



wwPDB EM Validation Summary Report ⓘ

Mar 20, 2026 – 05:00 AM UTC

PDB ID : 9B1E / pdb_00009b1e
EMDB ID : EMD-44075
Title : Cryo-EM structure of native SWR1 bound to nucleosome (composite structure)
Authors : Louder, R.K.; Park, G.; Wu, C.
Deposited on : 2024-03-13
Resolution : 4.40 Å (reported)
Based on initial models : 6GEJ, .

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev132
Mogul : 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 EMDb archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

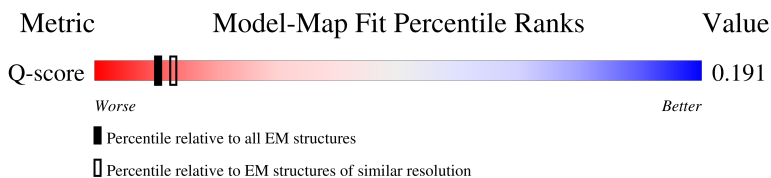
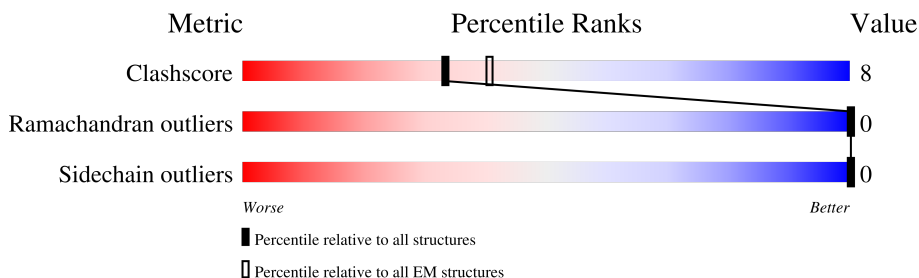
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.40 Å.

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



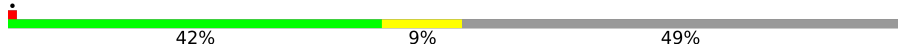
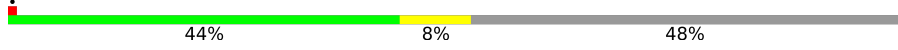
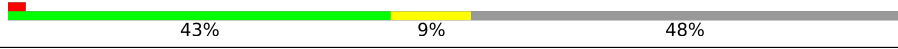
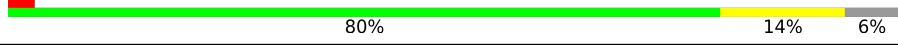
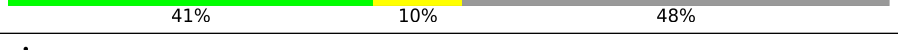
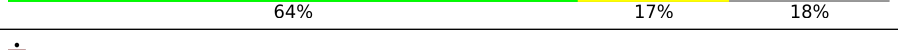
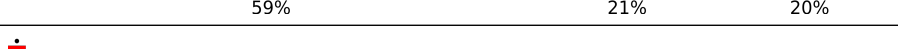
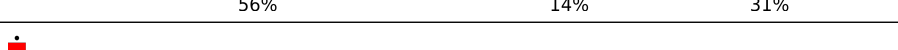
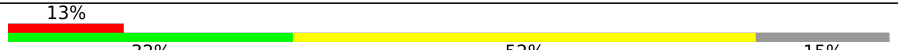
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	3132 (3.91 - 4.90)

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

Mol	Chain	Length	Quality of chain
1	A	1544	
2	B	795	
3	C	438	
4	D	280	

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Mol	Chain	Length	Quality of chain
5	E	837	
5	G	837	
5	I	837	
6	F	471	
6	H	471	
6	J	471	
7	K	625	
8	Q	132	
8	S	132	
9	R	131	
9	T	131	
10	U	136	
10	W	136	
11	V	103	
11	X	103	
12	Y	214	
13	Z	214	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 49842 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 Helicase SWR1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	720	Total	C	N	O	S	0	0
			5894	3757	1041	1069	27		

- Molecule 2 is a protein called Vacuolar protein sorting-associated protein 72.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	303	Total	C	N	O	S	0	0
			2513	1598	441	466	8		

- Molecule 3 is a protein called Actin-like protein ARP6.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	411	Total	C	N	O	S	0	0
			3336	2156	544	620	16		

- Molecule 4 is a protein called Vacuolar protein sorting-associated protein 71.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	206	Total	C	N	O	S	0	0
			1671	1054	296	311	10		

- Molecule 5 is a protein called RuvB-like protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	426	Total	C	N	O	S	0	0
			3281	2072	565	634	10		
5	G	434	Total	C	N	O	S	0	0
			3334	2104	575	645	10		
5	I	436	Total	C	N	O	S	0	0
			3351	2115	577	649	10		

- Molecule 6 is a protein called RuvB-like protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	443	Total	C	N	O	S	0	0
			3410	2131	591	676	12		
6	H	441	Total	C	N	O	S	0	0
			3393	2119	588	674	12		
6	J	426	Total	C	N	O	S	0	0
			3279	2052	566	650	11		

- Molecule 7 is a protein called SWR1-complex protein 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	322	Total	C	N	O	S	0	0
			2671	1699	470	489	13		

- Molecule 8 is a protein called Histone H2A.

Mol	Chain	Residues	Atoms				AltConf	Trace
8	Q	108	Total	C	N	O	0	0
			833	523	164	146		
8	S	106	Total	C	N	O	0	0
			819	514	161	144		

- Molecule 9 is a protein called Histone H2B.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	91	Total	C	N	O	S	0	0
			713	449	125	138	1		
9	T	93	Total	C	N	O	S	0	0
			726	456	127	142	1		

- Molecule 10 is a protein called Histone H3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	107	Total	C	N	O	S	0	0
			864	544	167	150	3		
10	W	98	Total	C	N	O	S	0	0
			807	508	156	140	3		

- Molecule 11 is a protein called Histone H4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

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Mol	Chain	Residues	Atoms					AltConf	Trace
11	X	81	Total	C	N	O	S	0	0
			646	407	126	112	1		

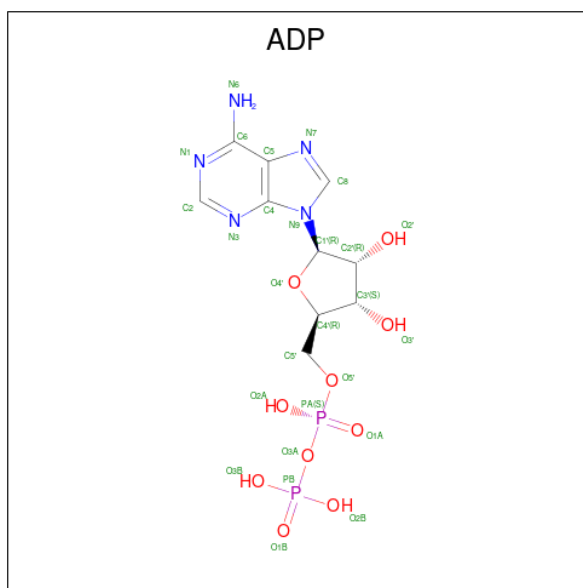
- Molecule 12 is a DNA chain called DNA (214-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
12	Y	181	Total	C	N	O	P	0	0
			3688	1751	667	1089	181		

- Molecule 13 is a DNA chain called DNA (214-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
13	Z	181	Total	C	N	O	P	0	0
			3733	1765	704	1083	181		

