



Full wwPDB EM Validation Report ⓘ

Mar 28, 2026 – 03:41 PM UTC

PDB ID : 7TQT / pdb_00007tqt
EMDB ID : EMD-26071
Title : Coxsackievirus A21 capsid subdomain in complex with mouse polyclonal antibody pAbC-5
Authors : Antanasijevic, A.; Ward, A.B.
Deposited on : 2022-01-27
Resolution : 4.10 Å(reported)
Based on initial model : 1Z7S

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

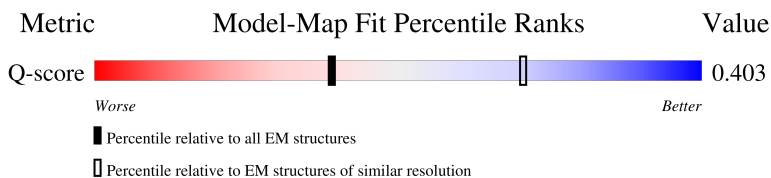
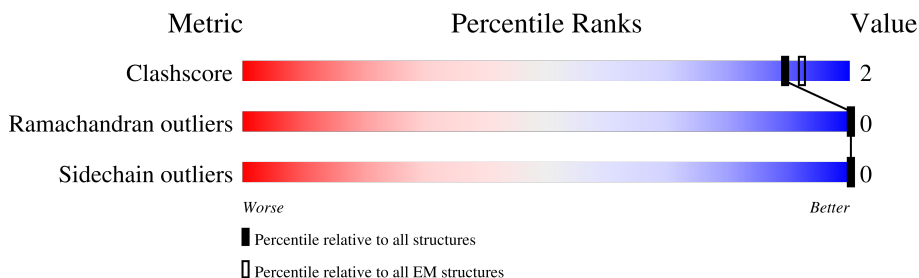
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb archive up until May 2025)
MapQ : 1.9.13
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 4.10 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	6458 (3.60 - 4.60)

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	L	98	49% 95% 5%
2	H	108	30% 98% .
3	a	298	40% 86% 7% 6%
3	e	298	34% 85% 9% 5%

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Mol	Chain	Length	Quality of chain
3	i	298	
3	m	298	
3	q	298	
4	b	272	
4	f	272	
4	j	272	
4	n	272	
4	r	272	
5	c	240	
5	g	240	
5	k	240	
5	o	240	
5	s	240	
6	d	69	
6	h	69	
6	l	69	
6	p	69	
6	t	69	

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 33877 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 pAbC-5 light chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	L	98	Total	C	N	O	0	0
			490	294	98	98		

- Molecule 2 is a protein called pAbC-5 heavy chain.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	H	108	Total	C	N	O	0	0
			540	324	108	108		

- Molecule 3 is a protein called VP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	a	281	Total	C	N	O	S	0	0
			2213	1402	378	423	10		
3	e	282	Total	C	N	O	S	0	0
			2219	1405	379	425	10		
3	i	283	Total	C	N	O	S	0	0
			2226	1410	380	426	10		
3	m	276	Total	C	N	O	S	0	0
			2176	1382	371	413	10		
3	q	283	Total	C	N	O	S	0	0
			2226	1410	380	426	10		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
a	290	ALA	THR	conflict	UNP Q7T7N6
e	290	ALA	THR	conflict	UNP Q7T7N6
i	290	ALA	THR	conflict	UNP Q7T7N6
m	290	ALA	THR	conflict	UNP Q7T7N6
q	290	ALA	THR	conflict	UNP Q7T7N6

- Molecule 4 is a protein called VP2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	b	264	Total	C	N	O	S	0	0
			2053	1306	346	390	11		
4	f	258	Total	C	N	O	S	0	0
			2008	1279	339	379	11		
4	j	257	Total	C	N	O	S	0	0
			2003	1276	339	377	11		
4	n	261	Total	C	N	O	S	0	0
			2029	1290	343	385	11		
4	r	253	Total	C	N	O	S	0	0
			1975	1261	333	370	11		

- Molecule 5 is a protein called VP3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	c	239	Total	C	N	O	S	0	0
			1848	1178	307	343	20		
5	g	234	Total	C	N	O	S	0	0
			1810	1154	299	337	20		
5	k	233	Total	C	N	O	S	0	0
			1801	1148	297	336	20		
5	o	234	Total	C	N	O	S	0	0
			1810	1154	299	337	20		
5	s	235	Total	C	N	O	S	0	0
			1818	1160	300	338	20		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
c	225	ARG	LYS	conflict	UNP Q7T7N6
g	225	ARG	LYS	conflict	UNP Q7T7N6
k	225	ARG	LYS	conflict	UNP Q7T7N6
o	225	ARG	LYS	conflict	UNP Q7T7N6
s	225	ARG	LYS	conflict	UNP Q7T7N6

- Molecule 6 is a protein called VP4.

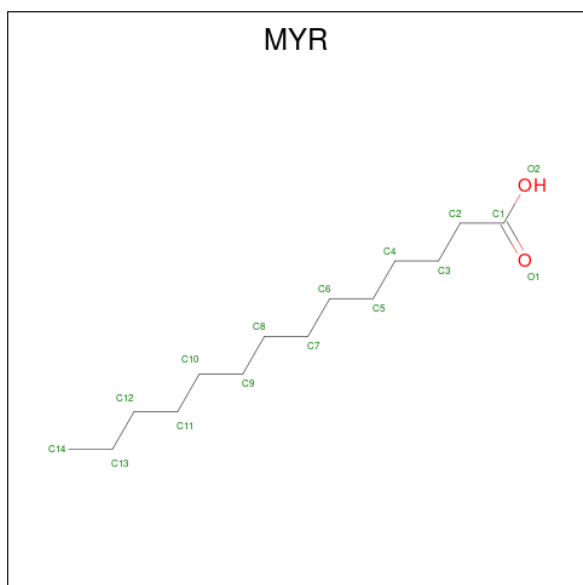
Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	h	68	Total	C	N	O	S	0	0
			512	311	90	110	1		
6	l	68	Total	C	N	O	S	0	0
			512	311	90	110	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	p	67	Total	C	N	O	S	0	0
			504	307	88	108	1		
6	t	68	Total	C	N	O	S	0	0
			512	311	90	110	1		

- Molecule 7 is MYRISTIC ACID (CCD ID: MYR) (formula: $C_{14}H_{28}O_2$).

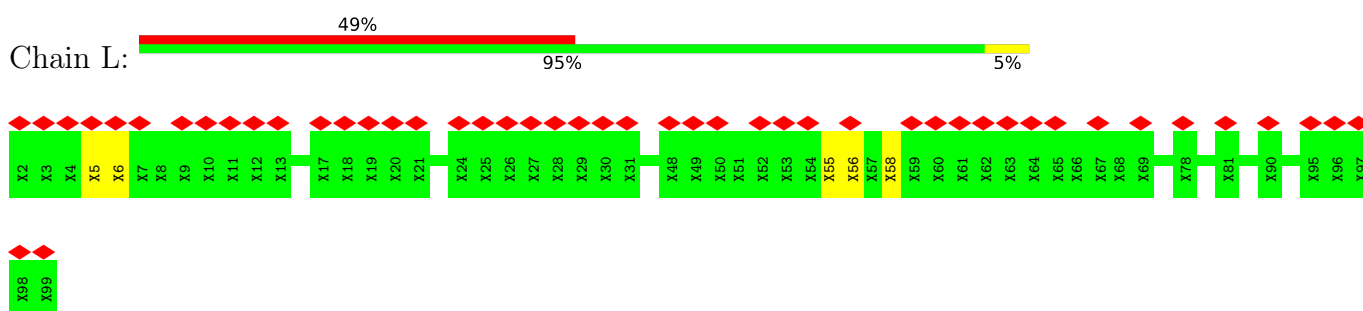


Mol	Chain	Residues	Atoms			AltConf
7	a	1	Total	C	O	0
			16	14	2	
7	e	1	Total	C	O	0
			16	14	2	
7	i	1	Total	C	O	0
			16	14	2	
7	m	1	Total	C	O	0
			16	14	2	
7	q	1	Total	C	O	0
			16	14	2	

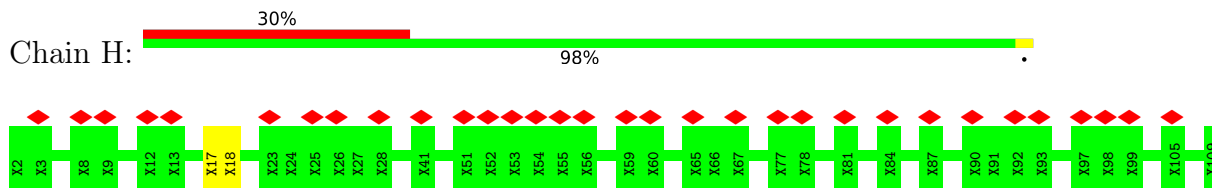
3 Residue-property plots

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.

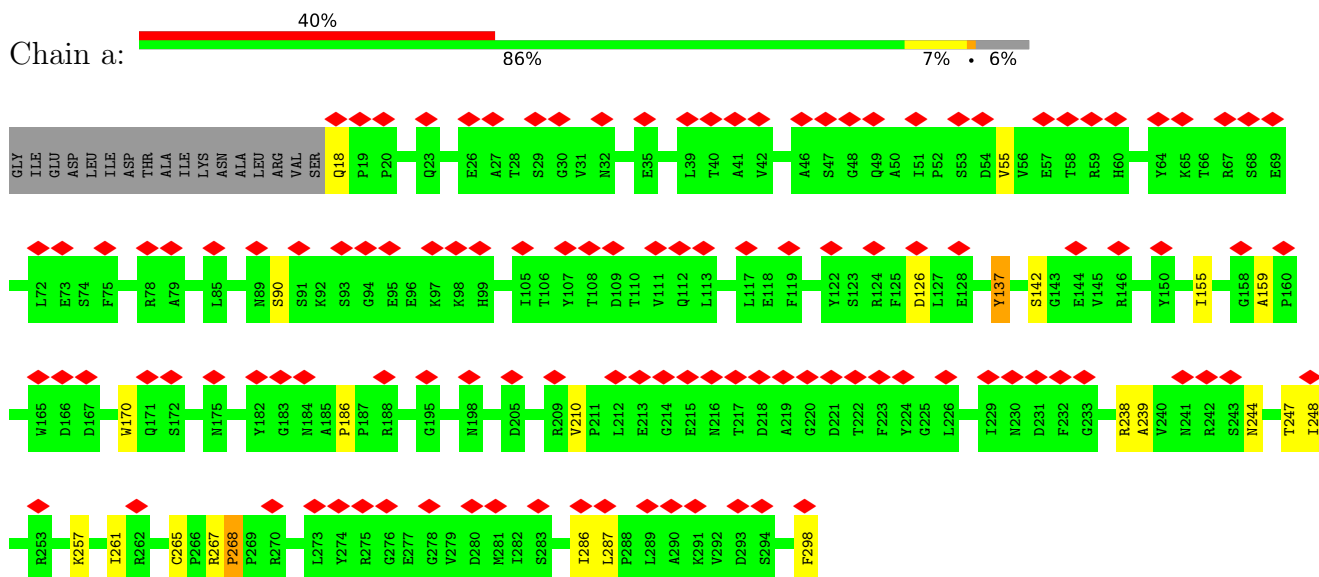
- Molecule 1: pAbC-5 light chain



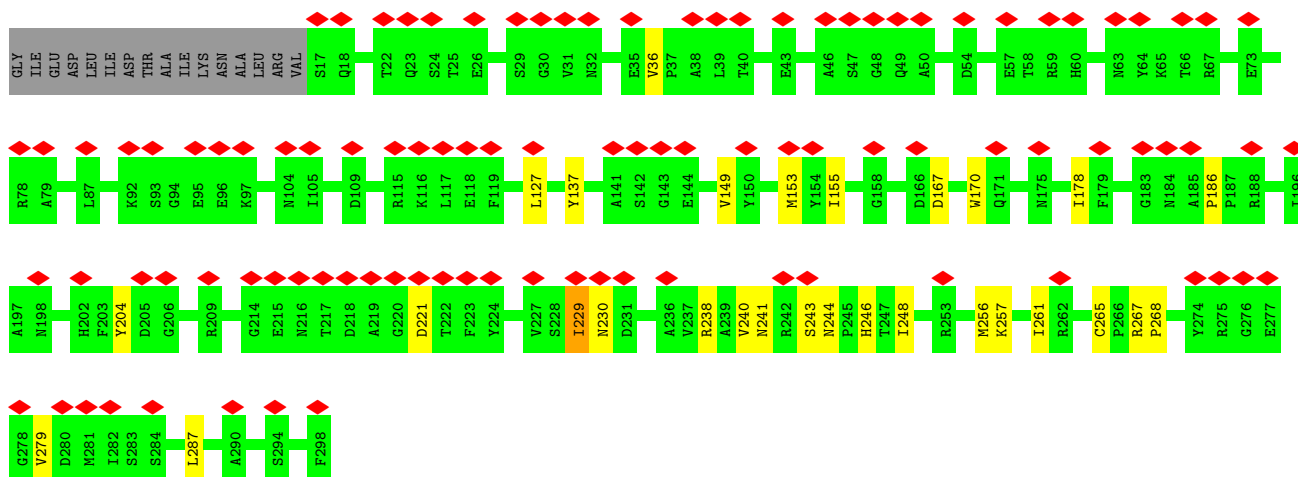
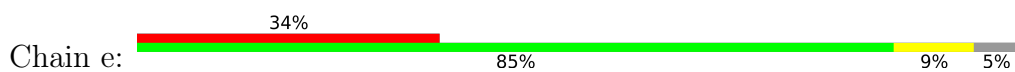
- Molecule 2: pAbC-5 heavy chain



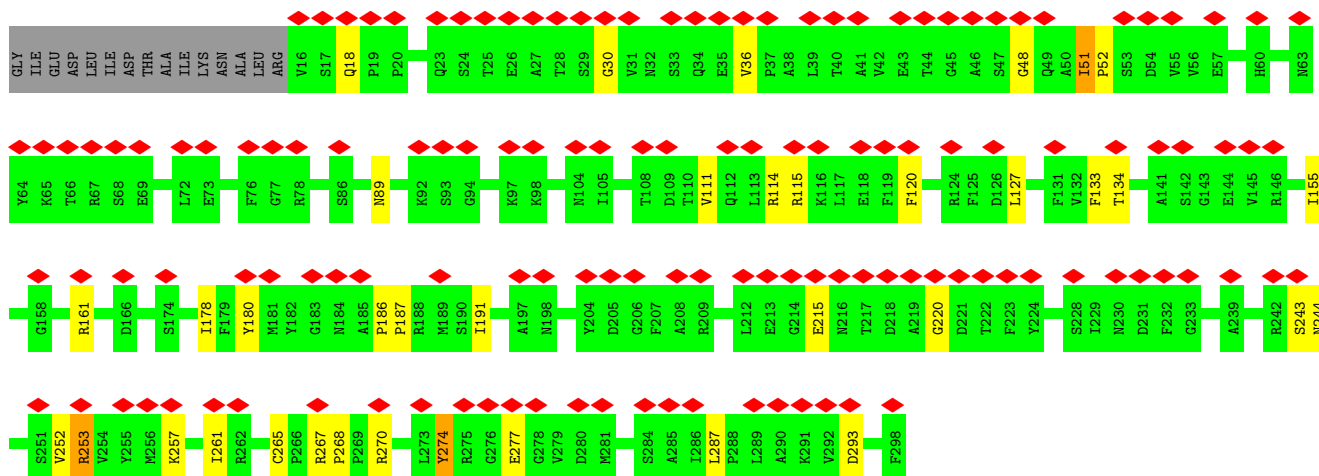
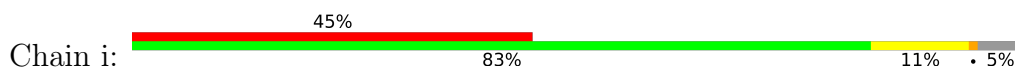
- Molecule 3: VP1



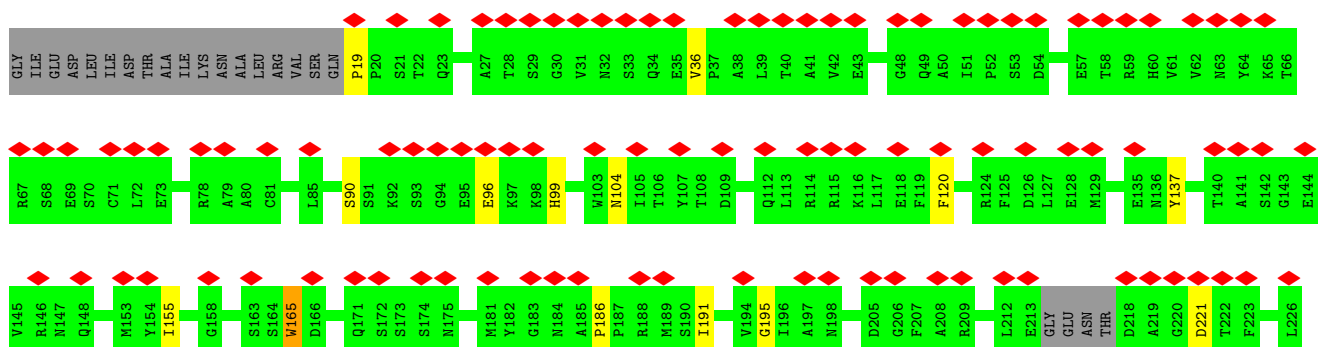
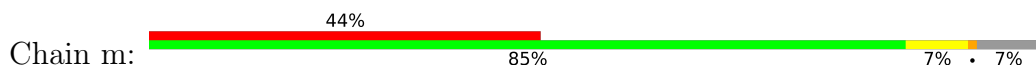
- Molecule 3: VP1

