wwPDB EM Validation Summary Report (i)

Aug 26, 2026 – 01:47 pm BST

PDB ID	:	9Q93 / pdb_00009q93
EMDB ID	:	EMD-52916
Title	:	CryoEM structure of bacterial transcription intermediate complex mediated by activator PspF containing nifH promoter DNA containing mismatch from -11 to -8 - conformation 4
Authors	:	Gao, F.; Zhang, X.
Deposited on	:	2025-02-26
Resolution	:	6.60 Å(reported)

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 (i) 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 (i)) were used in the production of this report:

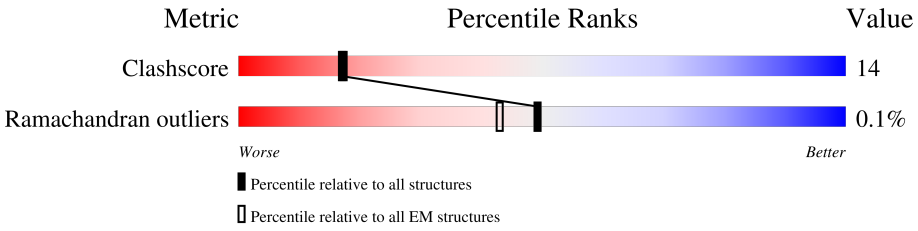
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

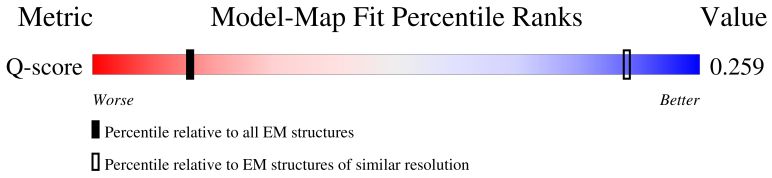
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.60 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.





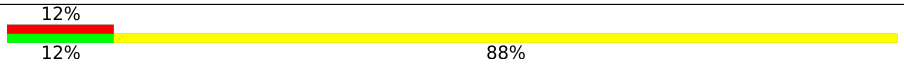
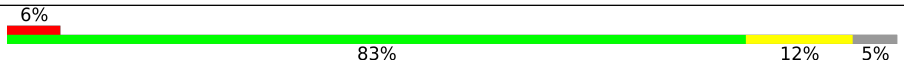
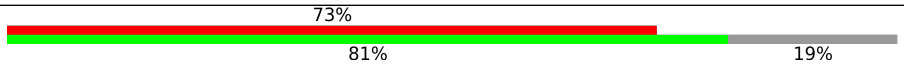
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Q-score	-	25397	531 (6.10 - 7.10)

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 <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	1	259	89% 8%
1	2	259	83% 15%
1	3	259	84% 14%
1	4	259	80% 19%
1	5	259	82% 17%

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Mol	Chain	Length	Quality of chain
1	6	259	
2	M	497	
3	N	34	
4	T	34	
5	A	329	
5	B	329	
6	C	1341	
7	D	1407	
8	E	91	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	AF3	3	602	-	-	X	-
10	AF3	4	602	-	-	X	-
9	ADP	3	601	-	-	X	-
9	ADP	5	601	-	-	X	-

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 26918 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 Psp operon transcriptional activator.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	6	253	Total 1247	C 741	N 253	O 253	0	0
1	1	253	Total 1247	C 741	N 253	O 253	0	0
1	2	255	Total 1257	C 747	N 255	O 255	0	0
1	3	255	Total 1257	C 747	N 255	O 255	0	0
1	4	259	Total 1277	C 759	N 259	O 259	0	0
1	5	257	Total 1267	C 753	N 257	O 257	0	0

- Molecule 2 is a protein called RNA polymerase sigma-54 factor.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	M	413	Total 2050	C 1223	N 413	O 414	0	0

There are 45 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	-19	MET	-	initiating methionine	UNP A0A377VEN9
M	-18	GLY	-	expression tag	UNP A0A377VEN9
M	-17	SER	-	expression tag	UNP A0A377VEN9
M	-16	SER	-	expression tag	UNP A0A377VEN9
M	-15	HIS	-	expression tag	UNP A0A377VEN9
M	-14	HIS	-	expression tag	UNP A0A377VEN9
M	-13	HIS	-	expression tag	UNP A0A377VEN9
M	-12	HIS	-	expression tag	UNP A0A377VEN9
M	-11	HIS	-	expression tag	UNP A0A377VEN9
M	-10	HIS	-	expression tag	UNP A0A377VEN9
M	-9	SER	-	expression tag	UNP A0A377VEN9

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-8	SER	-	expression tag	UNP A0A377VEN9
M	-7	GLY	-	expression tag	UNP A0A377VEN9
M	-6	LEU	-	expression tag	UNP A0A377VEN9
M	-5	VAL	-	expression tag	UNP A0A377VEN9
M	-4	PRO	-	expression tag	UNP A0A377VEN9
M	-3	ARG	-	expression tag	UNP A0A377VEN9
M	-2	GLY	-	expression tag	UNP A0A377VEN9
M	-1	SER	-	expression tag	UNP A0A377VEN9
M	0	HIS	-	expression tag	UNP A0A377VEN9
M	1	MET	-	expression tag	UNP A0A377VEN9
M	2	LYS	-	expression tag	UNP A0A377VEN9
M	3	GLN	-	expression tag	UNP A0A377VEN9
M	4	GLY	-	expression tag	UNP A0A377VEN9
M	5	LEU	-	expression tag	UNP A0A377VEN9
M	6	GLN	-	expression tag	UNP A0A377VEN9
M	7	LEU	-	expression tag	UNP A0A377VEN9
M	8	ARG	-	expression tag	UNP A0A377VEN9
M	9	LEU	-	expression tag	UNP A0A377VEN9
M	10	SER	-	expression tag	UNP A0A377VEN9
M	11	GLN	-	expression tag	UNP A0A377VEN9
M	12	GLN	-	expression tag	UNP A0A377VEN9
M	13	LEU	-	expression tag	UNP A0A377VEN9
M	14	ALA	-	expression tag	UNP A0A377VEN9
M	15	MET	-	expression tag	UNP A0A377VEN9
M	16	THR	-	expression tag	UNP A0A377VEN9
M	17	PRO	-	expression tag	UNP A0A377VEN9
M	18	GLN	-	expression tag	UNP A0A377VEN9
M	19	LEU	-	expression tag	UNP A0A377VEN9
M	20	GLN	-	expression tag	UNP A0A377VEN9
M	21	GLN	-	expression tag	UNP A0A377VEN9
M	22	ALA	-	expression tag	UNP A0A377VEN9
M	23	ILE	-	expression tag	UNP A0A377VEN9
M	24	ARG	-	expression tag	UNP A0A377VEN9
M	25	LEU	-	expression tag	UNP A0A377VEN9

- Molecule 3 is a DNA chain called Non-template DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	N	34	Total	C	N	O	P	0	0
			694	329	127	204	34		

- Molecule 4 is a DNA chain called Template DNA (34-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
4	T	34	Total	C	N	O	P	0	0
			700	331	131	204	34		

- Molecule 5 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	A	229	Total	C	N	O	0	0
			1130	672	229	229		
5	B	223	Total	C	N	O	0	0
			1101	655	223	223		

- Molecule 6 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	C	1341	Total	C	N	O	0	0
			6599	3917	1341	1341		

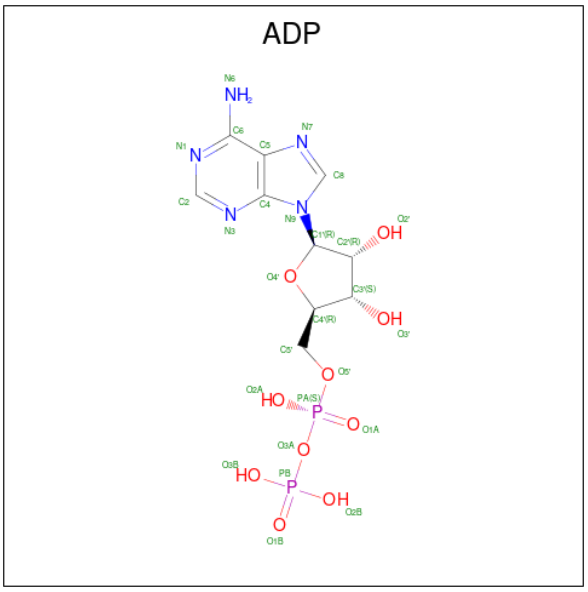
- Molecule 7 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms				AltConf	Trace
7	D	1334	Total	C	N	O	0	0
			6566	3898	1334	1334		

- Molecule 8 is a protein called DNA-directed RNA polymerase subunit omega.

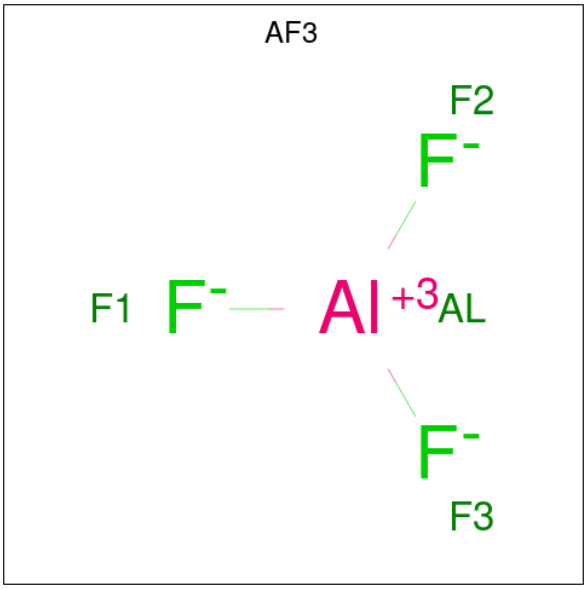
Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	74	Total	C	N	O	0	0
			366	218	74	74		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
9	1	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	2	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	3	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	4	1	Total	C	N	O	P	0
			27	10	5	10	2	
9	5	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 10 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).



