



wwPDB EM Validation Summary Report ⓘ

Jun 10, 2026 – 01:41 pm BST

PDB ID : 30GT / pdb_000030gt
EMDB ID : EMD-57765
Title : Cryo-EM structure of the PseCascade-TniQ-TnsC complex
Authors : Finocchio, G.; Oberli, S.; Schmitz, M.; Jinek, M.
Deposited on : 2026-04-24
Resolution : 3.30 Å(reported)
Based on initial model : .

This is a wwPDB EM Validation Summary 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:

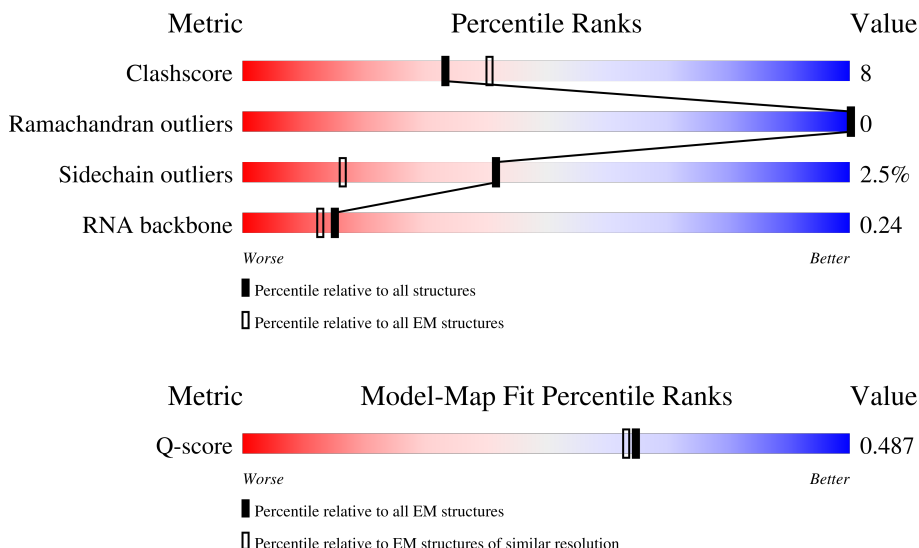
EMDB validation analysis : 0.0.1.dev132
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.














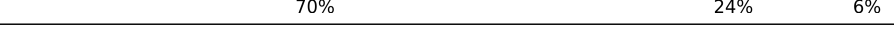





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	15087 (2.80 - 3.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	1	93	
2	2	144	
3	3	95	

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Mol	Chain	Length	Quality of chain
4	A	350	 73%19%8%
4	B	350	 77%21%..
4	C	350	 79%20%.
4	D	350	 78%20%..
4	E	350	 81%17%..
4	F	350	 81%16%..
5	G	695	 81%17%.
6	H	237	 66%17%16%
7	I	432	 72%22%. 6%
7	J	432	 78%16%6%
8	K	333	 76%23%.
8	L	333	 70%24%6%
8	M	333	 71%22%. 7%
8	N	333	 62%32%. 6%
8	O	333	 70%26%.
8	P	333	 75%19%. 6%
8	Q	333	 74%21%. .

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 51759 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 RNA chain called CRISPR RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	60	Total	C	N	O	P	0	0
			1291	577	243	412	59		

- Molecule 2 is a DNA chain called TS.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	65	Total	C	N	O	P	0	0
			1311	621	232	393	65		

- Molecule 3 is a DNA chain called NTS.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	3	40	Total	C	N	O	P	0	0
			784	374	144	229	37		

- Molecule 4 is a protein called Cas7.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	321	Total	C	N	O	S	0	0
			2580	1649	429	490	12		
4	B	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
4	C	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
4	D	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
4	E	346	Total	C	N	O	S	0	0
			2777	1774	462	529	12		
4	F	344	Total	C	N	O	S	0	0
			2763	1766	460	525	12		

- Molecule 5 is a protein called Cas8.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	G	684	Total	C	N	O	S	0	0
			5489	3525	945	994	25		

- Molecule 6 is a protein called Cas6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	H	198	Total	C	N	O	S	0	0
			1599	1019	278	293	9		

There are 34 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	204	SER	-	expression tag	UNP A0ABF7PQC0
H	205	ALA	-	expression tag	UNP A0ABF7PQC0
H	206	TRP	-	expression tag	UNP A0ABF7PQC0
H	207	SER	-	expression tag	UNP A0ABF7PQC0
H	208	HIS	-	expression tag	UNP A0ABF7PQC0
H	209	PRO	-	expression tag	UNP A0ABF7PQC0
H	210	GLN	-	expression tag	UNP A0ABF7PQC0
H	211	PHE	-	expression tag	UNP A0ABF7PQC0
H	212	GLU	-	expression tag	UNP A0ABF7PQC0
H	213	LYS	-	expression tag	UNP A0ABF7PQC0
H	214	GLY	-	expression tag	UNP A0ABF7PQC0
H	215	GLY	-	expression tag	UNP A0ABF7PQC0
H	216	GLY	-	expression tag	UNP A0ABF7PQC0
H	217	SER	-	expression tag	UNP A0ABF7PQC0
H	218	GLY	-	expression tag	UNP A0ABF7PQC0
H	219	GLY	-	expression tag	UNP A0ABF7PQC0
H	220	GLY	-	expression tag	UNP A0ABF7PQC0
H	221	SER	-	expression tag	UNP A0ABF7PQC0
H	222	GLY	-	expression tag	UNP A0ABF7PQC0
H	223	GLY	-	expression tag	UNP A0ABF7PQC0
H	224	SER	-	expression tag	UNP A0ABF7PQC0
H	225	ALA	-	expression tag	UNP A0ABF7PQC0
H	226	TRP	-	expression tag	UNP A0ABF7PQC0
H	227	SER	-	expression tag	UNP A0ABF7PQC0
H	228	HIS	-	expression tag	UNP A0ABF7PQC0
H	229	PRO	-	expression tag	UNP A0ABF7PQC0
H	230	GLN	-	expression tag	UNP A0ABF7PQC0
H	231	PHE	-	expression tag	UNP A0ABF7PQC0
H	232	GLU	-	expression tag	UNP A0ABF7PQC0
H	233	LYS	-	expression tag	UNP A0ABF7PQC0
H	234	SER	-	expression tag	UNP A0ABF7PQC0

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Chain	Residue	Modelled	Actual	Comment	Reference
H	235	GLY	-	expression tag	UNP A0ABF7PQC0
H	236	GLY	-	expression tag	UNP A0ABF7PQC0
H	237	GLY	-	expression tag	UNP A0ABF7PQC0

- Molecule 7 is a protein called TniQ.1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	I	408	Total	C	N	O	S	0	0
			3311	2120	561	614	16		
7	J	404	Total	C	N	O	S	0	0
			3271	2094	556	604	17		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-22	MET	-	initiating methionine	UNP A0ABF7PQC1
I	-21	GLY	-	expression tag	UNP A0ABF7PQC1
I	-20	HIS	-	expression tag	UNP A0ABF7PQC1
I	-19	HIS	-	expression tag	UNP A0ABF7PQC1
I	-18	HIS	-	expression tag	UNP A0ABF7PQC1
I	-17	HIS	-	expression tag	UNP A0ABF7PQC1
I	-16	HIS	-	expression tag	UNP A0ABF7PQC1
I	-15	HIS	-	expression tag	UNP A0ABF7PQC1
I	-14	HIS	-	expression tag	UNP A0ABF7PQC1
I	-13	HIS	-	expression tag	UNP A0ABF7PQC1
I	-12	HIS	-	expression tag	UNP A0ABF7PQC1
I	-11	HIS	-	expression tag	UNP A0ABF7PQC1
I	-10	GLY	-	expression tag	UNP A0ABF7PQC1
I	-9	GLY	-	expression tag	UNP A0ABF7PQC1
I	-8	SER	-	expression tag	UNP A0ABF7PQC1
I	-7	GLU	-	expression tag	UNP A0ABF7PQC1
I	-6	ASN	-	expression tag	UNP A0ABF7PQC1
I	-5	LEU	-	expression tag	UNP A0ABF7PQC1
I	-4	TYR	-	expression tag	UNP A0ABF7PQC1
I	-3	PHE	-	expression tag	UNP A0ABF7PQC1
I	-2	GLN	-	expression tag	UNP A0ABF7PQC1
I	-1	SER	-	expression tag	UNP A0ABF7PQC1
I	0	GLY	-	expression tag	UNP A0ABF7PQC1
J	-22	MET	-	initiating methionine	UNP A0ABF7PQC1
J	-21	GLY	-	expression tag	UNP A0ABF7PQC1
J	-20	HIS	-	expression tag	UNP A0ABF7PQC1
J	-19	HIS	-	expression tag	UNP A0ABF7PQC1

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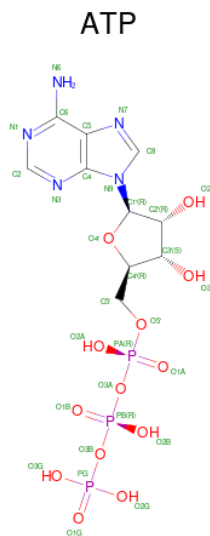
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Chain	Residue	Modelled	Actual	Comment	Reference
J	-18	HIS	-	expression tag	UNP A0ABF7PQC1
J	-17	HIS	-	expression tag	UNP A0ABF7PQC1
J	-16	HIS	-	expression tag	UNP A0ABF7PQC1
J	-15	HIS	-	expression tag	UNP A0ABF7PQC1
J	-14	HIS	-	expression tag	UNP A0ABF7PQC1
J	-13	HIS	-	expression tag	UNP A0ABF7PQC1
J	-12	HIS	-	expression tag	UNP A0ABF7PQC1
J	-11	HIS	-	expression tag	UNP A0ABF7PQC1
J	-10	GLY	-	expression tag	UNP A0ABF7PQC1
J	-9	GLY	-	expression tag	UNP A0ABF7PQC1
J	-8	SER	-	expression tag	UNP A0ABF7PQC1
J	-7	GLU	-	expression tag	UNP A0ABF7PQC1
J	-6	ASN	-	expression tag	UNP A0ABF7PQC1
J	-5	LEU	-	expression tag	UNP A0ABF7PQC1
J	-4	TYR	-	expression tag	UNP A0ABF7PQC1
J	-3	PHE	-	expression tag	UNP A0ABF7PQC1
J	-2	GLN	-	expression tag	UNP A0ABF7PQC1
J	-1	SER	-	expression tag	UNP A0ABF7PQC1
J	0	GLY	-	expression tag	UNP A0ABF7PQC1