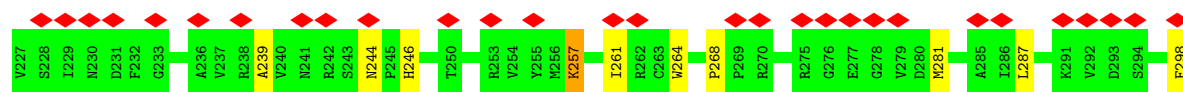


• Molecule 3: VP1

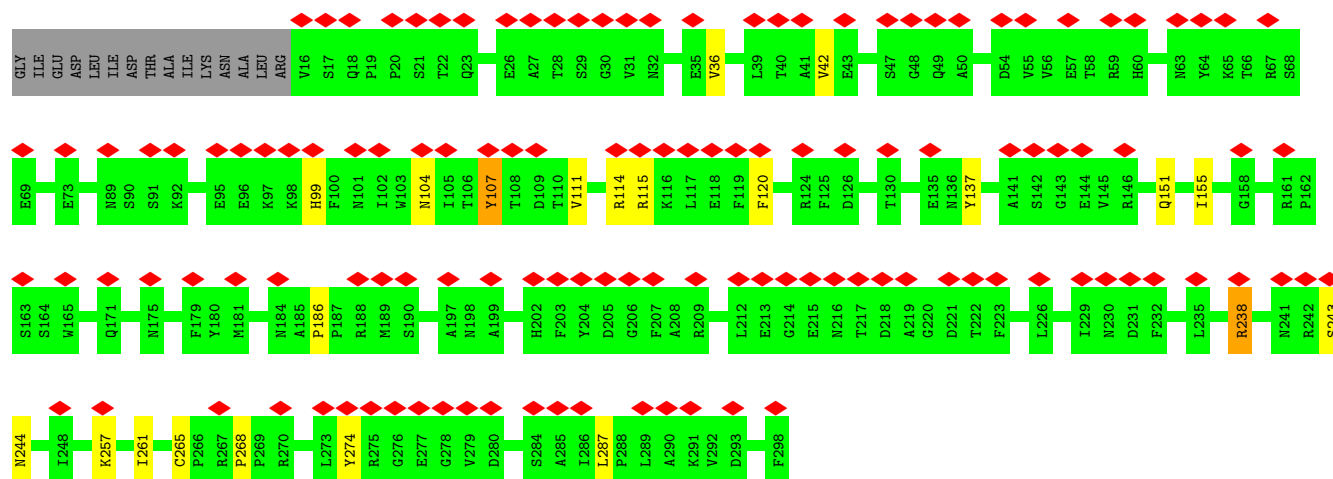
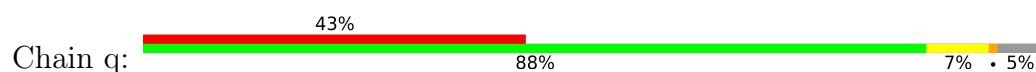


• Molecule 3: VP1

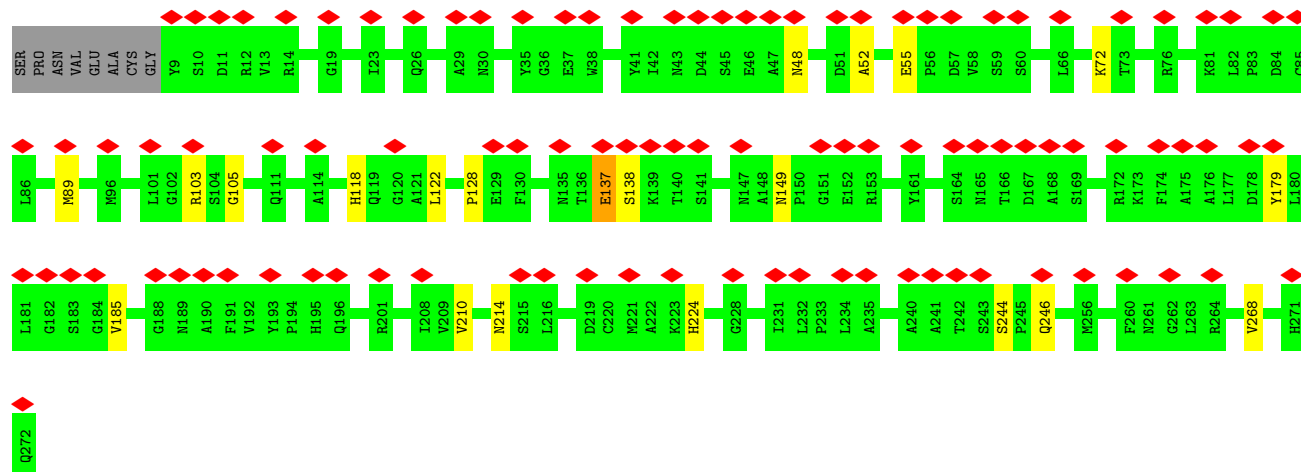
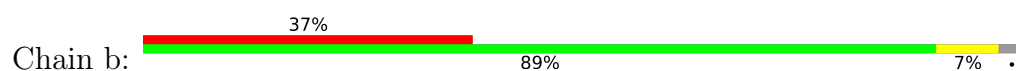




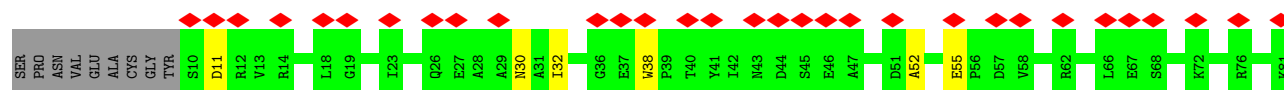
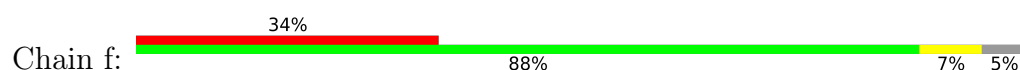
• Molecule 3: VP1

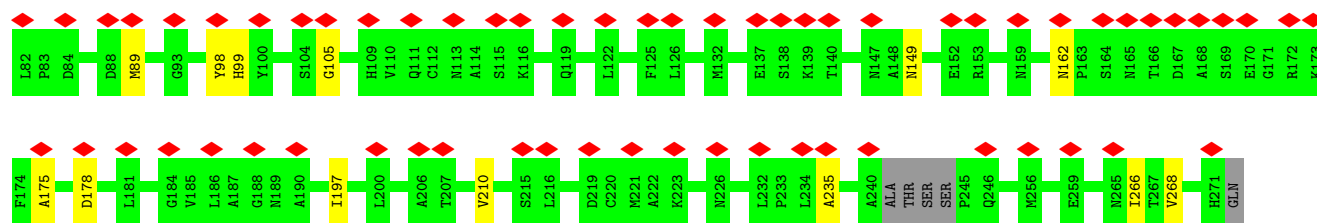


• Molecule 4: VP2

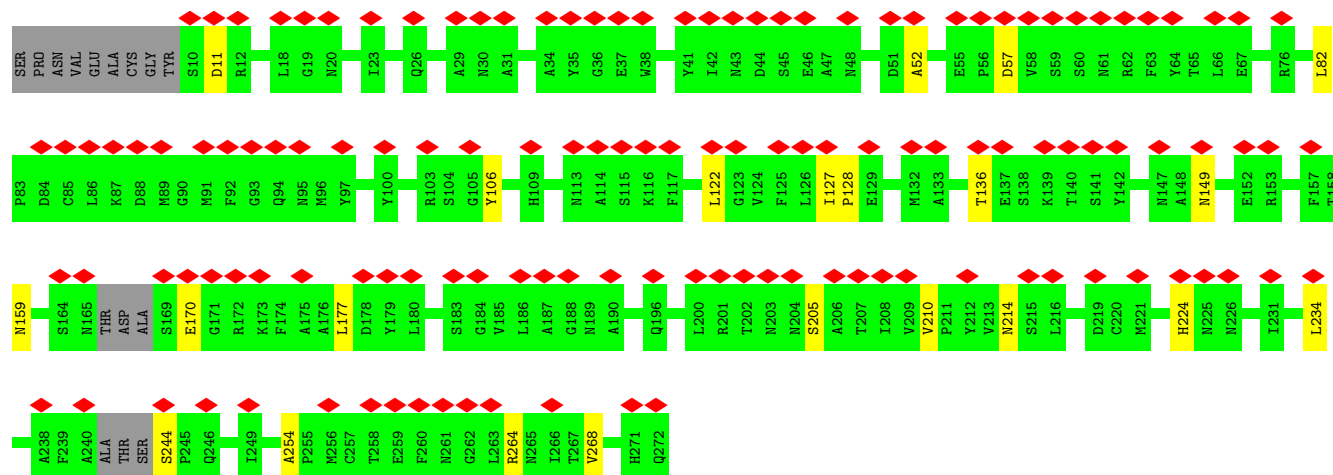
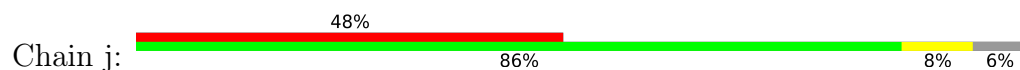


• Molecule 4: VP2

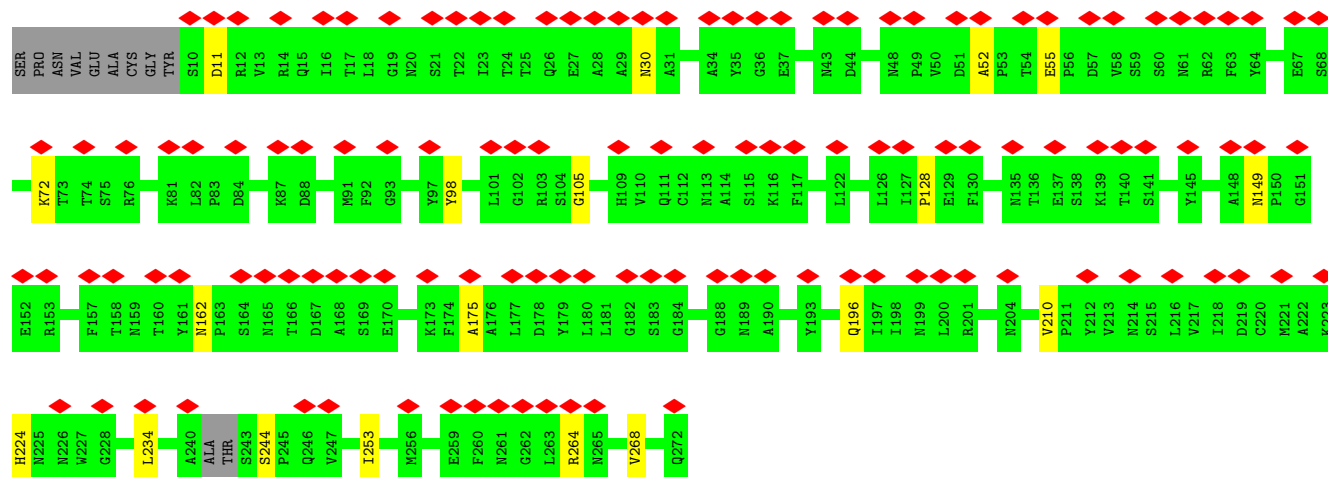
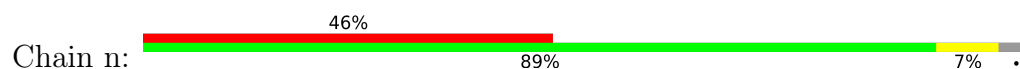




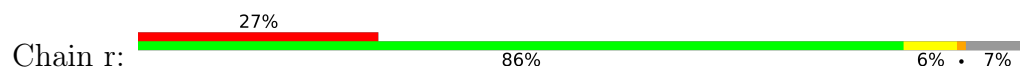
• Molecule 4: VP2

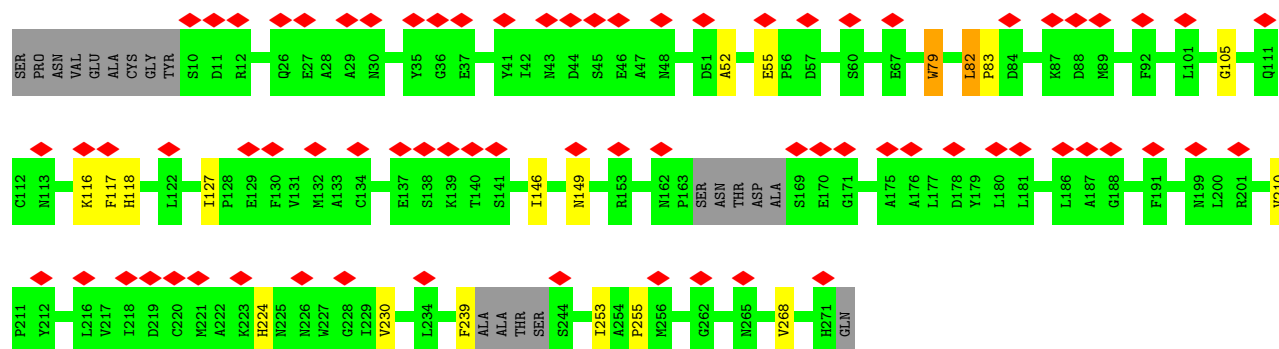


• Molecule 4: VP2

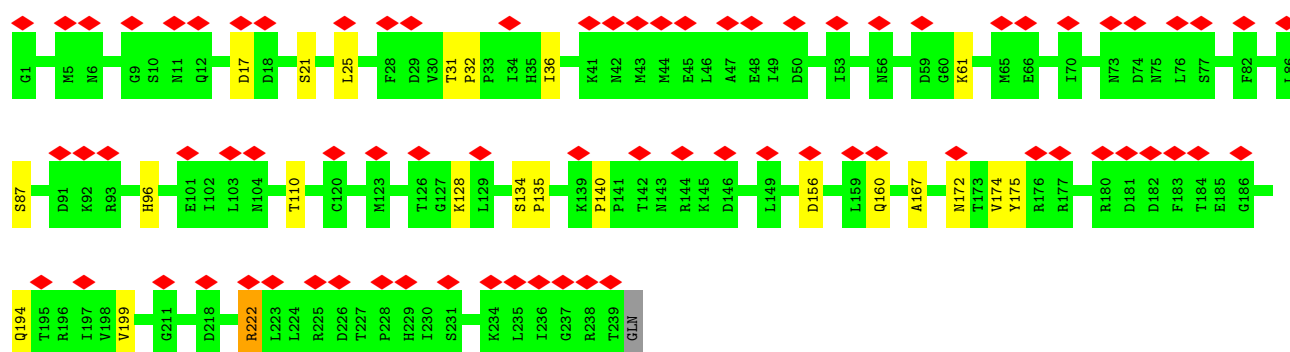


• Molecule 4: VP2

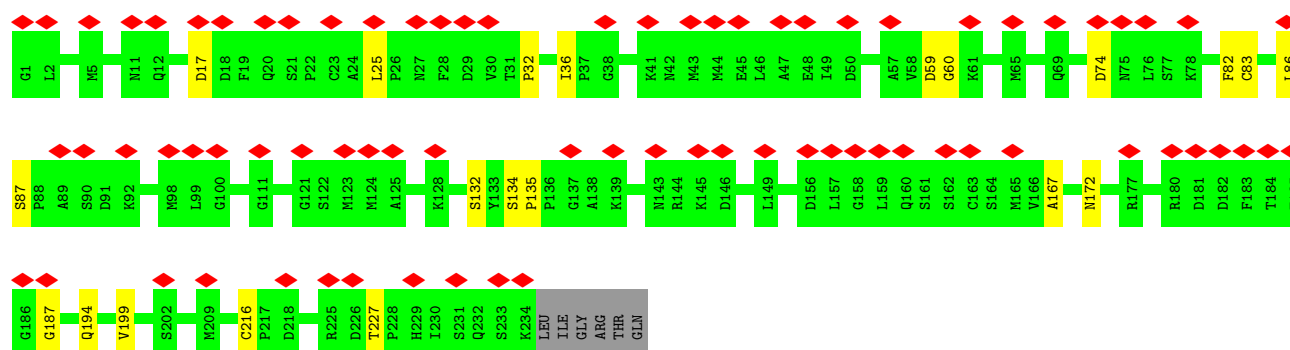
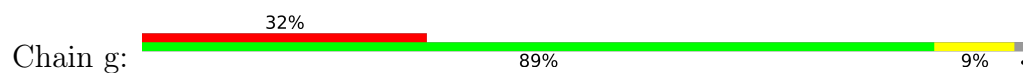