- Molecule 14 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



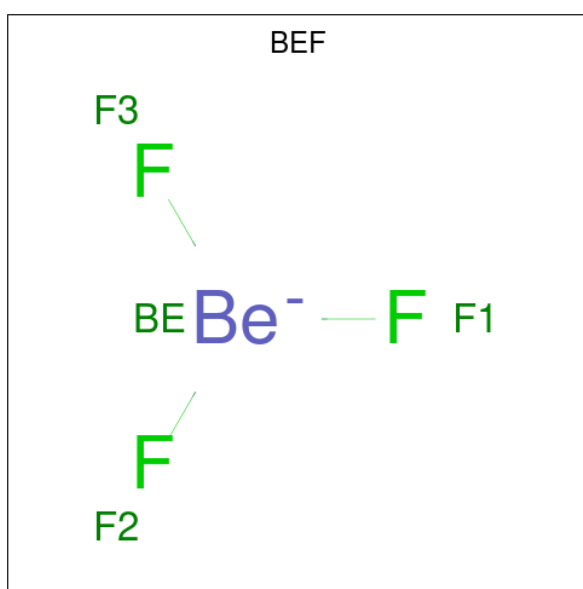
Mol	Chain	Residues	Atoms					AltConf
14	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
14	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
14	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 15 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			AltConf
15	A	1	Total	Be	F	0
			4	1	3	
15	C	1	Total	Be	F	0
			4	1	3	

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

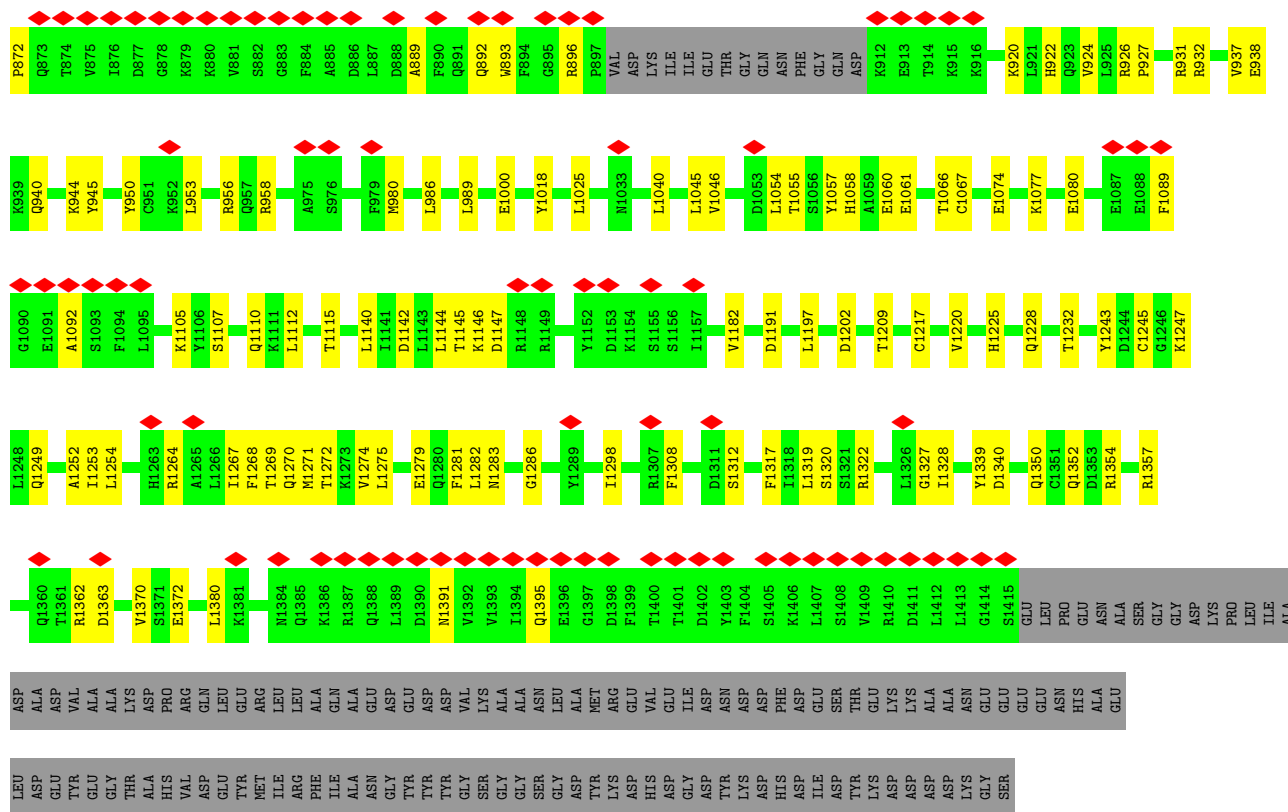
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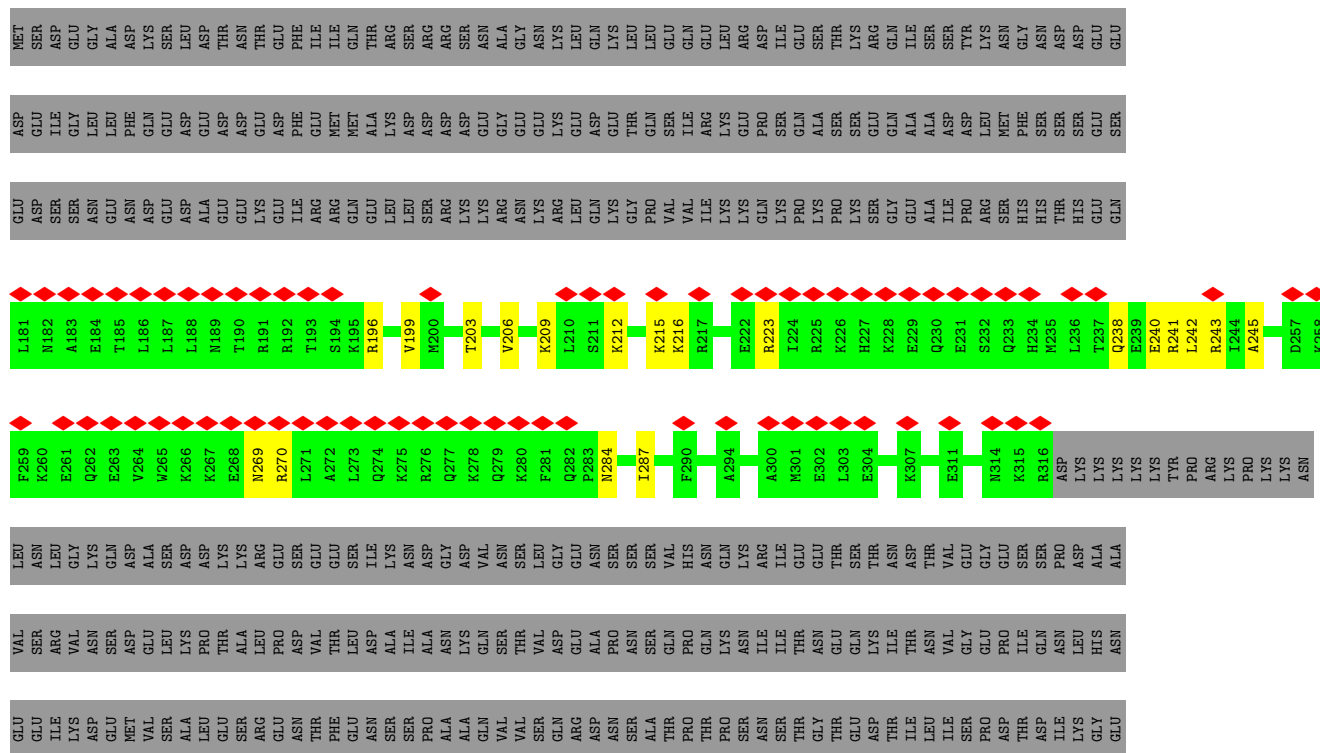
Mol	Chain	Residues	Atoms		AltConf
16	F	1	Total 1	Mg 1	0
16	G	1	Total 1	Mg 1	0
16	H	1	Total 1	Mg 1	0
16	I	1	Total 1	Mg 1	0
16	J	1	Total 1	Mg 1	0