- Molecule 8 is a protein called TnsC.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	327	Total	C	N	O	S	0	0
			2658	1704	455	486	13		
8	L	313	Total	C	N	O	S	0	0
			2545	1631	434	467	13		
8	M	311	Total	C	N	O	S	0	0
			2529	1622	432	463	12		
8	N	313	Total	C	N	O	S	0	0
			2547	1635	435	465	12		
8	O	319	Total	C	N	O	S	0	0
			2592	1664	443	473	12		
8	P	314	Total	C	N	O	S	0	0
			2559	1644	436	467	12		
8	Q	319	Total	C	N	O	S	0	0
			2598	1669	445	472	12		

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	K	1	Total 31	C 10	N 5	O 13	P 3	0
9	L	1	Total 31	C 10	N 5	O 13	P 3	0
9	M	1	Total 31	C 10	N 5	O 13	P 3	0
9	N	1	Total 31	C 10	N 5	O 13	P 3	0
9	O	1	Total 31	C 10	N 5	O 13	P 3	0
9	P	1	Total 31	C 10	N 5	O 13	P 3	0
9	Q	1	Total 31	C 10	N 5	O 13	P 3	0

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
10	K	1	Total Mg 1 1	0
10	L	1	Total Mg 1 1	0
10	M	1	Total Mg 1 1	0
10	N	1	Total Mg 1 1	0

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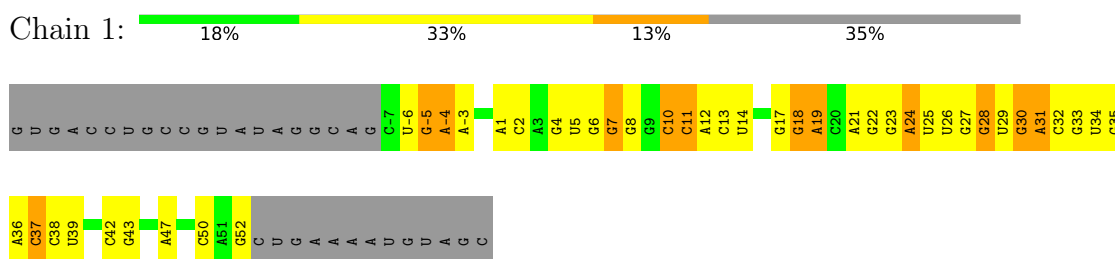
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Mol	Chain	Residues	Atoms		AltConf
10	O	1	Total 1	Mg 1	0
10	P	1	Total 1	Mg 1	0
10	Q	1	Total 1	Mg 1	0

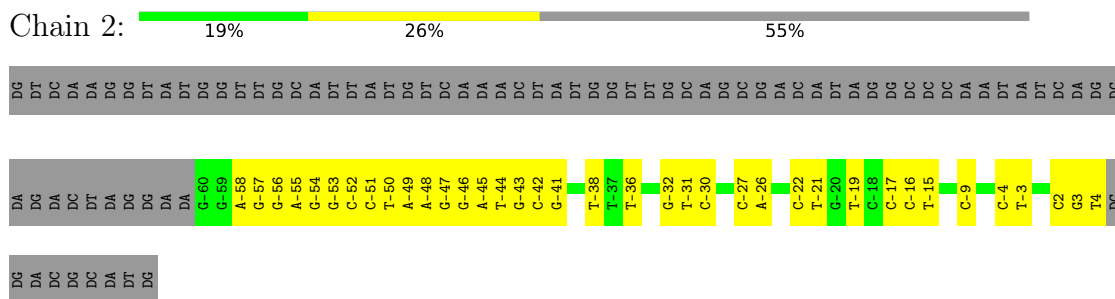
3 Residue-property plots [i](#)

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.

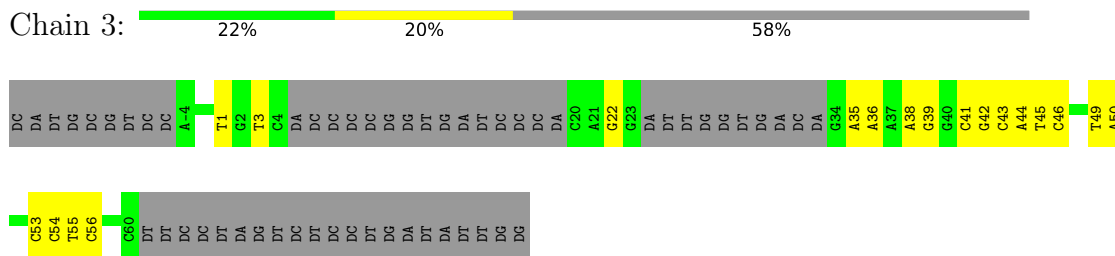
• Molecule 1: CRISPR RNA



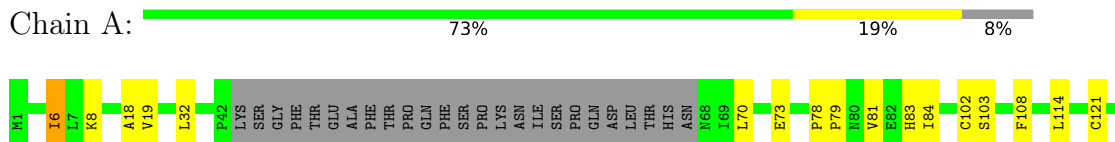
• Molecule 2: TS

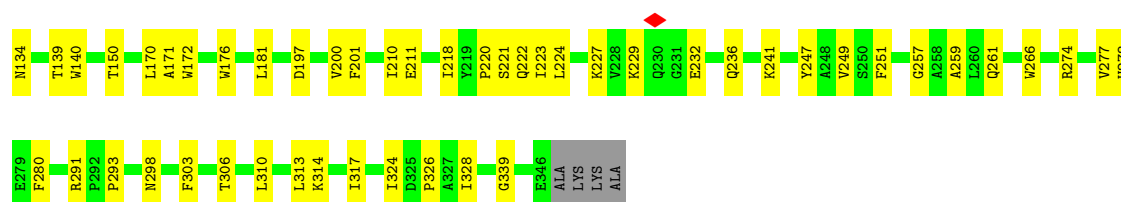


• Molecule 3: NTS



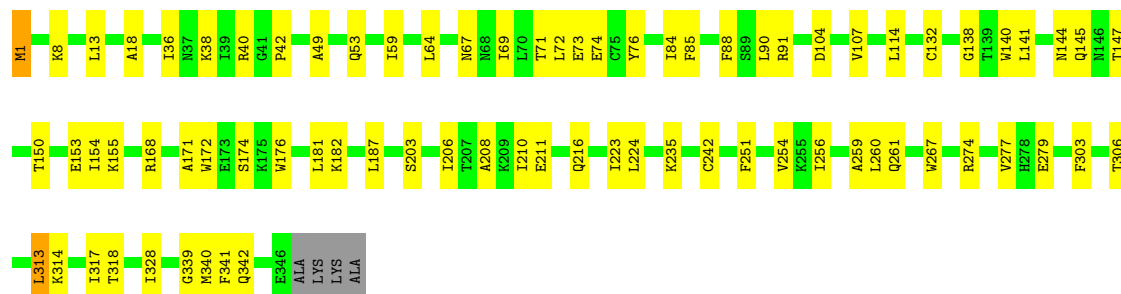
• Molecule 4: Cas7.1





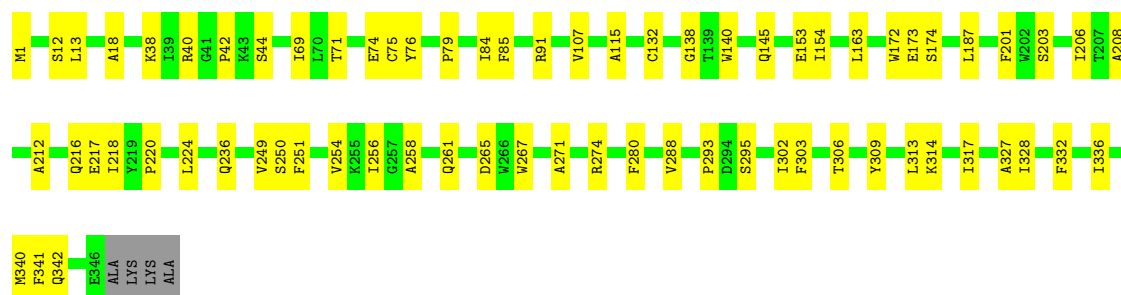
• Molecule 4: Cas7.1

Chain B: 77% 21% ..



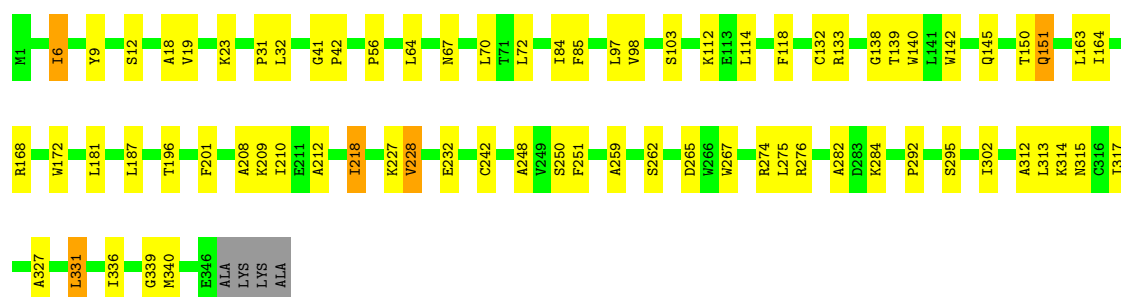
• Molecule 4: Cas7.1

Chain C: 79% 20% .