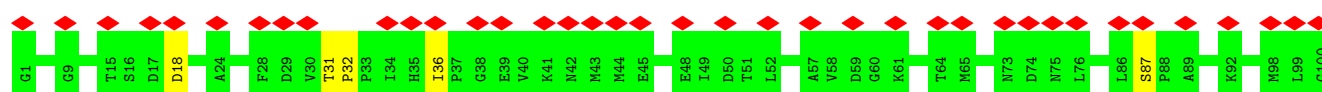
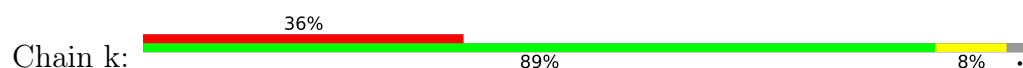
• Molecule 5: VP3

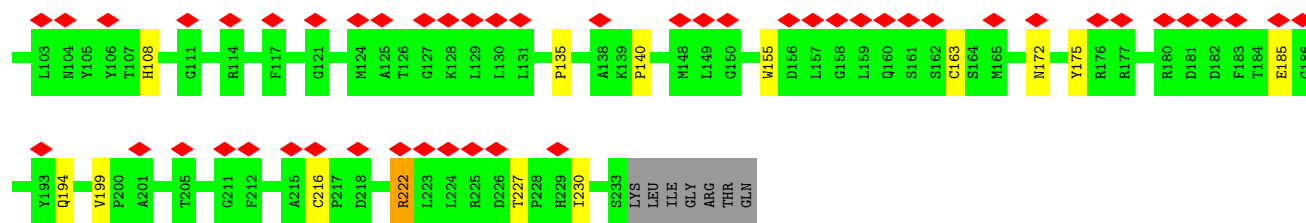


• Molecule 5: VP3

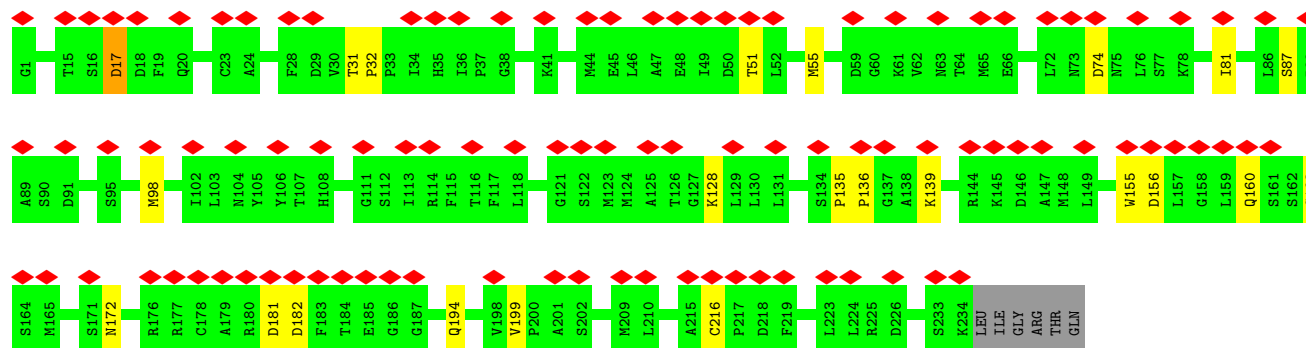
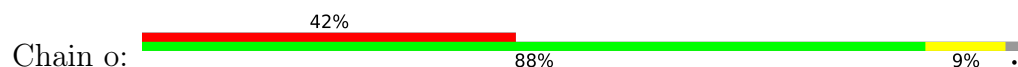


• Molecule 5: VP3

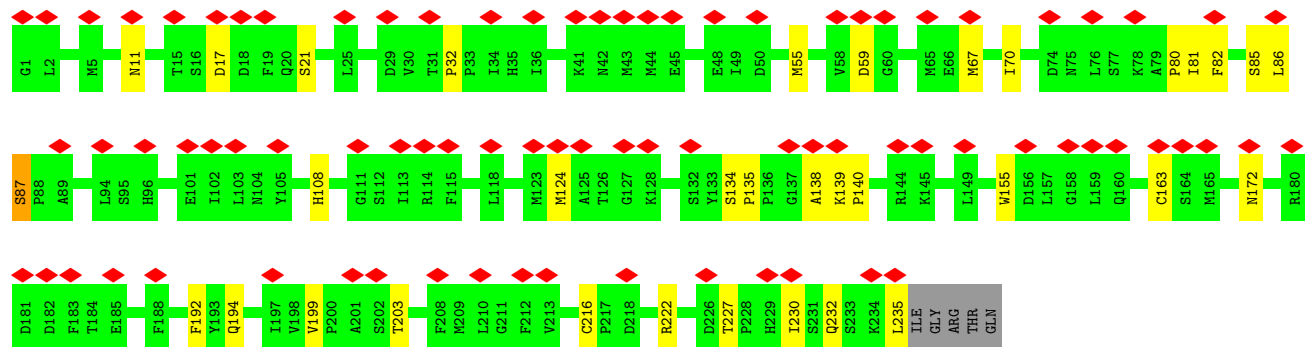
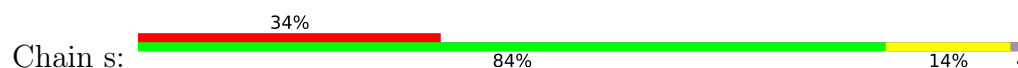




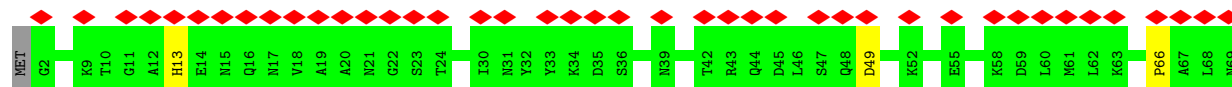
• Molecule 5: VP3



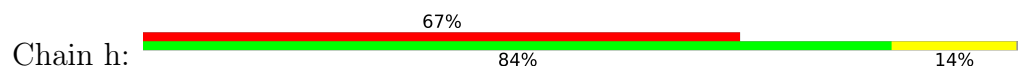
• Molecule 5: VP3

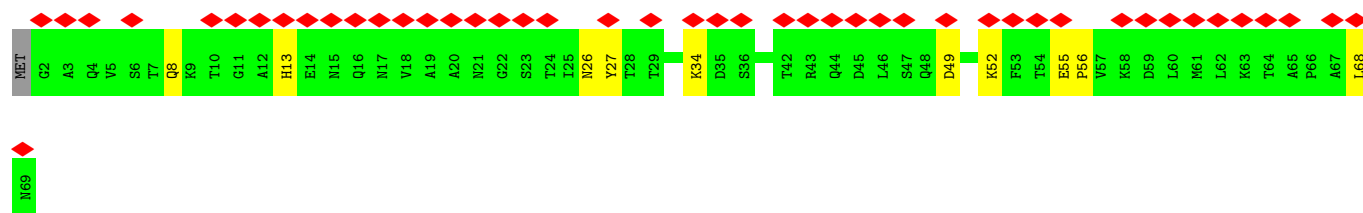


• Molecule 6: VP4

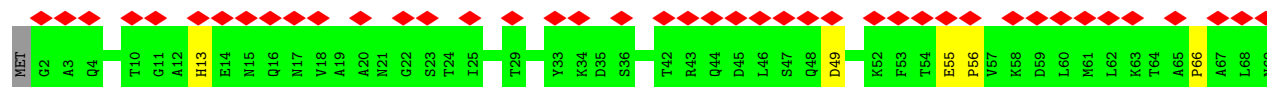


• Molecule 6: VP4

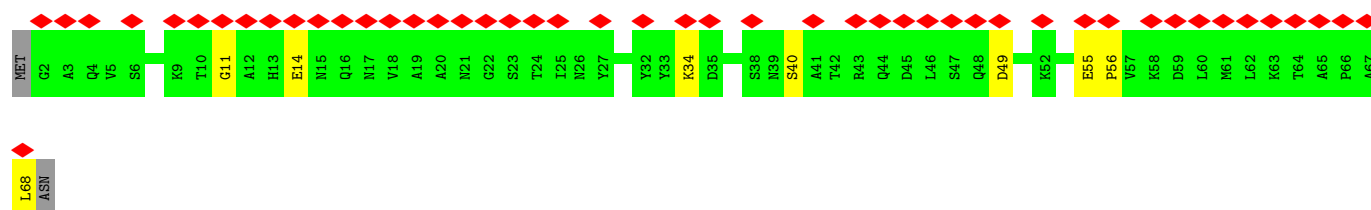
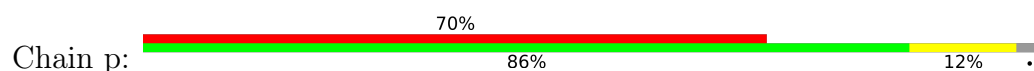




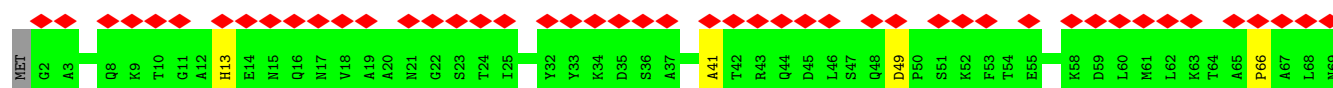
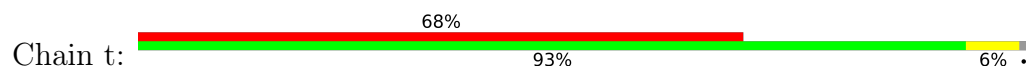
• Molecule 6: VP4



• Molecule 6: VP4



• Molecule 6: VP4



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	12654	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.019	Depositor
Minimum map value	-0.013	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.007	Depositor
Map size ($\text{\AA}$)	292.59998, 292.59998, 292.59998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.045, 1.045, 1.045	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MYR

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	$\# Z > 5$
3	a	1.16	3/2275 (0.1%)	1.37	26/3102 (0.8%)
3	e	1.14	1/2281 (0.0%)	1.39	27/3111 (0.9%)
3	i	1.14	0/2288	1.40	38/3121 (1.2%)
3	m	1.13	2/2237 (0.1%)	1.39	34/3048 (1.1%)
3	q	1.13	1/2288 (0.0%)	1.37	25/3121 (0.8%)
4	b	1.22	2/2110 (0.1%)	1.32	23/2887 (0.8%)
4	f	1.09	1/2063 (0.0%)	1.30	24/2821 (0.9%)
4	j	1.12	1/2057 (0.0%)	1.35	24/2811 (0.9%)
4	n	1.09	1/2084 (0.0%)	1.33	20/2850 (0.7%)
4	r	1.11	1/2029 (0.0%)	1.28	19/2773 (0.7%)
5	c	1.08	0/1897	1.36	26/2582 (1.0%)
5	g	1.14	0/1859	1.34	23/2531 (0.9%)
5	k	1.14	1/1850 (0.1%)	1.34	21/2520 (0.8%)
5	o	1.13	0/1859	1.38	20/2531 (0.8%)
5	s	1.15	3/1867 (0.2%)	1.39	28/2542 (1.1%)
6	d	1.02	0/519	1.29	3/705 (0.4%)
6	h	1.05	0/519	1.24	4/705 (0.6%)
6	l	1.11	0/519	1.29	3/704 (0.4%)
6	p	1.05	1/511 (0.2%)	1.12	3/694 (0.4%)
6	t	1.07	0/519	1.20	3/705 (0.4%)
All	All	1.13	18/33631 (0.1%)	1.35	394/45864 (0.9%)

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	224	HIS	CB-CG	-11.07	1.34	1.50
4	b	103	ARG	CD-NE	-6.48	1.37	1.46
3	q	238	ARG	CD-NE	-6.31	1.37	1.46
3	e	246	HIS	CB-CG	-6.26	1.41	1.50
4	r	224	HIS	CB-CG	-6.21	1.41	1.50
4	n	224	HIS	CB-CG	-6.13	1.41	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	k	108	HIS	CB-CG	-5.88	1.42	1.50
5	s	235	LEU	CB-CG	5.80	1.65	1.53
3	m	246	HIS	CB-CG	-5.58	1.42	1.50
3	m	298	PHE	CG-CD1	5.32	1.50	1.38
6	p	68	LEU	CB-CG	5.27	1.64	1.53
5	s	67	MET	CG-SD	-5.16	1.67	1.80
3	a	137	TYR	CB-CG	-5.15	1.40	1.51
3	a	18	GLN	C-N	5.12	1.39	1.33
4	j	224	HIS	CB-CG	-5.07	1.43	1.50
3	a	298	PHE	CG-CD2	5.05	1.49	1.38
4	f	99	HIS	CB-CG	-5.05	1.43	1.50
5	s	222	ARG	CD-NE	-5.02	1.39	1.46