Mol	Chain	Residues	Atoms	AltConf
10	1	1	Total Al F 4 1 3	0
10	2	1	Total Al F 4 1 3	0
10	3	1	Total Al F 4 1 3	0
10	4	1	Total Al F 4 1 3	0
10	5	1	Total Al F 4 1 3	0

- Molecule 11 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
11	1	1	Total Mg 1 1	0
11	2	1	Total Mg 1 1	0
11	3	1	Total Mg 1 1	0
11	4	1	Total Mg 1 1	0
11	5	1	Total Mg 1 1	0

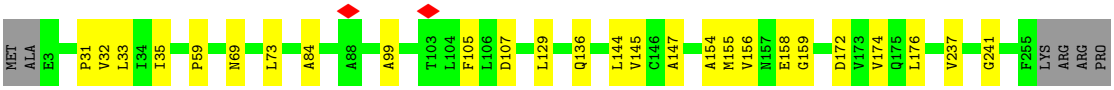
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Psp operon transcriptional activator

Chain 6:

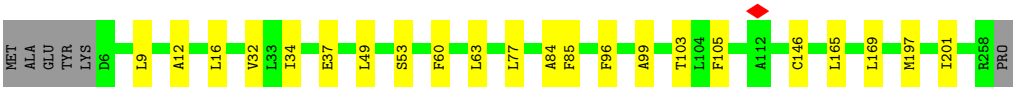




• Molecule 1: Psp operon transcriptional activator

Chain 1:

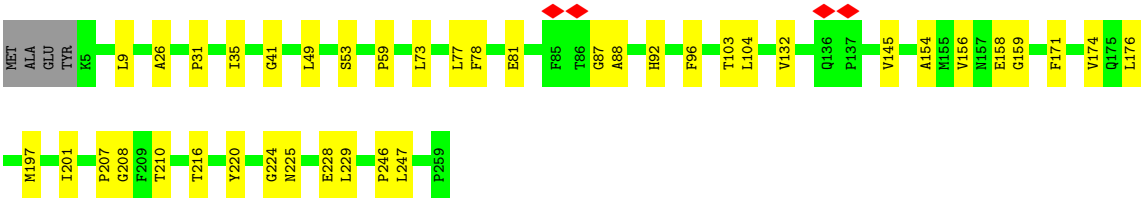




• Molecule 1: Psp operon transcriptional activator

Chain 2:

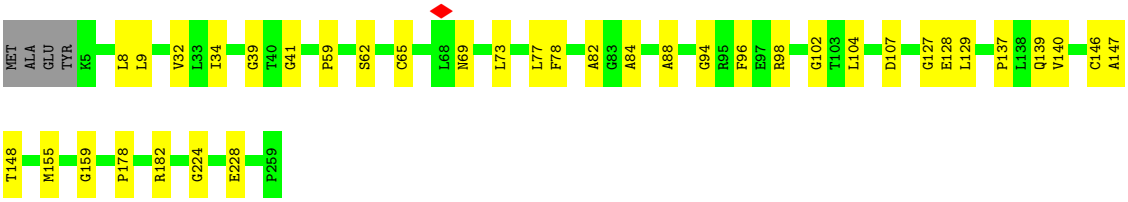




• Molecule 1: Psp operon transcriptional activator

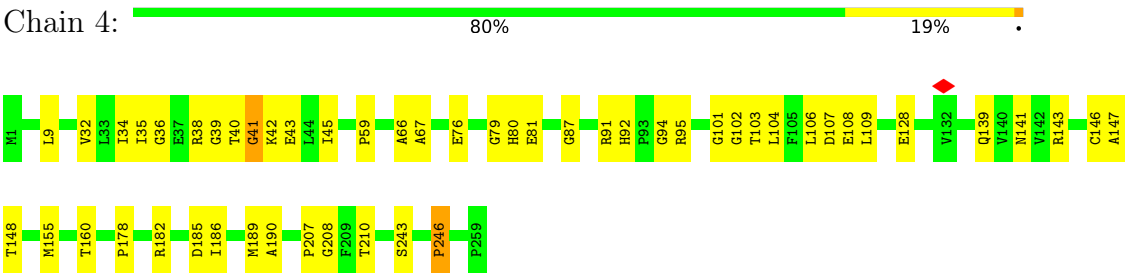
Chain 3:





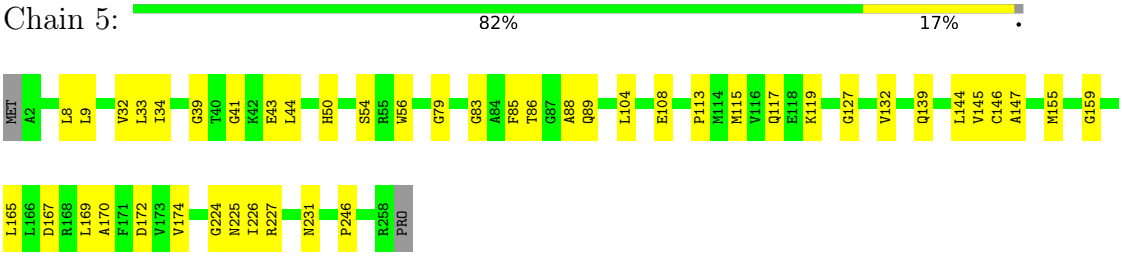
• Molecule 1: Psp operon transcriptional activator

Chain 4:



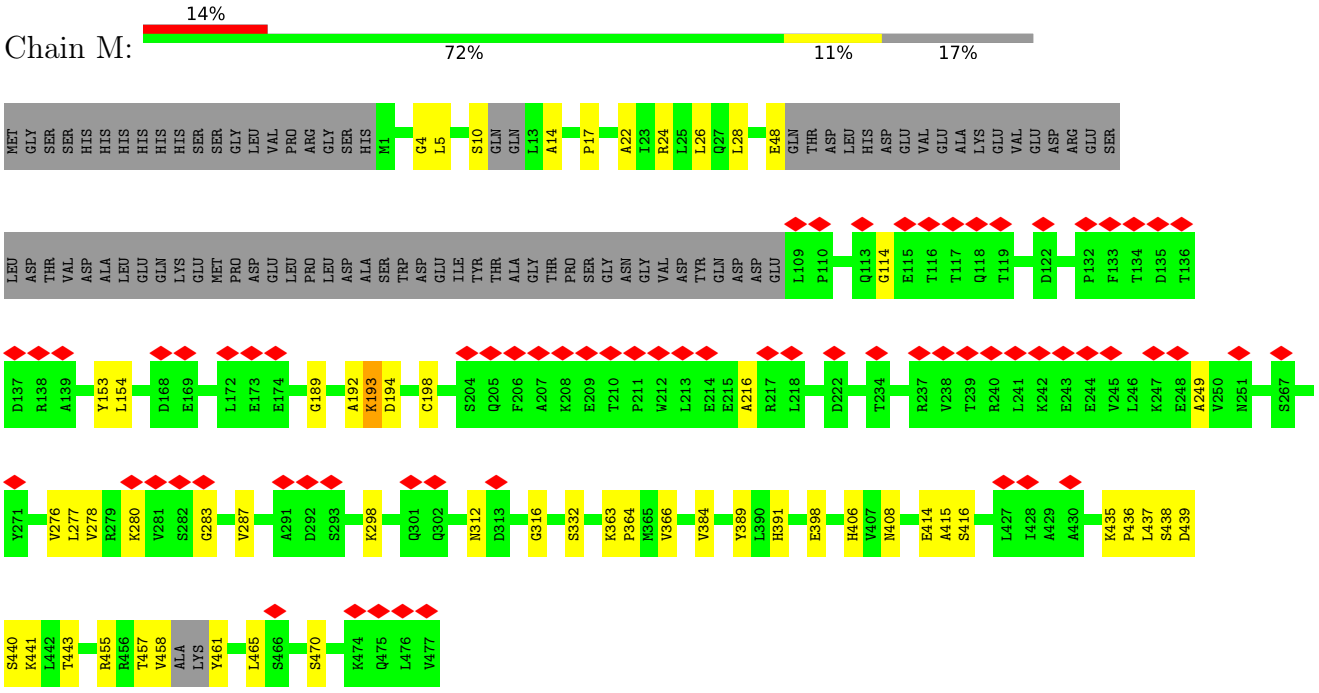
• Molecule 1: Psp operon transcriptional activator

Chain 5:



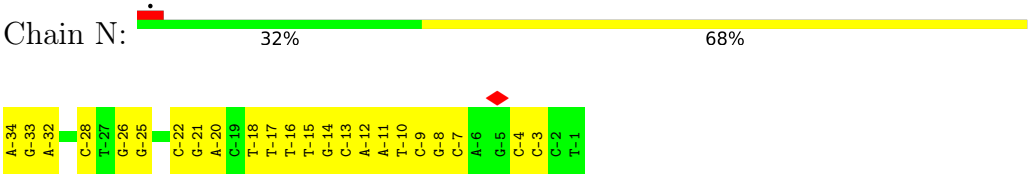
• Molecule 2: RNA polymerase sigma-54 factor

Chain M:



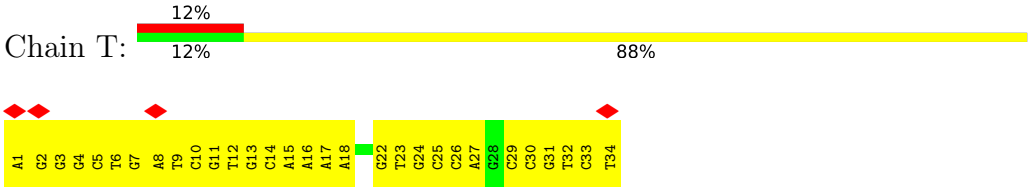
• Molecule 3: Non-template DNA (34-MER)

Chain N:



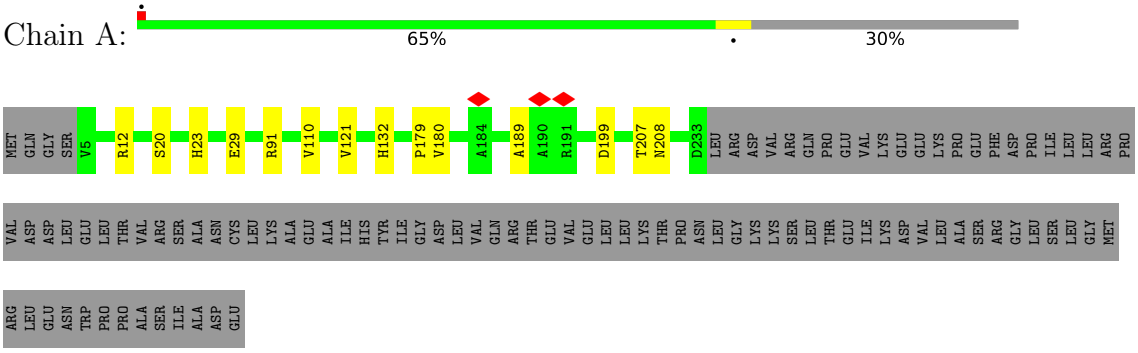
• Molecule 4: Template DNA (34-MER)

Chain T:



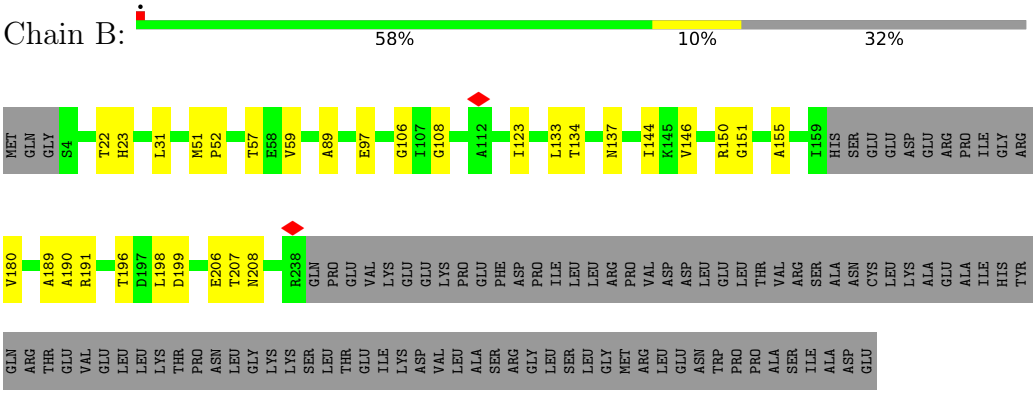
• Molecule 5: DNA-directed RNA polymerase subunit alpha

Chain A:



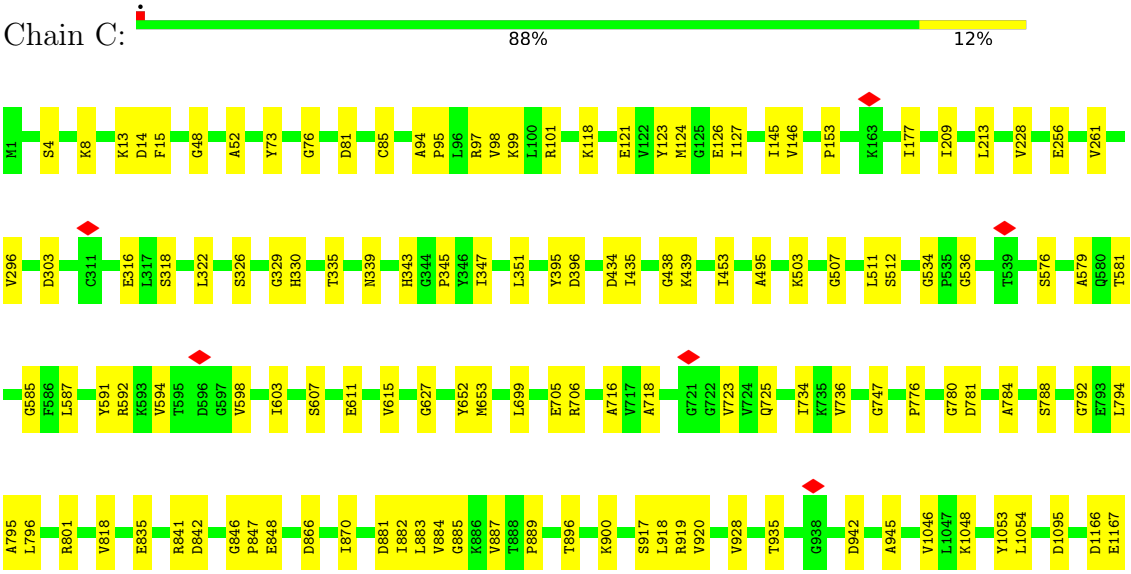
• Molecule 5: DNA-directed RNA polymerase subunit alpha

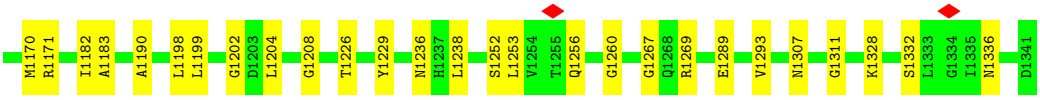
Chain B:



• Molecule 6: DNA-directed RNA polymerase subunit beta

Chain C:

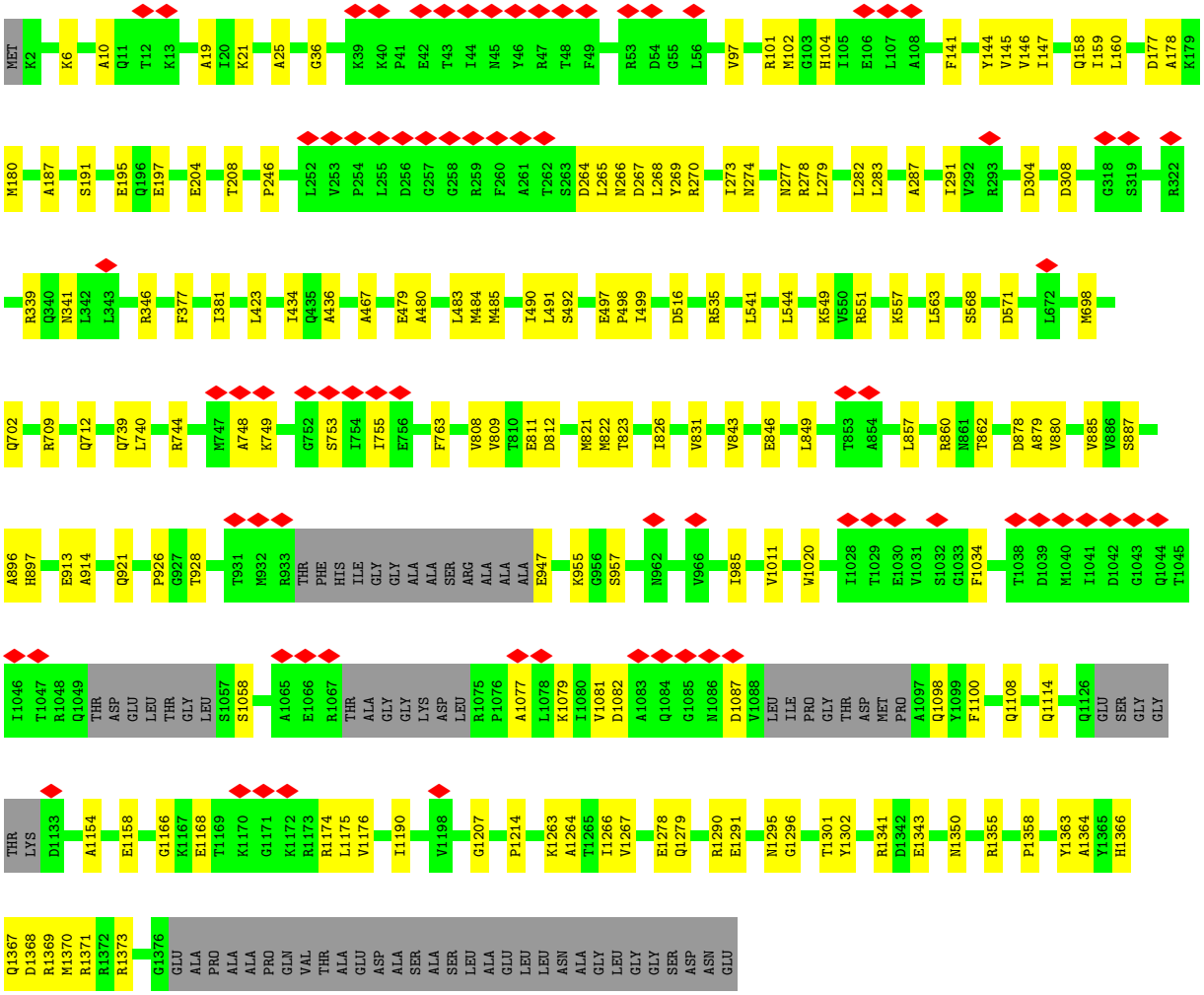




• Molecule 7: DNA-directed RNA polymerase subunit beta'

Chain D:

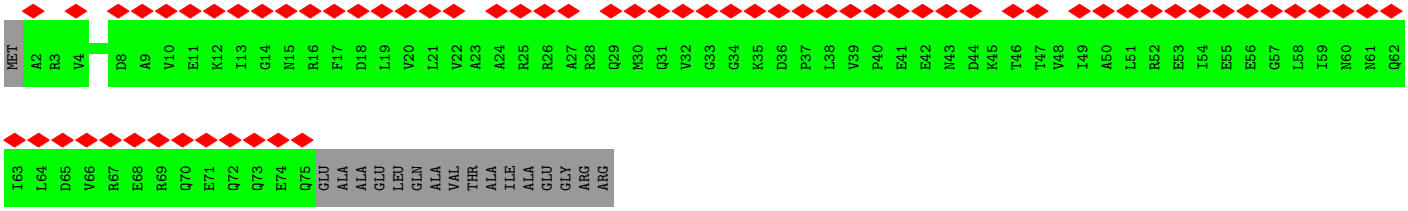




• Molecule 8: DNA-directed RNA polymerase subunit omega

Chain E:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	18337	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.050	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0175	Depositor
Map size (Å)	330.0, 330.0, 330.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: AF3, ADP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	1	0.25	0/1246	0.51	0/1732
1	2	0.19	0/1256	0.46	0/1746
1	3	0.20	0/1256	0.49	0/1746
1	4	0.24	0/1276	0.56	0/1774
1	5	0.24	0/1266	0.50	0/1760
1	6	0.21	0/1246	0.47	1/1732 (0.1%)
2	M	0.25	0/2046	0.55	0/2847
3	N	0.34	0/777	0.55	0/1196
4	T	0.35	0/785	0.58	0/1210
5	A	0.22	0/1129	0.48	0/1570
5	B	0.18	0/1099	0.41	0/1527
6	C	0.22	0/6598	0.49	0/9172
7	D	0.19	0/6560	0.46	1/9112 (0.0%)
8	E	0.13	0/365	0.35	0/507
All	All	0.22	0/26905	0.49	2/37631 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	921	GLN	N-CA-C	-8.17	103.84	113.88
1	6	84	ALA	CB-CA-C	-5.72	109.96	116.54

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	1	1247	0	566	15	0
1	2	1257	0	569	29	0
1	3	1257	0	569	45	0
1	4	1277	0	583	45	0
1	5	1267	0	576	62	0
1	6	1247	0	566	15	0
2	M	2050	0	914	42	0
3	N	694	0	382	44	0
4	T	700	0	382	62	0
5	A	1130	0	514	7	0
5	B	1101	0	501	18	0
6	C	6599	0	2971	88	0
7	D	6566	0	3043	95	0
8	E	366	0	167	0	0
9	1	27	0	12	1	0
9	2	27	0	11	8	0
9	3	27	0	12	22	0
9	4	27	0	12	6	0
9	5	27	0	12	36	0
10	1	4	0	0	1	0
10	2	4	0	0	0	0
10	3	4	0	0	3	0
10	4	4	0	0	8	0
10	5	4	0	0	1	0
11	1	1	0	0	0	0
11	2	1	0	0	0	0
11	3	1	0	0	0	0
11	4	1	0	0	0	0
11	5	1	0	0	0	0
All	All	26918	0	12362	528	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 14.

The worst 5 of 528 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)
1:3:8:LEU:CB	9:3:601:ADP:C5	1.88	1.52
1:5:8:LEU:HA	9:5:601:ADP:N6	1.12	1.42
1:5:8:LEU:CA	9:5:601:ADP:N6	1.85	1.36
1:5:44:LEU:N	9:5:601:ADP:O1A	1.61	1.34
1:3:41:GLY:HA2	9:3:601:ADP:O1B	1.27	1.28

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	1	251/259 (97%)	223 (89%)	28 (11%)	0	100	100
1	2	253/259 (98%)	235 (93%)	17 (7%)	1 (0%)	30	67
1	3	253/259 (98%)	225 (89%)	28 (11%)	0	100	100
1	4	257/259 (99%)	217 (84%)	38 (15%)	2 (1%)	16	54
1	5	255/259 (98%)	222 (87%)	32 (12%)	1 (0%)	30	67
1	6	251/259 (97%)	229 (91%)	22 (9%)	0	100	100
2	M	405/497 (82%)	372 (92%)	31 (8%)	2 (0%)	24	63
5	A	227/329 (69%)	207 (91%)	20 (9%)	0	100	100
5	B	219/329 (67%)	208 (95%)	11 (5%)	0	100	100
6	C	1339/1341 (100%)	1222 (91%)	117 (9%)	0	100	100
7	D	1322/1407 (94%)	1196 (90%)	126 (10%)	0	100	100
8	E	72/91 (79%)	71 (99%)	1 (1%)	0	100	100
All	All	5104/5548 (92%)	4627 (91%)	471 (9%)	6 (0%)	49	83

5 of 6 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	4	246	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	5	246	PRO
2	M	17	PRO
2	M	193	LYS
1	2	132	VAL

5.3.2 Protein sidechains (i)

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

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 15 ligands modelled in this entry, 5 are monoatomic - leaving 10 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	601	11,10	27,29,29	1.37	4 (14%)	42,45,45	1.99	12 (28%)
10	AF3	2	602	9	0,3,3	-	-	-		
10	AF3	1	602	1	0,3,3	-	-	-		
10	AF3	3	602	9	0,3,3	-	-	-		
9	ADP	2	601	11,10	27,29,29	1.37	4 (14%)	42,45,45	2.02	11 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
9	ADP	1	601	11	27,29,29	1.41	4 (14%)	42,45,45	2.11	8 (19%)
9	ADP	4	601	11,10	27,29,29	1.36	4 (14%)	42,45,45	1.98	10 (23%)
9	ADP	3	601	11,10	27,29,29	1.36	4 (14%)	42,45,45	2.00	10 (23%)
10	AF3	4	602	9	0,3,3	-	-	-		
10	AF3	5	602	9	0,3,3	-	-	-		

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	601	11,10	-	1/16/32/32	0/3/3/3
9	ADP	2	601	11,10	-	1/16/32/32	0/3/3/3
9	ADP	1	601	11	-	4/16/32/32	0/3/3/3
9	ADP	4	601	11,10	-	2/16/32/32	0/3/3/3
9	ADP	3	601	11,10	-	5/16/32/32	0/3/3/3

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	1	601	ADP	C5-C4	4.70	1.47	1.39
9	3	601	ADP	C5-C4	4.55	1.47	1.39
9	2	601	ADP	C5-C4	4.52	1.47	1.39
9	4	601	ADP	C5-C4	4.52	1.47	1.39
9	5	601	ADP	C5-C4	4.51	1.47	1.39

The worst 5 of 51 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	1	601	ADP	C5-C4-N3	-7.26	117.28	126.75
9	3	601	ADP	C5-C4-N3	-6.37	118.44	126.75
9	2	601	ADP	C5-C4-N3	-6.34	118.48	126.75
9	4	601	ADP	C5-C4-N3	-6.30	118.53	126.75
9	5	601	ADP	C5-C4-N3	-6.21	118.65	126.75

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	1	601	ADP	C5'-O5'-PA-O1A
9	1	601	ADP	C5'-O5'-PA-O3A
9	3	601	ADP	PA-O3A-PB-O3B
9	3	601	ADP	C5'-O5'-PA-O1A
9	4	601	ADP	C5'-O5'-PA-O3A

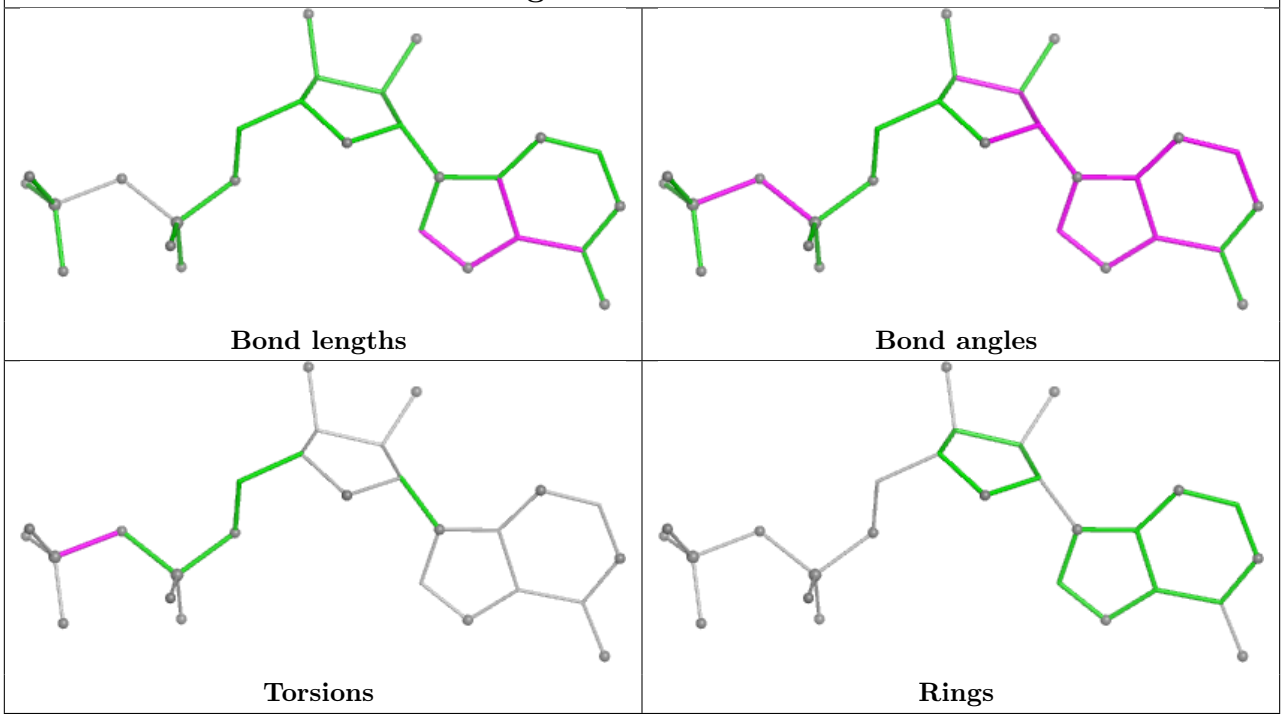
There are no ring outliers.