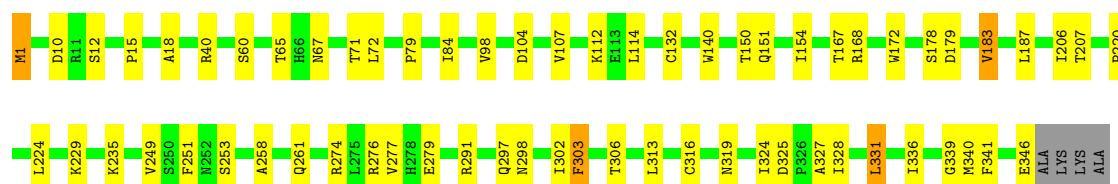
• Molecule 4: Cas7.1

Chain D: 78% 20% ..



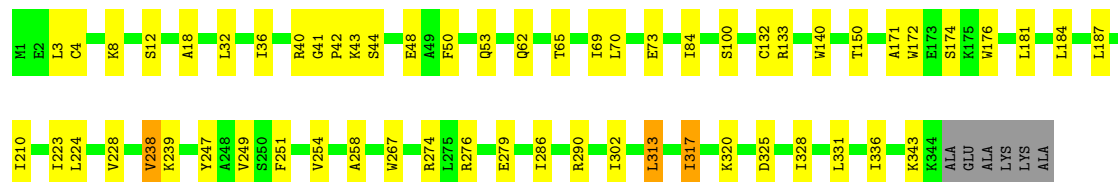
• Molecule 4: Cas7.1

Chain E: 81% 17% ..



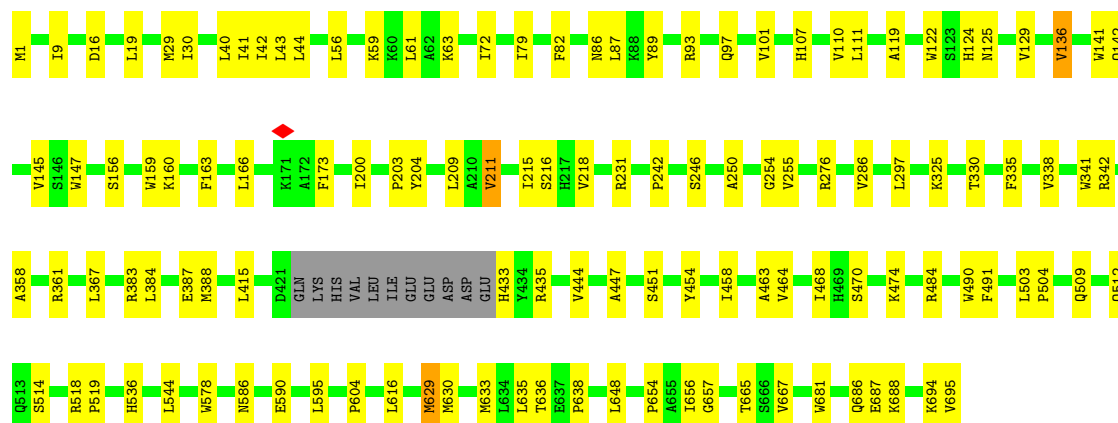
• Molecule 4: Cas7.1

Chain F: 81% 16% ..



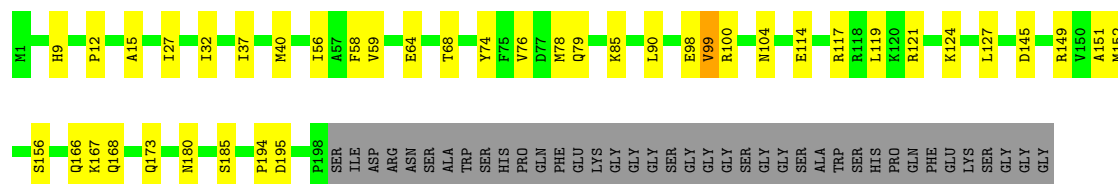
• Molecule 5: Cas8

Chain G: 81% 17% .



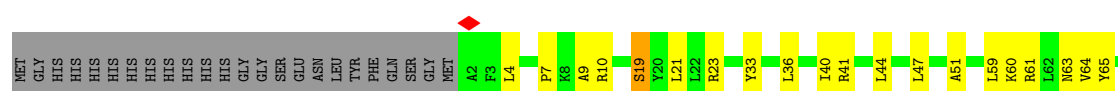
• Molecule 6: Cas6

Chain H: 66% 17% 16%



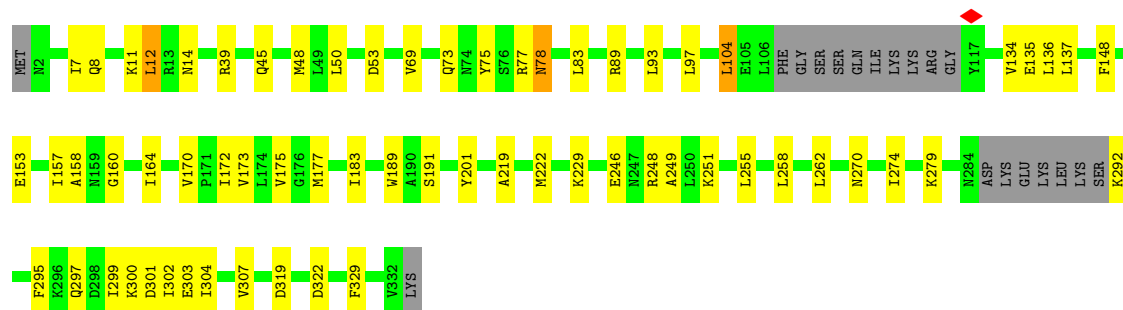
• Molecule 7: TniQ.1

Chain I: 72% 22% . 6%



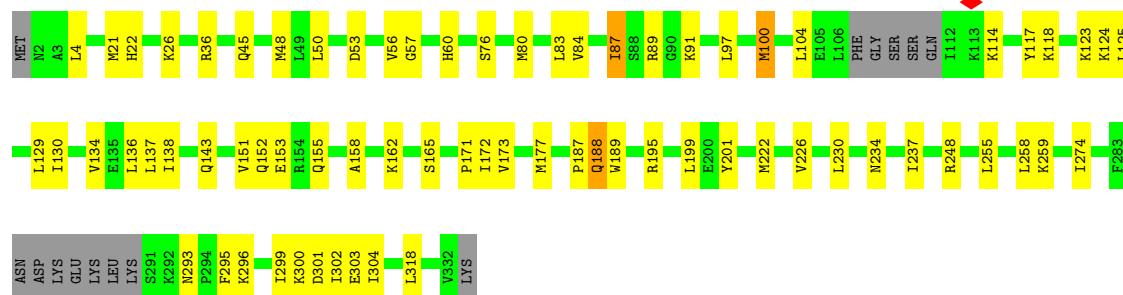
- Molecule 8: TnsC

Chain P:  75% 19% 6%



- Molecule 8: TnsC

Chain Q:  74% 21% 5%



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	76400	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 ($e^-/\text{\AA}^2$)	59.672	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	39.248	Depositor
Minimum map value	-15.587	Depositor
Average map value	0.011	Depositor
Map value standard deviation	1.118	Depositor
Recommended contour level	4.18	Depositor
Map size (\AA)	390.0, 390.0, 390.0	wwPDB
Map dimensions	600, 600, 600	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	0.65, 0.65, 0.65	Depositor

5 Model quality

5.1 Standard geometry

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

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	1	0.25	0/1447	0.41	0/2258
2	2	0.25	0/1467	0.48	0/2261
3	3	0.22	0/876	0.54	0/1345
4	A	0.21	0/2637	0.26	0/3565
4	B	0.23	0/2842	0.28	0/3846
4	C	0.22	0/2842	0.27	0/3846
4	D	0.21	0/2842	0.28	0/3846
4	E	0.21	0/2842	0.26	0/3846
4	F	0.20	0/2828	0.28	0/3827
5	G	0.18	0/5617	0.27	0/7609
6	H	0.14	0/1634	0.26	0/2201
7	I	0.16	0/3392	0.32	0/4595
7	J	0.18	0/3349	0.28	0/4534
8	K	0.25	0/2704	0.33	0/3635
8	L	0.22	0/2588	0.34	0/3481
8	M	0.15	0/2572	0.31	0/3460
8	N	0.17	0/2590	0.35	0/3484
8	O	0.21	0/2636	0.34	0/3543
8	P	0.21	0/2603	0.31	0/3502
8	Q	0.23	0/2642	0.33	0/3551
All	All	0.20	0/52950	0.32	0/72235

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	1	1291	0	648	34	0
2	2	1311	0	721	33	0
3	3	784	0	437	15	0
4	A	2580	0	2544	43	0
4	B	2777	0	2730	48	0
4	C	2777	0	2730	42	0
4	D	2777	0	2730	51	0
4	E	2777	0	2730	35	0
4	F	2763	0	2719	36	0
5	G	5489	0	5543	80	0
6	H	1599	0	1588	26	0
7	I	3311	0	3241	66	0
7	J	3271	0	3212	49	0
8	K	2658	0	2734	54	0
8	L	2545	0	2610	54	0
8	M	2529	0	2594	48	0
8	N	2547	0	2619	69	0
8	O	2592	0	2663	52	0
8	P	2559	0	2629	40	0
8	Q	2598	0	2681	51	0
9	K	31	0	12	4	0
9	L	31	0	12	4	0
9	M	31	0	12	1	0
9	N	31	0	12	2	0
9	O	31	0	12	0	0
9	P	31	0	12	1	0
9	Q	31	0	12	3	0
10	K	1	0	0	0	0
10	L	1	0	0	0	0
10	M	1	0	0	0	0
10	N	1	0	0	0	0
10	O	1	0	0	0	0
10	P	1	0	0	0	0
10	Q	1	0	0	0	0
All	All	51759	0	50187	841	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 8.