All (394) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	135	PRO	CA-C-N	9.34	129.18	120.21
5	g	135	PRO	C-N-CA	9.34	129.18	120.21
5	o	135	PRO	CA-C-N	9.20	129.13	120.03
5	o	135	PRO	C-N-CA	9.20	129.13	120.03
5	s	135	PRO	CA-C-N	9.11	128.95	120.21
5	s	135	PRO	C-N-CA	9.11	128.95	120.21
5	k	135	PRO	CA-C-N	9.10	129.66	119.92
5	k	135	PRO	C-N-CA	9.10	129.66	119.92
5	o	17	ASP	CA-CB-CG	8.96	121.56	112.60
4	n	234	LEU	N-CA-C	-8.61	102.70	113.55
3	m	165	TRP	CA-C-N	-8.51	111.63	123.03
3	m	165	TRP	C-N-CA	-8.51	111.63	123.03
4	j	149	ASN	CA-C-N	8.13	127.86	119.56
4	j	149	ASN	C-N-CA	8.13	127.86	119.56
4	j	268	VAL	CA-C-N	8.02	127.97	120.03
4	j	268	VAL	C-N-CA	8.02	127.97	120.03
3	e	267	ARG	CA-C-N	7.98	125.48	119.66
3	e	267	ARG	C-N-CA	7.98	125.48	119.66
5	k	199	VAL	CA-C-N	7.92	127.81	120.21
5	k	199	VAL	C-N-CA	7.92	127.81	120.21
3	m	261	ILE	N-CA-C	7.90	119.23	108.17
3	q	120	PHE	CA-CB-CG	-7.89	105.91	113.80
5	c	87	SER	CA-C-N	7.87	127.59	119.56
5	c	87	SER	C-N-CA	7.87	127.59	119.56
3	m	264	TRP	N-CA-C	7.87	122.64	112.41
4	r	127	ILE	N-CA-C	7.80	116.62	107.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	a	268	PRO	CA-C-N	7.58	127.74	120.31
3	a	268	PRO	C-N-CA	7.58	127.74	120.31
4	n	55	GLU	CA-C-N	7.57	127.28	119.56
4	n	55	GLU	C-N-CA	7.57	127.28	119.56
4	f	89	MET	N-CA-C	7.55	120.84	108.99
4	b	268	VAL	CA-C-N	7.50	127.41	120.21
4	b	268	VAL	C-N-CA	7.50	127.41	120.21
4	r	79	TRP	N-CA-C	7.48	120.68	108.26
3	i	36	VAL	CA-C-N	7.47	127.64	119.87
3	i	36	VAL	C-N-CA	7.47	127.64	119.87
3	a	261	ILE	N-CA-C	7.45	118.60	108.17
3	q	261	ILE	N-CA-C	7.43	118.57	108.17
3	m	36	VAL	N-CA-C	7.37	116.13	107.73
3	q	99	HIS	CA-CB-CG	7.33	121.13	113.80
3	e	265	CYS	CA-C-N	7.30	127.22	119.85
3	e	265	CYS	C-N-CA	7.30	127.22	119.85
3	m	36	VAL	CA-C-N	7.27	126.90	119.56
3	m	36	VAL	C-N-CA	7.27	126.90	119.56
5	g	134	SER	CA-C-N	7.21	124.92	119.66
5	g	134	SER	C-N-CA	7.21	124.92	119.66
4	f	55	GLU	CA-C-N	7.17	126.88	119.56
4	f	55	GLU	C-N-CA	7.17	126.88	119.56
4	n	268	VAL	CA-C-N	7.07	127.03	120.03
4	n	268	VAL	C-N-CA	7.07	127.03	120.03
3	i	267	ARG	CA-C-N	7.04	124.73	119.66
3	i	267	ARG	C-N-CA	7.04	124.73	119.66
3	q	244	ASN	CA-C-N	7.02	126.72	119.56
3	q	244	ASN	C-N-CA	7.02	126.72	119.56
4	b	128	PRO	N-CA-C	-7.00	100.19	111.19
4	r	55	GLU	CA-C-N	6.99	126.69	119.56
4	r	55	GLU	C-N-CA	6.99	126.69	119.56
4	b	55	GLU	CA-C-N	6.98	126.68	119.56
4	b	55	GLU	C-N-CA	6.98	126.68	119.56
4	r	268	VAL	CA-C-N	6.96	126.95	119.78
4	r	268	VAL	C-N-CA	6.96	126.95	119.78
4	f	268	VAL	CA-C-N	6.95	126.91	120.03
4	f	268	VAL	C-N-CA	6.95	126.91	120.03
6	l	49	ASP	CA-C-N	6.91	126.59	119.82
6	l	49	ASP	C-N-CA	6.91	126.59	119.82
3	a	265	CYS	CA-C-N	6.89	126.81	119.85
3	a	265	CYS	C-N-CA	6.89	126.81	119.85
4	n	149	ASN	CA-C-N	6.88	127.03	119.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	n	149	ASN	C-N-CA	6.88	127.03	119.87
3	i	51	ILE	N-CA-C	-6.88	100.21	107.84
5	c	222	ARG	CB-CA-C	-6.84	98.82	110.24
4	n	52	ALA	CA-C-N	6.83	126.79	120.03
4	n	52	ALA	C-N-CA	6.83	126.79	120.03
3	m	19	PRO	CA-C-N	6.81	126.79	119.78
3	m	19	PRO	C-N-CA	6.81	126.79	119.78
3	q	36	VAL	CA-C-N	6.80	126.50	119.56
3	q	36	VAL	C-N-CA	6.80	126.50	119.56
3	e	229	ILE	N-CA-C	6.78	117.56	110.72
4	f	52	ALA	CA-C-N	6.77	126.73	120.03
4	f	52	ALA	C-N-CA	6.77	126.73	120.03
5	s	134	SER	CA-C-N	6.75	124.59	119.66
5	s	134	SER	C-N-CA	6.75	124.59	119.66
4	j	52	ALA	CA-C-N	6.71	126.68	120.03
4	j	52	ALA	C-N-CA	6.71	126.68	120.03
3	m	186	PRO	CA-C-N	6.71	126.88	120.31
3	m	186	PRO	C-N-CA	6.71	126.88	120.31
5	k	185	GLU	CB-CG-CD	-6.67	101.26	112.60
5	s	227	THR	CA-C-N	6.65	126.78	119.87
5	s	227	THR	C-N-CA	6.65	126.78	119.87
5	o	199	VAL	CA-C-N	6.64	126.58	120.21
5	o	199	VAL	C-N-CA	6.64	126.58	120.21
3	e	248	ILE	N-CA-C	6.60	117.35	108.11
3	i	261	ILE	N-CA-C	6.59	117.40	108.17
3	e	244	ASN	CA-C-N	6.59	127.11	119.47
3	e	244	ASN	C-N-CA	6.59	127.11	119.47
5	s	11	ASN	CA-CB-CG	6.52	119.12	112.60
4	b	149	ASN	CA-C-N	6.50	126.63	119.87
4	b	149	ASN	C-N-CA	6.50	126.63	119.87
5	s	87	SER	CA-C-N	6.50	126.12	119.56
5	s	87	SER	C-N-CA	6.50	126.12	119.56
5	o	216	CYS	CA-C-N	6.49	126.18	119.56
5	o	216	CYS	C-N-CA	6.49	126.18	119.56
4	r	52	ALA	CA-C-N	6.46	126.42	120.03
4	r	52	ALA	C-N-CA	6.46	126.42	120.03
5	o	194	GLN	N-CA-C	-6.44	104.11	112.23
4	r	149	ASN	CA-C-N	6.43	126.11	119.56
4	r	149	ASN	C-N-CA	6.43	126.11	119.56
3	e	287	LEU	CA-C-N	6.42	126.04	119.56
3	e	287	LEU	C-N-CA	6.42	126.04	119.56
3	i	120	PHE	CA-CB-CG	-6.41	107.39	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	m	195	GLY	CA-C-N	6.40	129.22	120.46
3	m	195	GLY	C-N-CA	6.40	129.22	120.46
5	o	31	THR	CA-C-N	6.38	124.31	119.66
5	o	31	THR	C-N-CA	6.38	124.31	119.66
3	e	268	PRO	CA-C-N	6.37	126.29	119.85
3	e	268	PRO	C-N-CA	6.37	126.29	119.85
3	e	261	ILE	N-CA-C	6.37	117.77	108.53
5	s	140	PRO	CA-C-N	6.36	126.85	119.47
5	s	140	PRO	C-N-CA	6.36	126.85	119.47
5	c	135	PRO	CA-C-N	6.36	127.79	119.84
5	c	135	PRO	C-N-CA	6.36	127.79	119.84
3	a	267	ARG	CA-C-N	6.36	124.24	119.66
3	a	267	ARG	C-N-CA	6.36	124.24	119.66
5	c	25	LEU	CA-C-N	6.36	126.31	119.76
5	c	25	LEU	C-N-CA	6.36	126.31	119.76
4	n	128	PRO	N-CA-C	-6.35	101.22	111.19
4	f	30	ASN	CB-CA-C	-6.35	109.24	116.54
5	s	81	ILE	N-CA-C	-6.34	104.67	110.82
3	q	107	TYR	CB-CA-C	6.30	121.28	111.13
3	i	244	ASN	CA-C-N	6.27	125.96	119.56
3	i	244	ASN	C-N-CA	6.27	125.96	119.56
3	i	287	LEU	CA-C-N	6.26	125.94	119.56
3	i	287	LEU	C-N-CA	6.26	125.94	119.56
5	c	134	SER	CA-C-N	6.25	126.81	120.38
5	c	134	SER	C-N-CA	6.25	126.81	120.38
6	d	49	ASP	CA-C-N	6.24	125.86	119.56
6	d	49	ASP	C-N-CA	6.24	125.86	119.56
3	a	55	VAL	N-CA-C	6.24	117.17	111.81
4	n	253	ILE	N-CA-C	6.24	117.10	108.12
5	c	167	ALA	CA-C-N	6.22	126.19	120.03
5	c	167	ALA	C-N-CA	6.22	126.19	120.03
5	g	216	CYS	CA-C-N	6.22	125.91	119.56
5	g	216	CYS	C-N-CA	6.22	125.91	119.56
4	f	210	VAL	CA-C-N	6.22	126.41	120.31
4	f	210	VAL	C-N-CA	6.22	126.41	120.31
5	s	85	SER	N-CA-C	-6.17	101.34	110.48
4	f	149	ASN	CA-C-N	6.17	127.30	120.45
4	f	149	ASN	C-N-CA	6.17	127.30	120.45
4	j	57	ASP	N-CA-C	6.15	117.98	111.28
5	s	194	GLN	N-CA-C	-6.15	103.91	112.45
5	k	194	GLN	N-CA-C	-6.14	104.86	112.90
3	i	268	PRO	CA-C-N	6.12	126.03	119.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	i	268	PRO	C-N-CA	6.12	126.03	119.85
4	j	254	ALA	CA-C-N	6.09	126.00	119.85
4	j	254	ALA	C-N-CA	6.09	126.00	119.85
5	k	140	PRO	N-CA-C	-6.08	104.08	110.58
3	m	244	ASN	CA-C-N	6.08	125.76	119.56
3	m	244	ASN	C-N-CA	6.08	125.76	119.56
5	g	132	SER	N-CA-C	6.06	119.37	109.06
3	m	120	PHE	CA-CB-CG	-6.05	107.75	113.80
5	g	32	PRO	CA-C-N	6.05	126.02	120.03
5	g	32	PRO	C-N-CA	6.05	126.02	120.03
3	i	155	ILE	CA-C-N	6.01	126.57	120.38
3	i	155	ILE	C-N-CA	6.01	126.57	120.38
5	c	140	PRO	N-CA-C	-6.01	103.37	110.70
3	m	155	ILE	CA-C-N	6.01	126.57	120.38
3	m	155	ILE	C-N-CA	6.01	126.57	120.38
3	a	137	TYR	CA-C-N	6.00	125.62	119.56
3	a	137	TYR	C-N-CA	6.00	125.62	119.56
5	k	32	PRO	CA-C-N	6.00	125.97	120.03
5	k	32	PRO	C-N-CA	6.00	125.97	120.03
5	k	87	SER	CA-C-N	5.99	125.67	119.56
5	k	87	SER	C-N-CA	5.99	125.67	119.56
4	b	105	GLY	N-CA-C	-5.97	103.14	112.58
5	c	61	LYS	N-CA-C	-5.97	106.64	114.04
4	j	128	PRO	N-CA-C	-5.97	101.89	111.38
4	j	244	SER	CA-C-N	5.96	126.15	120.31
4	j	244	SER	C-N-CA	5.96	126.15	120.31
3	q	265	CYS	CA-C-N	5.96	125.92	119.78
3	q	265	CYS	C-N-CA	5.96	125.92	119.78
4	b	52	ALA	CA-C-N	5.94	125.84	119.85
4	b	52	ALA	C-N-CA	5.94	125.84	119.85
6	t	49	ASP	CA-C-N	5.93	126.04	119.87
6	t	49	ASP	C-N-CA	5.93	126.04	119.87
5	c	21	SER	CA-C-N	5.93	125.88	119.78
5	c	21	SER	C-N-CA	5.93	125.88	119.78
3	a	210	VAL	CB-CA-C	-5.92	103.97	110.78
3	i	161	ARG	CA-C-N	5.92	125.83	119.85
3	i	161	ARG	C-N-CA	5.92	125.83	119.85
5	k	36	ILE	CA-C-N	5.91	125.87	119.78
5	k	36	ILE	C-N-CA	5.91	125.87	119.78
5	c	160	GLN	N-CA-C	-5.90	98.91	108.41
6	p	49	ASP	CA-C-N	5.90	125.58	119.56
6	p	49	ASP	C-N-CA	5.90	125.58	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	q	287	LEU	CA-C-N	5.90	125.52	119.56
3	q	287	LEU	C-N-CA	5.90	125.52	119.56
3	a	244	ASN	CA-C-N	5.88	126.03	119.32
3	a	244	ASN	C-N-CA	5.88	126.03	119.32
3	i	265	CYS	CA-C-N	5.87	125.78	119.85
3	i	265	CYS	C-N-CA	5.87	125.78	119.85
3	e	137	TYR	CA-C-N	5.84	125.46	119.56
3	e	137	TYR	C-N-CA	5.84	125.46	119.56
4	b	48	ASN	CA-C-N	5.84	125.81	120.03
4	b	48	ASN	C-N-CA	5.84	125.81	120.03
5	o	87	SER	CA-C-N	5.83	125.45	119.56
5	o	87	SER	C-N-CA	5.83	125.45	119.56
4	r	255	PRO	N-CA-C	-5.83	101.94	111.68
3	e	155	ILE	CA-C-N	5.82	126.37	120.38
3	e	155	ILE	C-N-CA	5.82	126.37	120.38
5	k	216	CYS	CA-C-N	5.81	125.49	119.56
5	k	216	CYS	C-N-CA	5.81	125.49	119.56
5	k	227	THR	CA-C-N	5.81	126.32	120.04
5	k	227	THR	C-N-CA	5.81	126.32	120.04
4	j	234	LEU	N-CA-C	-5.81	106.74	113.88
3	i	18	GLN	CA-C-N	5.80	123.84	119.66
3	i	18	GLN	C-N-CA	5.80	123.84	119.66
4	f	98	TYR	CB-CA-C	5.80	118.82	109.07
3	i	257	LYS	CA-C-N	5.79	125.73	119.76
3	i	257	LYS	C-N-CA	5.79	125.73	119.76
4	f	235	ALA	N-CA-C	-5.79	101.41	110.14
4	n	210	VAL	N-CA-C	5.78	113.78	107.60
5	s	199	VAL	CA-C-N	5.77	126.23	120.52
5	s	199	VAL	C-N-CA	5.77	126.23	120.52
5	c	31	THR	CA-C-N	5.72	123.78	119.66
5	c	31	THR	C-N-CA	5.72	123.78	119.66
3	q	186	PRO	CA-C-N	5.72	125.63	119.85
3	q	186	PRO	C-N-CA	5.72	125.63	119.85
3	e	256	MET	N-CA-C	5.72	118.10	109.23
4	n	11	ASP	CA-CB-CG	-5.71	106.89	112.60
5	c	199	VAL	CA-C-N	5.71	126.17	120.52
5	c	199	VAL	C-N-CA	5.71	126.17	120.52
5	g	83	CYS	N-CA-C	5.71	118.46	107.44
5	g	167	ALA	CA-C-N	5.68	126.00	119.92
5	g	167	ALA	C-N-CA	5.68	126.00	119.92
3	q	243	SER	N-CA-C	5.68	118.51	110.50
3	q	137	TYR	CA-C-N	5.67	126.17	120.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	q	137	TYR	C-N-CA	5.67	126.17	120.04
3	i	111	VAL	N-CA-C	5.67	118.17	111.09
5	s	21	SER	CA-C-N	5.66	125.61	119.78
5	s	21	SER	C-N-CA	5.66	125.61	119.78
3	m	287	LEU	CA-C-N	5.66	125.28	119.56
3	m	287	LEU	C-N-CA	5.66	125.28	119.56
5	g	194	GLN	N-CA-C	-5.65	105.11	112.23
4	b	137	GLU	N-CA-C	-5.65	99.23	108.67
4	n	244	SER	CA-C-N	5.64	125.26	119.56
4	n	244	SER	C-N-CA	5.64	125.26	119.56
3	q	42	VAL	N-CA-C	-5.64	107.77	113.47
4	j	177	LEU	N-CA-C	-5.63	102.14	110.48
3	q	104	ASN	CA-C-N	-5.62	113.94	121.80
3	q	104	ASN	C-N-CA	-5.62	113.94	121.80
3	i	274	TYR	CB-CA-C	-5.60	97.98	110.19
3	i	191	ILE	CA-C-N	5.59	125.57	120.03
3	i	191	ILE	C-N-CA	5.59	125.57	120.03
3	m	257	LYS	CA-C-N	5.59	125.50	119.85
3	m	257	LYS	C-N-CA	5.59	125.50	119.85
5	s	55	MET	N-CA-C	5.58	119.82	112.89
3	q	265	CYS	N-CA-C	5.58	122.14	109.81
3	e	230	ASN	N-CA-C	5.55	118.55	107.62
3	i	127	LEU	N-CA-C	5.54	118.26	109.50
6	h	68	LEU	CA-C-N	5.54	131.68	121.70
6	h	68	LEU	C-N-CA	5.54	131.68	121.70
4	n	105	GLY	N-CA-C	-5.53	103.85	112.58
5	s	216	CYS	CA-C-N	5.53	126.75	119.84
5	s	216	CYS	C-N-CA	5.53	126.75	119.84
3	a	155	ILE	CA-C-N	5.53	126.07	120.38
3	a	155	ILE	C-N-CA	5.53	126.07	120.38
5	s	70	ILE	CB-CA-C	-5.52	104.80	110.71
4	r	105	GLY	N-CA-C	-5.51	103.87	112.58
4	r	79	TRP	N-CA-CB	-5.50	101.81	110.77
5	k	31	THR	CA-C-N	5.49	123.67	119.66
5	k	31	THR	C-N-CA	5.49	123.67	119.66
3	m	268	PRO	CA-C-N	5.49	125.69	120.31
3	m	268	PRO	C-N-CA	5.49	125.69	120.31
3	a	186	PRO	CA-C-N	5.46	125.37	119.85
3	a	186	PRO	C-N-CA	5.46	125.37	119.85
4	j	170	GLU	N-CA-C	-5.46	106.75	113.41
3	i	48	GLY	N-CA-C	-5.43	105.13	112.14
5	c	194	GLN	N-CA-C	-5.43	104.90	112.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	n	175	ALA	N-CA-C	-5.42	102.26	110.28
5	g	227	THR	CA-C-N	5.41	126.46	120.45
5	g	227	THR	C-N-CA	5.41	126.46	120.45
5	s	32	PRO	CA-C-N	5.41	125.88	120.14
5	s	32	PRO	C-N-CA	5.41	125.88	120.14
3	a	287	LEU	CA-C-N	5.41	125.02	119.56
3	a	287	LEU	C-N-CA	5.41	125.02	119.56
4	f	175	ALA	CA-C-N	-5.40	114.73	122.67
4	f	175	ALA	C-N-CA	-5.40	114.73	122.67
4	b	224	HIS	N-CA-C	5.40	117.88	108.76
3	m	191	ILE	CA-C-N	5.39	125.33	119.78
3	m	191	ILE	C-N-CA	5.39	125.33	119.78
4	f	105	GLY	N-CA-C	-5.38	103.31	112.51
4	b	210	VAL	CA-C-N	5.37	125.58	120.31
4	b	210	VAL	C-N-CA	5.37	125.58	120.31
3	a	90	SER	N-CA-C	5.37	117.27	108.52
4	j	127	ILE	N-CA-C	5.36	113.84	107.73
6	l	66	PRO	N-CA-C	-5.35	102.79	111.14
5	g	199	VAL	CA-C-N	5.35	125.34	120.21
5	g	199	VAL	C-N-CA	5.35	125.34	120.21
3	e	243	SER	N-CA-C	5.34	117.58	110.53
3	q	268	PRO	CA-C-N	5.34	125.32	120.03
3	q	268	PRO	C-N-CA	5.34	125.32	120.03
3	i	253	ARG	NE-CZ-NH1	-5.33	116.17	121.50
4	r	210	VAL	CA-C-N	5.32	125.53	120.31
4	r	210	VAL	C-N-CA	5.32	125.53	120.31
5	s	80	PRO	CA-C-N	5.31	128.33	120.74
5	s	80	PRO	C-N-CA	5.31	128.33	120.74
5	o	160	GLN	CA-C-N	5.30	129.09	120.60
5	o	160	GLN	C-N-CA	5.30	129.09	120.60
3	a	159	ALA	CA-C-N	5.30	125.21	119.85
3	a	159	ALA	C-N-CA	5.30	125.21	119.85
3	e	186	PRO	CA-C-N	5.29	125.19	119.85
3	e	186	PRO	C-N-CA	5.29	125.19	119.85
4	b	244	SER	CA-C-N	5.26	125.18	119.76
4	b	244	SER	C-N-CA	5.26	125.18	119.76
3	e	178	ILE	N-CA-C	5.26	115.47	108.11
5	k	222	ARG	CB-CA-C	-5.25	101.20	109.34
4	j	11	ASP	CA-CB-CG	-5.24	107.36	112.60
3	i	215	GLU	N-CA-C	5.23	116.23	108.86
4	j	210	VAL	CA-C-N	5.21	125.42	120.31
4	j	210	VAL	C-N-CA	5.21	125.42	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	g	36	ILE	CA-C-N	5.21	125.19	120.03
5	g	36	ILE	C-N-CA	5.21	125.19	120.03
3	i	253	ARG	CB-CG-CD	-5.21	99.32	111.30
3	i	243	SER	N-CA-C	5.20	117.83	110.50
3	m	191	ILE	N-CA-C	5.20	113.16	107.60
3	i	220	GLY	N-CA-C	-5.19	107.83	114.37
5	o	139	LYS	CA-C-N	5.19	123.45	119.66
5	o	139	LYS	C-N-CA	5.19	123.45	119.66
3	a	247	THR	N-CA-C	5.19	117.56	110.55
5	c	32	PRO	CA-C-N	5.19	125.09	119.85
5	c	32	PRO	C-N-CA	5.19	125.09	119.85
6	h	26	ASN	CA-C-N	-5.19	115.56	122.72
6	h	26	ASN	C-N-CA	-5.19	115.56	122.72
3	q	155	ILE	CA-C-N	5.19	125.73	120.38
3	q	155	ILE	C-N-CA	5.19	125.73	120.38
4	r	146	ILE	CB-CA-C	-5.19	105.22	112.02
3	m	104	ASN	CA-C-N	-5.19	113.92	120.98
3	m	104	ASN	C-N-CA	-5.19	113.92	120.98
3	e	36	VAL	CA-C-N	5.18	124.80	119.56
3	e	36	VAL	C-N-CA	5.18	124.80	119.56
3	e	127	LEU	N-CA-C	5.18	117.34	108.90
3	m	90	SER	N-CA-C	5.18	118.00	109.72
4	j	136	THR	N-CA-C	5.16	117.97	109.76
4	b	122	LEU	CA-C-N	-5.16	116.56	121.57
4	b	122	LEU	C-N-CA	-5.16	116.56	121.57
3	a	126	ASP	N-CA-C	-5.15	102.89	110.52
4	f	38	TRP	CA-C-N	5.15	125.06	119.76
4	f	38	TRP	C-N-CA	5.15	125.06	119.76
5	c	96	HIS	CA-CB-CG	-5.14	108.66	113.80
4	f	162	ASN	CA-C-N	5.14	125.06	119.76
4	f	162	ASN	C-N-CA	5.14	125.06	119.76
3	m	281	MET	N-CA-C	5.14	117.63	109.50
3	i	186	PRO	CA-C-N	5.14	125.05	119.85
3	i	186	PRO	C-N-CA	5.14	125.05	119.85
3	a	248	ILE	N-CA-C	5.14	116.12	108.46
4	j	122	LEU	CA-C-N	-5.14	117.38	122.36
4	j	122	LEU	C-N-CA	-5.14	117.38	122.36
4	r	230	VAL	N-CA-C	5.14	115.30	108.11
4	j	205	SER	N-CA-C	5.13	116.61	108.96
5	k	222	ARG	N-CA-C	5.13	120.01	113.55
4	f	32	ILE	N-CA-C	5.12	115.34	108.17
4	f	197	ILE	CA-C-N	-5.12	116.22	122.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	197	ILE	C-N-CA	-5.12	116.22	122.93
3	i	30	GLY	N-CA-C	-5.12	105.76	112.82
5	c	36	ILE	CA-C-N	5.11	125.04	119.78
5	c	36	ILE	C-N-CA	5.11	125.04	119.78
3	m	137	TYR	CA-C-N	5.11	125.56	120.04
3	m	137	TYR	C-N-CA	5.11	125.56	120.04
4	r	82	LEU	N-CA-C	5.11	119.12	112.17
4	n	162	ASN	CA-C-N	5.10	125.01	119.76
4	n	162	ASN	C-N-CA	5.10	125.01	119.76
4	n	72	LYS	N-CA-C	-5.09	103.68	110.55
5	s	59	ASP	N-CA-C	5.08	118.41	111.39
6	d	66	PRO	N-CA-C	-5.07	103.22	111.14
3	m	246	HIS	CA-CB-CG	-5.07	108.73	113.80
5	o	55	MET	N-CA-C	5.07	116.89	111.36
4	b	118	HIS	CA-CB-CG	5.07	118.87	113.80
3	i	178	ILE	N-CA-C	5.07	115.20	108.11
5	g	82	PHE	CA-CB-CG	5.06	118.86	113.80
6	t	66	PRO	N-CA-C	-5.06	103.24	111.03
4	b	89	MET	N-CA-C	5.05	117.32	108.52
4	j	214	ASN	CA-CB-CG	5.05	117.65	112.60
4	b	214	ASN	CA-CB-CG	5.05	117.65	112.60
3	a	239	ALA	N-CA-C	-5.04	103.40	110.50
5	g	187	GLY	N-CA-C	-5.03	104.90	112.84
5	o	32	PRO	CA-C-N	5.02	124.92	119.85
5	o	32	PRO	C-N-CA	5.02	124.92	119.85
6	p	40	SER	N-CA-C	-5.02	104.24	110.41
4	r	253	ILE	N-CA-C	5.02	115.94	108.46
5	s	108	HIS	CA-CB-CG	5.02	118.82	113.80
5	g	25	LEU	CA-C-N	5.01	124.92	119.76
5	g	25	LEU	C-N-CA	5.01	124.92	119.76
3	e	279	VAL	N-CA-C	-5.01	107.41	112.17
5	o	81	ILE	N-CA-C	-5.01	105.96	110.82

