



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 12:07 AM UTC

PDB ID : 8RIF / pdb_00008rif
EMDB ID : EMD-19186
Title : Cryo-EM structure of the MCM double hexamer loaded onto dsDNA.
Authors : Miller, T.C.R.; Lim, C.T.; Diffley, J.F.X.; Costa, A.
Deposited on : 2023-12-18
Resolution : 2.79 Å(reported)
Based on initial model : 7P30

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
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 EMD 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

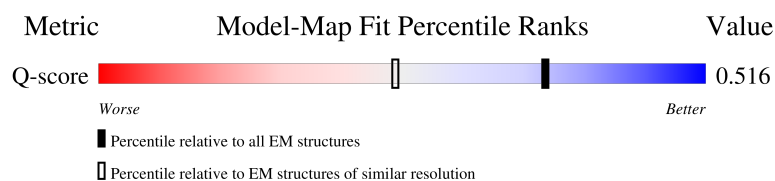
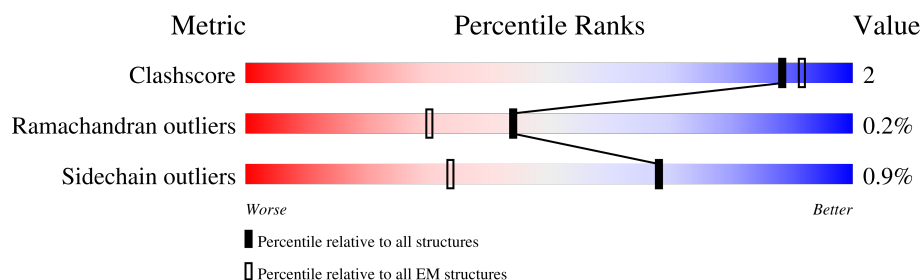
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.79 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.



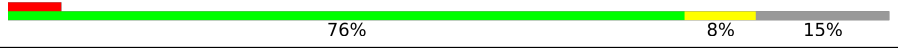
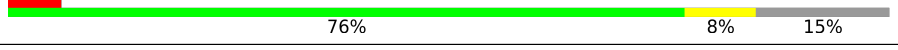
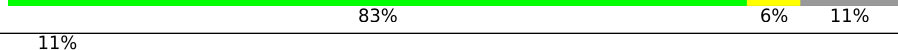
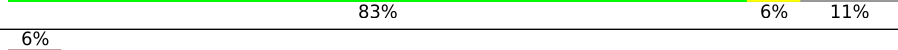
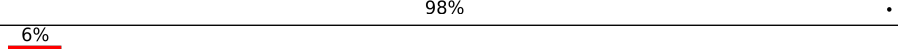
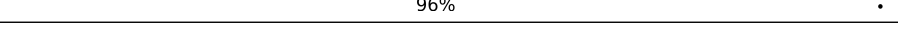
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	10811 (2.29 - 3.29)

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	2	868	
1	A	868	
2	3	1006	
2	B	1006	

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Mol	Chain	Length	Quality of chain
3	4	933	
3	C	933	
4	5	775	
4	D	775	
5	6	1017	
5	E	1017	
6	7	845	
6	F	845	
7	X	53	
8	Y	53	

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 64125 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 DNA replication licensing factor MCM2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	2	624	Total	C	N	O	S	0	0
			4938	3114	878	927	19		
1	A	624	Total	C	N	O	S	0	0
			4938	3114	878	927	19		

- Molecule 2 is a protein called DNA replication licensing factor MCM3.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	614	Total	C	N	O	S	0	0
			4811	3037	858	903	13		
2	B	614	Total	C	N	O	S	0	0
			4811	3037	858	903	13		

There are 70 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

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Chain	Residue	Modelled	Actual	Comment	Reference
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
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
B	-34	MET	-	initiating methionine	UNP P24279
B	-33	LYS	-	expression tag	UNP P24279
B	-32	ARG	-	expression tag	UNP P24279
B	-31	ARG	-	expression tag	UNP P24279
B	-30	TRP	-	expression tag	UNP P24279
B	-29	LYS	-	expression tag	UNP P24279
B	-28	LYS	-	expression tag	UNP P24279
B	-27	ASN	-	expression tag	UNP P24279
B	-26	PHE	-	expression tag	UNP P24279
B	-25	ILE	-	expression tag	UNP P24279
B	-24	ALA	-	expression tag	UNP P24279
B	-23	VAL	-	expression tag	UNP P24279
B	-22	SER	-	expression tag	UNP P24279
B	-21	ALA	-	expression tag	UNP P24279
B	-20	ALA	-	expression tag	UNP P24279
B	-19	ASN	-	expression tag	UNP P24279
B	-18	ARG	-	expression tag	UNP P24279
B	-17	PHE	-	expression tag	UNP P24279
B	-16	LYS	-	expression tag	UNP P24279
B	-15	LYS	-	expression tag	UNP P24279
B	-14	ILE	-	expression tag	UNP P24279
B	-13	SER	-	expression tag	UNP P24279
B	-12	SER	-	expression tag	UNP P24279
B	-11	SER	-	expression tag	UNP P24279

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	GLY	-	expression tag	UNP P24279
B	-9	ALA	-	expression tag	UNP P24279
B	-8	LEU	-	expression tag	UNP P24279
B	-7	GLU	-	expression tag	UNP P24279
B	-6	ASN	-	expression tag	UNP P24279
B	-5	LEU	-	expression tag	UNP P24279
B	-4	TYR	-	expression tag	UNP P24279
B	-3	PHE	-	expression tag	UNP P24279
B	-2	GLN	-	expression tag	UNP P24279
B	-1	GLY	-	expression tag	UNP P24279
B	0	GLU	-	expression tag	UNP P24279

- Molecule 3 is a protein called DNA replication licensing factor MCM4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	645	Total	C	N	O	S	0	0
			5120	3211	886	993	30		
3	C	645	Total	C	N	O	S	0	0
			5120	3211	886	993	30		

- Molecule 4 is a protein called Minichromosome maintenance protein 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	656	Total	C	N	O	S	0	0
			5136	3219	878	1014	25		
4	D	656	Total	C	N	O	S	0	0
			5136	3219	878	1014	25		

- Molecule 5 is a protein called DNA replication licensing factor MCM6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	615	Total	C	N	O	S	0	0
			4874	3077	851	921	25		
5	E	615	Total	C	N	O	S	0	0
			4874	3077	851	921	25		

- Molecule 6 is a protein called DNA replication licensing factor MCM7.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	755	Total	C	N	O	S	0	0
			5976	3771	1031	1142	32		

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Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	755	Total	C	N	O	S	0	0
			5976	3771	1031	1142	32		

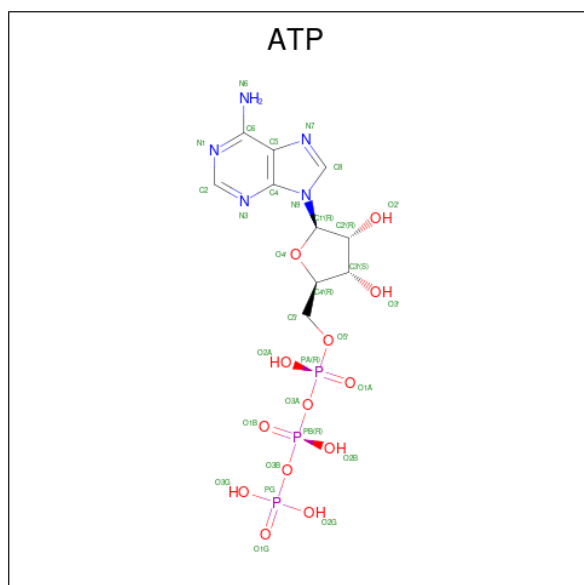
- Molecule 7 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	X	53	Total	C	N	O	P	0	0
			1086	515	199	319	53		

- Molecule 8 is a DNA chain called DNA (53-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	53	Total	C	N	O	P	0	0
			1087	515	202	317	53		

- 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).

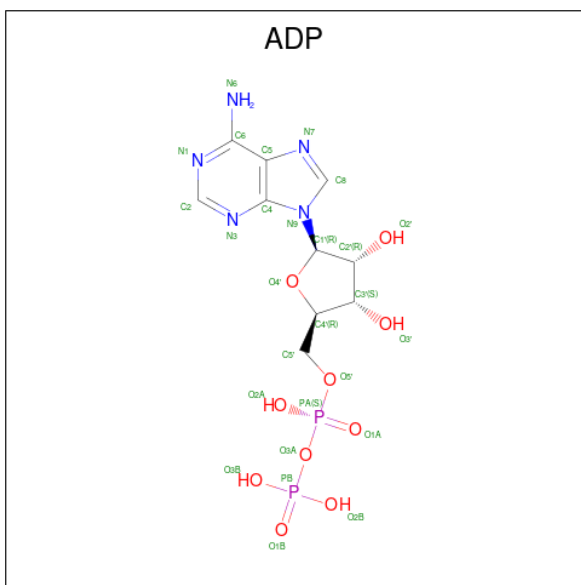


Mol	Chain	Residues	Atoms	AltConf
10	2	1	Total Mg 1 1	0
10	3	1	Total Mg 1 1	0
10	5	1	Total Mg 1 1	0
10	7	1	Total Mg 1 1	0
10	A	1	Total Mg 1 1	0
10	B	1	Total Mg 1 1	0
10	D	1	Total Mg 1 1	0
10	F	1	Total Mg 1 1	0

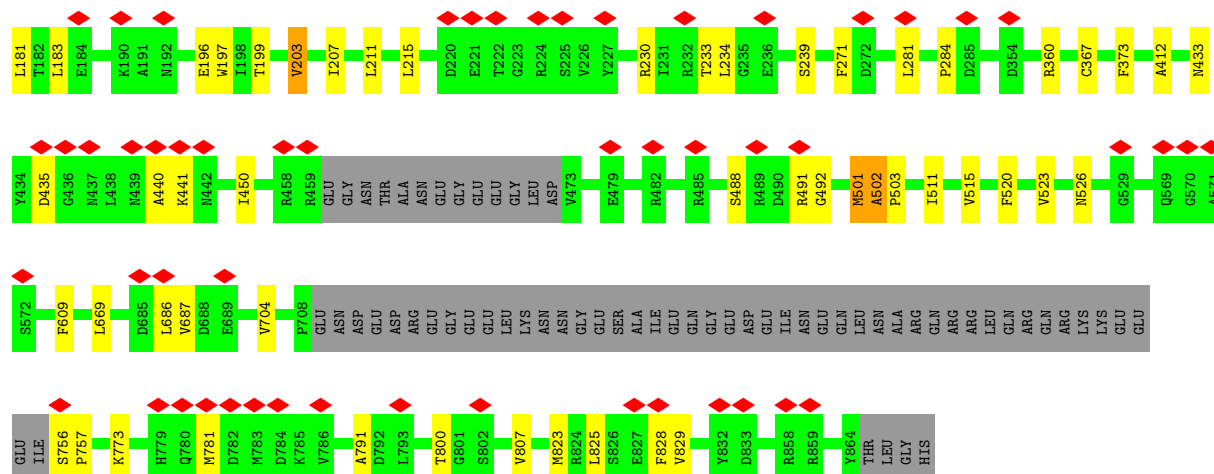
- Molecule 11 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms	AltConf
11	2	1	Total Zn 1 1	0
11	4	1	Total Zn 1 1	0
11	5	1	Total Zn 1 1	0
11	6	1	Total Zn 1 1	0
11	7	1	Total Zn 1 1	0
11	A	1	Total Zn 1 1	0
11	C	1	Total Zn 1 1	0
11	D	1	Total Zn 1 1	0
11	E	1	Total Zn 1 1	0
11	F	1	Total Zn 1 1	0

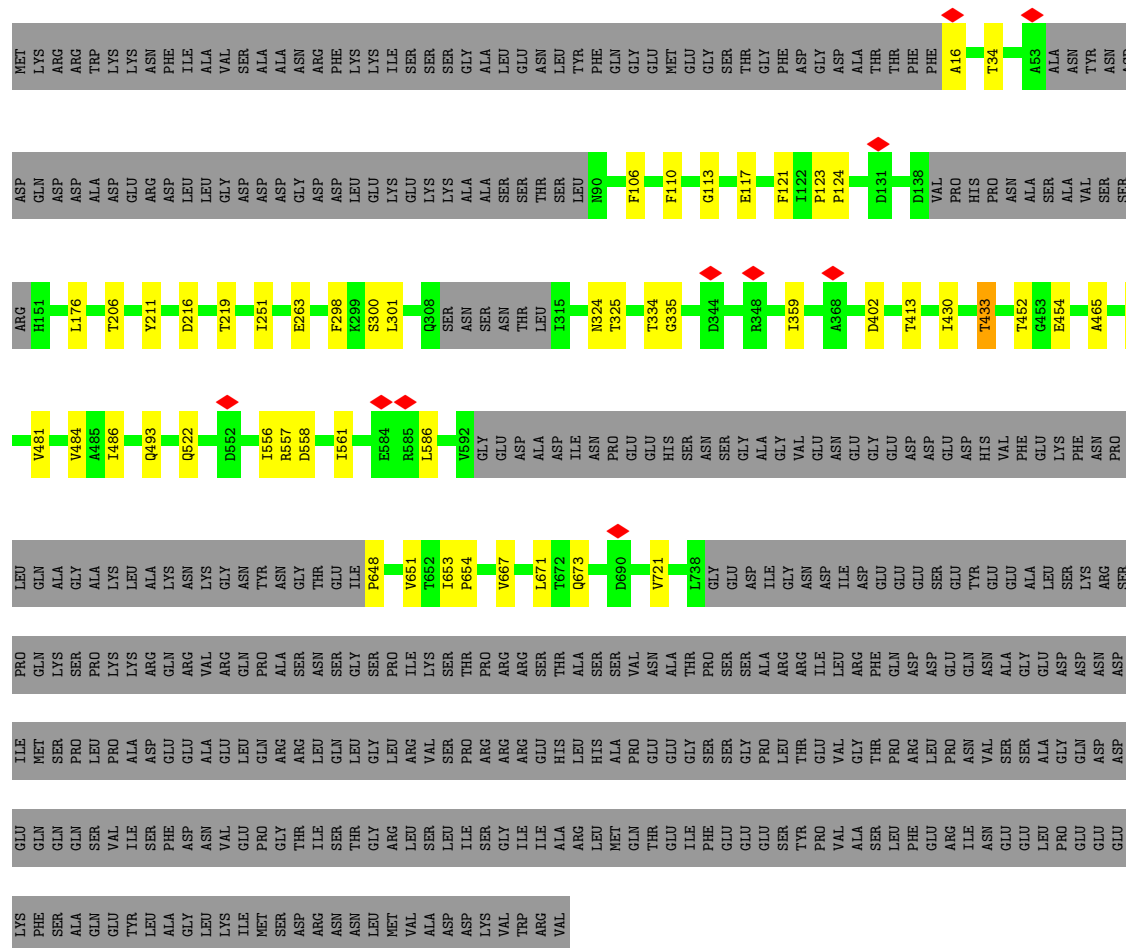
- Molecule 12 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
12	3	1	Total 27	C 10	N 5	O 10	P 2	0
12	5	1	Total 27	C 10	N 5	O 10	P 2	0
12	7	1	Total 27	C 10	N 5	O 10	P 2	0
12	B	1	Total 27	C 10	N 5	O 10	P 2	0
12	D	1	Total 27	C 10	N 5	O 10	P 2	0
12	F	1	Total 27	C 10	N 5	O 10	P 2	0