The worst 5 of 841 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)
7:I:136:CYS:SG	7:I:165:LEU:HD23	1.49	1.50
7:I:136:CYS:SG	7:I:165:LEU:CD2	2.26	1.23
7:I:136:CYS:HG	7:I:165:LEU:CD2	1.77	0.82
8:P:219:ALA:HA	8:P:222:MET:HE2	1.62	0.81
8:L:158:ALA:HB1	8:L:189:TRP:HE1	1.47	0.80

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	
4	A	317/350 (91%)	307 (97%)	10 (3%)	0	100	100
4	B	344/350 (98%)	337 (98%)	7 (2%)	0	100	100
4	C	344/350 (98%)	332 (96%)	12 (4%)	0	100	100
4	D	344/350 (98%)	333 (97%)	11 (3%)	0	100	100
4	E	344/350 (98%)	336 (98%)	8 (2%)	0	100	100
4	F	342/350 (98%)	336 (98%)	6 (2%)	0	100	100
5	G	680/695 (98%)	666 (98%)	14 (2%)	0	100	100
6	H	196/237 (83%)	194 (99%)	2 (1%)	0	100	100
7	I	406/432 (94%)	383 (94%)	23 (6%)	0	100	100
7	J	400/432 (93%)	390 (98%)	10 (2%)	0	100	100
8	K	323/333 (97%)	320 (99%)	3 (1%)	0	100	100
8	L	307/333 (92%)	298 (97%)	9 (3%)	0	100	100
8	M	305/333 (92%)	298 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	N	307/333 (92%)	300 (98%)	7 (2%)	0	100	100
8	O	313/333 (94%)	304 (97%)	9 (3%)	0	100	100
8	P	308/333 (92%)	300 (97%)	8 (3%)	0	100	100
8	Q	313/333 (94%)	306 (98%)	7 (2%)	0	100	100
All	All	5893/6227 (95%)	5740 (97%)	153 (3%)	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	
4	A	282/307 (92%)	277 (98%)	5 (2%)	51	70
4	B	305/307 (99%)	294 (96%)	11 (4%)	31	58
4	C	305/307 (99%)	296 (97%)	9 (3%)	36	61
4	D	305/307 (99%)	296 (97%)	9 (3%)	36	61
4	E	305/307 (99%)	290 (95%)	15 (5%)	22	51
4	F	304/307 (99%)	296 (97%)	8 (3%)	40	64
5	G	603/614 (98%)	594 (98%)	9 (2%)	57	72
6	H	174/200 (87%)	169 (97%)	5 (3%)	37	62
7	I	363/383 (95%)	353 (97%)	10 (3%)	38	62
7	J	359/383 (94%)	353 (98%)	6 (2%)	53	71
8	K	295/301 (98%)	292 (99%)	3 (1%)	68	76
8	L	283/301 (94%)	277 (98%)	6 (2%)	47	67
8	M	281/301 (93%)	276 (98%)	5 (2%)	51	70
8	N	283/301 (94%)	276 (98%)	7 (2%)	42	64
8	O	288/301 (96%)	280 (97%)	8 (3%)	38	62
8	P	284/301 (94%)	277 (98%)	7 (2%)	42	64
8	Q	288/301 (96%)	280 (97%)	8 (3%)	38	62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	5307/5529 (96%)	5176 (98%)	131 (2%)	42 64

5 of 131 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
8	O	302	ILE
8	P	104	LEU
8	Q	304	ILE
4	E	341	PHE
4	E	340	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
8	L	265	ASN
8	O	265	ASN
8	Q	64	HIS
8	L	284	ASN
8	M	272	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	1	59/93 (63%)	26 (44%)	3 (5%)

5 of 26 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	1	-5	G
1	1	-4	A
1	1	1	A
1	1	2	C
1	1	6	G

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	1	-5	G
1	1	10	C
1	1	31	A

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](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

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	$\# Z > 2$
9	ATP	N	402	10	29,33,33	0.36	0	44,52,52	0.53	0
9	ATP	K	401	10	29,33,33	0.39	0	44,52,52	0.55	0
9	ATP	L	402	10	29,33,33	0.35	0	44,52,52	0.52	0
9	ATP	O	402	10	29,33,33	0.35	0	44,52,52	0.48	0
9	ATP	M	401	10	29,33,33	0.35	0	44,52,52	0.53	0
9	ATP	Q	401	10	29,33,33	0.39	0	44,52,52	0.53	1 (2%)
9	ATP	P	401	10	29,33,33	0.38	0	44,52,52	0.52	1 (2%)

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
9	ATP	N	402	10	-	2/22/38/38	0/3/3/3
9	ATP	K	401	10	-	4/22/38/38	0/3/3/3
9	ATP	L	402	10	-	4/22/38/38	0/3/3/3
9	ATP	O	402	10	-	3/22/38/38	0/3/3/3
9	ATP	M	401	10	-	2/22/38/38	0/3/3/3
9	ATP	Q	401	10	-	3/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ATP	P	401	10	-	4/22/38/38	0/3/3/3

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	Q	401	ATP	PB-O3B-PG	2.02	139.77	132.83
9	P	401	ATP	PB-O3B-PG	2.01	139.71	132.83

There are no chirality outliers.

5 of 22 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	K	401	ATP	PB-O3B-PG-O2G
9	K	401	ATP	O4'-C4'-C5'-O5'
9	L	402	ATP	C5'-O5'-PA-O1A
9	P	401	ATP	PB-O3B-PG-O2G
9	P	401	ATP	O4'-C4'-C5'-O5'

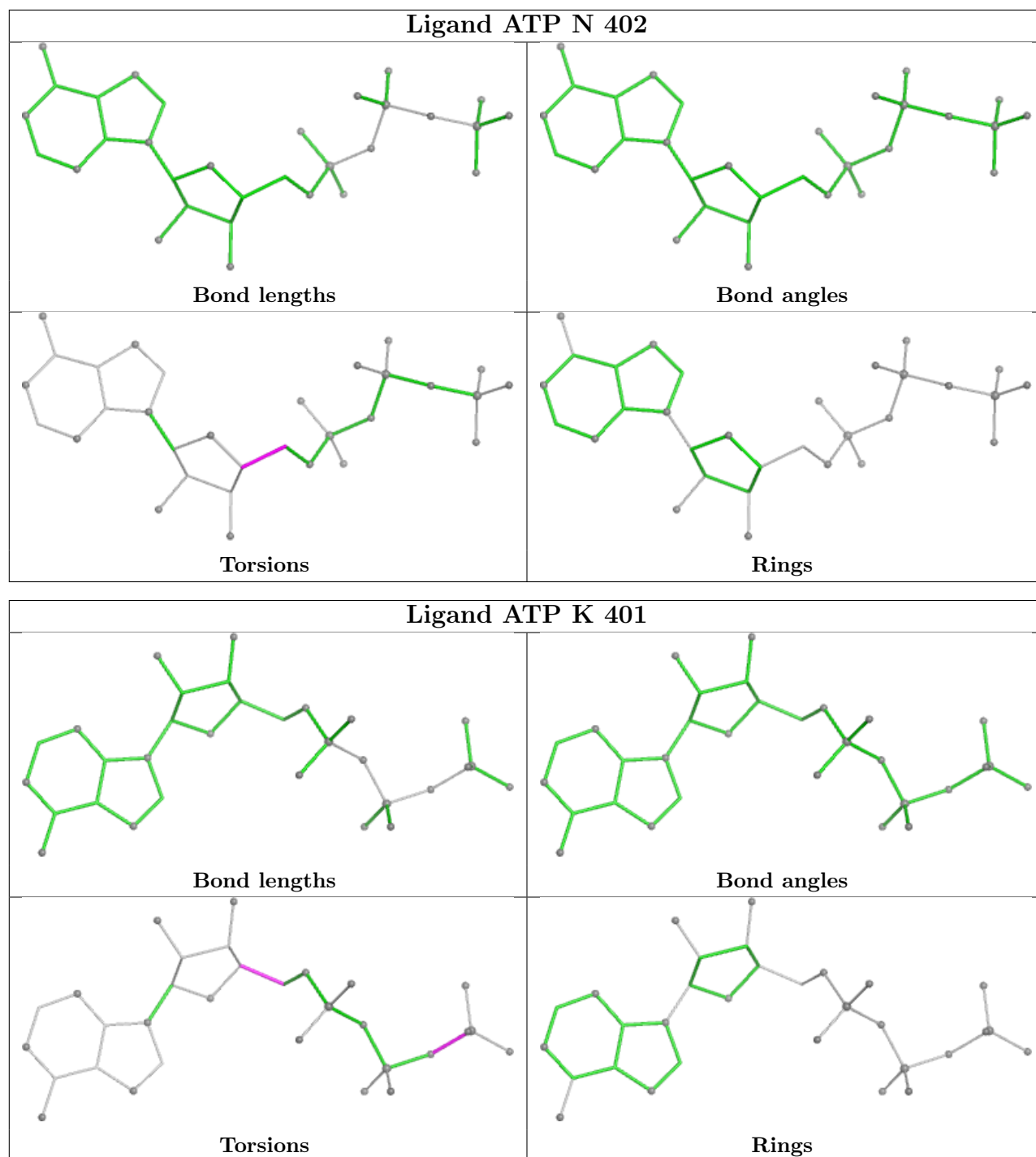
There are no ring outliers.