There are no chirality outliers.

There are no planarity outliers.

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

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	490	0	118	3	0
2	H	540	0	130	1	0
3	a	2213	0	2132	5	0
3	e	2219	0	2137	11	0
3	i	2226	0	2146	16	0
3	m	2176	0	2102	7	0
3	q	2226	0	2146	13	0
4	b	2053	0	1975	4	0
4	f	2008	0	1936	3	0
4	j	2003	0	1931	3	0
4	n	2029	0	1953	3	0
4	r	1975	0	1907	9	0
5	c	1848	0	1836	11	0
5	g	1810	0	1791	5	0
5	k	1801	0	1778	7	0
5	o	1810	0	1791	8	0
5	s	1818	0	1802	19	0
6	d	512	0	493	1	0
6	h	512	0	493	6	0
6	l	512	0	493	3	0
6	p	504	0	487	4	0
6	t	512	0	493	2	0
7	a	16	0	27	0	0
7	e	16	0	27	0	0
7	i	16	0	27	0	0
7	m	16	0	27	0	0
7	q	16	0	27	0	0
All	All	33877	0	32205	118	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 (118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:r:116:LYS:HB3	5:s:124:MET:HE3	1.79	0.65
3:q:115:ARG:HD2	5:s:230:ILE:HD13	1.80	0.63
3:m:99:HIS:CE1	3:m:239:ALA:O	2.53	0.62
3:i:274:TYR:CD1	5:k:230:ILE:HD11	2.35	0.62
3:e:170:TRP:CE2	3:e:238:ARG:HD3	2.36	0.61
4:f:11:ASP:OD1	4:f:11:ASP:N	2.30	0.61
3:e:149:VAL:HG13	3:e:240:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:n:264:ARG:HD2	5:s:138:ALA:HB2	1.85	0.59
3:i:180:TYR:CD1	3:i:187:PRO:HD3	2.38	0.59
3:m:99:HIS:HE1	3:m:239:ALA:O	1.87	0.58
5:s:155:TRP:CG	5:s:163:CYS:HG	2.23	0.57
3:e:240:VAL:HG13	3:i:253:ARG:NH1	2.18	0.57
6:h:34:LYS:NZ	5:k:18:ASP:OD2	2.38	0.57
6:l:13:HIS:O	6:l:13:HIS:CG	2.57	0.57
3:m:221:ASP:N	3:m:221:ASP:OD1	2.37	0.57
3:q:114:ARG:HD3	3:q:274:TYR:CZ	2.41	0.56
3:m:96:GLU:O	3:m:99:HIS:HB2	2.06	0.56
4:r:116:LYS:HD3	5:s:124:MET:HE3	1.88	0.56
5:o:128:LYS:NZ	5:o:156:ASP:OD1	2.39	0.55
3:e:153:MET:SD	3:e:170:TRP:CE3	2.99	0.55
3:e:241:ASN:ND2	3:i:134:THR:OG1	2.39	0.55
5:c:175:TYR:CZ	5:c:222:ARG:HD3	2.43	0.53
5:c:128:LYS:NZ	5:c:156:ASP:OD1	2.41	0.53
3:q:107:TYR:CE1	3:q:114:ARG:HG3	2.44	0.53
1:L:5:UNK:O	1:L:6:UNK:C	2.54	0.52
3:i:133:PHE:CE1	3:i:252:VAL:HG22	2.43	0.52
4:r:118:HIS:ND1	4:r:239:PHE:HB2	2.24	0.52
4:r:118:HIS:CE1	4:r:239:PHE:HB2	2.44	0.52
5:c:175:TYR:CE2	5:c:222:ARG:HD3	2.44	0.52
5:c:174:VAL:HG12	5:c:175:TYR:CE1	2.45	0.51
6:h:49:ASP:OD2	6:h:52:LYS:NZ	2.43	0.51
3:q:257:LYS:NZ	5:s:17:ASP:O	2.44	0.51
3:q:111:VAL:HG22	5:s:232:GLN:OE1	2.10	0.51
5:o:74:ASP:N	5:o:74:ASP:OD1	2.41	0.51
6:p:34:LYS:NZ	6:t:41:ALA:O	2.43	0.51
3:e:241:ASN:CG	3:i:134:THR:OG1	2.54	0.50
5:s:172:ASN:N	5:s:172:ASN:OD1	2.44	0.50
5:o:155:TRP:CG	5:o:163:CYS:HG	2.28	0.50
1:L:55:UNK:O	1:L:58:UNK:N	2.44	0.50
3:e:170:TRP:CD2	3:e:238:ARG:HD3	2.46	0.50
3:i:293:ASP:N	3:i:293:ASP:OD1	2.43	0.49
3:a:257:LYS:NZ	5:c:17:ASP:O	2.45	0.49
3:e:257:LYS:NZ	5:g:17:ASP:O	2.46	0.49
6:h:8:GLN:HG2	6:h:27:TYR:HB3	1.95	0.49
3:q:107:TYR:HE1	3:q:114:ARG:HG3	1.78	0.49
3:i:270:ARG:HD2	3:i:274:TYR:CE2	2.48	0.49
3:m:257:LYS:NZ	5:o:17:ASP:O	2.46	0.49
3:i:114:ARG:HD3	3:i:274:TYR:CZ	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:q:107:TYR:N	3:q:107:TYR:CD2	2.81	0.48
4:b:72:LYS:HG2	4:b:246:GLN:HG2	1.95	0.48
3:m:99:HIS:HB3	3:m:165:TRP:HB3	1.96	0.48
5:c:110:THR:HG21	5:c:175:TYR:CE2	2.49	0.48
3:i:274:TYR:CE1	5:k:230:ILE:HD11	2.50	0.47
5:c:110:THR:CG2	5:c:175:TYR:CE2	2.98	0.47
3:e:221:ASP:OD1	3:e:221:ASP:N	2.45	0.47
5:g:172:ASN:N	5:g:172:ASN:OD1	2.47	0.46
6:p:11:GLY:H	6:p:14:GLU:HG3	1.79	0.46
6:t:13:HIS:O	6:t:13:HIS:ND1	2.49	0.46
6:h:13:HIS:O	6:h:13:HIS:ND1	2.49	0.46
5:c:174:VAL:CG1	5:c:175:TYR:CE1	2.99	0.46
4:b:137:GLU:O	4:b:138:SER:C	2.59	0.45
5:o:172:ASN:OD1	5:o:172:ASN:N	2.49	0.45
3:q:111:VAL:HG13	5:s:232:GLN:CD	2.42	0.45
5:c:174:VAL:HG12	5:c:175:TYR:CD1	2.52	0.44
6:d:13:HIS:O	6:d:13:HIS:ND1	2.51	0.44
6:h:55:GLU:N	6:h:56:PRO:CD	2.81	0.44
3:i:180:TYR:CE1	3:i:187:PRO:HD3	2.53	0.44
3:q:111:VAL:HG11	5:s:232:GLN:HB2	2.00	0.43
4:r:116:LYS:HD3	5:s:124:MET:CE	2.48	0.43
4:f:178:ASP:OD1	4:f:178:ASP:N	2.50	0.43
1:L:55:UNK:O	1:L:56:UNK:C	2.66	0.43
4:f:266:ILE:O	4:f:266:ILE:HG23	2.19	0.43
5:g:86:LEU:O	5:g:87:SER:C	2.61	0.43
4:r:117:PHE:HD1	5:s:203:THR:CG2	2.31	0.43
5:c:172:ASN:OD1	5:c:172:ASN:N	2.51	0.43
3:a:170:TRP:CE2	3:a:238:ARG:HD3	2.54	0.43
3:q:115:ARG:HA	3:q:274:TYR:OH	2.18	0.43
4:r:79:TRP:CD1	4:r:79:TRP:C	2.97	0.43
3:a:286:ILE:HB	4:b:179:TYR:OH	2.19	0.42
5:g:74:ASP:OD1	5:g:74:ASP:N	2.50	0.42
4:j:82:LEU:HD21	4:j:106:TYR:CD1	2.54	0.42
6:p:55:GLU:N	6:p:56:PRO:CD	2.82	0.42
3:q:151:GLN:OE1	3:q:238:ARG:NH2	2.52	0.42
4:r:82:LEU:HB2	4:r:83:PRO:HD3	2.01	0.42
6:p:55:GLU:N	6:p:56:PRO:HD3	2.35	0.42
3:e:167:ASP:O	3:e:170:TRP:HD1	2.01	0.42
6:h:55:GLU:N	6:h:56:PRO:HD3	2.34	0.42
3:i:51:ILE:HG12	3:i:52:PRO:HD2	2.02	0.42
3:a:137:TYR:CE2	3:a:142:SER:HA	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:n:98:TYR:O	4:n:264:ARG:HG2	2.20	0.42
5:s:192:PHE:CD2	5:s:192:PHE:N	2.86	0.42
5:k:155:TRP:CD1	5:k:163:CYS:HB2	2.55	0.41
5:k:172:ASN:OD1	5:k:172:ASN:N	2.53	0.41
4:n:30:ASN:O	4:n:196:GLN:NE2	2.54	0.41
5:s:86:LEU:O	5:s:87:SER:C	2.61	0.41
3:i:115:ARG:HA	3:i:274:TYR:OH	2.21	0.41
5:k:175:TYR:CZ	5:k:222:ARG:HD3	2.55	0.41
5:o:51:THR:HG21	5:o:98:MET:H	1.86	0.41
4:r:239:PHE:O	4:r:239:PHE:CD2	2.74	0.41
4:j:264:ARG:NH1	5:o:136:PRO:O	2.54	0.41
3:q:111:VAL:CG1	5:s:232:GLN:HB2	2.51	0.41
4:j:159:ASN:OD1	4:j:159:ASN:N	2.54	0.41
3:e:204:TYR:CD2	3:e:229:ILE:HG13	2.55	0.41
6:l:55:GLU:N	6:l:56:PRO:HD3	2.36	0.41
3:a:268:PRO:HG2	4:b:185:VAL:HG11	2.03	0.41
3:i:89:ASN:OD1	3:i:89:ASN:C	2.64	0.41
3:i:274:TYR:CE1	5:k:230:ILE:CD1	3.04	0.41
3:i:277:GLU:OE1	3:i:277:GLU:N	2.54	0.40
2:H:17:UNK:O	2:H:18:UNK:C	2.70	0.40
5:o:181:ASP:CG	5:o:182:ASP:N	2.79	0.40
5:s:82:PHE:CD1	5:s:82:PHE:C	2.99	0.40
5:s:138:ALA:O	5:s:139:LYS:C	2.62	0.40
5:g:59:ASP:OD1	5:g:60:GLY:N	2.55	0.40
3:m:99:HIS:HB3	3:m:165:TRP:CB	2.51	0.40
3:q:111:VAL:HG21	5:s:232:GLN:HB2	2.04	0.40
5:c:175:TYR:CE1	5:c:222:ARG:HD3	2.56	0.40
6:l:55:GLU:N	6:l:56:PRO:CD	2.84	0.40
5:s:230:ILE:HD12	5:s:230:ILE:HA	1.89	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	
3	a	279/298 (94%)	274 (98%)	5 (2%)	0	100	100
3	e	280/298 (94%)	273 (98%)	7 (2%)	0	100	100
3	i	281/298 (94%)	276 (98%)	5 (2%)	0	100	100
3	m	272/298 (91%)	267 (98%)	5 (2%)	0	100	100
3	q	281/298 (94%)	276 (98%)	5 (2%)	0	100	100
4	b	262/272 (96%)	256 (98%)	6 (2%)	0	100	100
4	f	254/272 (93%)	247 (97%)	7 (3%)	0	100	100
4	j	251/272 (92%)	247 (98%)	4 (2%)	0	100	100
4	n	257/272 (94%)	252 (98%)	5 (2%)	0	100	100
4	r	247/272 (91%)	241 (98%)	6 (2%)	0	100	100
5	c	237/240 (99%)	236 (100%)	1 (0%)	0	100	100
5	g	232/240 (97%)	225 (97%)	7 (3%)	0	100	100
5	k	231/240 (96%)	228 (99%)	3 (1%)	0	100	100
5	o	232/240 (97%)	231 (100%)	1 (0%)	0	100	100
5	s	233/240 (97%)	227 (97%)	6 (3%)	0	100	100
6	d	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
6	h	66/69 (96%)	64 (97%)	2 (3%)	0	100	100
6	l	66/69 (96%)	65 (98%)	1 (2%)	0	100	100
6	p	65/69 (94%)	61 (94%)	4 (6%)	0	100	100
6	t	66/69 (96%)	66 (100%)	0	0	100	100
All	All	4158/4395 (95%)	4076 (98%)	82 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	
3	a	246/260 (95%)	246 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	e	247/260 (95%)	247 (100%)	0	100	100
3	i	248/260 (95%)	248 (100%)	0	100	100
3	m	242/260 (93%)	242 (100%)	0	100	100
3	q	248/260 (95%)	248 (100%)	0	100	100
4	b	224/230 (97%)	224 (100%)	0	100	100
4	f	219/230 (95%)	219 (100%)	0	100	100
4	j	219/230 (95%)	219 (100%)	0	100	100
4	n	222/230 (96%)	222 (100%)	0	100	100
4	r	216/230 (94%)	216 (100%)	0	100	100
5	c	212/213 (100%)	212 (100%)	0	100	100
5	g	208/213 (98%)	208 (100%)	0	100	100
5	k	207/213 (97%)	207 (100%)	0	100	100
5	o	208/213 (98%)	208 (100%)	0	100	100
5	s	209/213 (98%)	209 (100%)	0	100	100
6	d	57/58 (98%)	57 (100%)	0	100	100
6	h	57/58 (98%)	57 (100%)	0	100	100
6	l	57/58 (98%)	57 (100%)	0	100	100
6	p	56/58 (97%)	56 (100%)	0	100	100
6	t	57/58 (98%)	57 (100%)	0	100	100
All	All	3659/3805 (96%)	3659 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
3	a	18	GLN
3	a	198	ASN
4	b	119	GLN
5	c	194	GLN
5	c	229	HIS
3	e	136	ASN
3	e	171	GLN
4	f	162	ASN
4	f	226	ASN

