



wwPDB EM Validation Summary Report ⓘ

Sep 15, 2026 – 07:26 am BST

PDB ID : 9TGM / pdb_00009tgm
EMDB ID : EMD-55904
Title : Cryo-EM structure of MCM2-7 DH bound to Sld3-Sld7
Authors : Saleh, A.; Noguchi, Y.; Ivanova, M.E.; Aramayo, R.; Speck, C.
Deposited on : 2025-12-02
Resolution : 3.60 Å(reported)
Based on initial models : 7PT6, 5BK4, 7P30, 3WI3, 3X38

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:

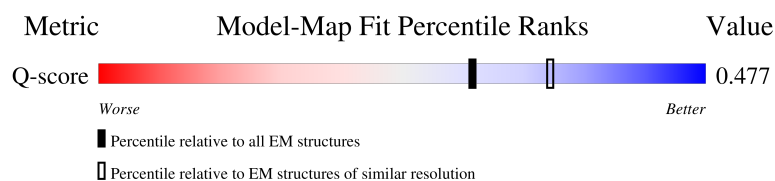
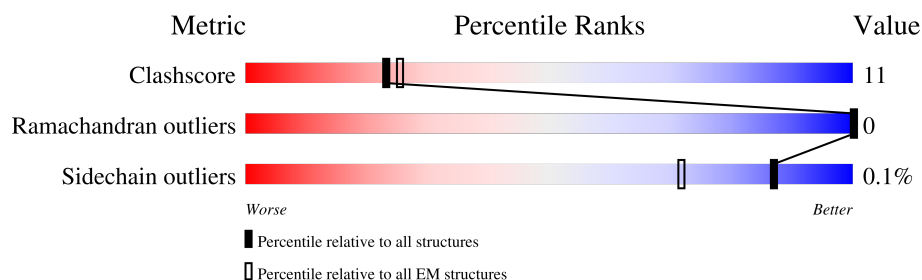
EMDB validation analysis : 0.0.1.dev133
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

1 Overall quality at a glance

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

The reported resolution of this entry is 3.60 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	12797 (3.10 - 4.10)

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	 7% 50% 22% 28%
1	B	868	 1% 50% 22% 28%
2	3	971	 1% 50% 15% 35%
2	C	971	 54% 11% 35%

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Mol	Chain	Length	Quality of chain
3	4	933	
3	D	933	
4	5	775	
4	E	775	
5	6	1017	
5	F	1017	
6	7	845	
6	G	845	
7	8	668	
7	X	668	
8	Y	257	

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 63086 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
			4947	3116	876	936	19		
1	B	624	Total	C	N	O	S	0	0
			4947	3116	876	936	19		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	631	Total	C	N	O	S	0	0
			4947	3130	880	924	13		
2	C	631	Total	C	N	O	S	0	0
			4947	3130	880	924	13		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	668	Total	C	N	O	S	0	0
			5326	3343	919	1035	29		
3	D	668	Total	C	N	O	S	0	0
			5326	3343	919	1035	29		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	5	643	Total	C	N	O	S	0	0
			5033	3160	863	986	24		
4	E	643	Total	C	N	O	S	0	0
			5033	3160	863	986	24		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	6	647	Total	C	N	O	S	0	0
			5127	3226	895	980	26		
5	F	647	Total	C	N	O	S	0	0
			5127	3226	895	980	26		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	7	690	Total	C	N	O	S	0	0
			5438	3424	942	1042	30		
6	G	690	Total	C	N	O	S	0	0
			5438	3424	942	1042	30		

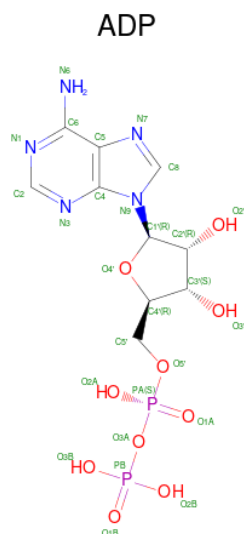
- Molecule 7 is a protein called DNA replication regulator SLD3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	8	29	Total	C	N	O	S	0	0
			236	144	40	51	1		
7	X	29	Total	C	N	O	S	0	0
			236	144	40	51	1		

- Molecule 8 is a protein called Mitochondrial morphogenesis protein SLD7.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	Y	94	Total	C	N	O	S	0	0
			752	466	137	148	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	2	1	Total 27	C 10	N 5	O 10	P 2	0
9	3	1	Total 27	C 10	N 5	O 10	P 2	0
9	5	1	Total 27	C 10	N 5	O 10	P 2	0
9	7	1	Total 27	C 10	N 5	O 10	P 2	0
9	B	1	Total 27	C 10	N 5	O 10	P 2	0
9	C	1	Total 27	C 10	N 5	O 10	P 2	0
9	E	1	Total 27	C 10	N 5	O 10	P 2	0
9	G	1	Total 27	C 10	N 5	O 10	P 2	0

- Molecule 10 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

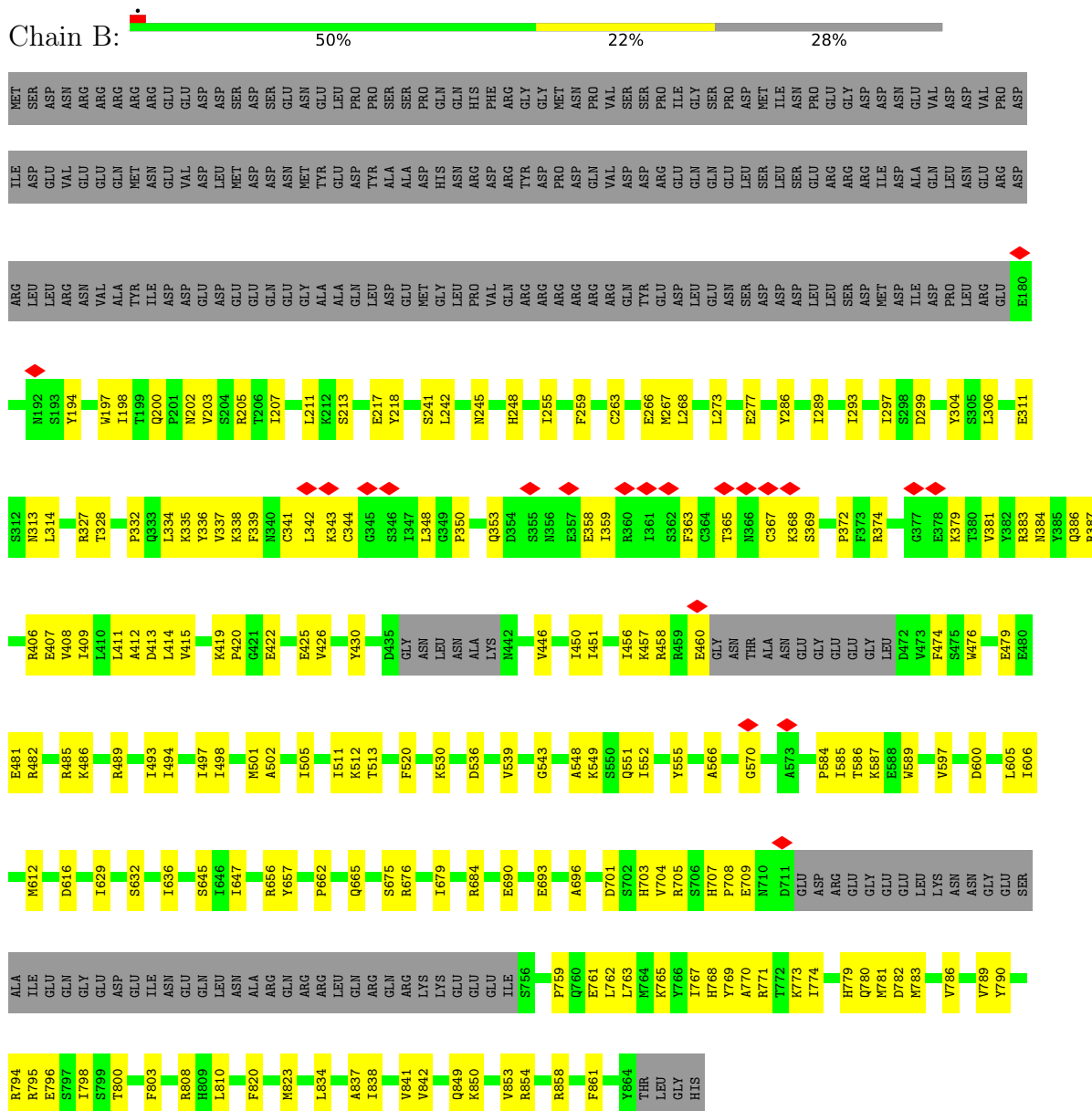
Mol	Chain	Residues	Atoms	AltConf
10	2	1	Total Zn 1 1	0
10	4	1	Total Zn 1 1	0
10	5	1	Total Zn 1 1	0

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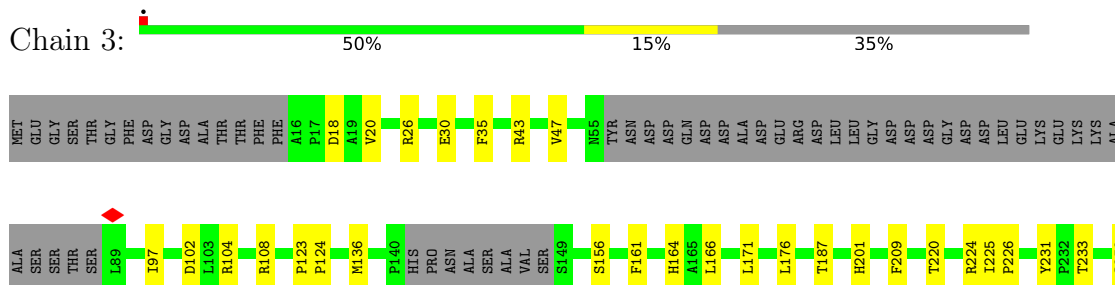
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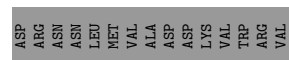
Mol	Chain	Residues	Atoms		AltConf
10	6	1	Total 1	Zn 1	0
10	7	1	Total 1	Zn 1	0
10	B	1	Total 1	Zn 1	0
10	D	1	Total 1	Zn 1	0
10	E	1	Total 1	Zn 1	0
10	F	1	Total 1	Zn 1	0
10	G	1	Total 1	Zn 1	0