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

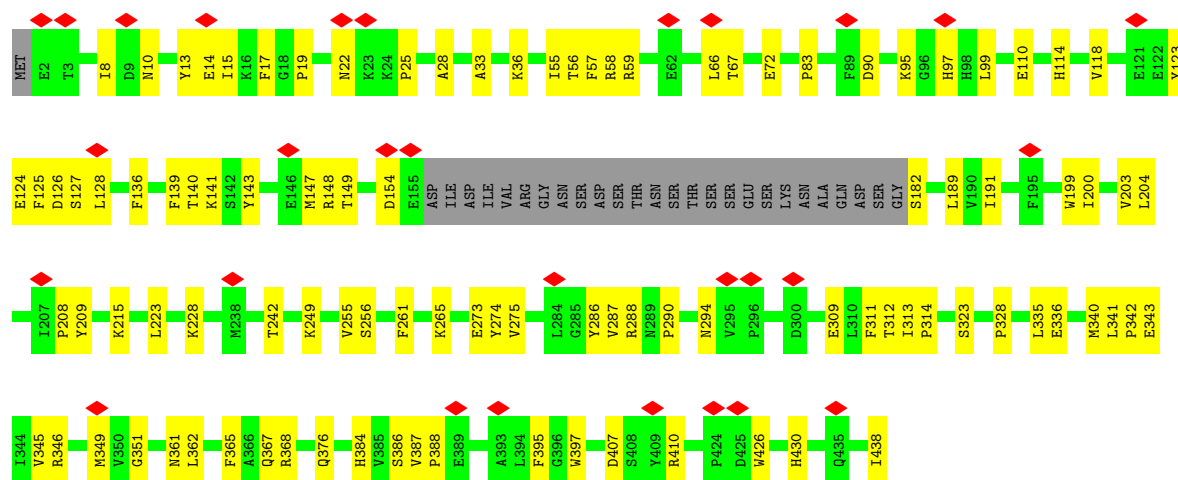
Mol	Chain	Residues	Atoms		AltConf
17	D	2	Total 2	Zn 2	0



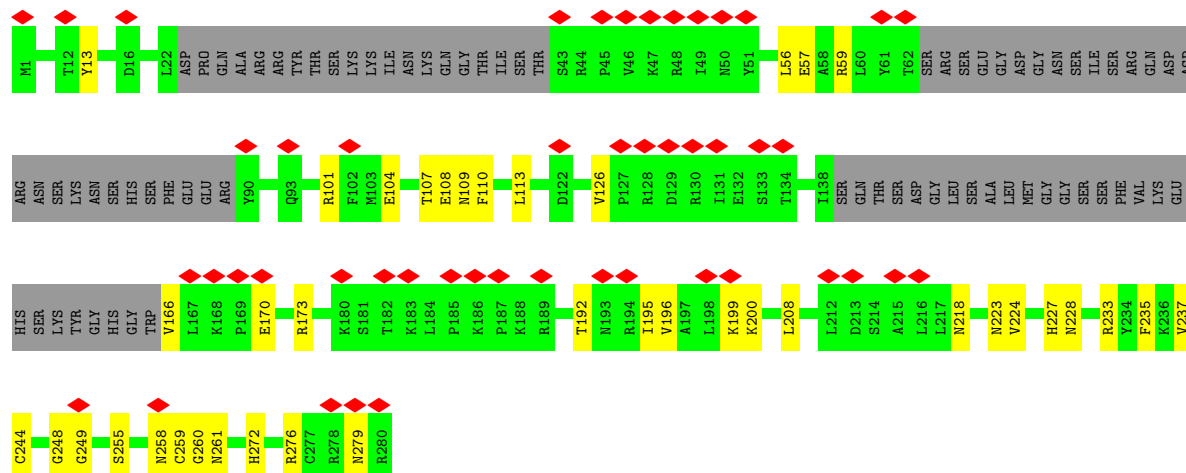
• Molecule 2: Vacuolar protein sorting-associated protein 72