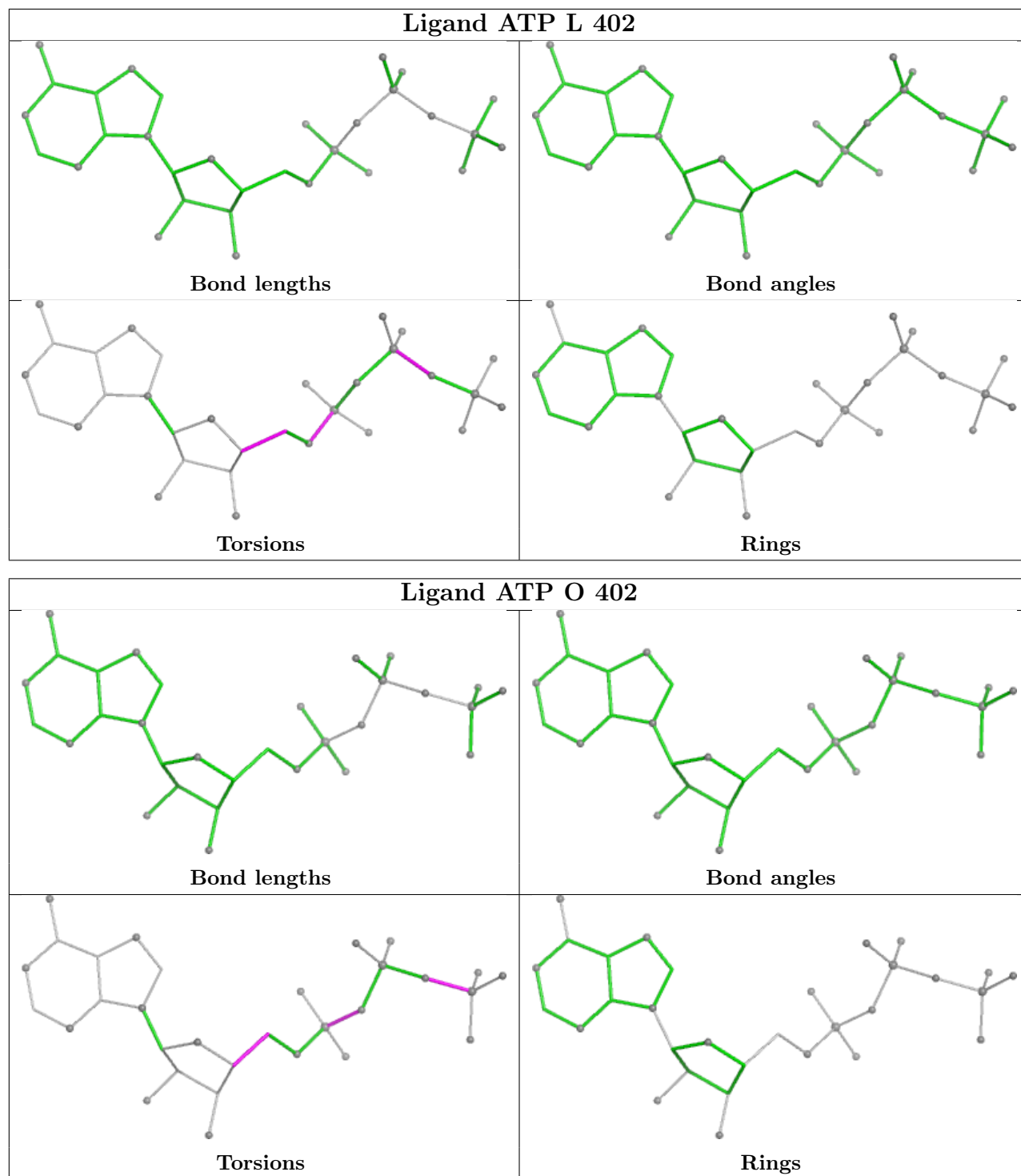
6 monomers are involved in 15 short contacts:

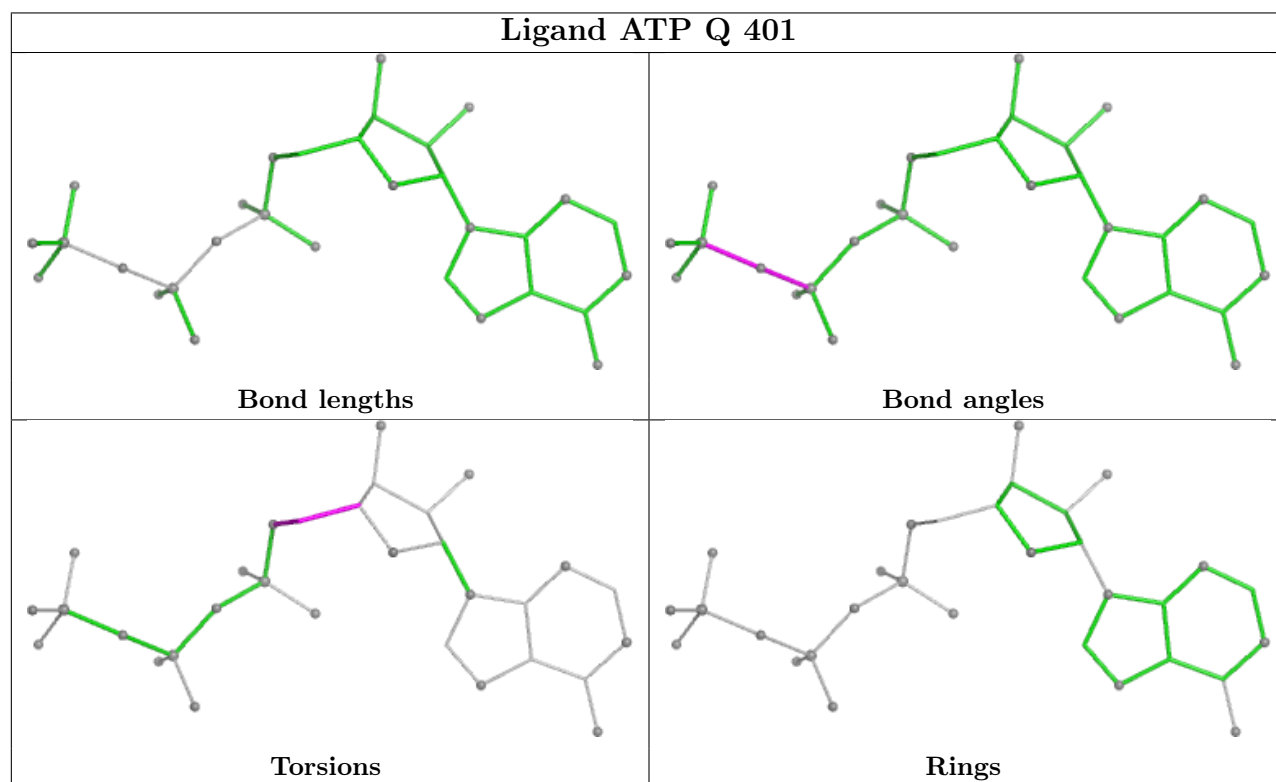
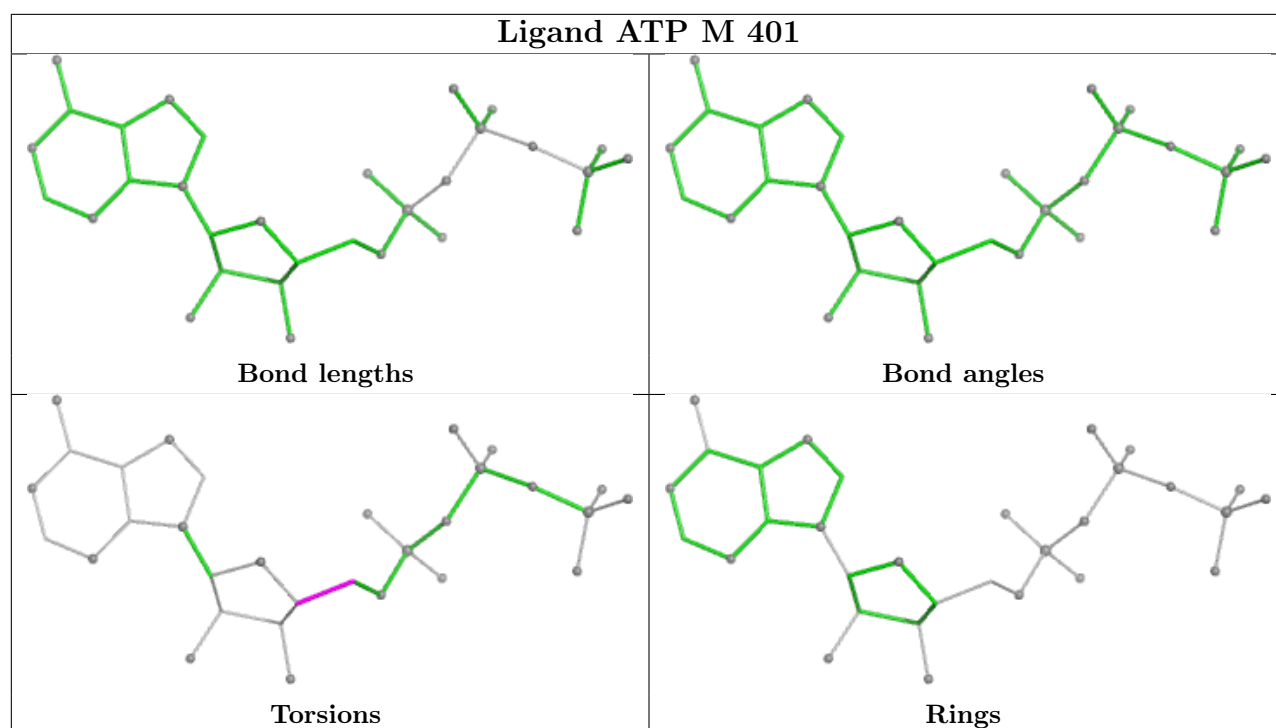
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	N	402	ATP	2	0
9	K	401	ATP	4	0
9	L	402	ATP	4	0
9	M	401	ATP	1	0
9	Q	401	ATP	3	0
9	P	401	ATP	1	0

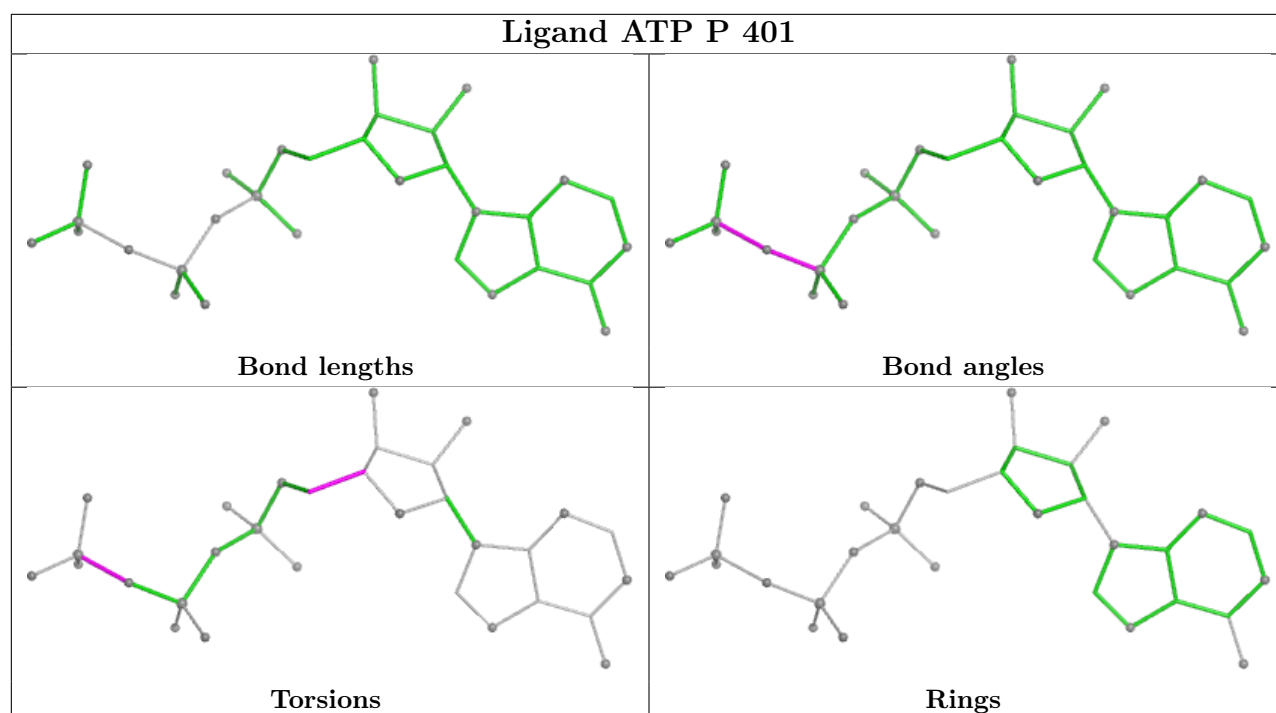
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.