- Molecule 1: DNA replication licensing factor MCM2



- Molecule 2: DNA replication licensing factor MCM3



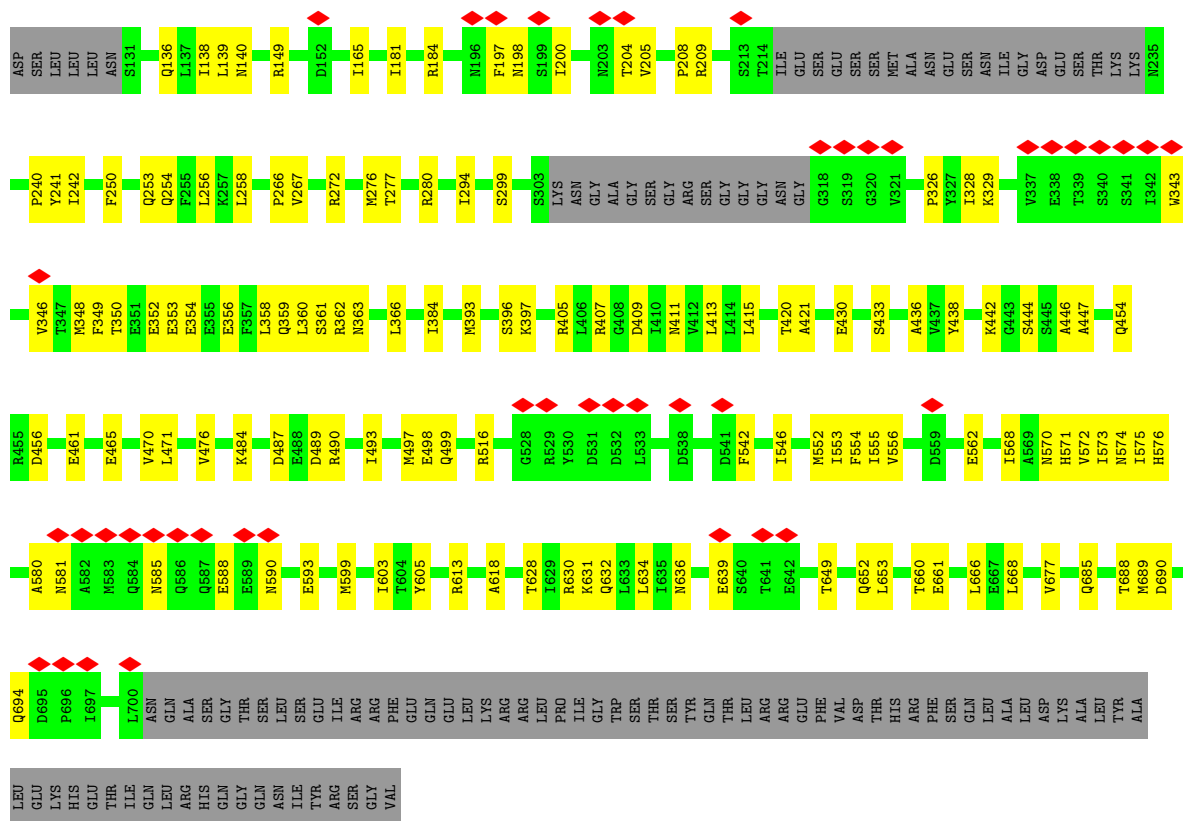


Chain C: 54% 11% 35%

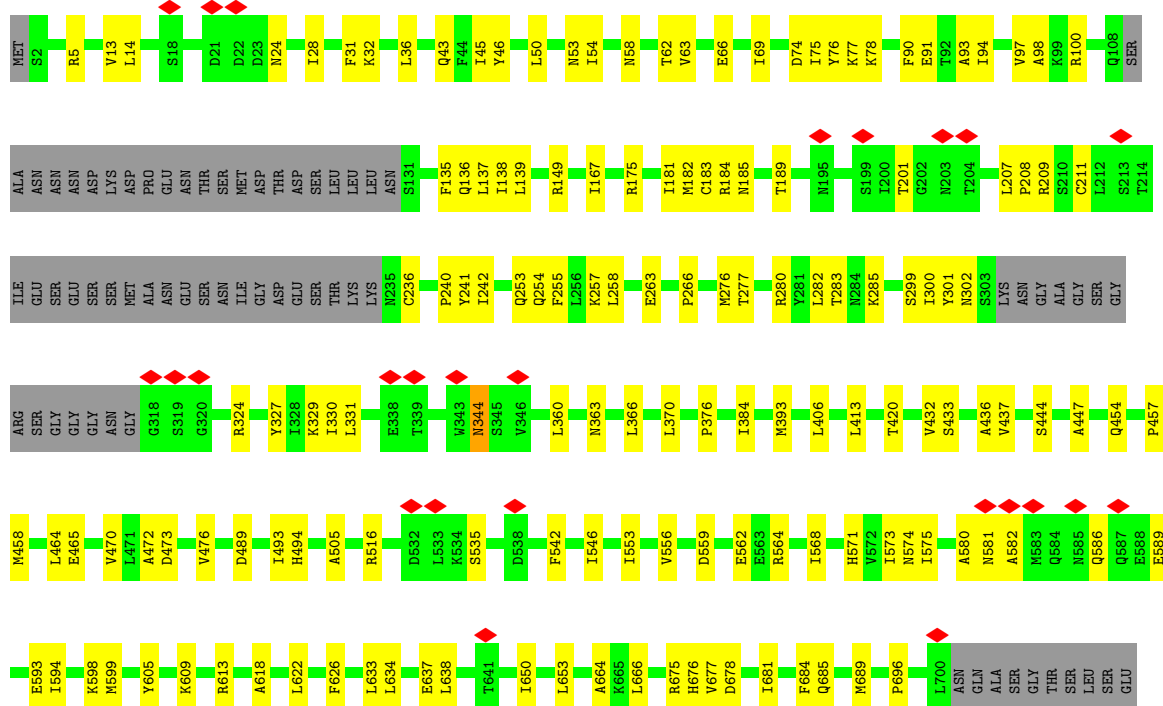


Frequency	Percentage
Daily	50%
Weekly	21%
Monthly	28%





• Molecule 4: Minichromosome maintenance protein 5

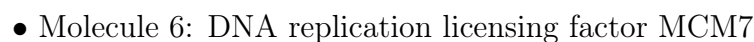


- Molecule 5: DNA replication licensing factor MCM6



PHE	LYS	THR	ASP	K737	V613	M484	L412	R315	Q139	PHE	VAL
VAL	GLU	VAL	VAL	R738	R614	M487	P413	R316	I140	ASN	ASN
ILE	GLU	THR	MET	E740	D615	M487	Q414	I317	E141	GLY	GLY
ARG	GLU	TYR	ASP	E741	E616	L488	V415	V318	ASP	SER	SER
LEU	GLU	ASP	GLU	I742	E617	L488	K416		LEU	LEU	THR
VAL	PHE	LYS	GLU		E618	Q489	L421	F325	PRO	ARG	GLN
LYS	THR	VAL	ASP	P745	Q618	A490	D422		T150	ASP	PHE
ASP	ASN	VAL	ASP	A748	Q619	M491	T423	T328	SER	SER	THR
ARG	MET	MET	ASN	M492	D620	M492	T423	E329	GLY	GLN	PRO
ILE	MET	MET	ILE	M493	T622	V493	R424	P330	ASP	ASP	THR
LEU	ASN	ASN	SER				G425		L158	ARG	SER
MET	GLN	ASN	SER		G626	Q494	I426	T331	R161	LEU	ASN
GLY	GLN	ILE	GLN			Q495	SER	F332	ALA	GLN	ARG
HIS	HIS	VAL	HIS	M629	ARG	D496	LYS	C333	PRO	THR	PRO
THR	ALA	LYS	ALA	L630	ALA	M497	THR	P334	GLY	ASP	SER
ARG	SER	ILE	SER	C637	GLY	E498	GLU	M335	ASN	SER	SER
THR	ALA	THR	GLY	F641	GLY	R499	LEU	P336	GLY	ALA	PRO
HIS	ASN	VAL	ASN			D500	ASN	S337	THR	THR	ASN
LEU	ASP	VAL	ASP	F641	ASN	Q501	ASN		S171	ASP	PRO
ARG	ASP	ARG	ASP	D648	GLY	E502	GLY	R341	E172	MET	PRO
ASP	ASN	GLY	ASN	H653	THR	V503	SER	A342	R176	GLU	SER
LEU	ASP	GLY	ASP		GLY	L505	THR	F343	F177	ALA	ILE
GLY	ALA	GLY	ASP		GLY	M506	GLY	W344	ASN	GLY	GLY
GLU	GLU	GLU	ASP	E657	LEU		ARG		G184	GLU	ALA
ASN	GLY	GLU	GLY	Q658	ARG		LEU	R350	L185	GLU	GLY
GLU	THR	GLU	THR	L780	THR	S509	SER	S351	R186	PRO	PHE
ASN	THR	GLU	SER	R781	GLY	S510	ARG	R352	R187	ALA	GLY
GLY	ALA	GLY	GLY	K782	THR	D511	LEU		V188	ARG	SER
VAL	VAL	VAL	VAL	D783	ASN	E512	ARG	D355	K191	SER	SER
ASN	ASN	ASN	ASN	D784	ILE		THR	W356	V192	LYS	SER
LYS	ILE	ILE	ILE		THR	L516	GLY		GLN	GLY	LEU
THR	THR	VAL	SER	G787	THR		ARG	V359	L196	ALA	ASP
VAL	VAL	ASP	GLU	PHE	L672	K521	LEU	E363	S200	ASN	GLN
VAL	TRP	TRP	PRO	SER	M673	A674	T449	Q264	ASP	HIS	ILE
TYR	TYR	TYR	PRO	R790	R675	R675		L265	LEU	ASN	GLY
VAL	VAL	VAL	VAL				L452	E367	LYS	GLY	GLY
ILE	ILE	ILE	ILE	S791	G686	G686	S453	I368	ARG	V100	SER
HIS	PRO	GLN	ILE	S792			F454	P369	LEU	K101	SER
ASN	LYS	LYS	GLU	S793	R696			T370	ARG	K102	ARG
CYS	GLU	GLU	GLU	R794			T462	G371	SER	V103	HIS
GLU	ASN	GLY	GLY		A703	P535	GLY	S372	GLU	D104	PHE
VAL	VAL	GLN	GLN	R798	P704	A536	SER	S373	ASP	K110	SER
LEU	LEU	LEU	SER	I705	I705	V537	ASN	P374	GLY	GLY	SER
ASP	ASP	GLY	GLU	L800	M706	F538	ILE	R375	GLY	GLY	PRO
GLN	GLN	SER	ALA	E801	S707		GLY		ASP	GLY	SER
LEU	LEU	LEU	THR		R708	K544	THR		GLY	GLY	SER
LEU	GLU	ALA	ALA	L806			ALA	V379	GLY	GLY	SER
PRO	PRO	GLU	ALA		R709	L548	SER		GLN	GLN	GLN
GLN	GLN	TYR	PRO	T810	D710	L549	SER	D384	ALA	ASP	HIS
ASP	ASP	TRP	GLY	A811	L711		PRO	R295	ASP	GLU	VAL
SER	SER	GLY	THR	R812	F712		ASP	T297	ASP	GLU	SER
SER	SER	GLU	SER		T725	I571	ALA	R301	GLU	GLN	SER
		GLU	THR	Y828	E726	C572	ASN		GLN	GLN	THR
		ARG	GLY				SER	G392	ASP	GLN	GLY
		ARG	ARG	V838		F584	ASN	E401	ASP	ASP	THR
		LEU	LEU	ASP	D732	L585	ASN		GLY	GLY	GLY
		ALA	LVS	VAL	V733		ARG	V407	ASP	ASP	PRO
			LVS	ASP	W736		ARG	T408	ASP	ASP	
							E479	Q409	ASP	ASP	
							T480	L410	ASP	ASP	
							E481	Q411	ASP	ASP	
									ASP	ASP	
									R137	ASP	
									I138	ASP	