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Mol	Chain	Res	Type
4	f	246	GLN
4	j	15	GLN
4	j	272	GLN
6	l	69	ASN
3	m	99	HIS
3	m	147	ASN
3	q	198	ASN
4	r	149	ASN
4	r	225	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	MYR	i	300	-	15,15,15	1.46	2 (13%)	15,15,15	0.95	2 (13%)
7	MYR	a	300	-	15,15,15	1.44	2 (13%)	15,15,15	0.98	2 (13%)
7	MYR	m	300	-	15,15,15	1.53	2 (13%)	15,15,15	0.78	0
7	MYR	q	300	-	15,15,15	1.43	2 (13%)	15,15,15	0.92	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	MYR	e	300	-	15,15,15	1.44	2 (13%)	15,15,15	0.76	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	MYR	i	300	-	-	6/13/13/13	-
7	MYR	a	300	-	-	4/13/13/13	-
7	MYR	m	300	-	-	6/13/13/13	-
7	MYR	q	300	-	-	3/13/13/13	-
7	MYR	e	300	-	-	4/13/13/13	-

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	e	300	MYR	O2-C1	-3.41	1.19	1.30
7	m	300	MYR	O1-C1	3.39	1.33	1.22
7	q	300	MYR	O1-C1	3.36	1.33	1.22
7	i	300	MYR	O2-C1	-3.36	1.19	1.30
7	m	300	MYR	O2-C1	-3.24	1.20	1.30
7	a	300	MYR	O2-C1	-3.11	1.20	1.30
7	a	300	MYR	O1-C1	3.10	1.32	1.22
7	e	300	MYR	O1-C1	3.06	1.32	1.22
7	q	300	MYR	O2-C1	-3.01	1.20	1.30
7	i	300	MYR	O1-C1	2.98	1.31	1.22

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	q	300	MYR	O2-C1-C2	2.67	122.45	114.00
7	i	300	MYR	O2-C1-O1	-2.59	116.68	123.33
7	a	300	MYR	O2-C1-C2	2.58	122.15	114.00
7	a	300	MYR	O2-C1-O1	-2.38	117.22	123.33
7	i	300	MYR	O2-C1-C2	2.31	121.31	114.00
7	e	300	MYR	O2-C1-O1	-2.20	117.67	123.33

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	i	300	MYR	C4-C5-C6-C7
7	a	300	MYR	C3-C4-C5-C6
7	i	300	MYR	C10-C11-C12-C13
7	e	300	MYR	C11-C10-C9-C8
7	e	300	MYR	C5-C6-C7-C8
7	m	300	MYR	C6-C7-C8-C9
7	q	300	MYR	C11-C10-C9-C8
7	e	300	MYR	C7-C8-C9-C10
7	q	300	MYR	C4-C5-C6-C7
7	m	300	MYR	C11-C12-C13-C14
7	i	300	MYR	O2-C1-C2-C3
7	m	300	MYR	O2-C1-C2-C3
7	q	300	MYR	C5-C6-C7-C8
7	i	300	MYR	O1-C1-C2-C3
7	m	300	MYR	O1-C1-C2-C3
7	a	300	MYR	O1-C1-C2-C3
7	i	300	MYR	C3-C4-C5-C6
7	a	300	MYR	O2-C1-C2-C3
7	a	300	MYR	C11-C10-C9-C8
7	e	300	MYR	C11-C12-C13-C14
7	i	300	MYR	C5-C6-C7-C8
7	m	300	MYR	C5-C6-C7-C8
7	m	300	MYR	C7-C8-C9-C10

There are no ring outliers.

No monomer is involved in short contacts.

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.

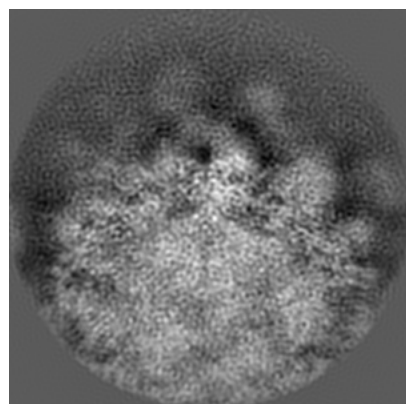
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-26071. These allow visual inspection of the internal detail of the map and identification of artifacts.

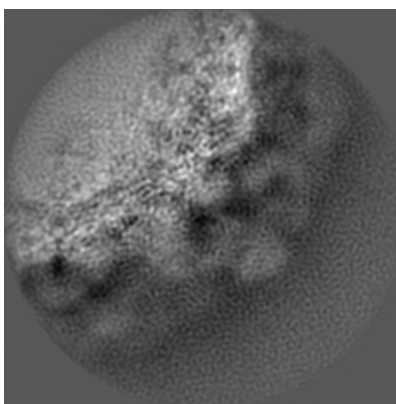
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

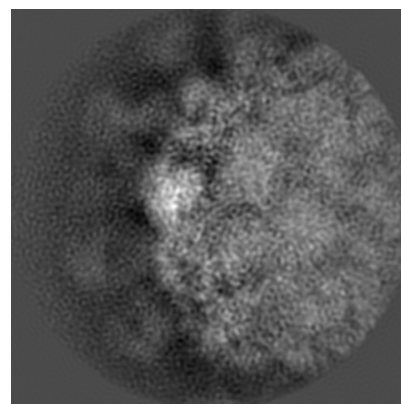
6.1.1 Primary map



X

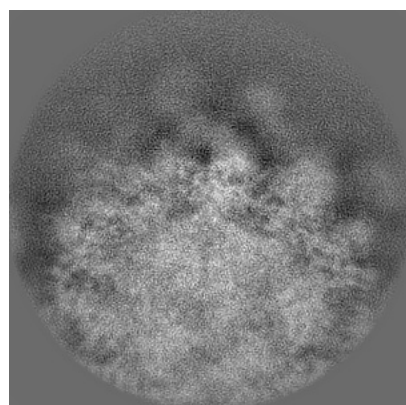


Y

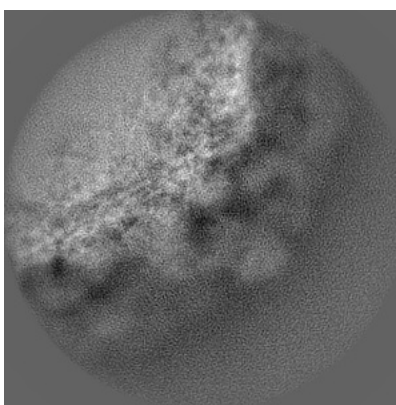


Z

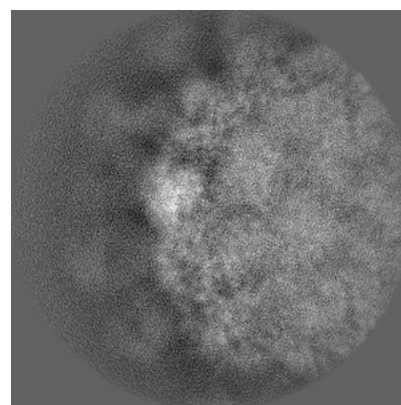
6.1.2 Raw map



X



Y

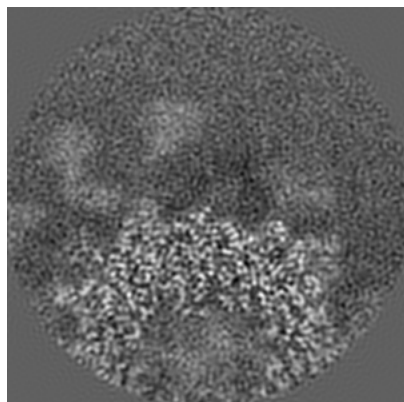


Z

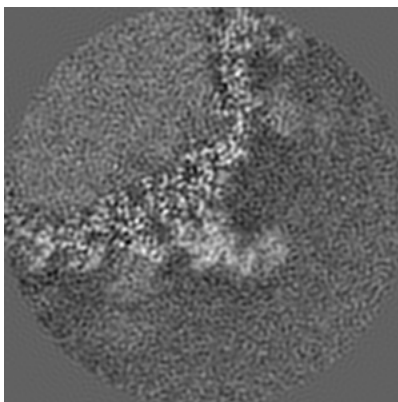
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

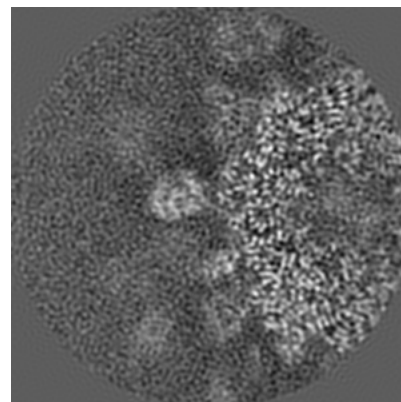
6.2.1 Primary map



X Index: 140

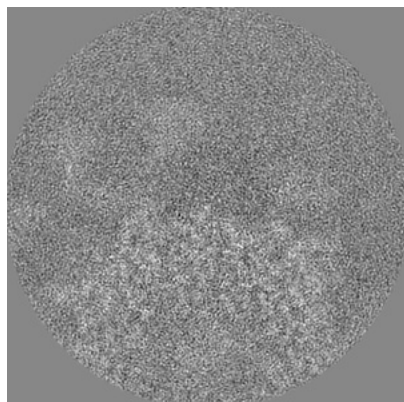


Y Index: 140

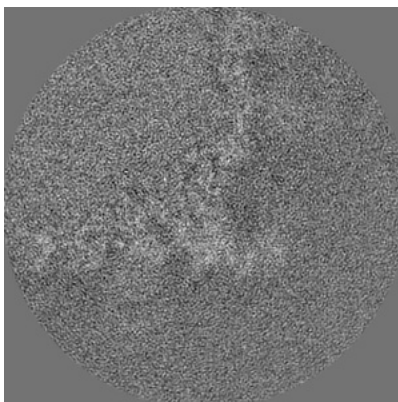


Z Index: 140

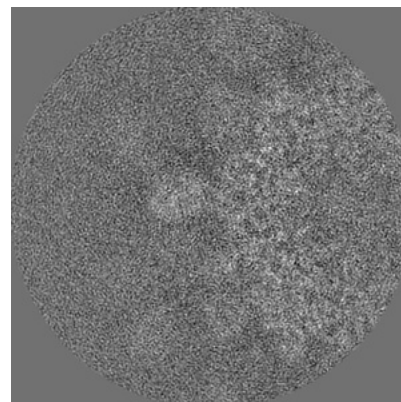
6.2.2 Raw map



X Index: 140



Y Index: 140

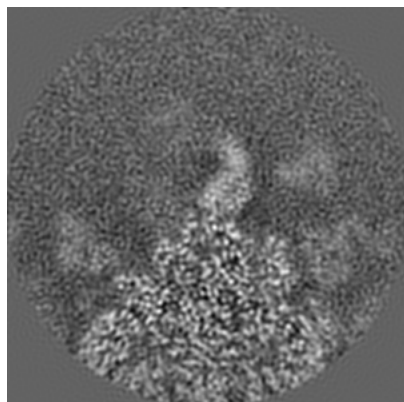


Z Index: 140

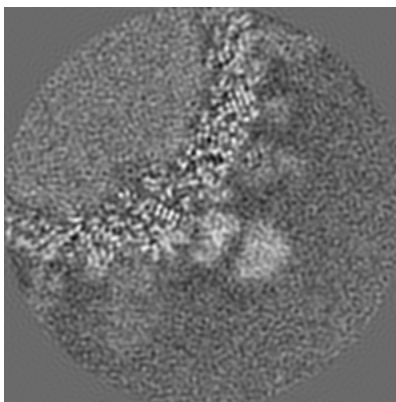
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

