% 90% 9% .
6	R	458	 100% 95% 5%
6	S	458	 97% 91% 7% .
7	T	587	 86% 6% 8%
7	U	587	 89% 5% 6%
7	V	587	 6% 90% 5% 6%
7	W	587	 90% . 6%
7	X	587	 88% 5% . 6%
7	Y	587	 90% . 6%

## 2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 98678 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 ORF61.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	234	Total	C	N	O	S	0	0
			1871	1174	314	377	6		

- Molecule 2 is a protein called ORF62.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	348	Total	C	N	O	S	0	0
			2760	1734	459	560	7		
2	C	347	Total	C	N	O	S	0	0
			2752	1729	458	559	6		

- Molecule 3 is a protein called ORF63.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	457	Total	C	N	O	S	0	0
			3769	2412	610	738	9		

- Molecule 4 is a protein called ORF64.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	E	170	Total	C	N	O	S	0	0
			1336	849	219	267	1		
4	F	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
4	G	170	Total	C	N	O	S	0	0
			1336	849	219	267	1		
4	H	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
4	I	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		
4	J	172	Total	C	N	O	S	0	0
			1349	858	221	269	1		

- Molecule 5 is a protein called ORF65.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	L	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	M	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	N	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	O	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		
5	P	908	Total	C	N	O	S	0	0
			7166	4511	1184	1453	18		

- Molecule 6 is a protein called ORF68.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Q	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
6	R	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		
6	S	458	Total	C	N	O	S	0	0
			3548	2224	592	719	13		

- Molecule 7 is a protein called ORF49.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	T	540	Total	C	N	O	S	0	0
			4213	2653	714	839	7		
7	U	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
7	V	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
7	W	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
7	X	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		
7	Y	553	Total	C	N	O	S	0	0
			4321	2723	734	857	7		

### 3 Residue-property plots

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

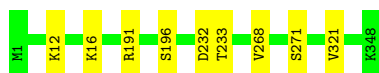
- Molecule 1: ORF61

Chain A:  95%



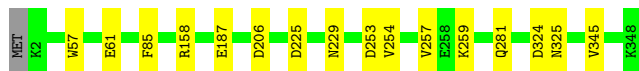
- Molecule 2: ORF62

Chain B:  97%




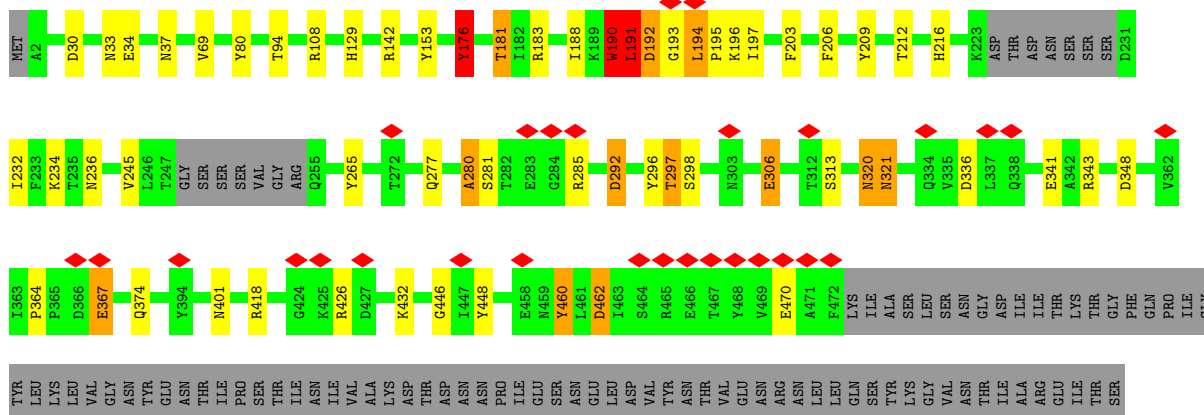
- Molecule 2: ORF62

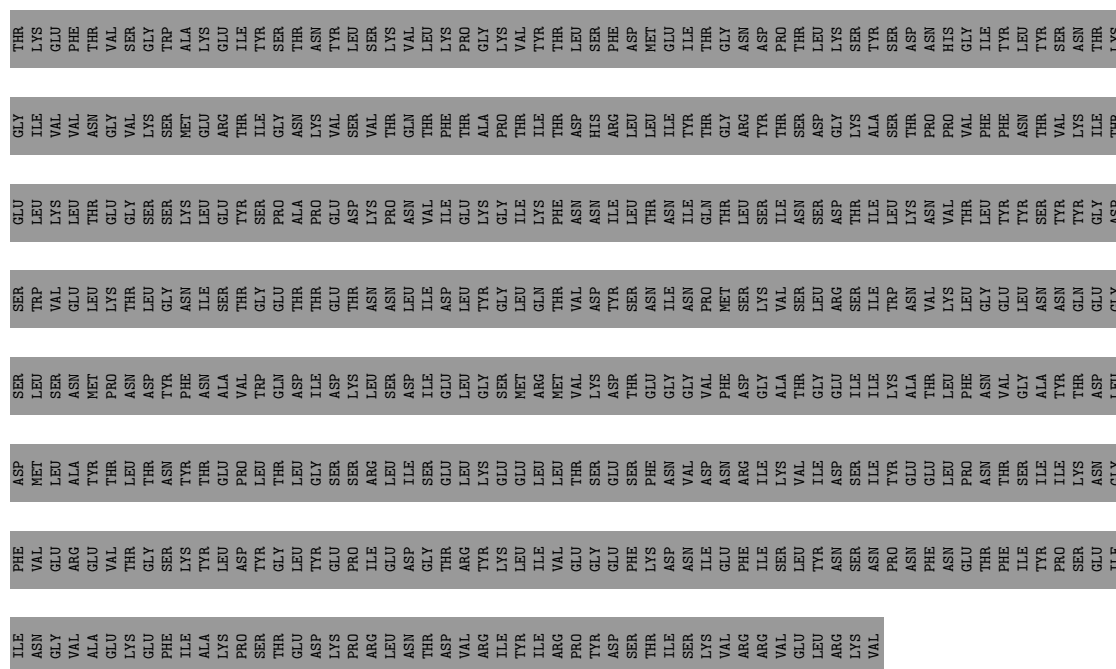
Chain C:  95% 5%



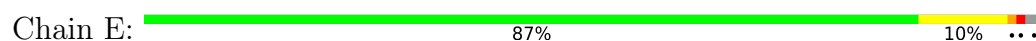
- Molecule 3: ORF63

Chain D:  39% 5% 55%

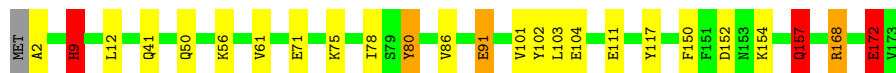
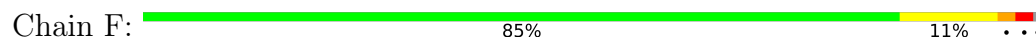




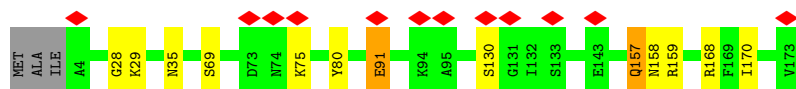
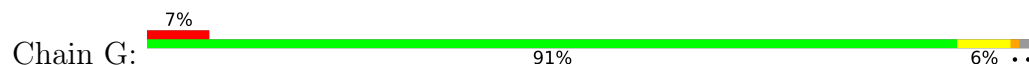
- Molecule 4: ORF64



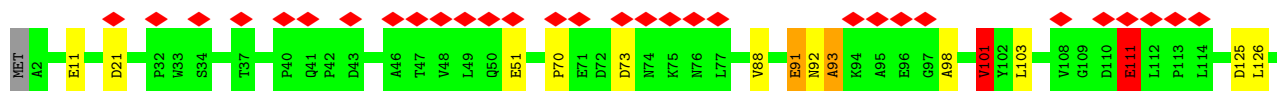
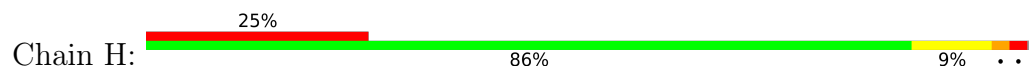
- Molecule 4: ORF64



- Molecule 4: ORF64



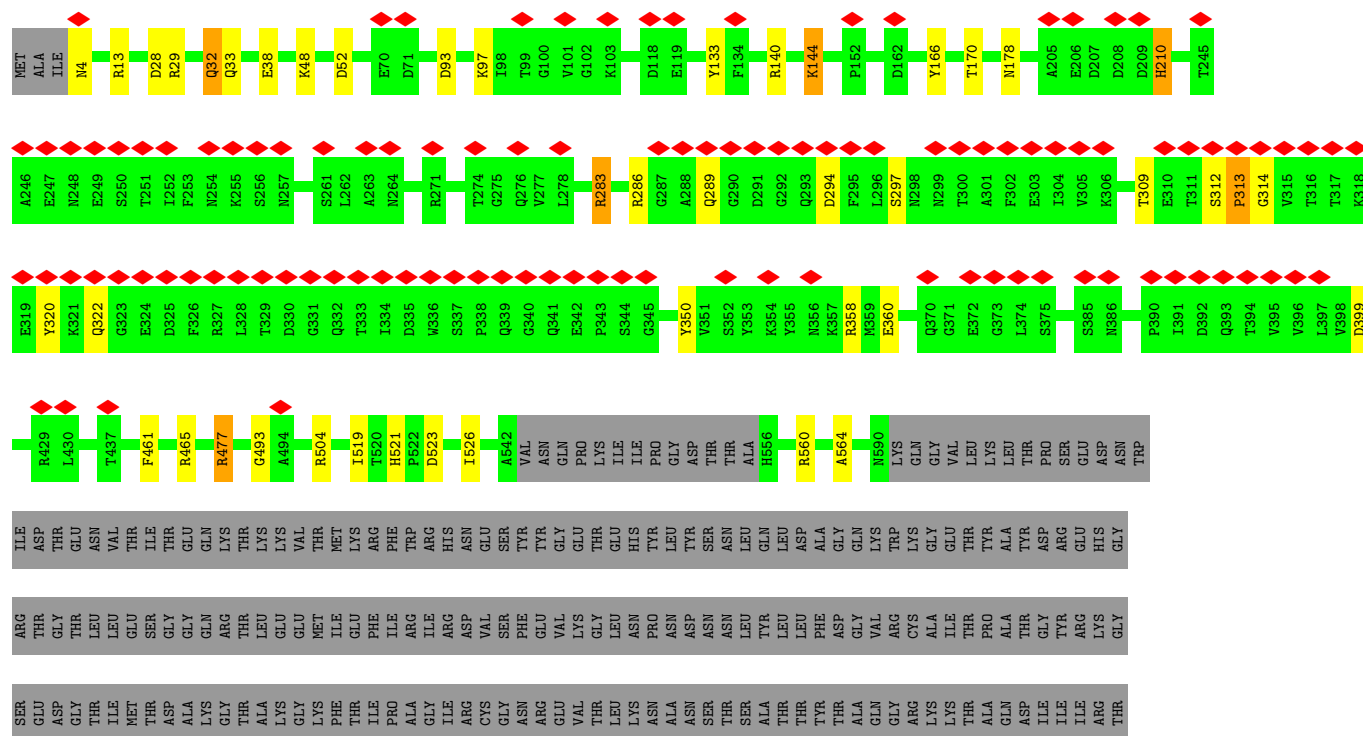
- Molecule 4: ORF64











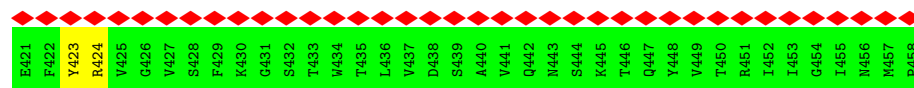


T121	G181	R241	T301	D361	E421
N122	V182	D242	P302	I362	F422
N123	S183	D243	N303	S363	Y423
N124	S184	G244	T304	N364	R424
Q125	G185	A246	S306	Y365	Y425
I126	F186	S247	S307	S366	G426
K127	L187	F248	H308	Y367	V427
M128	D188	P249	G309	V368	S428
L129	L189	G309	V310	E369	F429
Y130	S190	L250	V311	V370	K430
R131	V191	L251	Y311	Y371	G431
F132	D192	V252	N312	T372	S432
V133	A193	Y253	A313	T373	T433
S134	N194	T254	I314	H374	W434
G135	D195	S255	G315	K375	T435
N136	N196	D256	T316	T376	L436
S137	R197	S257	D317	T377	V437
S138	L198	K258	G318	E378	D438
S139	A199	T259	R319	K379	S439
E140	R200	F260	N320	T380	A440
W141	L201	Q261	V321	K381	V441
Q142	T202	Q262	T322	G382	Q442
F143	D203	A263	G323	N383	M443
I144	A204	I264	S324	D384	S444
Q145	E205	I265	V325	N385	K445
G146	T206	D266	V326	T386	T446
L147	G207	H267	G327	G387	Q447
P148	K208	I268	S328	T388	Y448
S149	E209	D269	N329	I389	V449
N150	Y210	R270	W330	C390	T450
K151	T211	T271	T331	H391	R451
N152	S212	G272	S332	K392	L452
A153	I213	Q273	P333	F393	L453
V154	K214	T274	K334	Y394	G454
I155	K215	T275	T335	L395	I455
S156	P216	F276	S336	D396	N456
G157	T217	T277	P337	G397	M457
T158	G218	F278	S338	S398	P458
N159	T219	Y279	H339	G399	
I160	Y220	V280	K340	T400	
L161	T221	Q281	E341	Y401	
D162	A222	Q282	L342	V402	
I163	W223	G283	W343	C403	
A164	K224	V284	T344	S404	
S165	K225	S285	G345	G405	
P166	E226	G286	A346	T406	
G167	F227	S287	Q347	F407	
V168	E228	P288	S348	V408	
Y169	P229	M289	F349	S409	
F170	K230	S290	L350	G410	
V171	D231	N291	S351	D411	
M172	M232	S292	T352	R412	
G173	E233	C293	G353	T413	
M174	K234	R294	T354	D414	
T175	Y235	G295	T355	T415	
G176	L236	L296	K356	K416	
M177	L237	F297	N357	P417	
G178	M238	M298	L358	P418	
P179	S239	S299	S359	I419	
S180	I240	D300	D360	T420	

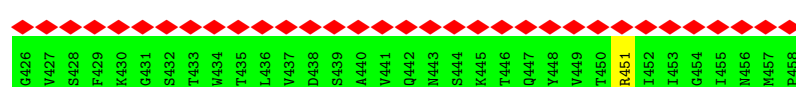
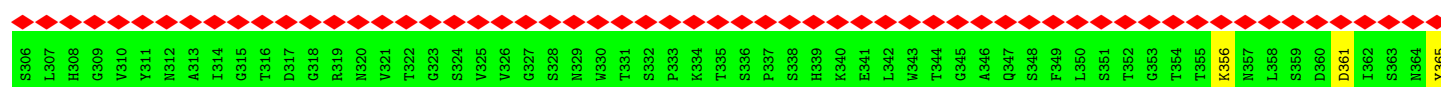
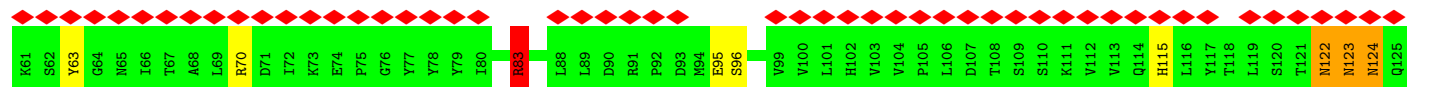
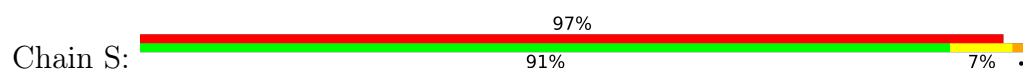
## ● Molecule 6: ORF68



