



wwPDB EM Validation Summary Report ⓘ

Dec 11, 2022 – 04:04 am GMT

PDB ID : 6RQC
EMDB ID : EMD-4980
Title : Cryo-EM structure of an MCM loading intermediate
Authors : Miller, T.C.R.; Locke, J.; Costa, A.
Deposited on : 2019-05-15
Resolution : 4.40 Å(reported)
Based on initial models : 5BK4, 6EYC, 6F0L, 5ZR1

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.dev43
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

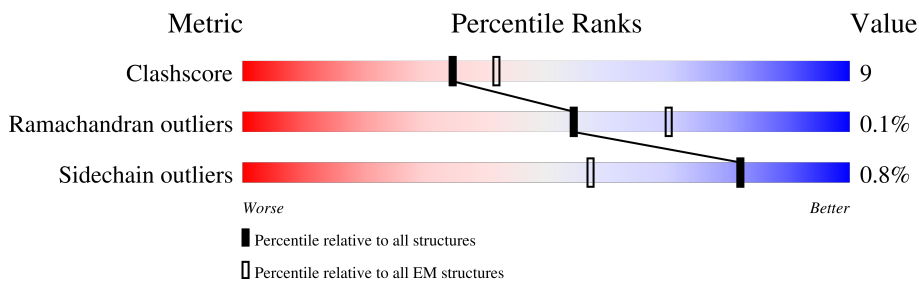
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



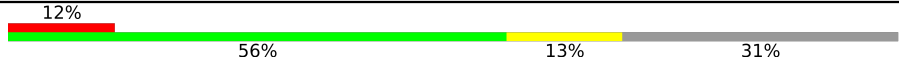
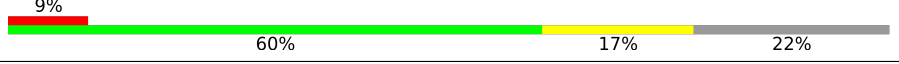
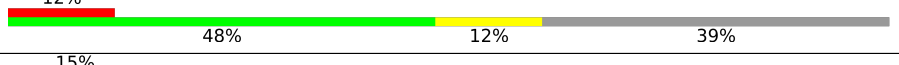


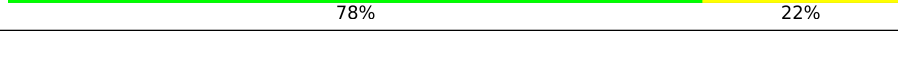
Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	A	949	
2	B	620	
3	C	616	
4	D	529	
5	E	479	
6	F	435	
7	2	868	
8	3	1006	

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Mol	Chain	Length	Quality of chain
9	4	933	
10	5	775	
11	6	1017	
12	7	845	
13	X	88	
14	Y	88	

2 Entry composition

There are 18 unique types of molecules in this entry. The entry contains 105307 atoms, of which 52062 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 Origin recognition complex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	494	8028	2527	4070	676	736	19	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	MET	-	initiating methionine	UNP P54784
A	-33	LYS	-	expression tag	UNP P54784
A	-32	ARG	-	expression tag	UNP P54784
A	-31	ARG	-	expression tag	UNP P54784
A	-30	TRP	-	expression tag	UNP P54784
A	-29	LYS	-	expression tag	UNP P54784
A	-28	LYS	-	expression tag	UNP P54784
A	-27	ASN	-	expression tag	UNP P54784
A	-26	PHE	-	expression tag	UNP P54784
A	-25	ILE	-	expression tag	UNP P54784
A	-24	ALA	-	expression tag	UNP P54784
A	-23	VAL	-	expression tag	UNP P54784
A	-22	SER	-	expression tag	UNP P54784
A	-21	ALA	-	expression tag	UNP P54784
A	-20	ALA	-	expression tag	UNP P54784
A	-19	ASN	-	expression tag	UNP P54784
A	-18	ARG	-	expression tag	UNP P54784
A	-17	PHE	-	expression tag	UNP P54784
A	-16	LYS	-	expression tag	UNP P54784
A	-15	LYS	-	expression tag	UNP P54784
A	-14	ILE	-	expression tag	UNP P54784
A	-13	SER	-	expression tag	UNP P54784
A	-12	SER	-	expression tag	UNP P54784
A	-11	SER	-	expression tag	UNP P54784
A	-10	GLY	-	expression tag	UNP P54784
A	-9	ALA	-	expression tag	UNP P54784
A	-8	LEU	-	expression tag	UNP P54784
A	-7	GLU	-	expression tag	UNP P54784

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASN	-	expression tag	UNP P54784
A	-5	LEU	-	expression tag	UNP P54784
A	-4	TYR	-	expression tag	UNP P54784
A	-3	PHE	-	expression tag	UNP P54784
A	-2	GLN	-	expression tag	UNP P54784
A	-1	GLY	-	expression tag	UNP P54784
A	0	GLU	-	expression tag	UNP P54784

- Molecule 2 is a protein called Origin recognition complex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
2	B	247	4067	1330	2018	339	372	8	0	0

- Molecule 3 is a protein called Origin recognition complex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
3	C	582	9579	3102	4766	794	901	16	0	0

- Molecule 4 is a protein called Origin recognition complex subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
4	D	437	7193	2285	3627	605	663	13	0	0

- Molecule 5 is a protein called Origin recognition complex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
5	E	459	7529	2431	3780	609	695	14	0	0

- Molecule 6 is a protein called Origin recognition complex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
6	F	242	4046	1274	2051	343	358	20	0	0

- Molecule 7 is a protein called DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
7	2	601	9573	2998	4820	845	891	19	0	0

- Molecule 8 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
8	3	599	9448	2956	4752	840	887	13	0	0

There are 35 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
3	-34	MET	-	initiating methionine	UNP P24279
3	-33	LYS	-	expression tag	UNP P24279
3	-32	ARG	-	expression tag	UNP P24279
3	-31	ARG	-	expression tag	UNP P24279
3	-30	TRP	-	expression tag	UNP P24279
3	-29	LYS	-	expression tag	UNP P24279
3	-28	LYS	-	expression tag	UNP P24279
3	-27	ASN	-	expression tag	UNP P24279
3	-26	PHE	-	expression tag	UNP P24279
3	-25	ILE	-	expression tag	UNP P24279
3	-24	ALA	-	expression tag	UNP P24279
3	-23	VAL	-	expression tag	UNP P24279
3	-22	SER	-	expression tag	UNP P24279
3	-21	ALA	-	expression tag	UNP P24279
3	-20	ALA	-	expression tag	UNP P24279
3	-19	ASN	-	expression tag	UNP P24279
3	-18	ARG	-	expression tag	UNP P24279
3	-17	PHE	-	expression tag	UNP P24279
3	-16	LYS	-	expression tag	UNP P24279
3	-15	LYS	-	expression tag	UNP P24279
3	-14	ILE	-	expression tag	UNP P24279
3	-13	SER	-	expression tag	UNP P24279
3	-12	SER	-	expression tag	UNP P24279
3	-11	SER	-	expression tag	UNP P24279
3	-10	GLY	-	expression tag	UNP P24279
3	-9	ALA	-	expression tag	UNP P24279
3	-8	LEU	-	expression tag	UNP P24279
3	-7	GLU	-	expression tag	UNP P24279
3	-6	ASN	-	expression tag	UNP P24279
3	-5	LEU	-	expression tag	UNP P24279
3	-4	TYR	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
3	-3	PHE	-	expression tag	UNP P24279
3	-2	GLN	-	expression tag	UNP P24279
3	-1	GLY	-	expression tag	UNP P24279
3	0	GLU	-	expression tag	UNP P24279

- Molecule 9 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
9	4	641	10282	3210	5172	883	989	28	0	0

- Molecule 10 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
10	5	602	9532	2976	4802	813	917	24	0	0

- Molecule 11 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
11	6	616	9782	3072	4908	853	924	25	0	0

- Molecule 12 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
12	7	654	10353	3244	5215	886	979	29	0	0

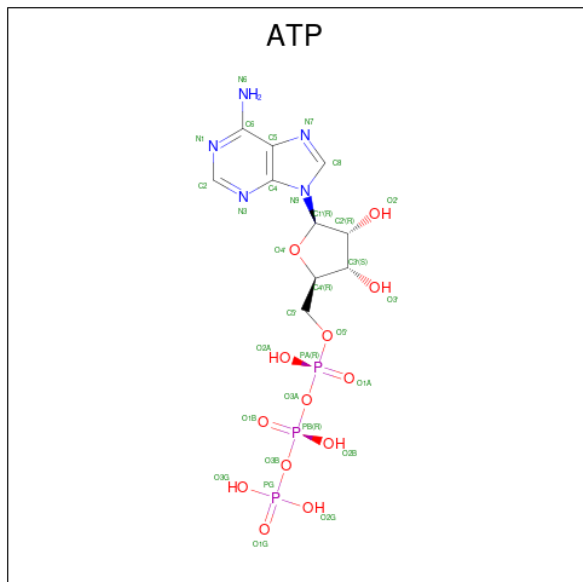
- Molecule 13 is a DNA chain called DNA (88-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
13	X	88	2806	867	1010	294	548	87	0	0

- Molecule 14 is a DNA chain called DNA (88-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			P
14	Y	88	2796	863	987	352	506	88	0	0

- Molecule 15 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
15	A	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
15	D	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	
15	E	1	Total	C	H	N	O	P	0
			43	10	12	5	13	3	

- Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
16	A	1	Total	Mg	0
			1	1	
16	D	1	Total	Mg	0
			1	1	
16	E	1	Total	Mg	0
			1	1	

- Molecule 17 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
17	2	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
17	3	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
17	5	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	
17	7	1	Total	C	H	N	O	P	0
			39	10	12	5	10	2	

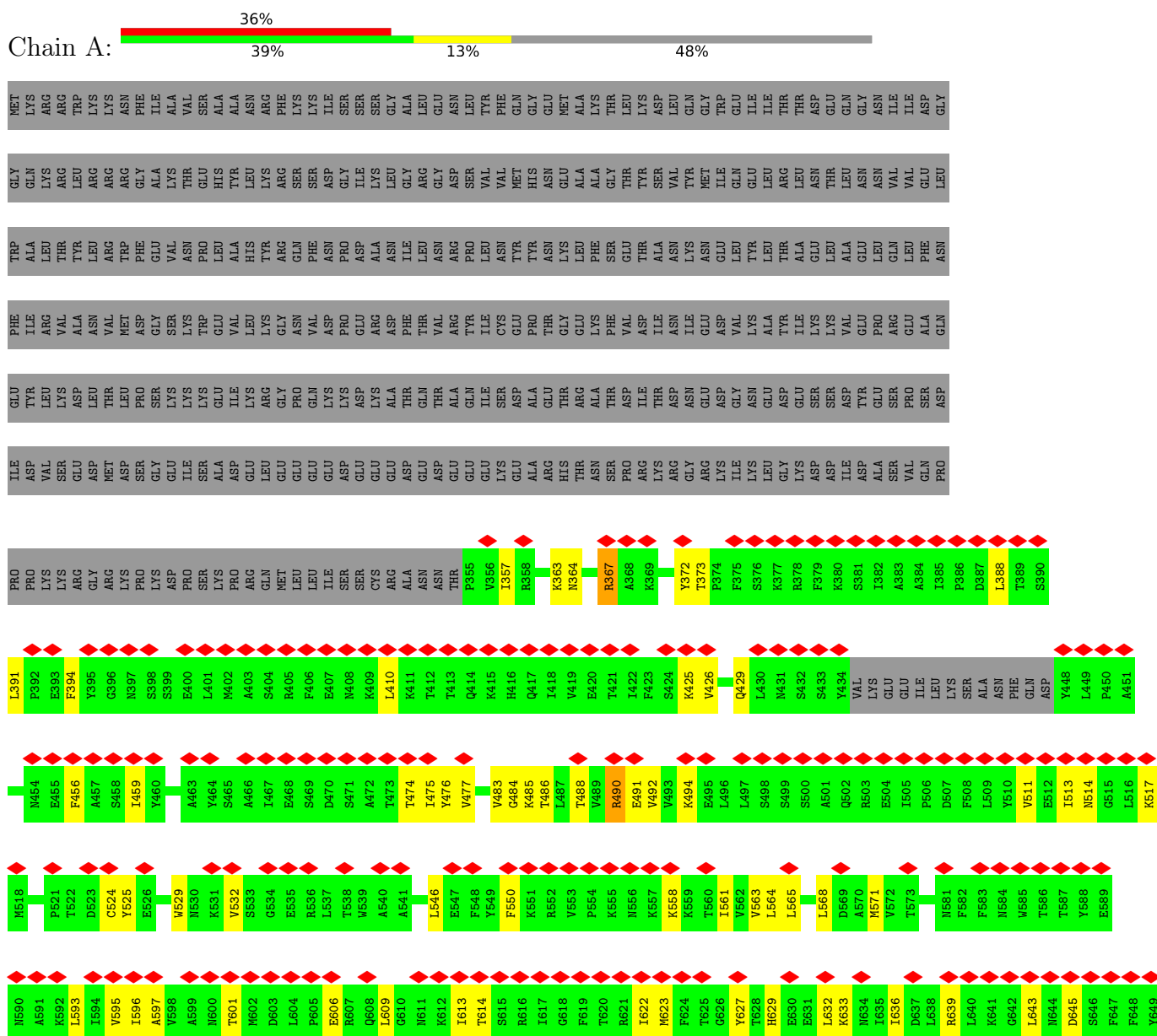
- Molecule 18 is ZINC ION (three-letter code: ZN) (formula: Zn).

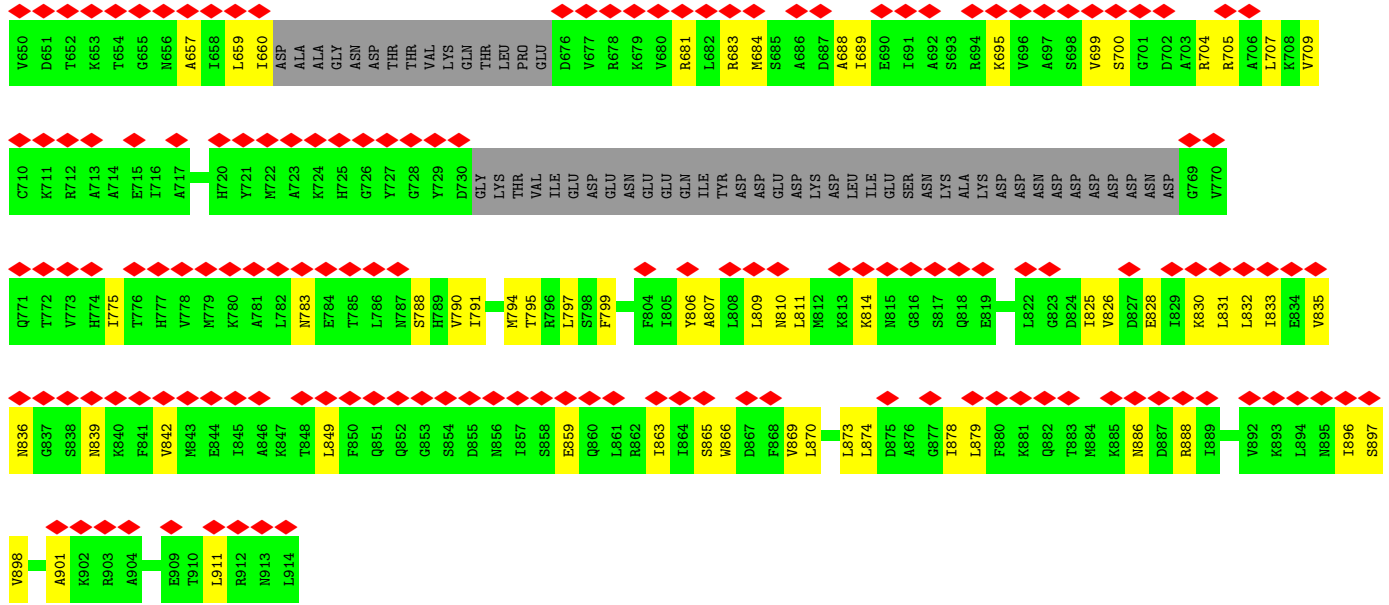
Mol	Chain	Residues	Atoms		AltConf
18	2	1	Total	Zn	0
			1	1	
18	4	1	Total	Zn	0
			1	1	
18	5	1	Total	Zn	0
			1	1	
18	6	1	Total	Zn	0
			1	1	
18	7	1	Total	Zn	0
			1	1	