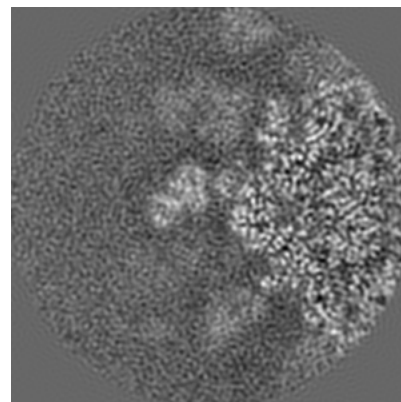
6.3.1 Primary map



X Index: 125

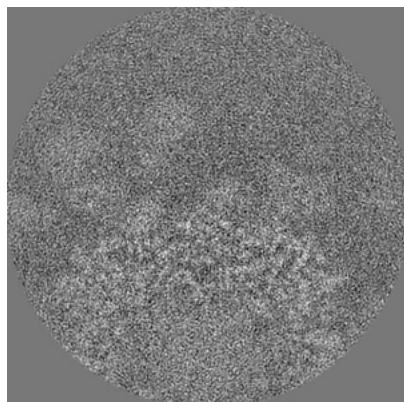


Y Index: 152

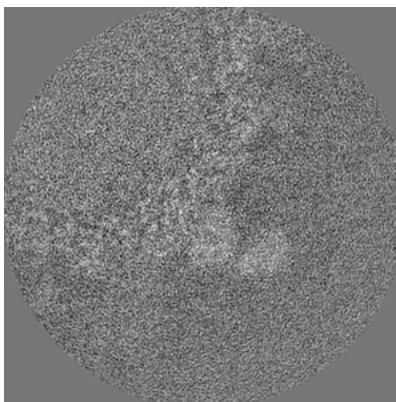


Z Index: 153

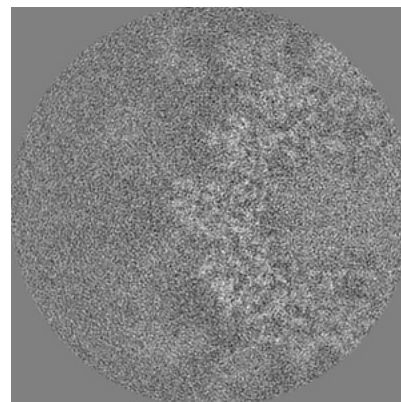
6.3.2 Raw map



X Index: 145



Y Index: 144

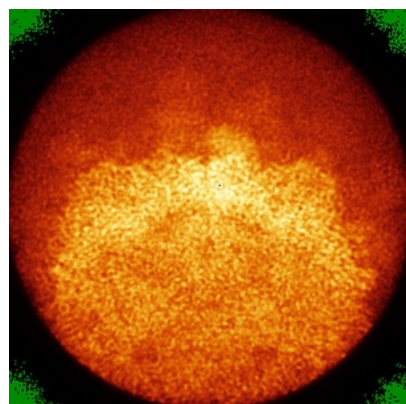


Z Index: 128

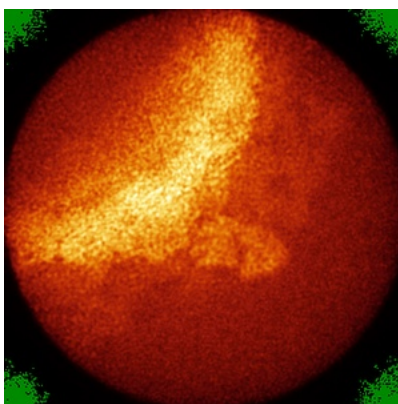
The images above show the largest variance slices of the map in three orthogonal directions.

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

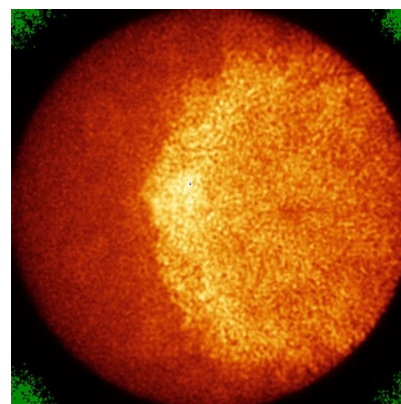
6.4.1 Primary map



X

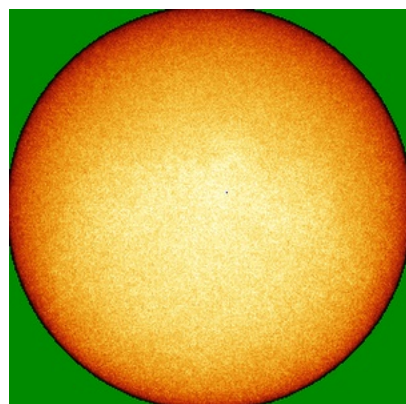


Y

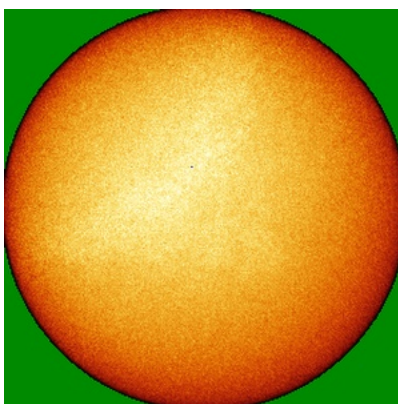


Z

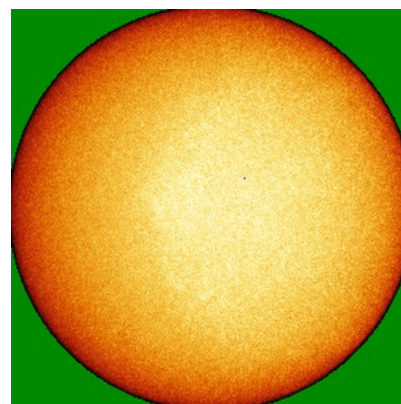
6.4.2 Raw map



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.

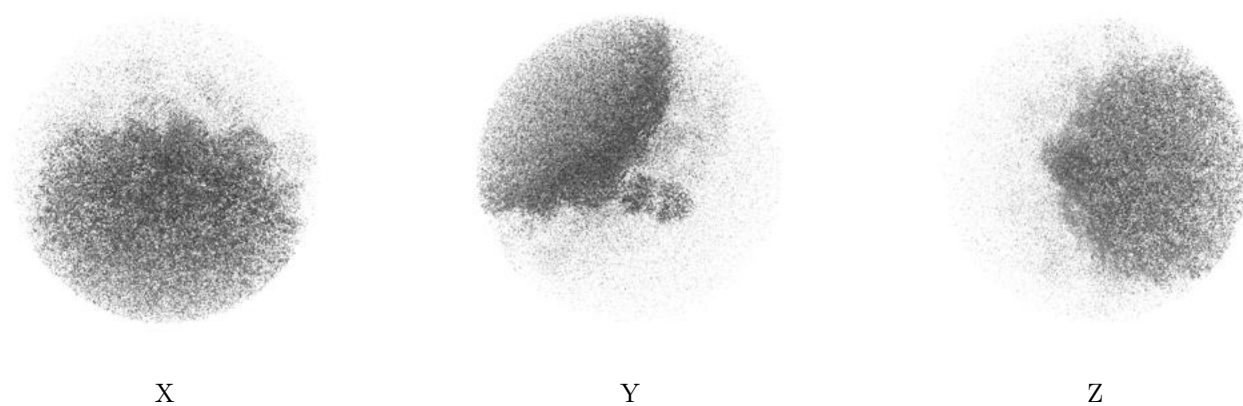
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.007. 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.

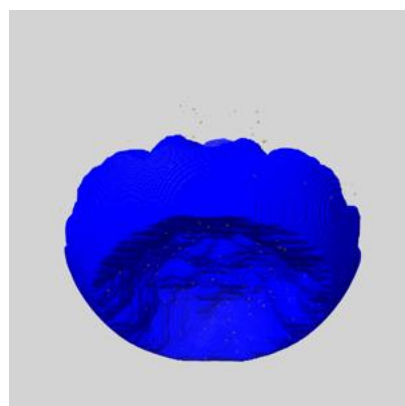
6.6 Mask visualisation [i](#)

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

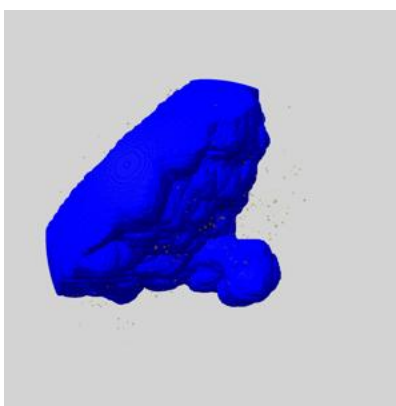
A mask typically either:

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

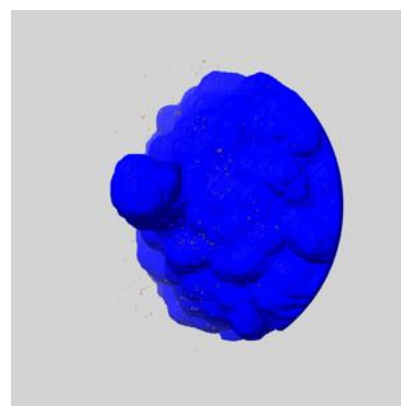
6.6.1 emd_26071_msk_1.map [i](#)



X



Y

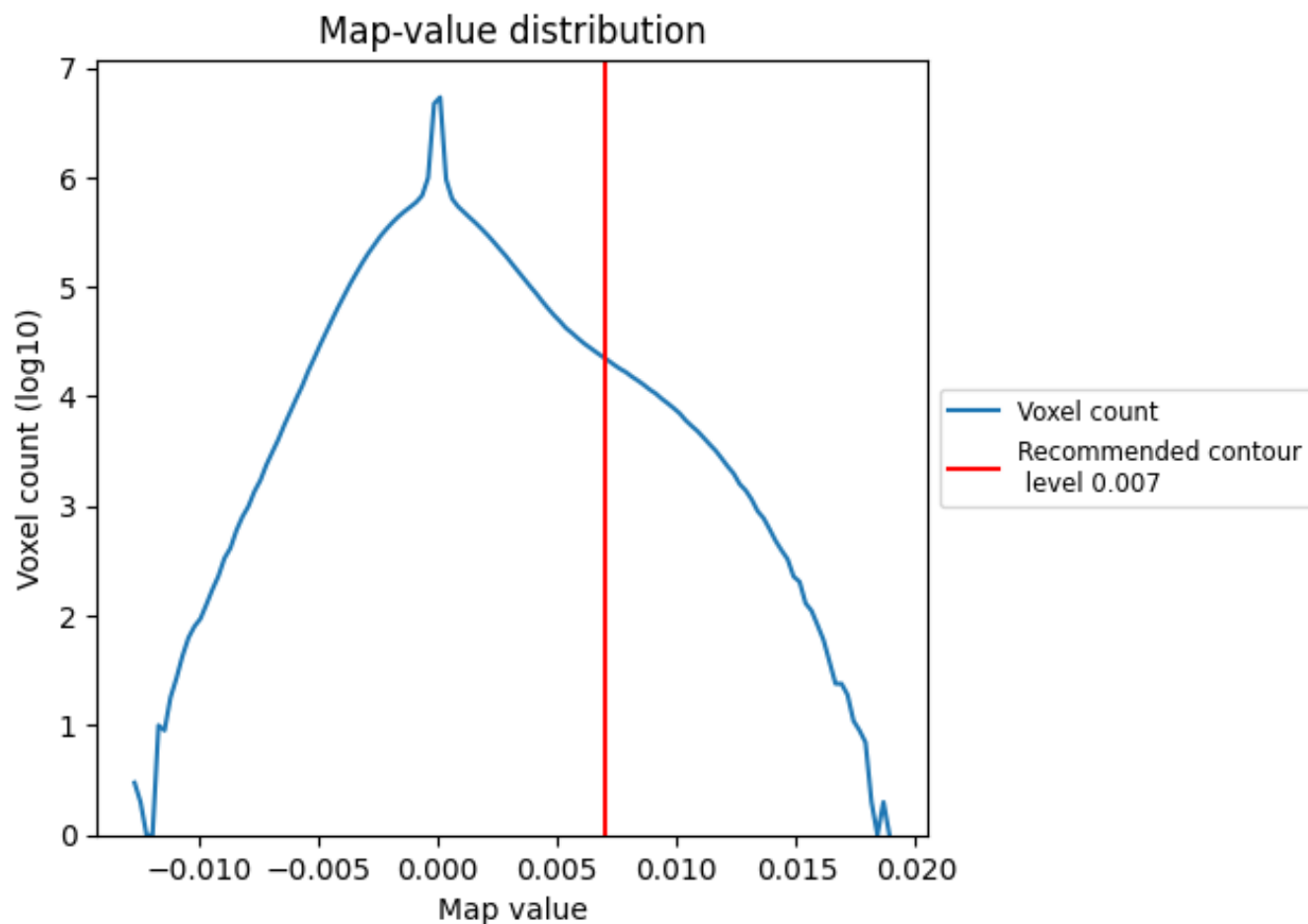


Z

7 Map analysis [i](#)

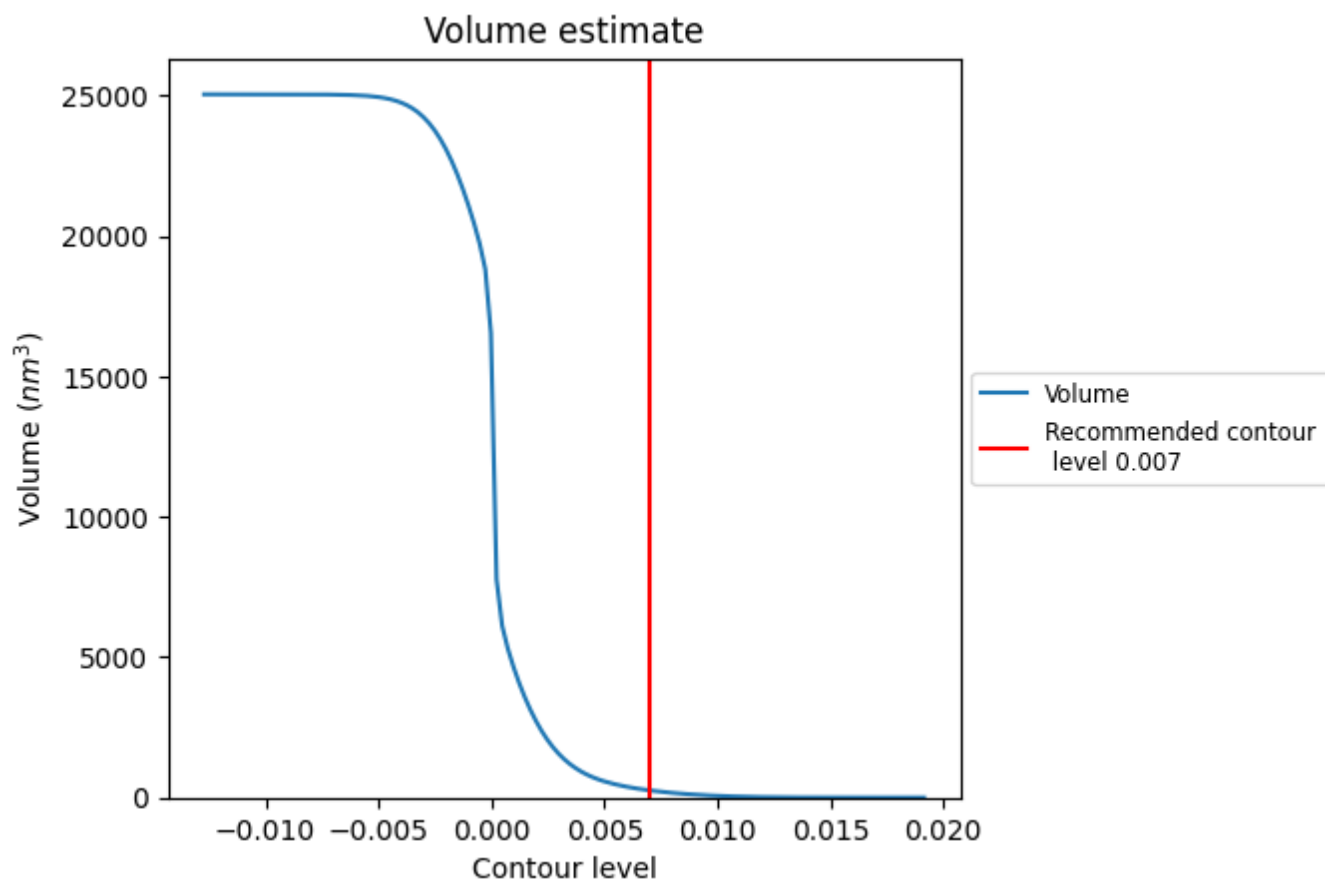
This section contains the results of statistical analysis of the map.

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.