- Molecule 3: Actin-like protein ARP6

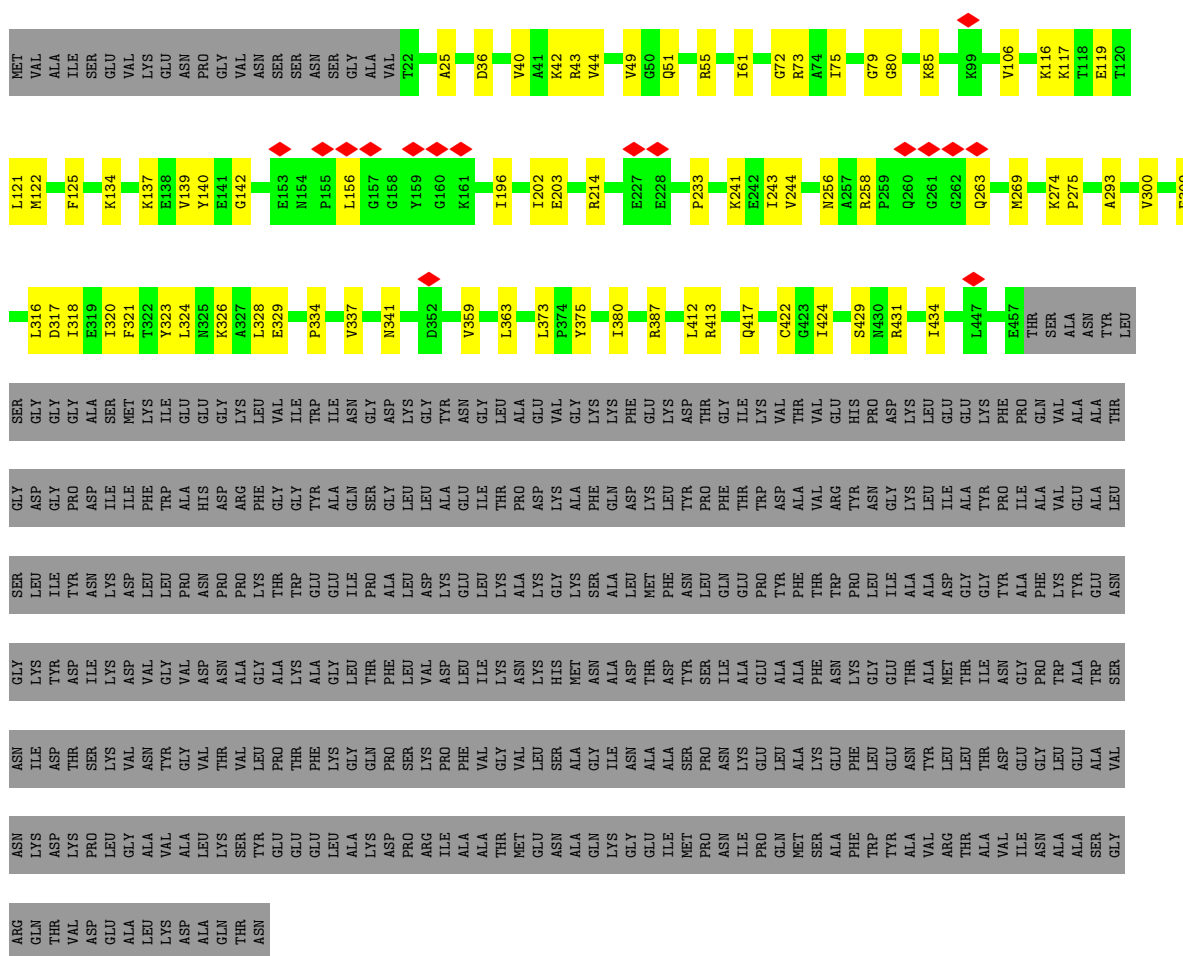


- Molecule 4: Vacuolar protein sorting-associated protein 71

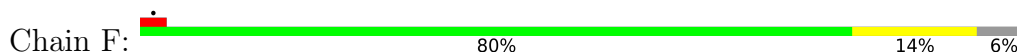


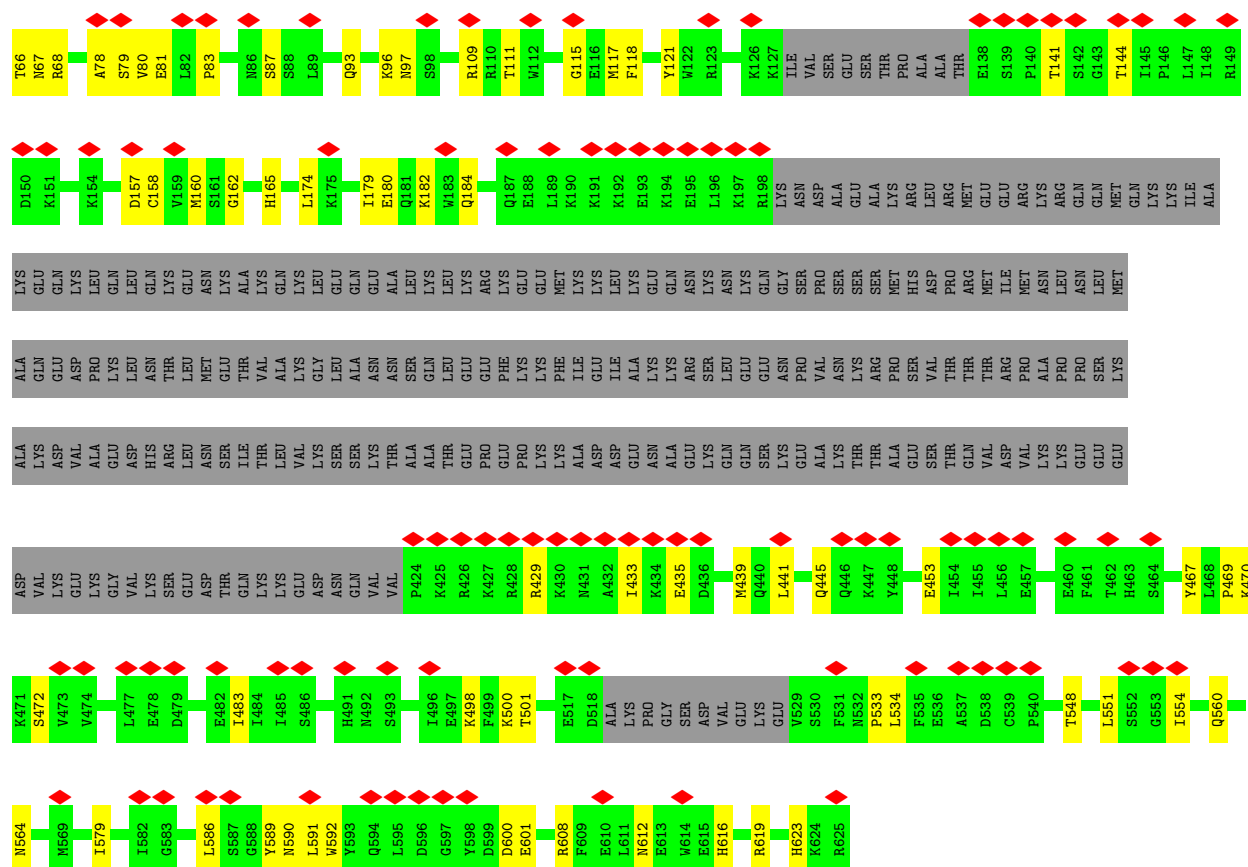
ALA	THR	ALA	THR	GLY	VAL	ILE	LEU
THR	MET	GLU	VAL	LEU	VAL	LYS	LYS
GLU	ASN	SER	ASN	GLY	ALA	MET	LYS
ALA	GLN	LYS	GLY	ILE	ASN	THR	GLY
GLY	GLY	ASN	ILE	ASN	ALA	ASP	SER
GLY	GLY	ALA	ASN	ALA	ASP	THR	LEU
ILE	ILE	ALA	ALA	ALA	ASP	ASP	PHE
MET	MET	PRO	PRO	SER	SER	TYR	ASN
PRO	ASN	ASN	ASN	PRO	ILE	SER	LEU
ASN	ILE	PRO	GLN	GLY	LYS	GLY	GLN
GLN	GLN	GLN	LEU	LEU	ALA	ALA	PRO
MET	MET	ALA	ALA	ASN	THR	THR	ALA
SER	SER	LYS	LYS	TYR	PHE	PHE	PHE
ALA	ALA	GLU	GLU	LEU	ASN	ASN	THR
PHE	PHE	THR	THR	LEU	MET	LYS	TRP
ALA	ALA	ALA	ALA	THR	ILE	ILE	ALA
VAL	VAL	VAL	VAL	ASP	ASN	ASN	ALA
ILE	ILE	ASN	ASN	GLY	GLY	GLY	ALA
ASN	ASN	GLY	GLY	GLY	PRO	PRO	ALA
ALA	ALA	GLU	GLU	LEU	LEU	TRP	TYR
ALA	ALA	ALA	ALA	VAL	ASN	GLU	GLY
GLY	GLY	GLY	GLY	ASN	ASN	ASN	ASN
ARG	ARG	GLN	GLN	LYS	ILE	ILE	LYS
THR	THR	VAL	VAL	ASP	THR	THR	TYR
ASP	ASP	GLU	GLU	PRO	SER	SER	ASP
GLY	GLY	LEU	LEU	LEU	LYS	LYS	LYS
ALA	ALA	GLY	GLY	VAL	VAL	VAL	ASP
LEU	LEU	ALA	ALA	ASN	ASN	ASN	VAL
LYS	LYS	VAL	VAL	VAL	GLY	GLY	GLY
ASP	ASP	ALA	ALA	ALA	THR	THR	ALA
ALA	ALA	LEU	LEU	LYS	THR	THR	ASN
GLN	GLN	LYS	LYS	SER	VAL	VAL	ALA
THR	THR	TYR	TYR	TYR	LEU	LEU	GLY
ASN	ASN	GLU	GLU	GLU	PRO	PRO	ALA
		GLU	GLU	THR	THR	THR	LYS
		LEU	LEU	LEU	PHE	PHE	ALA
		ALA	ALA	ALA	LYS	LYS	GLY
		LEU	LEU	LEU	GLY	GLY	LEU
		LYS	LYS	LYS	GLN	GLN	THR
		ASP	ASP	ASP	ASP	ASP	PHE
		PRO	PRO	PRO	SER	SER	LEU
		ARG	ARG	ARG	LYS	LYS	VAL
		ILE	ILE	ILE	PRO	PRO	ASP
		ALA	ALA	ALA	PHE	PHE	LEU