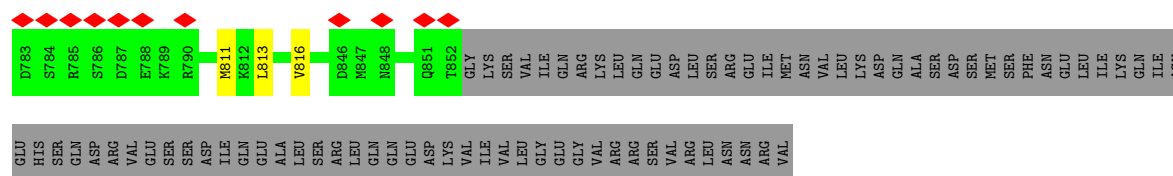


• Molecule 2: DNA replication licensing factor MCM3



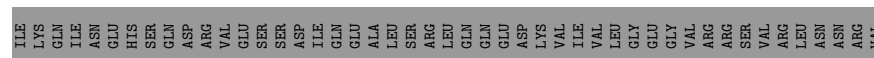
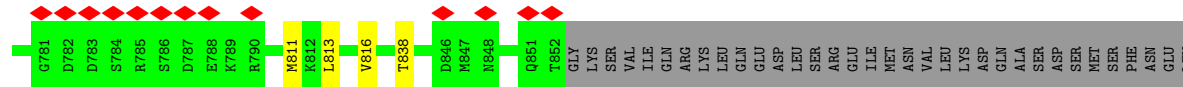
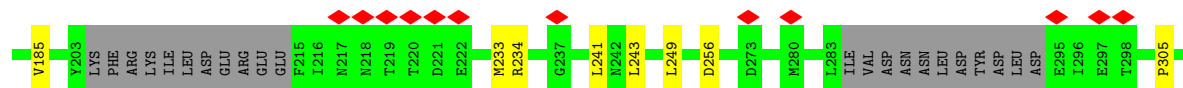
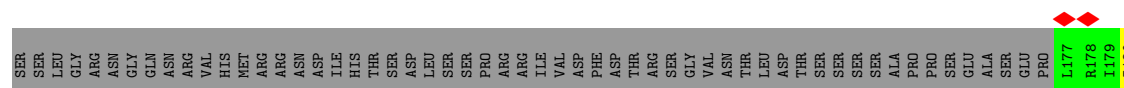
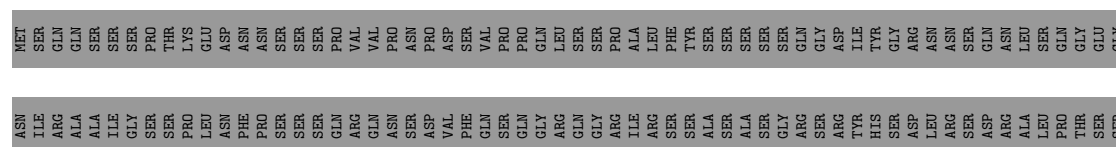
• Molecule 2: DNA replication licensing factor MCM3





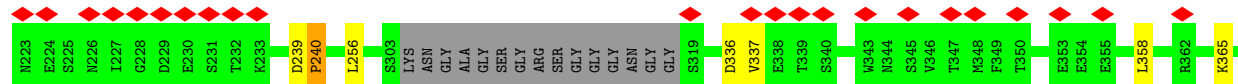
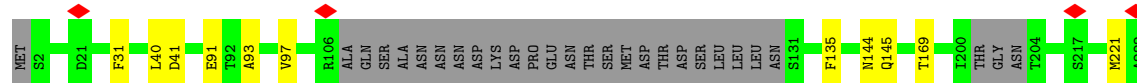
• Molecule 3: DNA replication licensing factor MCM4

Chain C:

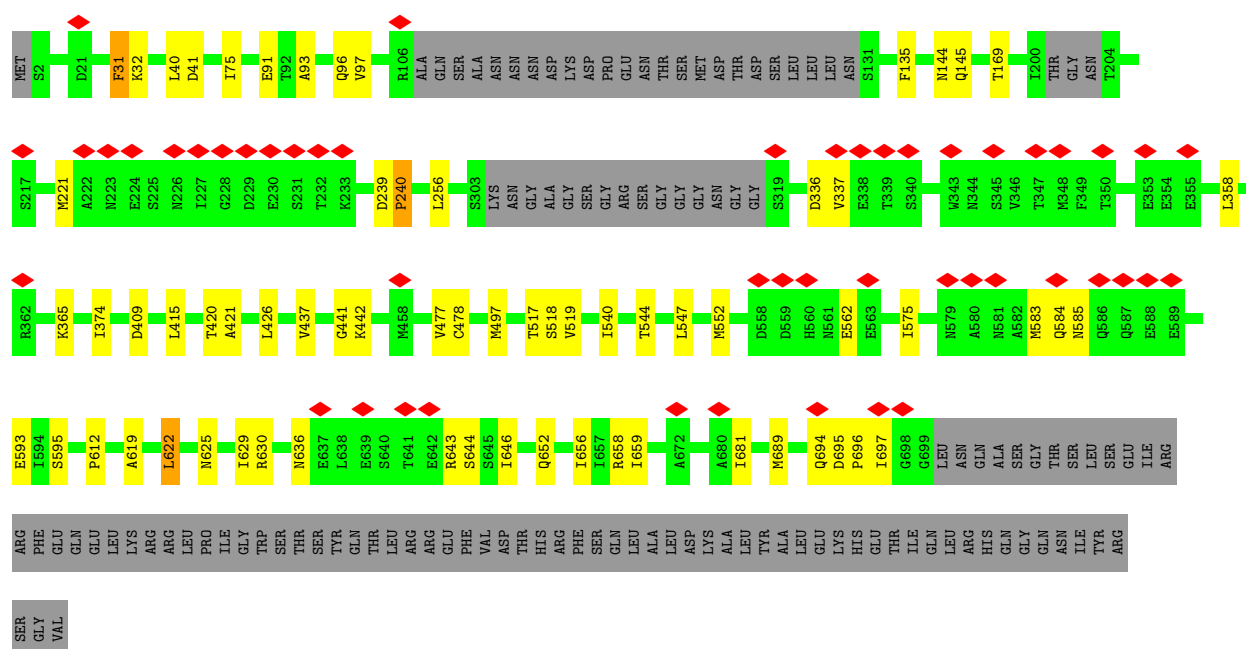


• Molecule 4: Minichromosome maintenance protein 5

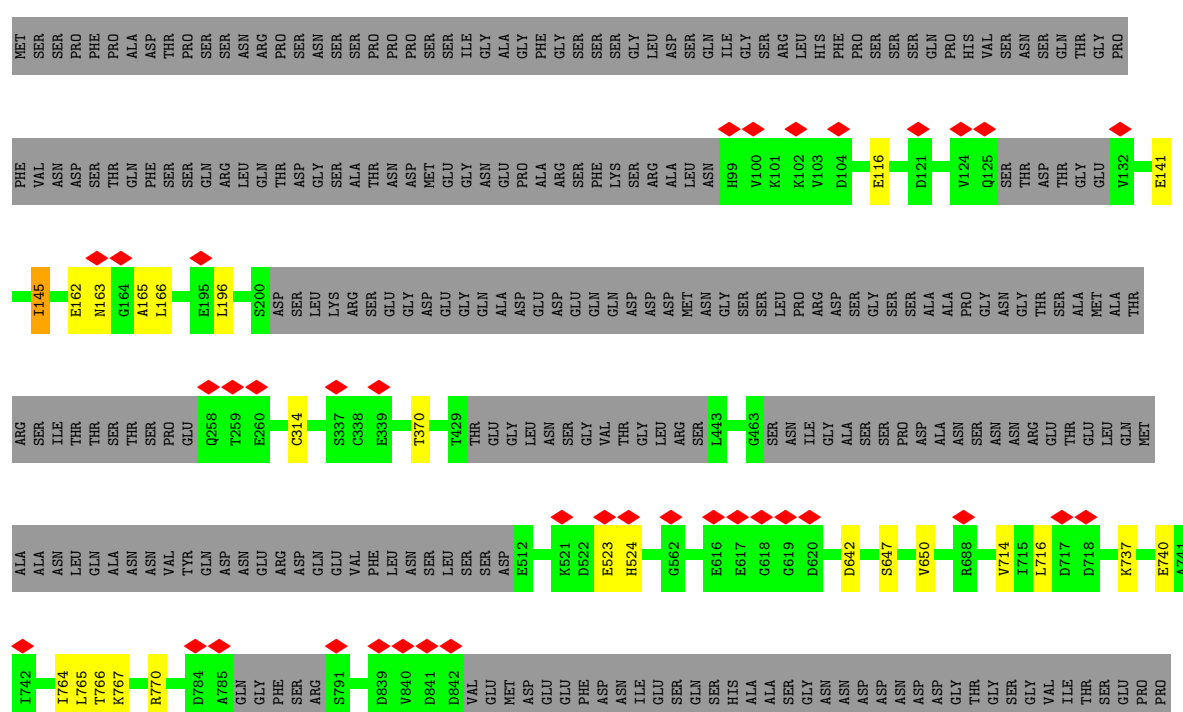
Chain 5:

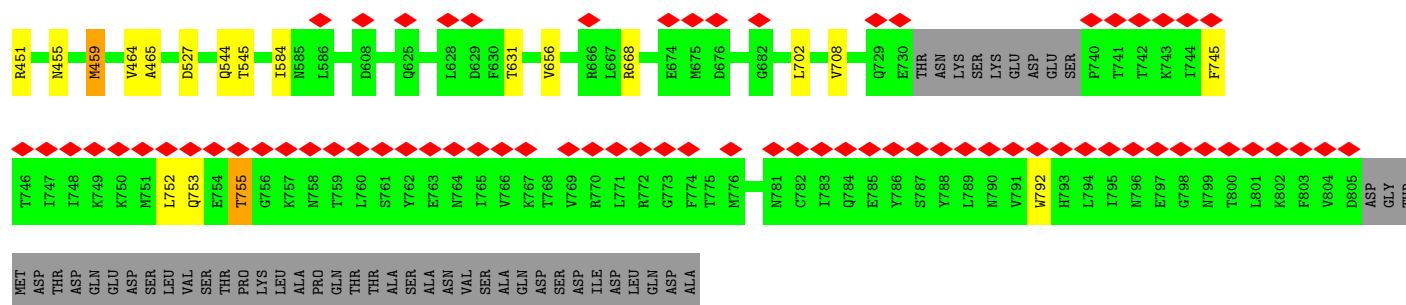


Chain D: 6% 76% 8% 15%

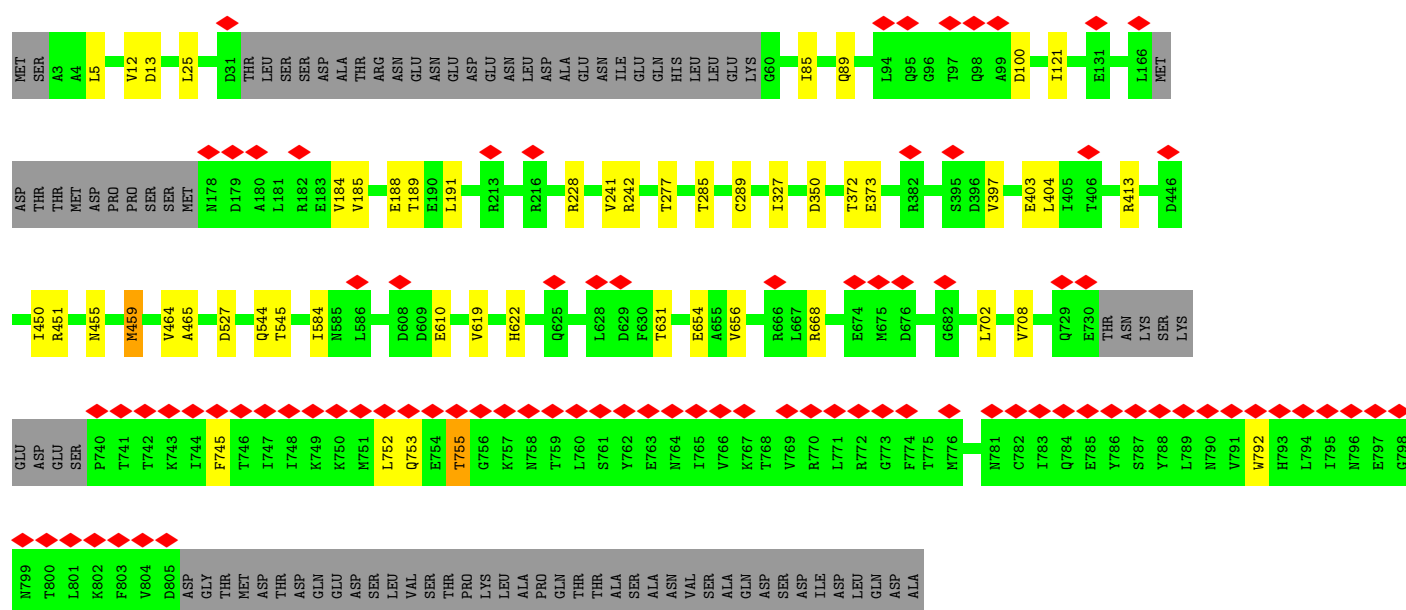
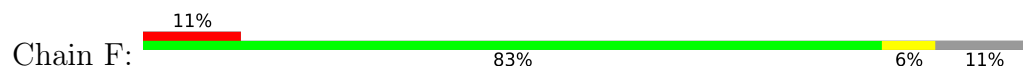


Chain 6: 58% 40%

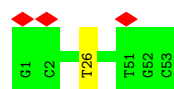




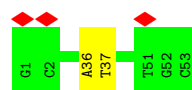
• Molecule 6: DNA replication licensing factor MCM7



• Molecule 7: DNA (53-MER)



• Molecule 8: DNA (53-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	135143	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 ($e^-/\text{\AA}^2$)	51.2	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	4500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.039	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	453.6, 453.6, 453.6	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.08, 1.08, 1.08	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, ADP, MG, ZN

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	2	0.48	1/5025 (0.0%)	0.70	6/6790 (0.1%)
1	A	0.48	1/5025 (0.0%)	0.70	5/6790 (0.1%)
2	3	0.33	2/4894 (0.0%)	0.51	2/6635 (0.0%)
2	B	0.33	2/4894 (0.0%)	0.51	2/6635 (0.0%)
3	4	0.44	1/5192 (0.0%)	0.66	3/7016 (0.0%)
3	C	0.44	1/5192 (0.0%)	0.66	3/7016 (0.0%)
4	5	0.46	3/5210 (0.1%)	0.69	9/7046 (0.1%)
4	D	0.46	3/5210 (0.1%)	0.69	9/7046 (0.1%)
5	6	0.35	0/4952	0.55	2/6679 (0.0%)
5	E	0.35	0/4952	0.55	2/6679 (0.0%)
6	7	0.42	1/6068 (0.0%)	0.68	11/8199 (0.1%)
6	F	0.42	1/6068 (0.0%)	0.68	11/8199 (0.1%)
7	X	0.28	0/1217	0.52	0/1876
8	Y	0.28	0/1219	0.55	0/1879
All	All	0.41	16/65118 (0.0%)	0.63	65/88485 (0.1%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	5	584	GLN	C-O	-7.04	1.14	1.24
4	D	584	GLN	C-O	-7.04	1.14	1.24
4	D	658	ARG	C-O	-6.08	1.16	1.24
4	5	658	ARG	C-O	-6.02	1.16	1.24
2	3	251	ILE	C-O	-5.68	1.18	1.24
2	B	251	ILE	C-O	-5.68	1.18	1.24
3	4	349	CYS	C-O	-5.48	1.17	1.24
3	C	349	CYS	C-O	-5.48	1.17	1.24
2	3	433	THR	C-O	-5.48	1.17	1.24
2	B	433	THR	C-O	-5.48	1.17	1.24
4	5	374	ILE	N-CA	5.29	1.52	1.46
1	2	207	ILE	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	ILE	C-O	-5.29	1.17	1.24
4	D	374	ILE	N-CA	5.29	1.52	1.46
6	7	373	GLU	C-O	-5.20	1.17	1.23
6	F	373	GLU	C-O	-5.19	1.17	1.23