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.

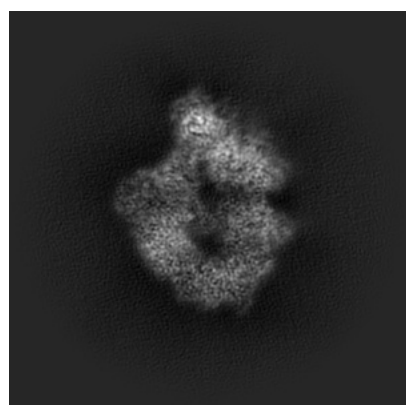
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-57765. These allow visual inspection of the internal detail of the map and identification of artifacts.

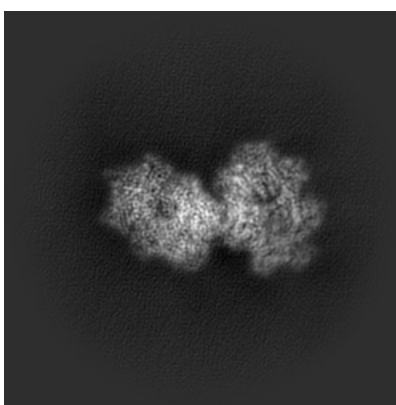
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

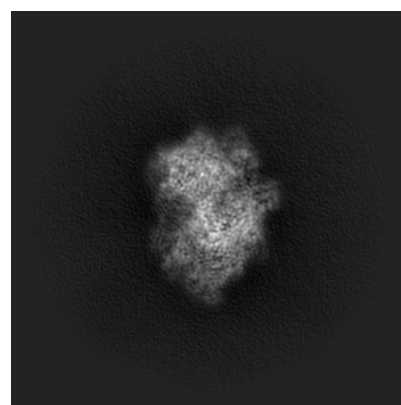
6.1.1 Primary map



X



Y

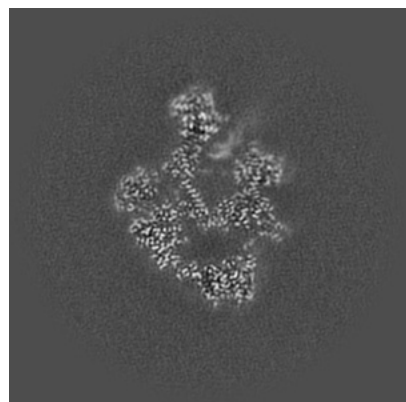


Z

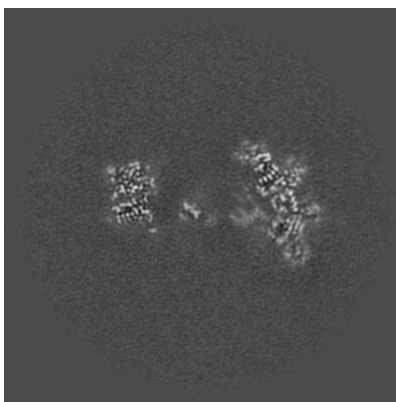
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

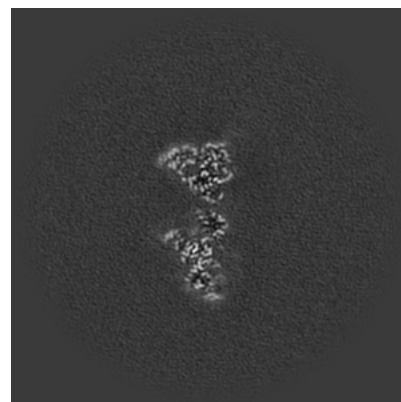
6.2.1 Primary map



X Index: 300



Y Index: 300

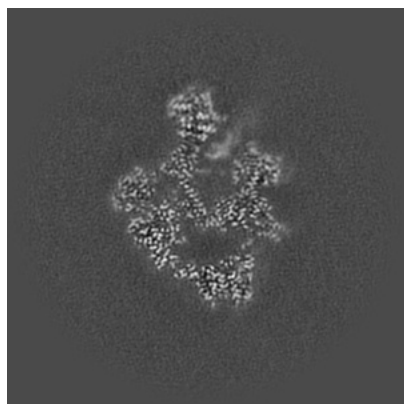


Z Index: 300

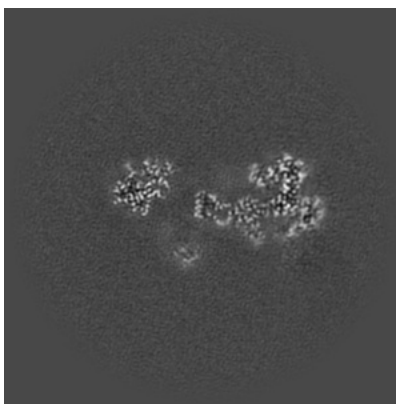
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

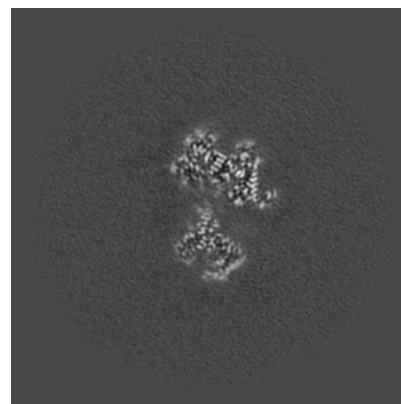
6.3.1 Primary map



X Index: 299



Y Index: 274

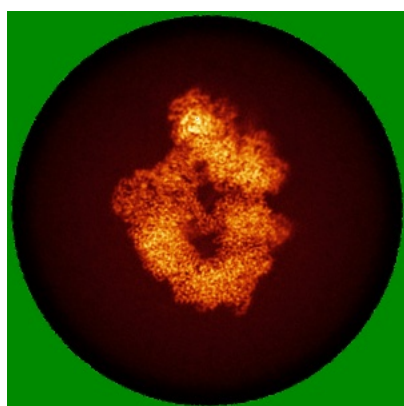


Z Index: 355

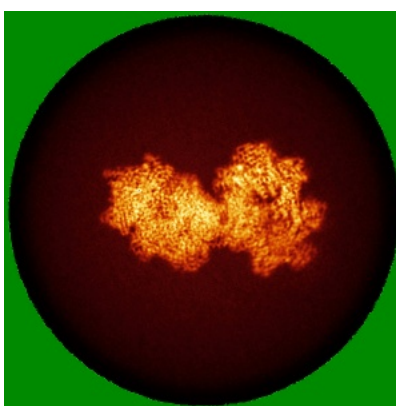
The images above show the largest variance slices of the map in three orthogonal directions.

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

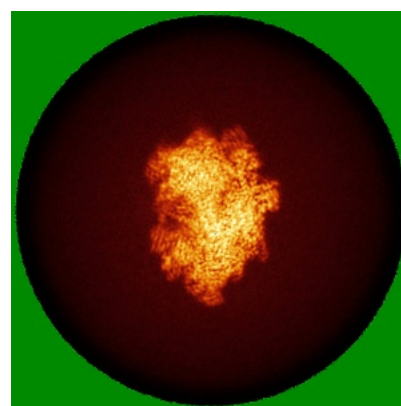
6.4.1 Primary map



X



Y

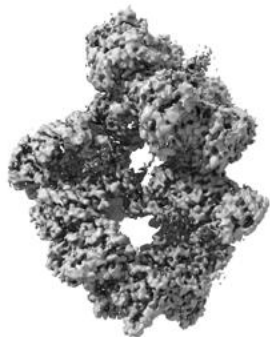


Z

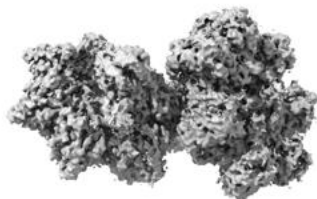
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.18. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