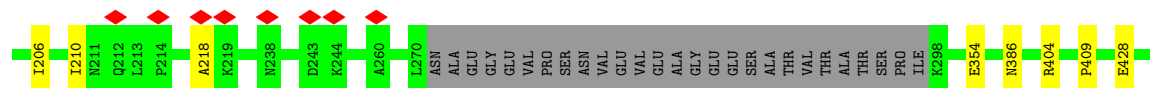
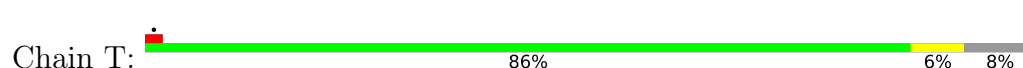
M1	K61	T121	G181	R241	T301	D361
A2	S62	N122	V182	D242	P302	I362
L3	Y63	N123	S183	D243	N303	S363
N4	G64	N124	S184	G244	T304	N364
F5	N65	Q125	G185	S245	S306	Y365
T6	I66	I126	F186	A246	S307	Y366
T7	T67	K127	L187	S247	L307	Y367
I8	A68	M128	D188	F248	H308	V368
T9	L69	L129	L189	P249	G309	E369
E10	R70	Y130	S190	L250	V310	V370
N11	D71	R131	V191	L251	Y311	Y371
N12	I72	F132	D192	V252	N312	T372
V13	K73	V133	A193	Y253	A313	T373
I14	E74	S134	N194	T254	I314	H374
R15	P75	G135	D195	S255	G315	K375
D16	G76	N136	N196	D256	T316	T376
L17	Y77	S137	R197	S257	D317	T377
T18	Y78	S138	L198	K258	G318	E378
T19	Y79	S139	A199	T259	R319	K379
Q20	I80	E140	R200	F260	N320	T380
V21	G81	W141	L201	Q261	V321	K381
N22	A82	Q142	T202	Q262	T322	G382
N23	R83	F143	D203	A263	G323	N383
I24	T84	I144	A204	I264	S324	D384
G25	L85	Q145	E205	I265	V325	N385
E26	A86	G146	T206	D266	V326	T386
E27	T87	L147	G207	H267	G327	G387
L28	L88	P148	K208	I268	S328	T388
T29	L89	S149	E209	D269	N329	I389
K30	D90	N150	Y210	R270	W330	C390
E31	R91	K151	T211	T271	T331	H391
R32	P92	N152	S212	G272	S332	K392
N33	D93	A153	I213	Q273	P333	F393
I34	M94	V154	K214	T274	K334	Y394
F35	E95	I155	K215	T275	T335	L395
D36	S96	S156	P216	F276	S336	D396
I37	L97	G157	T217	T277	P337	G397
T38	D98	T158	G218	F278	S338	S398
D39	V99	N159	T219	Y279	H339	G399
D40	V100	I160	Y220	V280	K340	T400
L41	L101	L161	T221	Q281	E341	Y401
H102	H102	D162	A222	Q282	L342	V402
V103	V103	I163	W223	G283	W343	C403
N104	V104	A164	K224	V284	T344	S404
F105	P105	S165	K225	S285	G345	G405
N106	L106	P166	E226	G286	A346	T406
K107	D107	G167	F227	S287	Q347	F407
S108	T108	V168	E228	P288	S348	V408
S109	S109	Y169	P229	M289	F349	S409
K110	S110	F170	K230	S290	L350	G410
V111	K111	V171	D231	N291	S351	D411
V112	V112	M172	M232	S292	T352	R412
Q113	T113	G173	E233	C293	G353	T413
T114	Q114	M174	K234	R294	T354	D414
H115	H115	T175	Y235	G295	T355	T415
L116	L116	G176	L236	L296	K356	K416
Y117	Y117	G177	L237	F297	N357	P417
T118	T118	M178	M238	M298	L358	P418
L119	L119	P179	S239	S299	S359	I419
S120		S180	I240	D300	D360	T420




• Molecule 6: ORF68

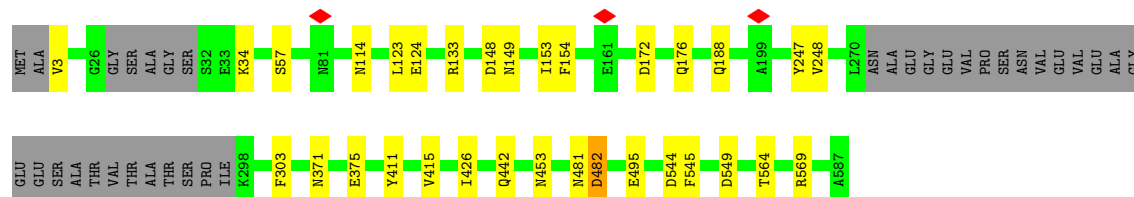


• Molecule 7: ORF49




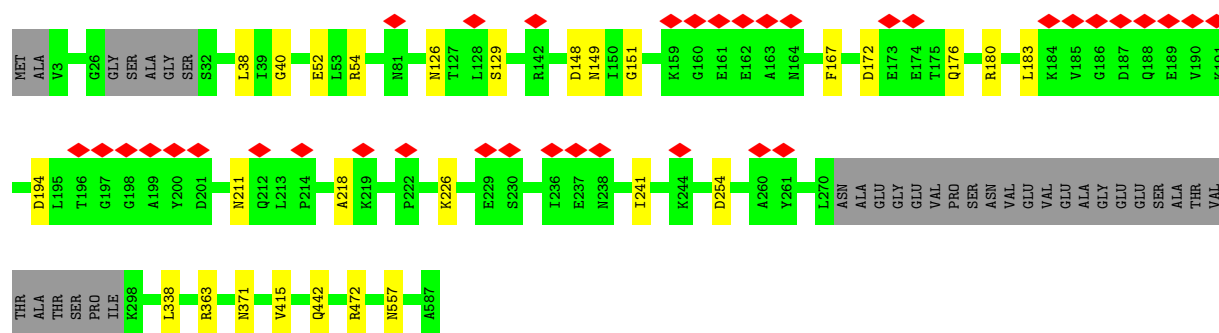
- Molecule 7: ORF49

Chain U: 



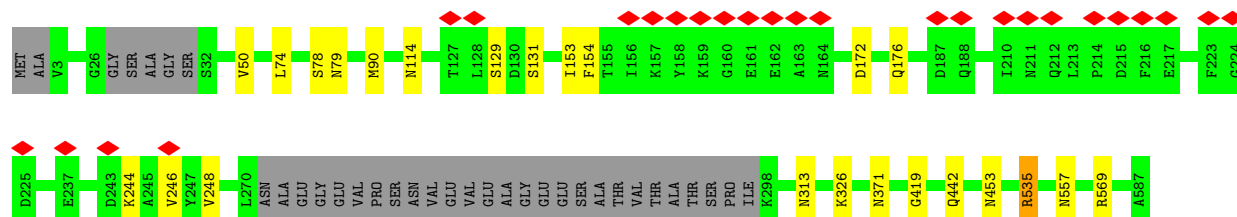
- Molecule 7: ORF49

Chain V: 




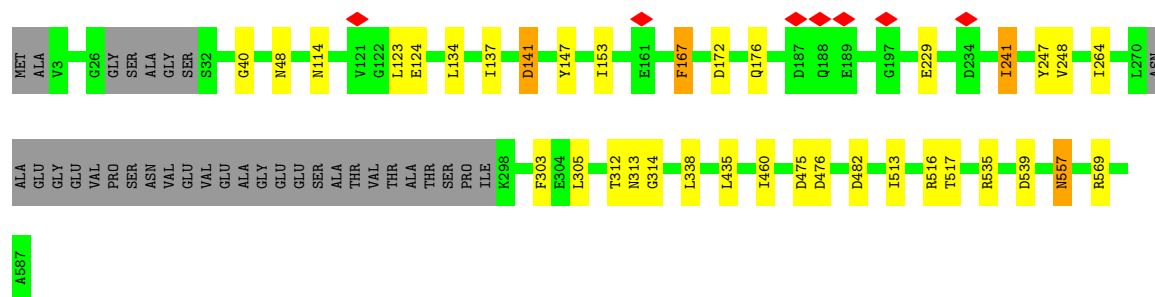
- Molecule 7: ORF49

Chain W: 

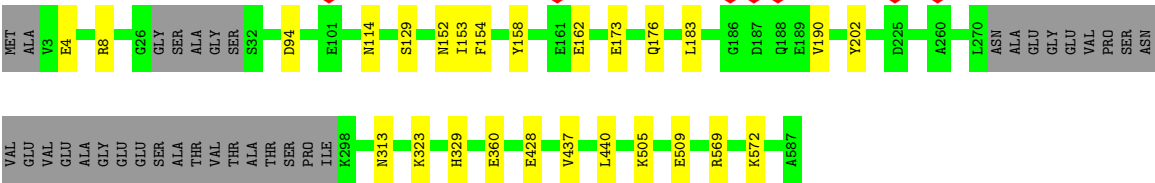
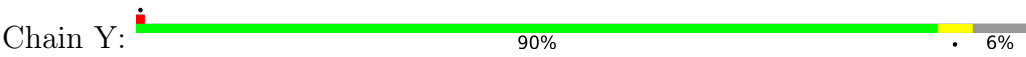


- Molecule 7: ORF49

Chain X: 



- Molecule 7: ORF49



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	21264	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	42	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.110	Depositor
Minimum map value	-0.043	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	1352.9601, 1352.9601, 1352.9601	wwPDB
Map dimensions	640, 640, 640	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.114, 2.114, 2.114	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	A	0.23	0/1902	0.49	0/2572
2	B	0.41	0/2803	0.74	0/3794
2	C	0.21	0/2795	0.44	0/3784
3	D	0.70	1/3852 (0.0%)	1.30	30/5218 (0.6%)
4	E	0.72	0/1364	1.40	7/1854 (0.4%)
4	F	0.79	0/1377	1.44	7/1872 (0.4%)
4	G	0.72	0/1364	1.36	5/1854 (0.3%)
4	H	0.72	0/1377	1.39	8/1872 (0.4%)
4	I	0.73	0/1377	1.41	11/1872 (0.6%)
4	J	0.75	0/1377	1.42	6/1872 (0.3%)
5	K	0.71	0/7308	1.26	17/9911 (0.2%)
5	L	0.71	0/7308	1.27	18/9911 (0.2%)
5	M	0.71	0/7308	1.25	16/9911 (0.2%)
5	N	0.71	0/7308	1.28	29/9911 (0.3%)
5	O	0.75	0/7308	1.31	27/9911 (0.3%)
5	P	0.72	0/7308	1.29	23/9911 (0.2%)
6	Q	0.77	0/3619	1.34	18/4913 (0.4%)
6	R	0.76	0/3619	1.29	13/4913 (0.3%)
6	S	0.78	0/3619	1.34	17/4913 (0.3%)
7	T	0.24	0/4280	0.48	0/5777
7	U	0.33	0/4392	0.63	0/5930
7	V	0.35	0/4392	0.64	1/5930 (0.0%)
7	W	0.32	0/4392	0.62	1/5930 (0.0%)
7	X	0.28	0/4392	0.56	0/5930
7	Y	0.21	0/4392	0.45	0/5930
All	All	0.62	1/100533 (0.0%)	1.11	254/136196 (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
3	D	0	7
4	E	0	2
4	F	0	3
4	G	0	2
4	H	0	1
4	I	0	1
4	J	0	1
5	K	0	10
5	L	0	6
5	M	0	7
5	N	0	8
5	O	0	13
5	P	0	5
6	Q	0	7
6	R	0	6
6	S	0	7
7	V	0	1
7	W	0	1
All	All	0	88

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	364	PRO	CA-C	5.34	1.54	1.51