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	7	753	GLN	N-CA-C	-7.16	101.08	110.53
6	F	753	GLN	N-CA-C	-7.15	101.09	110.53
3	4	256	ASP	CA-CB-CG	7.08	119.68	112.60
3	C	256	ASP	CA-CB-CG	7.08	119.68	112.60
4	5	584	GLN	N-CA-C	-6.93	103.85	112.72
4	D	584	GLN	N-CA-C	-6.93	103.85	112.72
4	5	31	PHE	CA-CB-CG	6.55	120.35	113.80
4	D	31	PHE	CA-CB-CG	6.55	120.35	113.80
4	D	656	ILE	N-CA-C	-6.43	104.24	110.42
4	5	656	ILE	N-CA-C	-6.40	104.27	110.42
3	4	555	GLY	CA-C-O	-6.30	116.53	122.39
3	C	555	GLY	CA-C-O	-6.26	116.56	122.39
6	F	397	VAL	N-CA-C	-6.23	104.42	110.72
6	7	397	VAL	N-CA-C	-6.22	104.44	110.72
6	F	289	CYS	N-CA-C	-6.21	104.58	111.36
6	7	289	CYS	N-CA-C	-6.20	104.60	111.36
6	F	527	ASP	CA-CB-CG	6.18	118.78	112.60
6	7	527	ASP	CA-CB-CG	6.16	118.76	112.60
1	2	781	MET	N-CA-C	-6.14	104.58	111.28
1	A	781	MET	N-CA-C	-6.14	104.58	111.28
1	2	271	PHE	CA-CB-CG	6.09	119.89	113.80
1	A	271	PHE	CA-CB-CG	6.08	119.89	113.80
6	F	404	LEU	N-CA-C	-6.00	104.74	111.28
6	7	404	LEU	N-CA-C	-5.97	104.78	111.28
1	2	373	PHE	CA-CB-CG	5.94	119.74	113.80
1	A	373	PHE	CA-CB-CG	5.94	119.74	113.80
6	7	668	ARG	N-CA-C	-5.84	105.00	111.36
6	F	668	ARG	N-CA-C	-5.83	105.01	111.36
5	E	314	CYS	CA-C-O	-5.79	115.11	121.89
5	6	314	CYS	CA-C-O	-5.77	115.14	121.89
6	7	459	MET	CA-C-O	-5.76	114.60	121.11
6	F	459	MET	CA-C-O	-5.76	114.60	121.11
4	5	409	ASP	CA-C-O	-5.72	115.11	121.23
4	D	409	ASP	CA-C-O	-5.71	115.12	121.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	5	595	SER	CA-C-O	-5.64	114.45	121.50
4	D	595	SER	CA-C-O	-5.64	114.45	121.50
1	A	501	MET	CA-C-O	-5.60	116.13	122.01
4	5	612	PRO	O-C-N	-5.57	116.87	123.10
4	D	612	PRO	O-C-N	-5.57	116.87	123.10
1	2	501	MET	CA-C-O	-5.56	116.17	122.01
2	3	110	PHE	N-CA-C	-5.49	105.38	111.36
2	B	110	PHE	N-CA-C	-5.49	105.38	111.36
4	5	575	ILE	N-CA-C	-5.46	105.18	110.42
4	D	575	ILE	N-CA-C	-5.46	105.18	110.42
5	6	116	GLU	CA-C-O	-5.43	115.12	120.82
5	E	116	GLU	CA-C-O	-5.43	115.12	120.82
6	7	752	LEU	N-CA-C	-5.31	105.41	111.14
3	C	552	PHE	CA-CB-CG	5.29	119.09	113.80
6	F	752	LEU	N-CA-C	-5.29	105.42	111.14
3	4	552	PHE	CA-CB-CG	5.26	119.06	113.80
6	7	451	ARG	N-CA-C	5.25	118.84	112.23
6	F	451	ARG	N-CA-C	5.25	118.84	112.23
6	7	450	ILE	N-CA-C	-5.25	100.93	108.48
6	F	450	ILE	N-CA-C	-5.25	100.93	108.48
4	5	240	PRO	N-CA-CB	-5.23	97.75	103.25
4	D	240	PRO	N-CA-CB	-5.23	97.76	103.25
1	2	284	PRO	CA-C-O	-5.23	115.29	121.67
4	D	583	MET	N-CA-C	-5.22	106.30	113.30
2	B	413	THR	CB-CA-C	5.21	119.40	111.02
1	A	284	PRO	CA-C-O	-5.20	115.33	121.67
2	3	413	THR	CB-CA-C	5.19	119.37	111.02
4	5	583	MET	N-CA-C	-5.18	106.36	113.30
6	7	455	ASN	CA-C-O	-5.15	114.77	120.38
6	F	455	ASN	CA-C-O	-5.15	114.77	120.38
1	2	503	PRO	N-CA-CB	-5.02	97.98	103.25

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	2	4938	0	4997	27	0
1	A	4938	0	4997	27	0
2	3	4811	0	4893	26	0
2	B	4811	0	4893	26	0
3	4	5120	0	5187	15	0
3	C	5120	0	5187	17	0
4	5	5136	0	5177	27	0
4	D	5136	0	5177	29	0
5	6	4874	0	4918	14	0
5	E	4874	0	4918	14	0
6	7	5976	0	6057	19	0
6	F	5976	0	6057	21	0
7	X	1086	0	596	1	0
8	Y	1087	0	595	1	0
9	2	31	0	12	0	0
9	A	31	0	12	0	0
10	2	1	0	0	0	0
10	3	1	0	0	0	0
10	5	1	0	0	0	0
10	7	1	0	0	0	0
10	A	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
10	F	1	0	0	0	0
11	2	1	0	0	0	0
11	4	1	0	0	0	0
11	5	1	0	0	0	0
11	6	1	0	0	0	0
11	7	1	0	0	0	0
11	A	1	0	0	0	0
11	C	1	0	0	0	0
11	D	1	0	0	0	0
11	E	1	0	0	0	0
11	F	1	0	0	0	0
12	3	27	0	12	0	0
12	5	27	0	12	0	0
12	7	27	0	12	0	0
12	B	27	0	12	0	0
12	D	27	0	12	0	0
12	F	27	0	12	0	0
All	All	64125	0	63745	247	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 (247) 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)
1:2:501:MET:O	1:2:502:ALA:C	2.41	0.63
1:A:501:MET:O	1:A:502:ALA:C	2.41	0.62
3:C:729:LEU:O	3:C:730:GLU:C	2.50	0.55
3:4:729:LEU:O	3:4:730:GLU:C	2.50	0.53
5:6:165:ALA:O	5:6:166:LEU:C	2.55	0.49
6:F:654:GLU:OE1	6:F:654:GLU:N	2.38	0.48
5:6:141:GLU:O	5:6:145:ILE:HD12	2.13	0.48
5:E:165:ALA:O	5:E:166:LEU:C	2.55	0.48
5:E:141:GLU:O	5:E:145:ILE:HD12	2.13	0.48
3:4:243:LEU:O	3:4:305:PRO:HA	2.14	0.48
3:C:519:TYR:HD1	3:C:811:MET:HE1	1.79	0.48
4:D:441:GLY:O	4:D:442:LYS:HB2	2.14	0.48
2:B:113:GLY:O	2:B:117:GLU:N	2.37	0.47
3:4:519:TYR:HD1	3:4:811:MET:HE1	1.79	0.47
2:3:113:GLY:O	2:3:117:GLU:N	2.37	0.47
6:7:459:MET:SD	6:7:584:ILE:HD13	2.55	0.47
4:D:497:MET:HG2	4:D:519:VAL:HG21	1.97	0.47
5:6:766:THR:HG22	5:6:767:LYS:N	2.30	0.47
6:F:459:MET:SD	6:F:584:ILE:HD13	2.55	0.47
3:C:243:LEU:O	3:C:305:PRO:HA	2.14	0.47
1:2:234:LEU:HD11	1:2:239:SER:O	2.15	0.47
2:3:556:ILE:HG23	2:3:557:ARG:N	2.30	0.47
2:B:556:ILE:HG23	2:B:557:ARG:N	2.30	0.47
3:C:452:VAL:CG1	6:F:277:THR:HB	2.45	0.47
6:F:745:PHE:CE1	6:F:792:TRP:HZ3	2.33	0.47
1:2:704:VAL:HG21	5:6:770:ARG:HE	1.80	0.47
4:5:497:MET:HG2	4:5:519:VAL:HG21	1.97	0.47
1:2:523:VAL:HG23	1:2:523:VAL:O	2.14	0.47
6:7:631:THR:O	6:7:631:THR:HG23	2.15	0.47
2:B:433:THR:O	2:B:433:THR:HG23	2.15	0.47
2:B:481:VAL:O	2:B:484:VAL:HG22	2.15	0.47
3:4:452:VAL:CG1	6:7:277:THR:HB	2.45	0.46
4:5:441:GLY:O	4:5:442:LYS:HB2	2.14	0.46
1:A:704:VAL:HG21	5:E:770:ARG:HE	1.80	0.46
3:C:233:MET:HE1	3:C:241:LEU:HB2	1.97	0.46
5:6:647:SER:O	5:6:650:VAL:HG22	2.16	0.46
1:A:234:LEU:HD11	1:A:239:SER:O	2.15	0.46
4:5:91:GLU:OE1	4:5:135:PHE:O	2.34	0.46
6:7:745:PHE:CE1	6:7:792:TRP:HZ3	2.33	0.46
3:4:233:MET:HE1	3:4:241:LEU:HB2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:523:VAL:HG23	1:A:523:VAL:O	2.14	0.46
5:E:647:SER:O	5:E:650:VAL:HG22	2.16	0.46
5:E:766:THR:HG22	5:E:767:LYS:N	2.30	0.46
2:3:433:THR:HG23	2:3:433:THR:O	2.15	0.46
6:7:656:VAL:HG11	6:7:708:VAL:O	2.16	0.46
5:E:714:VAL:HG12	5:E:716:LEU:CD2	2.46	0.46
6:F:656:VAL:HG11	6:F:708:VAL:O	2.16	0.45
1:2:199:THR:O	1:2:199:THR:HG22	2.16	0.45
5:6:714:VAL:HG12	5:6:716:LEU:CD2	2.46	0.45
2:3:478:MET:HE1	2:3:486:ILE:CD1	2.47	0.45
1:A:211:LEU:O	1:A:215:LEU:HD23	2.17	0.45
4:D:420:THR:O	4:D:421:ALA:HB3	2.16	0.45
2:B:478:MET:HE1	2:B:486:ILE:CD1	2.47	0.45
6:F:85:ILE:HG22	6:F:89:GLN:OE1	2.17	0.45
1:2:807:VAL:HG12	1:2:807:VAL:O	2.16	0.45
2:3:481:VAL:O	2:3:484:VAL:HG22	2.15	0.45
2:3:211:TYR:OH	2:B:16:ALA:HB3	2.17	0.45
1:A:234:LEU:HD12	1:A:239:SER:OG	2.17	0.45
1:2:440:ALA:O	1:2:441:LYS:C	2.60	0.45
6:7:85:ILE:HG22	6:7:89:GLN:OE1	2.17	0.45
5:E:370:THR:HG23	5:E:370:THR:O	2.16	0.45
6:F:413:ARG:NH2	6:F:631:THR:HG21	2.31	0.45
1:2:488:SER:HB3	1:2:825:LEU:HD12	1.98	0.45
4:5:420:THR:O	4:5:421:ALA:HB3	2.16	0.45
1:A:807:VAL:O	1:A:807:VAL:HG12	2.16	0.45
2:B:653:ILE:N	2:B:654:PRO:HD2	2.32	0.45
4:D:91:GLU:OE1	4:D:135:PHE:O	2.34	0.45
6:F:631:THR:HG23	6:F:631:THR:O	2.15	0.45
1:A:440:ALA:O	1:A:441:LYS:C	2.60	0.45
4:D:644:SER:OG	4:D:697:ILE:HD11	2.17	0.45
1:2:433:ASN:OD1	1:2:450:ILE:HG23	2.16	0.44
4:5:415:LEU:HD11	4:5:540:ILE:CG2	2.47	0.44
6:7:413:ARG:NH2	6:7:631:THR:HG21	2.32	0.44
1:A:199:THR:HG22	1:A:199:THR:O	2.16	0.44
1:2:211:LEU:O	1:2:215:LEU:HD23	2.17	0.44
1:2:234:LEU:HD12	1:2:239:SER:OG	2.17	0.44
2:B:176:LEU:HD23	2:B:298:PHE:CD2	2.53	0.44
6:7:12:VAL:HG12	6:7:13:ASP:N	2.33	0.44
1:A:488:SER:HB3	1:A:825:LEU:HD12	1.98	0.44
2:3:16:ALA:HB3	2:B:211:TYR:OH	2.17	0.44
4:D:437:VAL:HG13	4:D:477:VAL:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:544:THR:O	4:D:544:THR:HG22	2.18	0.44
4:5:40:LEU:O	4:5:41:ASP:HB2	2.17	0.44
4:5:625:ASN:ND2	4:5:681:ILE:HD12	2.33	0.44
1:A:433:ASN:OD1	1:A:450:ILE:HG23	2.16	0.44
4:5:437:VAL:HG13	4:5:477:VAL:HG23	2.00	0.44
5:6:766:THR:HG22	5:6:767:LYS:H	1.82	0.44
2:B:452:THR:HG23	2:B:454:GLU:H	1.83	0.44
2:3:206:THR:O	2:3:206:THR:HG22	2.18	0.44
4:5:544:THR:HG22	4:5:544:THR:O	2.18	0.44
4:D:40:LEU:O	4:D:41:ASP:HB2	2.17	0.44
4:D:625:ASN:ND2	4:D:681:ILE:HD12	2.33	0.44
5:E:766:THR:HG22	5:E:767:LYS:H	1.82	0.44
2:3:176:LEU:HD23	2:3:298:PHE:CD2	2.52	0.44
2:3:653:ILE:N	2:3:654:PRO:HD2	2.32	0.44
3:4:435:VAL:HG13	3:4:463:VAL:HG13	2.00	0.44
4:5:547:LEU:HD13	4:5:646:ILE:CD1	2.48	0.44
5:6:196:LEU:HD23	5:6:196:LEU:O	2.18	0.44
6:7:464:VAL:O	6:7:465:ALA:HB3	2.18	0.44
6:F:12:VAL:HG12	6:F:13:ASP:N	2.33	0.44
7:X:26:DT:OP1	1:A:360:ARG:NH2	2.50	0.43
2:B:324:ASN:OD1	2:B:325:THR:N	2.51	0.43
3:C:435:VAL:HG13	3:C:463:VAL:HG13	2.00	0.43
4:5:644:SER:OG	4:5:697:ILE:HD11	2.17	0.43
1:A:197:TRP:O	1:A:203:VAL:HG21	2.18	0.43
3:C:816:VAL:O	3:C:816:VAL:HG23	2.18	0.43
5:E:196:LEU:HD23	5:E:196:LEU:O	2.18	0.43
2:3:216:ASP:OD1	2:3:219:THR:HG23	2.18	0.43
3:4:435:VAL:HG11	3:4:463:VAL:HG22	2.00	0.43
3:4:758:ILE:HD13	3:4:813:LEU:HA	2.01	0.43
5:6:370:THR:O	5:6:370:THR:HG23	2.16	0.43
2:3:452:THR:HG23	2:3:454:GLU:H	1.83	0.43
3:C:180:ILE:HD12	3:C:185:VAL:O	2.18	0.43
4:D:415:LEU:HD11	4:D:540:ILE:CG2	2.47	0.43
3:4:180:ILE:HD12	3:4:185:VAL:O	2.18	0.43
4:5:552:MET:HE1	4:5:659:ILE:HD11	2.00	0.43
2:B:206:THR:O	2:B:206:THR:HG22	2.18	0.43
1:2:197:TRP:O	1:2:203:VAL:HG21	2.18	0.43
1:2:791:ALA:HB1	4:5:562:GLU:OE2	2.18	0.43
1:A:791:ALA:HB1	4:D:562:GLU:OE2	2.18	0.43
6:F:464:VAL:O	6:F:465:ALA:HB3	2.18	0.43
6:F:544:GLN:O	6:F:545:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:2:828:PHE:O	1:2:829:VAL:C	2.61	0.43
6:7:372:THR:HG22	4:D:221:MET:HE1	2.01	0.43
4:D:547:LEU:HD13	4:D:646:ILE:CD1	2.48	0.43
2:3:558:ASP:OD1	4:5:630:ARG:HD3	2.19	0.43
1:A:511:ILE:O	1:A:515:VAL:HG23	2.19	0.43
1:2:686:LEU:HD23	1:2:686:LEU:H	1.84	0.43
1:A:686:LEU:H	1:A:686:LEU:HD23	1.84	0.43
2:B:216:ASP:OD1	2:B:219:THR:HG23	2.18	0.43
3:C:758:ILE:HD13	3:C:813:LEU:HA	2.01	0.43
4:D:32:LYS:NZ	4:D:96:GLN:OE1	2.45	0.43
1:A:687:VAL:HG13	1:A:687:VAL:O	2.19	0.42
4:D:552:MET:HE1	4:D:659:ILE:HD11	2.00	0.42
5:E:737:LYS:HE2	5:E:740:GLU:O	2.20	0.42
2:3:324:ASN:OD1	2:3:325:THR:N	2.51	0.42
3:C:180:ILE:HD12	3:C:180:ILE:H	1.85	0.42
4:5:694:GLN:NE2	4:5:696:PRO:HD2	2.34	0.42
5:6:764:ILE:HG22	5:6:765:LEU:N	2.35	0.42
1:A:609:PHE:HD2	1:A:669:LEU:HD11	1.84	0.42
3:C:435:VAL:HG11	3:C:463:VAL:HG22	2.00	0.42
3:C:696:PRO:N	3:C:697:PRO:CD	2.83	0.42
6:7:544:GLN:O	6:7:545:THR:HG23	2.19	0.42
1:2:687:VAL:HG13	1:2:687:VAL:O	2.19	0.42
1:A:828:PHE:O	1:A:829:VAL:C	2.61	0.42
4:5:169:THR:HG22	4:5:256:LEU:HD22	2.01	0.42
1:A:773:LYS:O	1:A:773:LYS:HG2	2.19	0.42
2:B:558:ASP:OD1	4:D:630:ARG:HD3	2.19	0.42
3:C:694:LEU:HD22	3:C:698:LEU:HD23	2.01	0.42
6:F:185:VAL:O	6:F:189:THR:HG22	2.19	0.42
6:F:241:VAL:O	6:F:350:ASP:HA	2.20	0.42
1:2:281:LEU:HD23	1:2:281:LEU:O	2.20	0.42
3:4:180:ILE:HD12	3:4:180:ILE:H	1.85	0.42
2:B:300:SER:C	2:B:301:LEU:HD22	2.45	0.42
4:D:169:THR:HG22	4:D:256:LEU:HD22	2.01	0.42
5:E:523:GLU:OE2	5:E:524:HIS:CE1	2.73	0.42
1:2:609:PHE:HD2	1:2:669:LEU:HD11	1.84	0.42
2:3:430:ILE:HD12	2:3:465:ALA:HB2	2.02	0.42
4:5:93:ALA:O	4:5:97:VAL:HG23	2.20	0.42
4:5:695:ASP:CB	4:5:696:PRO:CD	2.98	0.42
2:B:522:GLN:OE1	4:D:643:ARG:NE	2.53	0.42
3:C:349:CYS:HB2	3:C:382:MET:HE1	2.02	0.42
1:2:511:ILE:O	1:2:515:VAL:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:5:221:MET:HE1	6:F:372:THR:HG22	2.02	0.42
4:D:695:ASP:HB2	4:D:696:PRO:CD	2.50	0.42
1:2:183:LEU:C	1:2:183:LEU:HD23	2.45	0.41
3:4:816:VAL:O	3:4:816:VAL:HG23	2.18	0.41
4:5:629:ILE:HG23	4:5:689:MET:HE3	2.02	0.41
1:A:230:ARG:HA	1:A:233:THR:HG22	2.02	0.41
4:D:426:LEU:HD22	4:D:478:CYS:HB3	2.02	0.41
4:D:695:ASP:CB	4:D:696:PRO:CD	2.98	0.41
5:E:162:GLU:O	5:E:163:ASN:C	2.63	0.41
1:2:230:ARG:HA	1:2:233:THR:HG22	2.02	0.41
2:3:263:GLU:CG	2:3:586:LEU:HD11	2.50	0.41
2:3:402:ASP:OD2	2:3:493:GLN:NE2	2.53	0.41
2:3:522:GLN:OE1	4:5:643:ARG:NE	2.53	0.41
1:A:281:LEU:HD23	1:A:281:LEU:O	2.20	0.41
4:D:93:ALA:O	4:D:97:VAL:HG23	2.20	0.41
4:D:517:THR:HG22	4:D:518:SER:N	2.35	0.41
1:2:520:PHE:CE2	1:2:823:MET:HG2	2.55	0.41
1:2:773:LYS:O	1:2:773:LYS:HG2	2.19	0.41
2:3:673:GLN:O	2:3:673:GLN:HG3	2.20	0.41
1:A:183:LEU:C	1:A:183:LEU:HD23	2.45	0.41
1:A:800:THR:O	1:A:800:THR:HG22	2.20	0.41
6:F:184:VAL:O	6:F:188:GLU:HG2	2.20	0.41
5:6:737:LYS:HE2	5:6:740:GLU:O	2.19	0.41
6:7:185:VAL:O	6:7:189:THR:HG22	2.19	0.41
2:B:557:ARG:O	2:B:561:ILE:HG22	2.20	0.41
6:F:619:VAL:O	6:F:622:HIS:O	2.39	0.41
2:3:300:SER:C	2:3:301:LEU:HD22	2.45	0.41
4:5:144:ASN:OD1	4:5:145:GLN:N	2.54	0.41
6:7:25:LEU:HD13	6:7:121:ILE:HG12	2.02	0.41
6:F:25:LEU:HD13	6:F:121:ILE:HG12	2.03	0.41
2:3:334:THR:HG22	2:3:335:GLY:N	2.36	0.41
3:4:696:PRO:N	3:4:697:PRO:CD	2.83	0.41
4:5:426:LEU:HD22	4:5:478:CYS:HB3	2.02	0.41
4:5:619:ALA:HA	4:5:622:LEU:HD12	2.02	0.41
6:7:228:ARG:NH2	6:7:327:ILE:O	2.54	0.41
5:E:764:ILE:HG22	5:E:765:LEU:N	2.34	0.41
2:3:557:ARG:O	2:3:561:ILE:HG22	2.20	0.41
3:4:694:LEU:HD22	3:4:698:LEU:HD23	2.01	0.41
1:A:520:PHE:CE2	1:A:823:MET:HG2	2.55	0.41
2:B:263:GLU:CG	2:B:586:LEU:HD11	2.50	0.41
4:D:144:ASN:OD1	4:D:145:GLN:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:694:GLN:NE2	4:D:696:PRO:HD2	2.34	0.41
4:5:336:ASP:O	4:5:337:VAL:HG23	2.21	0.41
2:B:334:THR:HG22	2:B:335:GLY:N	2.36	0.41
2:B:671:LEU:HD23	2:B:721:VAL:HG11	2.03	0.41
3:C:374:ILE:HD12	3:C:374:ILE:H	1.86	0.41
1:2:800:THR:HG22	1:2:800:THR:O	2.20	0.41
2:3:34:THR:HG21	2:3:106:PHE:CD2	2.56	0.41
3:4:374:ILE:H	3:4:374:ILE:HD12	1.86	0.41
4:5:517:THR:HG22	4:5:518:SER:N	2.35	0.41
5:6:162:GLU:O	5:6:163:ASN:C	2.63	0.41
6:7:184:VAL:O	6:7:188:GLU:HG2	2.21	0.41
6:7:241:VAL:HG12	6:7:242:ARG:N	2.36	0.41
6:7:241:VAL:O	6:7:350:ASP:HA	2.20	0.41
8:Y:36:DA:C8	8:Y:37:DT:H71	2.56	0.41
1:A:491:ARG:HE	1:A:492:GLY:H	1.69	0.41
1:A:756:SER:N	1:A:757:PRO:CD	2.84	0.41
2:B:34:THR:HG21	2:B:106:PHE:CD2	2.56	0.41
3:C:774:TYR:HD2	5:E:728:ALA:HB2	1.86	0.41
4:D:336:ASP:O	4:D:337:VAL:HG23	2.21	0.41
2:3:671:LEU:HD23	2:3:721:VAL:HG11	2.03	0.41
4:5:695:ASP:HB2	4:5:696:PRO:CD	2.50	0.41
5:6:523:GLU:OE2	5:6:524:HIS:CE1	2.73	0.41
2:B:123:PRO:HB2	2:B:124:PRO:HD3	2.03	0.41
6:F:228:ARG:NH2	6:F:327:ILE:O	2.54	0.41
6:7:160:GLU:O	6:7:164:GLU:OE1	2.39	0.40
2:B:402:ASP:OD2	2:B:493:GLN:NE2	2.53	0.40
2:B:430:ILE:HD12	2:B:465:ALA:HB2	2.02	0.40
4:D:619:ALA:HA	4:D:622:LEU:HD12	2.02	0.40
1:2:390:LEU:HD23	1:2:390:LEU:HA	1.98	0.40
1:2:485:ARG:HD2	1:2:485:ARG:N	2.37	0.40
2:3:671:LEU:HA	2:3:721:VAL:HG12	2.03	0.40
5:6:642:ASP:OD1	5:6:642:ASP:N	2.55	0.40
2:B:684:THR:HG21	6:F:610:GLU:OE2	2.22	0.40
1:2:417:VAL:HG23	1:2:418:SER:N	2.37	0.40
2:3:123:PRO:HB2	2:3:124:PRO:HD3	2.03	0.40
3:4:187:ILE:HG23	3:4:188:GLN:N	2.36	0.40
6:7:97:THR:HG22	6:7:98:GLN:H	1.87	0.40
2:B:673:GLN:O	2:B:673:GLN:HG3	2.20	0.40
3:C:249:LEU:O	3:C:249:LEU:HG	2.22	0.40
4:D:31:PHE:CE1	4:D:75:ILE:HD12	2.57	0.40
4:D:629:ILE:HG23	4:D:689:MET:HE3	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:5:LEU:HD12	6:F:5:LEU:HA	1.99	0.40
6:F:241:VAL:HG12	6:F:242:ARG:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	2	618/868 (71%)	583 (94%)	32 (5%)	3 (0%)	24	55
1	A	618/868 (71%)	583 (94%)	32 (5%)	3 (0%)	24	55
2	3	604/1006 (60%)	582 (96%)	22 (4%)	0	100	100
2	B	604/1006 (60%)	582 (96%)	22 (4%)	0	100	100
3	4	637/933 (68%)	604 (95%)	33 (5%)	0	100	100
3	C	637/933 (68%)	604 (95%)	33 (5%)	0	100	100
4	5	648/775 (84%)	603 (93%)	43 (7%)	2 (0%)	36	66
4	D	648/775 (84%)	603 (93%)	43 (7%)	2 (0%)	36	66
5	6	603/1017 (59%)	570 (94%)	33 (6%)	0	100	100
5	E	603/1017 (59%)	570 (94%)	33 (6%)	0	100	100
6	7	747/845 (88%)	718 (96%)	28 (4%)	1 (0%)	48	77
6	F	747/845 (88%)	718 (96%)	28 (4%)	1 (0%)	48	77
All	All	7714/10888 (71%)	7320 (95%)	382 (5%)	12 (0%)	44	72