- Molecule 5: DNA replication licensing factor MCM6



96%

- Molecule 7: DNA replication regulator SLD3

96%

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	344362	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3200	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	39.670	Depositor
Minimum map value	-19.985	Depositor
Average map value	0.010	Depositor
Map value standard deviation	1.022	Depositor
Recommended contour level	4	Depositor
Map size (Å)	542.7184, 542.7184, 542.7184	wwPDB
Map dimensions	376, 376, 376	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4433999, 1.4433999, 1.4433999	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, 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	0.16	0/5033	0.40	0/6800
1	B	0.16	0/5033	0.40	0/6800
2	3	0.18	0/5033	0.35	0/6823
2	C	0.19	0/5033	0.34	0/6823
3	4	0.16	0/5405	0.37	0/7310
3	D	0.18	0/5405	0.38	0/7310
4	5	0.17	0/5107	0.39	0/6910
4	E	0.18	0/5107	0.40	0/6910
5	6	0.15	0/5207	0.36	0/7026
5	F	0.17	0/5207	0.39	0/7026
6	7	0.18	0/5521	0.37	0/7460
6	G	0.18	0/5521	0.38	0/7460
7	8	0.13	0/237	0.36	0/316
7	X	0.15	0/237	0.48	0/316
8	Y	0.16	0/756	0.48	0/1006
All	All	0.17	0/63842	0.38	0/86296

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	4	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	4	420	TYR	Peptide

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	4947	0	4984	148	0
1	B	4947	0	4984	138	0
2	3	4947	0	5032	106	0
2	C	4947	0	5032	68	0
3	4	5326	0	5385	131	0
3	D	5326	0	5385	150	0
4	5	5033	0	5083	115	0
4	E	5033	0	5083	115	0
5	6	5127	0	5148	125	0
5	F	5127	0	5148	136	0
6	7	5438	0	5507	135	0
6	G	5438	0	5507	123	0
7	8	236	0	221	5	0
7	X	236	0	221	7	0
8	Y	752	0	780	38	0
9	2	27	0	12	0	0
9	3	27	0	12	1	0
9	5	27	0	12	1	0
9	7	27	0	12	1	0
9	B	27	0	12	0	0
9	C	27	0	12	1	0
9	E	27	0	12	0	0
9	G	27	0	12	1	0
10	2	1	0	0	0	0
10	4	1	0	0	0	0
10	5	1	0	0	0	0
10	6	1	0	0	0	0
10	7	1	0	0	0	0
10	B	1	0	0	0	0
10	D	1	0	0	0	0
10	E	1	0	0	0	0
10	F	1	0	0	0	0
10	G	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	63086	0	63596	1405	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 11.

The worst 5 of 1405 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:211:CYS:HB2	4:E:236:CYS:SG	2.03	0.98
2:3:259:GLN:HE21	2:3:271:PRO:HG2	1.31	0.95
1:2:338:LYS:HD3	1:2:379:LYS:HZ1	1.32	0.92
2:3:585:ARG:HD2	2:3:586:LEU:H	1.37	0.87
5:6:535:PRO:HB2	5:6:742:ILE:HD11	1.57	0.86

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	616/868 (71%)	598 (97%)	18 (3%)	0	100	100
1	B	616/868 (71%)	600 (97%)	16 (3%)	0	100	100
2	3	617/971 (64%)	601 (97%)	16 (3%)	0	100	100
2	C	617/971 (64%)	603 (98%)	14 (2%)	0	100	100
3	4	664/933 (71%)	647 (97%)	17 (3%)	0	100	100
3	D	664/933 (71%)	645 (97%)	19 (3%)	0	100	100
4	5	635/775 (82%)	616 (97%)	19 (3%)	0	100	100
4	E	635/775 (82%)	617 (97%)	18 (3%)	0	100	100
5	6	637/1017 (63%)	619 (97%)	18 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	F	637/1017 (63%)	624 (98%)	13 (2%)	0	100	100
6	7	684/845 (81%)	667 (98%)	17 (2%)	0	100	100
6	G	684/845 (81%)	670 (98%)	14 (2%)	0	100	100
7	8	25/668 (4%)	25 (100%)	0	0	100	100
7	X	25/668 (4%)	25 (100%)	0	0	100	100
8	Y	90/257 (35%)	87 (97%)	3 (3%)	0	100	100
All	All	7846/12411 (63%)	7644 (97%)	202 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	2	550/770 (71%)	549 (100%)	1 (0%)	87	85
1	B	550/770 (71%)	550 (100%)	0	100	100
2	3	546/835 (65%)	545 (100%)	1 (0%)	87	85
2	C	546/835 (65%)	546 (100%)	0	100	100
3	4	608/848 (72%)	608 (100%)	0	100	100
3	D	608/848 (72%)	607 (100%)	1 (0%)	87	85
4	5	575/688 (84%)	574 (100%)	1 (0%)	87	85
4	E	575/688 (84%)	574 (100%)	1 (0%)	87	85
5	6	566/886 (64%)	565 (100%)	1 (0%)	87	85
5	F	566/886 (64%)	566 (100%)	0	100	100
6	7	609/753 (81%)	609 (100%)	0	100	100
6	G	609/753 (81%)	609 (100%)	0	100	100
7	8	29/628 (5%)	29 (100%)	0	100	100
7	X	29/628 (5%)	29 (100%)	0	100	100
8	Y	87/234 (37%)	87 (100%)	0	100	100

Continued on next page...

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7053/11050 (64%)	7047 (100%)	6 (0%)	87 87

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	6	673	ASN
3	D	488	ASN
4	E	344	ASN
2	3	293	ASN
1	2	551	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	581	ASN
4	E	676	HIS
6	G	311	GLN
4	5	584	GLN
4	5	576	HIS

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 18 ligands modelled in this entry, 10 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
9	ADP	5	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.93	10 (23%)
9	ADP	E	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.95	10 (23%)
9	ADP	7	1001	-	27,29,29	1.32	4 (14%)	42,45,45	1.99	9 (21%)
9	ADP	B	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.97	9 (21%)
9	ADP	2	1001	-	27,29,29	1.34	4 (14%)	42,45,45	2.00	11 (26%)
9	ADP	C	1001	-	27,29,29	1.35	4 (14%)	42,45,45	1.96	10 (23%)
9	ADP	G	1001	-	27,29,29	1.33	4 (14%)	42,45,45	1.97	9 (21%)
9	ADP	3	1001	-	27,29,29	1.34	4 (14%)	42,45,45	1.95	11 (26%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	5	1001	-	-	5/16/32/32	0/3/3/3
9	ADP	E	1001	-	-	5/16/32/32	0/3/3/3
9	ADP	7	1001	-	-	5/16/32/32	0/3/3/3
9	ADP	B	1001	-	-	5/16/32/32	0/3/3/3
9	ADP	2	1001	-	-	7/16/32/32	0/3/3/3
9	ADP	C	1001	-	-	4/16/32/32	0/3/3/3
9	ADP	G	1001	-	-	4/16/32/32	0/3/3/3
9	ADP	3	1001	-	-	5/16/32/32	0/3/3/3

The worst 5 of 32 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	1001	ADP	C5-C4	4.43	1.47	1.39
9	B	1001	ADP	C5-C4	4.39	1.47	1.39
9	G	1001	ADP	C5-C4	4.38	1.47	1.39
9	7	1001	ADP	C5-C4	4.36	1.47	1.39
9	C	1001	ADP	C5-C4	4.36	1.47	1.39

The worst 5 of 79 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	7	1001	ADP	C5-C4-N3	-6.37	118.44	126.75
9	B	1001	ADP	C5-C4-N3	-6.22	118.64	126.75
9	5	1001	ADP	C5-C4-N3	-6.16	118.71	126.75
9	2	1001	ADP	C5-C4-N3	-6.13	118.75	126.75
9	G	1001	ADP	C5-C4-N3	-6.12	118.77	126.75

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

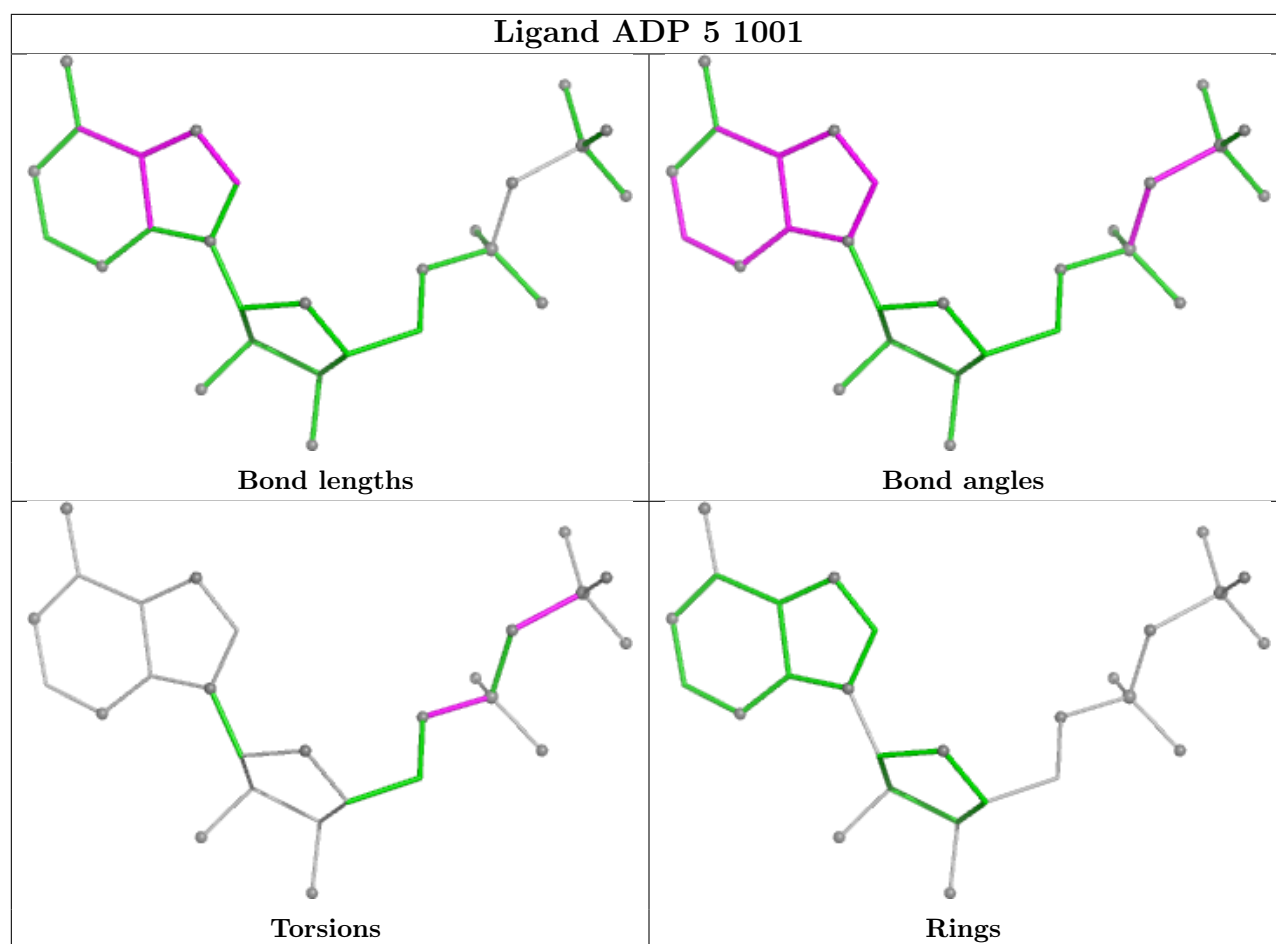
Mol	Chain	Res	Type	Atoms
9	2	1001	ADP	C5'-O5'-PA-O1A
9	2	1001	ADP	C5'-O5'-PA-O2A
9	3	1001	ADP	PA-O3A-PB-O2B
9	3	1001	ADP	C5'-O5'-PA-O1A
9	3	1001	ADP	C5'-O5'-PA-O2A