- Molecule 5: RuvB-like protein 1

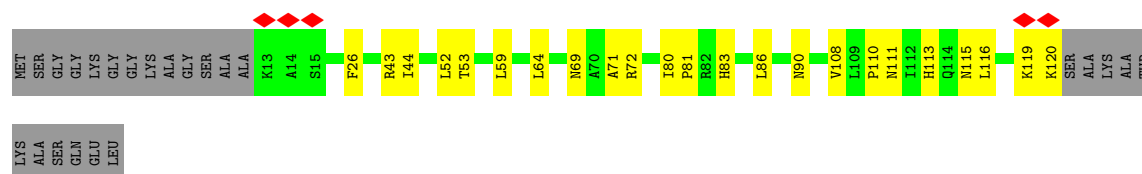


- Molecule 6: RuvB-like protein 2

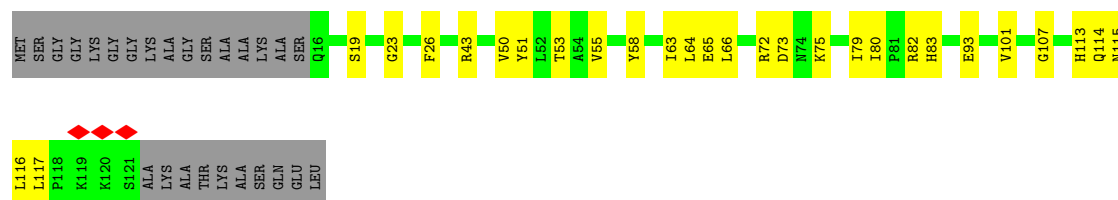




- Molecule 8: Histone H2A

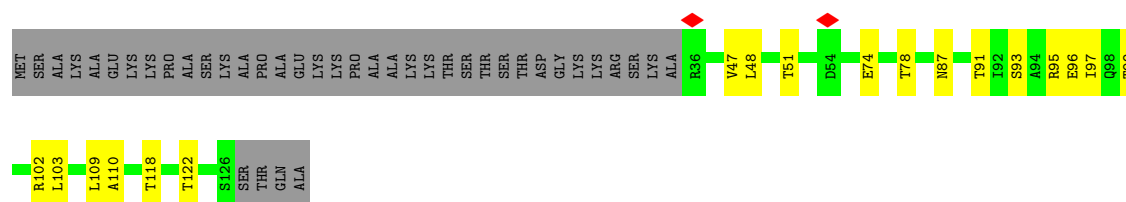


- Molecule 8: Histone H2A

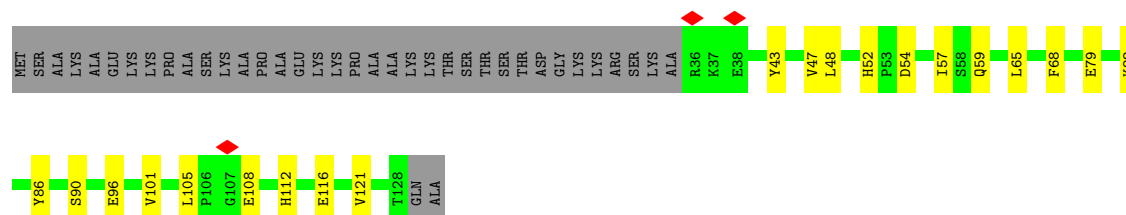


- Molecule 9: Histone H2B

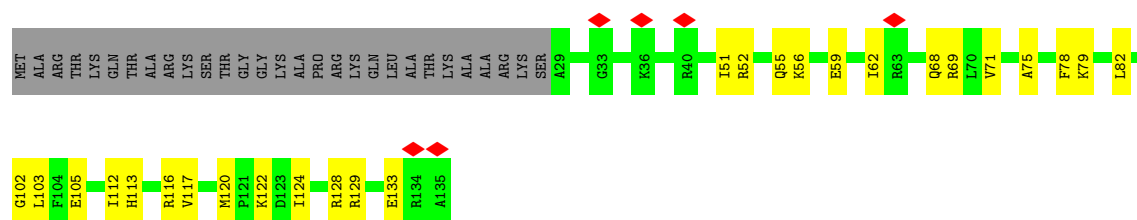




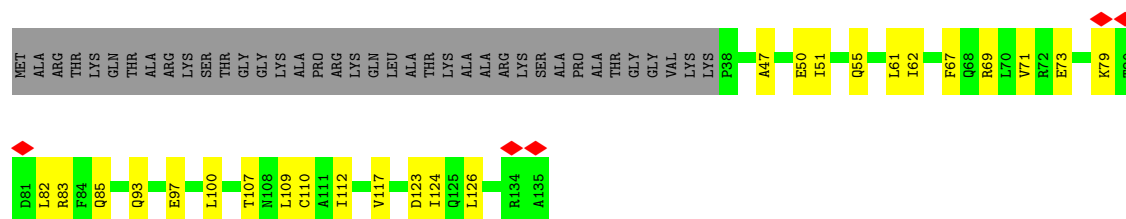
• Molecule 9: Histone H2B



• Molecule 10: Histone H3



• Molecule 10: Histone H3

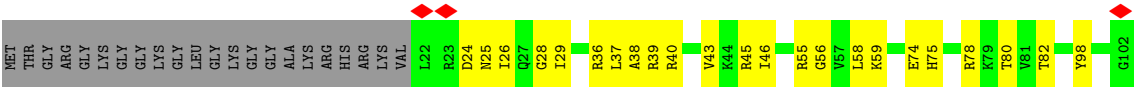


• Molecule 11: Histone H4

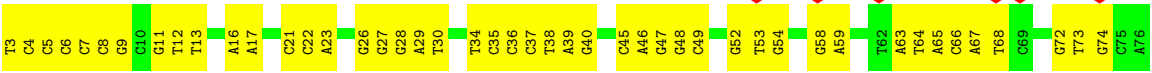
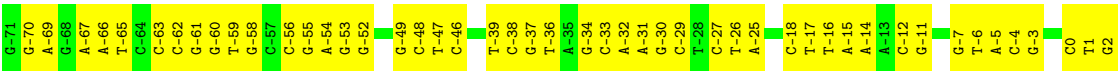


• Molecule 11: Histone H4

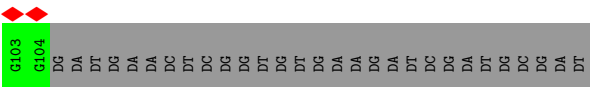
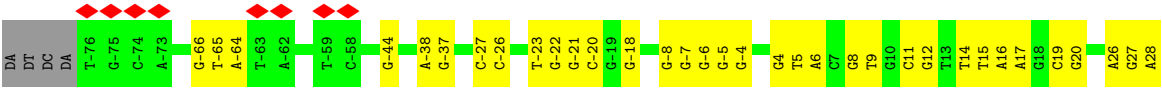




• Molecule 12: DNA (214-MER)



• Molecule 13: DNA (214-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	16524	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 ($e^-/\text{\AA}^2$)	54	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3600	Depositor
Magnification	48543	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.114	Depositor
Minimum map value	-0.005	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	395.52, 395.52, 395.52	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.03, 1.03, 1.03	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, BEF, 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	A	0.11	0/6007	0.34	0/8104
2	B	0.13	0/2559	0.36	0/3432
3	C	0.10	0/3430	0.30	0/4650
4	D	0.12	0/1696	0.35	0/2283
5	E	0.10	0/3319	0.27	0/4487
5	G	0.10	0/3375	0.30	0/4564
5	I	0.09	0/3392	0.24	0/4587
6	F	0.09	0/3448	0.27	0/4648
6	H	0.09	0/3430	0.24	0/4623
6	J	0.09	0/3312	0.28	0/4462
7	K	0.13	0/2724	0.37	0/3650
8	Q	0.12	0/844	0.33	0/1139
8	S	0.14	0/830	0.38	0/1121
9	R	0.13	0/723	0.38	0/973
9	T	0.15	0/736	0.38	0/991
10	U	0.13	0/877	0.36	0/1176
10	W	0.12	0/819	0.34	0/1097
11	V	0.13	0/653	0.37	0/873
11	X	0.14	0/653	0.37	0/873
12	Y	0.28	0/4131	0.85	0/6368
13	Z	0.28	0/4193	0.83	0/6475
All	All	0.15	0/51151	0.46	0/70576

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5894	0	5984	119	0
2	B	2513	0	2547	47	0
3	C	3336	0	3256	67	0
4	D	1671	0	1722	28	0
5	E	3281	0	3425	51	0
5	G	3334	0	3472	41	0
5	I	3351	0	3490	52	0
6	F	3410	0	3484	42	0
6	H	3393	0	3456	63	0
6	J	3279	0	3371	60	0
7	K	2671	0	2721	53	0
8	Q	833	0	883	21	0
8	S	819	0	865	24	0
9	R	713	0	736	14	0
9	T	726	0	748	22	0
10	U	864	0	908	27	0
10	W	807	0	844	24	0
11	V	646	0	687	16	0
11	X	646	0	687	28	0
12	Y	3688	0	2032	96	0
13	Z	3733	0	2029	67	0
14	A	27	0	12	3	0
14	C	27	0	12	1	0
14	E	27	0	12	2	0
14	F	27	0	12	4	0
14	G	27	0	12	0	0
14	H	27	0	12	4	0
14	I	27	0	12	2	0
14	J	27	0	12	1	0
15	A	4	0	0	1	0
15	C	4	0	0	1	0
16	A	1	0	0	0	0
16	C	1	0	0	0	0
16	E	1	0	0	0	0
16	F	1	0	0	0	0
16	G	1	0	0	0	0
16	H	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
16	I	1	0	0	0	0
16	J	1	0	0	0	0
17	D	2	0	0	0	0
All	All	49842	0	47443	807	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

The worst 5 of 807 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)
6:H:17:LEU:HB2	5:I:293:ALA:HB2	1.57	0.84
4:D:259:CYS:SG	4:D:261:ASN:ND2	2.55	0.80
8:Q:64:LEU:HD22	9:R:48:LEU:HD13	1.65	0.78
2:B:688:LEU:HD12	4:D:233:ARG:HE	1.49	0.77
3:C:15:ILE:HB	3:C:28:ALA:HB3	1.66	0.75