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	435	ASP
6	7	755	THR

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Mol	Chain	Res	Type
1	A	435	ASP
6	F	755	THR
1	2	412	ALA
1	2	502	ALA
4	5	593	GLU
1	A	412	ALA
1	A	502	ALA
4	D	593	GLU
4	5	240	PRO
4	D	240	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	548/770 (71%)	541 (99%)	7 (1%)	61	86
1	A	548/770 (71%)	542 (99%)	6 (1%)	65	87
2	3	530/864 (61%)	525 (99%)	5 (1%)	70	89
2	B	530/864 (61%)	525 (99%)	5 (1%)	70	89
3	4	584/848 (69%)	580 (99%)	4 (1%)	76	91
3	C	584/848 (69%)	579 (99%)	5 (1%)	70	89
4	5	589/688 (86%)	582 (99%)	7 (1%)	63	87
4	D	589/688 (86%)	582 (99%)	7 (1%)	63	87
5	6	538/886 (61%)	537 (100%)	1 (0%)	87	96
5	E	538/886 (61%)	537 (100%)	1 (0%)	87	96
6	7	671/753 (89%)	665 (99%)	6 (1%)	70	89
6	F	671/753 (89%)	665 (99%)	6 (1%)	70	89
All	All	6920/9618 (72%)	6860 (99%)	60 (1%)	68	89

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	2	181	LEU
1	2	196	GLU
1	2	203	VAL
1	2	283	TYR
1	2	367	CYS
1	2	503	PRO
1	2	526	ASN
2	3	121	PHE
2	3	359	ILE
2	3	648	PRO
2	3	651	VAL
2	3	667	VAL
3	4	234	ARG
3	4	312	LYS
3	4	553	THR
3	4	572	THR
4	5	239	ASP
4	5	358	LEU
4	5	365	LYS
4	5	585	ASN
4	5	622	LEU
4	5	636	ASN
4	5	652	GLN
5	6	145	ILE
6	7	100	ASP
6	7	191	LEU
6	7	285	THR
6	7	403	GLU
6	7	702	LEU
6	7	755	THR
1	A	181	LEU
1	A	196	GLU
1	A	203	VAL
1	A	367	CYS
1	A	503	PRO
1	A	526	ASN
2	B	121	PHE
2	B	359	ILE
2	B	648	PRO
2	B	651	VAL
2	B	667	VAL
3	C	234	ARG
3	C	312	LYS

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Mol	Chain	Res	Type
3	C	553	THR
3	C	572	THR
3	C	838	THR
4	D	239	ASP
4	D	358	LEU
4	D	365	LYS
4	D	585	ASN
4	D	622	LEU
4	D	636	ASN
4	D	652	GLN
5	E	145	ILE
6	F	100	ASP
6	F	191	LEU
6	F	285	THR
6	F	403	GLU
6	F	702	LEU
6	F	755	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	2	248	HIS
1	2	405	HIS
1	2	526	ASN
1	2	531	HIS
1	2	768	HIS
2	3	151	HIS
2	3	175	HIS
2	3	210	HIS
2	3	253	HIS
2	3	376	HIS
2	3	587	ASN
2	3	673	GLN
2	3	682	ASN
2	3	688	ASN
2	3	691	ASN
2	3	712	HIS
3	4	318	ASN
3	4	500	GLN
3	4	549	ASN
3	4	808	HIS
4	5	245	HIS

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Mol	Chain	Res	Type
4	5	254	GLN
4	5	359	GLN
4	5	539	ASN
4	5	571	HIS
4	5	585	ASN
4	5	632	GLN
4	5	636	ASN
4	5	694	GLN
5	6	156	GLN
5	6	274	HIS
5	6	364	ASN
5	6	524	HIS
5	6	540	HIS
5	6	653	HIS
5	6	750	GLN
6	7	144	ASN
6	7	209	GLN
6	7	554	ASN
1	A	188	ASN
1	A	248	HIS
1	A	405	HIS
1	A	526	ASN
1	A	531	HIS
1	A	621	HIS
1	A	768	HIS
2	B	151	HIS
2	B	253	HIS
2	B	376	HIS
2	B	587	ASN
2	B	673	GLN
2	B	682	ASN
2	B	688	ASN
2	B	691	ASN
2	B	712	HIS
3	C	318	ASN
3	C	500	GLN
3	C	549	ASN
3	C	683	ASN
3	C	685	ASN
3	C	808	HIS
3	C	815	ASN
4	D	245	HIS

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Mol	Chain	Res	Type
4	D	254	GLN
4	D	359	GLN
4	D	539	ASN
4	D	571	HIS
4	D	625	ASN
4	D	632	GLN
4	D	636	ASN
4	D	694	GLN
5	E	139	GLN
5	E	156	GLN
5	E	274	HIS
5	E	364	ASN
5	E	524	HIS
5	E	540	HIS
5	E	633	ASN
5	E	653	HIS
5	E	730	HIS
5	E	750	GLN
6	F	90	ASN
6	F	144	ASN
6	F	209	GLN
6	F	468	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 26 ligands modelled in this entry, 18 are monoatomic - leaving 8 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
12	ADP	3	1000	10	28,29,29	0.58	0	43,45,45	0.57	0
9	ATP	A	1000	10	32,33,33	0.65	0	48,52,52	0.64	0
9	ATP	2	1000	10	32,33,33	0.64	0	48,52,52	0.64	0
12	ADP	F	1000	10	28,29,29	0.59	0	43,45,45	0.50	0
12	ADP	7	1000	10	28,29,29	0.59	0	43,45,45	0.50	0
12	ADP	B	1000	10	28,29,29	0.58	0	43,45,45	0.57	0
12	ADP	D	1000	10	28,29,29	0.87	1 (3%)	43,45,45	0.69	0
12	ADP	5	1000	10	28,29,29	0.87	1 (3%)	43,45,45	0.69	0

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
12	ADP	3	1000	10	-	1/16/32/32	0/3/3/3
9	ATP	A	1000	10	-	4/22/38/38	0/3/3/3
9	ATP	2	1000	10	-	4/22/38/38	0/3/3/3
12	ADP	F	1000	10	-	1/16/32/32	0/3/3/3
12	ADP	7	1000	10	-	1/16/32/32	0/3/3/3
12	ADP	B	1000	10	-	1/16/32/32	0/3/3/3
12	ADP	D	1000	10	-	3/16/32/32	0/3/3/3
12	ADP	5	1000	10	-	3/16/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	1000	ADP	PB-O2B	-3.25	1.42	1.54
12	5	1000	ADP	PB-O2B	-3.25	1.42	1.54

There are no bond angle outliers.

There are no chirality outliers.