All (254) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	227	PHE	N-CA-C	11.22	126.72	108.55
3	D	462	ASP	CA-CB-CG	11.11	123.71	112.60
3	D	191	LEU	N-CA-C	10.90	125.94	112.87
5	N	311	THR	CA-CB-CG2	9.89	127.31	110.50
3	D	280	ALA	CB-CA-C	9.55	131.02	110.19
6	Q	231	ASP	CA-CB-CG	9.24	121.84	112.60
4	E	69	SER	CA-C-N	9.22	131.37	119.84
4	E	69	SER	C-N-CA	9.22	131.37	119.84
4	E	70	PRO	CA-N-CD	-8.90	99.54	112.00
5	L	1144	ARG	NE-CZ-NH2	8.74	127.07	119.20
5	N	1144	ARG	NE-CZ-NH2	8.64	126.97	119.20
6	Q	266	ASP	CA-CB-CG	8.06	120.67	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	1144	ARG	NE-CZ-NH2	8.05	126.44	119.20
5	O	1144	ARG	NE-CZ-NH2	7.93	126.34	119.20
5	O	477	ARG	NE-CZ-NH2	7.91	126.32	119.20
5	M	1144	ARG	NE-CZ-NH2	7.70	126.13	119.20
6	S	83	ARG	NE-CZ-NH2	7.54	125.99	119.20
3	D	94	THR	O-C-N	-7.54	114.66	123.25
5	P	1144	ARG	NE-CZ-NH2	7.50	125.95	119.20
6	Q	136	ASN	N-CA-C	7.44	122.39	113.16
6	S	122	ASN	CA-CB-CG	7.43	120.03	112.60
5	L	520	THR	OG1-CB-CG2	-7.41	94.49	109.30
4	I	136	ASN	CA-CB-CG	7.40	120.00	112.60
3	D	94	THR	CA-C-N	7.38	130.18	120.28
3	D	94	THR	C-N-CA	7.38	130.18	120.28
4	H	21	ASP	CA-CB-CG	-7.30	105.30	112.60
5	P	477	ARG	NE-CZ-NH2	7.24	125.72	119.20
6	S	200	ARG	NE-CZ-NH2	7.21	125.69	119.20
5	L	29	ARG	NE-CZ-NH2	7.15	125.63	119.20
3	D	292	ASP	CA-CB-CG	7.11	119.71	112.60
6	R	266	ASP	CA-CB-CG	7.11	119.71	112.60
4	I	111	GLU	CB-CG-CD	7.04	124.56	112.60
5	N	310	GLU	CB-CA-C	7.04	123.19	114.40
6	S	267	HIS	CB-CG-CD2	-7.04	122.05	131.20
6	Q	200	ARG	NE-CZ-NH2	7.00	125.50	119.20
5	O	399	ASP	CA-CB-CG	6.97	119.57	112.60
3	D	321	ASN	OD1-CG-ND2	-6.92	115.67	122.60
4	F	157	GLN	OE1-CD-NE2	-6.90	115.70	122.60
6	S	123	ASN	CA-CB-CG	-6.90	105.70	112.60
3	D	181	THR	CA-CB-OG1	6.86	119.90	109.60
5	P	528	PHE	CA-CB-CG	6.82	120.62	113.80
5	N	311	THR	OG1-CB-CG2	-6.73	95.83	109.30
4	H	136	ASN	CA-CB-CG	6.73	119.33	112.60
5	M	477	ARG	NE-CZ-NH2	6.70	125.23	119.20
5	M	504	ARG	NE-CZ-NH2	6.67	125.20	119.20
5	L	477	ARG	NE-CZ-NH2	6.66	125.19	119.20
3	D	192	ASP	CB-CA-C	6.65	121.51	111.80
5	L	286	ARG	NE-CZ-NH2	6.59	125.13	119.20
5	N	429	ARG	NE-CZ-NH2	6.58	125.12	119.20
4	E	9	HIS	CB-CG-CD2	-6.57	122.66	131.20
3	D	194	LEU	CA-C-N	6.56	126.69	119.87
3	D	194	LEU	C-N-CA	6.56	126.69	119.87
3	D	297	THR	CA-C-N	6.54	131.81	120.68
3	D	297	THR	C-N-CA	6.54	131.81	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	O	32	GLN	N-CA-C	6.51	119.66	109.96
5	O	210	HIS	CB-CG-CD2	-6.44	122.82	131.20
7	W	535	ARG	NE-CZ-NH2	6.43	124.98	119.20
5	M	272	ARG	NE-CZ-NH2	6.40	124.96	119.20
5	P	321	LYS	CB-CG-CD	-6.40	96.58	111.30
5	L	1026	ARG	NE-CZ-NH2	6.39	124.95	119.20
5	O	804	ARG	NE-CZ-NH2	6.36	124.93	119.20
6	S	451	ARG	NE-CZ-NH2	6.36	124.92	119.20
5	M	286	ARG	NE-CZ-NH2	6.35	124.91	119.20
3	D	108	ARG	NE-CZ-NH2	6.30	124.87	119.20
5	O	1023	GLU	CB-CG-CD	-6.29	101.91	112.60
5	L	1023	GLU	CB-CG-CD	-6.28	101.93	112.60
5	P	184	ARG	NE-CZ-NH2	6.23	124.81	119.20
5	N	477	ARG	NE-CZ-NH2	6.22	124.80	119.20
5	P	1019	ARG	NE-CZ-NH2	6.21	124.79	119.20
6	S	23	ASN	CA-CB-CG	6.20	118.80	112.60
4	G	130	SER	N-CA-C	6.19	118.82	111.33
6	S	384	ASP	CA-CB-CG	6.18	118.78	112.60
5	P	996	LEU	CA-C-N	6.17	131.26	121.44
5	P	996	LEU	C-N-CA	6.17	131.26	121.44
5	P	321	LYS	CG-CD-CE	6.16	125.47	111.30
5	N	29	ARG	NE-CZ-NH2	6.14	124.73	119.20
4	I	158	ASN	OD1-CG-ND2	-6.12	116.47	122.60
3	D	190	TRP	CA-CB-CG	6.11	125.22	113.60
4	F	168	ARG	NE-CZ-NH2	6.10	124.69	119.20
6	Q	424	ARG	NE-CZ-NH2	6.07	124.66	119.20
5	P	895	ARG	NE-CZ-NH2	6.07	124.66	119.20
3	D	336	ASP	CA-CB-CG	-6.02	106.58	112.60
5	L	1150	ARG	NE-CZ-NH2	5.99	124.59	119.20
5	N	1026	ARG	NE-CZ-NH2	5.99	124.59	119.20
6	Q	319	ARG	NE-CZ-NH2	5.99	124.59	119.20
3	D	129	HIS	CB-CG-CD2	-5.98	123.43	131.20
5	K	286	ARG	NE-CZ-NH2	5.97	124.58	119.20
5	P	286	ARG	NE-CZ-NH2	5.97	124.58	119.20
6	S	424	ARG	NE-CZ-NH2	5.97	124.58	119.20
4	E	70	PRO	N-CA-C	5.96	124.75	112.47
6	Q	273	GLN	OE1-CD-NE2	-5.96	116.64	122.60
3	D	364	PRO	N-CA-CB	5.94	106.52	103.19
4	I	9	HIS	CA-CB-CG	5.91	119.71	113.80
5	P	1019	ARG	NE-CZ-NH1	-5.91	115.59	121.50
4	H	101	VAL	CA-CB-CG1	5.91	120.45	110.40
5	P	1104	ASN	CA-CB-CG	5.91	118.51	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	S	266	ASP	CA-CB-CG	5.91	118.51	112.60
5	K	504	ARG	NE-CZ-NH2	5.90	124.51	119.20
5	L	465	ARG	CD-NE-CZ	5.89	132.65	124.40
5	O	32	GLN	OE1-CD-NE2	-5.89	116.71	122.60
5	P	504	ARG	NE-CZ-NH2	5.89	124.50	119.20
4	F	9	HIS	CA-CB-CG	5.88	119.68	113.80
6	R	424	ARG	NE-CZ-NH2	5.88	124.49	119.20
4	G	157	GLN	OE1-CD-NE2	-5.86	116.74	122.60
5	K	477	ARG	NE-CZ-NH2	5.84	124.46	119.20
6	S	124	ASN	CA-CB-CG	5.84	118.44	112.60
5	K	804	ARG	NE-CZ-NH2	5.83	124.45	119.20
6	R	361	ASP	CA-CB-CG	-5.82	106.78	112.60
3	D	374	GLN	OE1-CD-NE2	-5.80	116.80	122.60
5	N	286	ARG	NE-CZ-NH2	5.80	124.42	119.20
6	Q	414	ASP	CA-CB-CG	5.79	118.39	112.60
5	K	826	GLN	OE1-CD-NE2	-5.78	116.82	122.60
5	M	321	LYS	CG-CD-CE	5.78	124.59	111.30
5	N	570	ARG	NE-CZ-NH2	5.78	124.40	119.20
6	Q	267	HIS	CB-CG-CD2	-5.76	123.71	131.20
3	D	183	ARG	NE-CZ-NH2	5.76	124.39	119.20
5	K	1143	ARG	NE-CZ-NH2	5.75	124.37	119.20
4	H	111	GLU	CB-CG-CD	5.73	122.34	112.60
5	O	914	GLN	OE1-CD-NE2	-5.72	116.88	122.60
6	Q	227	PHE	CA-CB-CG	-5.72	108.08	113.80
6	S	361	ASP	CA-CB-CG	-5.72	106.88	112.60
5	L	1019	ARG	NE-CZ-NH1	-5.72	115.78	121.50
5	M	826	GLN	OE1-CD-NE2	-5.71	116.89	122.60
4	J	21	ASP	CA-CB-CG	-5.71	106.89	112.60
5	M	868	PRO	N-CA-CB	5.67	106.10	102.92
5	O	13	ARG	NE-CZ-NH2	5.63	124.27	119.20
7	V	472	ARG	NE-CZ-NH2	5.63	124.27	119.20
6	Q	74	GLU	CB-CG-CD	-5.62	103.06	112.60
6	S	131	ARG	NE-CZ-NH2	5.60	124.24	119.20
3	D	192	ASP	CA-CB-CG	-5.59	107.00	112.60
3	D	343	ARG	NE-CZ-NH2	5.59	124.24	119.20
5	O	828	ARG	NE-CZ-NH1	-5.59	115.91	121.50
4	E	65	ARG	NE-CZ-NH2	5.58	124.23	119.20
6	Q	131	ARG	NE-CZ-NH2	5.58	124.22	119.20
4	J	38	ASN	CA-CB-CG	5.56	118.16	112.60
3	D	401	ASN	CA-CB-CG	-5.56	107.04	112.60
5	N	1023	GLU	CB-CG-CD	-5.55	103.16	112.60
5	M	321	LYS	CB-CG-CD	-5.55	98.53	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	142	ARG	NE-CZ-NH2	5.55	124.20	119.20
5	M	342	GLU	O-C-N	-5.55	118.16	121.71
6	R	424	ARG	CD-NE-CZ	5.54	132.16	124.40
5	O	826	GLN	OE1-CD-NE2	-5.54	117.06	122.60
5	N	918	PHE	CA-CB-CG	5.53	119.33	113.80
6	R	417	PRO	N-CA-CB	5.53	106.10	103.22
5	M	799	GLN	OE1-CD-NE2	-5.52	117.08	122.60
5	M	895	ARG	NE-CZ-NH2	5.51	124.16	119.20
5	N	272	ARG	NE-CZ-NH2	5.51	124.16	119.20
5	N	887	ASP	CA-CB-CG	-5.50	107.09	112.60
5	N	485	GLN	OE1-CD-NE2	-5.50	117.10	122.60
5	P	204	ASN	CA-CB-CG	5.50	118.10	112.60
5	N	1019	ARG	NE-CZ-NH2	5.49	124.14	119.20
4	G	35	ASN	OD1-CG-ND2	-5.49	117.11	122.60
5	O	564	ALA	CA-C-N	5.49	125.10	119.56
5	O	564	ALA	C-N-CA	5.49	125.10	119.56
5	M	1026	ARG	NE-CZ-NH2	5.48	124.13	119.20
5	K	1150	ARG	NE-CZ-NH2	5.46	124.11	119.20
5	P	822	ASN	OD1-CG-ND2	-5.46	117.14	122.60
3	D	181	THR	OG1-CB-CG2	5.44	120.19	109.30
5	P	1109	ARG	NE-CZ-NH2	5.43	124.09	119.20
5	K	13	ARG	NE-CZ-NH2	5.42	124.08	119.20
6	R	320	ASN	OD1-CG-ND2	-5.42	117.18	122.60
5	L	461	PHE	CA-CB-CG	5.42	119.22	113.80
5	L	833	GLN	OE1-CD-NE2	-5.41	117.19	122.60
5	O	1150	ARG	NE-CZ-NH2	5.41	124.07	119.20
5	K	184	ARG	NE-CZ-NH2	5.41	124.07	119.20
5	M	828	ARG	NE-CZ-NH1	-5.40	116.10	121.50
5	O	140	ARG	NE-CZ-NH2	5.40	124.06	119.20
5	M	1150	ARG	NE-CZ-NH2	5.39	124.05	119.20
5	N	358	ARG	NE-CZ-NH2	5.35	124.02	119.20
5	K	828	ARG	NE-CZ-NH1	-5.35	116.15	121.50
6	S	197	ARG	NE-CZ-NH2	5.34	124.00	119.20
3	D	190	TRP	CB-CG-CD1	-5.33	118.90	126.90
6	Q	162	ASP	CA-CB-CG	5.33	117.93	112.60
6	R	35	PHE	CA-CB-CG	5.33	119.13	113.80
4	G	28	GLY	CA-C-N	5.32	131.71	121.54
4	G	28	GLY	C-N-CA	5.32	131.71	121.54
5	N	289	GLN	CA-C-N	5.32	125.16	120.10
5	N	289	GLN	C-N-CA	5.32	125.16	120.10
6	Q	248	PHE	CA-CB-CG	5.32	119.12	113.80
5	O	358	ARG	NE-CZ-NH2	5.31	123.98	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	21	ASP	N-CA-C	5.29	119.00	112.54
4	H	93	ALA	CA-C-N	5.29	127.63	120.38
4	H	93	ALA	C-N-CA	5.29	127.63	120.38
5	P	19	ASP	CA-CB-CG	5.29	117.89	112.60
5	K	560	ARG	NE-CZ-NH2	5.29	123.96	119.20
6	S	241	ARG	NE-CZ-NH2	5.28	123.95	119.20
5	K	488	ASN	OD1-CG-ND2	-5.25	117.35	122.60
4	I	65	ARG	NE-CZ-NH1	-5.24	116.26	121.50
6	S	32	ARG	NE-CZ-NH2	5.24	123.91	119.20
5	K	399	ASP	CA-CB-CG	5.23	117.83	112.60
4	J	111	GLU	CB-CG-CD	5.22	121.48	112.60
6	R	384	ASP	CA-CB-CG	5.22	117.82	112.60
5	K	92	ASN	OD1-CG-ND2	-5.22	117.38	122.60
5	L	488	ASN	OD1-CG-ND2	-5.21	117.39	122.60
5	N	310	GLU	CA-C-N	5.21	131.50	121.54
5	N	310	GLU	C-N-CA	5.21	131.50	121.54
5	L	498	GLN	OE1-CD-NE2	-5.21	117.39	122.60
6	R	32	ARG	NE-CZ-NH2	5.19	123.87	119.20
4	E	162	GLN	OE1-CD-NE2	-5.18	117.42	122.60
5	K	1014	ARG	CD-NE-CZ	5.18	131.66	124.40
5	L	204	ASN	CA-CB-CG	5.18	117.78	112.60
4	I	111	GLU	CA-C-N	5.18	134.44	121.80
4	I	111	GLU	C-N-CA	5.18	134.44	121.80
5	N	895	ARG	NE-CZ-NH2	5.16	123.85	119.20
4	I	158	ASN	N-CA-C	5.16	117.69	111.40
5	L	828	ARG	NE-CZ-NH1	-5.16	116.34	121.50
5	P	272	ARG	CD-NE-CZ	5.16	131.62	124.40
5	N	335	ASP	CA-CB-CG	5.15	117.75	112.60
5	L	1014	ARG	NE-CZ-NH2	5.14	123.83	119.20
3	D	367	GLU	CB-CG-CD	-5.13	103.88	112.60
6	Q	384	ASP	CA-CB-CG	5.13	117.73	112.60
5	N	293	GLN	OE1-CD-NE2	-5.13	117.47	122.60
5	N	837	ASN	CA-CB-CG	5.13	117.73	112.60
5	M	234	ARG	NE-CZ-NH2	5.12	123.81	119.20
5	O	312	SER	CA-C-N	5.12	126.24	119.84
5	O	312	SER	C-N-CA	5.12	126.24	119.84
4	F	168	ARG	CD-NE-CZ	5.11	131.55	124.40
4	F	172	GLU	CB-CG-CD	5.11	121.28	112.60
5	O	289	GLN	CA-C-N	5.11	125.19	120.34
5	O	289	GLN	C-N-CA	5.11	125.19	120.34
4	F	50	GLN	OE1-CD-NE2	-5.10	117.50	122.60
5	P	868	PRO	N-CA-CB	5.10	105.78	102.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	833	GLN	OE1-CD-NE2	-5.10	117.50	122.60
5	O	862	ARG	NE-CZ-NH2	5.10	123.79	119.20
5	P	1015	GLN	OE1-CD-NE2	-5.09	117.51	122.60
5	O	833	GLN	OE1-CD-NE2	-5.09	117.51	122.60
4	H	156	PHE	CA-CB-CG	5.08	118.88	113.80
6	R	339	HIS	CB-CG-CD2	-5.08	124.59	131.20
5	N	1150	ARG	NE-CZ-NH2	5.08	123.77	119.20
4	I	101	VAL	CA-CB-CG1	5.07	119.03	110.40
6	Q	451	ARG	NE-CZ-NH2	5.07	123.77	119.20
5	N	234	ARG	NE-CZ-NH2	5.07	123.76	119.20
6	R	40	ASP	CA-CB-CG	5.07	117.67	112.60
3	D	341	GLU	CB-CG-CD	-5.07	103.99	112.60
3	D	348	ASP	CA-CB-CG	5.06	117.66	112.60
5	O	521	HIS	CB-CG-CD2	-5.06	124.62	131.20
5	N	1006	ASP	CA-CB-CG	5.06	117.66	112.60
5	P	822	ASN	CA-CB-CG	5.06	117.66	112.60
6	Q	11	ASN	OD1-CG-ND2	-5.06	117.54	122.60
6	R	131	ARG	NE-CZ-NH2	5.05	123.75	119.20
5	L	521	HIS	CB-CG-CD2	-5.05	124.63	131.20
4	J	9	HIS	CB-CG-CD2	-5.05	124.63	131.20
4	H	103	LEU	N-CA-CB	-5.05	103.08	110.86
5	N	498	GLN	OE1-CD-NE2	-5.04	117.56	122.60
6	Q	36	ASP	CA-CB-CG	5.04	117.64	112.60
5	P	166	TYR	N-CA-C	5.03	116.85	111.36
4	J	136	ASN	CA-CB-CG	5.03	117.63	112.60
4	I	136	ASN	OD1-CG-ND2	-5.02	117.58	122.60
4	I	69	SER	N-CA-C	5.02	120.90	109.81
5	O	178	ASN	CA-CB-CG	-5.02	107.58	112.60
4	F	86	VAL	N-CA-C	5.01	115.70	108.48
5	O	38	GLU	CA-C-N	5.01	127.30	120.54
5	O	38	GLU	C-N-CA	5.01	127.30	120.54
6	R	23	ASN	CA-CB-CG	5.00	117.60	112.60

There are no chirality outliers.

All (88) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	176	TYR	Sidechain
3	D	203	PHE	Sidechain
3	D	216	HIS	Sidechain
3	D	418	ARG	Sidechain
3	D	426	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	D	448	TYR	Sidechain
3	D	460	TYR	Sidechain
4	E	102	TYR	Sidechain
4	E	55	TYR	Sidechain
4	F	102	TYR	Sidechain
4	F	117	TYR	Sidechain
4	F	80	TYR	Sidechain
4	G	168	ARG	Sidechain
4	G	80	TYR	Sidechain
4	H	168	ARG	Sidechain
4	I	168	ARG	Sidechain
4	J	80	TYR	Sidechain
5	K	1004	TYR	Sidechain
5	K	1014	ARG	Sidechain
5	K	1083	TYR	Sidechain
5	K	166	TYR	Sidechain
5	K	192	TYR	Sidechain
5	K	286	ARG	Sidechain
5	K	350	TYR	Sidechain
5	K	46	TYR	Sidechain
5	K	477	ARG	Sidechain
5	K	570	ARG	Sidechain
5	L	1139	ARG	Sidechain
5	L	13	ARG	Sidechain
5	L	166	TYR	Sidechain
5	L	327	ARG	Sidechain
5	L	403	TYR	Sidechain
5	L	477	ARG	Sidechain
5	M	13	ARG	Sidechain
5	M	166	TYR	Sidechain
5	M	283	ARG	Sidechain
5	M	403	TYR	Sidechain
5	M	523	ASP	Sidechain
5	M	872	GLU	Sidechain
5	M	943	PHE	Sidechain
5	N	1019	ARG	Sidechain
5	N	1027	TYR	Sidechain
5	N	1128	ARG	Sidechain
5	N	1139	ARG	Sidechain
5	N	166	TYR	Sidechain
5	N	403	TYR	Sidechain
5	N	46	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	N	560	ARG	Sidechain
5	O	1004	TYR	Sidechain
5	O	1026	ARG	Sidechain
5	O	1041	THR	Peptide
5	O	133	TYR	Sidechain
5	O	166	TYR	Sidechain
5	O	210	HIS	Sidechain
5	O	286	ARG	Sidechain
5	O	29	ARG	Sidechain
5	O	350	TYR	Sidechain
5	O	465	ARG	Sidechain
5	O	477	ARG	Sidechain
5	O	523	ASP	Sidechain
5	O	560	ARG	Sidechain
5	P	1019	ARG	Sidechain
5	P	13	ARG	Sidechain
5	P	166	TYR	Sidechain
5	P	403	TYR	Sidechain
5	P	5	PHE	Sidechain
6	Q	117	TYR	Sidechain
6	Q	220	TYR	Sidechain
6	Q	365	TYR	Sidechain
6	Q	367	TYR	Sidechain
6	Q	401	TYR	Sidechain
6	Q	423	TYR	Sidechain
6	Q	78	TYR	Sidechain
6	R	220	TYR	Sidechain
6	R	365	TYR	Sidechain
6	R	367	TYR	Sidechain
6	R	401	TYR	Sidechain
6	R	423	TYR	Sidechain
6	R	79	TYR	Sidechain
6	S	115	HIS	Sidechain
6	S	200	ARG	Sidechain
6	S	235	TYR	Sidechain
6	S	365	TYR	Sidechain
6	S	394	TYR	Sidechain
6	S	412	ARG	Sidechain
6	S	63	TYR	Sidechain
7	V	363	ARG	Sidechain
7	W	535	ARG	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	1871	0	1828	9	0
2	B	2760	0	2729	6	0
2	C	2752	0	2717	8	0
3	D	3769	0	3640	64	0
4	E	1336	0	1323	14	0
4	F	1349	0	1339	26	0
4	G	1336	0	1323	5	0
4	H	1349	0	1339	7	0
4	I	1349	0	1339	5	0
4	J	1349	0	1339	6	0
5	K	7166	0	6971	6	0
5	L	7166	0	6971	16	0
5	M	7166	0	6971	16	0
5	N	7166	0	6971	30	0
5	O	7166	0	6971	24	0
5	P	7166	0	6971	23	0
6	Q	3548	0	3468	9	0
6	R	3548	0	3468	3	0
6	S	3548	0	3468	23	0
7	T	4213	0	4167	21	0
7	U	4321	0	4280	17	0
7	V	4321	0	4280	16	0
7	W	4321	0	4280	14	0
7	X	4321	0	4280	22	0
7	Y	4321	0	4280	14	0
All	All	98678	0	96713	295	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 2.