3 Residue-property plots

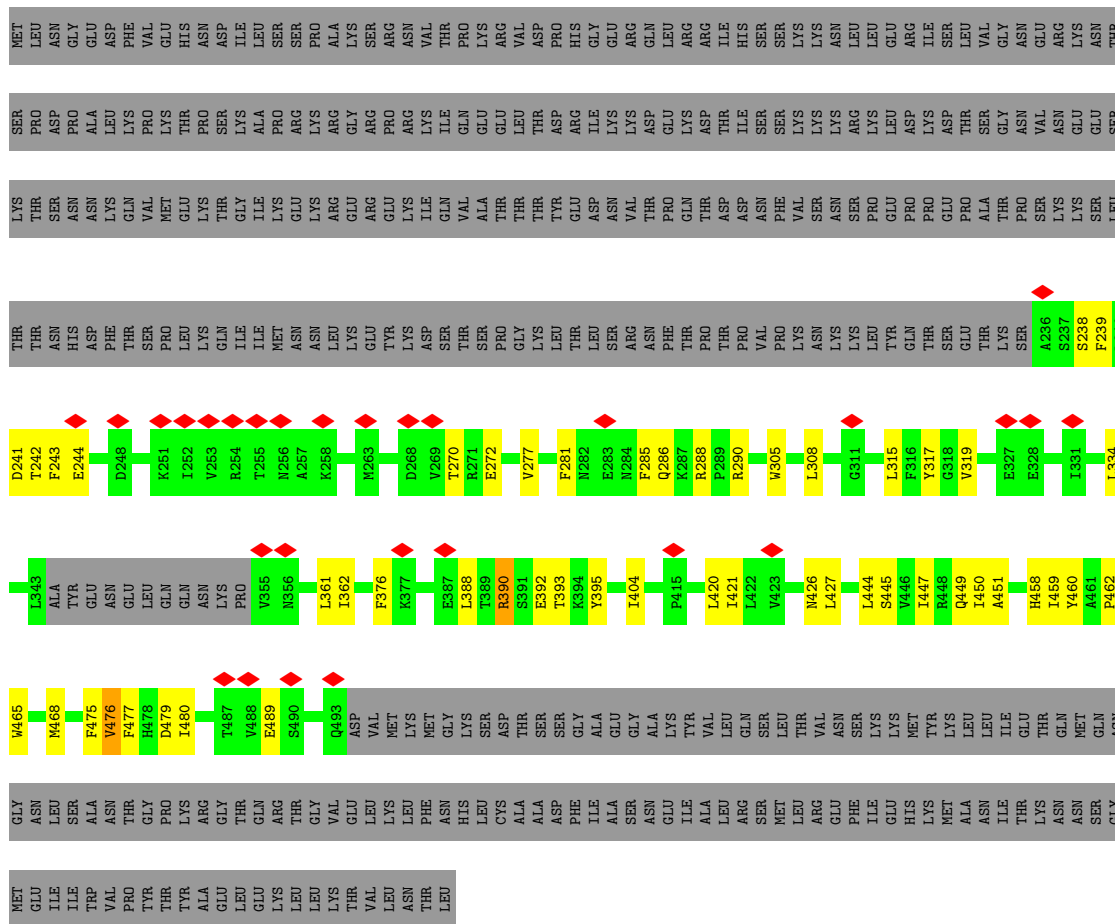
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Origin recognition complex subunit 1

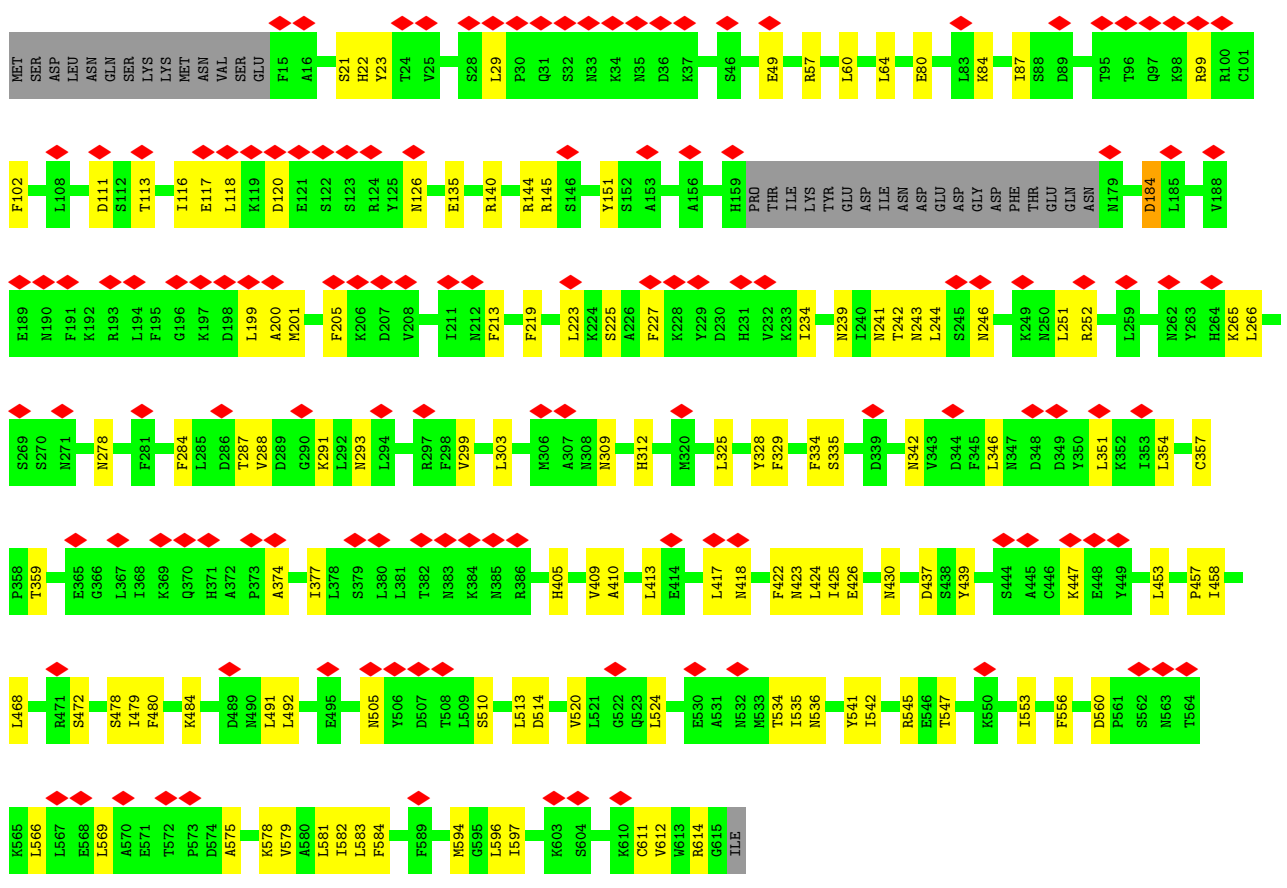
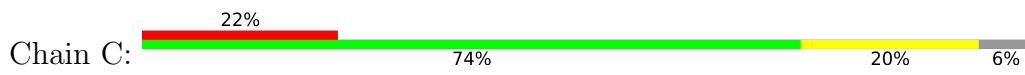




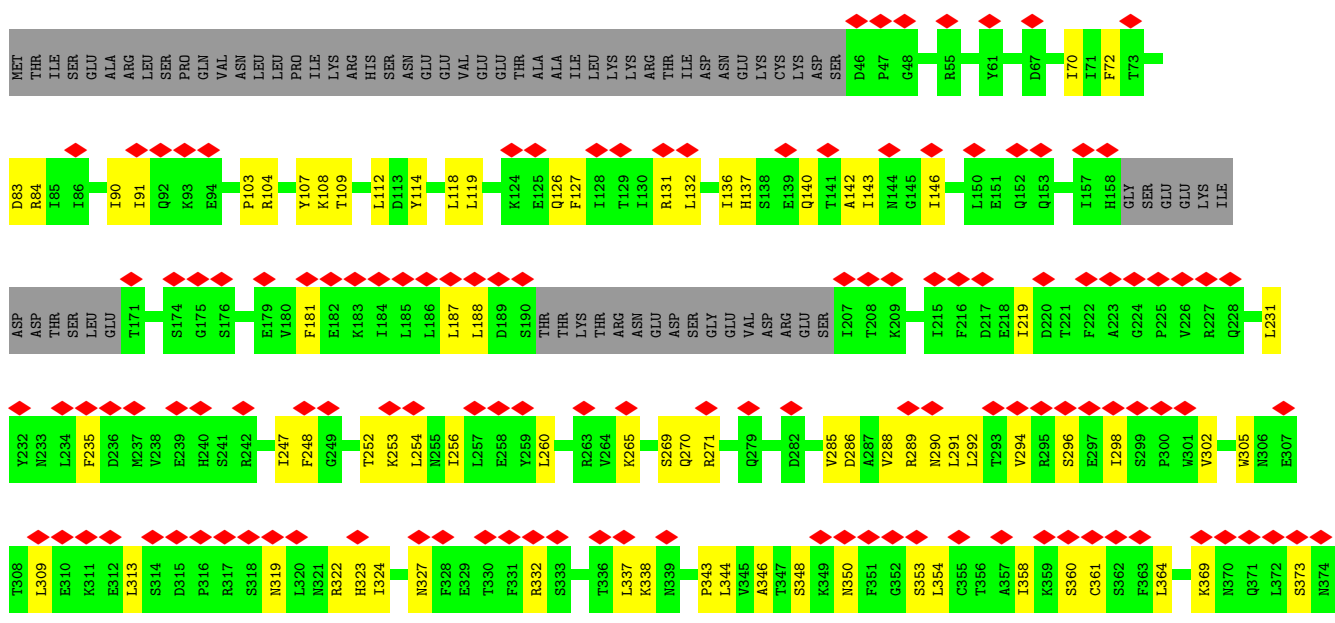
• Molecule 2: Origin recognition complex subunit 2

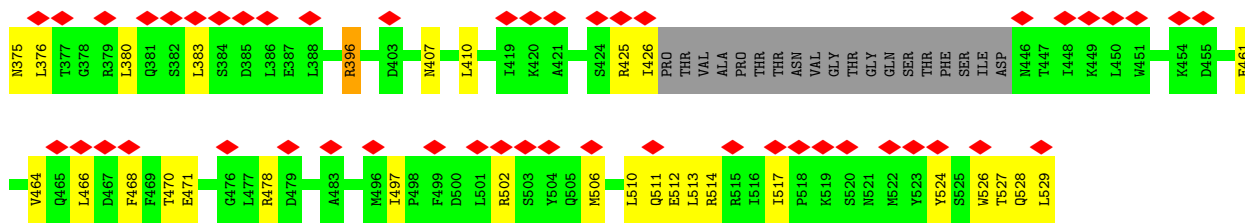


• Molecule 3: Origin recognition complex subunit 3

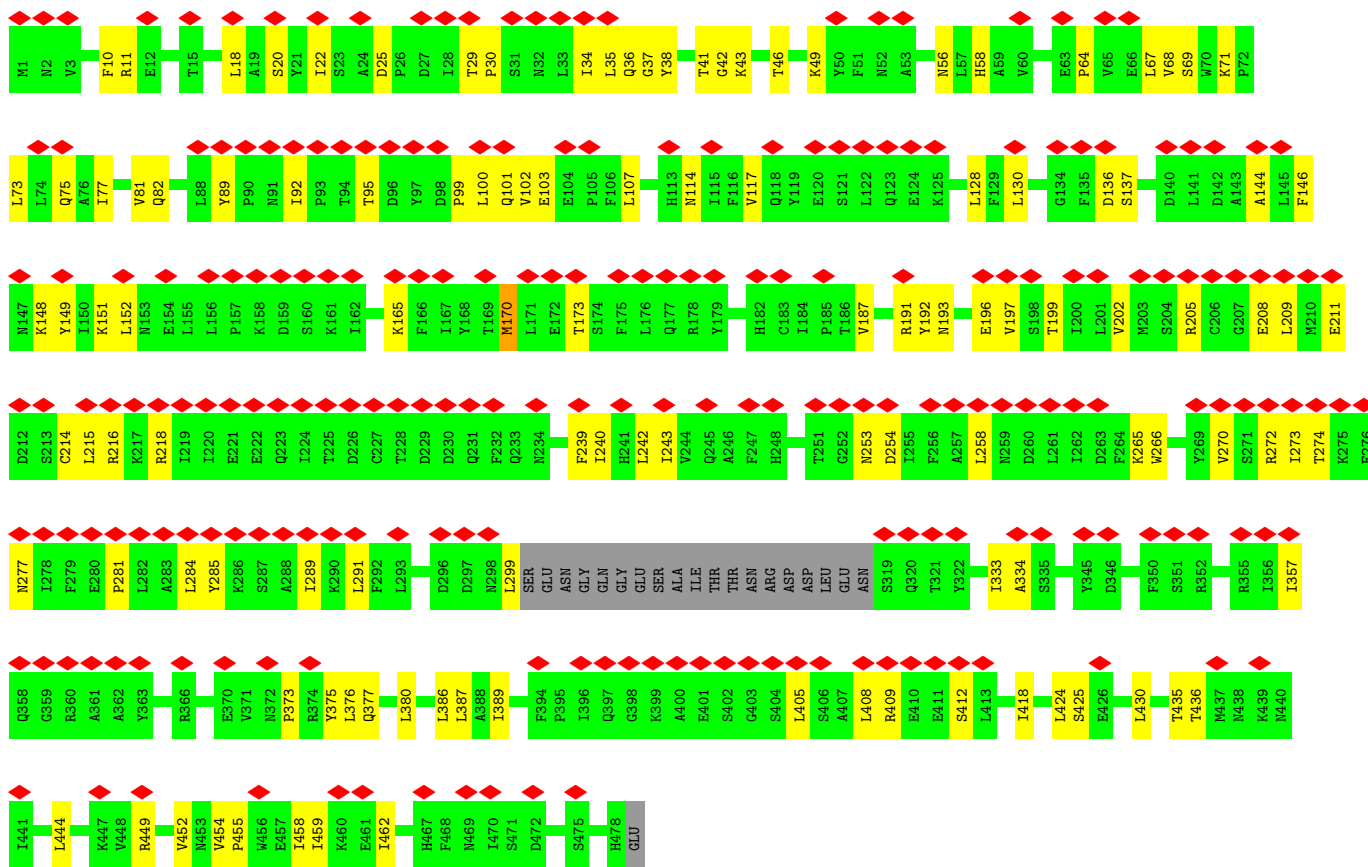


• Molecule 4: Origin recognition complex subunit 4

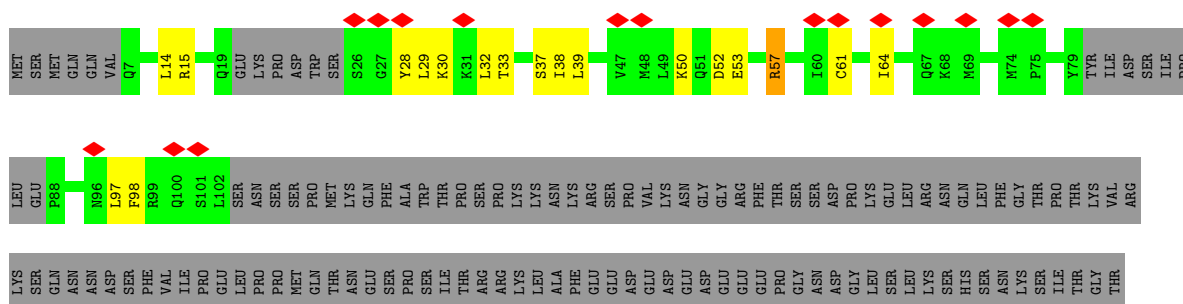
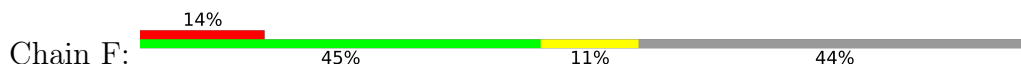