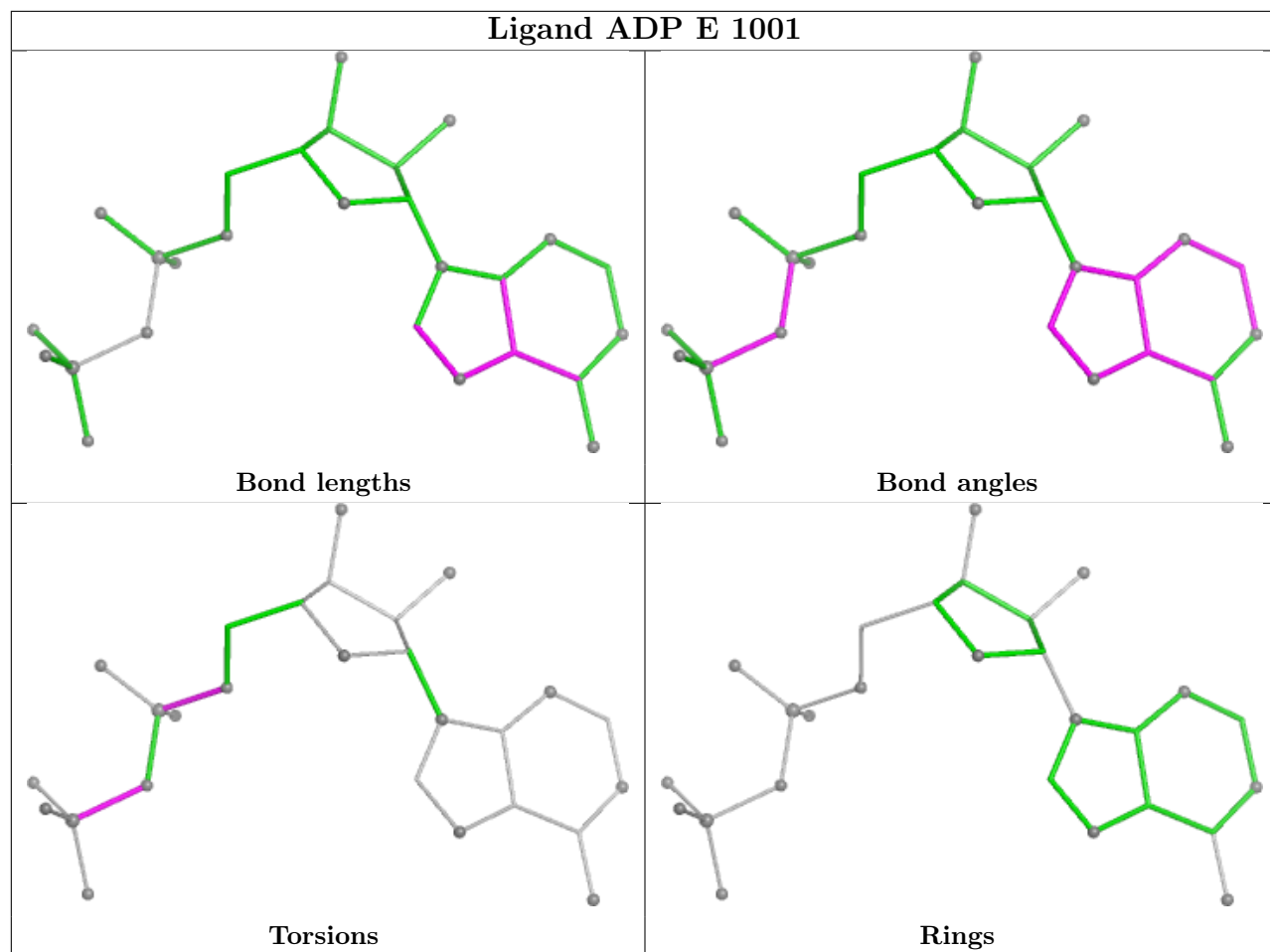
There are no ring outliers.

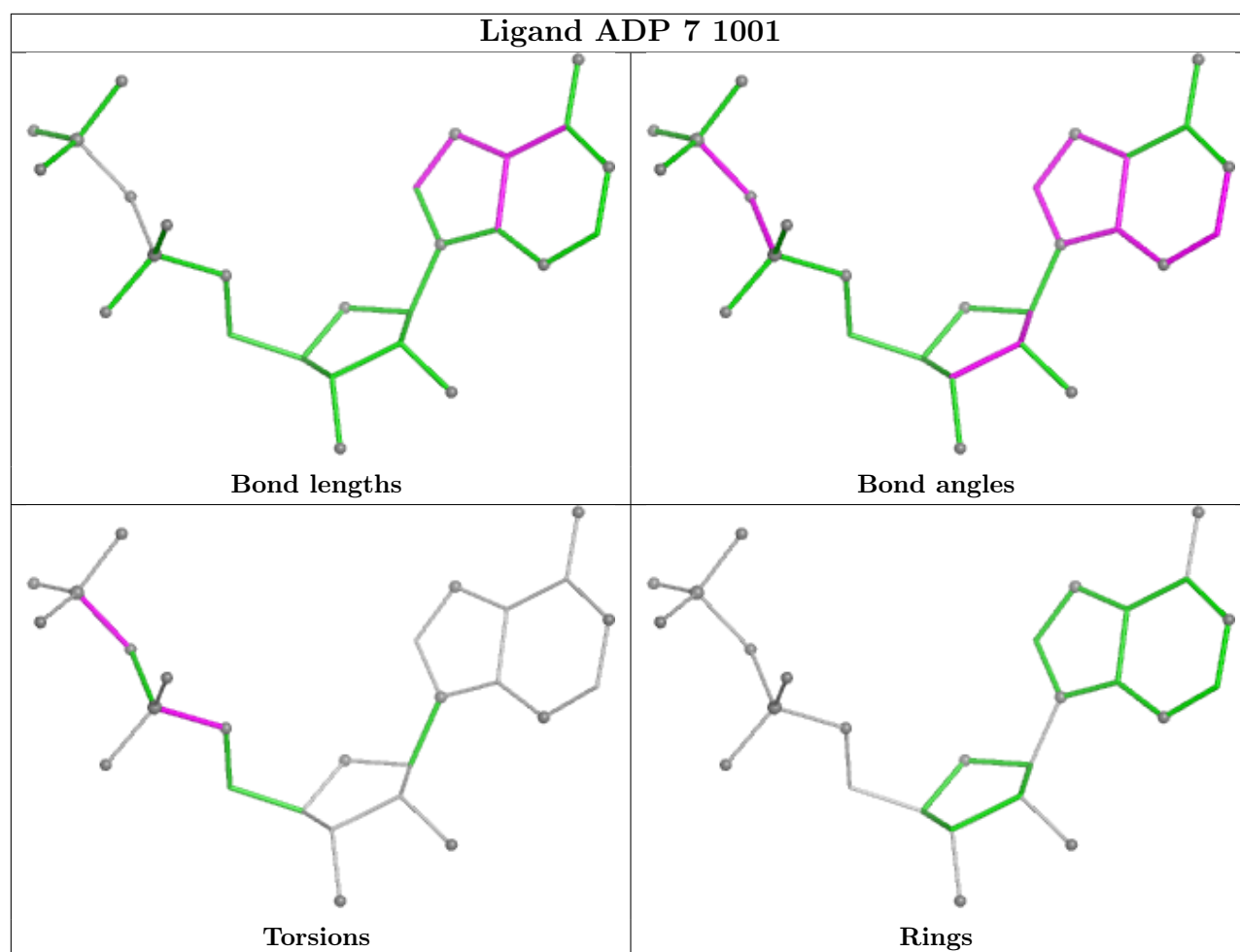
5 monomers are involved in 5 short contacts:

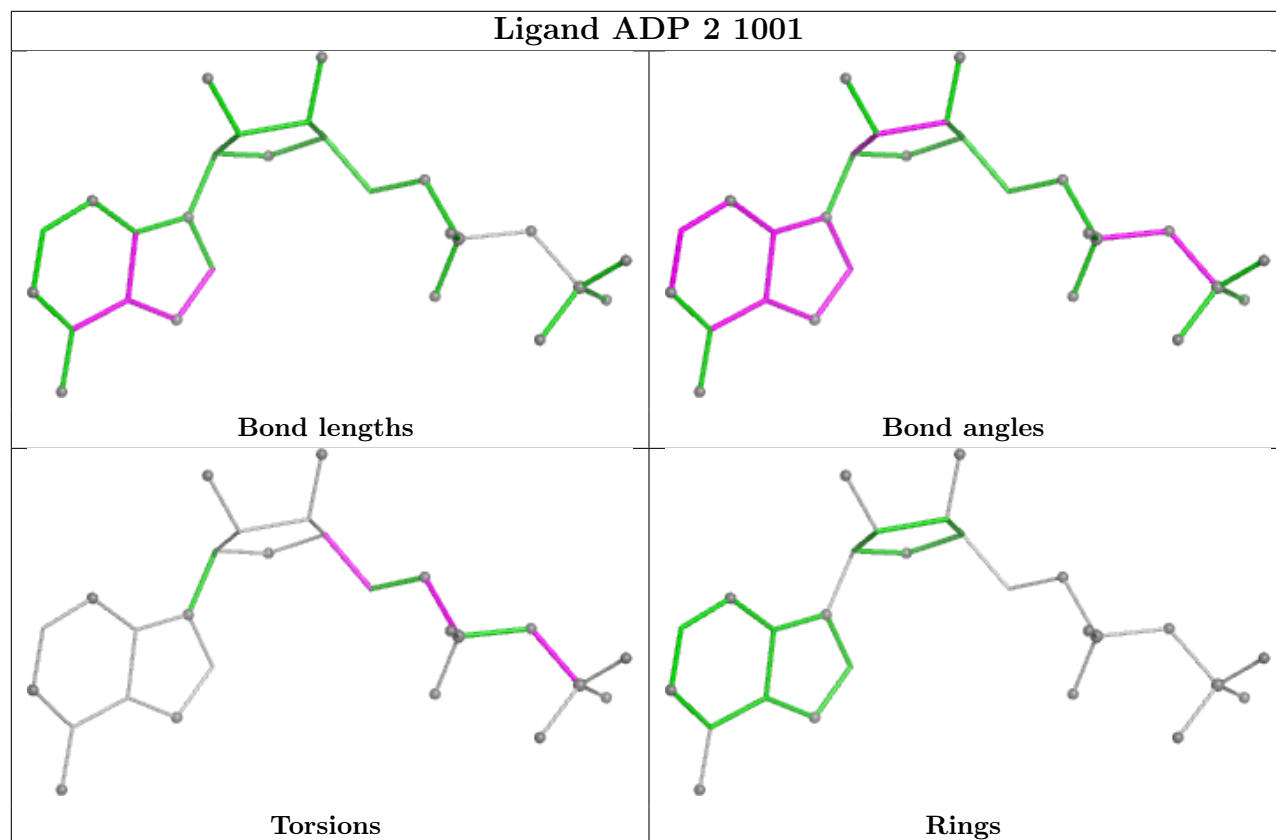
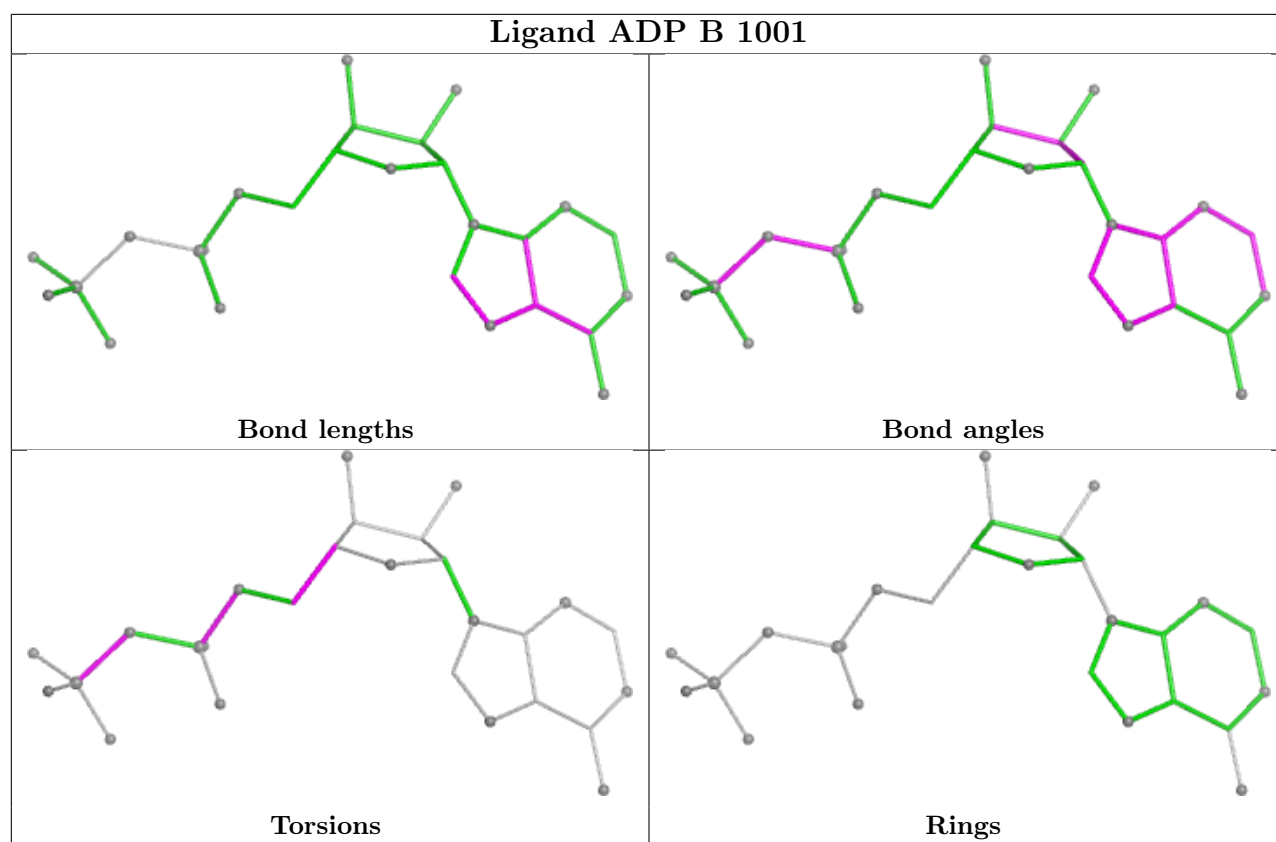
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	5	1001	ADP	1	0
9	7	1001	ADP	1	0
9	C	1001	ADP	1	0
9	G	1001	ADP	1	0
9	3	1001	ADP	1	0

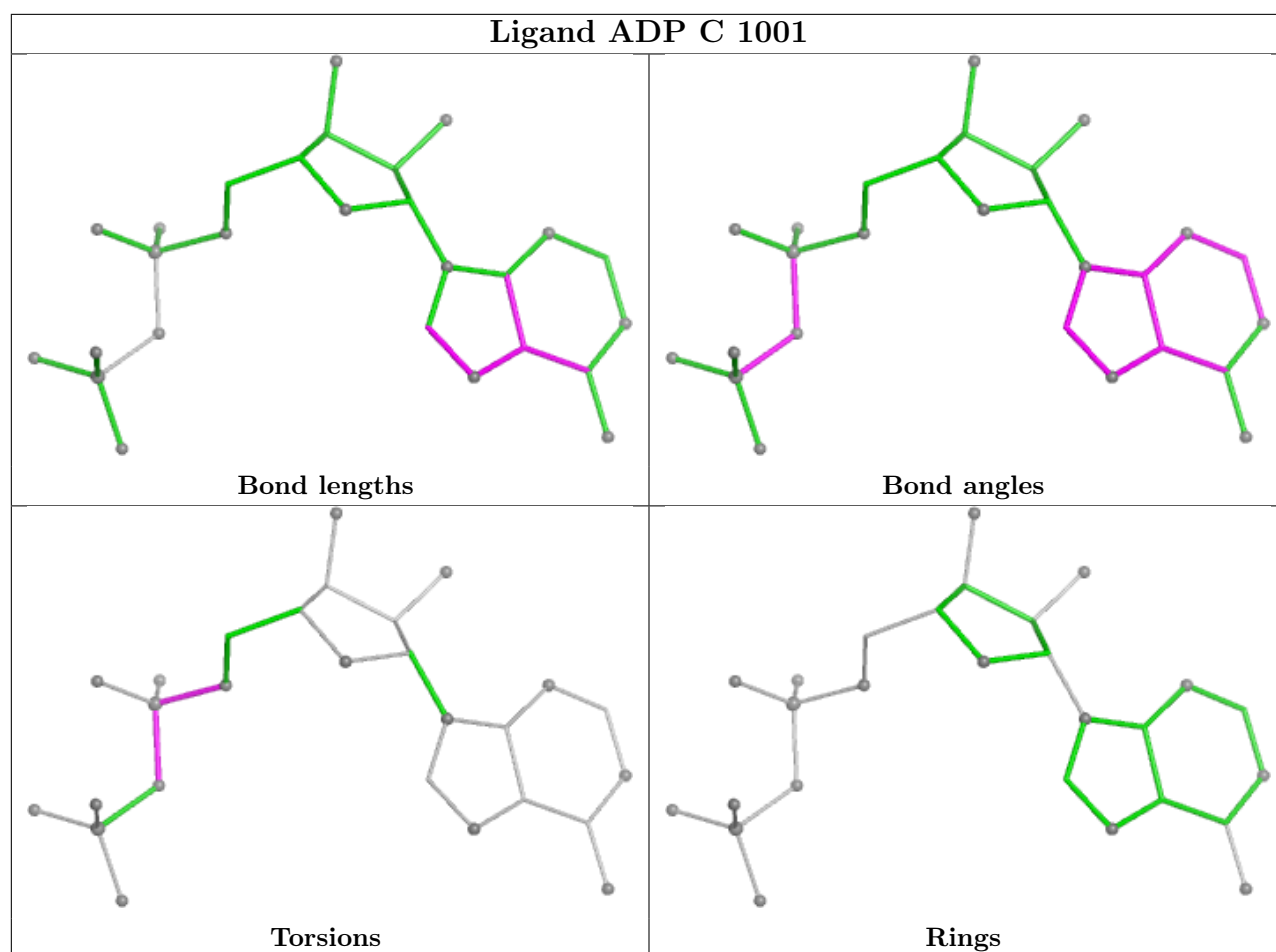
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