9 monomers are involved in 85 short contacts:

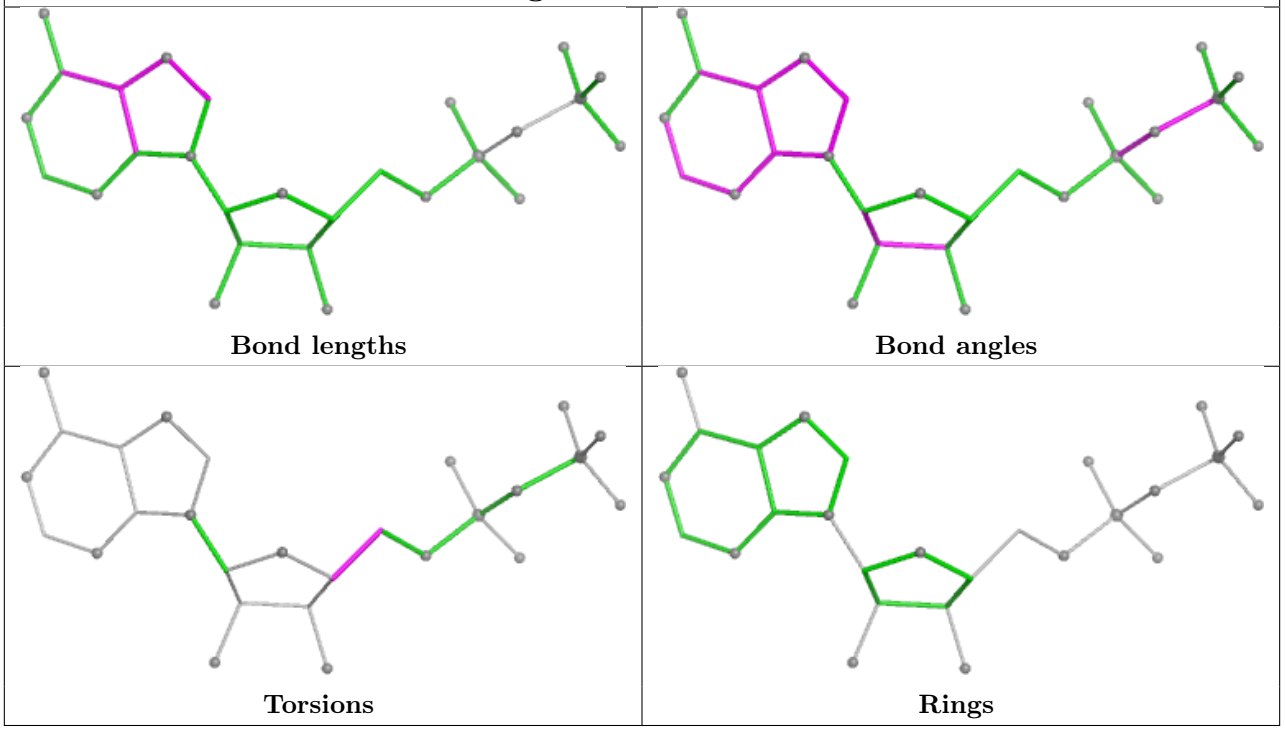
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	5	601	ADP	36	0
10	1	602	AF3	1	0
10	3	602	AF3	3	0
9	2	601	ADP	8	0
9	1	601	ADP	1	0
9	4	601	ADP	6	0
9	3	601	ADP	22	0
10	4	602	AF3	8	0
10	5	602	AF3	1	0

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 then 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.