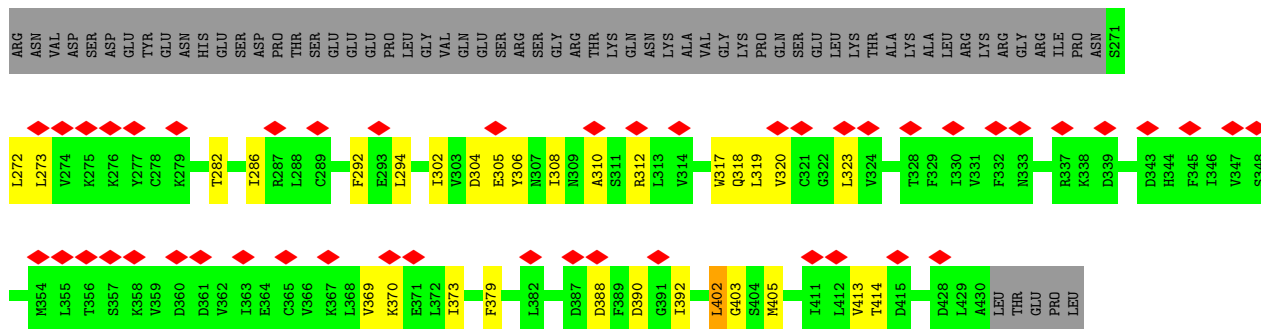


• Molecule 5: Origin recognition complex subunit 5

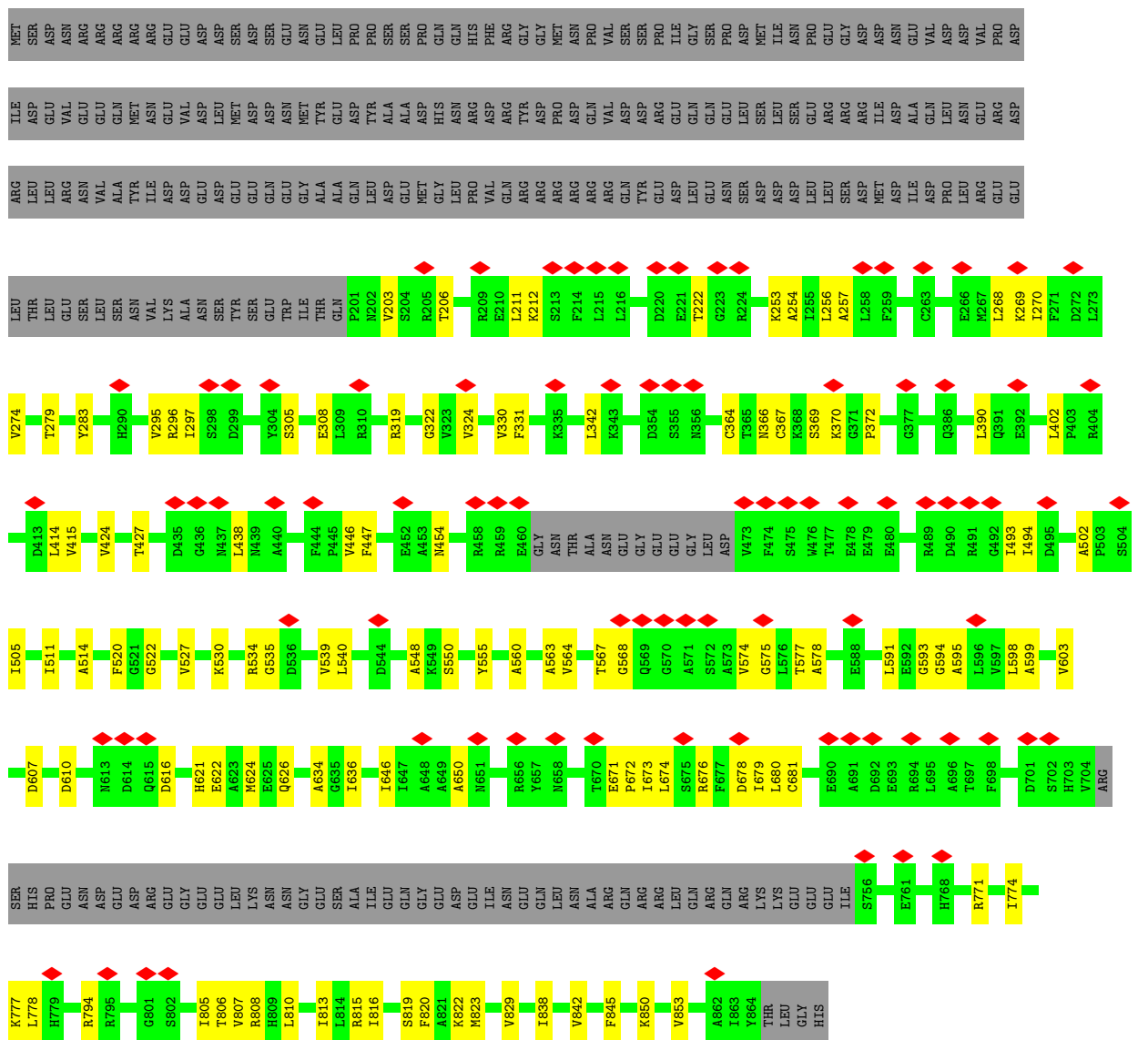


• Molecule 6: Origin recognition complex subunit 6



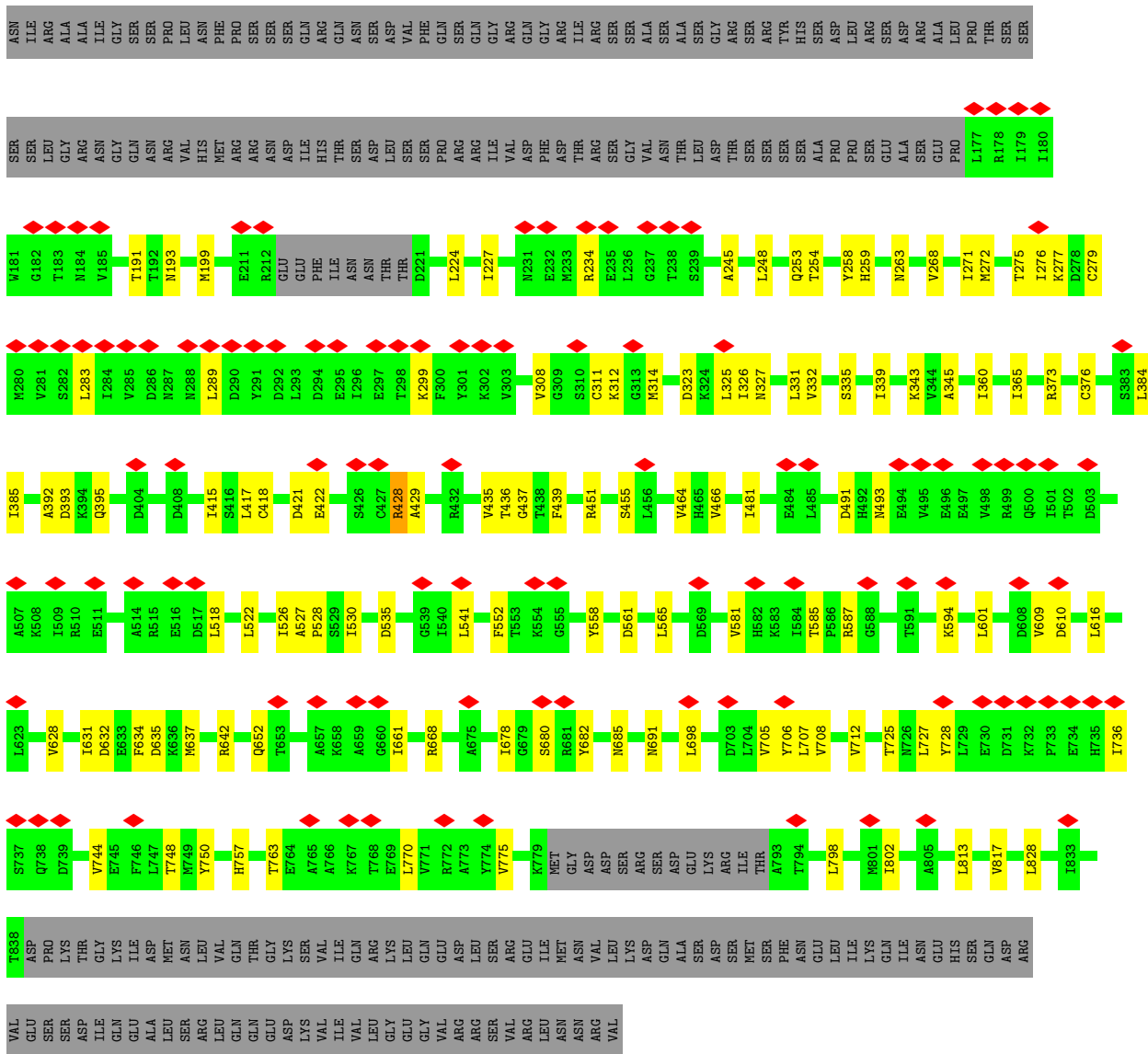


• Molecule 7: DNA replication licensing factor MCM2

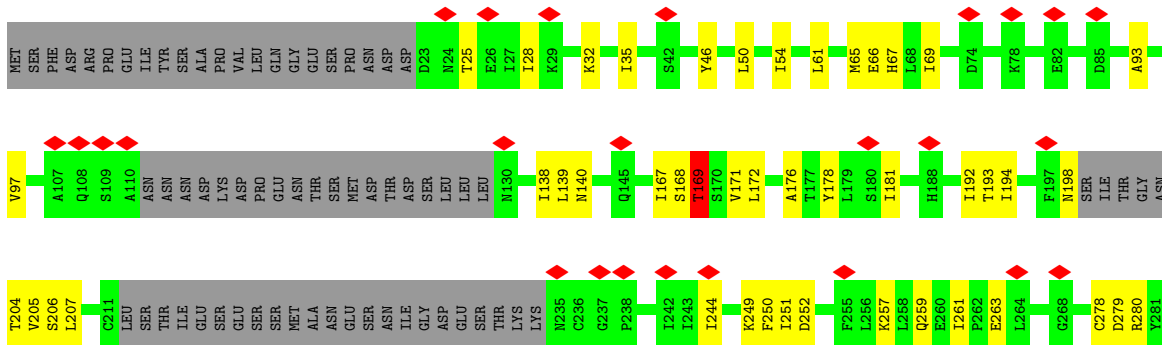


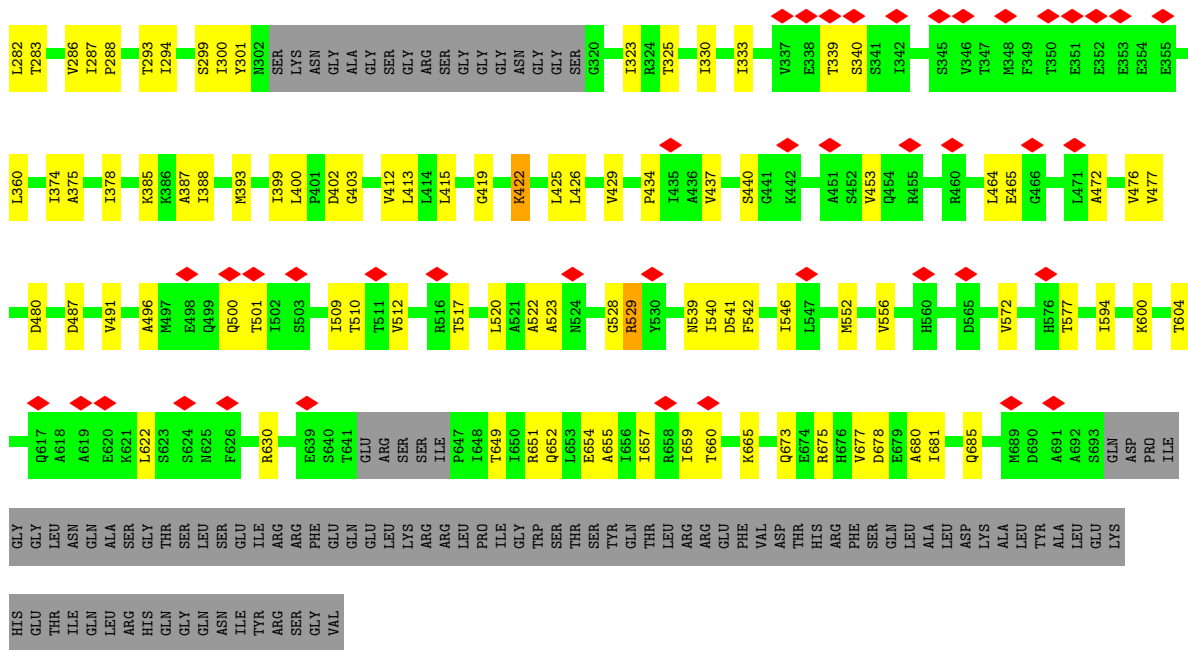
• Molecule 8: DNA replication licensing factor MCM3