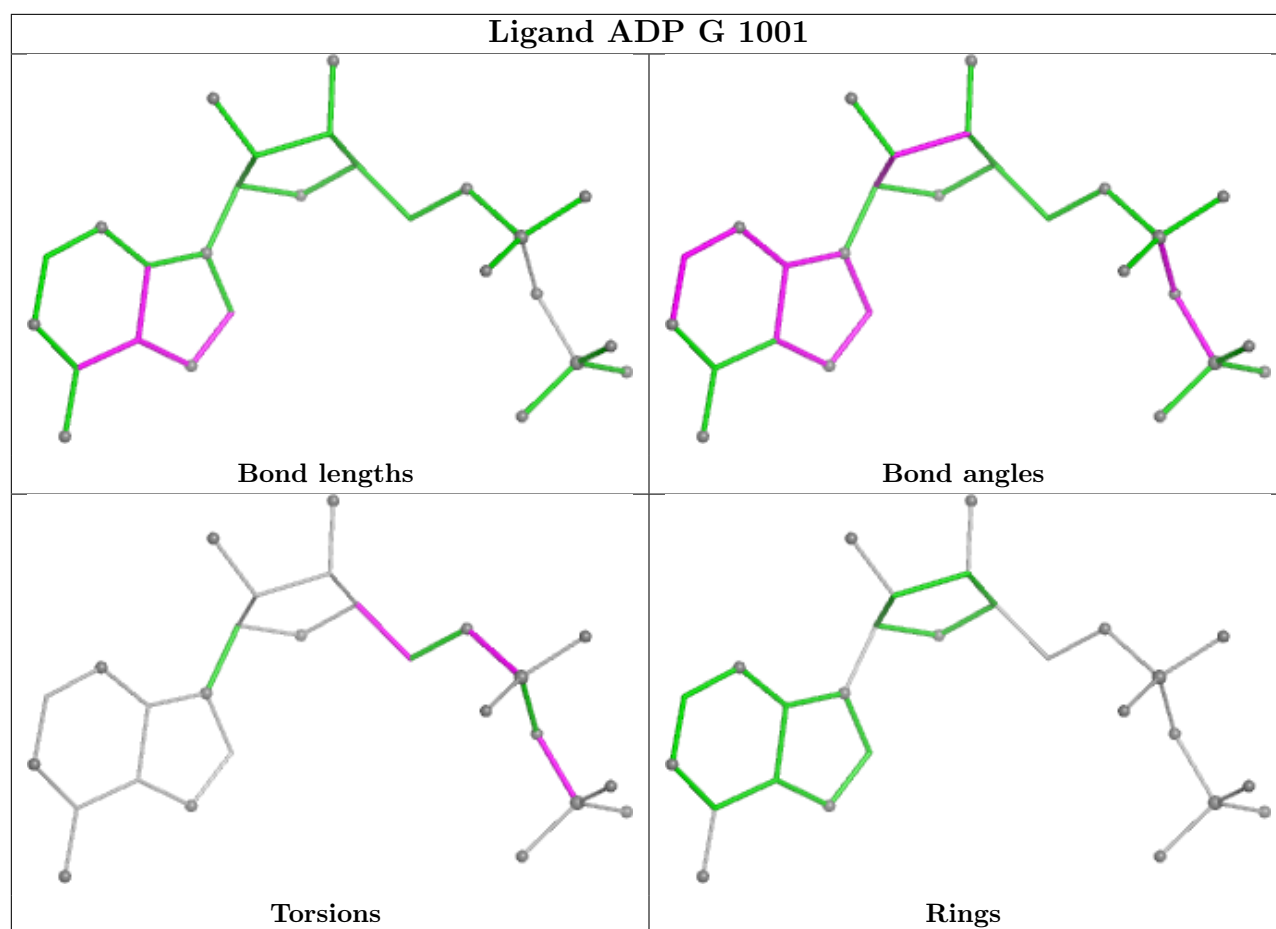


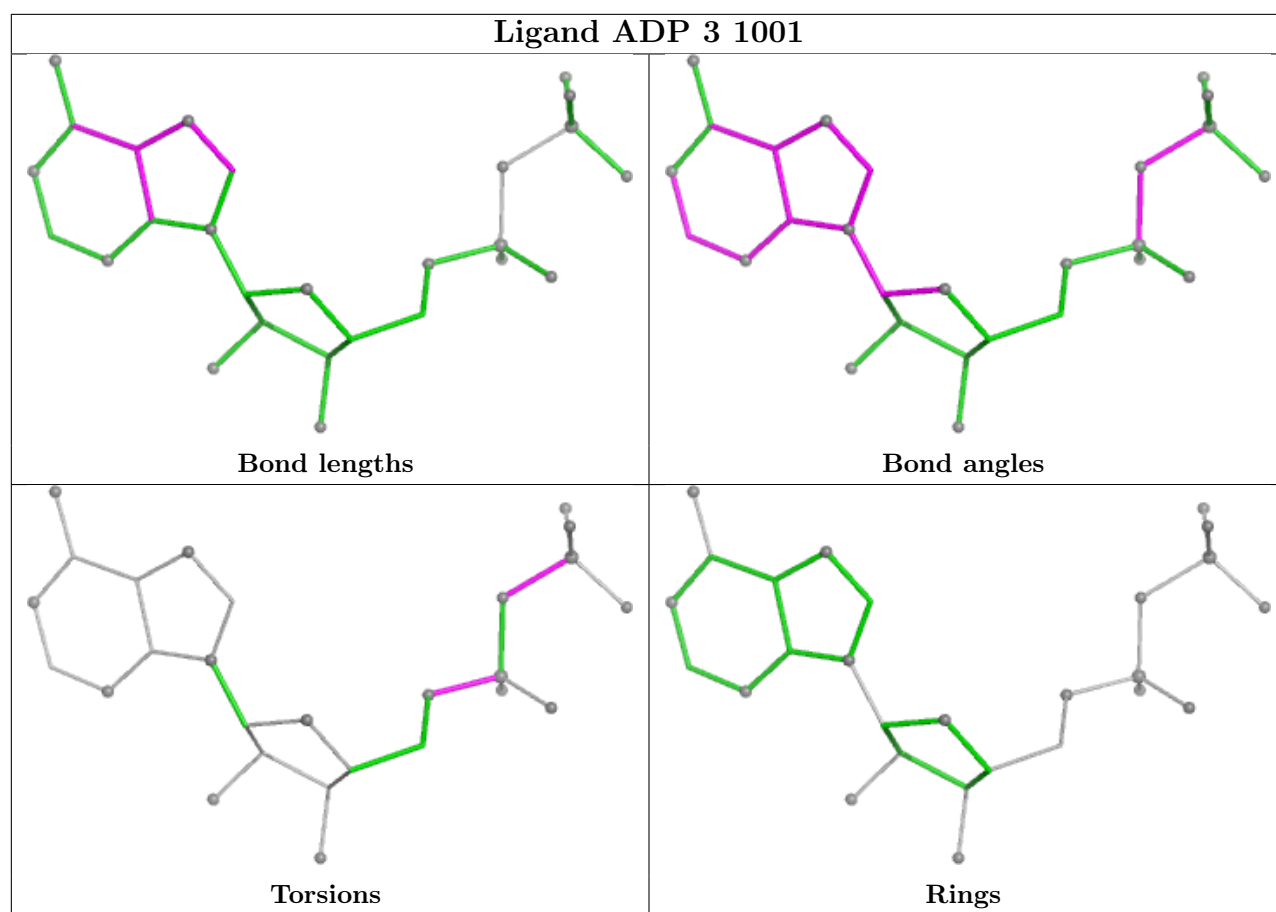












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

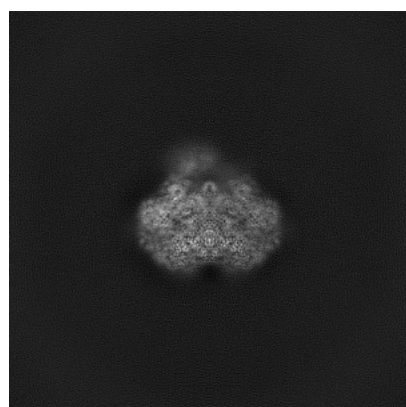
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-55904. These allow visual inspection of the internal detail of the map and identification of artifacts.

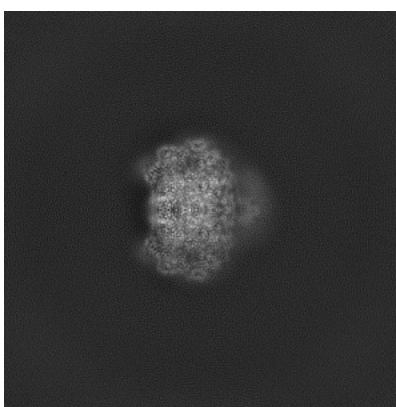
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

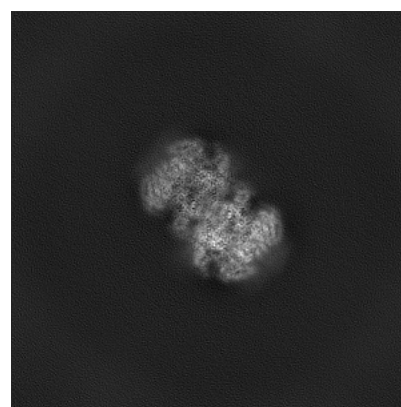
6.1.1 Primary map



X



Y

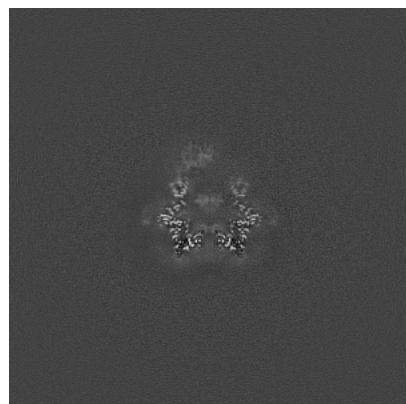


Z

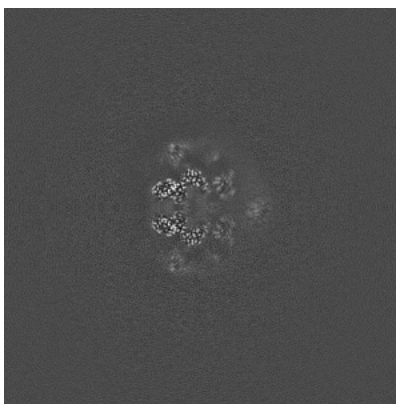
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

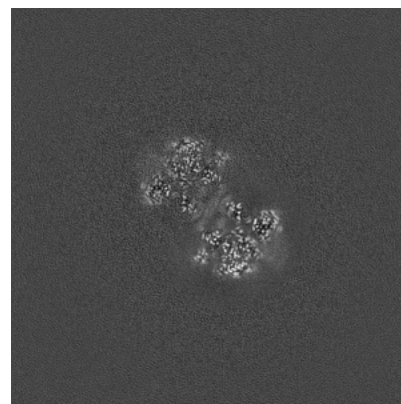
6.2.1 Primary map



X Index: 188



Y Index: 188

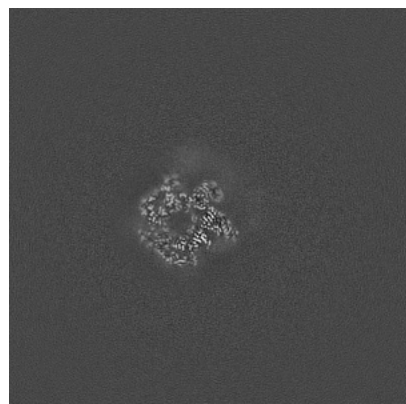


Z Index: 188

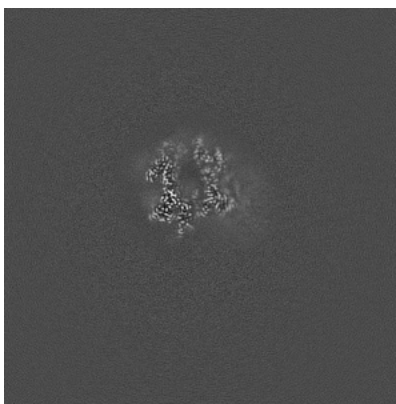
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

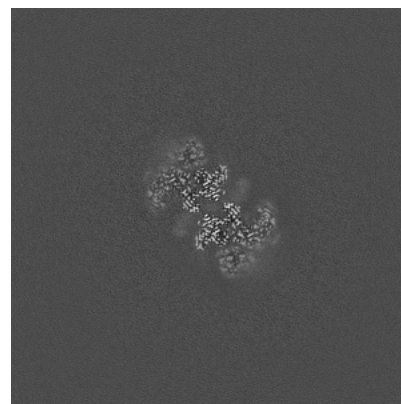
6.3.1 Primary map



X Index: 214



Y Index: 160

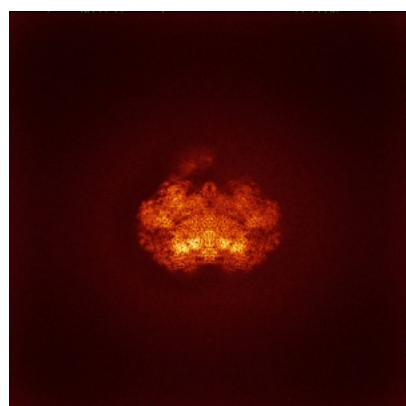


Z Index: 155

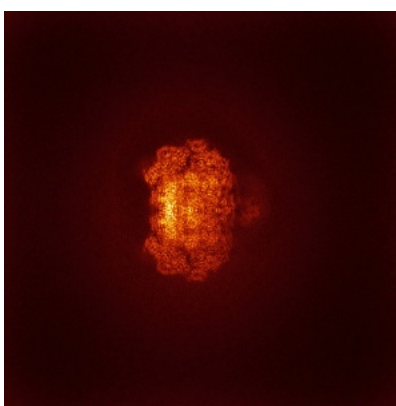
The images above show the largest variance slices of the map in three orthogonal directions.