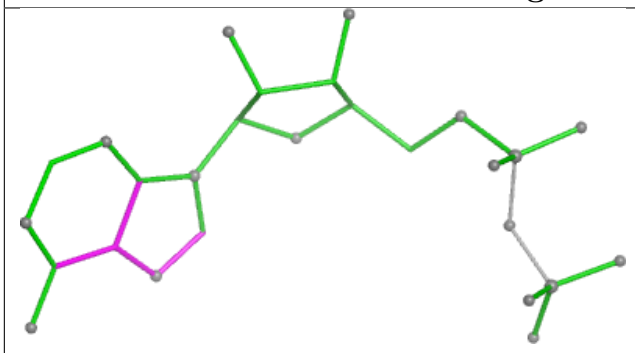
Ligand ADP 5 601



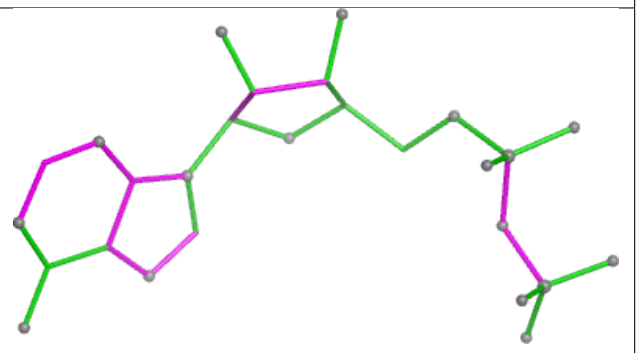
Ligand ADP 2 601



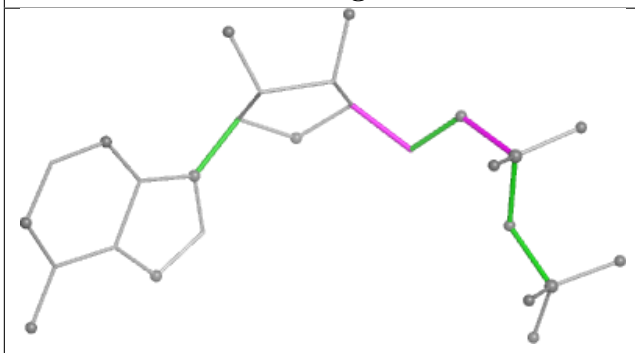
Ligand ADP 1 601



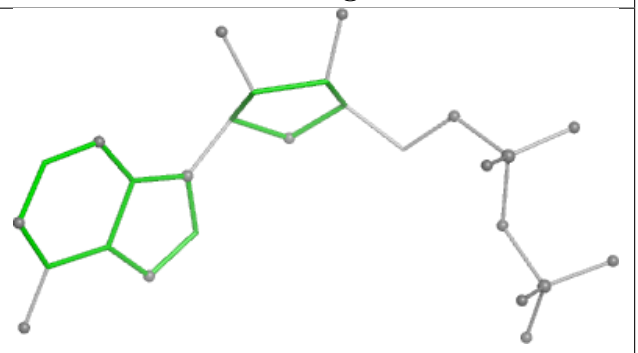
Bond lengths



Bond angles

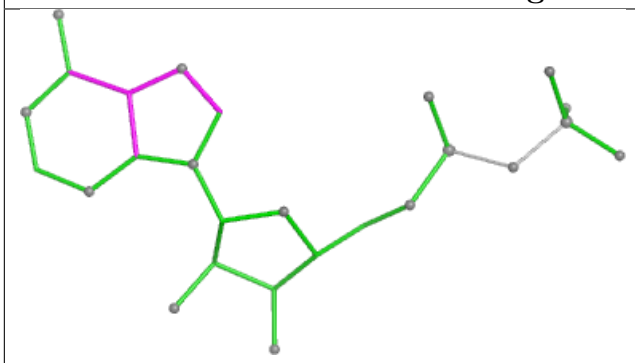


Torsions

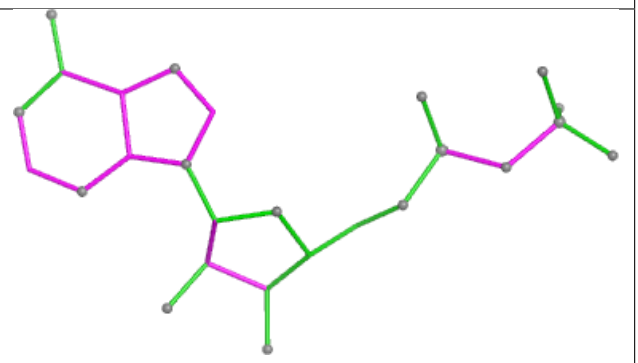


Rings

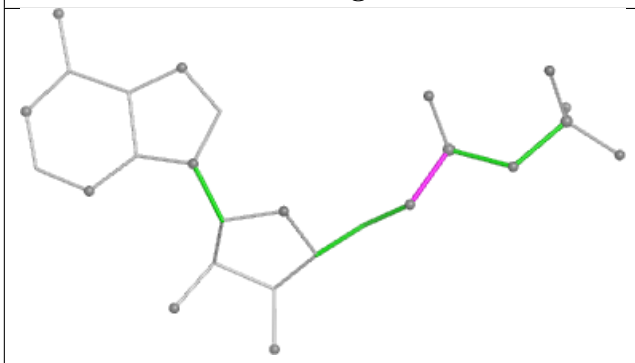
Ligand ADP 4 601



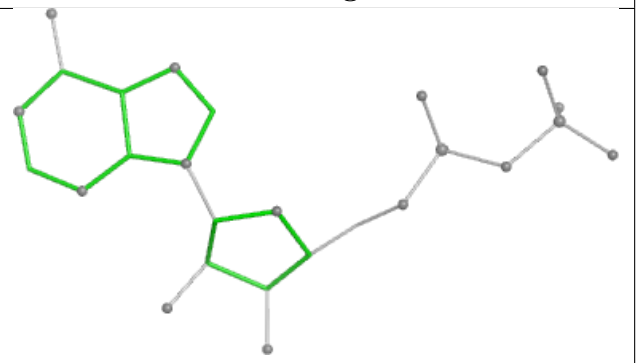
Bond lengths



Bond angles

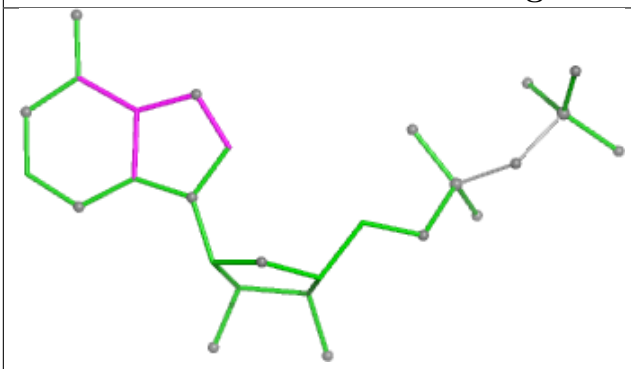


Torsions

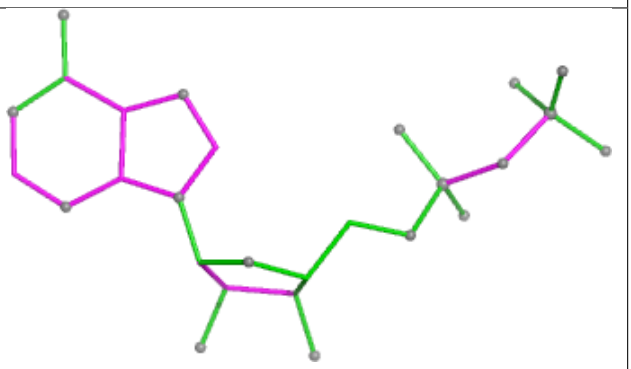


Rings

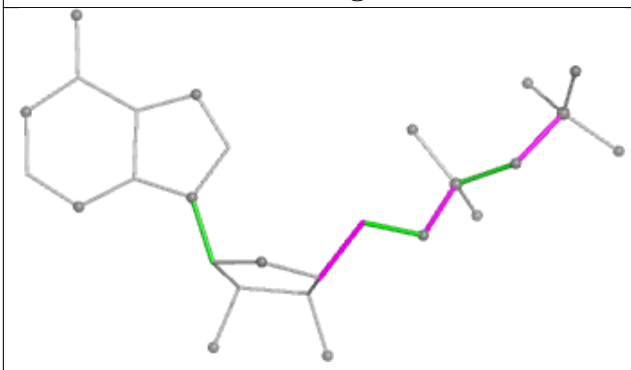
Ligand ADP 3 601



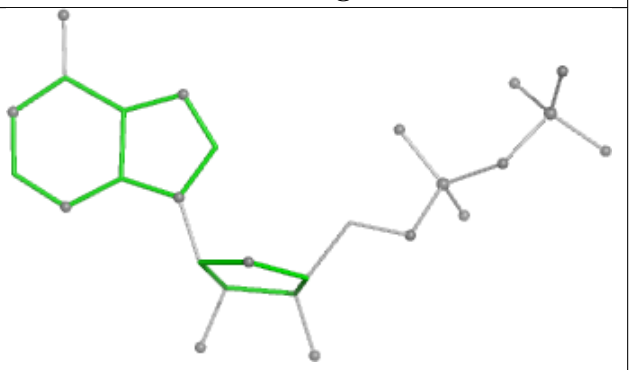
Bond lengths



Bond angles



Torsions



Rings

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.

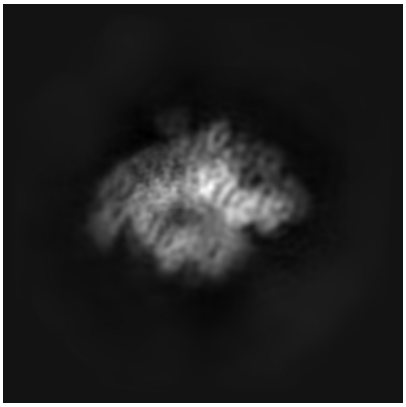
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-52916. These allow visual inspection of the internal detail of the map and identification of artifacts.

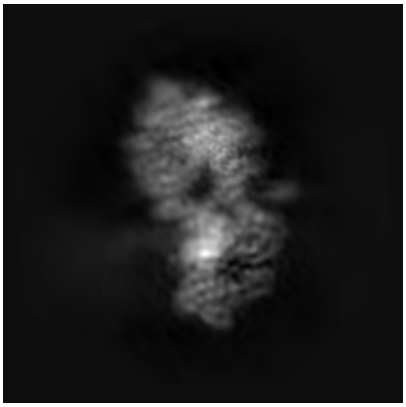
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

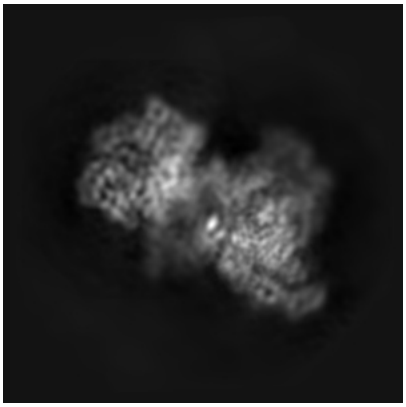
6.1.1 Primary map



X



Y

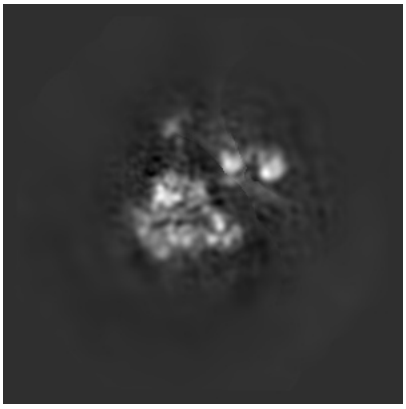


Z

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

6.2 Central slices

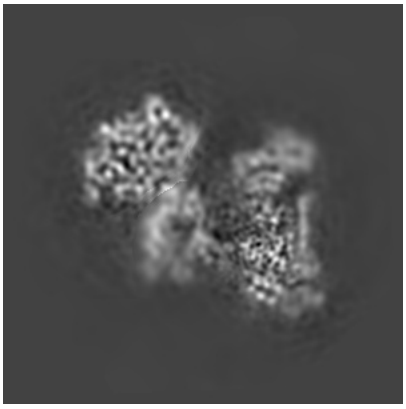
6.2.1 Primary map



X Index: 150



Y Index: 150

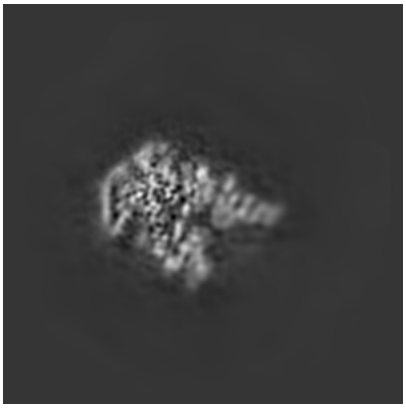


Z Index: 150

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

6.3 Largest variance slices (i)

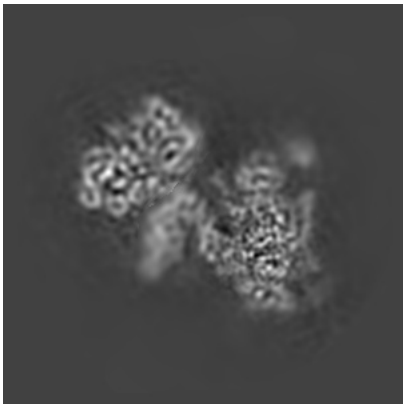
6.3.1 Primary map



X Index: 200



Y Index: 164

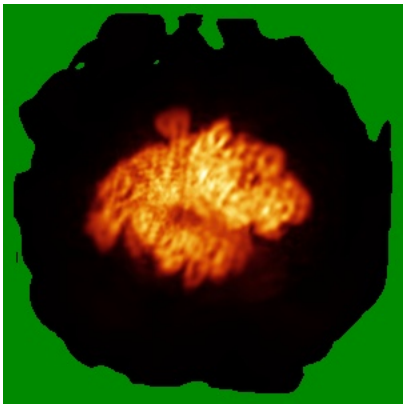


Z Index: 156

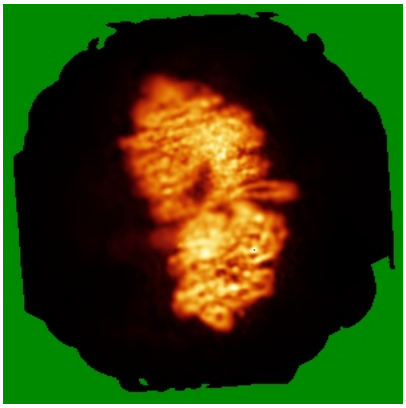
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

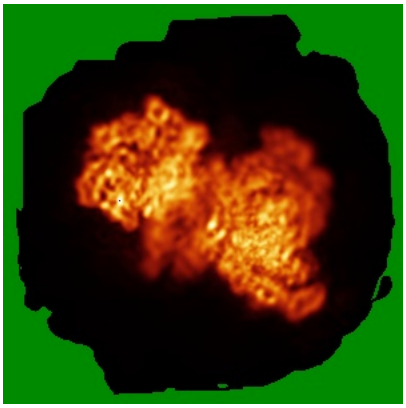
6.4.1 Primary map



X



Y

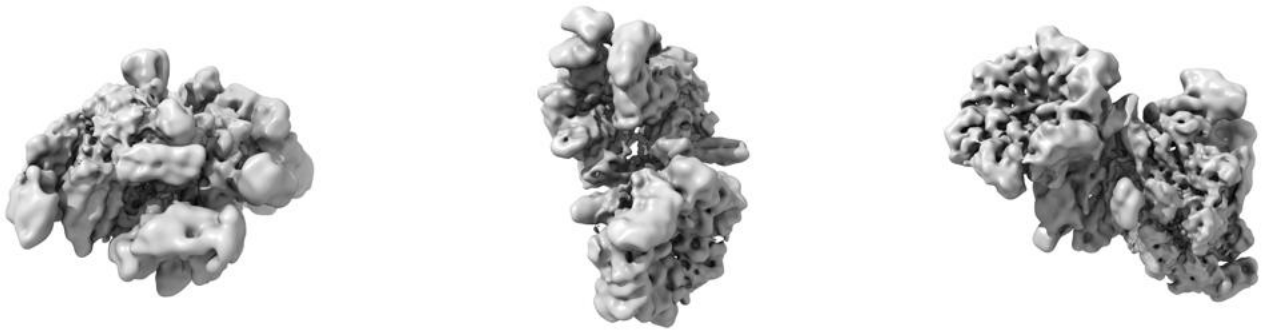


Z

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 0.0175. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