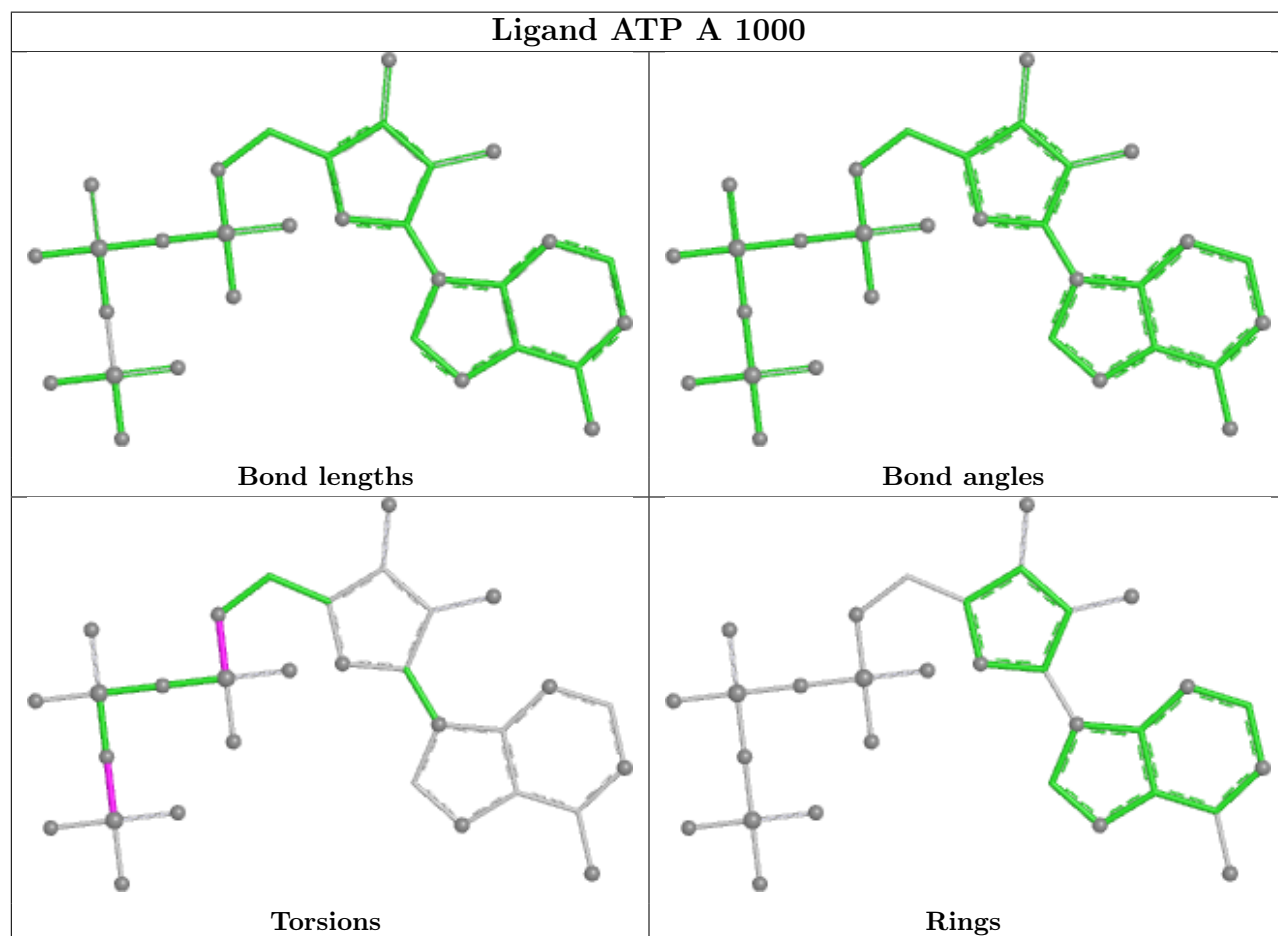
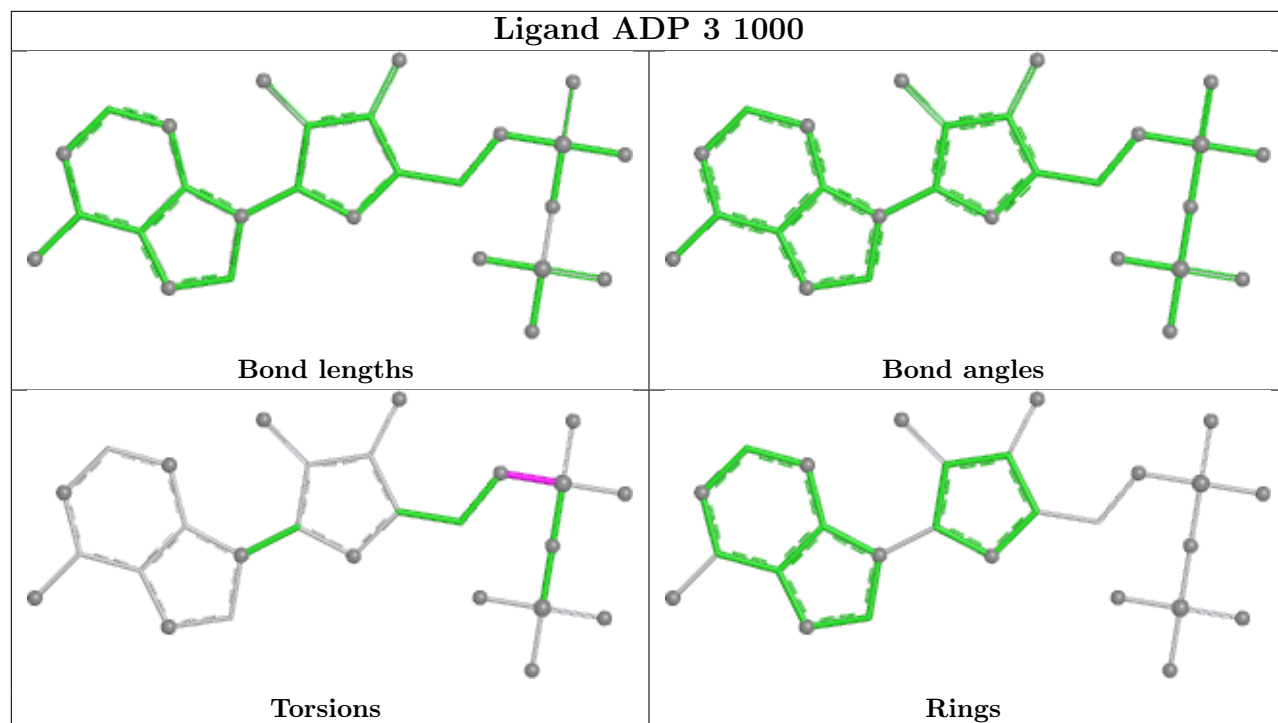
All (18) torsion outliers are listed below:

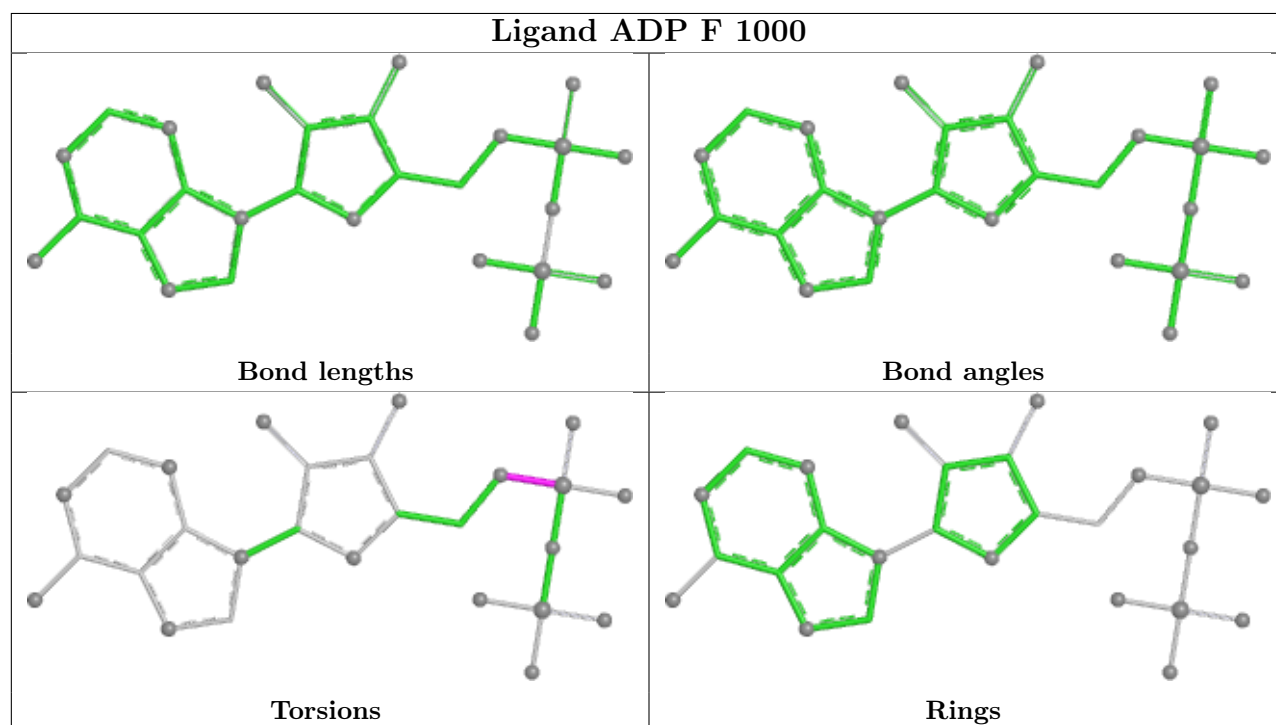
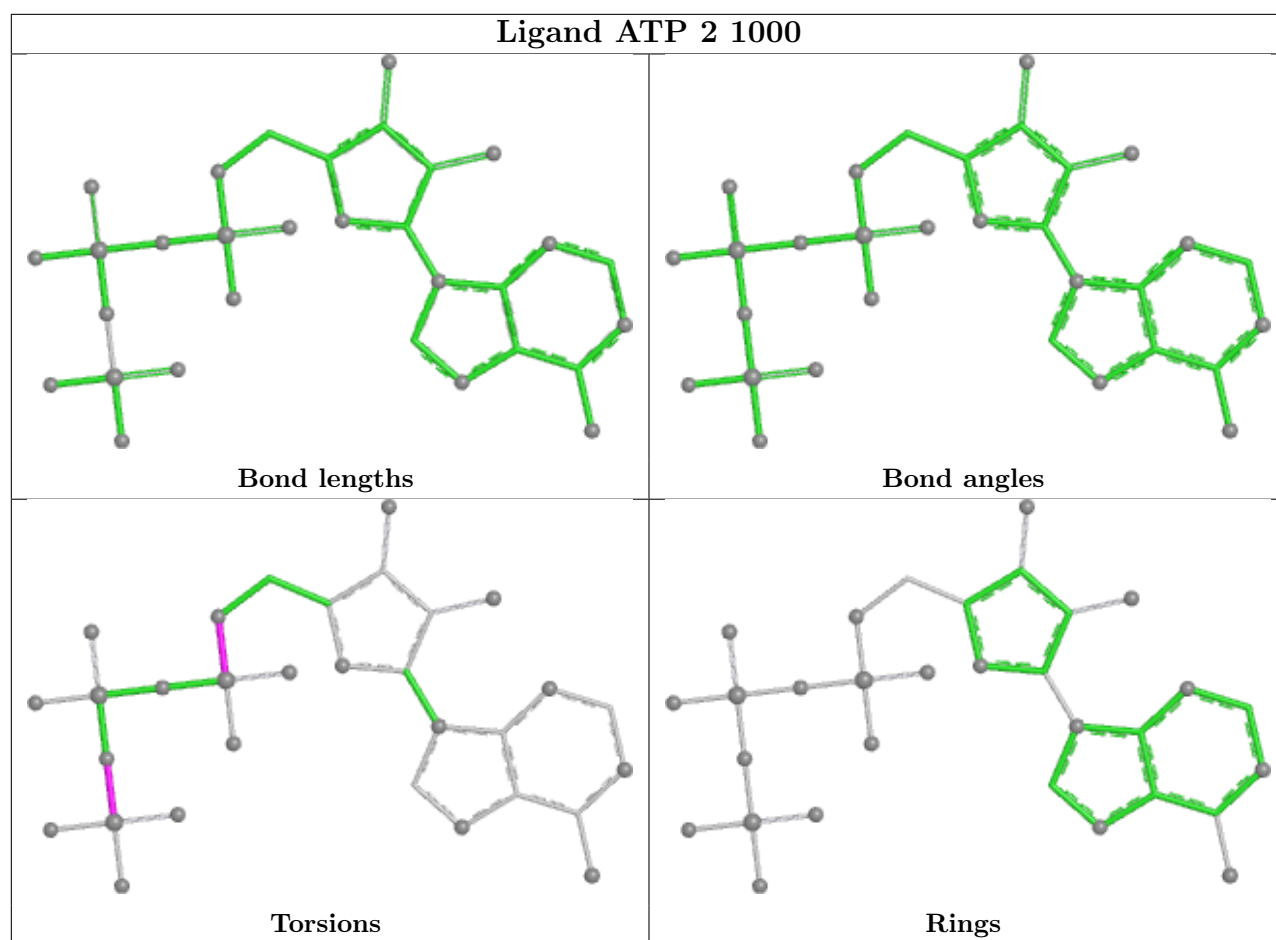
Mol	Chain	Res	Type	Atoms
9	2	1000	ATP	PB-O3B-PG-O3G
9	A	1000	ATP	PB-O3B-PG-O3G
12	7	1000	ADP	C5'-O5'-PA-O1A
12	F	1000	ADP	C5'-O5'-PA-O1A
9	2	1000	ATP	C5'-O5'-PA-O1A
9	A	1000	ATP	C5'-O5'-PA-O1A
12	3	1000	ADP	C5'-O5'-PA-O1A
12	B	1000	ADP	C5'-O5'-PA-O1A
12	5	1000	ADP	PB-O3A-PA-O2A
12	D	1000	ADP	PB-O3A-PA-O2A
12	5	1000	ADP	C4'-C5'-O5'-PA
12	D	1000	ADP	C4'-C5'-O5'-PA
9	2	1000	ATP	PB-O3B-PG-O2G
9	A	1000	ATP	PB-O3B-PG-O2G
9	2	1000	ATP	PB-O3B-PG-O1G
9	A	1000	ATP	PB-O3B-PG-O1G
12	5	1000	ADP	O4'-C4'-C5'-O5'
12	D	1000	ADP	O4'-C4'-C5'-O5'

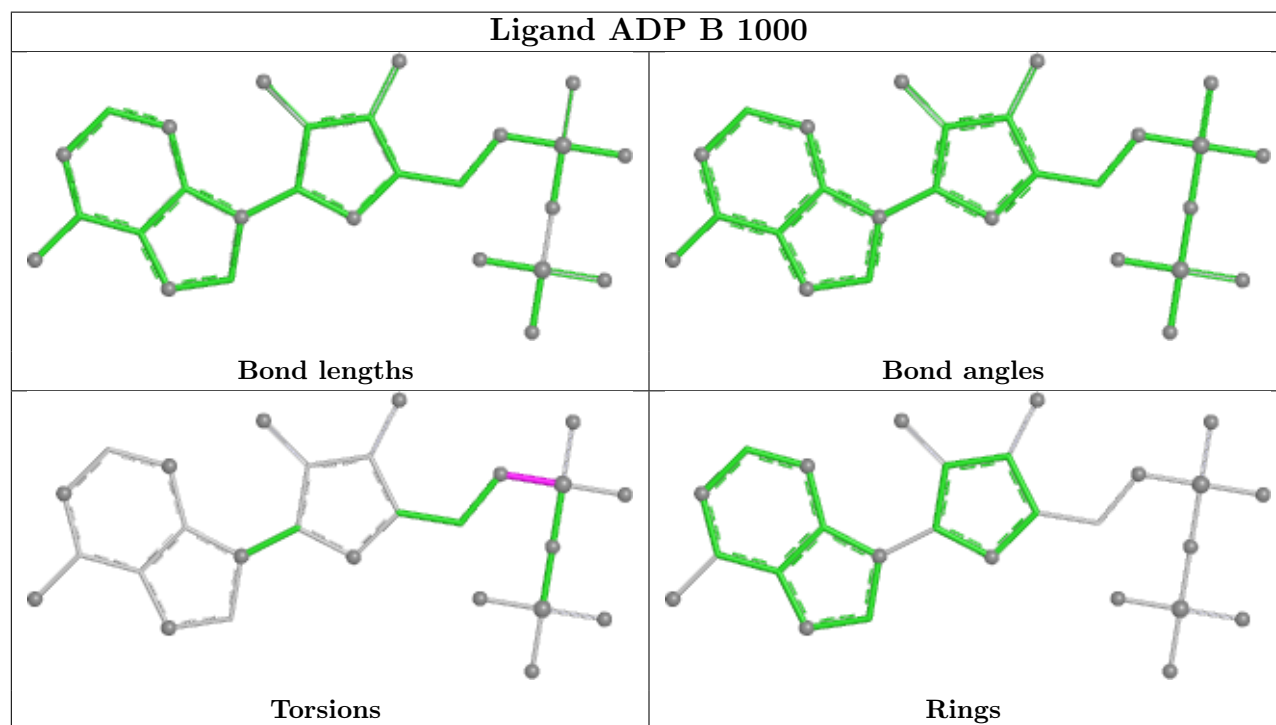
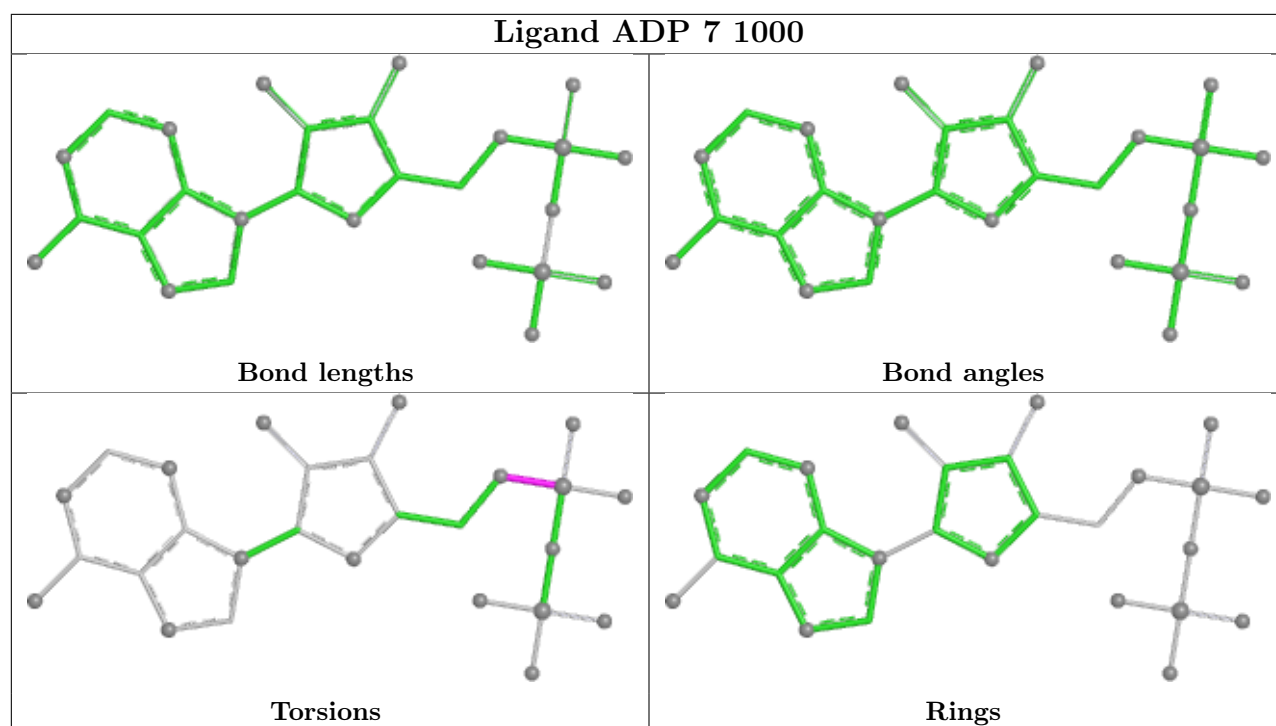
There are no ring outliers.