All (295) 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:O:314:GLY:CA	6:S:122:ASN:HD21	1.27	1.44
5:O:314:GLY:CA	6:S:122:ASN:ND2	2.01	1.24

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:280:ALA:HB3	5:P:130:VAL:HG21	1.31	1.08
5:O:314:GLY:N	6:S:122:ASN:ND2	2.07	1.00
5:O:314:GLY:HA3	6:S:122:ASN:HD21	0.87	1.00
5:O:314:GLY:HA3	6:S:122:ASN:ND2	1.69	0.99
3:D:280:ALA:HB3	5:P:130:VAL:CG2	1.92	0.97
5:K:272:ARG:NH1	5:N:248:ASN:OD1	2.00	0.94
3:D:192:ASP:HA	4:E:173:VAL:CB	1.98	0.93
3:D:192:ASP:HA	4:E:173:VAL:HB	1.50	0.91
3:D:245:VAL:HB	5:O:28:ASP:HA	1.58	0.84
3:D:192:ASP:CA	4:E:173:VAL:HB	2.10	0.80
3:D:192:ASP:HA	4:E:173:VAL:CG1	2.11	0.79
5:M:1105:ASN:HB2	5:N:291:ASP:CG	2.10	0.76
3:D:280:ALA:C	5:P:130:VAL:HG11	2.12	0.75
3:D:33:ASN:OD1	3:D:37:ASN:ND2	2.20	0.74
2:B:191:ARG:NH1	2:C:187:GLU:OE1	2.21	0.74
5:O:314:GLY:HA2	6:S:122:ASN:HD21	1.48	0.74
3:D:191:LEU:HD22	3:D:195:PRO:HD3	1.72	0.72
5:L:520:THR:HA	5:N:311:THR:HA	1.73	0.71
3:D:245:VAL:CB	5:O:28:ASP:HA	2.21	0.70
3:D:196:LYS:HB2	4:F:172:GLU:CG	2.22	0.70
3:D:190:TRP:CH2	4:F:9:HIS:HA	2.28	0.69
3:D:280:ALA:CB	5:P:130:VAL:CG2	2.70	0.68
2:C:85:PHE:O	2:C:158:ARG:NH2	2.26	0.68
7:V:557:ASN:OD1	7:W:569:ARG:NH2	2.25	0.68
3:D:192:ASP:HA	4:E:173:VAL:HG11	1.74	0.68
3:D:280:ALA:HB1	5:P:130:VAL:HB	1.77	0.67
3:D:281:SER:HB2	5:P:130:VAL:HG12	1.75	0.67
3:D:196:LYS:HB2	4:F:172:GLU:CB	2.25	0.66
3:D:196:LYS:HB2	4:F:172:GLU:HG2	1.77	0.66
4:G:91:GLU:CD	4:G:91:GLU:H	2.04	0.66
7:U:371:ASN:OD1	7:U:442:GLN:NE2	2.29	0.65
3:D:188:ILE:HG12	4:F:2:ALA:HB3	1.77	0.65
3:D:192:ASP:H	4:E:173:VAL:CG2	2.10	0.64
3:D:280:ALA:CB	5:P:130:VAL:HB	2.28	0.64
5:M:1105:ASN:CB	5:N:291:ASP:CG	2.71	0.64
7:T:557:ASN:OD1	7:U:569:ARG:NH2	2.31	0.64
7:X:141:ASP:N	7:X:141:ASP:OD1	2.27	0.64
4:F:157:GLN:HG2	4:G:158:ASN:HB3	1.81	0.63
5:L:318:LYS:HE3	5:L:320:TYR:CE2	2.34	0.63
3:D:197:ILE:HG21	4:F:150:PHE:CD1	2.34	0.63
5:O:314:GLY:HA2	6:S:122:ASN:ND2	2.08	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:943:PHE:CE2	5:N:339:GLN:HG3	2.35	0.62
7:W:371:ASN:OD1	7:W:442:GLN:NE2	2.33	0.62
3:D:196:LYS:HG3	4:F:172:GLU:HG3	1.82	0.62
7:X:124:GLU:OE1	7:X:124:GLU:N	2.33	0.61
3:D:280:ALA:CB	5:P:130:VAL:CB	2.78	0.61
7:Y:329:HIS:ND1	7:Y:360:GLU:OE2	2.35	0.60
7:X:516:ARG:NH1	7:Y:428:GLU:OE2	2.35	0.59
7:Y:129:SER:O	7:Y:152:ASN:ND2	2.35	0.59
5:M:1104:ASN:HA	5:N:290:GLY:HA3	1.83	0.59
2:C:57:TRP:NE1	2:C:61:GLU:OE1	2.35	0.59
3:D:191:LEU:HD22	3:D:195:PRO:CD	2.32	0.59
3:D:191:LEU:CD2	3:D:195:PRO:HD3	2.32	0.58
5:O:283:ARG:HD3	6:S:96:SER:O	2.02	0.58
7:W:74:LEU:O	7:W:78:SER:N	2.37	0.58
3:D:280:ALA:C	5:P:130:VAL:CG1	2.76	0.58
7:T:70:ASP:OD1	7:T:404:ARG:NH1	2.36	0.58
5:M:1104:ASN:HA	5:N:290:GLY:CA	2.34	0.58
7:T:386:ASN:O	7:T:479:THR:OG1	2.22	0.58
3:D:191:LEU:CD2	3:D:195:PRO:CD	2.82	0.58
2:B:12:LYS:NZ	3:D:34:GLU:OE2	2.36	0.58
1:A:80:ASN:ND2	7:T:83:THR:OG1	2.37	0.57
3:D:281:SER:CB	5:P:130:VAL:HG12	2.34	0.57
5:M:318:LYS:HE3	5:M:320:TYR:CE2	2.39	0.57
7:Y:4:GLU:OE2	7:Y:8:ARG:NH2	2.38	0.57
3:D:188:ILE:CG1	4:F:2:ALA:HB3	2.35	0.56
7:Y:94:ASP:OD1	7:Y:323:LYS:NZ	2.38	0.56
5:M:1105:ASN:HB2	5:N:291:ASP:OD1	2.06	0.56
7:Y:158:TYR:OH	7:Y:162:GLU:N	2.38	0.55
5:L:519:ILE:HG13	5:N:311:THR:HG22	1.88	0.55
3:D:192:ASP:CA	4:E:173:VAL:CB	2.73	0.55
1:A:131:ILE:HG21	7:T:22:THR:HG23	1.89	0.55
4:F:157:GLN:NE2	4:G:157:GLN:HE21	2.04	0.55
3:D:196:LYS:CA	4:F:172:GLU:HB3	2.37	0.54
7:U:482:ASP:OD1	7:U:482:ASP:N	2.39	0.54
5:M:1102:ARG:HH21	5:N:289:GLN:NE2	2.06	0.54
7:U:172:ASP:O	7:U:176:GLN:N	2.40	0.54
7:X:535:ARG:NH1	7:X:539:ASP:OD2	2.41	0.53
7:V:371:ASN:OD1	7:V:442:GLN:NE2	2.41	0.53
7:X:229:GLU:OE1	7:X:229:GLU:N	2.41	0.53
7:Y:153:ILE:HG23	7:Y:154:PHE:HD1	1.74	0.53
3:D:193:GLY:C	3:D:194:LEU:HG	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:M:1105:ASN:HB2	5:N:291:ASP:CB	2.39	0.53
7:W:153:ILE:HG23	7:W:154:PHE:HD1	1.72	0.53
4:F:91:GLU:CD	4:F:91:GLU:H	2.17	0.53
7:T:148:ASP:OD1	7:T:149:ASN:N	2.41	0.53
5:N:483:TYR:CE1	5:P:504:ARG:HD3	2.44	0.53
7:T:172:ASP:O	7:T:176:GLN:N	2.40	0.53
7:V:148:ASP:OD1	7:V:149:ASN:N	2.42	0.53
7:W:557:ASN:OD1	7:X:569:ARG:NH2	2.42	0.52
7:T:517:THR:N	7:U:569:ARG:O	2.41	0.52
7:W:153:ILE:HG22	7:W:248:VAL:O	2.09	0.52
7:T:164:ASN:OD1	7:T:165:ALA:N	2.42	0.52
7:T:153:ILE:HG23	7:T:154:PHE:CD1	2.44	0.51
7:T:206:ILE:HG22	7:T:210:ILE:CD1	2.39	0.51
7:T:34:LYS:NZ	7:T:495:GLU:OE2	2.31	0.51
7:V:167:PHE:HD1	7:V:241:ILE:HD11	1.75	0.51
5:O:309:THR:HG23	5:O:320:TYR:CE1	2.46	0.51
7:T:464:ARG:O	7:T:466:ARG:NH2	2.43	0.51
5:L:498:GLN:HA	5:N:344:SER:HA	1.91	0.51
5:O:283:ARG:CB	6:S:96:SER:O	2.59	0.51
3:D:196:LYS:HB2	4:F:172:GLU:HB2	1.91	0.51
4:H:157:GLN:HA	4:I:158:ASN:HD22	1.75	0.51
4:I:116:THR:HG22	4:I:158:ASN:HA	1.93	0.50
2:B:232:ASP:OD1	2:B:233:THR:N	2.44	0.50
5:L:520:THR:HA	5:N:311:THR:CA	2.42	0.50
5:M:357:LYS:HZ3	5:M:364:ASP:CG	2.19	0.50
5:P:1026:ARG:HG3	5:P:1026:ARG:HH21	1.76	0.50
6:R:168:VAL:HG11	6:S:190:SER:OG	2.11	0.50
6:S:209:GLU:HB3	6:S:226:GLU:HG2	1.94	0.50
7:X:513:ILE:HG23	7:Y:572:LYS:HA	1.92	0.50
5:L:520:THR:CA	5:N:311:THR:HA	2.42	0.49
7:W:172:ASP:O	7:W:176:GLN:N	2.42	0.49
3:D:196:LYS:C	4:F:172:GLU:HB3	2.37	0.49
3:D:153:TYR:CE2	4:E:155:GLN:HB2	2.47	0.49
5:N:291:ASP:OD1	5:N:337:SER:HA	2.11	0.49
5:L:497:GLY:CA	5:N:344:SER:OG	2.61	0.49
1:A:30:ASP:OD1	1:A:30:ASP:N	2.45	0.49
5:N:560:ARG:HH21	5:N:560:ARG:HA	1.78	0.49
7:U:123:LEU:HD12	7:U:303:PHE:CE2	2.47	0.49
4:H:101:VAL:HB	4:H:171:VAL:CG2	2.42	0.49
1:A:124:ASP:OD1	1:A:125:LEU:N	2.46	0.49
5:O:283:ARG:CG	6:S:96:SER:O	2.61	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:Q:233:GLU:HG2	6:Q:240:ILE:HD12	1.94	0.49
7:W:50:VAL:HG22	7:W:90:MET:HE3	1.95	0.49
2:B:16:LYS:NZ	3:D:30:ASP:OD2	2.45	0.49
1:A:131:ILE:HG21	7:T:22:THR:CG2	2.44	0.48
7:U:148:ASP:OD1	7:U:149:ASN:N	2.46	0.48
5:P:318:LYS:HE3	5:P:320:TYR:CD2	2.47	0.48
2:B:191:ARG:O	2:B:196:SER:OG	2.30	0.48
4:J:129:LYS:HE3	4:J:142:VAL:O	2.13	0.48
7:T:509:GLU:HA	7:T:513:ILE:HD12	1.95	0.48
7:U:124:GLU:O	7:U:133:ARG:N	2.47	0.48
7:W:90:MET:HE1	7:W:326:LYS:HB2	1.96	0.48
7:T:206:ILE:HG22	7:T:210:ILE:HD11	1.95	0.48
3:D:206:PHE:CZ	4:G:170:ILE:HD13	2.49	0.48
7:W:114:ASN:N	7:W:313:ASN:OD1	2.47	0.48
7:X:557:ASN:OD1	7:X:557:ASN:N	2.47	0.48
5:N:872:GLU:OE2	5:N:875:LYS:HE2	2.13	0.48
3:D:306:GLU:CD	3:D:432:LYS:HZ3	2.22	0.47
7:X:123:LEU:HD12	7:X:303:PHE:CE2	2.49	0.47
3:D:192:ASP:N	4:E:173:VAL:HB	2.28	0.47
1:A:142:LEU:O	1:A:157:SER:OG	2.31	0.47
3:D:320:ASN:C	3:D:321:ASN:HD22	2.21	0.47
5:M:943:PHE:CD2	5:N:339:GLN:HG3	2.49	0.47
5:K:998:TRP:CD1	5:K:999:GLU:H	2.32	0.47
4:E:172:GLU:C	4:E:173:VAL:HG22	2.40	0.47
6:Q:225:LYS:HG2	6:Q:228:GLU:HB2	1.96	0.47
7:X:517:THR:N	7:Y:569:ARG:O	2.45	0.47
7:V:151:GLY:O	7:V:226:LYS:NZ	2.36	0.47
7:X:40:GLY:HA3	7:X:338:LEU:HD12	1.97	0.47
7:V:167:PHE:CB	7:V:183:LEU:HD23	2.45	0.47
1:A:54:GLU:OE1	1:A:54:GLU:N	2.42	0.46
7:X:475:ASP:OD1	7:X:476:ASP:N	2.45	0.46
5:M:1105:ASN:HB2	5:N:291:ASP:HB2	1.97	0.46
7:X:435:LEU:HD22	7:X:460:ILE:HD13	1.96	0.46
4:J:116:THR:HG22	4:J:158:ASN:HA	1.98	0.46
4:H:91:GLU:H	4:H:91:GLU:CD	2.24	0.46
5:O:144:LYS:HE3	5:P:19:ASP:HB2	1.96	0.46
7:V:211:ASN:ND2	7:V:218:ALA:O	2.48	0.46
7:X:482:ASP:N	7:X:482:ASP:OD1	2.49	0.46
3:D:196:LYS:CB	4:F:172:GLU:CG	2.91	0.46
7:T:516:ARG:NH1	7:U:426:ILE:O	2.49	0.46
5:O:313:PRO:C	6:S:122:ASN:ND2	2.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:225:ASP:OD1	2:C:229:ASN:N	2.49	0.46
3:D:296:TYR:C	3:D:298:SER:H	2.24	0.46
5:L:885:ASN:HD21	5:L:887:ASP:HB3	1.80	0.46
5:O:309:THR:HG23	5:O:320:TYR:CD1	2.51	0.46
7:X:312:THR:HG22	7:X:314:GLY:H	1.81	0.46
3:D:153:TYR:CZ	4:E:155:GLN:HB2	2.51	0.45
3:D:460:TYR:CE2	4:I:162:GLN:HA	2.51	0.45
3:D:190:TRP:CH2	4:F:12:LEU:HB2	2.50	0.45
7:W:153:ILE:HG23	7:W:154:PHE:CD1	2.50	0.45
5:P:318:LYS:HE3	5:P:320:TYR:CE2	2.52	0.45
5:P:995:GLN:C	5:P:997:LYS:H	2.24	0.45
7:V:126:ASN:ND2	7:V:129:SER:OG	2.46	0.45
7:X:172:ASP:O	7:X:176:GLN:N	2.42	0.45
6:Q:213:ILE:HD13	6:Q:215:LYS:HE3	1.97	0.45
7:U:375:GLU:OE1	7:U:375:GLU:N	2.47	0.45
3:D:280:ALA:O	5:P:130:VAL:HG11	2.16	0.45
4:J:91:GLU:N	4:J:91:GLU:CD	2.75	0.45
2:C:324:ASP:OD1	2:C:325:ASN:N	2.49	0.45
6:S:123:ASN:HA	6:S:126:ILE:HG22	1.99	0.45
7:V:167:PHE:CD1	7:V:241:ILE:HD11	2.52	0.45
4:F:61:VAL:HG12	4:F:103:LEU:HA	1.98	0.45
7:V:40:GLY:HA3	7:V:338:LEU:HD12	1.99	0.45
7:W:129:SER:OG	7:W:131:SER:OG	2.33	0.45
3:D:153:TYR:CZ	3:D:181:THR:HB	2.52	0.45
4:H:101:VAL:HB	4:H:171:VAL:HG22	1.99	0.45
3:D:69:VAL:O	3:D:80:TYR:OH	2.34	0.45
7:V:180:ARG:NE	7:V:194:ASP:OD1	2.42	0.44
4:H:129:LYS:HE3	4:H:142:VAL:O	2.17	0.44
5:N:291:ASP:CG	5:N:337:SER:HA	2.43	0.44
7:T:74:LEU:O	7:T:78:SER:N	2.50	0.44
5:L:996:LEU:CD1	5:L:996:LEU:H	2.30	0.44
6:R:144:ILE:HG22	6:S:144:ILE:HD12	1.99	0.44
7:Y:114:ASN:OD1	7:Y:313:ASN:N	2.49	0.44
7:Y:183:LEU:O	7:Y:190:VAL:N	2.48	0.44
4:F:56:LYS:HZ2	4:F:111:GLU:CD	2.26	0.44
5:L:520:THR:HG22	5:N:310:GLU:O	2.18	0.44
6:Q:123:ASN:HA	6:Q:126:ILE:HG22	2.00	0.44
7:X:114:ASN:OD1	7:X:313:ASN:N	2.51	0.44
4:J:14:LYS:HE2	4:J:90:PRO:O	2.18	0.44
7:X:153:ILE:HG22	7:X:248:VAL:O	2.18	0.44
7:X:312:THR:HG22	7:X:314:GLY:N	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:104:GLU:CD	4:F:168:ARG:HE	2.25	0.44
5:N:186:TYR:CE1	5:N:223:LYS:HE2	2.53	0.44
5:K:560:ARG:HE	5:K:560:ARG:HA	1.82	0.43
7:T:577:SER:C	7:T:578:LEU:HD12	2.43	0.43
7:X:134:LEU:N	7:X:147:TYR:O	2.51	0.43
4:F:157:GLN:CD	4:G:158:ASN:H	2.26	0.43
5:L:996:LEU:H	5:L:996:LEU:HD12	1.82	0.43
7:W:79:ASN:ND2	7:W:419:GLY:O	2.50	0.43
3:D:190:TRP:HZ3	4:F:9:HIS:CG	2.37	0.43
5:L:497:GLY:HA2	5:N:344:SER:OG	2.17	0.43
6:Q:198:LEU:HD22	6:S:202:THR:HB	2.00	0.43
6:S:209:GLU:H	6:S:226:GLU:CD	2.26	0.43
3:D:209:TYR:CE1	3:D:446:GLY:HA2	2.54	0.43
4:F:152:ASP:CG	4:F:154:LYS:HZ3	2.27	0.43
6:Q:381:LYS:HZ2	6:Q:411:ASP:CG	2.25	0.43
5:L:318:LYS:HE3	5:L:320:TYR:CZ	2.54	0.43
1:A:214:VAL:HG12	1:A:218:ILE:HD12	2.00	0.43
5:K:318:LYS:NZ	5:P:802:GLU:OE2	2.42	0.43
7:U:153:ILE:HG22	7:U:248:VAL:O	2.19	0.43
7:X:137:ILE:HD12	7:X:305:LEU:HD21	2.01	0.43
7:V:52:GLU:OE2	7:V:54:ARG:NE	2.51	0.42
5:O:981:LYS:HZ3	5:O:981:LYS:N	2.17	0.42
7:T:210:ILE:HG21	7:T:218:ALA:HB2	2.00	0.42
3:D:176:TYR:OH	3:D:181:THR:HG21	2.19	0.42
7:T:185:VAL:HG23	7:T:190:VAL:CG2	2.48	0.42
4:I:14:LYS:HE2	4:I:93:ALA:HB3	2.01	0.42
7:V:226:LYS:HZ2	7:V:254:ASP:CG	2.27	0.42
1:A:48:GLU:OE1	1:A:48:GLU:N	2.52	0.42
2:C:253:ASP:OD1	2:C:254:VAL:N	2.52	0.42
5:K:60:LYS:HE3	5:K:60:LYS:H	1.85	0.42
7:U:544:ASP:OD1	7:U:545:PHE:N	2.52	0.42
7:V:38:LEU:HD21	7:V:415:VAL:HG13	2.01	0.42
3:D:196:LYS:CB	4:F:172:GLU:CB	2.96	0.42
3:D:245:VAL:HB	5:O:28:ASP:CA	2.40	0.42
5:O:297:SER:CB	6:S:83:ARG:HG2	2.50	0.42
4:E:129:LYS:HE3	4:E:143:GLU:HA	2.02	0.42
5:L:497:GLY:C	5:N:344:SER:OG	2.62	0.42
5:P:92:ASN:HD22	5:P:94:ASP:HB2	1.85	0.42
3:D:232:ILE:O	3:D:234:LYS:HE2	2.19	0.42
7:U:34:LYS:NZ	7:U:495:GLU:OE2	2.36	0.42
5:P:60:LYS:HE2	5:P:173:GLU:OE1	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:W:244:LYS:O	7:W:246:VAL:HG23	2.20	0.42
7:Y:505:LYS:NZ	7:Y:509:GLU:OE2	2.52	0.42
5:M:869:MET:HE1	5:M:877:TYR:CE1	2.55	0.41
6:Q:190:SER:HB3	6:S:186:PHE:CD1	2.54	0.41
7:U:153:ILE:HG23	7:U:154:PHE:CD1	2.54	0.41
7:X:167:PHE:HB3	7:X:241:ILE:HD11	2.02	0.41
3:D:265:TYR:CE2	3:D:285:ARG:HB3	2.55	0.41
4:J:129:LYS:HE3	4:J:142:VAL:C	2.45	0.41
5:L:497:GLY:HA2	5:N:344:SER:CB	2.50	0.41
5:N:483:TYR:CD1	5:P:504:ARG:HD3	2.55	0.41
7:V:172:ASP:O	7:V:176:GLN:N	2.52	0.41
3:D:196:LYS:N	4:F:172:GLU:HB3	2.35	0.41
7:U:549:ASP:OD2	7:U:564:THR:OG1	2.33	0.41
2:C:281:GLN:NE2	2:C:345:VAL:O	2.51	0.41
3:D:245:VAL:CG1	5:O:28:ASP:HA	2.50	0.41
2:B:268:VAL:HG23	2:B:321:VAL:HG22	2.01	0.41
3:D:192:ASP:N	4:E:173:VAL:CG2	2.82	0.41
4:H:156:PHE:CD1	4:H:156:PHE:N	2.89	0.41
4:I:11:GLU:OE2	4:I:94:LYS:HE3	2.19	0.41
7:U:411:TYR:O	7:U:415:VAL:HG23	2.21	0.41
4:E:172:GLU:HB2	4:E:173:VAL:HG22	2.03	0.41
5:O:504:ARG:HD3	5:P:483:TYR:CE2	2.56	0.41
2:C:257:VAL:O	2:C:259:LYS:N	2.54	0.41
5:O:48:LYS:HE2	5:O:52:ASP:OD2	2.20	0.41
6:R:240:ILE:HG12	6:S:235:TYR:CD1	2.56	0.41
3:D:196:LYS:C	4:F:172:GLU:CB	2.94	0.41
3:D:462:ASP:CB	4:H:168:ARG:HH22	2.34	0.41
5:O:996:LEU:CD1	5:O:996:LEU:H	2.34	0.41
7:U:188:GLN:N	7:U:188:GLN:OE1	2.54	0.41
4:F:157:GLN:HE21	4:F:157:GLN:HB3	1.75	0.41
4:J:125:ASP:O	4:J:146:GLY:HA3	2.22	0.41
5:K:324:GLU:OE2	5:P:942:LYS:NZ	2.54	0.41
5:N:311:THR:HG23	5:N:317:THR:OG1	2.21	0.41
7:Y:173:GLU:O	7:Y:176:GLN:NE2	2.54	0.41
5:M:369:THR:HG21	5:M:376:LYS:HE3	2.02	0.40
6:Q:402:VAL:HG13	6:Q:424:ARG:HD2	2.01	0.40
3:D:196:LYS:O	3:D:197:ILE:HG23	2.21	0.40
5:M:999:GLU:H	5:M:999:GLU:CD	2.29	0.40
5:N:999:GLU:H	5:N:999:GLU:CD	2.29	0.40
5:O:283:ARG:CD	6:S:96:SER:O	2.69	0.40
6:Q:342:LEU:HB3	6:Q:358:LEU:HD22	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:V:167:PHE:HB2	7:V:183:LEU:HD23	2.03	0.40
5:L:996:LEU:HD12	5:L:996:LEU:N	2.36	0.40
7:Y:437:VAL:HG11	7:Y:440:LEU:HD21	2.04	0.40
5:M:56:LYS:HE3	5:M:175:ASP:HB2	2.04	0.40
6:S:130:TYR:HE1	6:S:144:ILE:HD11	1.87	0.40
6:S:214:LYS:HE2	6:S:218:GLY:O	2.22	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	232/234 (99%)	223 (96%)	9 (4%)	0	100	100
2	B	346/348 (99%)	341 (99%)	5 (1%)	0	100	100
2	C	345/348 (99%)	339 (98%)	6 (2%)	0	100	100
3	D	451/1019 (44%)	407 (90%)	41 (9%)	3 (1%)	18	55
4	E	168/173 (97%)	156 (93%)	9 (5%)	3 (2%)	6	33
4	F	170/173 (98%)	160 (94%)	10 (6%)	0	100	100
4	G	168/173 (97%)	156 (93%)	9 (5%)	3 (2%)	6	33
4	H	170/173 (98%)	152 (89%)	11 (6%)	7 (4%)	2	18
4	I	170/173 (98%)	152 (89%)	13 (8%)	5 (3%)	3	23
4	J	170/173 (98%)	156 (92%)	10 (6%)	4 (2%)	4	27
5	K	900/1152 (78%)	851 (95%)	49 (5%)	0	100	100
5	L	900/1152 (78%)	846 (94%)	52 (6%)	2 (0%)	43	77
5	M	900/1152 (78%)	856 (95%)	43 (5%)	1 (0%)	48	83
5	N	900/1152 (78%)	845 (94%)	46 (5%)	9 (1%)	12	47
5	O	900/1152 (78%)	834 (93%)	58 (6%)	8 (1%)	14	49