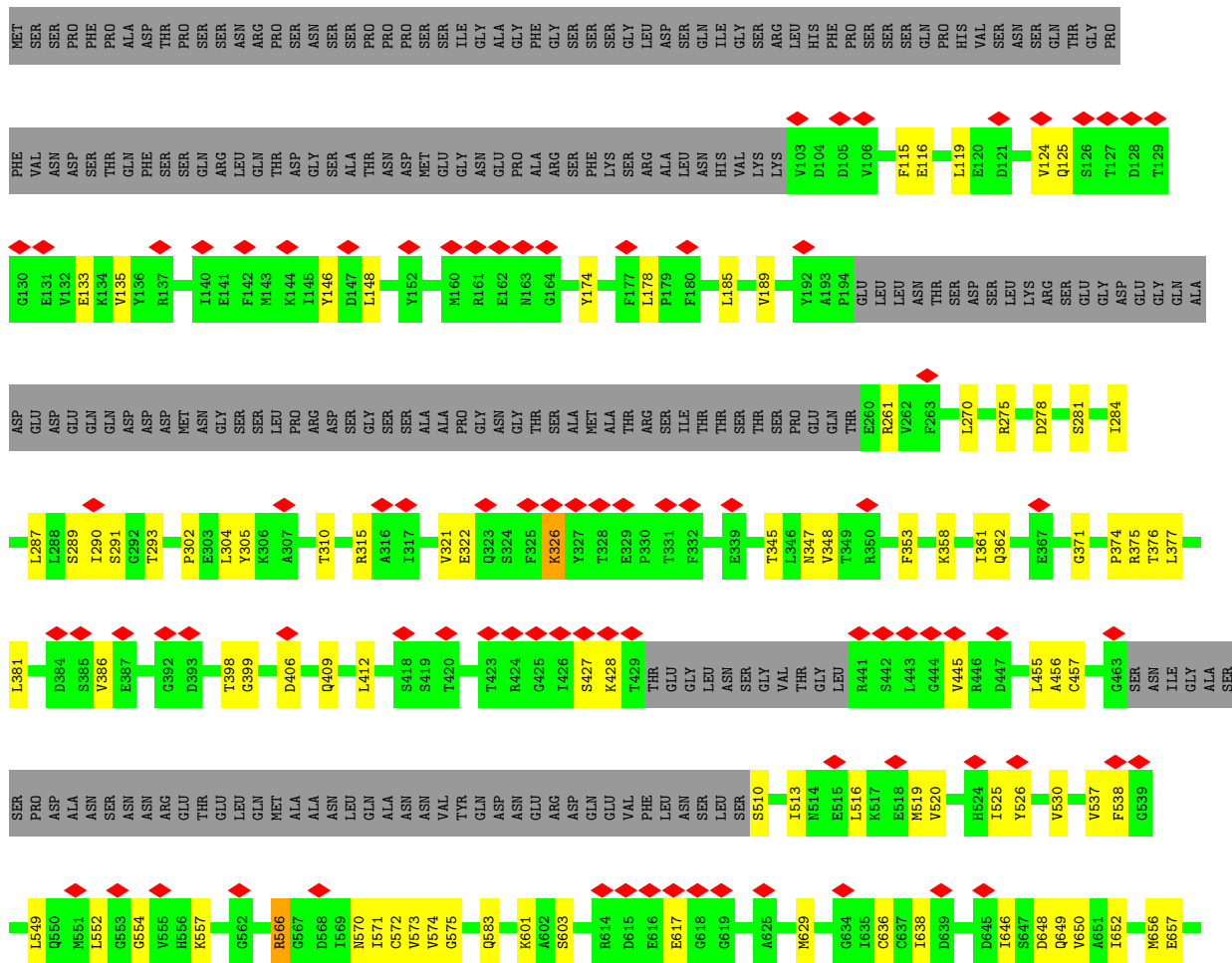


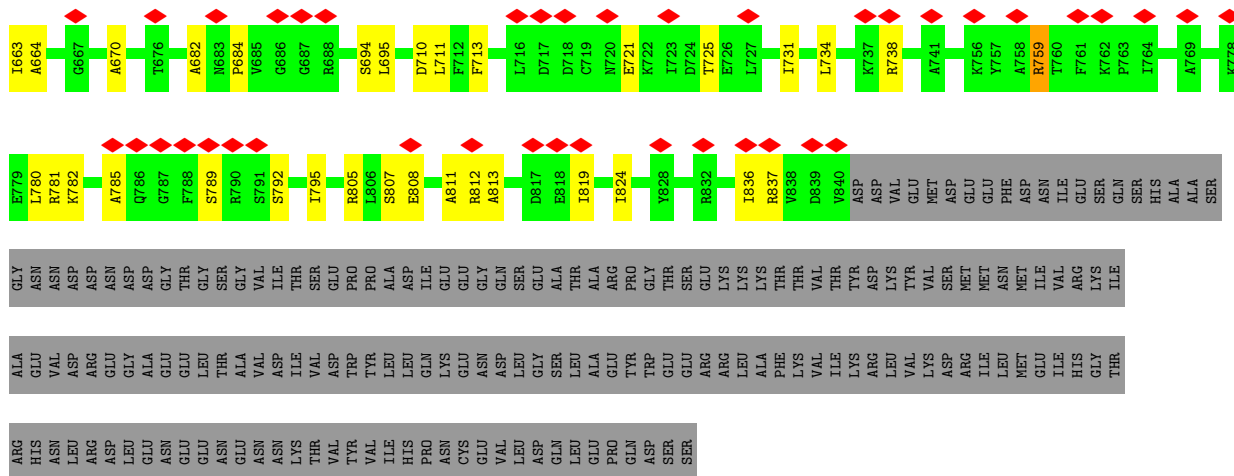
● Molecule 10: Minichromosome maintenance protein 5



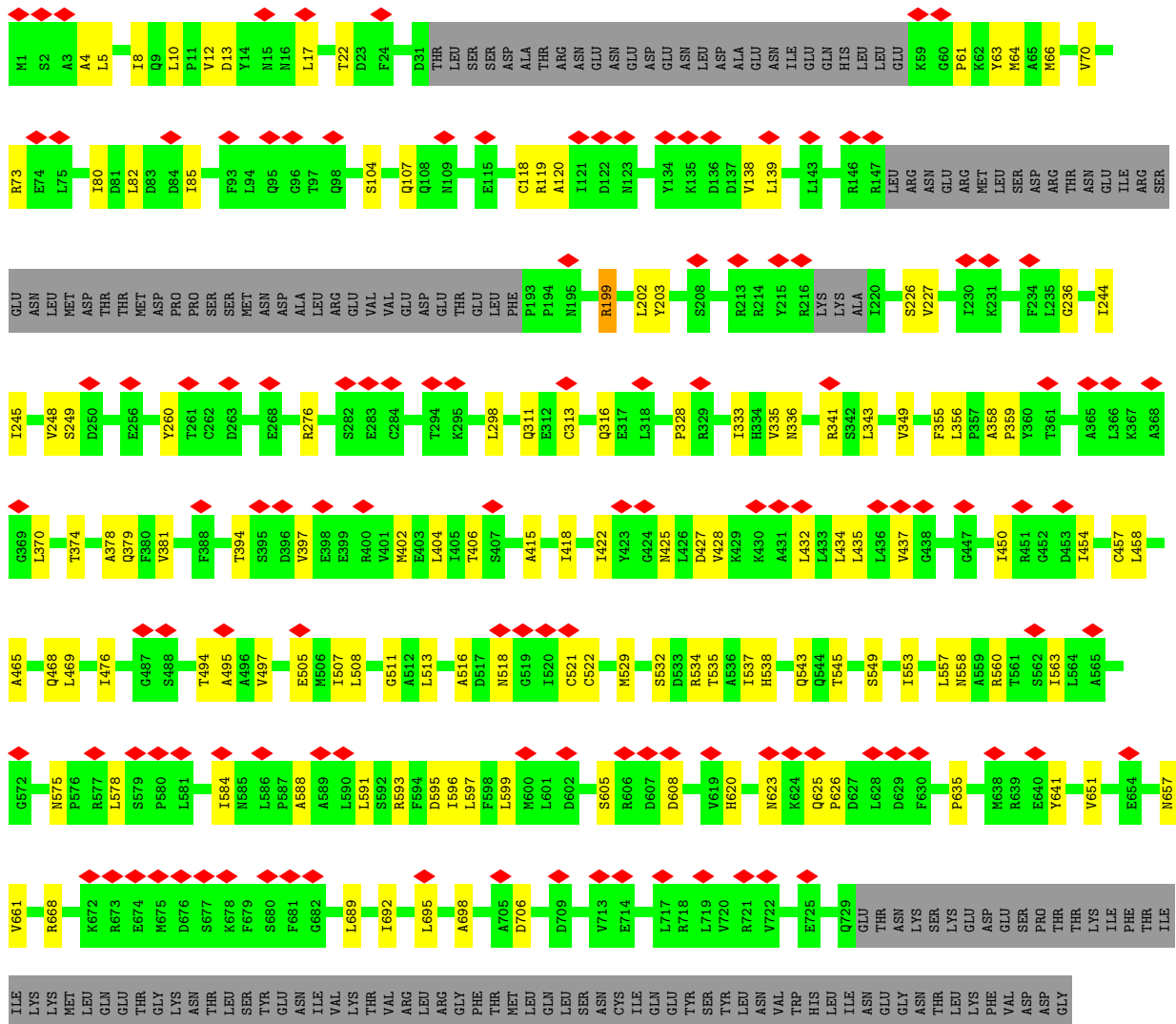


• Molecule 11: DNA replication licensing factor MCM6



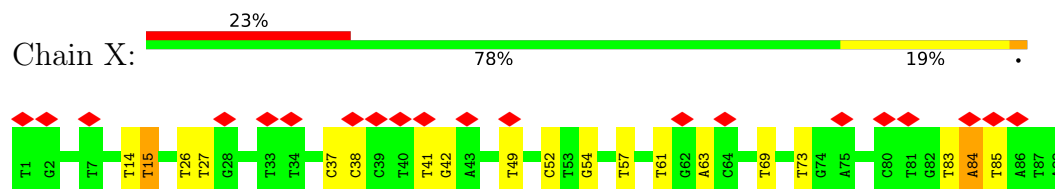


• Molecule 12: DNA replication licensing factor MCM7

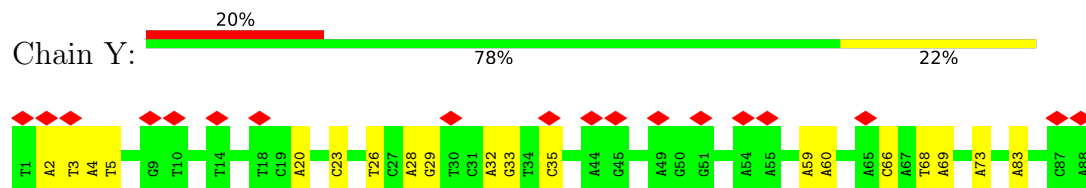


THR
MET
ASP
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GLN
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ASP
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SER
VAL
VAL
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THR
PRO
LYS
LEU
ALA
PRO
GLN
THR
THR
ALA
SER
ALA
ASN
VAL
SER
ALA
GLN
ASP
SER
ASP
ILE
ASP
LEU
GLN
ASP
ALA

- Molecule 13: DNA (88-MER)



- Molecule 14: DNA (88-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	177637	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.68	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.070	Depositor
Minimum map value	-0.037	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.016	Depositor
Map size (Å)	469.2, 469.2, 469.2	wwPDB
Map dimensions	340, 340, 340	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	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: ADP, ZN, MG, ATP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.41	0/4020	0.64	1/5407 (0.0%)
2	B	0.58	0/2102	0.72	1/2844 (0.0%)
3	C	0.51	0/4918	0.70	0/6641
4	D	0.49	0/3628	0.67	1/4901 (0.0%)
5	E	0.50	0/3835	0.68	1/5205 (0.0%)
6	F	0.57	0/2026	0.76	2/2722 (0.1%)
7	2	0.56	0/4835	0.75	0/6529
8	3	0.53	0/4775	0.74	0/6473
9	4	0.52	0/5185	0.72	1/7009 (0.0%)
10	5	0.57	0/4796	0.79	2/6482 (0.0%)
11	6	0.55	0/4954	0.79	5/6683 (0.1%)
12	7	0.52	0/5219	0.73	0/7053
13	X	1.15	4/2006 (0.2%)	1.31	12/3097 (0.4%)
14	Y	1.14	5/2037 (0.2%)	1.23	11/3139 (0.4%)
All	All	0.60	9/54336 (0.0%)	0.79	37/74185 (0.0%)

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	X	84	DA	O3'-P	-12.59	1.46	1.61
13	X	14	DT	C3'-O3'	-8.06	1.33	1.44
13	X	15	DT	C3'-O3'	-7.03	1.34	1.44
14	Y	66	DC	C3'-O3'	-5.69	1.36	1.44
14	Y	33	DG	C3'-O3'	-5.67	1.36	1.44

The worst 5 of 37 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	405	MET	CG-SD-CE	-7.70	87.89	100.20
14	Y	60	DA	O3'-P-O5'	6.89	117.09	104.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	Y	28	DA	O4'-C1'-N9	6.77	112.74	108.00
14	Y	59	DA	P-O3'-C3'	-6.53	111.87	119.70
11	6	322	GLU	CB-CA-C	6.46	123.33	110.40

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	A	3958	4070	4070	92	0
2	B	2049	2018	2018	51	0
3	C	4813	4766	4765	99	0
4	D	3566	3627	3627	76	0
5	E	3749	3780	3780	96	0
6	F	1995	2051	2051	34	0
7	2	4753	4820	4820	84	0
8	3	4696	4752	4752	101	0
9	4	5110	5172	5171	92	0
10	5	4730	4802	4803	95	0
11	6	4874	4908	4908	86	0
12	7	5138	5215	5214	105	0
13	X	1796	1010	1010	5	0
14	Y	1809	987	987	5	0
15	A	31	12	12	4	0
15	D	31	12	12	2	0
15	E	31	12	12	0	0
16	A	1	0	0	0	0
16	D	1	0	0	0	0
16	E	1	0	0	0	0
17	2	27	12	12	3	0
17	3	27	12	12	2	0
17	5	27	12	12	2	0
17	7	27	12	12	3	0
18	2	1	0	0	0	0
18	4	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	5	1	0	0	0	0
18	6	1	0	0	0	0
18	7	1	0	0	0	0
All	All	53245	52062	52060	922	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 9.

The worst 5 of 922 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)
1:A:550:PHE:O	1:A:558:LYS:NZ	2.09	0.86
6:F:302:ILE:HG23	6:F:323:LEU:HD13	1.60	0.83
3:C:80:GLU:OE2	3:C:84:LYS:HD2	1.79	0.81
8:3:488:GLU:O	8:3:493:GLN:N	2.15	0.79
9:4:775:VAL:HG21	11:6:725:THR:HG22	1.66	0.77

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/949 (51%)	447 (92%)	39 (8%)	0	100	100
2	B	243/620 (39%)	215 (88%)	28 (12%)	0	100	100
3	C	578/616 (94%)	514 (89%)	64 (11%)	0	100	100
4	D	429/529 (81%)	389 (91%)	40 (9%)	0	100	100
5	E	455/479 (95%)	409 (90%)	44 (10%)	2 (0%)	34	72
6	F	234/435 (54%)	208 (89%)	25 (11%)	1 (0%)	34	72
7	2	595/868 (68%)	528 (89%)	67 (11%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	3	589/1006 (58%)	521 (88%)	68 (12%)	0	100	100
9	4	635/933 (68%)	572 (90%)	61 (10%)	2 (0%)	41	76
10	5	590/775 (76%)	526 (89%)	63 (11%)	1 (0%)	47	81
11	6	608/1017 (60%)	541 (89%)	67 (11%)	0	100	100
12	7	646/845 (76%)	579 (90%)	67 (10%)	0	100	100
All	All	6088/9072 (67%)	5449 (90%)	633 (10%)	6 (0%)	54	85

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
9	4	373	ARG
9	4	668	ARG
5	E	412	SER
10	5	434	PRO
6	F	403	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	438/842 (52%)	435 (99%)	3 (1%)	84	90
2	B	230/573 (40%)	227 (99%)	3 (1%)	69	82
3	C	543/576 (94%)	534 (98%)	9 (2%)	60	78
4	D	404/488 (83%)	402 (100%)	2 (0%)	88	93
5	E	423/440 (96%)	422 (100%)	1 (0%)	93	96
6	F	228/406 (56%)	227 (100%)	1 (0%)	91	94
7	2	526/770 (68%)	523 (99%)	3 (1%)	86	92
8	3	518/864 (60%)	515 (99%)	3 (1%)	86	92
9	4	582/848 (69%)	577 (99%)	5 (1%)	78	88
10	5	539/688 (78%)	532 (99%)	7 (1%)	69	82
11	6	537/886 (61%)	531 (99%)	6 (1%)	73	85

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
12	7	575/753 (76%)	571 (99%)	4 (1%)	84	90
All	All	5543/8134 (68%)	5496 (99%)	47 (1%)	82	89

5 of 47 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
9	4	682	TYR
10	5	529	ARG
9	4	685	ASN
10	5	280	ARG
11	6	326	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
6	F	96	ASN
6	F	407	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 8 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$
15	ATP	D	2001	16	26,33,33	0.97	1 (3%)	31,52,52	1.81	5 (16%)
17	ADP	5	801	-	24,29,29	0.97	1 (4%)	29,45,45	1.51	4 (13%)
17	ADP	2	901	-	24,29,29	0.99	1 (4%)	29,45,45	1.77	4 (13%)
15	ATP	E	2001	16	26,33,33	1.00	2 (7%)	31,52,52	1.71	6 (19%)
17	ADP	3	2001	-	24,29,29	0.94	0	29,45,45	1.59	4 (13%)
17	ADP	7	901	-	24,29,29	0.95	1 (4%)	29,45,45	1.52	6 (20%)
15	ATP	A	2001	16	26,33,33	0.93	1 (3%)	31,52,52	1.70	5 (16%)

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
15	ATP	D	2001	16	-	2/18/38/38	0/3/3/3
17	ADP	5	801	-	-	6/12/32/32	0/3/3/3
17	ADP	2	901	-	-	3/12/32/32	0/3/3/3
15	ATP	E	2001	16	-	4/18/38/38	0/3/3/3
17	ADP	3	2001	-	-	5/12/32/32	0/3/3/3
17	ADP	7	901	-	-	3/12/32/32	0/3/3/3
15	ATP	A	2001	16	-	4/18/38/38	0/3/3/3

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	5	801	ADP	C5-C4	2.43	1.47	1.40
15	E	2001	ATP	C5-C4	2.34	1.47	1.40
15	D	2001	ATP	C5-C4	2.27	1.46	1.40
15	A	2001	ATP	C5-C4	2.22	1.46	1.40
17	7	901	ADP	C2'-C1'	-2.12	1.50	1.53

The worst 5 of 34 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	2001	ATP	PA-O3A-PB	-5.39	114.33	132.83
15	D	2001	ATP	PA-O3A-PB	-5.30	114.65	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	D	2001	ATP	PB-O3B-PG	-4.78	116.42	132.83
17	2	901	ADP	PA-O3A-PB	-4.70	116.69	132.83
17	3	2001	ADP	PA-O3A-PB	-4.14	118.63	132.83