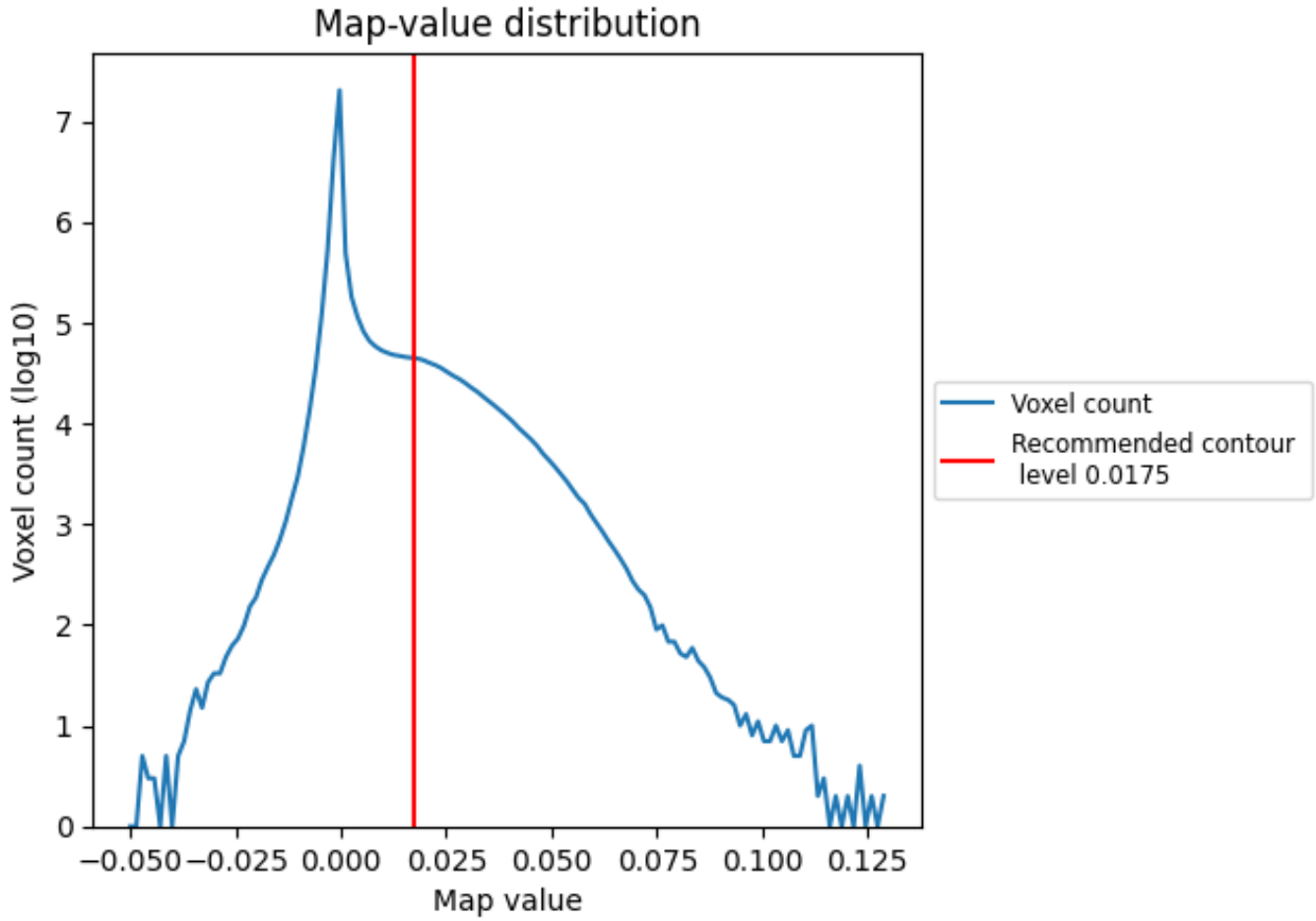
6.6 Mask visualisation (i)

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

7 Map analysis

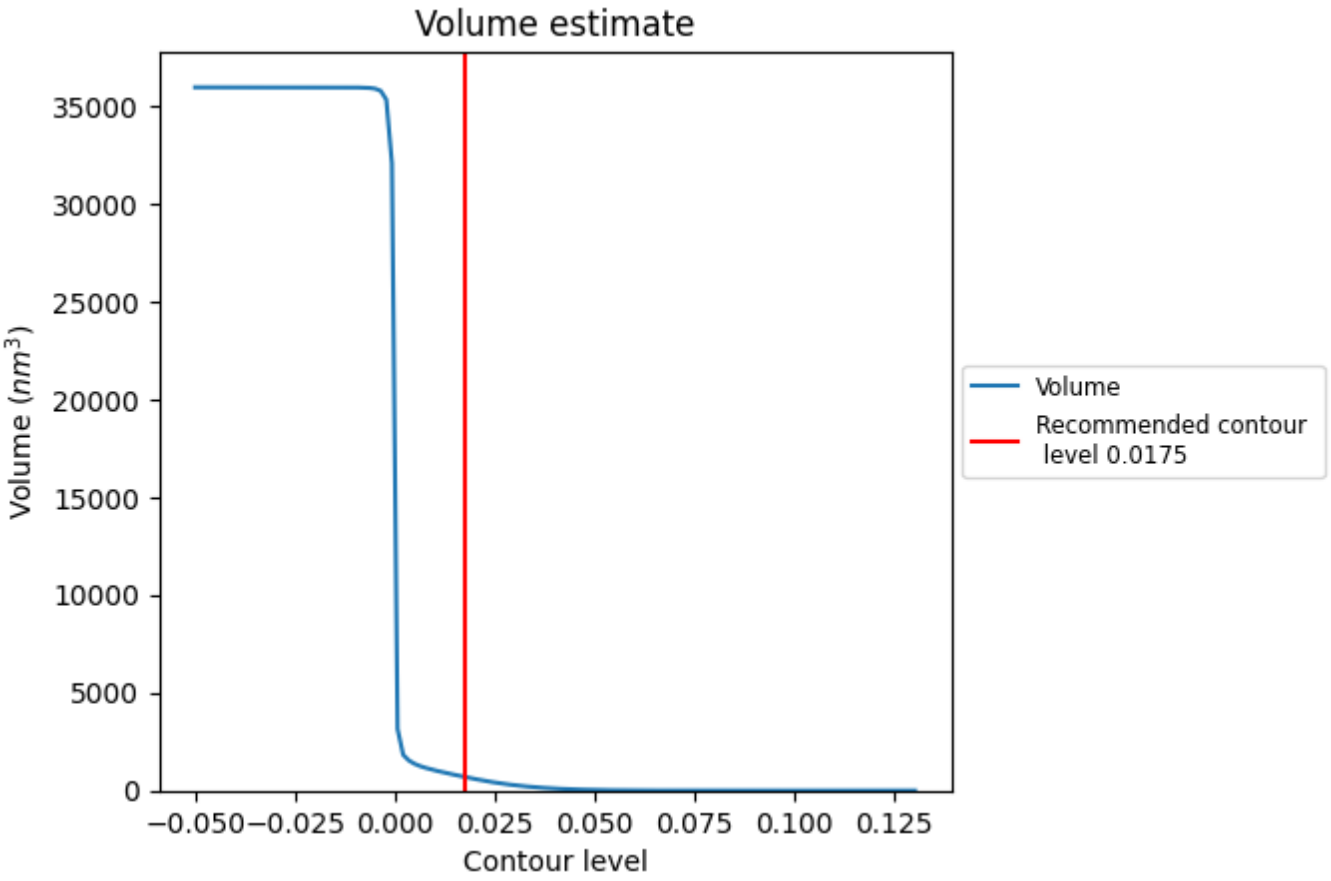
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