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	P	900/1152 (78%)	842 (94%)	52 (6%)	6 (1%)	18	55
6	Q	456/458 (100%)	431 (94%)	23 (5%)	2 (0%)	30	66
6	R	456/458 (100%)	431 (94%)	25 (6%)	0	100	100
6	S	456/458 (100%)	428 (94%)	26 (6%)	2 (0%)	30	66
7	T	534/587 (91%)	502 (94%)	31 (6%)	1 (0%)	43	77
7	U	547/587 (93%)	516 (94%)	31 (6%)	0	100	100
7	V	547/587 (93%)	521 (95%)	26 (5%)	0	100	100
7	W	547/587 (93%)	524 (96%)	23 (4%)	0	100	100
7	X	547/587 (93%)	526 (96%)	21 (4%)	0	100	100
7	Y	547/587 (93%)	522 (95%)	25 (5%)	0	100	100
All	All	12427/14795 (84%)	11717 (94%)	654 (5%)	56 (0%)	26	62

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	E	70	PRO
4	H	93	ALA
4	I	93	ALA
4	J	93	ALA
4	J	111	GLU
6	Q	227	PHE
6	S	157	GLY
3	D	190	TRP
4	E	161	GLU
4	G	29	LYS
4	J	73	ASP
5	N	311	THR
5	N	913	LEU
5	O	313	PRO
5	O	360	GLU
5	P	996	LEU
4	E	76	ASN
4	H	92	ASN
4	H	98	ALA
4	I	92	ASN
5	M	996	LEU
5	N	869	MET
5	N	996	LEU

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Mol	Chain	Res	Type
5	N	1116	VAL
5	O	461	PHE
5	O	519	ILE
6	S	83	ARG
3	D	297	THR
3	D	313	SER
4	G	159	ARG
4	H	73	ASP
4	H	111	GLU
4	H	156	PHE
4	I	70	PRO
5	P	1010	LEU
4	G	69	SER
4	I	69	SER
4	I	73	ASP
4	J	143	GLU
5	L	1003	ASN
5	N	28	ASP
5	N	340	GLY
5	O	93	ASP
5	O	833	GLN
5	O	1040	THR
5	P	340	GLY
6	Q	432	SER
4	H	70	PRO
5	N	337	SER
5	O	493	GLY
5	P	1043	LEU
5	L	340	GLY
5	P	557	ILE
7	T	409	PRO
5	N	583	VAL
5	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	209/209 (100%)	208 (100%)	1 (0%)	81	81
2	B	311/311 (100%)	310 (100%)	1 (0%)	86	84
2	C	310/311 (100%)	309 (100%)	1 (0%)	86	84
3	D	417/928 (45%)	406 (97%)	11 (3%)	40	60
4	E	151/153 (99%)	144 (95%)	7 (5%)	24	46
4	F	152/153 (99%)	142 (93%)	10 (7%)	15	37
4	G	151/153 (99%)	149 (99%)	2 (1%)	61	72
4	H	152/153 (99%)	141 (93%)	11 (7%)	13	35
4	I	152/153 (99%)	137 (90%)	15 (10%)	7	24
4	J	152/153 (99%)	142 (93%)	10 (7%)	15	37
5	K	800/1010 (79%)	790 (99%)	10 (1%)	61	72
5	L	800/1010 (79%)	786 (98%)	14 (2%)	51	67
5	M	800/1010 (79%)	791 (99%)	9 (1%)	65	74
5	N	800/1010 (79%)	781 (98%)	19 (2%)	43	63
5	O	800/1010 (79%)	785 (98%)	15 (2%)	50	66
5	P	800/1010 (79%)	781 (98%)	19 (2%)	43	63
6	Q	405/405 (100%)	396 (98%)	9 (2%)	45	64
6	R	405/405 (100%)	400 (99%)	5 (1%)	63	73
6	S	405/405 (100%)	394 (97%)	11 (3%)	39	59
7	T	459/495 (93%)	456 (99%)	3 (1%)	76	79
7	U	471/495 (95%)	464 (98%)	7 (2%)	57	70
7	V	471/495 (95%)	471 (100%)	0	100	100
7	W	471/495 (95%)	470 (100%)	1 (0%)	87	85
7	X	471/495 (95%)	464 (98%)	7 (2%)	57	70
7	Y	471/495 (95%)	470 (100%)	1 (0%)	87	85
All	All	10986/12922 (85%)	10787 (98%)	199 (2%)	51	67

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ASP
2	B	271	SER
2	C	206	ASP
3	D	176	TYR

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Mol	Chain	Res	Type
3	D	190	TRP
3	D	191	LEU
3	D	212	THR
3	D	236	ASN
3	D	277	GLN
3	D	292	ASP
3	D	306	GLU
3	D	320	ASN
3	D	367	GLU
3	D	470	GLU
4	E	9	HIS
4	E	70	PRO
4	E	150	PHE
4	E	151	PHE
4	E	157	GLN
4	E	159	ARG
4	E	166	LYS
4	F	9	HIS
4	F	41	GLN
4	F	71	GLU
4	F	75	LYS
4	F	78	ILE
4	F	80	TYR
4	F	91	GLU
4	F	101	VAL
4	F	157	GLN
4	F	172	GLU
4	G	75	LYS
4	G	91	GLU
4	H	11	GLU
4	H	51	GLU
4	H	88	VAL
4	H	91	GLU
4	H	101	VAL
4	H	111	GLU
4	H	125	ASP
4	H	126	LEU
4	H	136	ASN
4	H	143	GLU
4	H	156	PHE
4	I	3	ILE
4	I	38	ASN

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Mol	Chain	Res	Type
4	I	51	GLU
4	I	68	LYS
4	I	88	VAL
4	I	101	VAL
4	I	108	VAL
4	I	111	GLU
4	I	125	ASP
4	I	127	VAL
4	I	136	ASN
4	I	142	VAL
4	I	143	GLU
4	I	154	LYS
4	I	162	GLN
4	J	38	ASN
4	J	51	GLU
4	J	68	LYS
4	J	88	VAL
4	J	91	GLU
4	J	101	VAL
4	J	111	GLU
4	J	125	ASP
4	J	127	VAL
4	J	157	GLN
5	K	33	GLN
5	K	97	LYS
5	K	170	THR
5	K	269	GLU
5	K	560	ARG
5	K	945	GLU
5	K	981	LYS
5	K	1007	LEU
5	K	1078	LYS
5	K	1133	THR
5	L	97	LYS
5	L	103	LYS
5	L	144	LYS
5	L	198	GLU
5	L	257	ASN
5	L	342	GLU
5	L	358	ARG
5	L	366	GLU
5	L	465	ARG