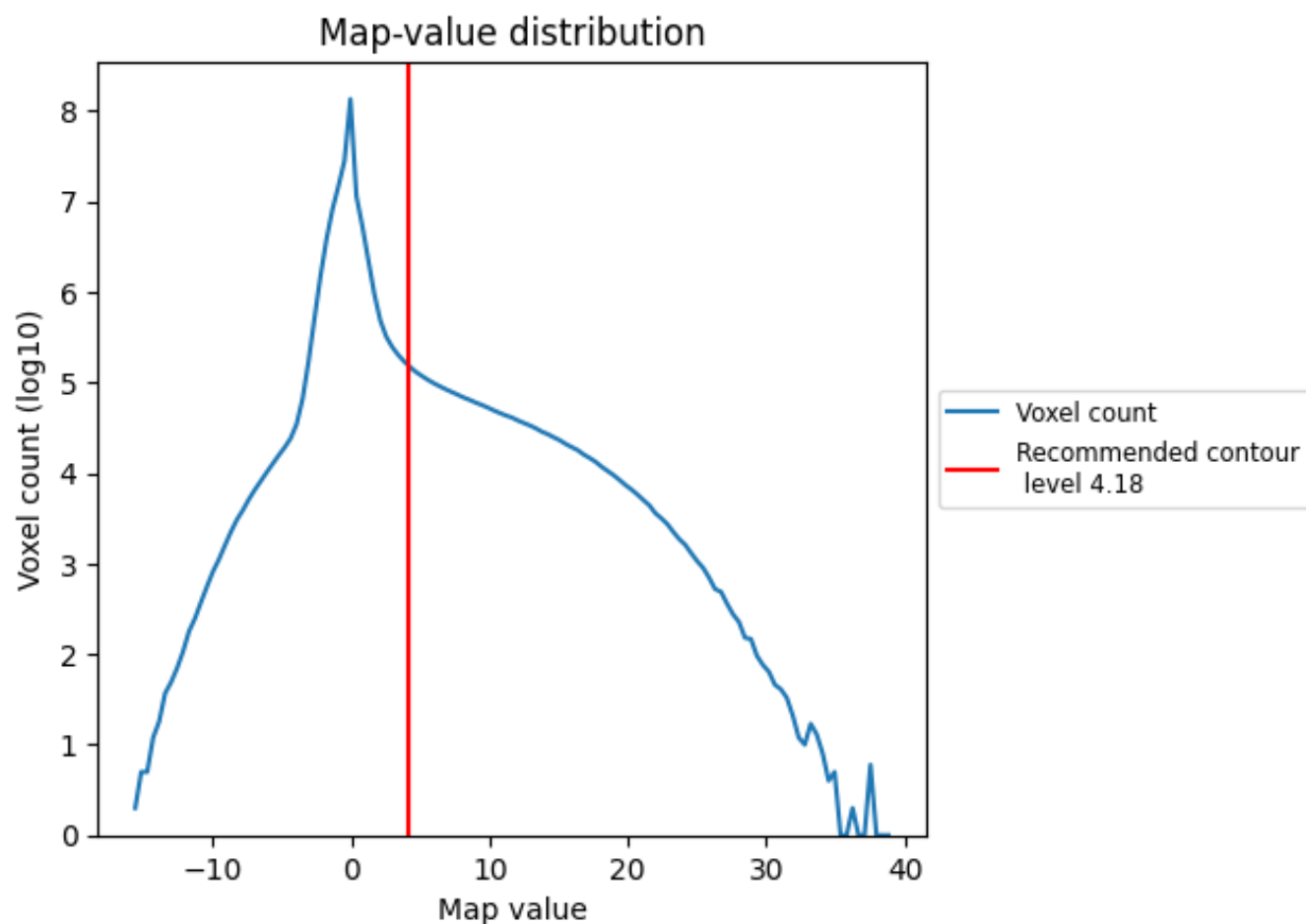
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

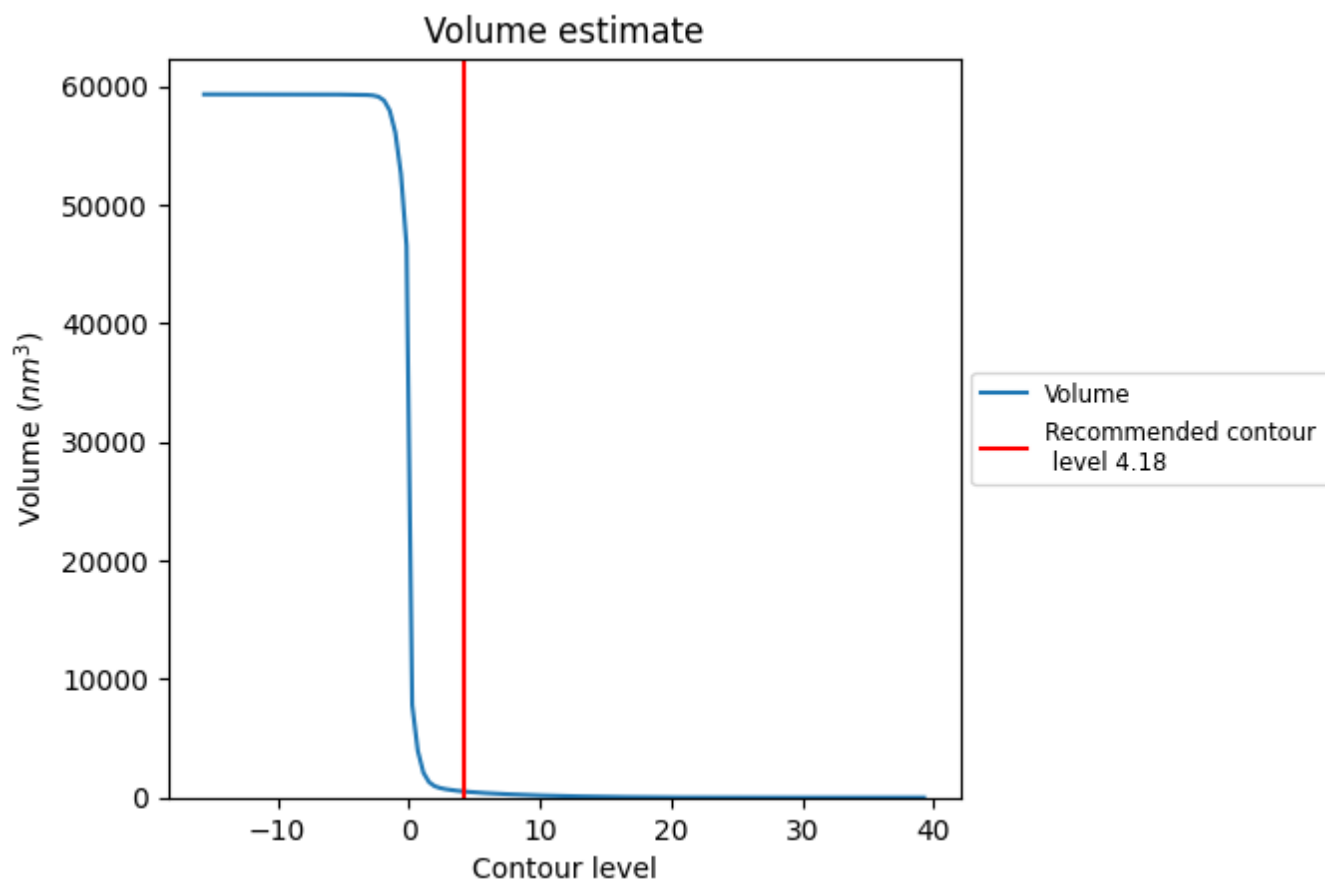
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

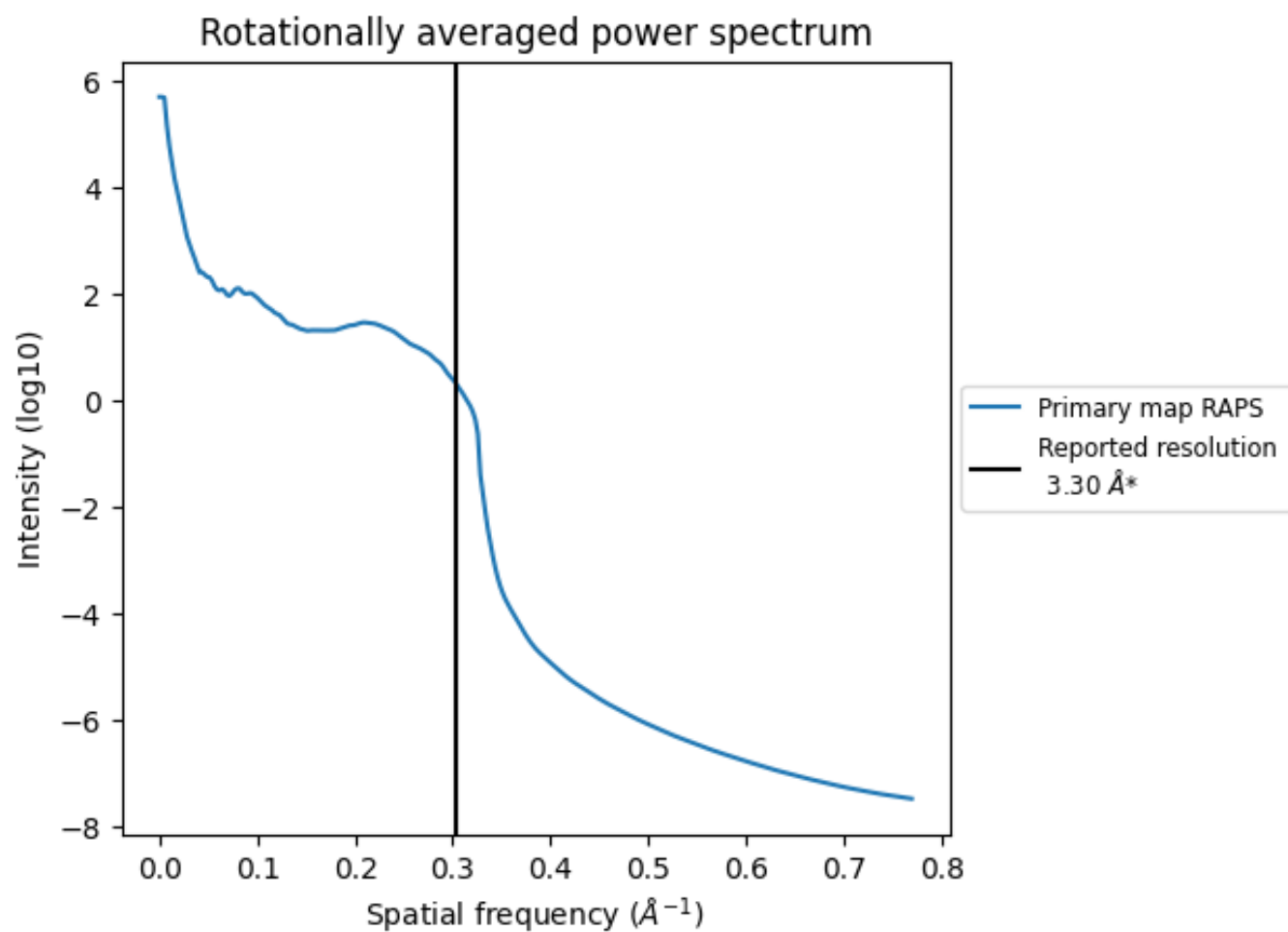
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 516 nm^3 ; this corresponds to an approximate mass of 467 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 0.303 Å⁻¹