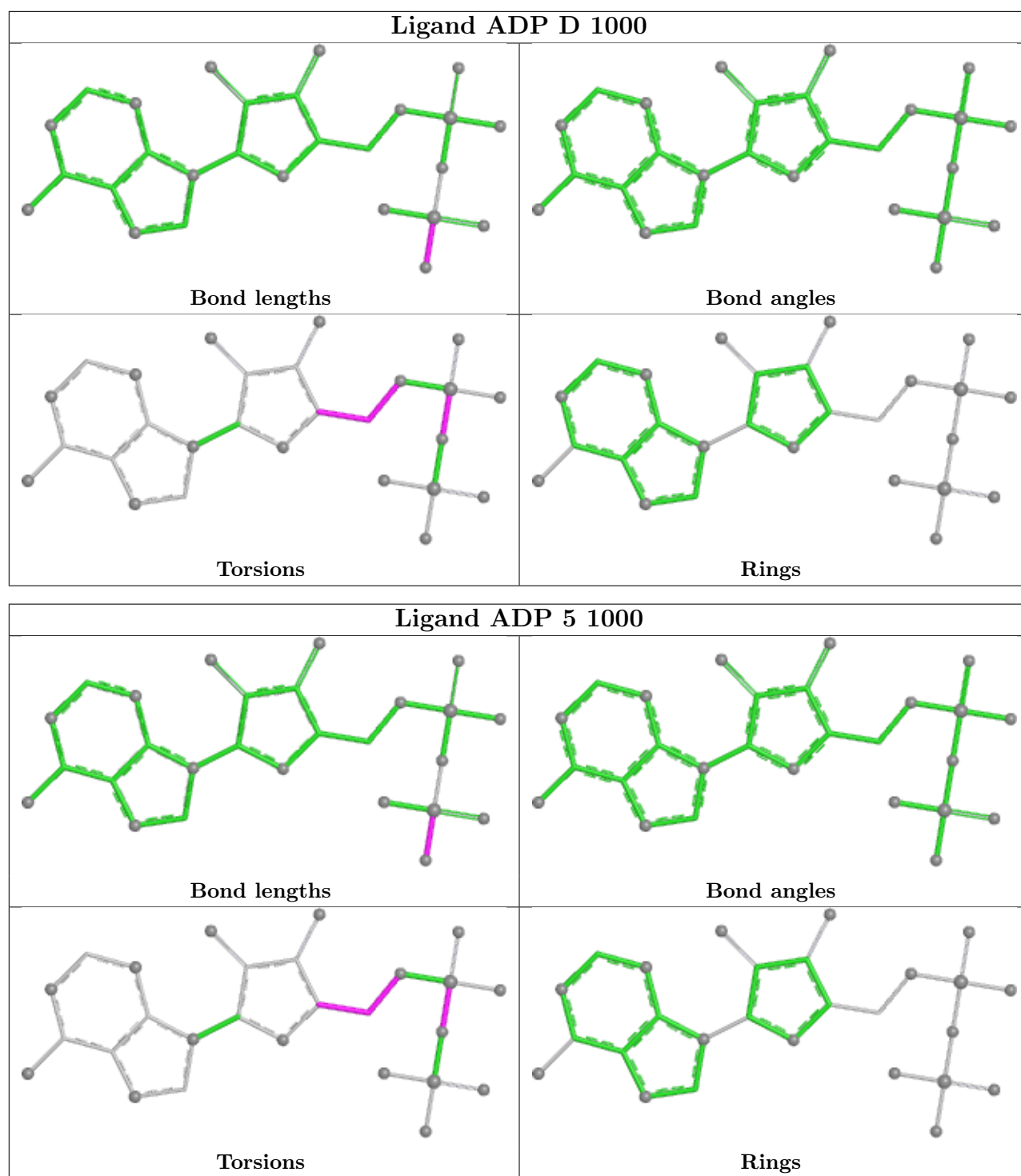
No monomer is involved in short contacts.

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

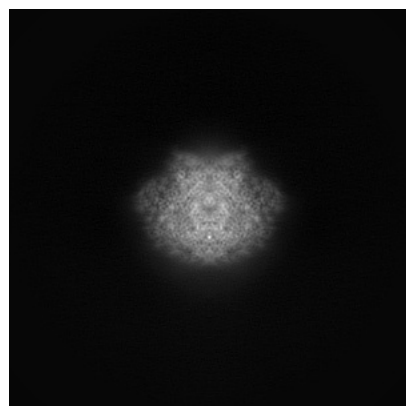
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-19186. These allow visual inspection of the internal detail of the map and identification of artifacts.

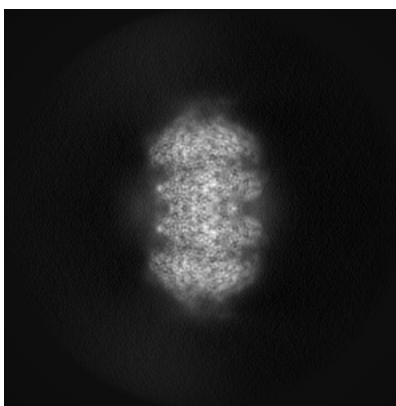
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

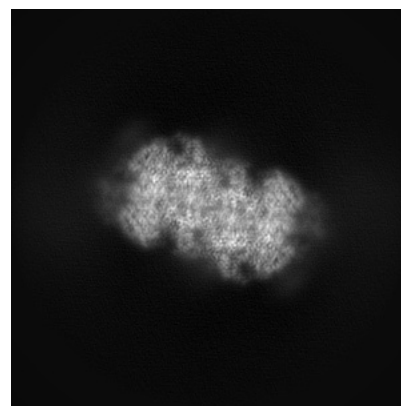
6.1.1 Primary map



X

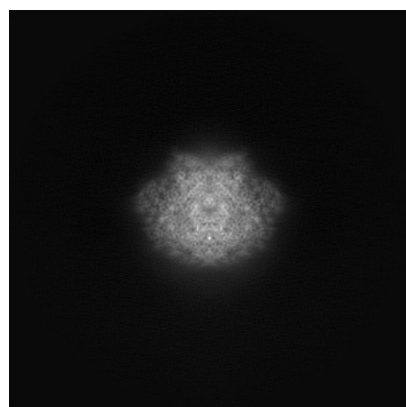


Y

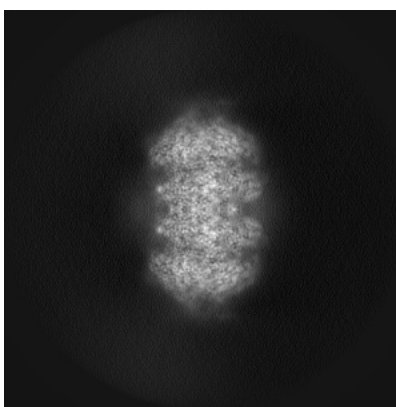


Z

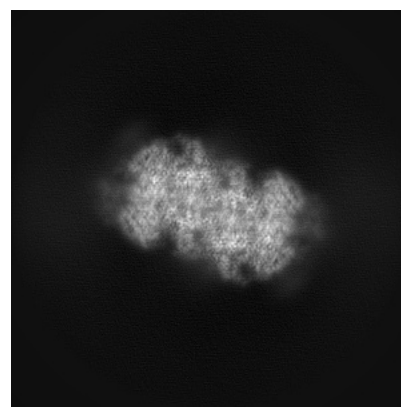
6.1.2 Raw map



X



Y

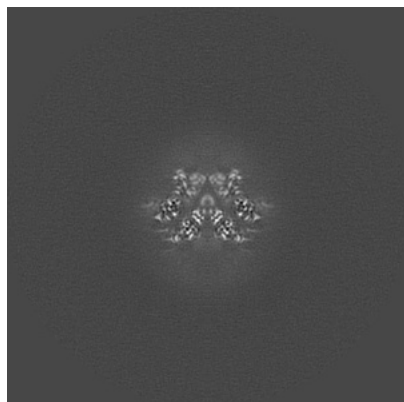


Z

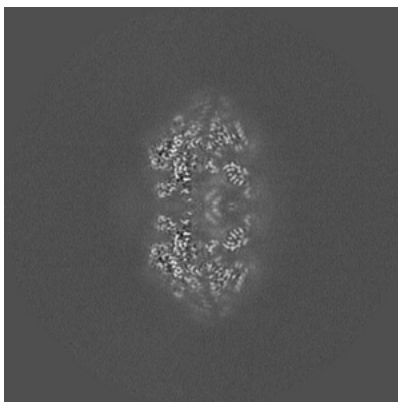
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

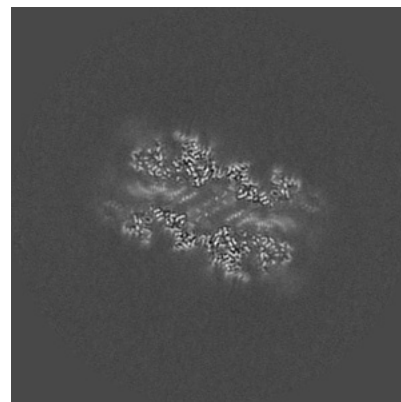
6.2.1 Primary map



X Index: 210

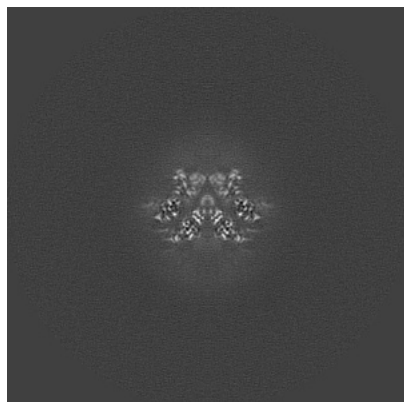


Y Index: 210

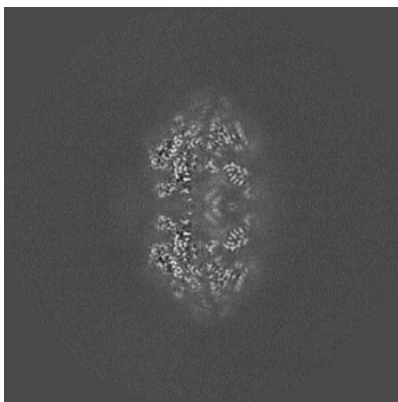


Z Index: 210

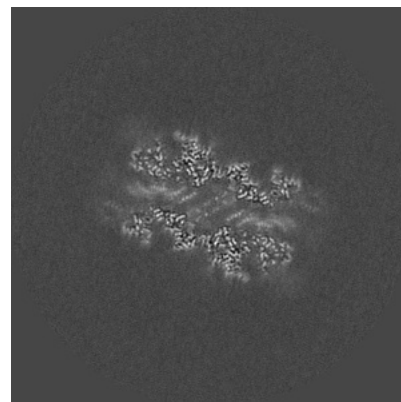
6.2.2 Raw map



X Index: 210



Y Index: 210

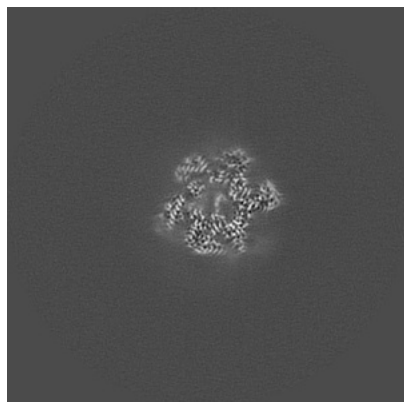


Z Index: 210

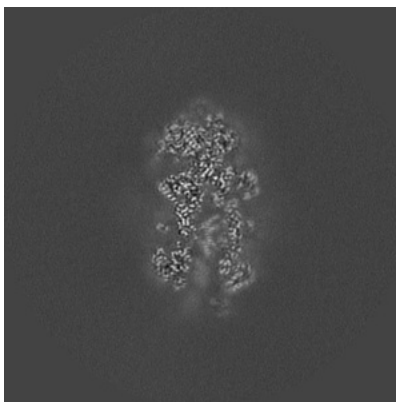
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

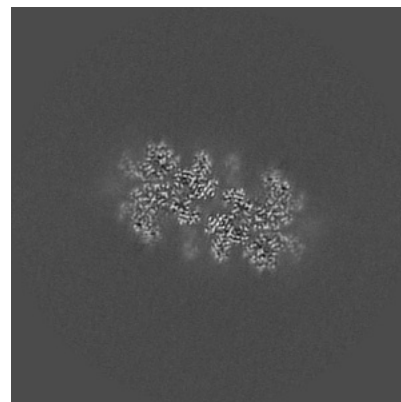
6.3.1 Primary map



X Index: 187

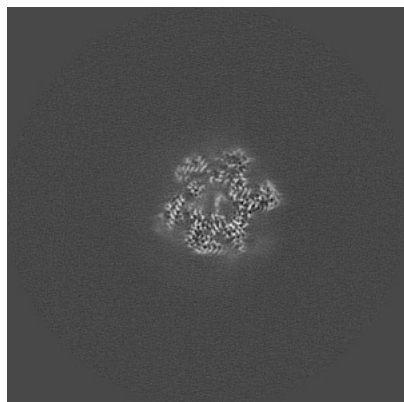


Y Index: 222

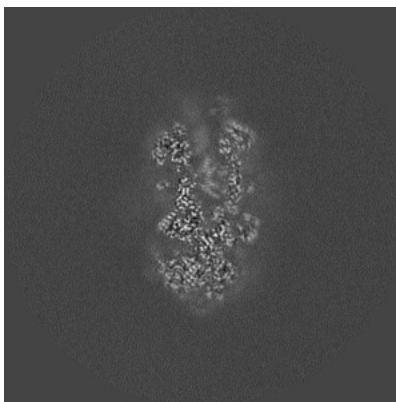


Z Index: 185

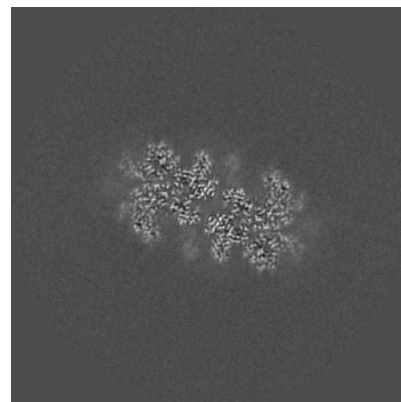
6.3.2 Raw map



X Index: 187



Y Index: 198

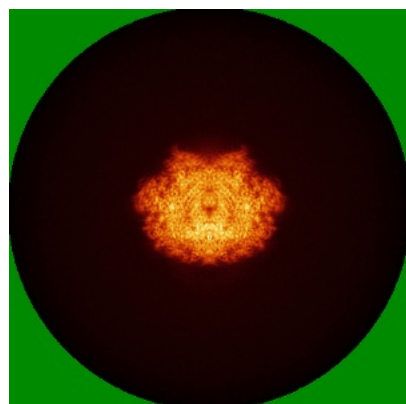


Z Index: 185

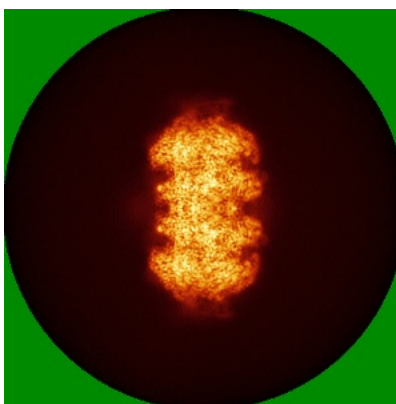
The images above show the largest variance slices of the map in three orthogonal directions.