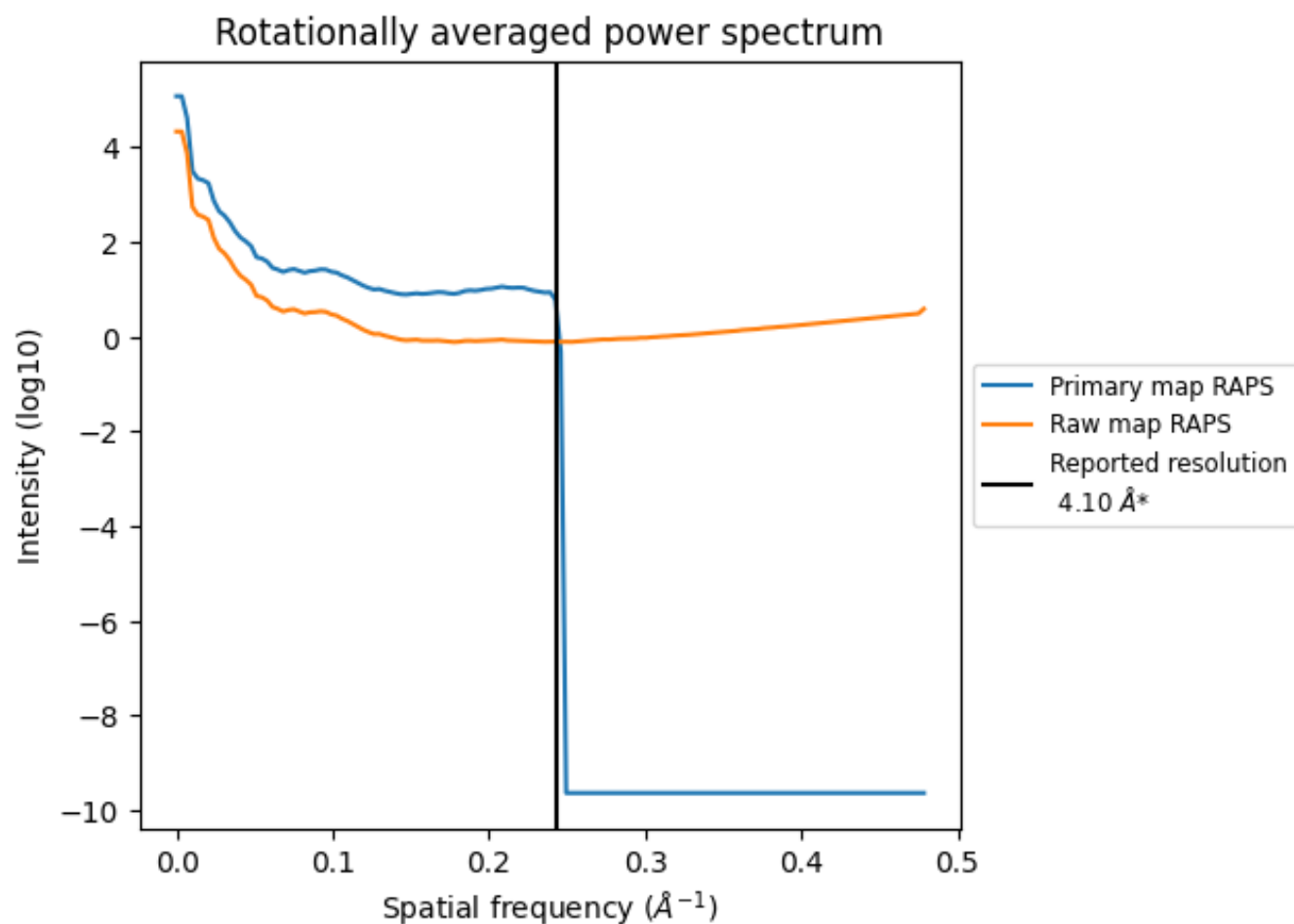
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 257 nm³; this corresponds to an approximate mass of 232 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 ⓘ

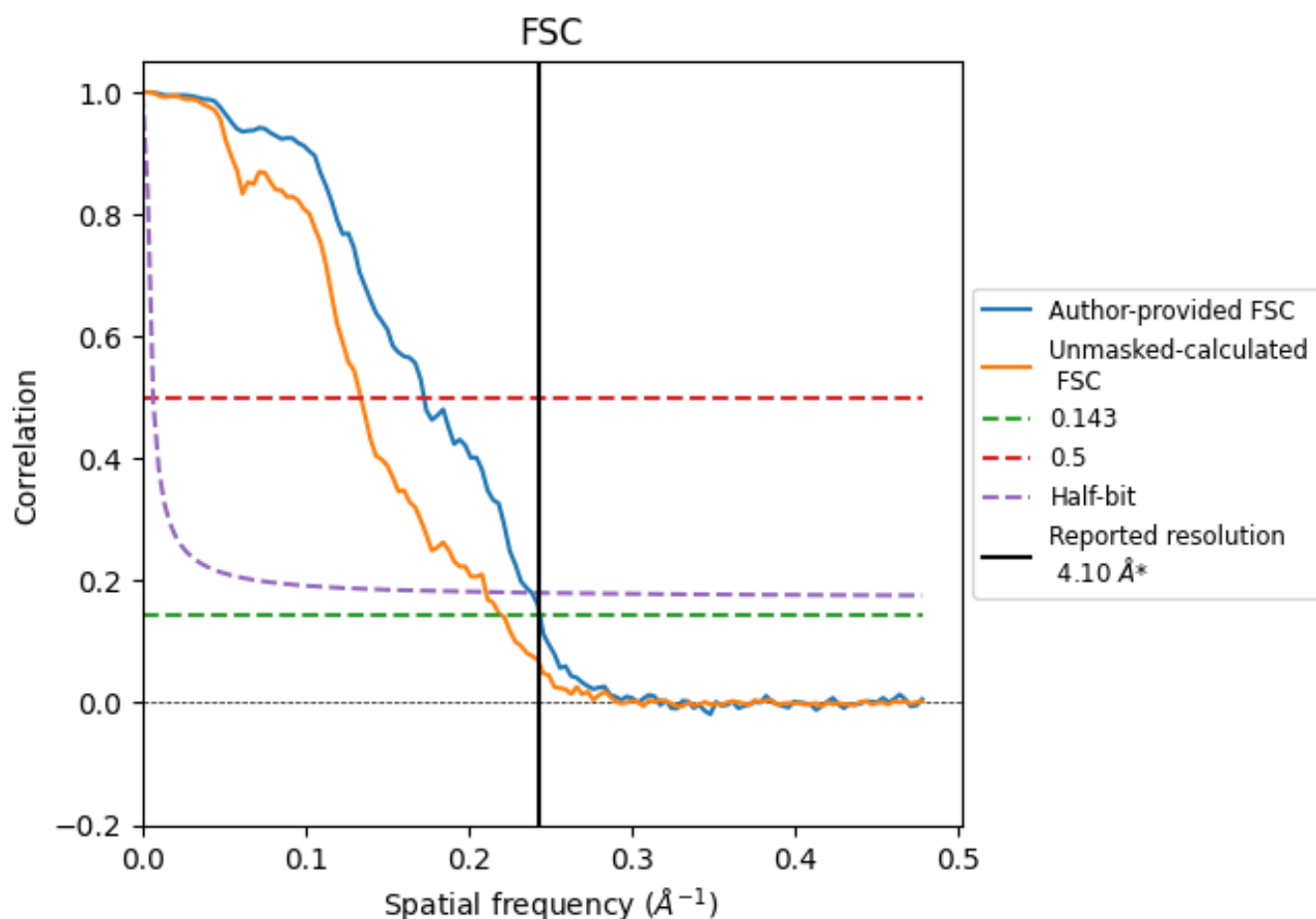


*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.244 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

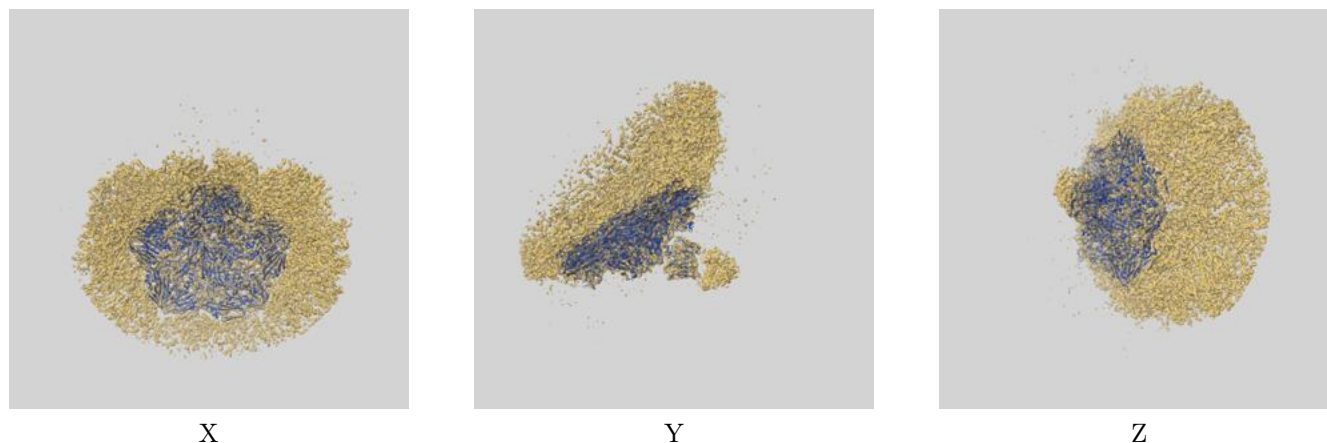
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.10	5.78	4.18
Unmasked-calculated*	4.53	7.46	4.74

*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 4.53 differs from the reported value 4.1 by more than 10 %

9 Map-model fit [i](#)

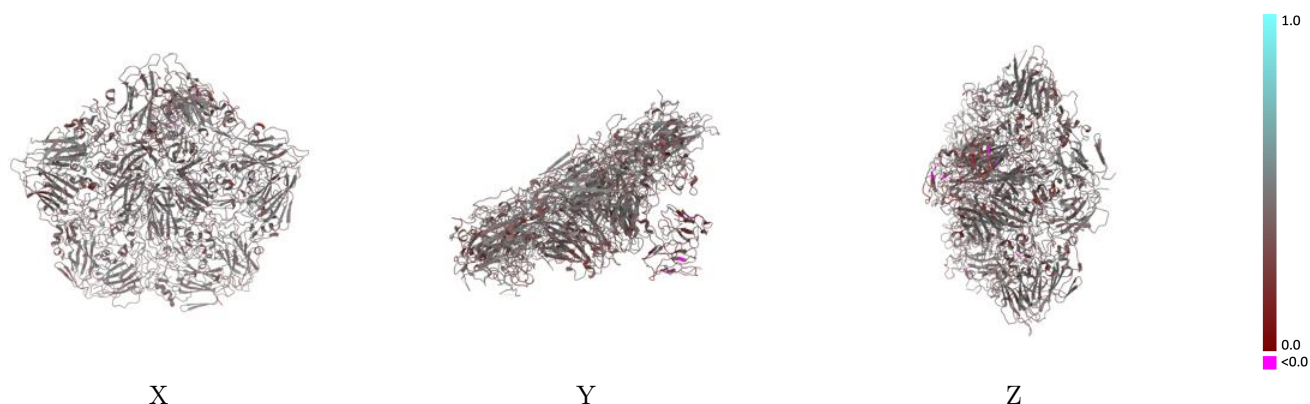
This section contains information regarding the fit between EMDB map EMD-26071 and PDB model 7TQT. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



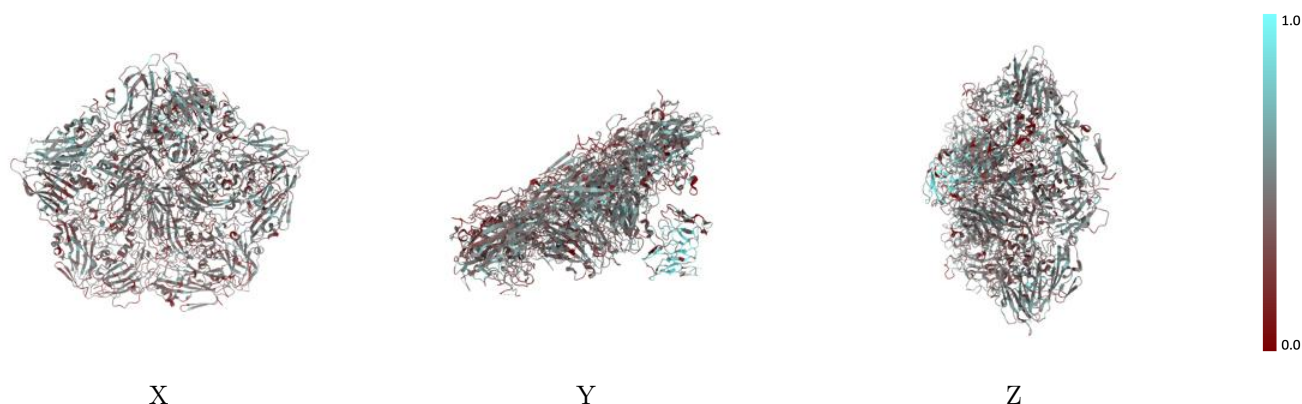
The images above show the 3D surface view of the map at the recommended contour level 0.007 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



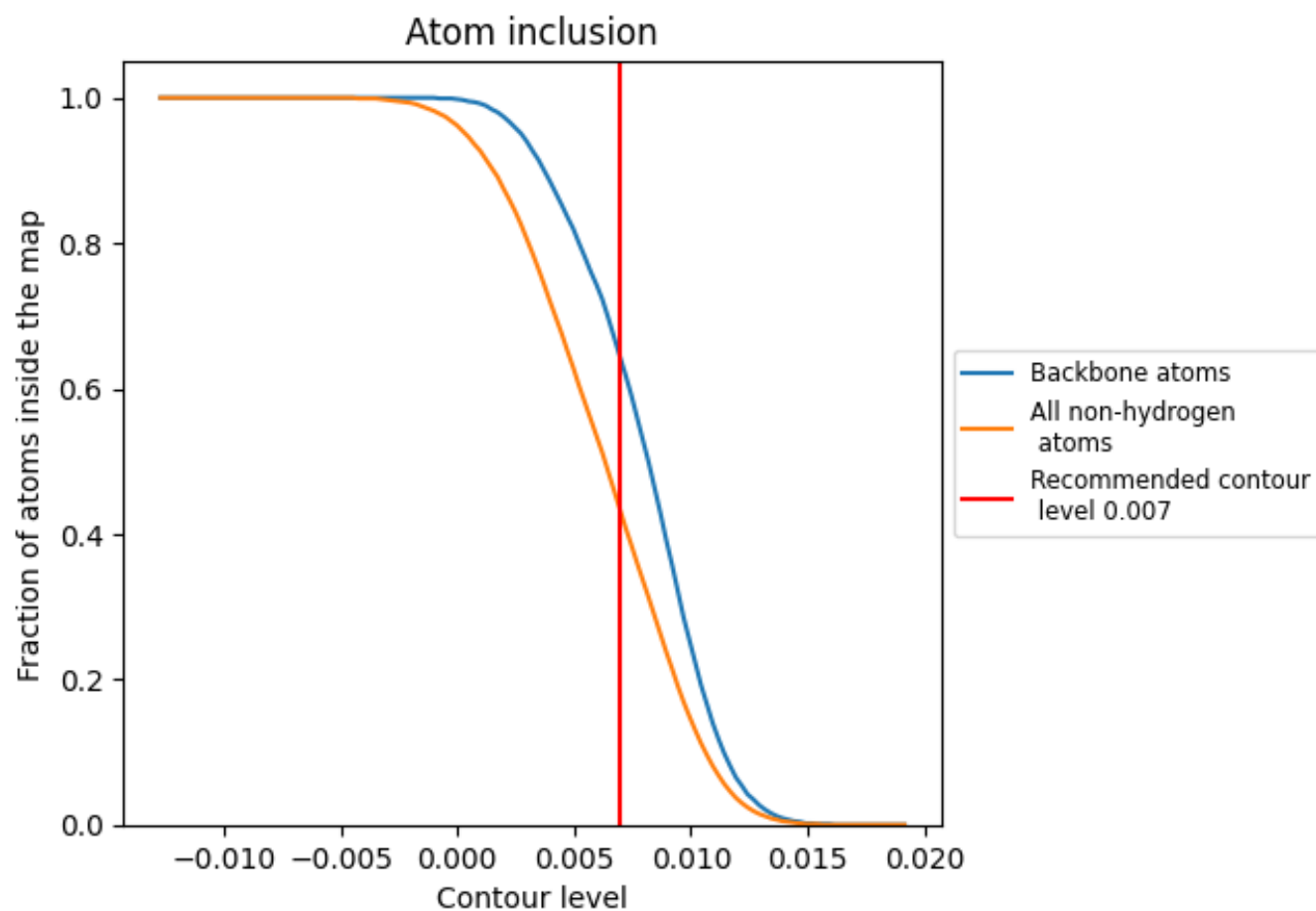
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.007).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 43% 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 (0.007) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.4300	 0.4030
H	 0.6240	 0.3120
L	 0.5000	 0.3340
a	 0.4320	 0.4050
b	 0.4460	 0.4150
c	 0.4610	 0.4090
d	 0.3390	 0.4170
e	 0.4430	 0.4120
f	 0.4520	 0.4180
g	 0.4680	 0.4080
h	 0.3100	 0.4040
i	 0.4060	 0.4020
j	 0.4050	 0.3980
k	 0.4450	 0.4060
l	 0.3000	 0.3970
m	 0.4150	 0.4020
n	 0.4070	 0.3930
o	 0.4280	 0.3970
p	 0.2830	 0.3940
q	 0.4160	 0.3980
r	 0.4810	 0.4170
s	 0.4490	 0.4070
t	 0.3020	 0.3970