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

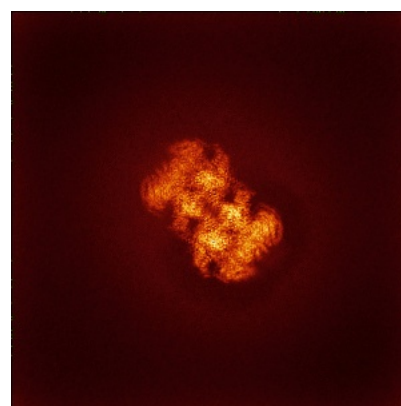
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.0. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

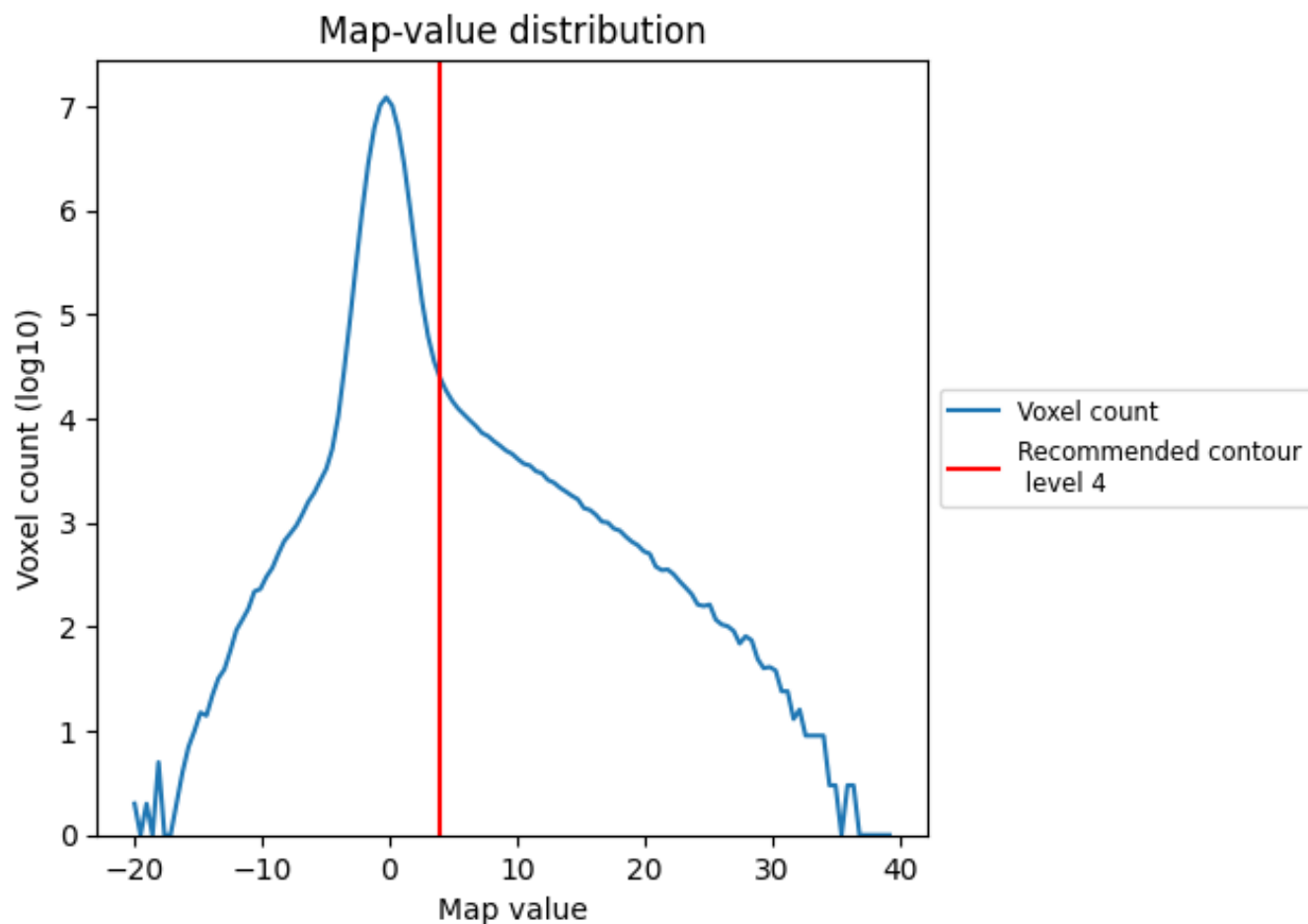
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

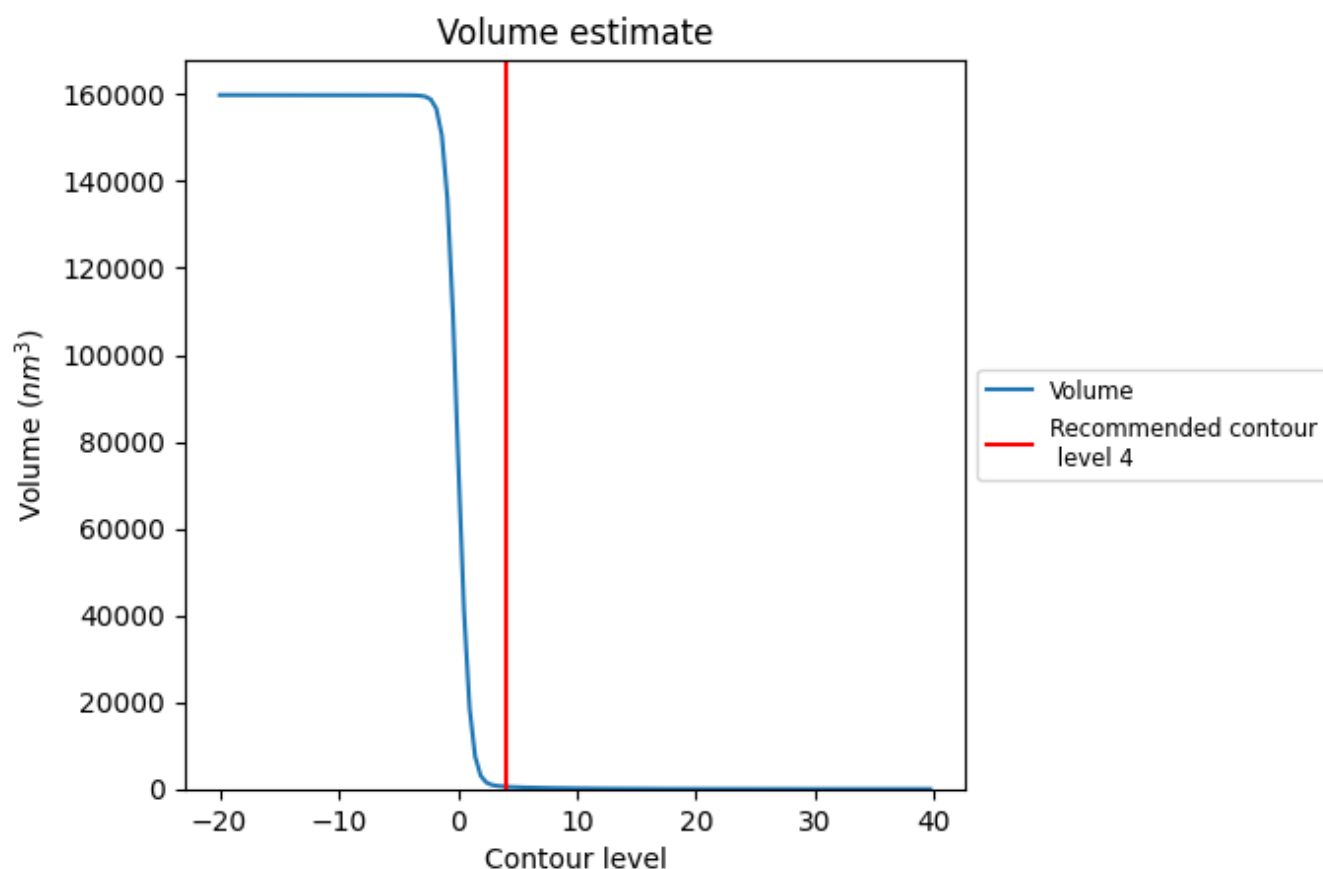
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

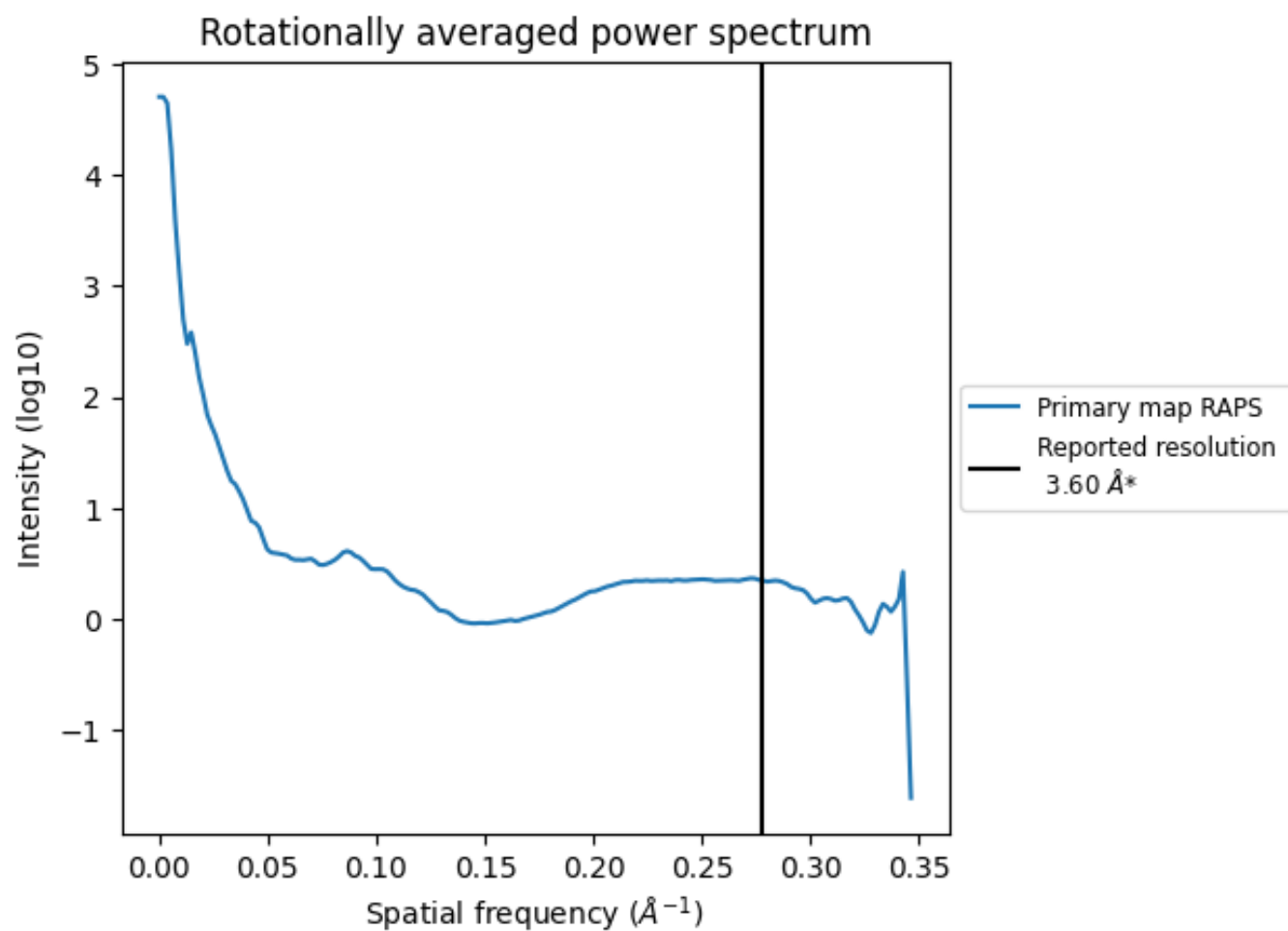
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 534 nm^3 ; this corresponds to an approximate mass of 482 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 0.278 Å⁻¹