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

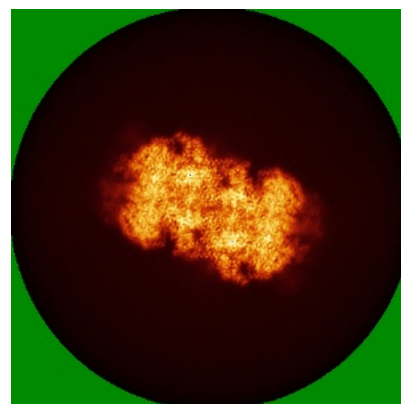
6.4.1 Primary map



X

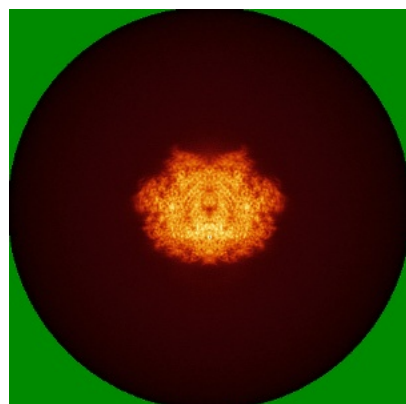


Y

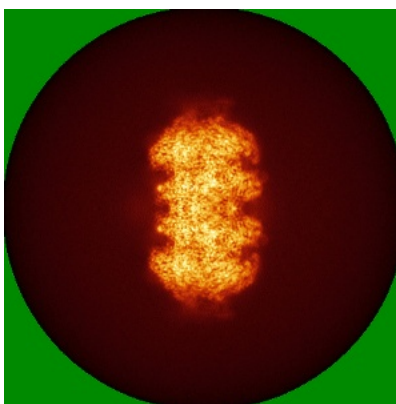


Z

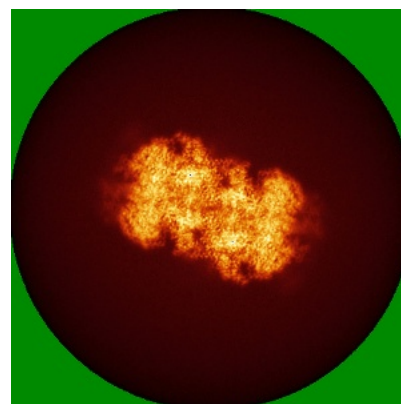
6.4.2 Raw map



X



Y

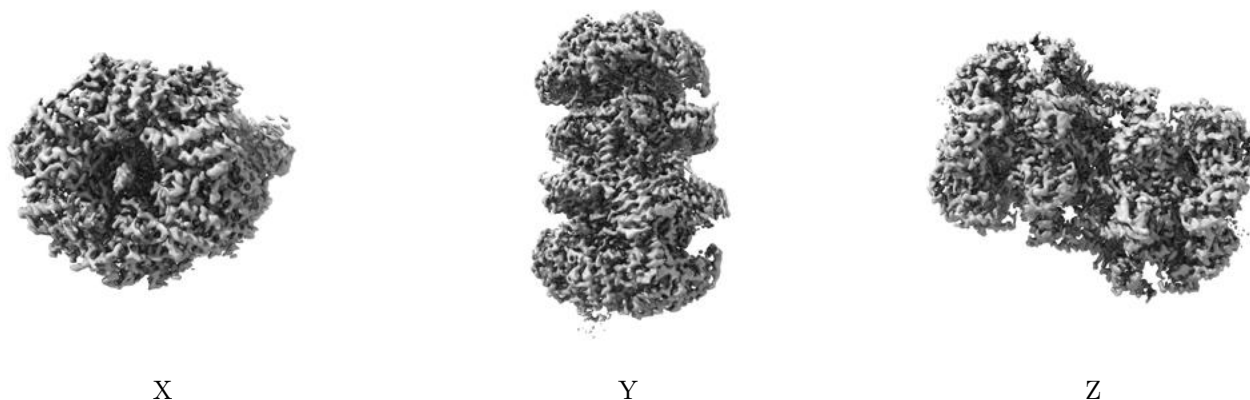


Z

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

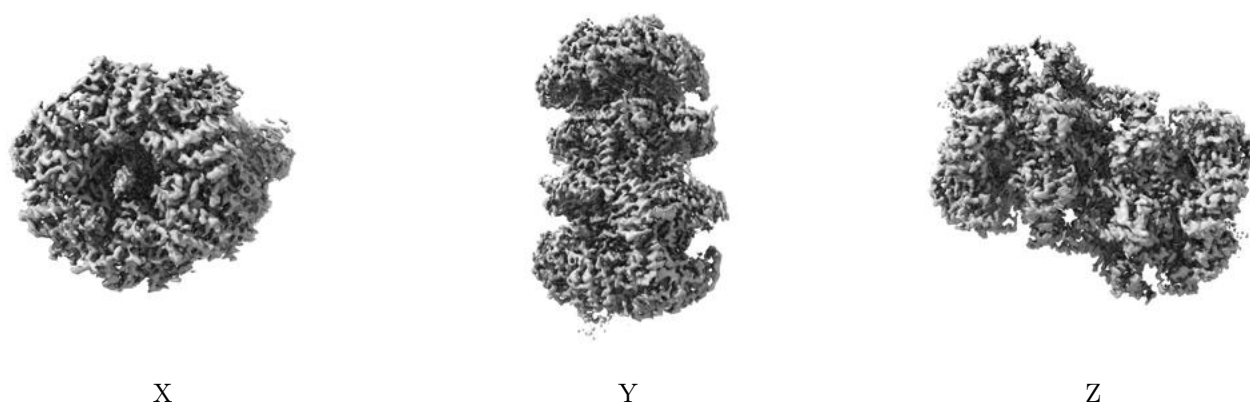
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

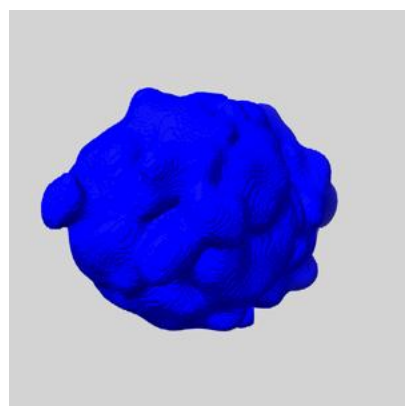
6.6 Mask visualisation [i](#)

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

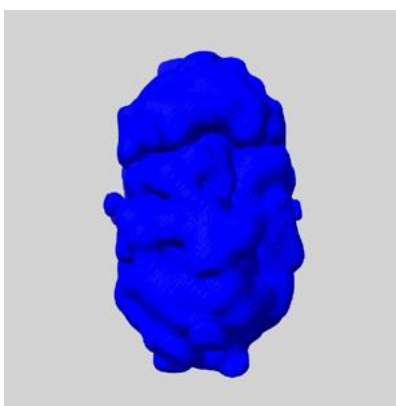
A mask typically either:

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

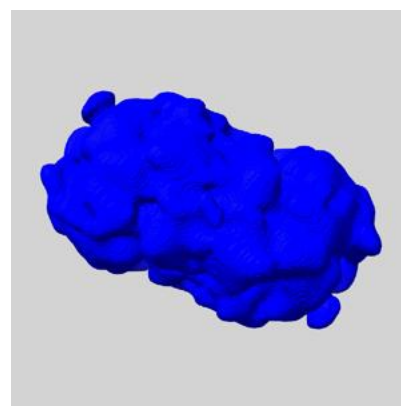
6.6.1 emd_19186_msk_1.map [i](#)



X



Y

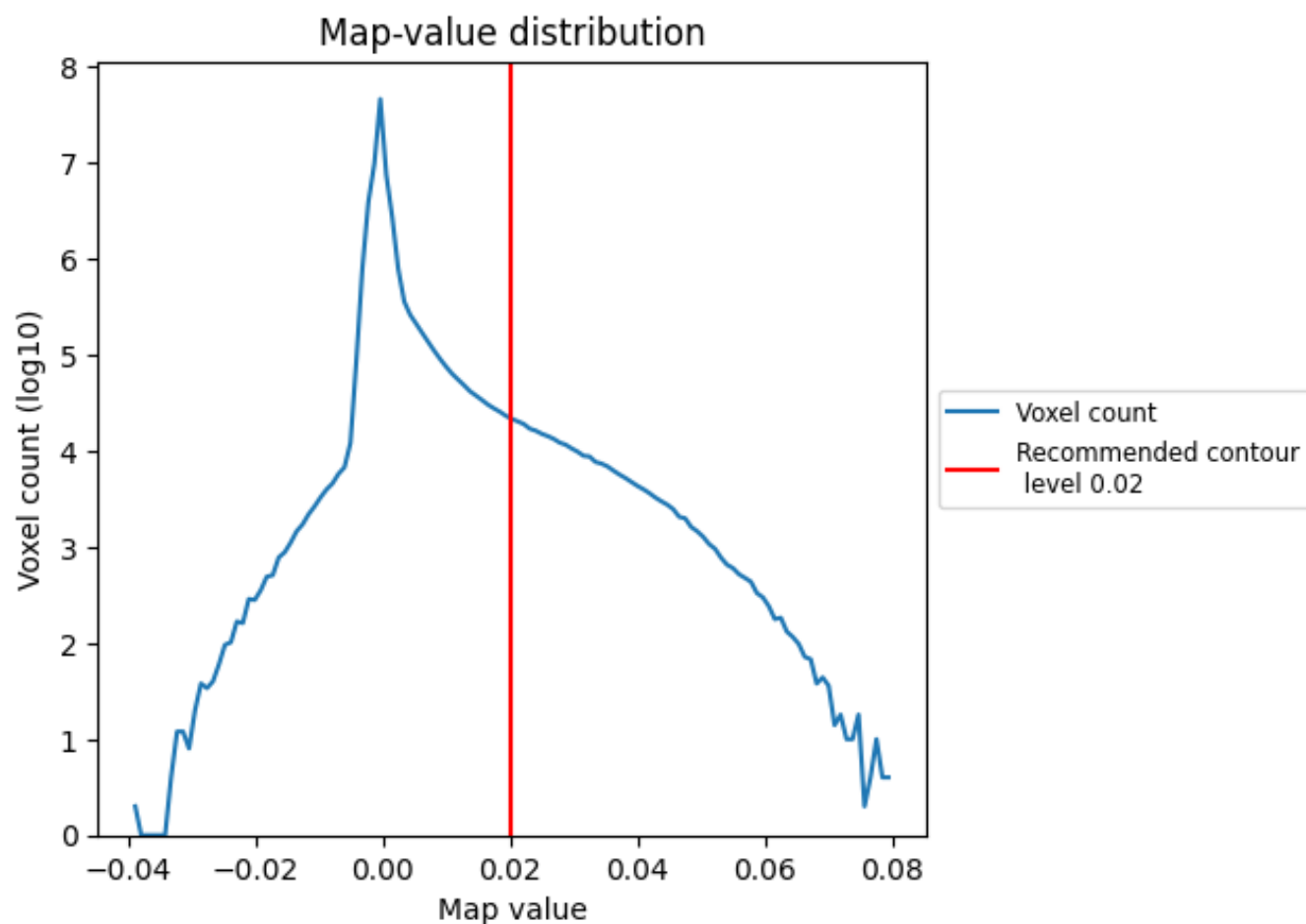


Z

7 Map analysis [i](#)

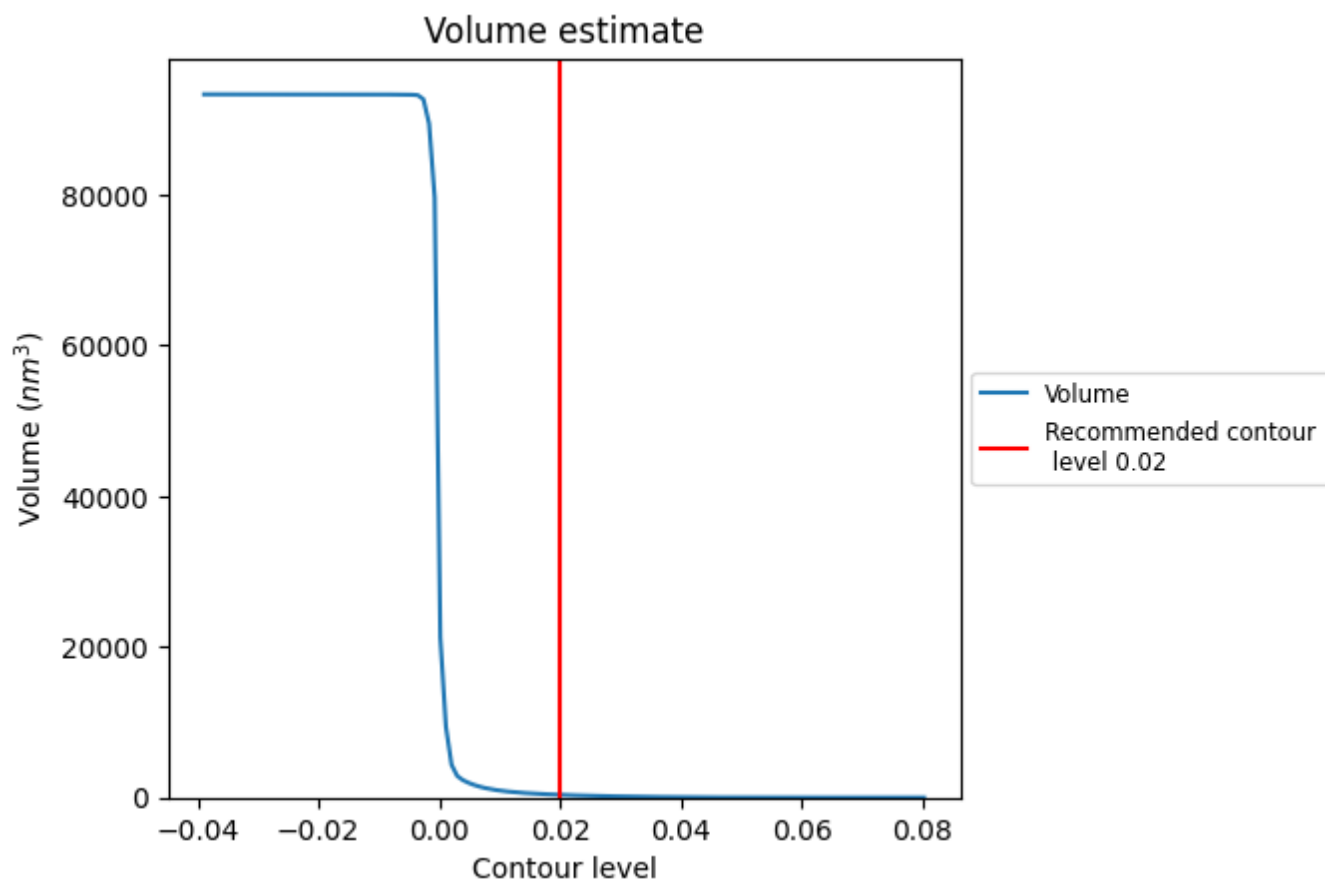
This section contains the results of statistical analysis of the map.

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.