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

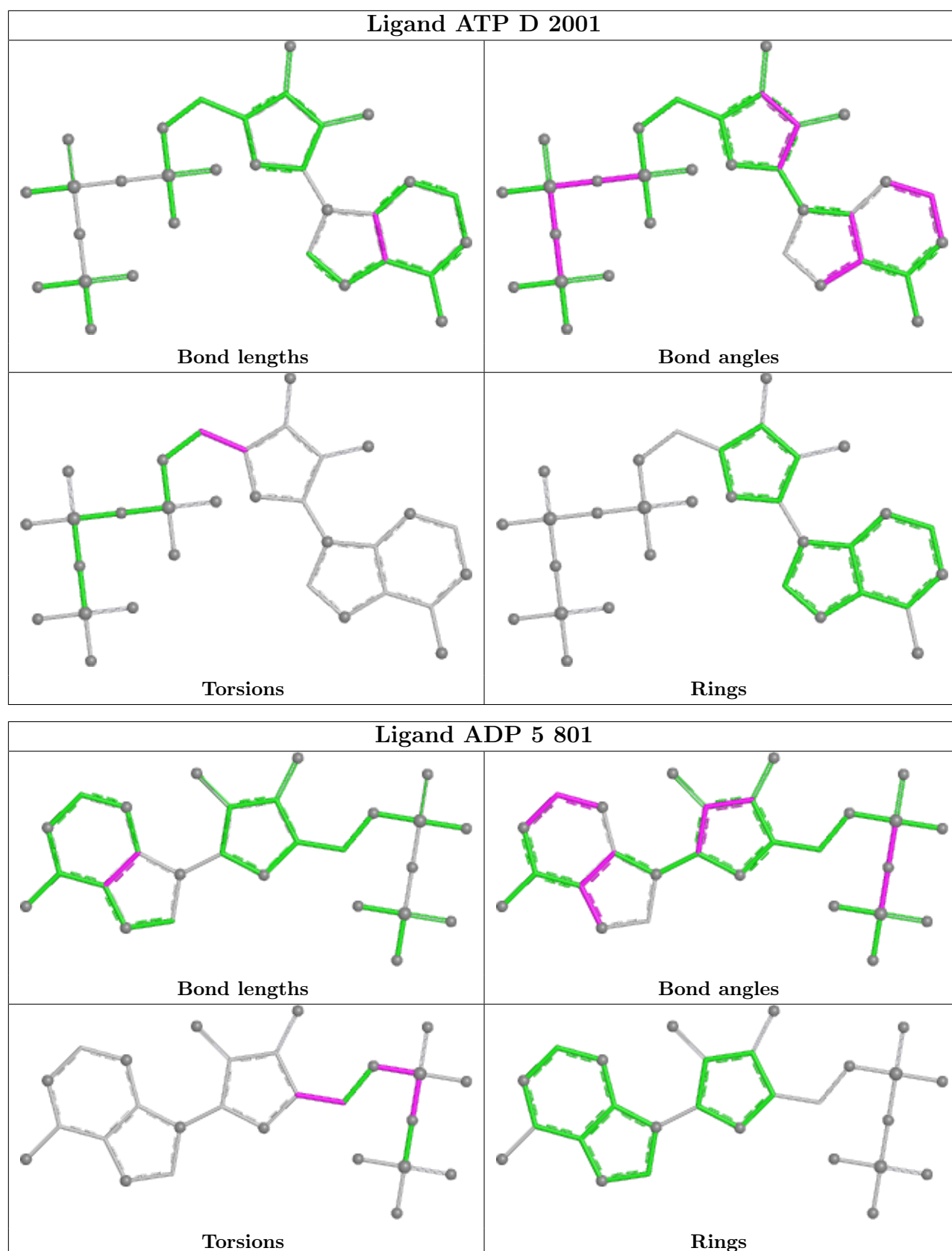
Mol	Chain	Res	Type	Atoms
15	A	2001	ATP	C5'-O5'-PA-O1A
15	A	2001	ATP	C5'-O5'-PA-O2A
15	E	2001	ATP	C5'-O5'-PA-O1A
15	E	2001	ATP	C5'-O5'-PA-O2A
15	E	2001	ATP	C5'-O5'-PA-O3A

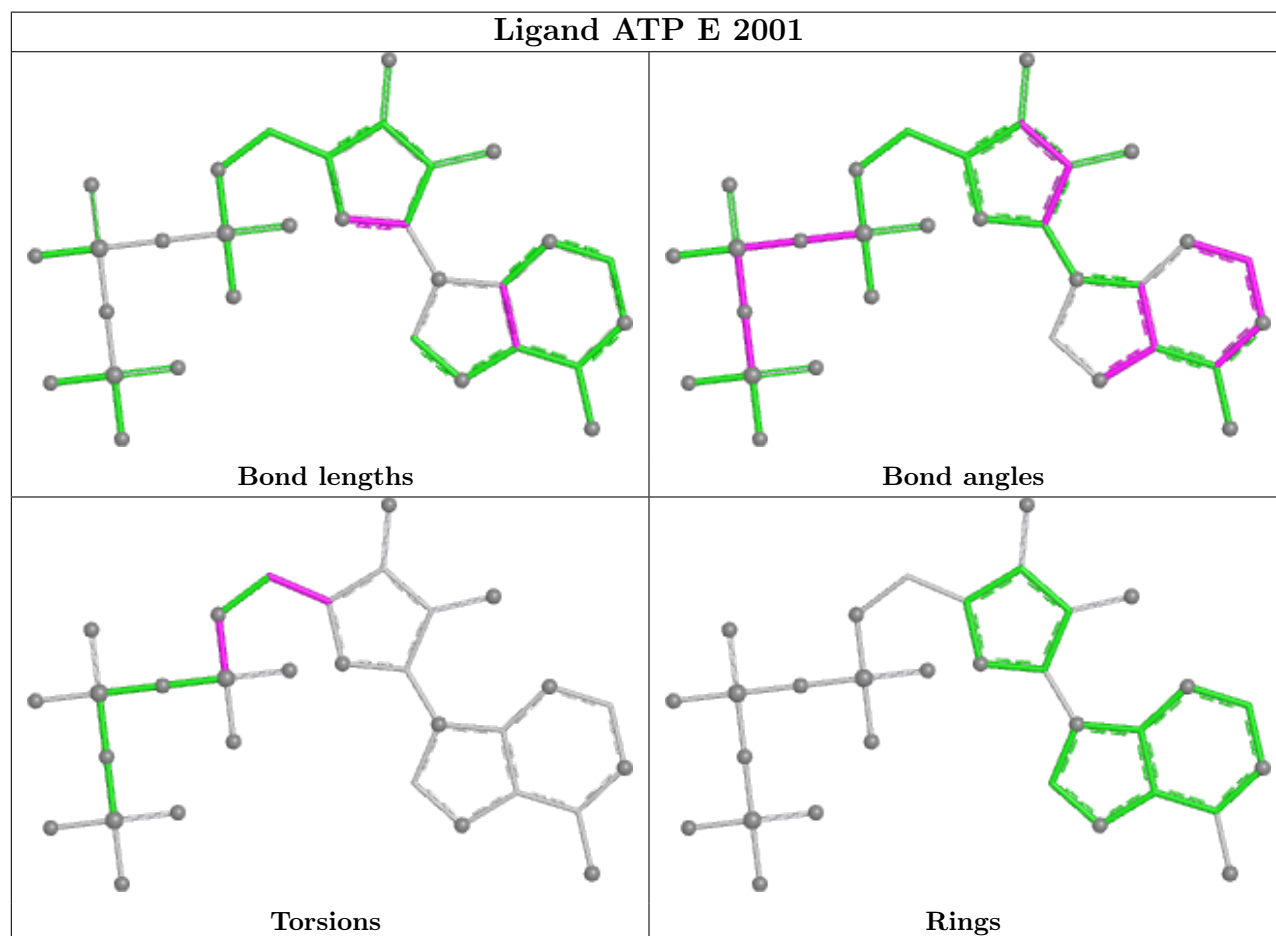
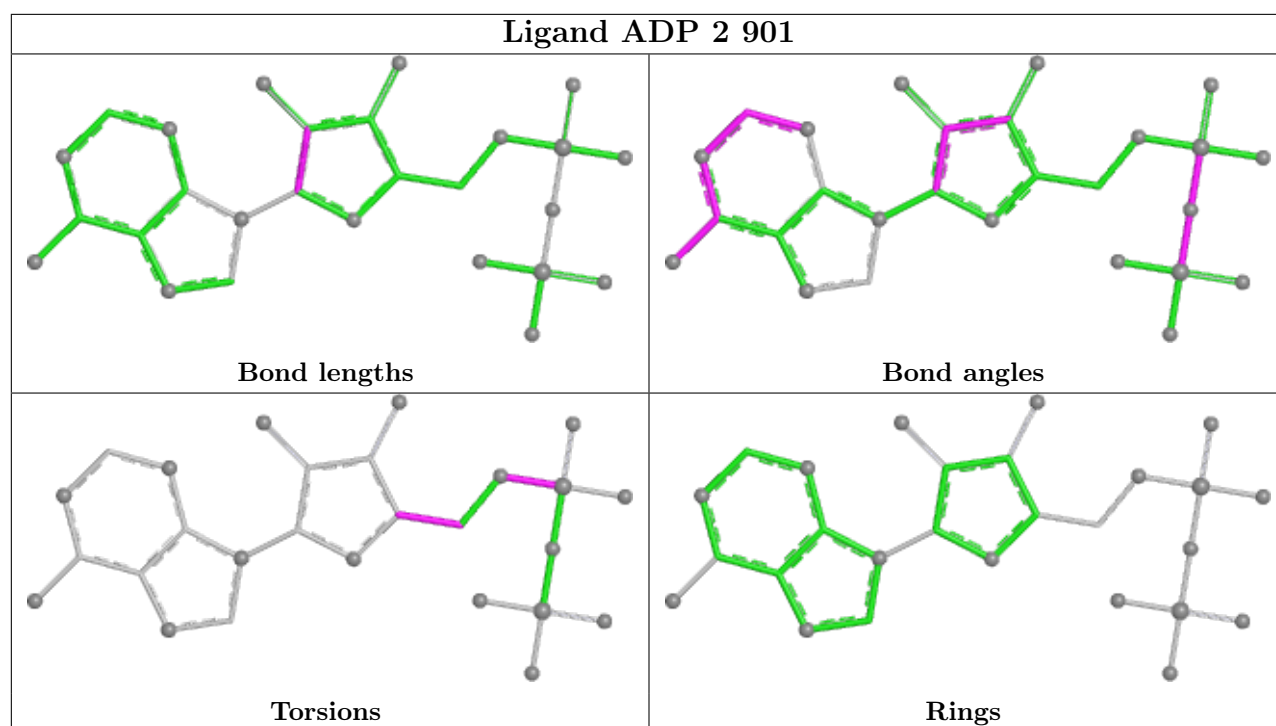
There are no ring outliers.

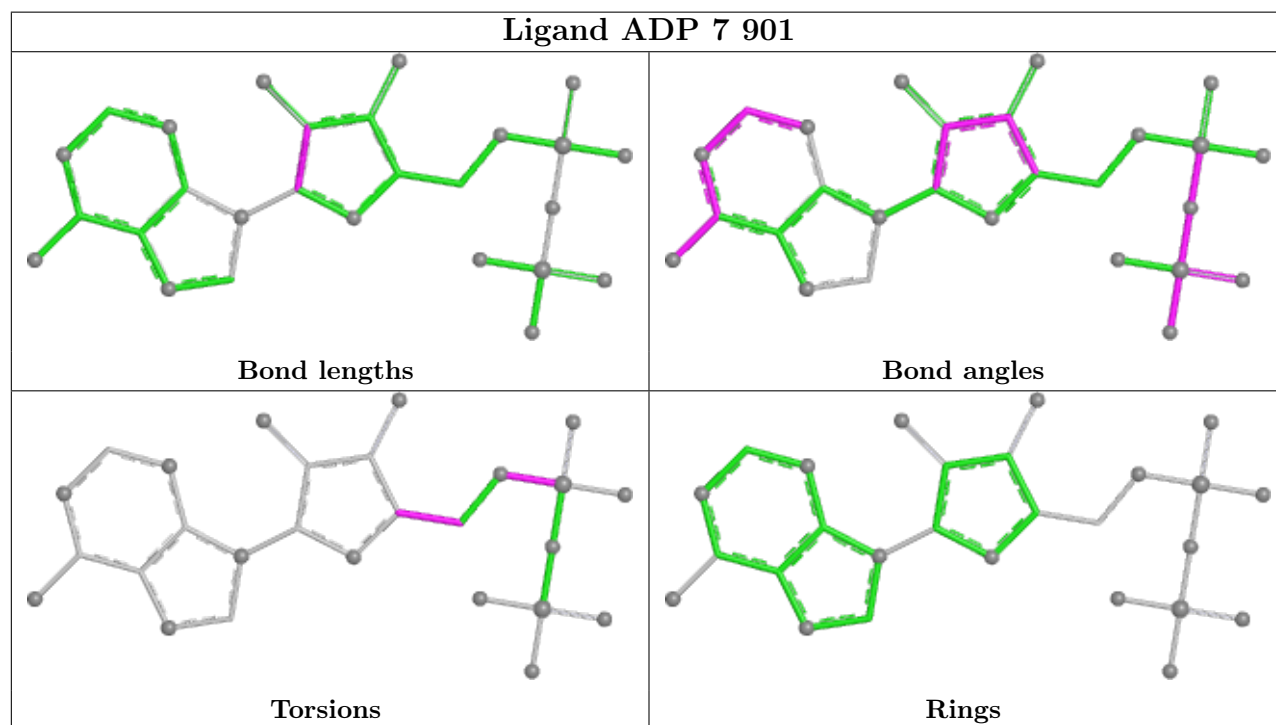
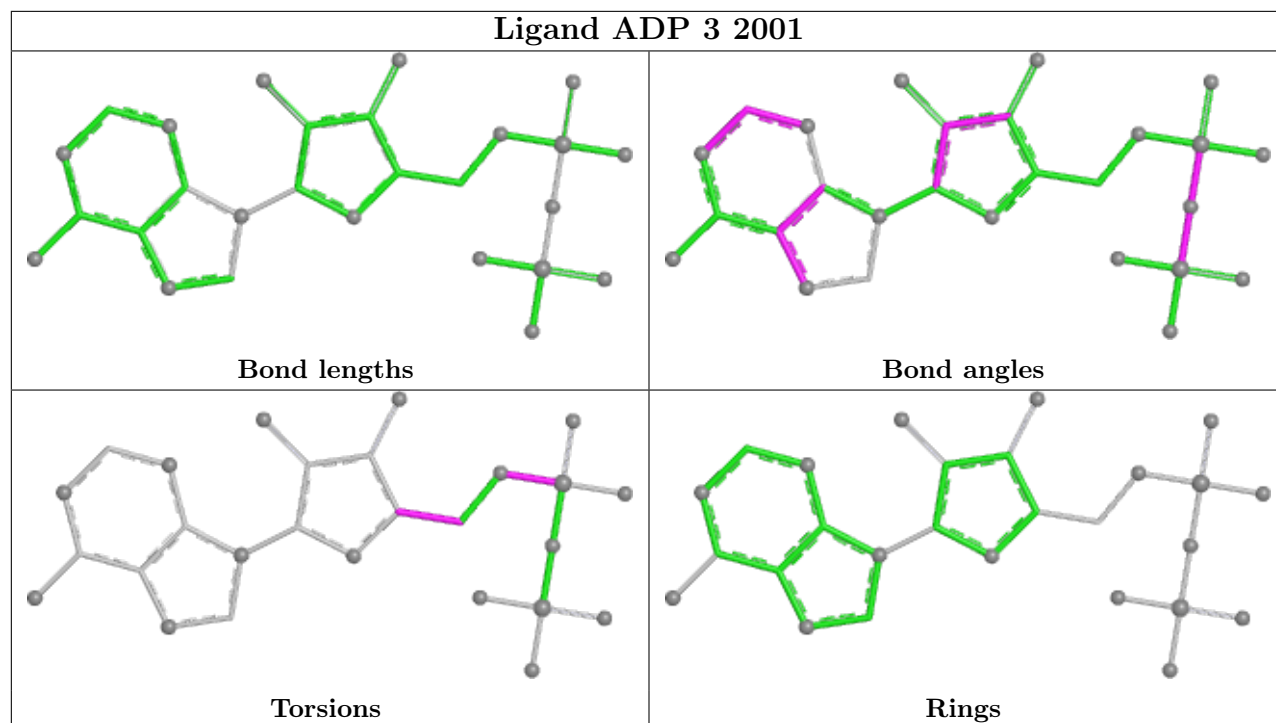
6 monomers are involved in 16 short contacts:

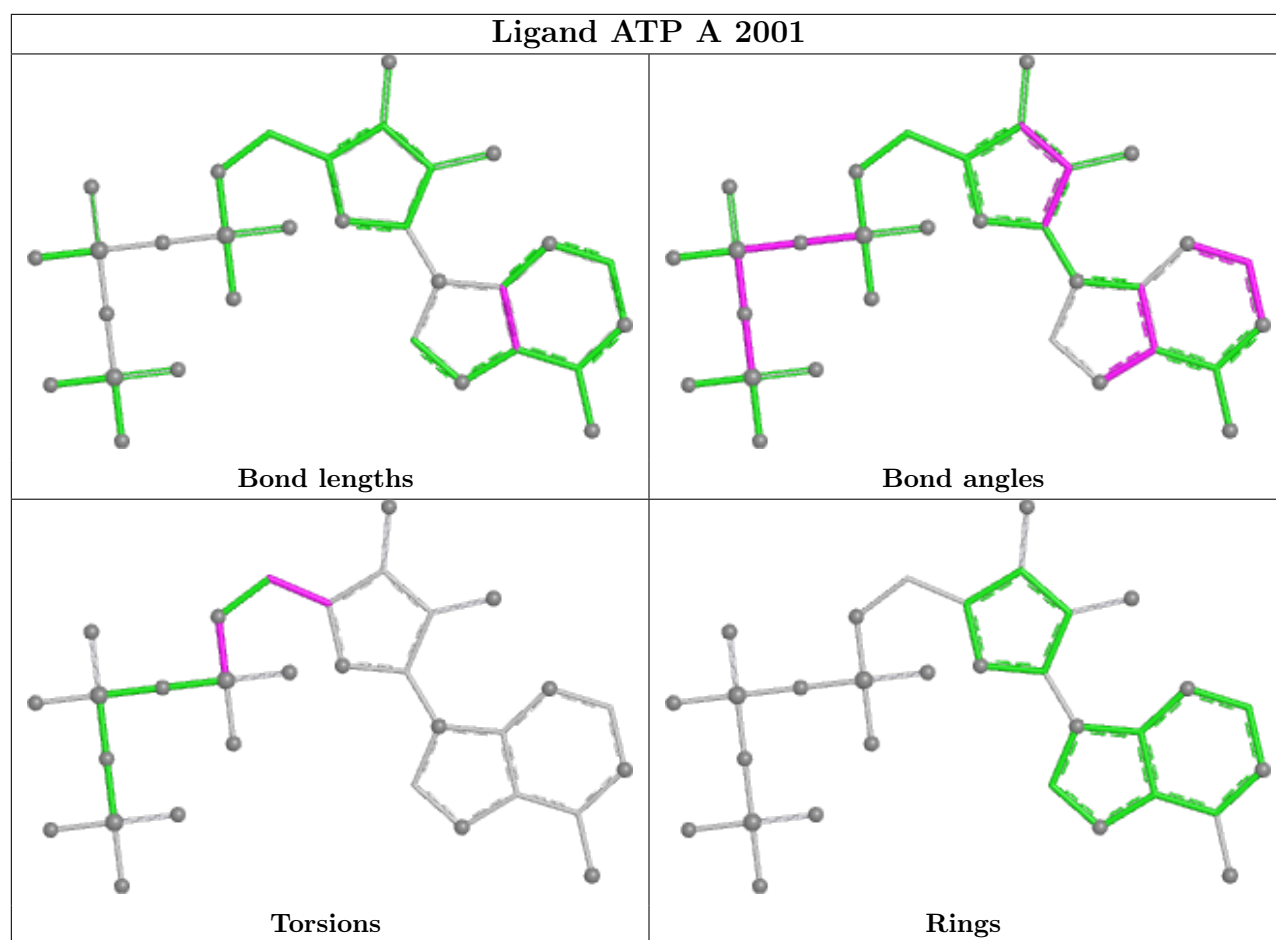
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	D	2001	ATP	2	0
17	5	801	ADP	2	0
17	2	901	ADP	3	0
17	3	2001	ADP	2	0
17	7	901	ADP	3	0
15	A	2001	ATP	4	0

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.

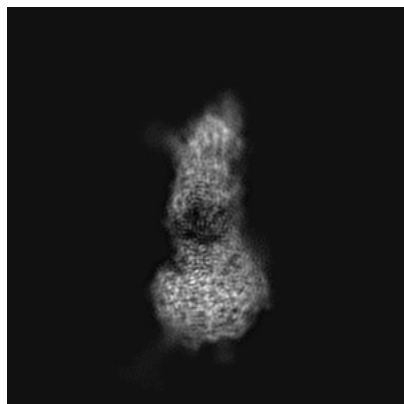
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-4980. These allow visual inspection of the internal detail of the map and identification of artifacts.

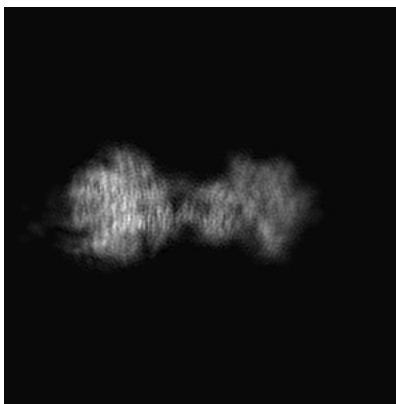
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

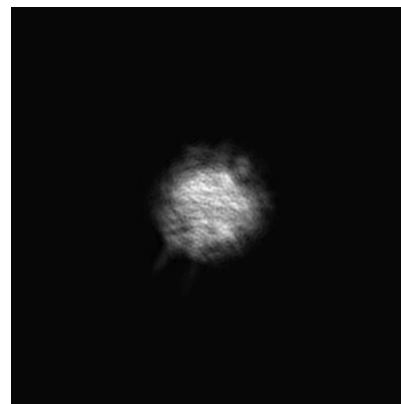
6.1.1 Primary map



X

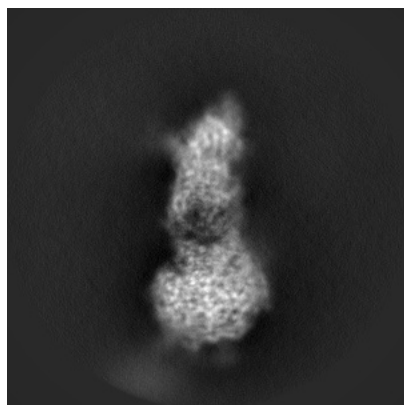


Y

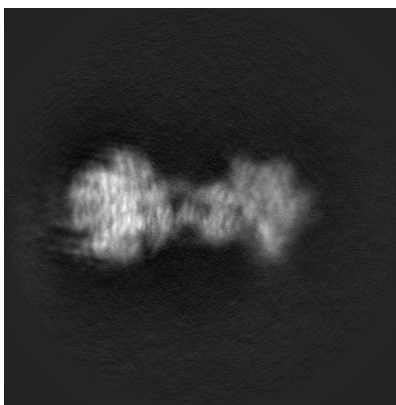


Z

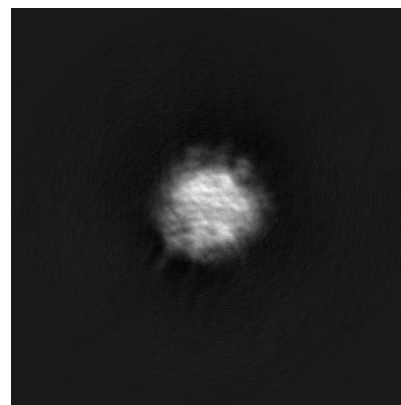
6.1.2 Raw map



X



Y

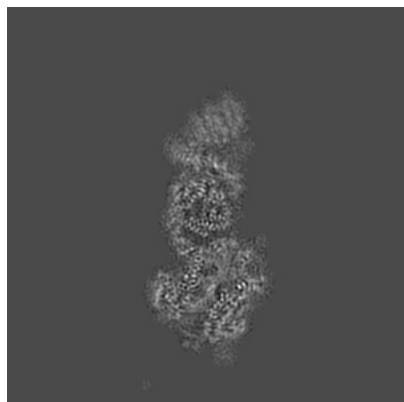


Z

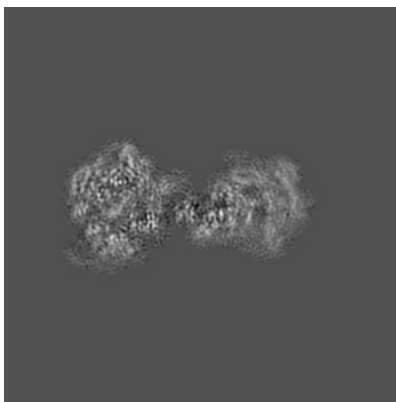
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

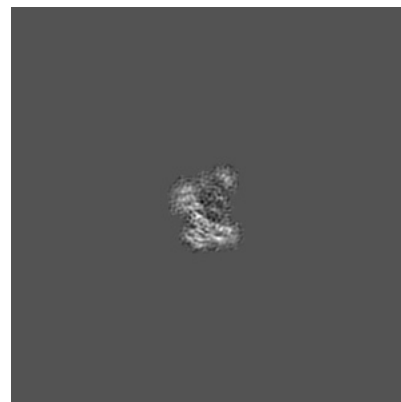
6.2.1 Primary map



X Index: 170

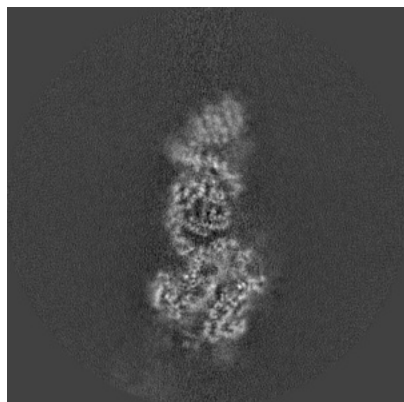


Y Index: 170

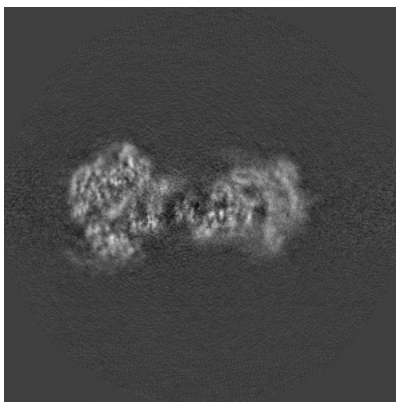


Z Index: 170

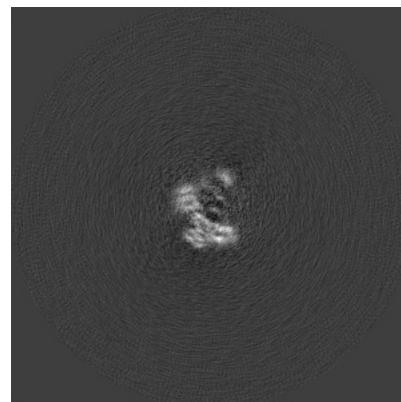
6.2.2 Raw map



X Index: 170



Y Index: 170

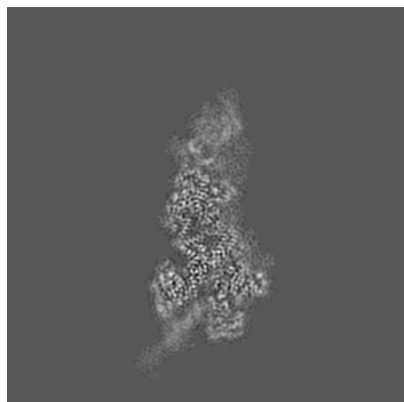


Z Index: 170

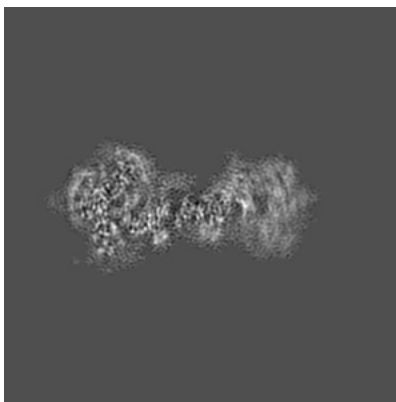
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

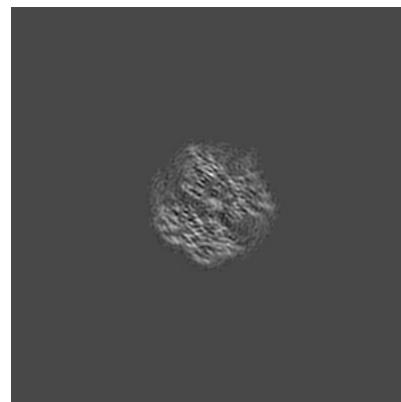
6.3.1 Primary map



X Index: 159

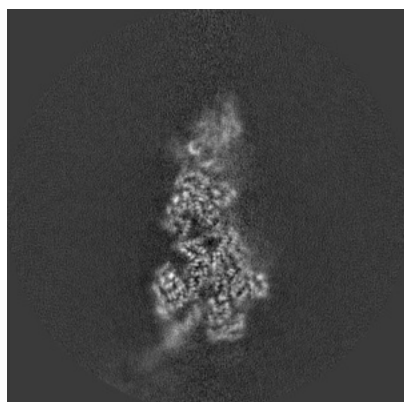


Y Index: 177

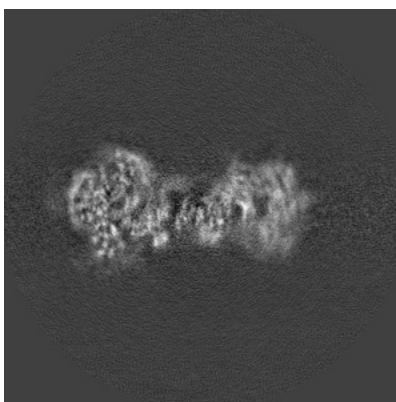


Z Index: 102

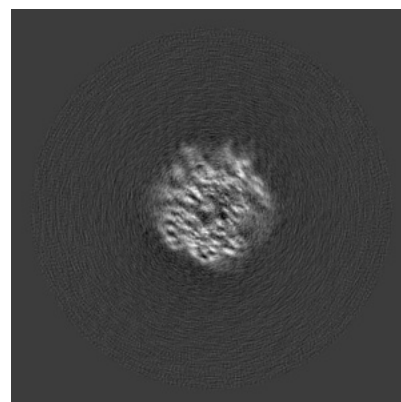
6.3.2 Raw map



X Index: 158



Y Index: 177

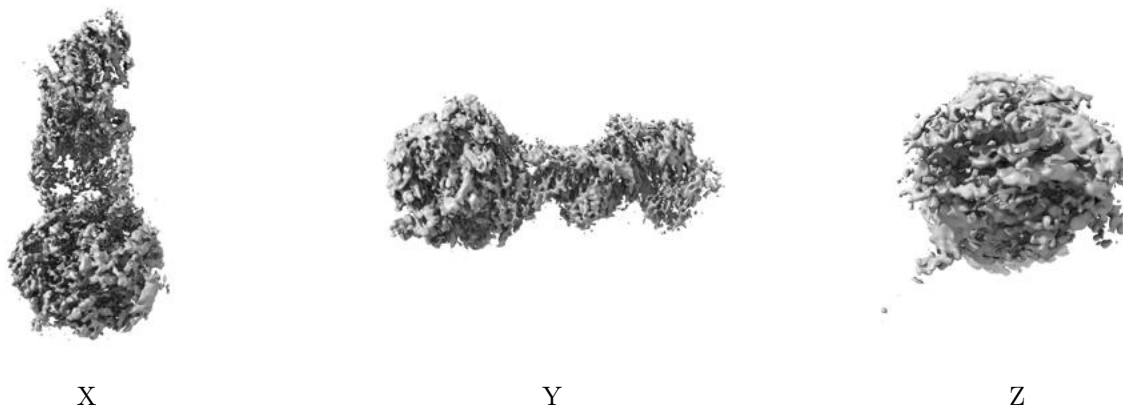


Z Index: 94

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

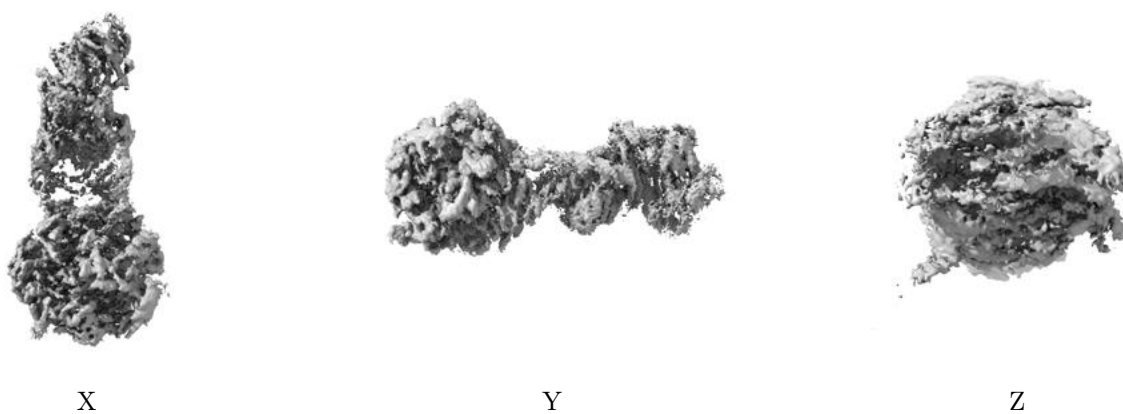
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.016. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