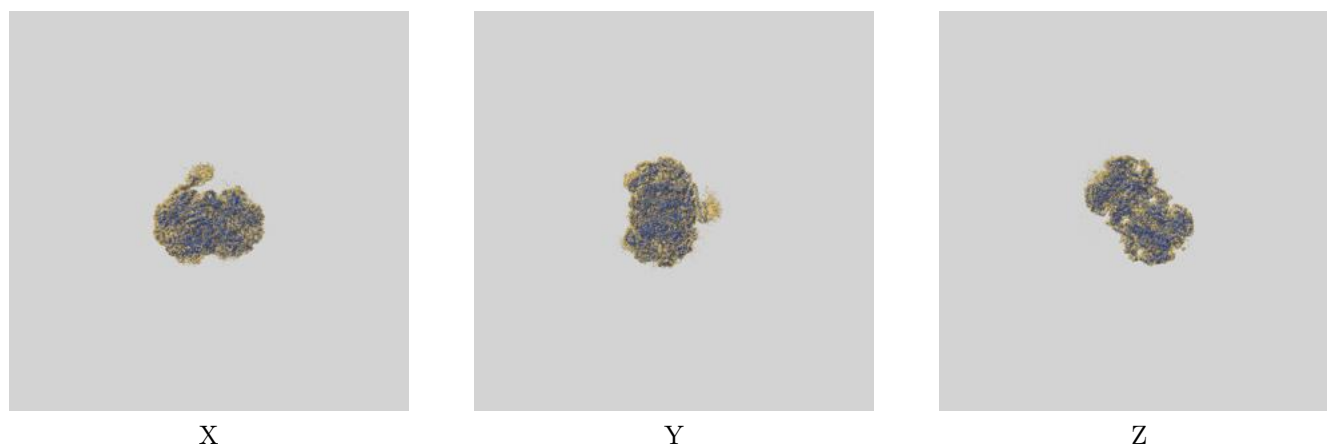
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

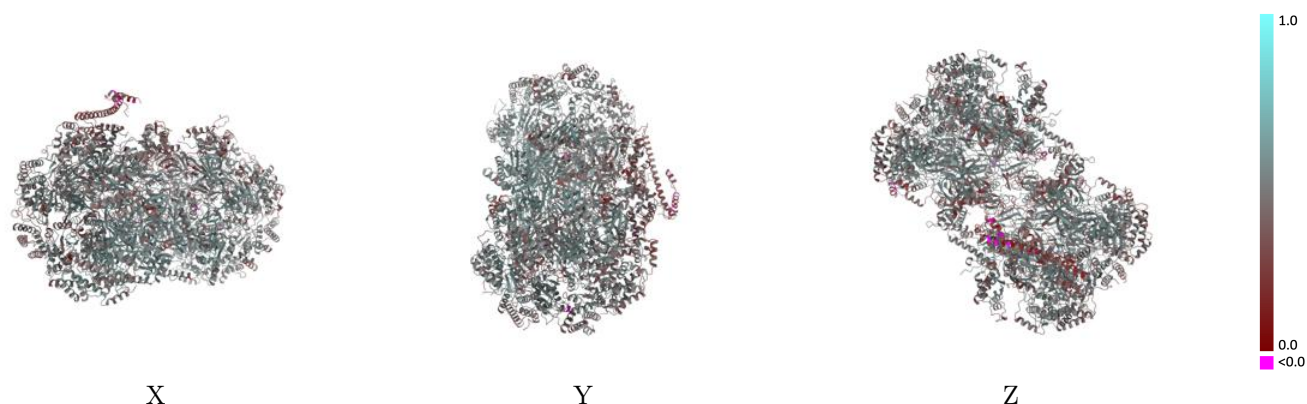
This section contains information regarding the fit between EMDB map EMD-55904 and PDB model 9TGM. Per-residue inclusion information can be found in section [3](#) on page [8](#).

9.1 Map-model overlay [i](#)



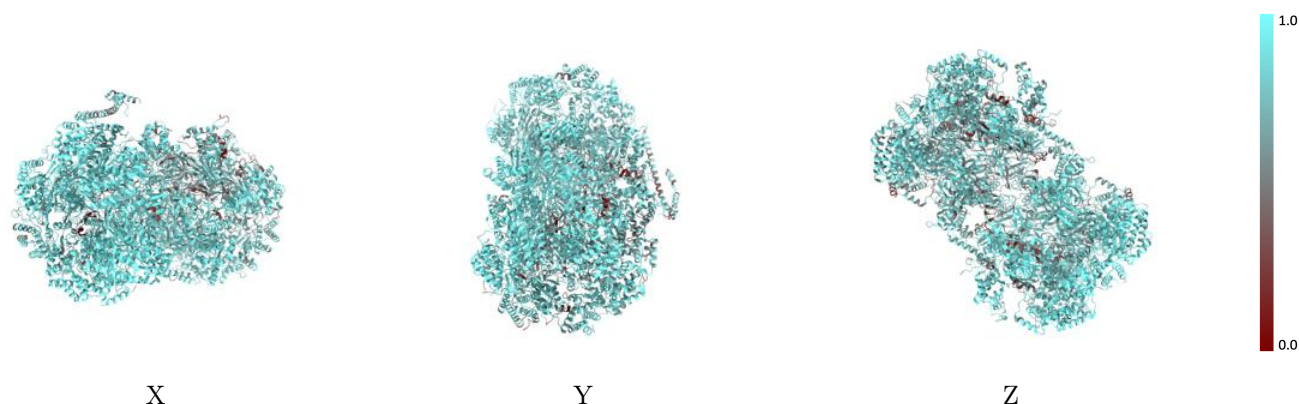
The images above show the 3D surface view of the map at the recommended contour level 4.0 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



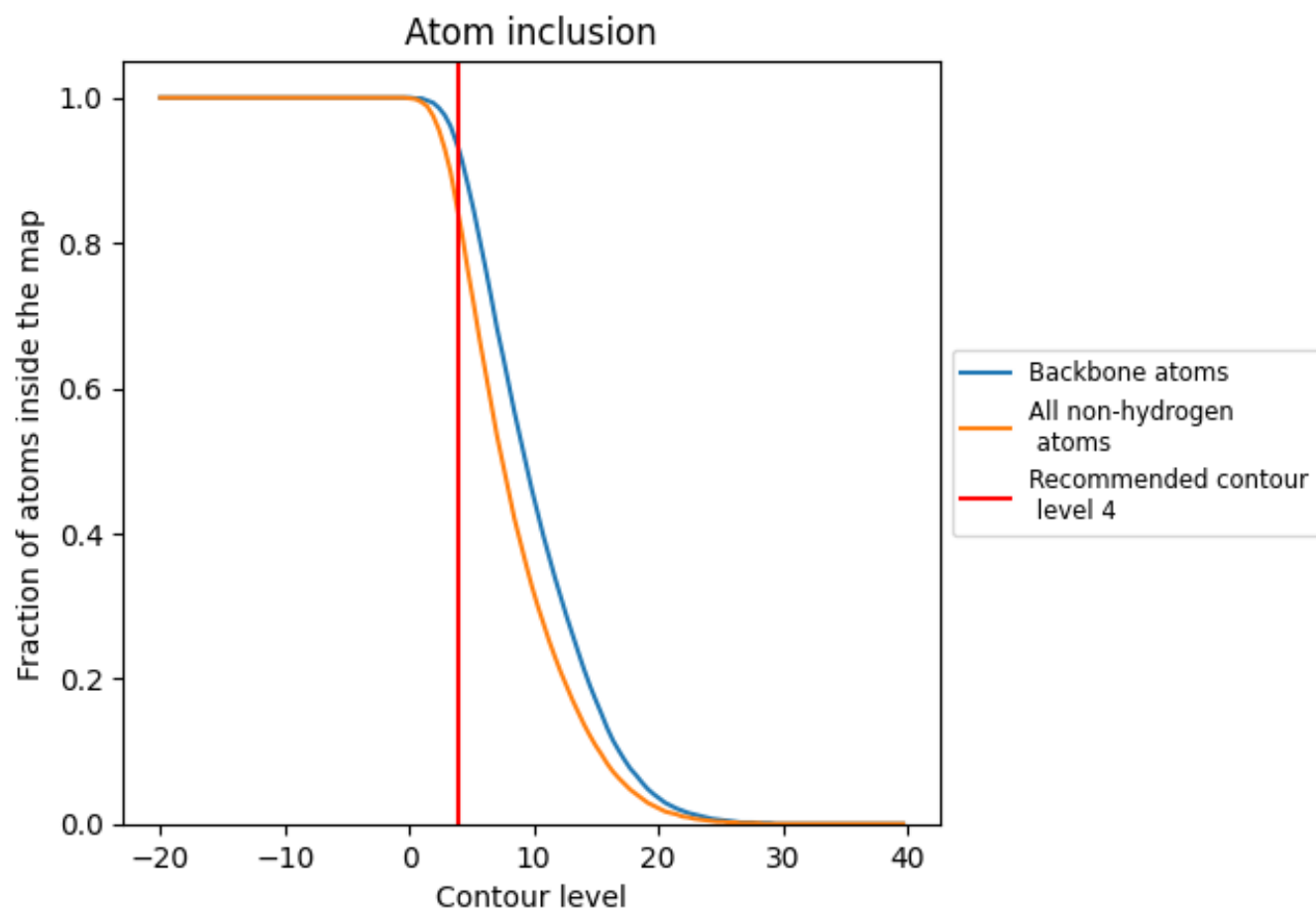
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (4).

9.4 Atom inclusion [i](#)



At the recommended contour level, 93% of all backbone atoms, 84% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8360	0.4770
2	0.7510	0.4530
3	0.8820	0.5270
4	0.7980	0.4780
5	0.8090	0.4880
6	0.7280	0.4530
7	0.8330	0.4880
8	0.3550	0.3700
B	0.8660	0.4530
C	0.9260	0.5310
D	0.8870	0.4710
E	0.8700	0.4920
F	0.8570	0.4450
G	0.8780	0.4910
X	0.5560	0.3680
Y	0.6930	0.2350