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Mol	Chain	Res	Type
5	L	560	ARG
5	L	942	LYS
5	L	945	GLU
5	L	1014	ARG
5	L	1075	LYS
5	M	33	GLN
5	M	269	GLU
5	M	291	ASP
5	M	342	GLU
5	M	358	ARG
5	M	833	GLN
5	M	981	LYS
5	M	1045	GLU
5	M	1134	GLU
5	N	33	GLN
5	N	185	THR
5	N	257	ASN
5	N	283	ARG
5	N	339	GLN
5	N	342	GLU
5	N	515	ASP
5	N	520	THR
5	N	541	GLU
5	N	584	ASN
5	N	822	ASN
5	N	833	GLN
5	N	942	LYS
5	N	1045	GLU
5	N	1075	LYS
5	N	1078	LYS
5	N	1086	ASP
5	N	1087	ASP
5	N	1134	GLU
5	O	4	ASN
5	O	32	GLN
5	O	33	GLN
5	O	97	LYS
5	O	144	LYS
5	O	170	THR
5	O	283	ARG
5	O	294	ASP
5	O	322	GLN

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Mol	Chain	Res	Type
5	O	526	ILE
5	O	942	LYS
5	O	981	LYS
5	O	1075	LYS
5	O	1078	LYS
5	O	1133	THR
5	P	19	ASP
5	P	97	LYS
5	P	144	LYS
5	P	269	GLU
5	P	283	ARG
5	P	822	ASN
5	P	861	THR
5	P	869	MET
5	P	884	GLU
5	P	892	VAL
5	P	981	LYS
5	P	987	MET
5	P	995	GLN
5	P	997	LYS
5	P	1045	GLU
5	P	1078	LYS
5	P	1087	ASP
5	P	1092	LYS
5	P	1143	ARG
6	Q	26	GLU
6	Q	32	ARG
6	Q	40	ASP
6	Q	70	ARG
6	Q	83	ARG
6	Q	192	ASP
6	Q	225	LYS
6	Q	231	ASP
6	Q	414	ASP
6	R	10	GLU
6	R	70	ARG
6	R	192	ASP
6	R	209	GLU
6	R	320	ASN
6	S	26	GLU
6	S	40	ASP
6	S	70	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
6	S	83	ARG
6	S	95	GLU
6	S	124	ASN
6	S	192	ASP
6	S	224	LYS
6	S	226	GLU
6	S	227	PHE
6	S	356	LYS
7	T	102	ILE
7	T	354	GLU
7	T	428	GLU
7	U	3	VAL
7	U	57	SER
7	U	114	ASN
7	U	247	TYR
7	U	453	ASN
7	U	481	ASN
7	U	482	ASP
7	W	453	ASN
7	X	48	ASN
7	X	141	ASP
7	X	167	PHE
7	X	241	ILE
7	X	247	TYR
7	X	264	ILE
7	X	557	ASN
7	Y	202	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (108) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	ASN
2	B	111	GLN
3	D	268	ASN
3	D	277	GLN
3	D	303	ASN
3	D	321	ASN
4	E	76	ASN
4	E	82	ASN
4	E	92	ASN
4	E	162	GLN
4	F	50	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
4	F	158	ASN
4	G	157	GLN
4	H	153	ASN
4	I	7	ASN
4	I	38	ASN
4	I	45	ASN
4	I	158	ASN
4	J	45	ASN
4	J	153	ASN
4	J	157	GLN
5	K	248	ASN
5	K	258	ASN
5	K	264	ASN
5	K	276	GLN
5	K	293	GLN
5	K	332	GLN
5	K	393	GLN
5	K	576	GLN
5	K	837	ASN
5	K	910	ASN
5	K	1003	ASN
5	K	1105	ASN
5	L	49	ASN
5	L	92	ASN
5	L	248	ASN
5	L	258	ASN
5	L	441	ASN
5	L	443	GLN
5	L	576	GLN
5	L	590	ASN
5	L	799	GLN
5	L	885	ASN
5	L	910	ASN
5	L	1126	GLN
5	M	92	ASN
5	M	254	ASN
5	M	258	ASN
5	M	393	GLN
5	M	799	GLN
5	M	833	GLN
5	M	910	ASN
5	N	195	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
5	N	257	ASN
5	N	276	GLN
5	N	289	GLN
5	N	339	GLN
5	N	356	ASN
5	N	441	ASN
5	N	799	GLN
5	N	833	GLN
5	N	944	ASN
5	N	995	GLN
5	O	195	ASN
5	O	254	ASN
5	O	276	GLN
5	O	356	ASN
5	O	393	GLN
5	O	443	GLN
5	O	499	ASN
5	O	576	GLN
5	O	590	ASN
5	O	1003	ASN
5	O	1105	ASN
5	P	92	ASN
5	P	126	GLN
5	P	386	ASN
5	P	441	ASN
5	P	556	HIS
5	P	590	ASN
5	P	822	ASN
5	P	914	GLN
6	Q	23	ASN
6	Q	320	ASN
6	R	20	GLN
6	S	20	GLN
6	S	102	HIS
6	S	122	ASN
6	S	267	HIS
7	T	269	GLN
7	T	342	GLN
7	T	376	GLN
7	T	543	GLN
7	U	407	HIS
7	U	497	ASN

*Continued on next page...*

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Mol	Chain	Res	Type
7	U	543	GLN
7	V	126	ASN
7	V	269	GLN
7	X	120	GLN
7	X	171	HIS
7	X	204	ASN
7	X	258	GLN
7	X	262	ASN
7	X	540	ASN
7	Y	120	GLN
7	Y	204	ASN
7	Y	262	ASN
7	Y	465	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.

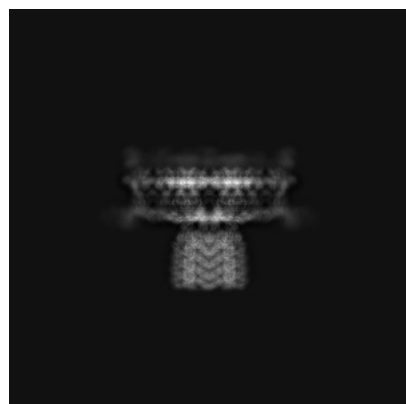
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55967. These allow visual inspection of the internal detail of the map and identification of artifacts.

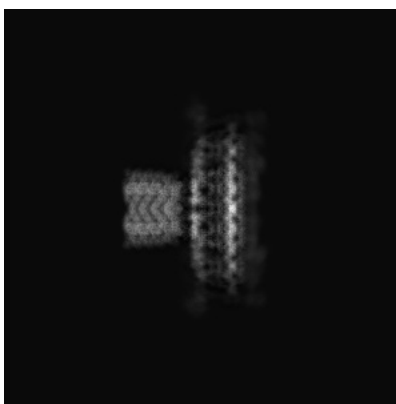
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

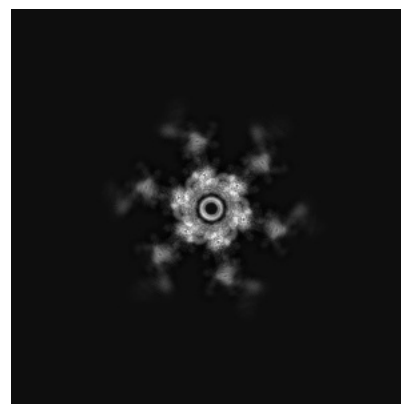
#### 6.1.1 Primary map



X

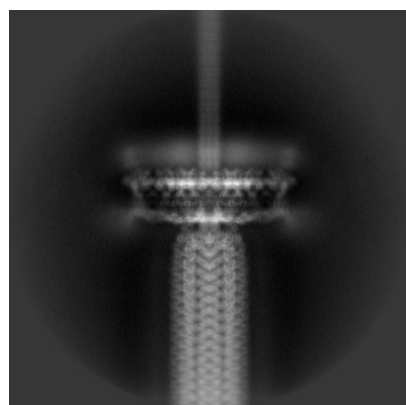


Y

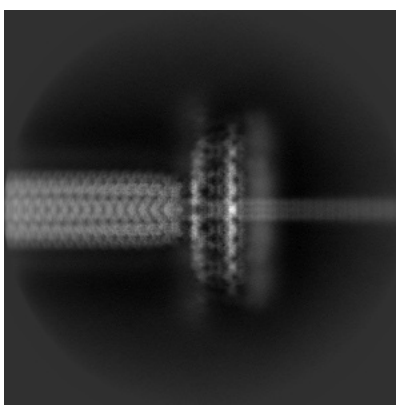


Z

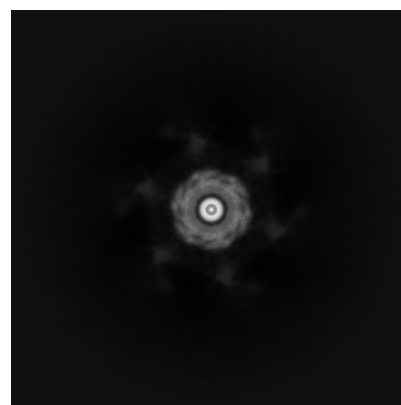
#### 6.1.2 Raw map



X



Y

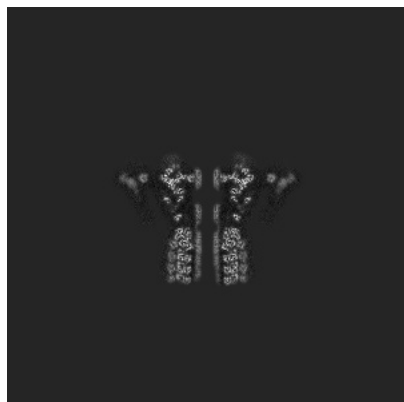


Z

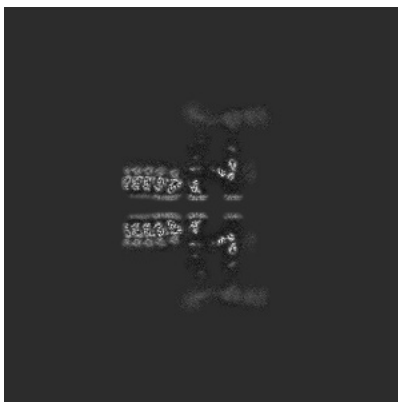
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

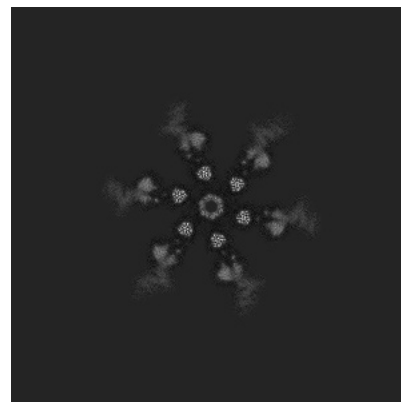
### 6.2.1 Primary map



X Index: 320

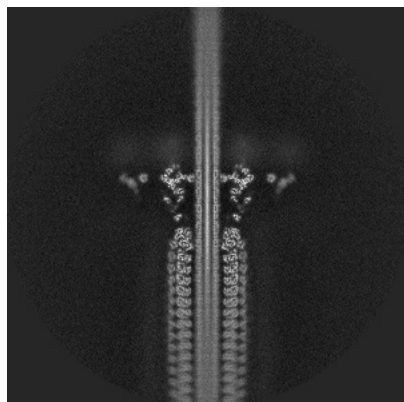


Y Index: 320

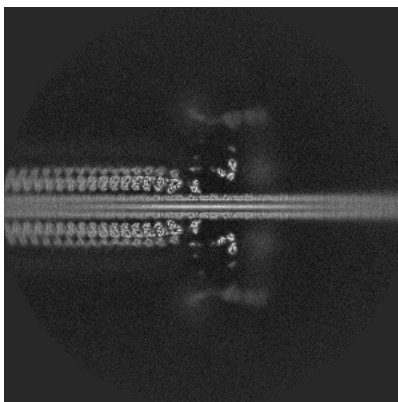


Z Index: 320

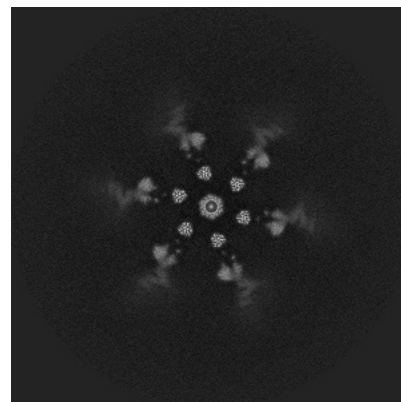
### 6.2.2 Raw map



X Index: 320



Y Index: 320



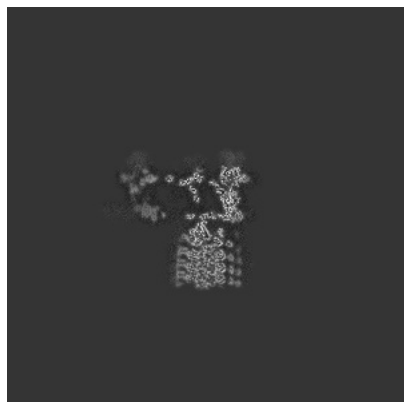
Z Index: 320

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

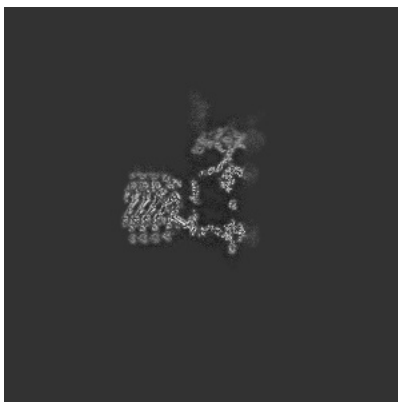


## 6.3 Largest variance slices [i](#)

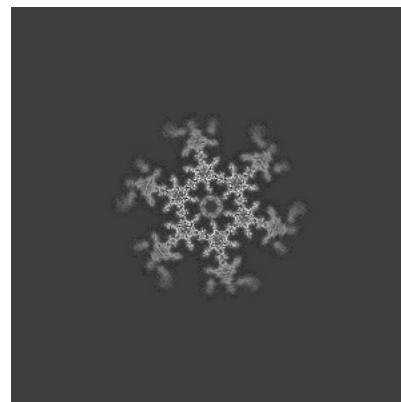
### 6.3.1 Primary map



X Index: 357

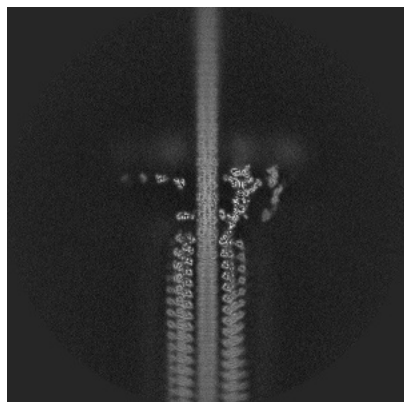


Y Index: 292

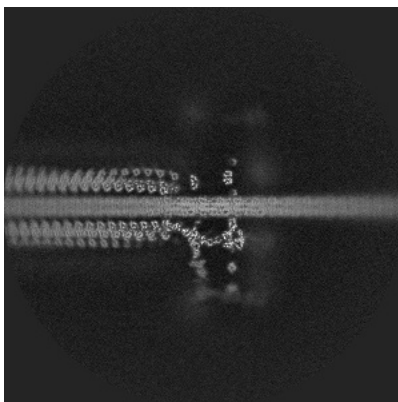


Z Index: 361

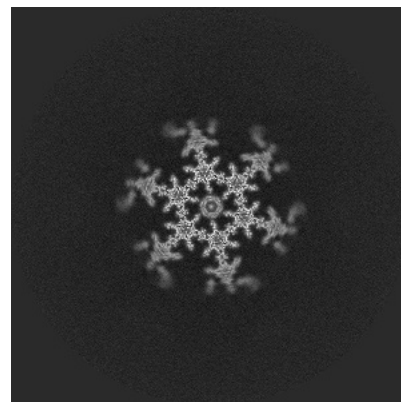
### 6.3.2 Raw map



X Index: 310



Y Index: 330

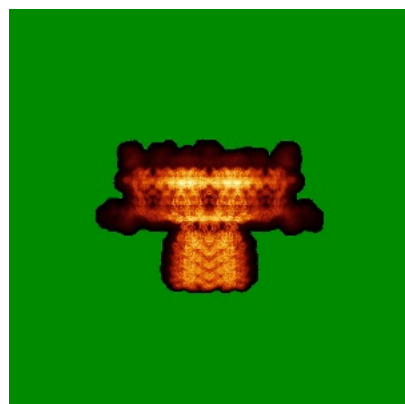


Z Index: 361

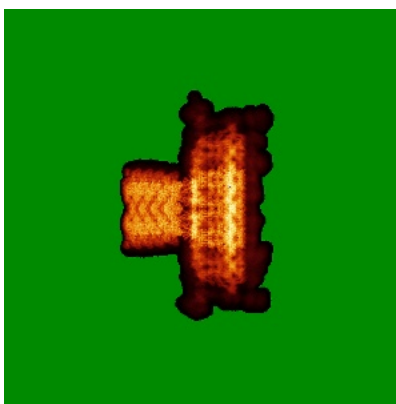
The images above show the largest variance slices of the map in three orthogonal directions.