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	716/1544 (46%)	698 (98%)	18 (2%)	0	100	100
2	B	293/795 (37%)	280 (96%)	13 (4%)	0	100	100
3	C	407/438 (93%)	392 (96%)	15 (4%)	0	100	100
4	D	198/280 (71%)	192 (97%)	6 (3%)	0	100	100
5	E	422/837 (50%)	411 (97%)	11 (3%)	0	100	100
5	G	432/837 (52%)	421 (98%)	11 (2%)	0	100	100
5	I	434/837 (52%)	425 (98%)	9 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	F	441/471 (94%)	431 (98%)	10 (2%)	0	100	100
6	H	437/471 (93%)	427 (98%)	10 (2%)	0	100	100
6	J	420/471 (89%)	407 (97%)	13 (3%)	0	100	100
7	K	314/625 (50%)	303 (96%)	11 (4%)	0	100	100
8	Q	106/132 (80%)	103 (97%)	3 (3%)	0	100	100
8	S	104/132 (79%)	101 (97%)	3 (3%)	0	100	100
9	R	89/131 (68%)	89 (100%)	0	0	100	100
9	T	91/131 (70%)	90 (99%)	1 (1%)	0	100	100
10	U	105/136 (77%)	103 (98%)	2 (2%)	0	100	100
10	W	96/136 (71%)	93 (97%)	3 (3%)	0	100	100
11	V	79/103 (77%)	76 (96%)	3 (4%)	0	100	100
11	X	79/103 (77%)	76 (96%)	3 (4%)	0	100	100
All	All	5263/8610 (61%)	5118 (97%)	145 (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	A	659/1400 (47%)	659 (100%)	0	100	100
2	B	280/732 (38%)	280 (100%)	0	100	100
3	C	372/396 (94%)	372 (100%)	0	100	100
4	D	197/261 (76%)	197 (100%)	0	100	100
5	E	363/688 (53%)	363 (100%)	0	100	100
5	G	367/688 (53%)	367 (100%)	0	100	100
5	I	369/688 (54%)	369 (100%)	0	100	100
6	F	377/403 (94%)	377 (100%)	0	100	100
6	H	375/403 (93%)	375 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	366/403 (91%)	366 (100%)	0	100	100
7	K	298/570 (52%)	298 (100%)	0	100	100
8	Q	86/99 (87%)	86 (100%)	0	100	100
8	S	85/99 (86%)	85 (100%)	0	100	100
9	R	79/109 (72%)	79 (100%)	0	100	100
9	T	81/109 (74%)	81 (100%)	0	100	100
10	U	90/111 (81%)	90 (100%)	0	100	100
10	W	85/111 (77%)	85 (100%)	0	100	100
11	V	66/79 (84%)	66 (100%)	0	100	100
11	X	66/79 (84%)	66 (100%)	0	100	100
All	All	4661/7428 (63%)	4661 (100%)	0	100	100

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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 31 such sidechains are listed below:

Mol	Chain	Res	Type
6	H	23	HIS
10	U	39	HIS
6	H	63	ASN
11	V	25	ASN
9	R	50	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

Of 20 ligands modelled in this entry, 10 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
14	ADP	E	901	16	28,29,29	1.39	4 (14%)	43,45,45	1.77	8 (18%)
14	ADP	C	501	16	28,29,29	1.41	4 (14%)	43,45,45	1.81	10 (23%)
14	ADP	A	1601	16,15	28,29,29	1.41	4 (14%)	43,45,45	1.80	9 (20%)
14	ADP	J	501	16	28,29,29	1.41	4 (14%)	43,45,45	1.78	9 (20%)
15	BEF	C	502	-	0,3,3	-	-	-	-	-
14	ADP	F	501	16	28,29,29	1.39	4 (14%)	43,45,45	1.81	7 (16%)
14	ADP	G	901	16	28,29,29	1.39	4 (14%)	43,45,45	1.87	8 (18%)
15	BEF	A	1602	14	0,3,3	-	-	-	-	-
14	ADP	I	901	16	28,29,29	1.41	4 (14%)	43,45,45	1.76	8 (18%)
14	ADP	H	501	16	28,29,29	1.40	4 (14%)	43,45,45	1.84	8 (18%)

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
14	ADP	E	901	16	-	4/16/32/32	0/3/3/3
14	ADP	C	501	16	-	3/16/32/32	0/3/3/3
14	ADP	A	1601	16,15	-	4/16/32/32	0/3/3/3
14	ADP	J	501	16	-	1/16/32/32	0/3/3/3
14	ADP	F	501	16	-	3/16/32/32	0/3/3/3
14	ADP	G	901	16	-	4/16/32/32	0/3/3/3
14	ADP	I	901	16	-	5/16/32/32	0/3/3/3
14	ADP	H	501	16	-	3/16/32/32	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)
14	A	1601	ADP	C5-C4	4.73	1.47	1.39
14	E	901	ADP	C5-C4	4.68	1.47	1.39
14	I	901	ADP	C5-C4	4.64	1.47	1.39
14	G	901	ADP	C5-C4	4.64	1.47	1.39
14	C	501	ADP	C5-C4	4.62	1.47	1.39

The worst 5 of 67 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	F	501	ADP	C5-C4-N3	-6.17	118.22	126.72
14	H	501	ADP	C5-C4-N3	-6.03	118.41	126.72
14	G	901	ADP	C5-C4-N3	-6.00	118.46	126.72
14	J	501	ADP	C5-C4-N3	-5.87	118.64	126.72
14	E	901	ADP	C5-C4-N3	-5.85	118.66	126.72

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
14	C	501	ADP	C5'-O5'-PA-O2A
14	E	901	ADP	PA-O3A-PB-O2B
14	F	501	ADP	C5'-O5'-PA-O1A
14	G	901	ADP	C5'-O5'-PA-O2A
14	G	901	ADP	C5'-O5'-PA-O3A

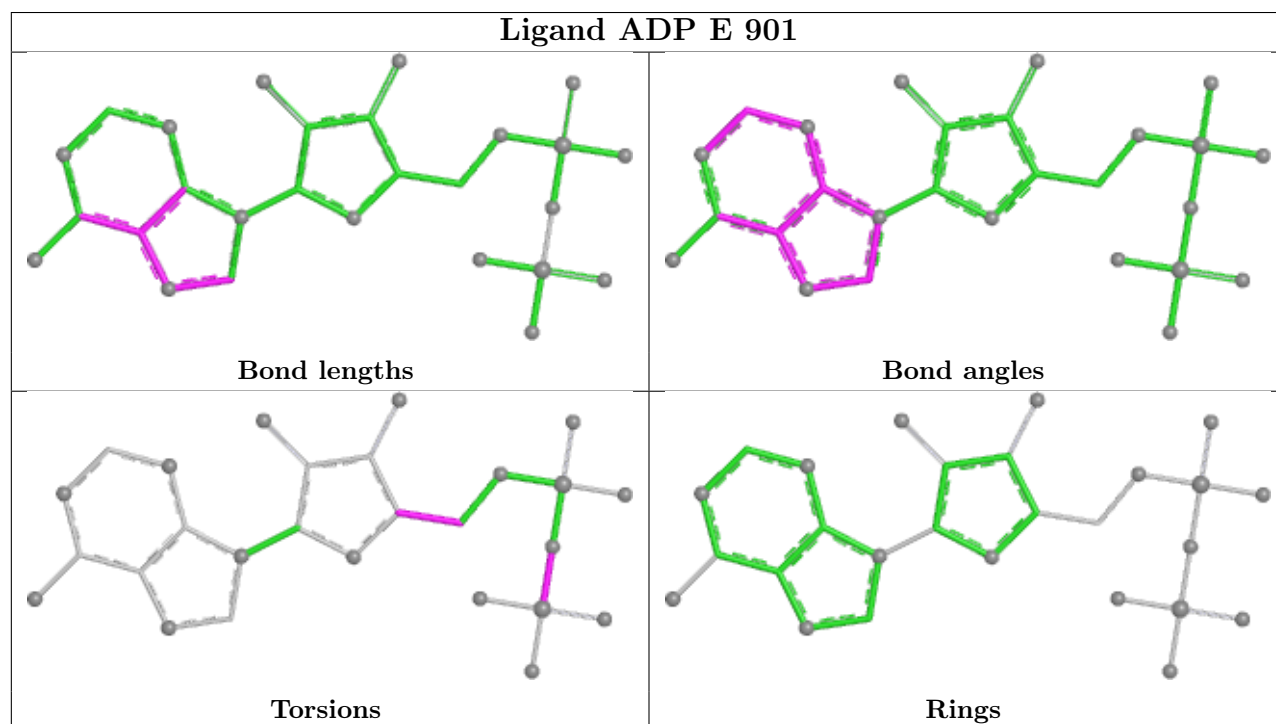
There are no ring outliers.