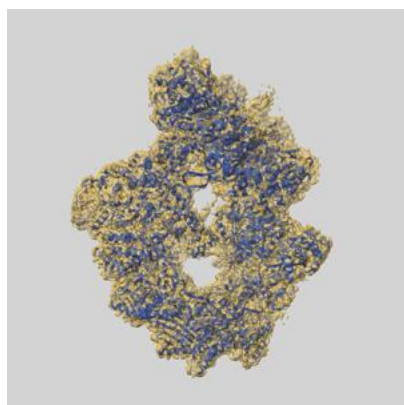
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

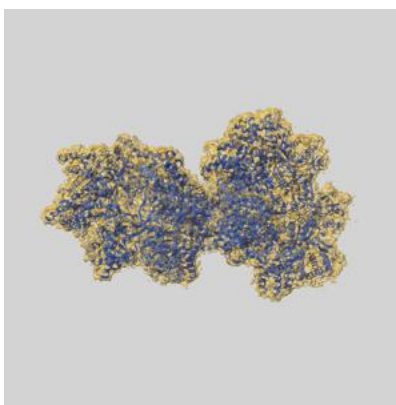
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-57765 and PDB model 30GT. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

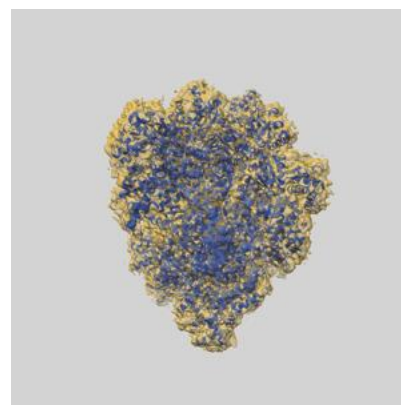
9.1 Map-model overlay [i](#)



X



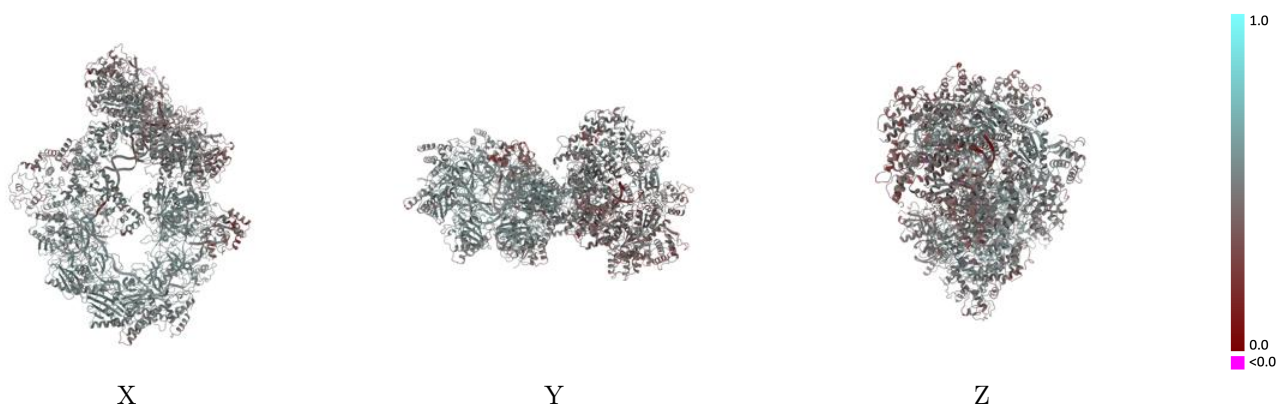
Y



Z

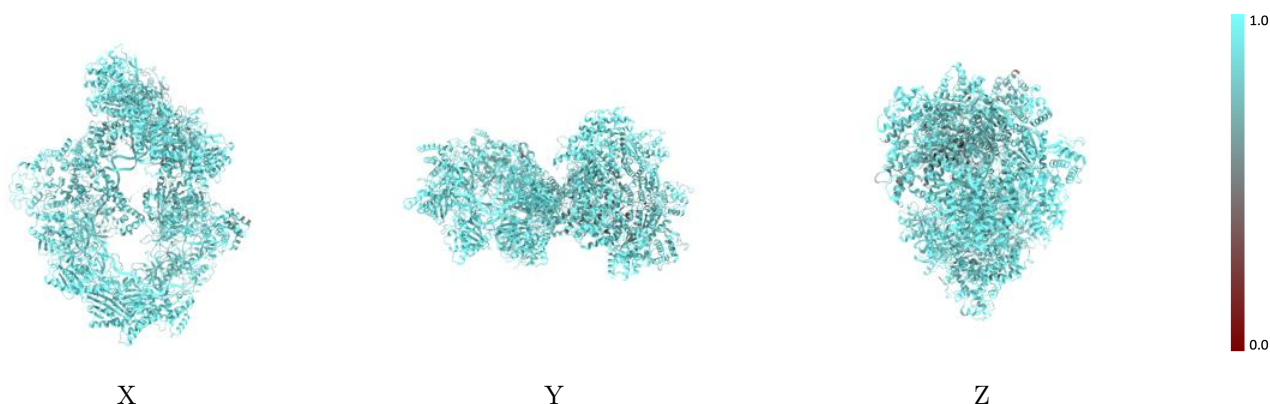
The images above show the 3D surface view of the map at the recommended contour level 4.18 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



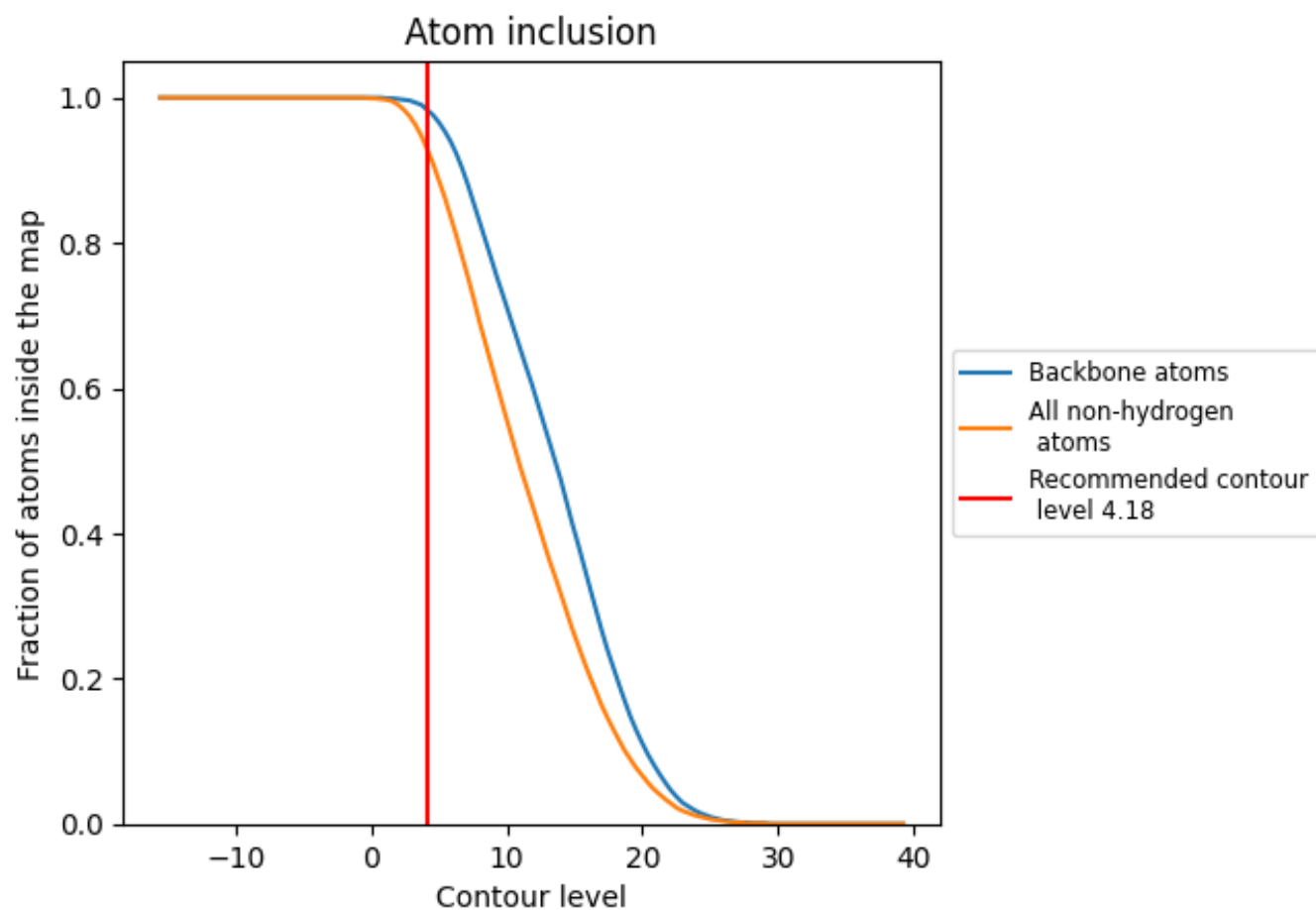
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4.18).











































9.4 Atom inclusion [i](#)



At the recommended contour level, 98% of all backbone atoms, 93% 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 (4.18) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.9260	 0.4870
1	 0.9800	 0.5140
2	 0.9550	 0.4620
3	 0.9170	 0.4100
A	 0.9470	 0.5360
B	 0.9670	 0.5460
C	 0.9510	 0.5330
D	 0.9520	 0.5320
E	 0.9500	 0.5350
F	 0.9450	 0.5290
G	 0.9170	 0.5020
H	 0.9330	 0.4670
I	 0.9080	 0.4660
J	 0.9200	 0.4980
K	 0.9550	 0.4730
L	 0.9050	 0.4080
M	 0.8110	 0.4130
N	 0.8700	 0.4110
O	 0.8960	 0.4480
P	 0.9430	 0.4720
Q	 0.9490	 0.4850