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

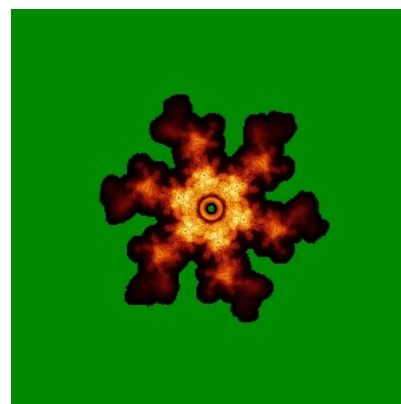
### 6.4.1 Primary map



X

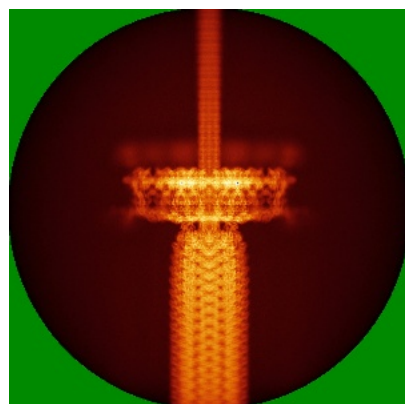


Y

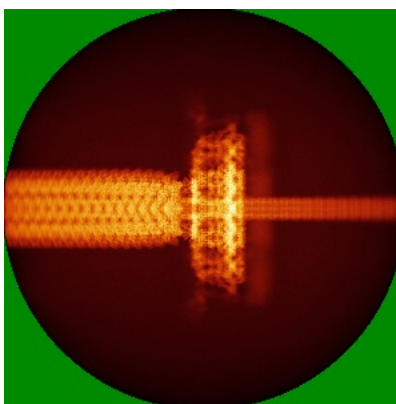


Z

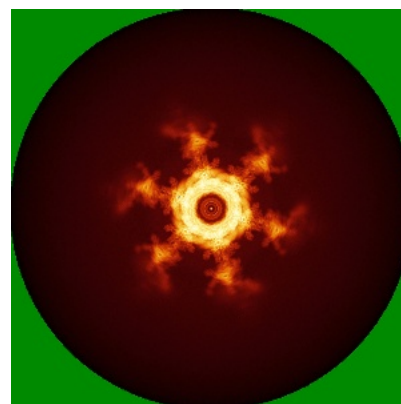
### 6.4.2 Raw map



X



Y

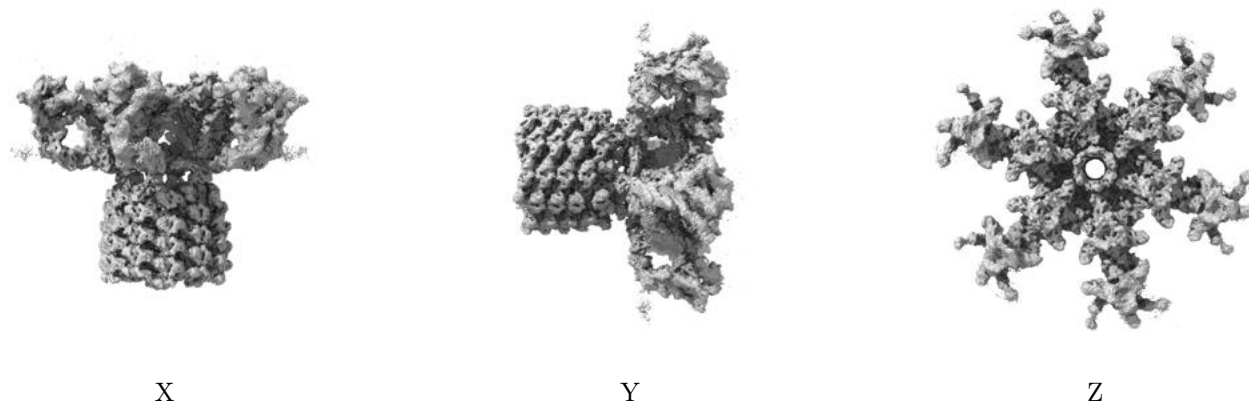


Z

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.

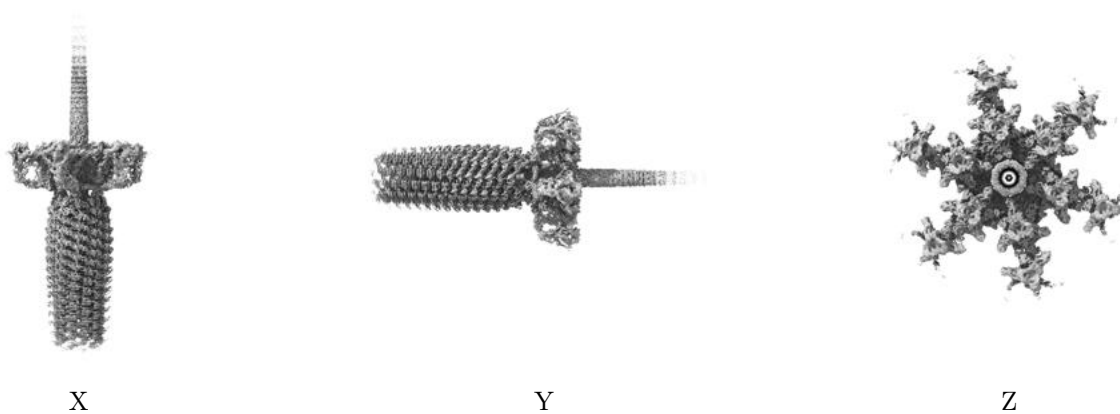
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. 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.

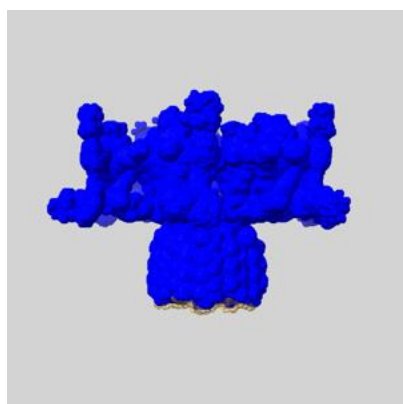
## 6.6 Mask visualisation [i](#)

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

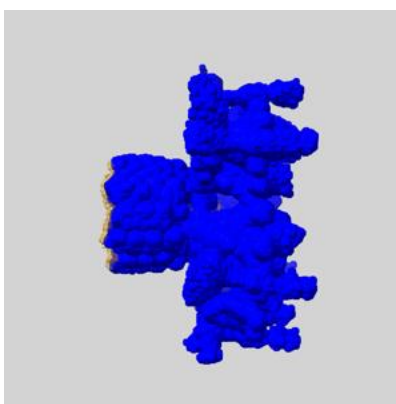
A mask typically either:

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

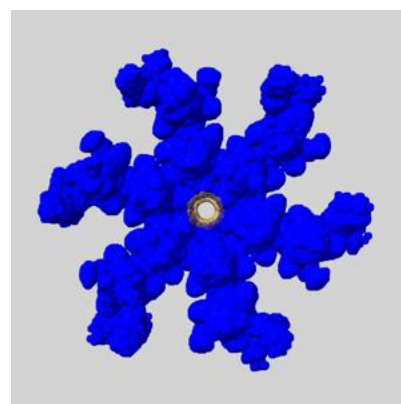
### 6.6.1 emd\_55967\_msk\_1.map [i](#)



X



Y

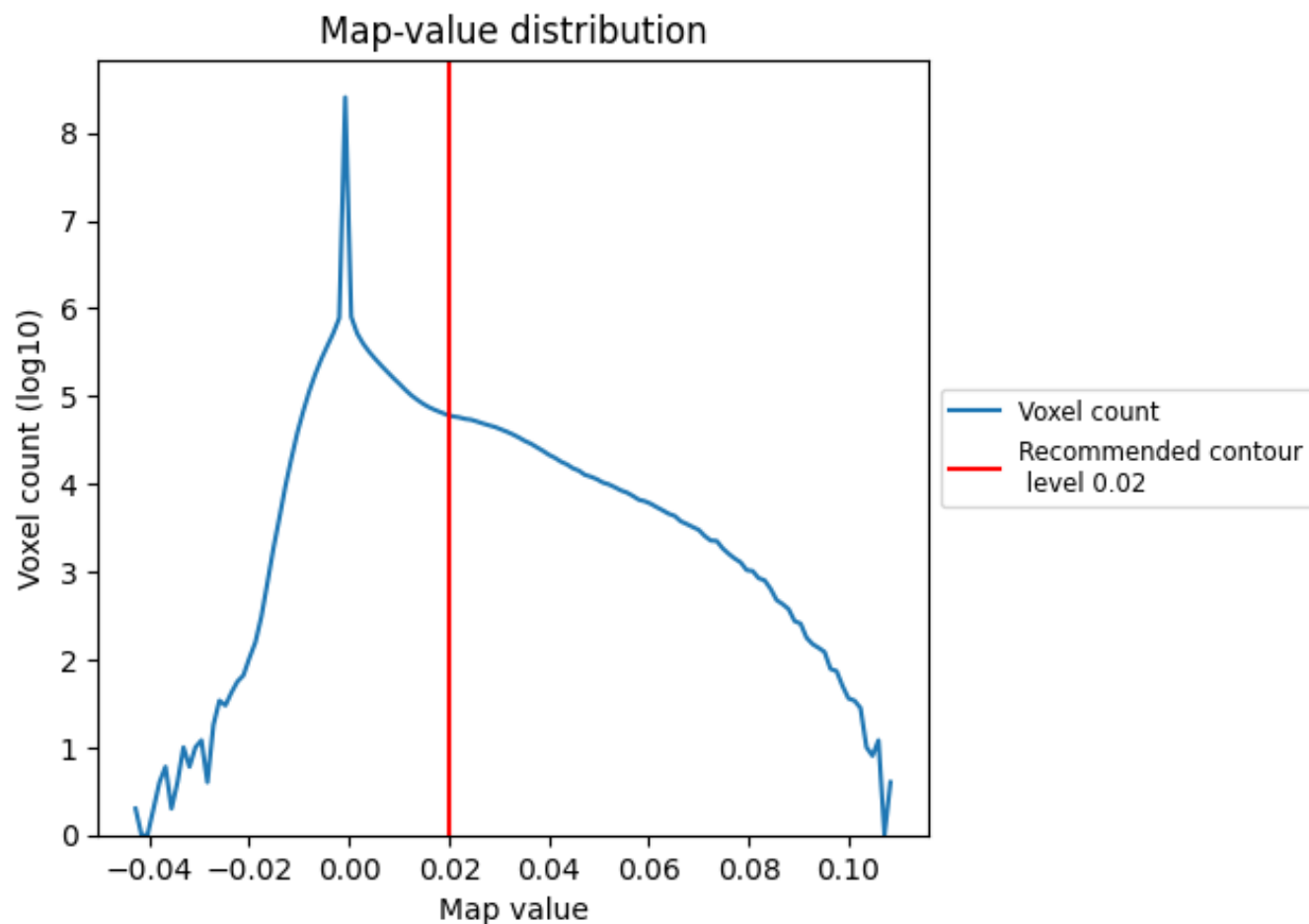


Z

## 7 Map analysis [i](#)

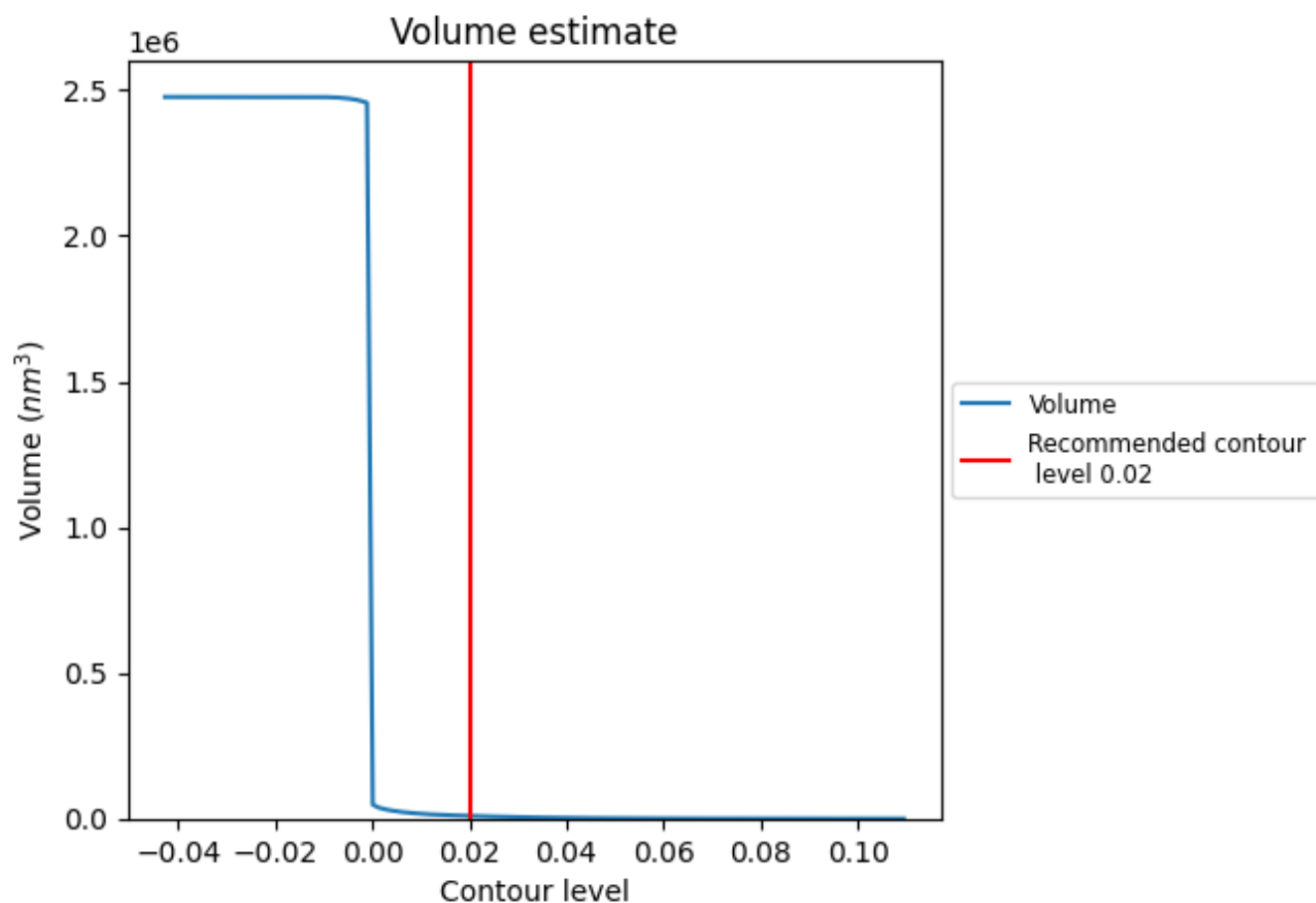
This section contains the results of statistical analysis of the map.