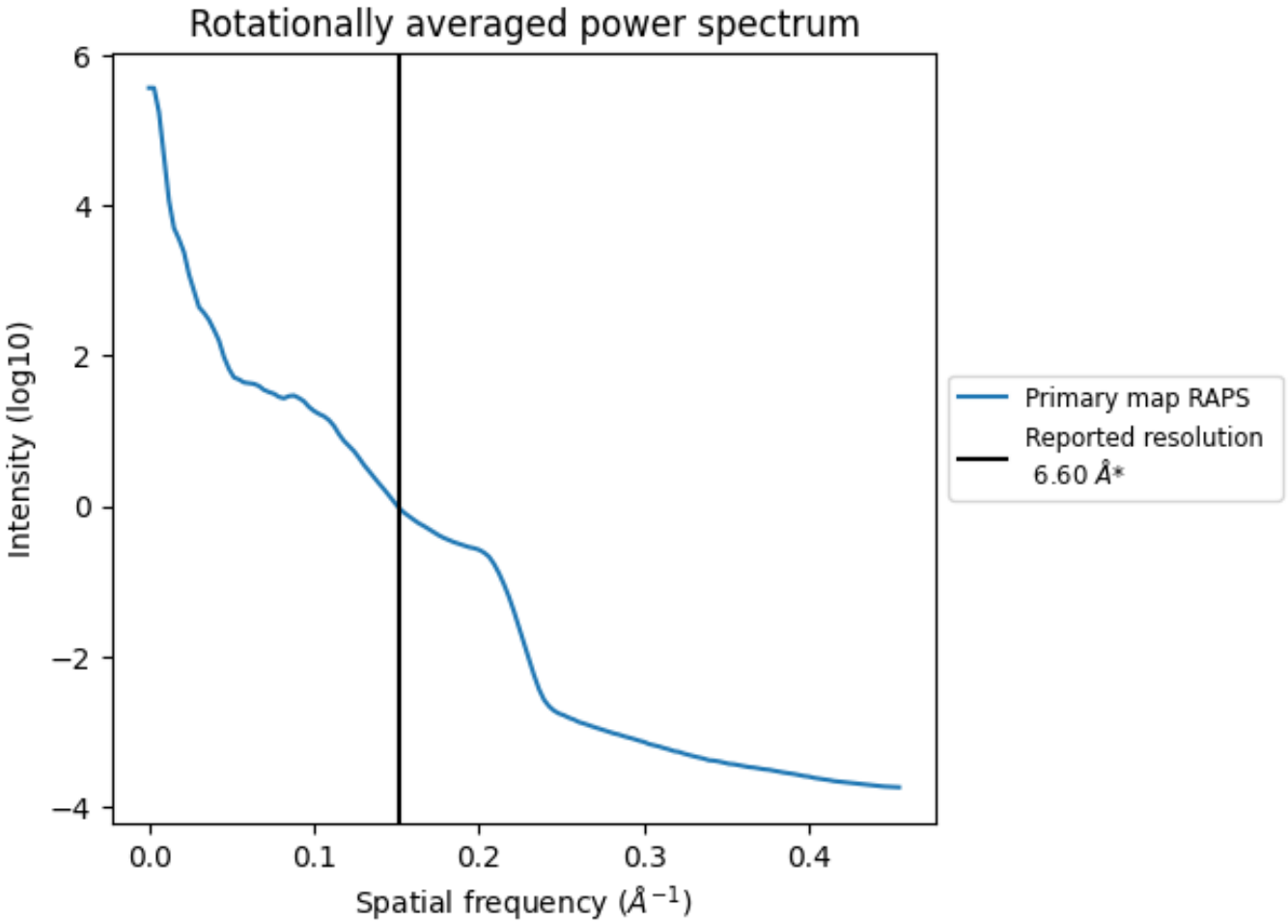
7.2 Volume estimate (i)



The volume at the recommended contour level is 699 nm^3; this corresponds to an approximate mass of 631 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 0.152 Å^{-1}

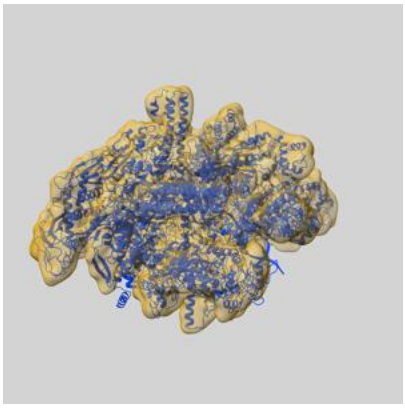
8 Fourier-Shell correlation (i)

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

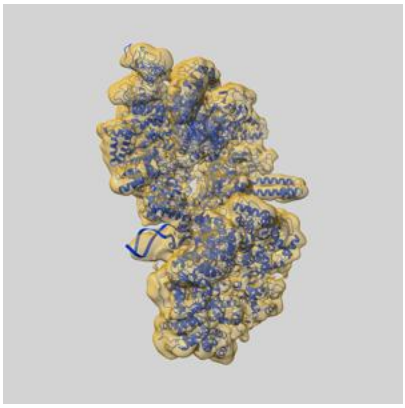
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-52916 and PDB model 9Q93. Per-residue inclusion information can be found in section 3 on page 9.

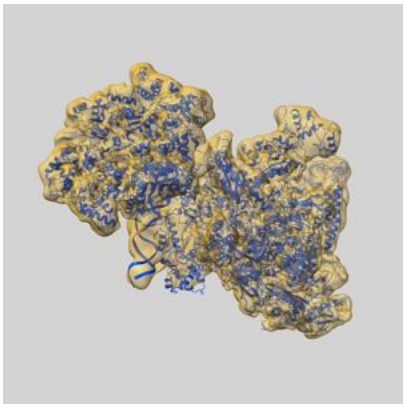
9.1 Map-model overlay



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0175 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.

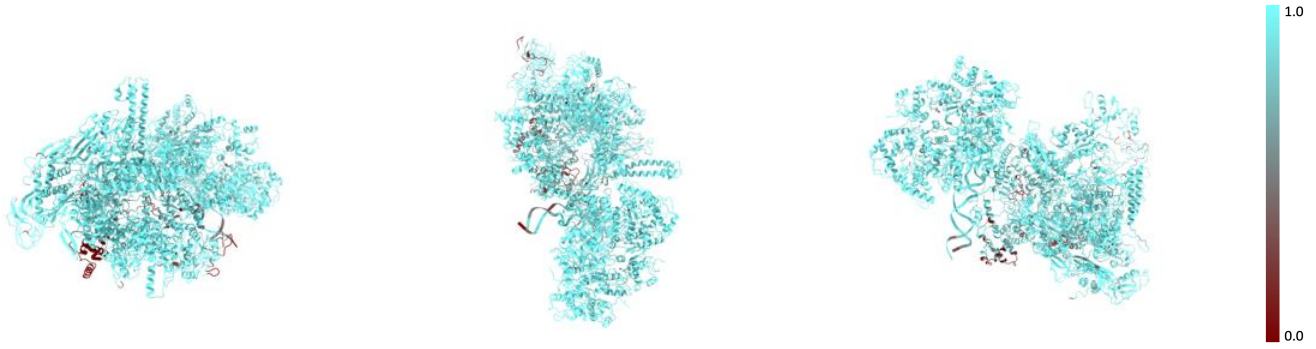
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

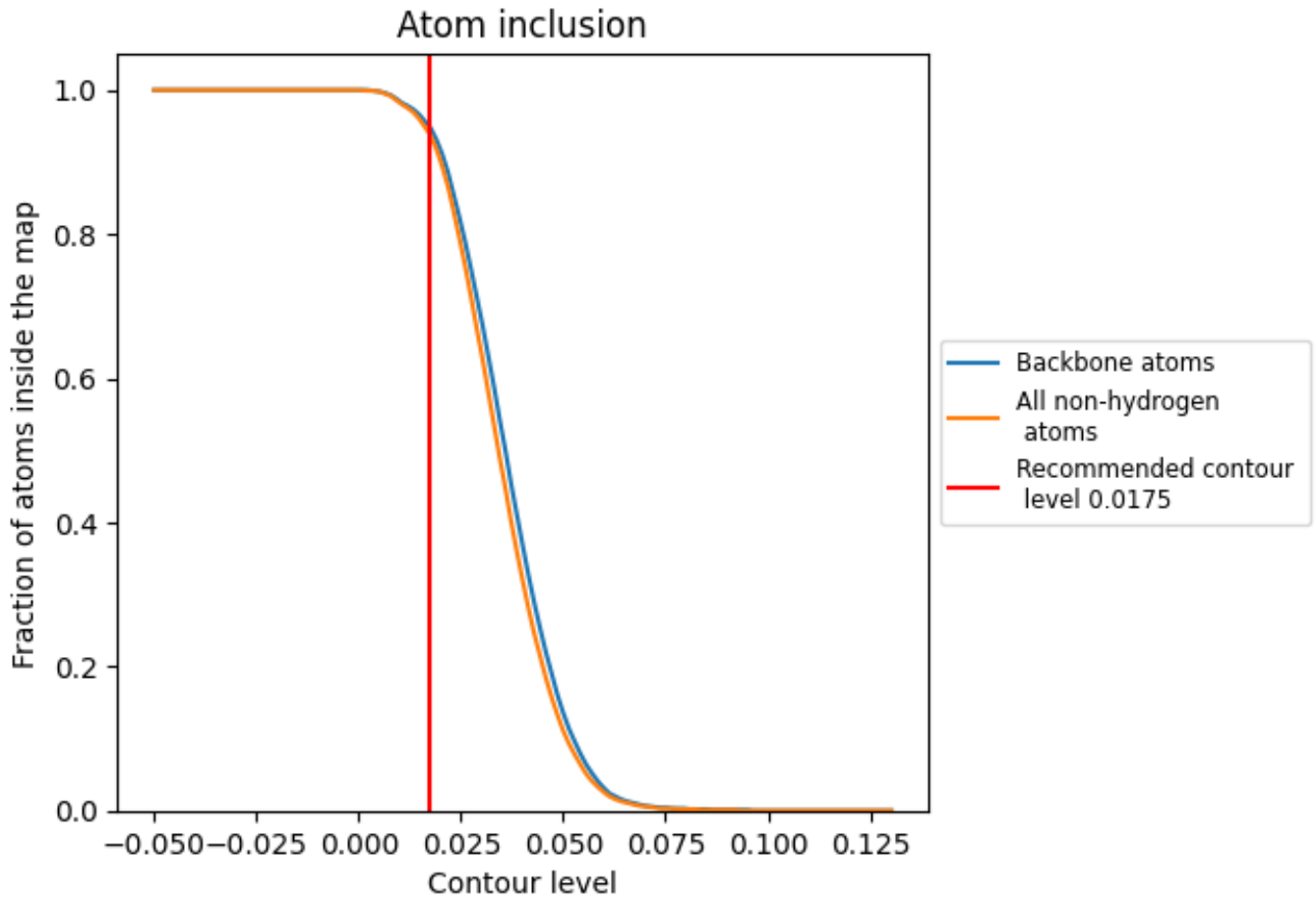
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.0175).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 94% 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 (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9380	0.2590
1	0.9830	0.2290
2	0.9710	0.2550
3	0.9900	0.2760
4	0.9850	0.2880
5	0.9930	0.2860
6	0.9820	0.2570
A	0.9830	0.3310
B	0.9770	0.2620
C	0.9830	0.3000
D	0.9250	0.2480
E	0.1260	0.1500
M	0.8060	0.1900
N	0.8790	0.1650
T	0.8430	0.1580