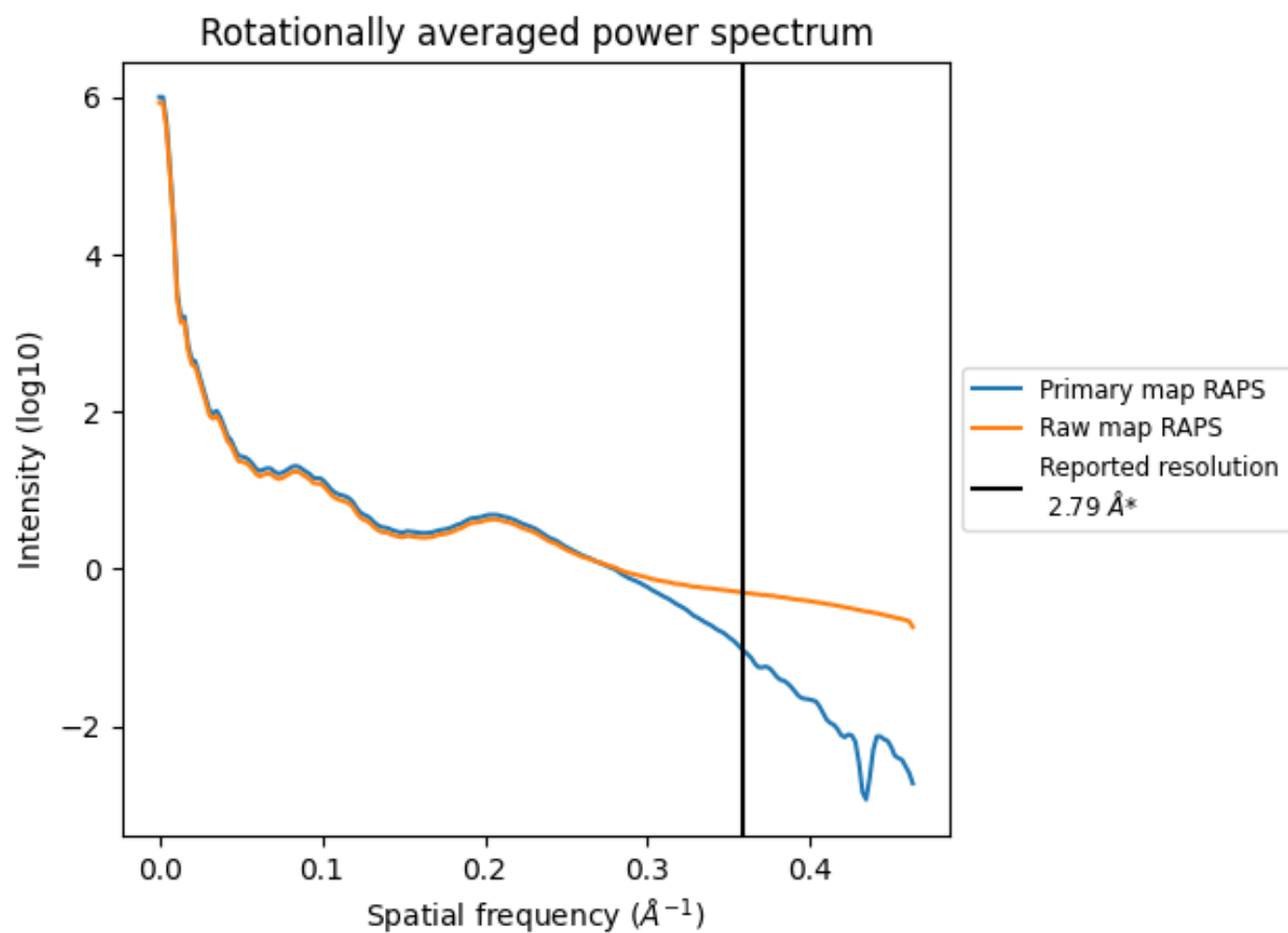
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 363 nm³; this corresponds to an approximate mass of 328 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 ⓘ

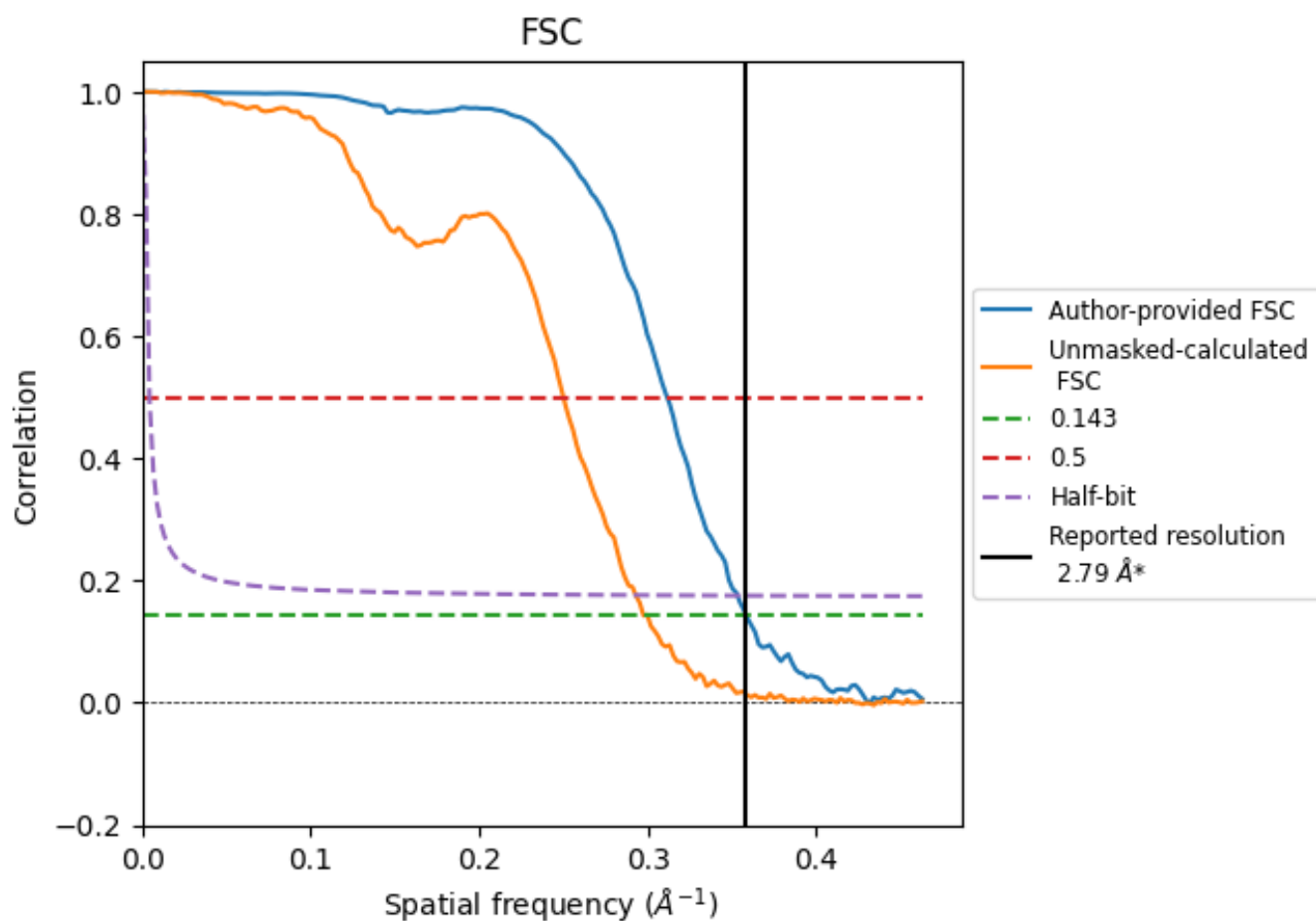


*Reported resolution corresponds to spatial frequency of 0.358 Å⁻¹

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 0.358 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

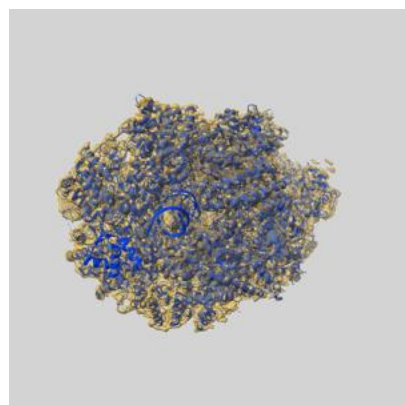
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.79	-	-
Author-provided FSC curve	2.79	3.21	2.83
Unmasked-calculated*	3.36	4.00	3.41

*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 3.36 differs from the reported value 2.79 by more than 10 %

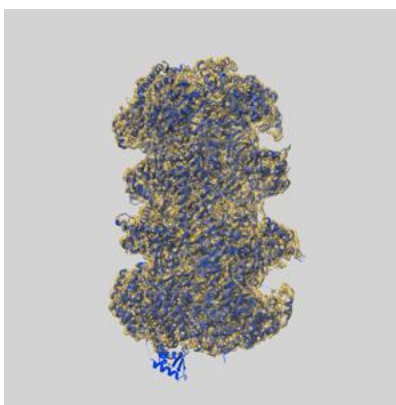
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-19186 and PDB model 8RIF. Per-residue inclusion information can be found in [section 3](#) on [page 10](#).

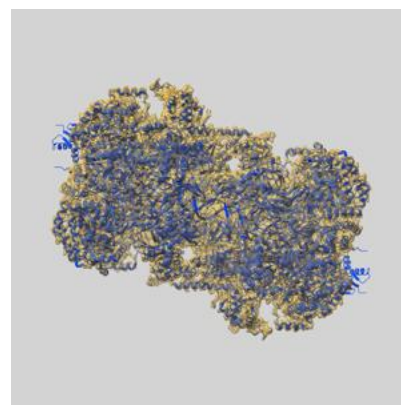
9.1 Map-model overlay [i](#)



X



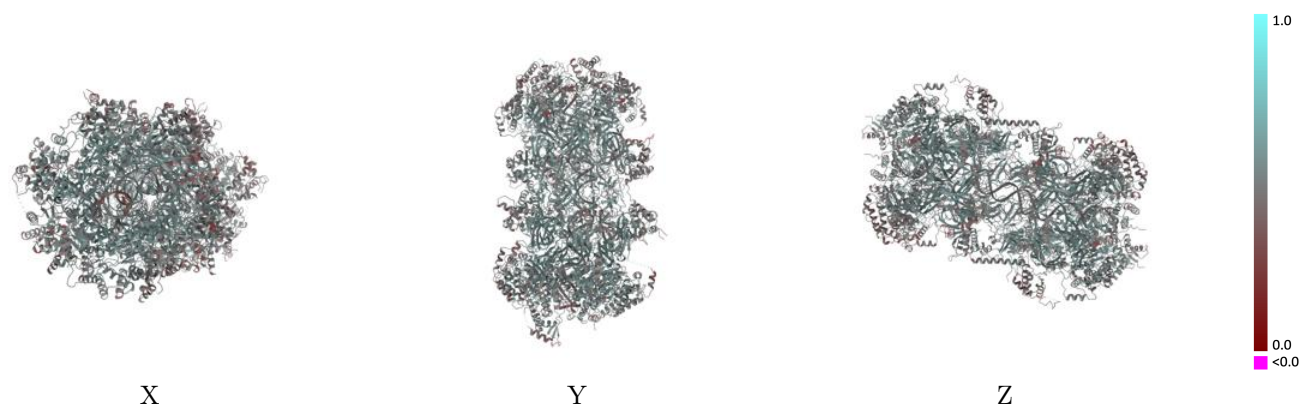
Y



Z

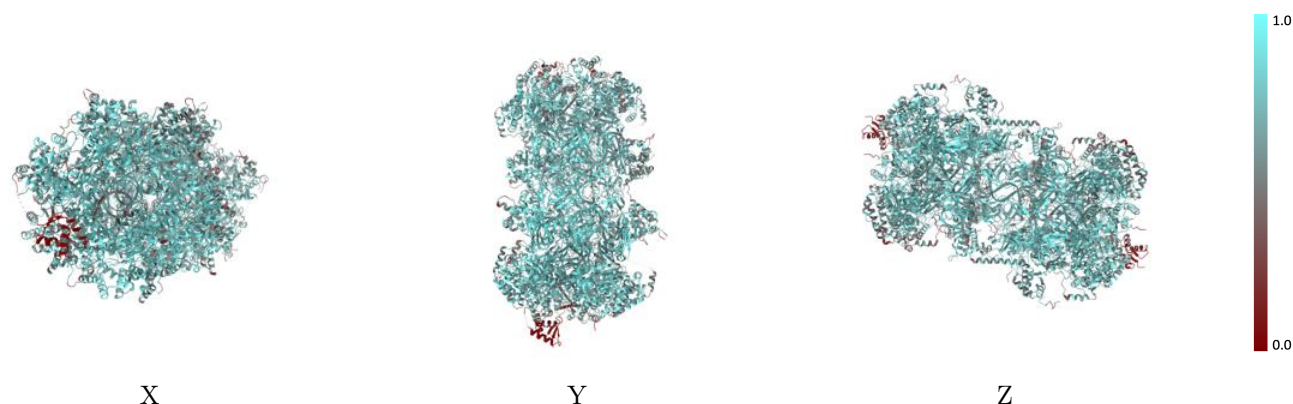
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



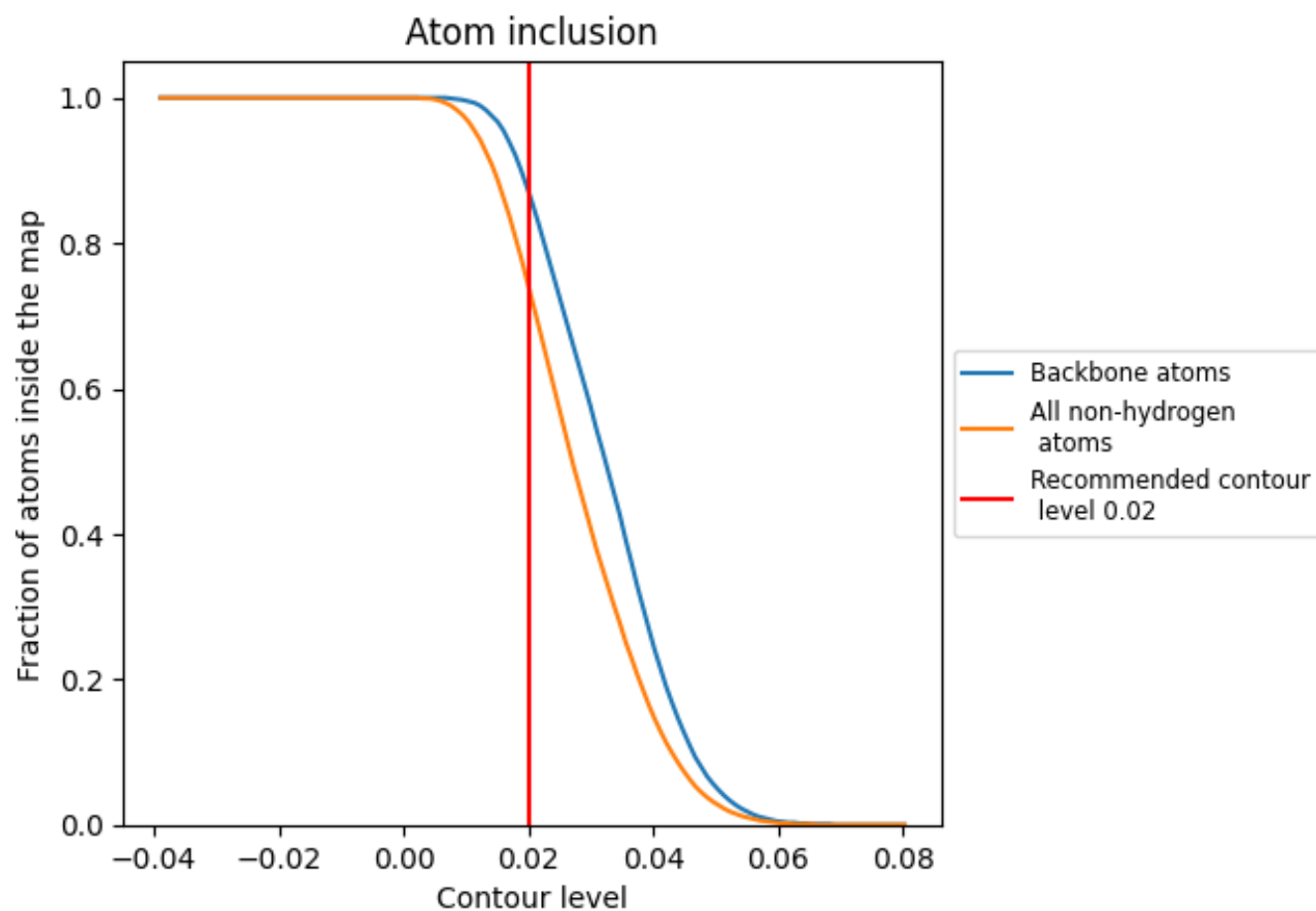
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 87% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7420	0.5160
2	0.7140	0.4990
3	0.8070	0.5360
4	0.7480	0.5180
5	0.7480	0.5060
6	0.7400	0.5220
7	0.7200	0.5210
A	0.7120	0.5000
B	0.8070	0.5380
C	0.7450	0.5170
D	0.7450	0.5080
E	0.7380	0.5230
F	0.7180	0.5210
X	0.6960	0.4630
Y	0.6960	0.4670

1.0

0.0

<0.0