### 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.

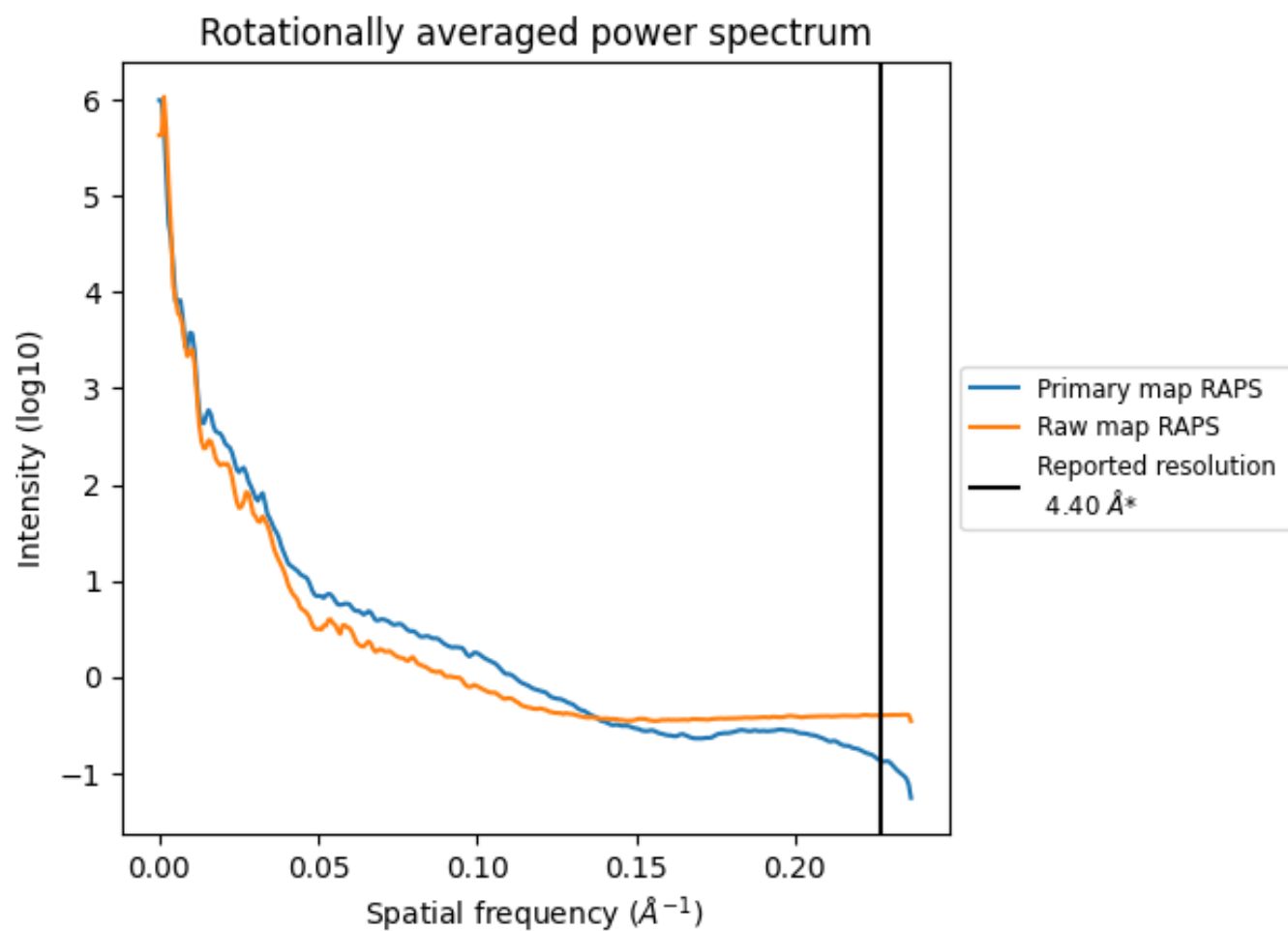
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is  $9334 \text{ nm}^3$ ; this corresponds to an approximate mass of  $8431 \text{ kDa}$ .

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 ⓘ

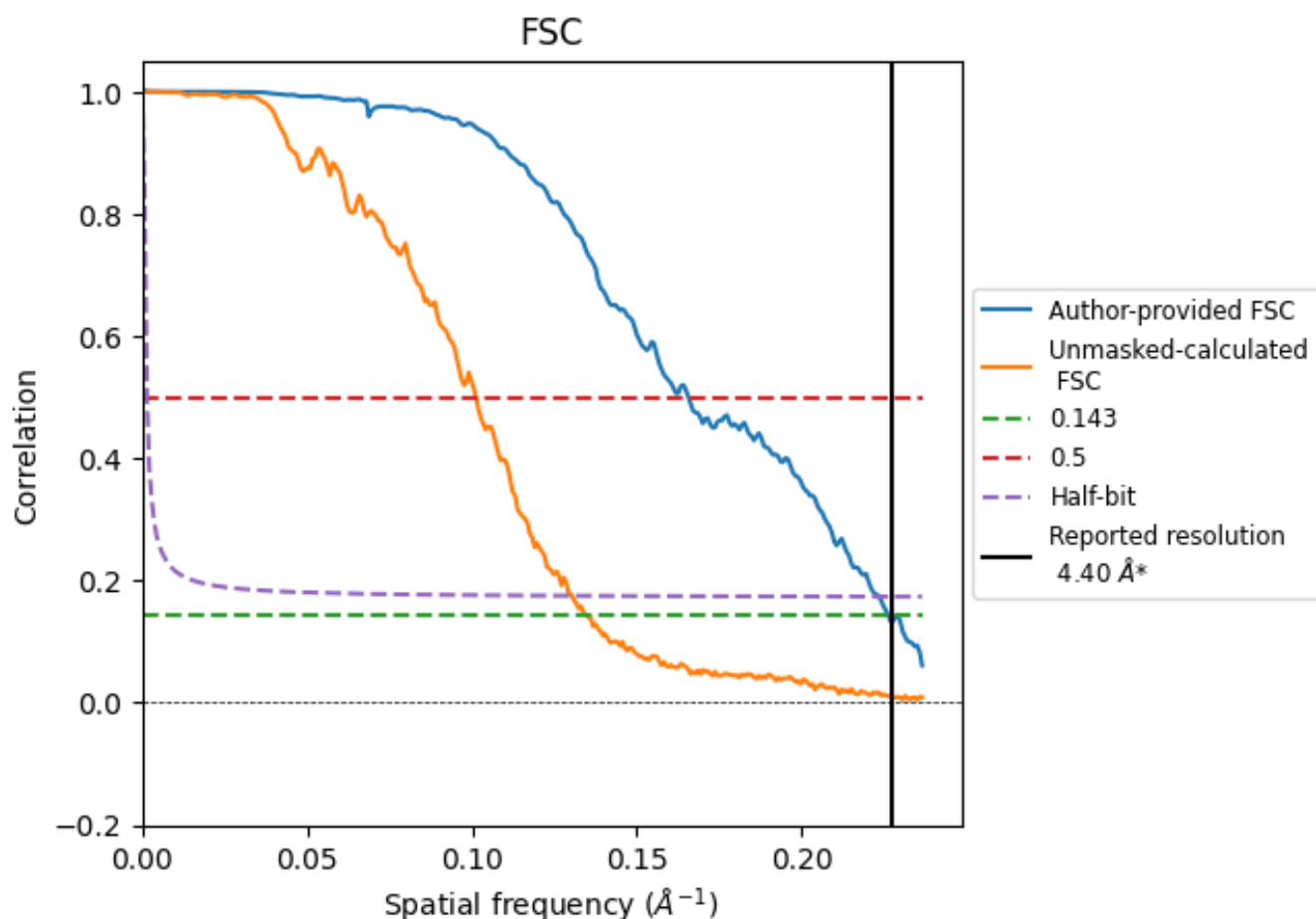


\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>

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

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

### 8.1 FSC [i](#)



\*Reported resolution corresponds to spatial frequency of 0.227 Å<sup>-1</sup>



## 8.2 Resolution estimates [i](#)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	4.42	6.04	4.48
Unmasked-calculated*	7.43	9.88	7.67

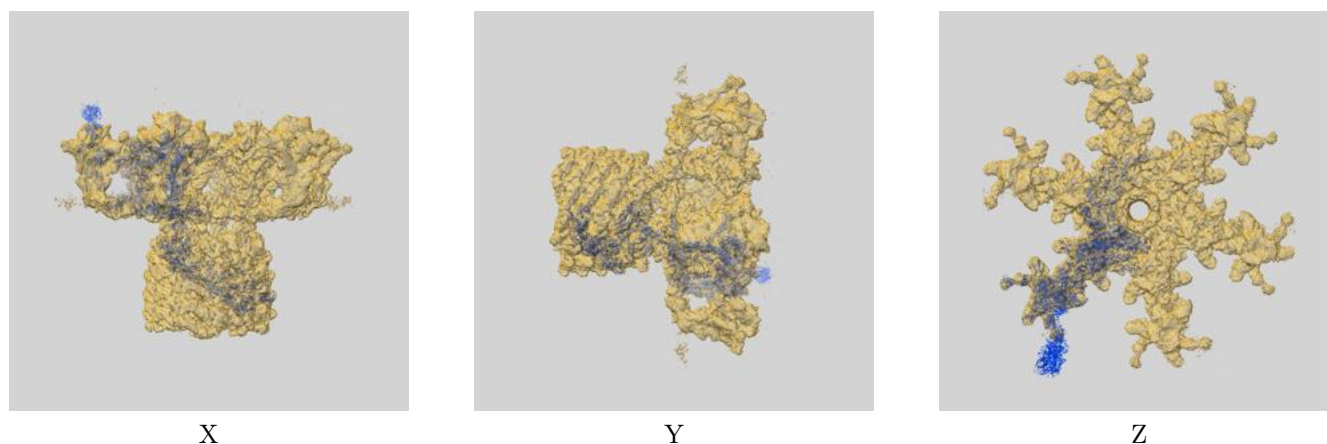
\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.43 differs from the reported value 4.4 by more than 10 %

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

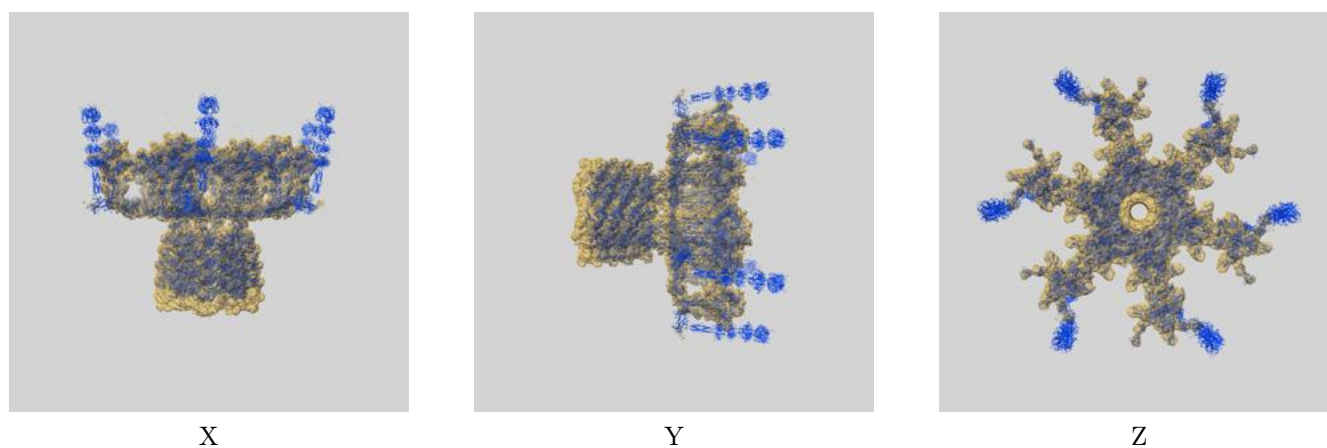
This section contains information regarding the fit between EMDB map EMD-55967 and PDB model 9TIR. Per-residue inclusion information can be found in section 3 on page 6.

### 9.1 Map-model overlays

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



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



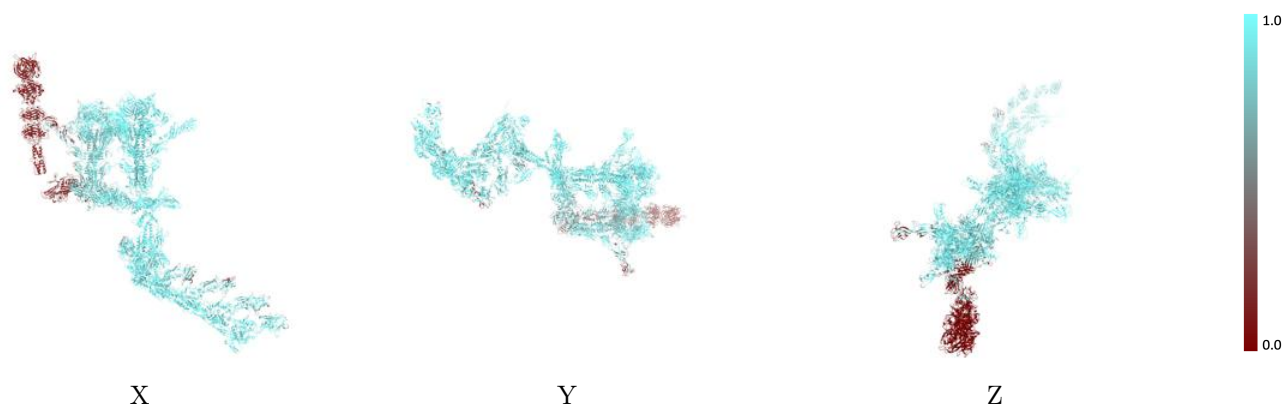
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



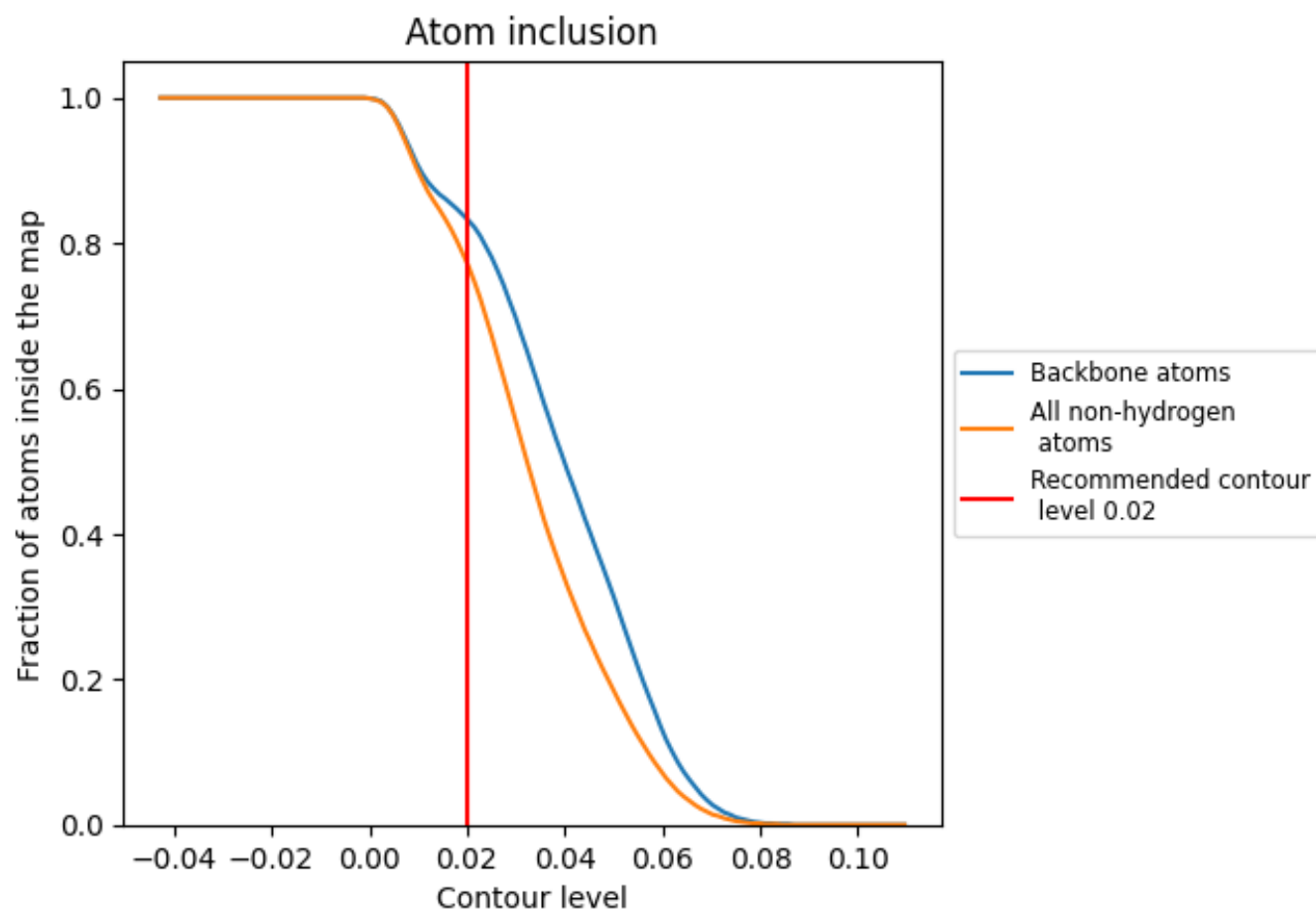
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).





















































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 77% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7730	 0.2190
A	 0.9240	 0.3200
B	 0.9360	 0.3200
C	 0.9410	 0.3320
D	 0.8400	 0.2060
E	 0.9410	 0.2920
F	 0.9340	 0.2140
G	 0.8070	 0.1600
H	 0.6440	 0.1270
I	 0.0440	 0.0340
J	 0.0110	 0.0390
K	 0.9480	 0.3330
L	 0.9500	 0.3430
M	 0.9510	 0.3430
N	 0.9100	 0.1620
O	 0.8080	 0.1270
P	 0.8560	 0.1270
Q	 0.0000	 0.0220
R	 0.0000	 0.0190
S	 0.0220	 0.0100
T	 0.8820	 0.2860
U	 0.9050	 0.2850
V	 0.8640	 0.2520
W	 0.8640	 0.2540
X	 0.8870	 0.2560
Y	 0.8940	 0.2520