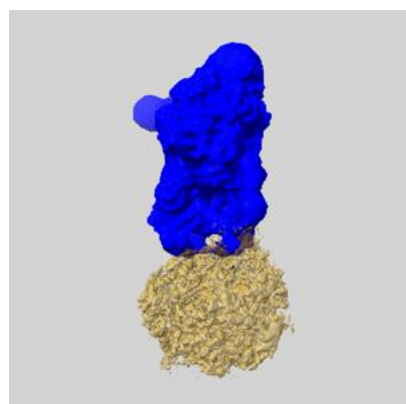
6.5 Mask visualisation [i](#)

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

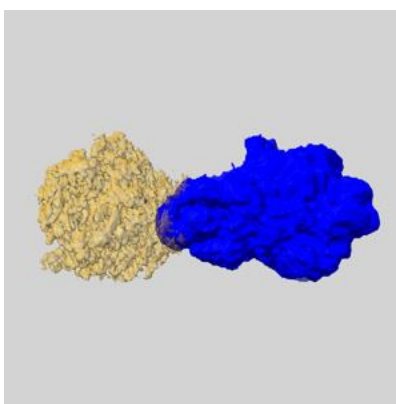
A mask typically either:

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

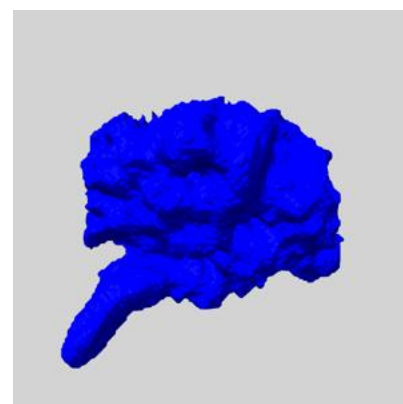
6.5.1 emd_4980_msk_2.map [i](#)



X

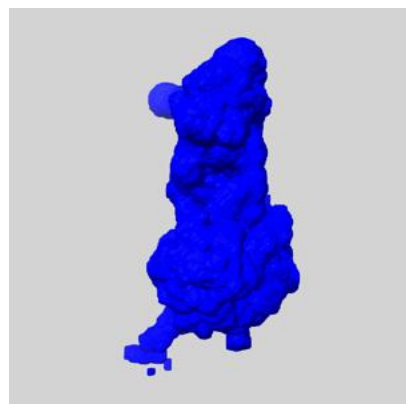


Y

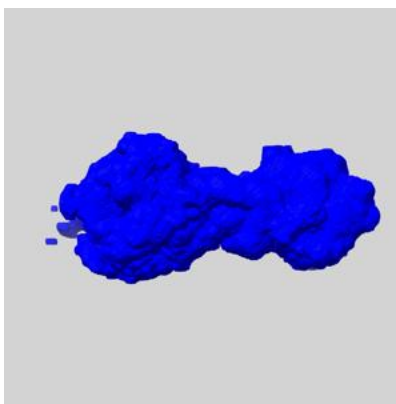


Z

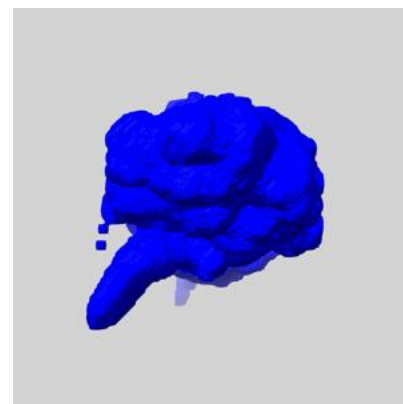
6.5.2 emd_4980_msk_3.map [i](#)



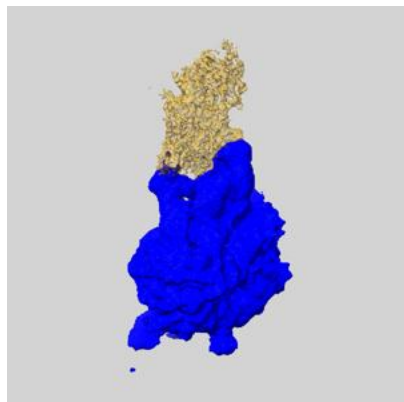
X



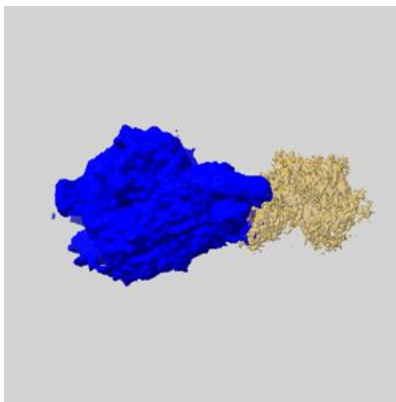
Y



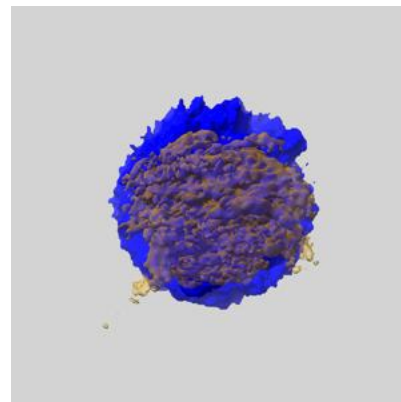
Z

6.5.3 emd_4980_msk_1.map [i](#)

X



Y

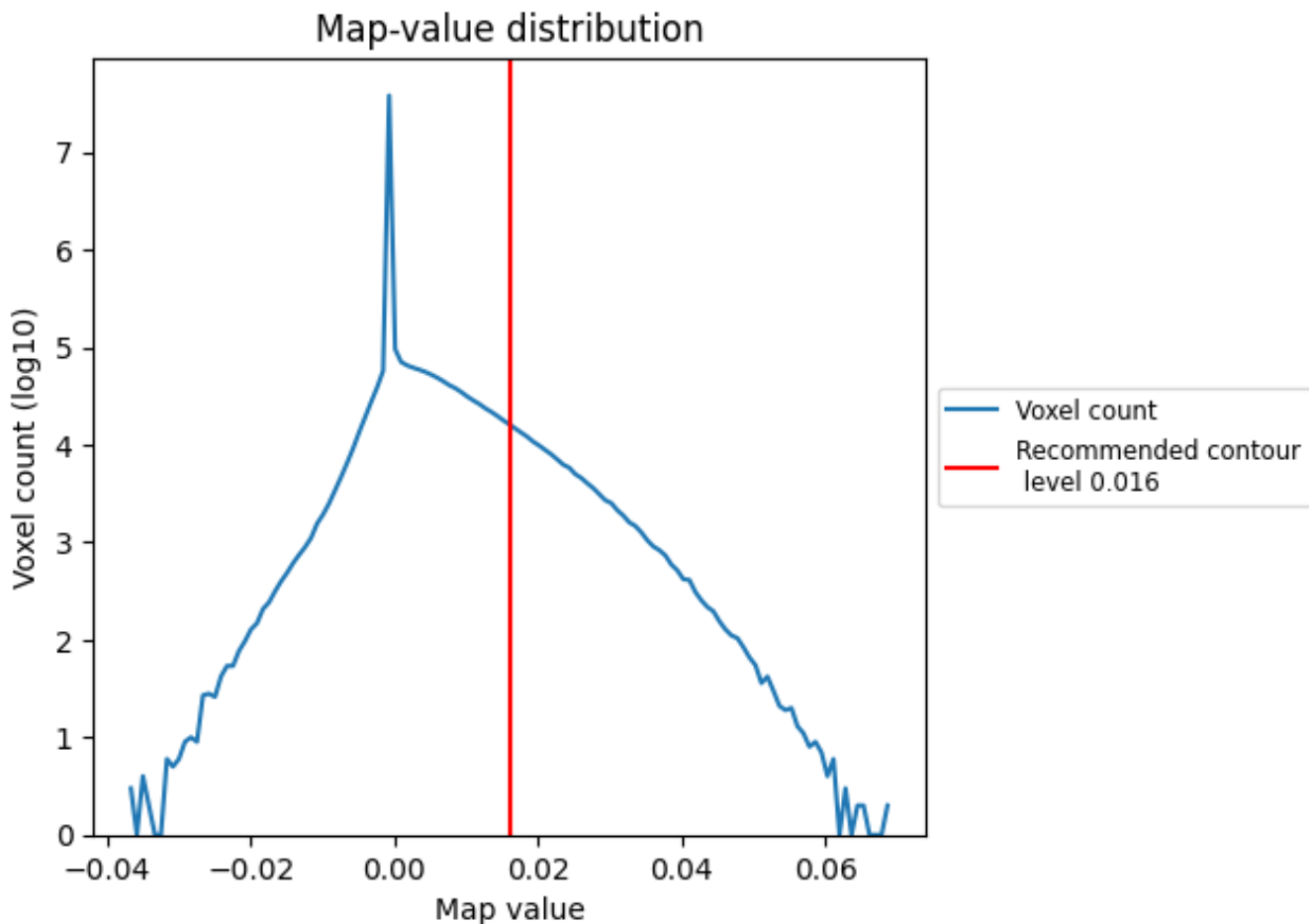


Z

7 Map analysis [i](#)

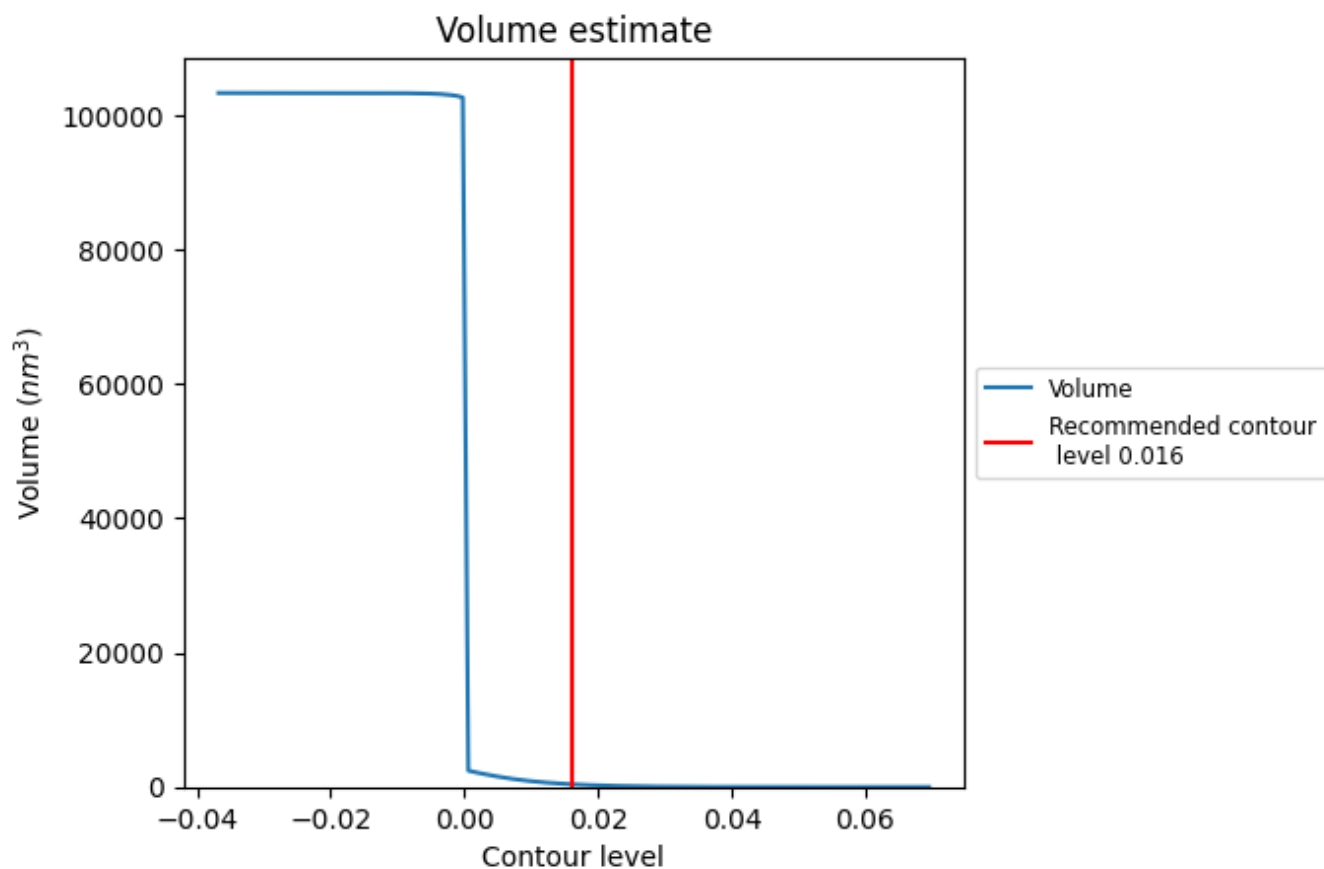
This section contains the results of statistical analysis of the map.

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.

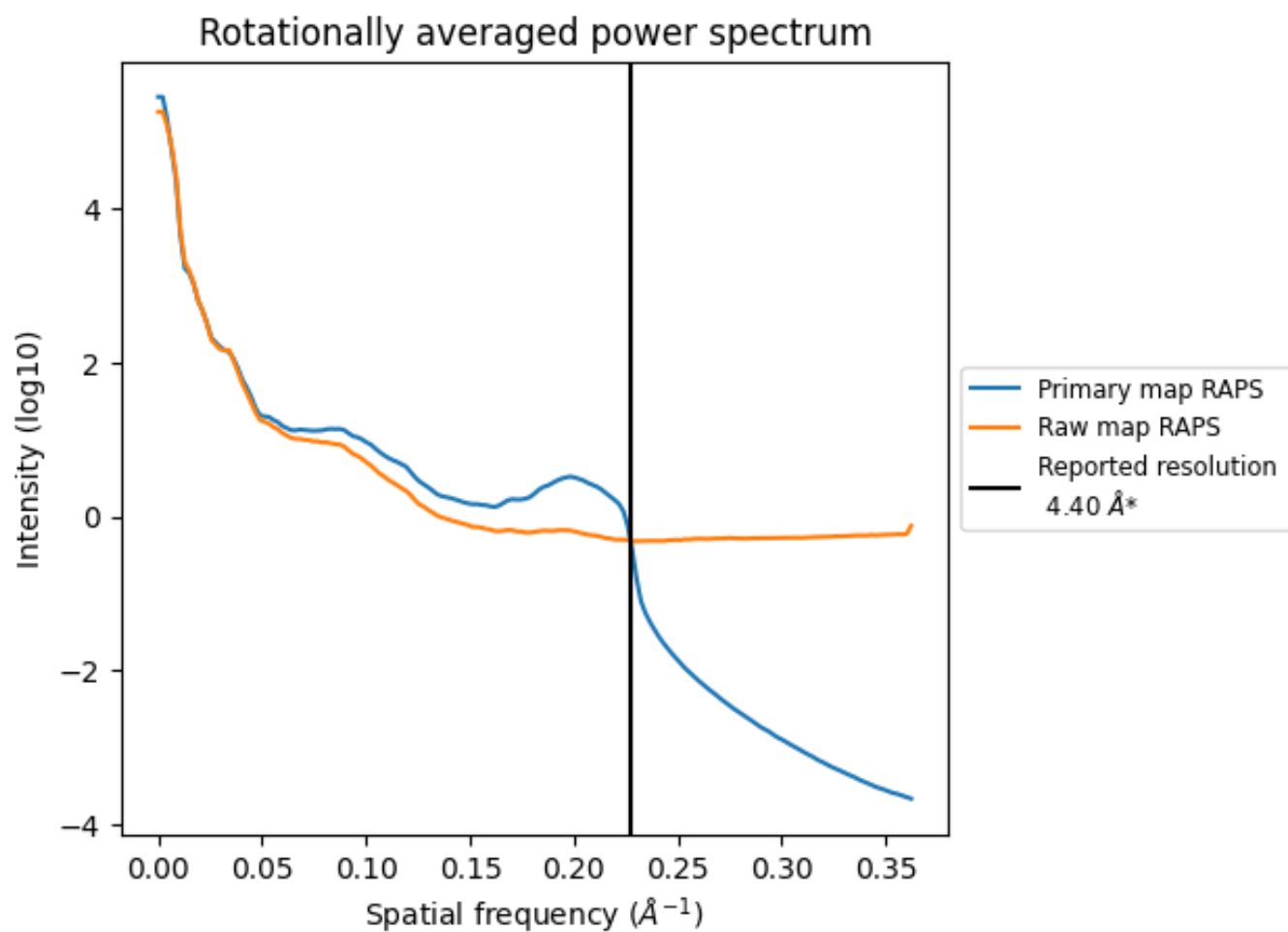
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 404 nm³; this corresponds to an approximate mass of 365 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 i

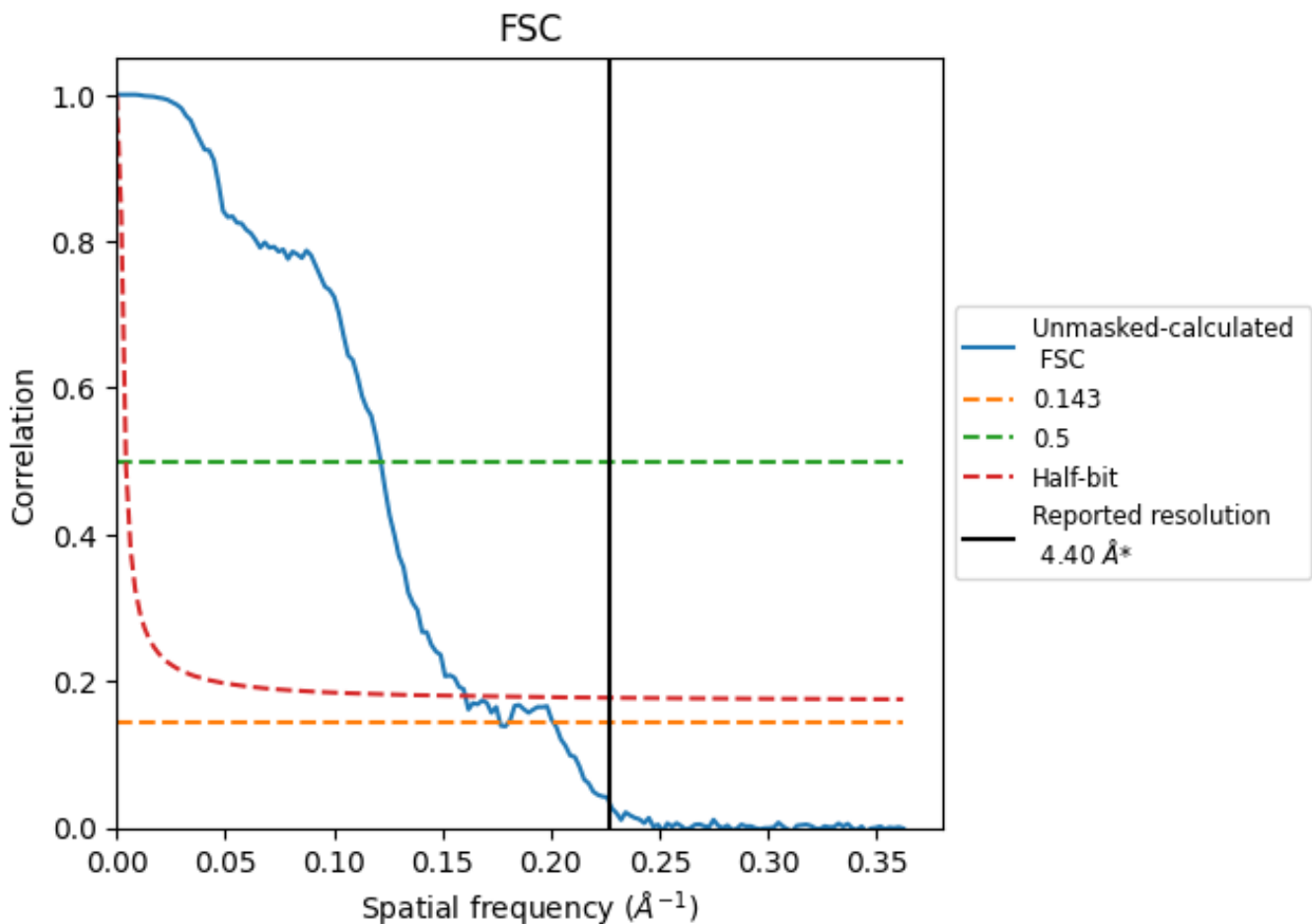


*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.227 Å⁻¹

8.2 Resolution estimates [i](#)

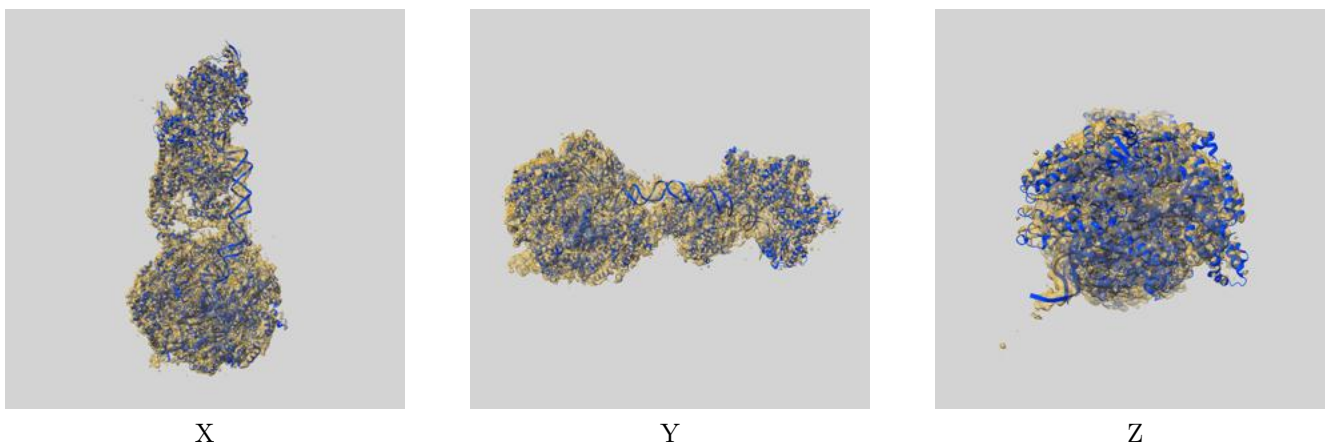
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	5.66	8.22	6.23

*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 5.66 differs from the reported value 4.4 by more than 10 %

9 Map-model fit [i](#)

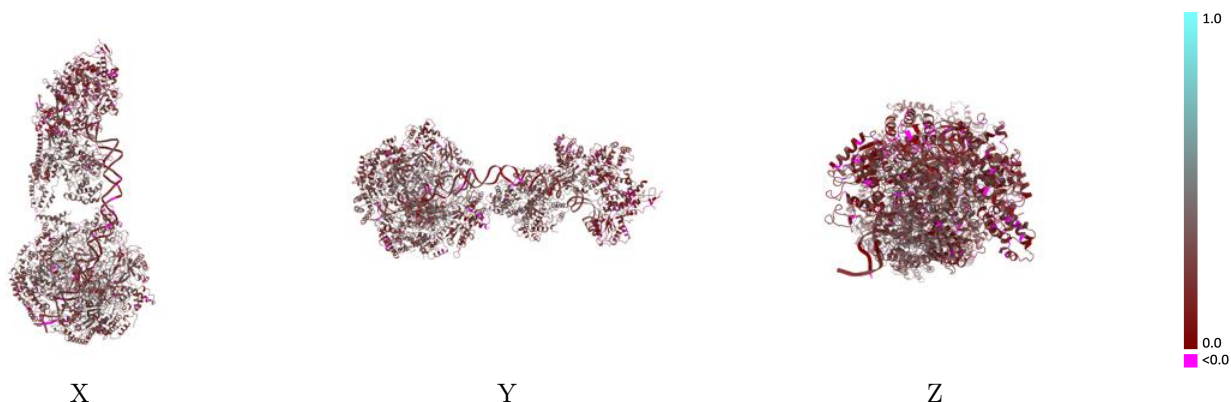
This section contains information regarding the fit between EMDB map EMD-4980 and PDB model 6RQC. Per-residue inclusion information can be found in section 3 on page 10.

9.1 Map-model overlay [i](#)



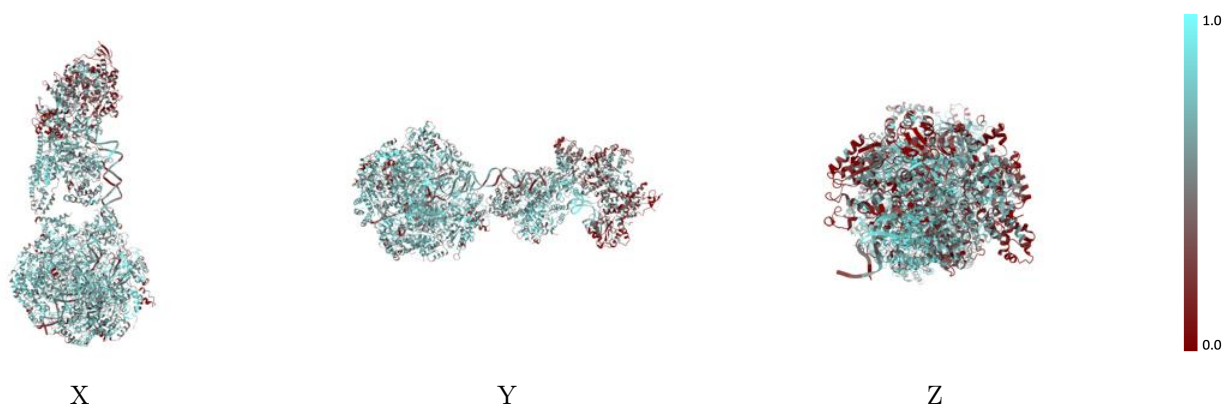
The images above show the 3D surface view of the map at the recommended contour level 0.016 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



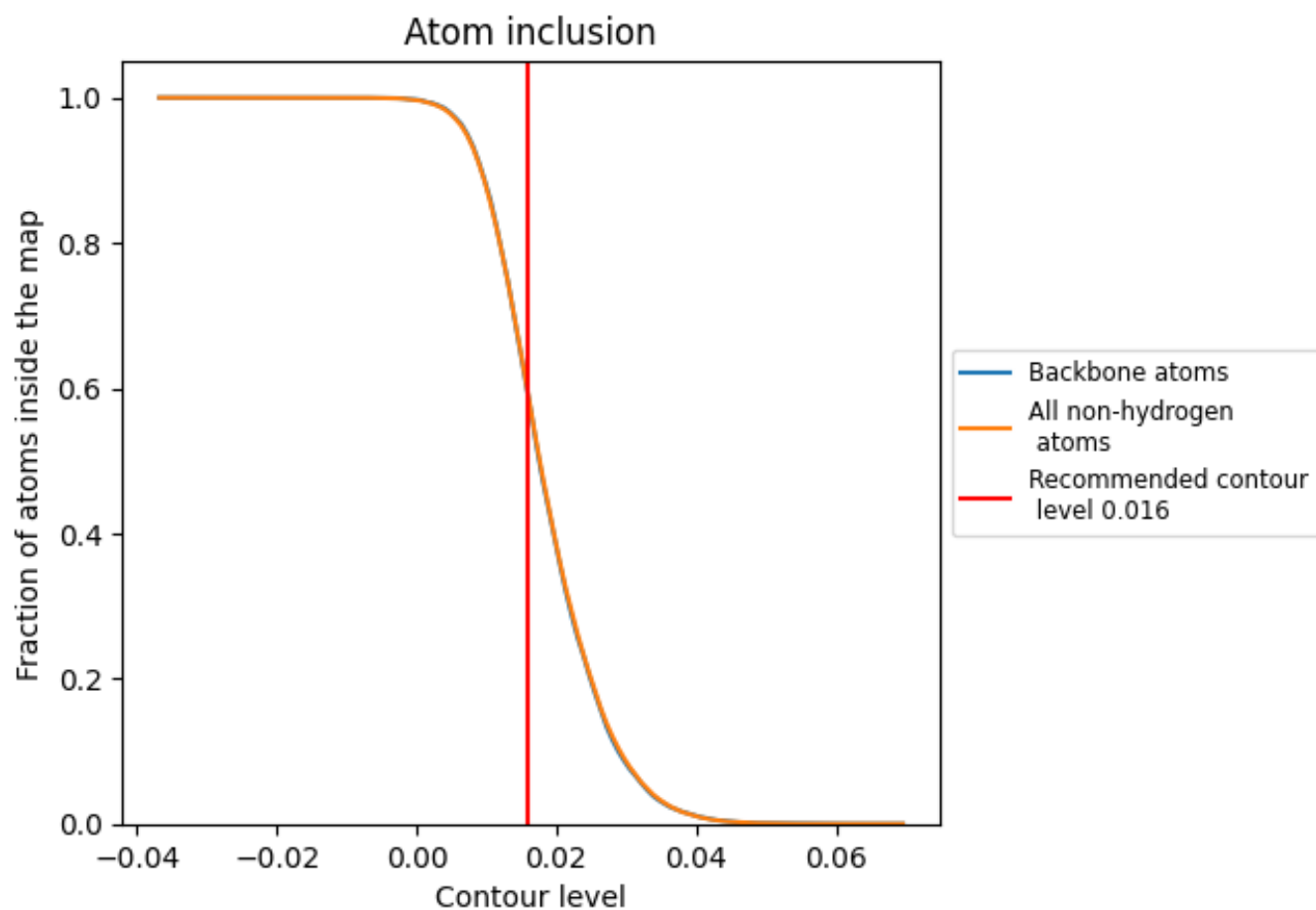
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.016).































9.4 Atom inclusion [i](#)



At the recommended contour level, 59% of all backbone atoms, 59% 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 (0.016) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5893	 0.2720
2	 0.6856	 0.3070
3	 0.6529	 0.3000
4	 0.6589	 0.3020
5	 0.7087	 0.3190
6	 0.6311	 0.2830
7	 0.6334	 0.2890
A	 0.2884	 0.1800
B	 0.7104	 0.3270
C	 0.6366	 0.2840
D	 0.4804	 0.2190
E	 0.4371	 0.2430
F	 0.5779	 0.2840
X	 0.5852	 0.1760
Y	 0.6031	 0.1800