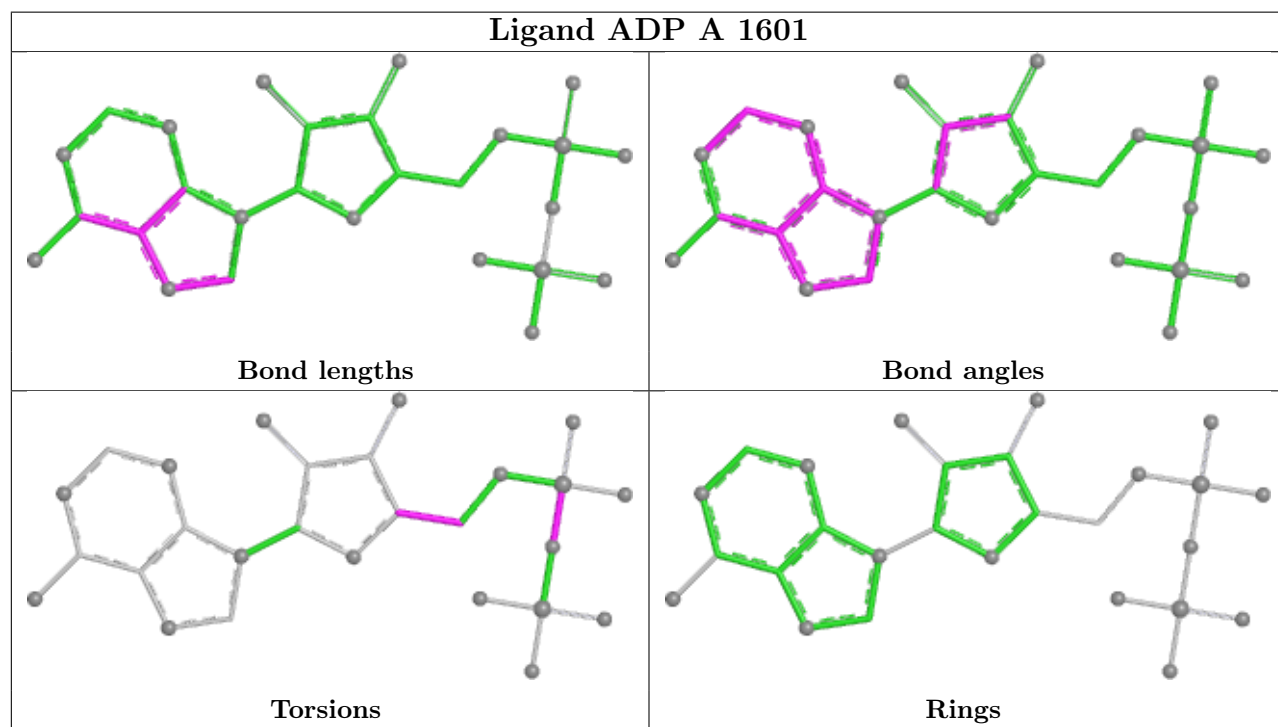
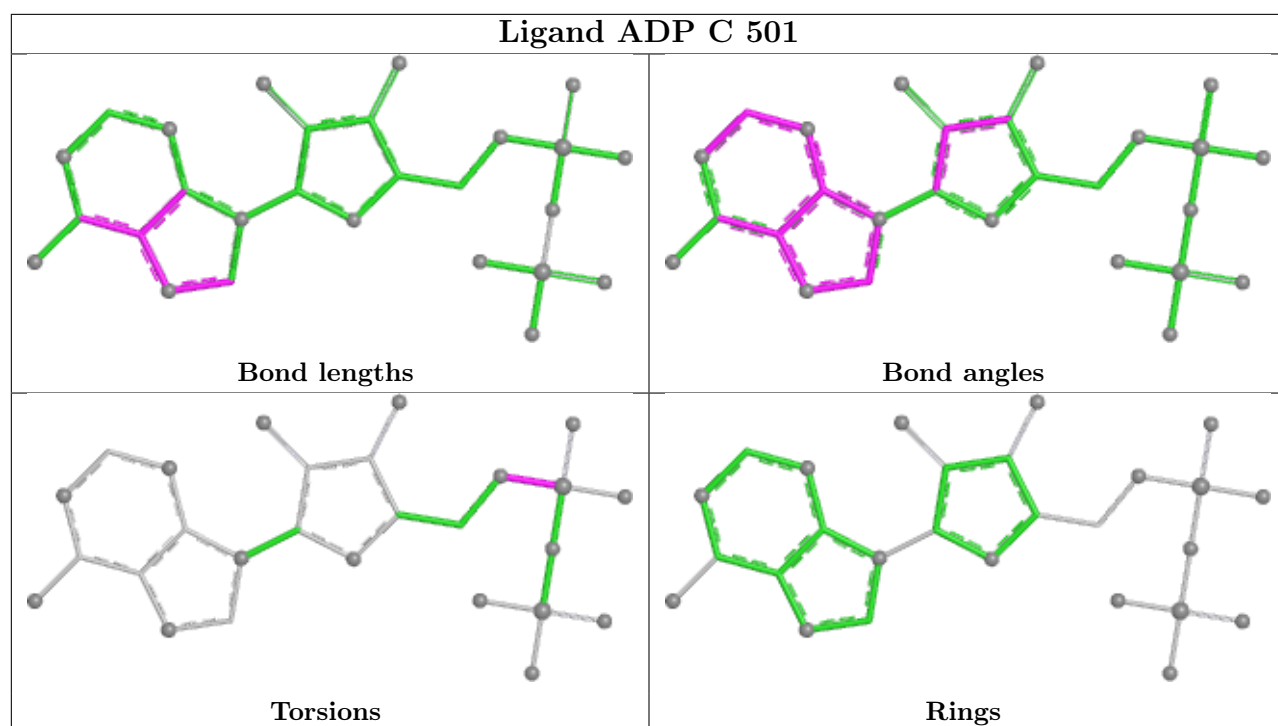
9 monomers are involved in 17 short contacts:

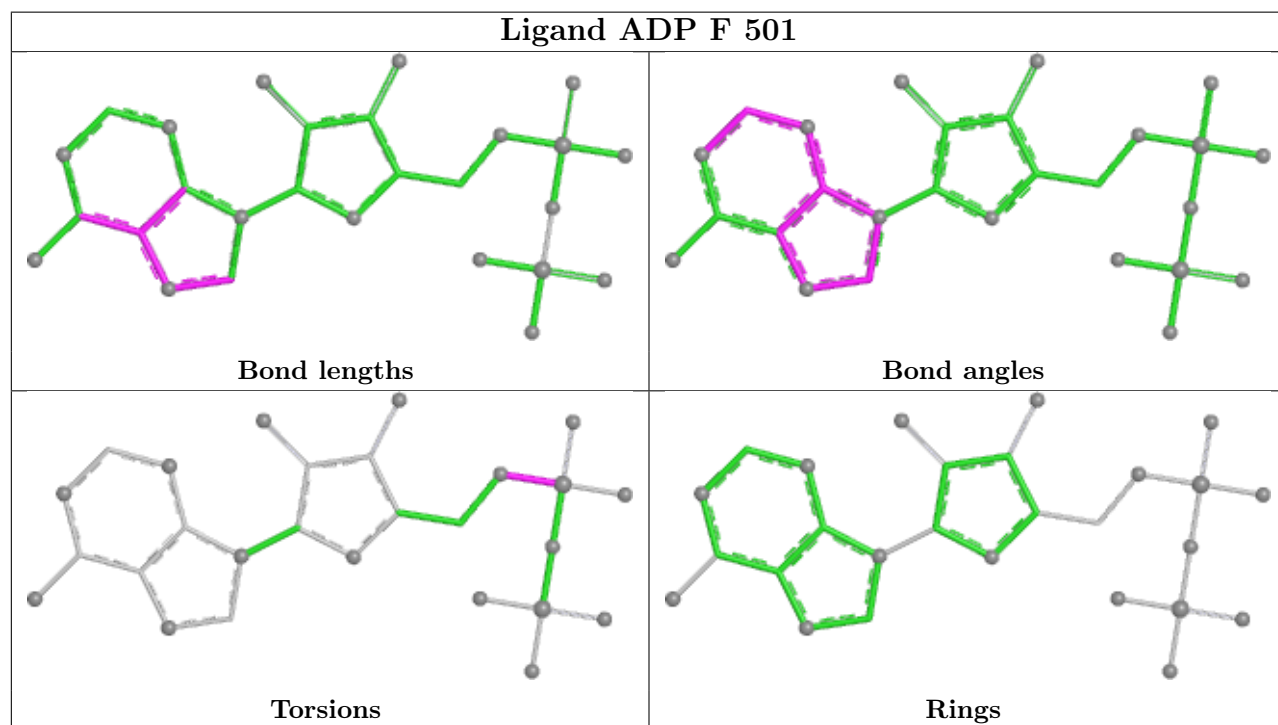
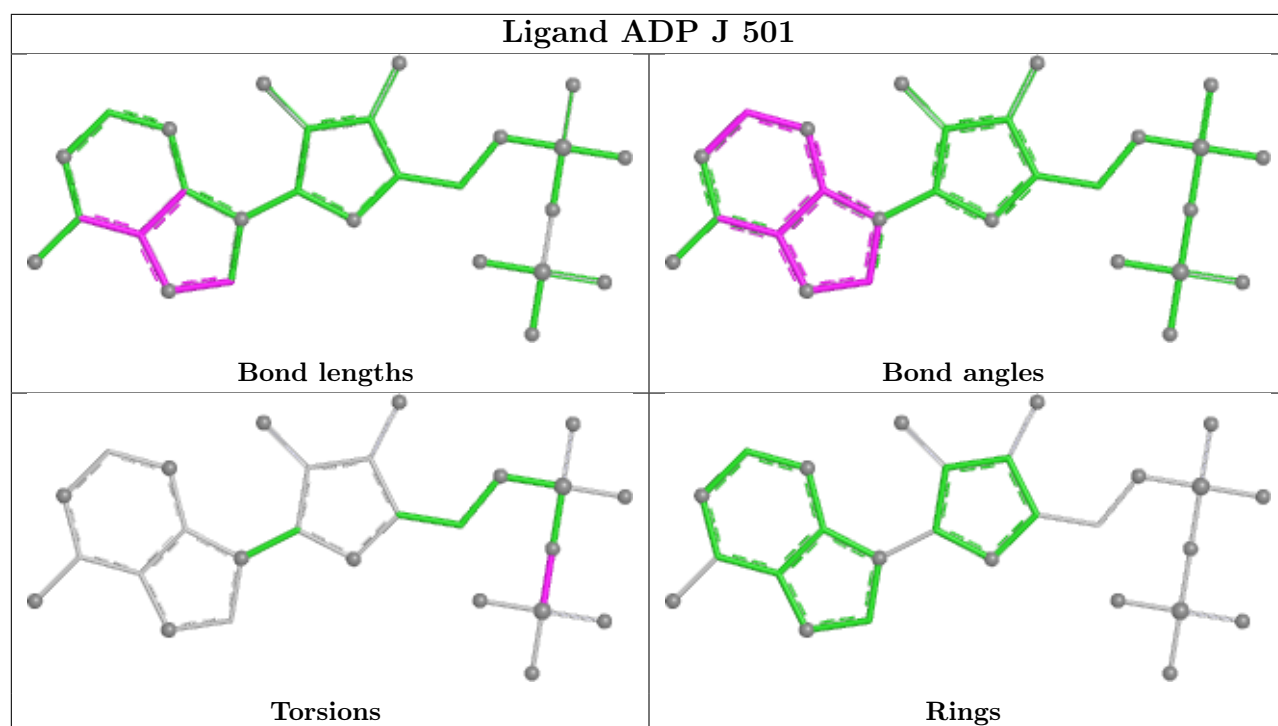
Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	E	901	ADP	2	0
14	C	501	ADP	1	0
14	A	1601	ADP	3	0
14	J	501	ADP	1	0
15	C	502	BEF	1	0
14	F	501	ADP	4	0
15	A	1602	BEF	1	0
14	I	901	ADP	2	0
14	H	501	ADP	4	0

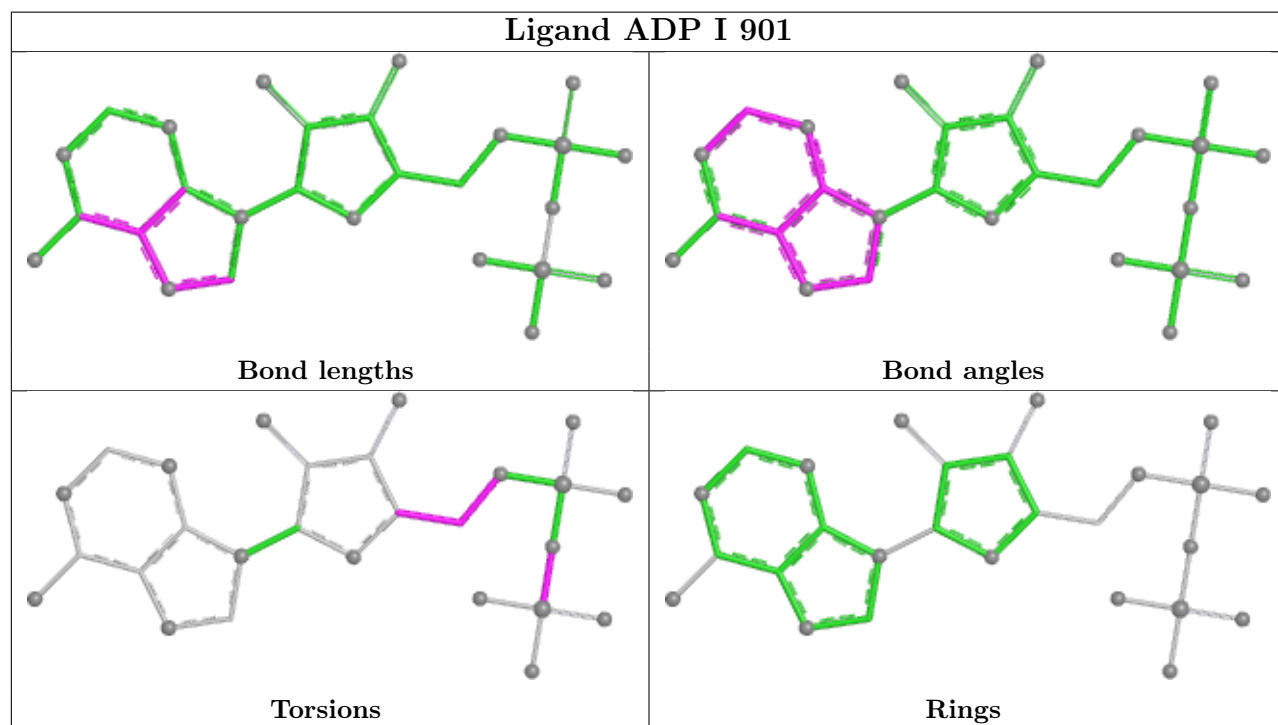
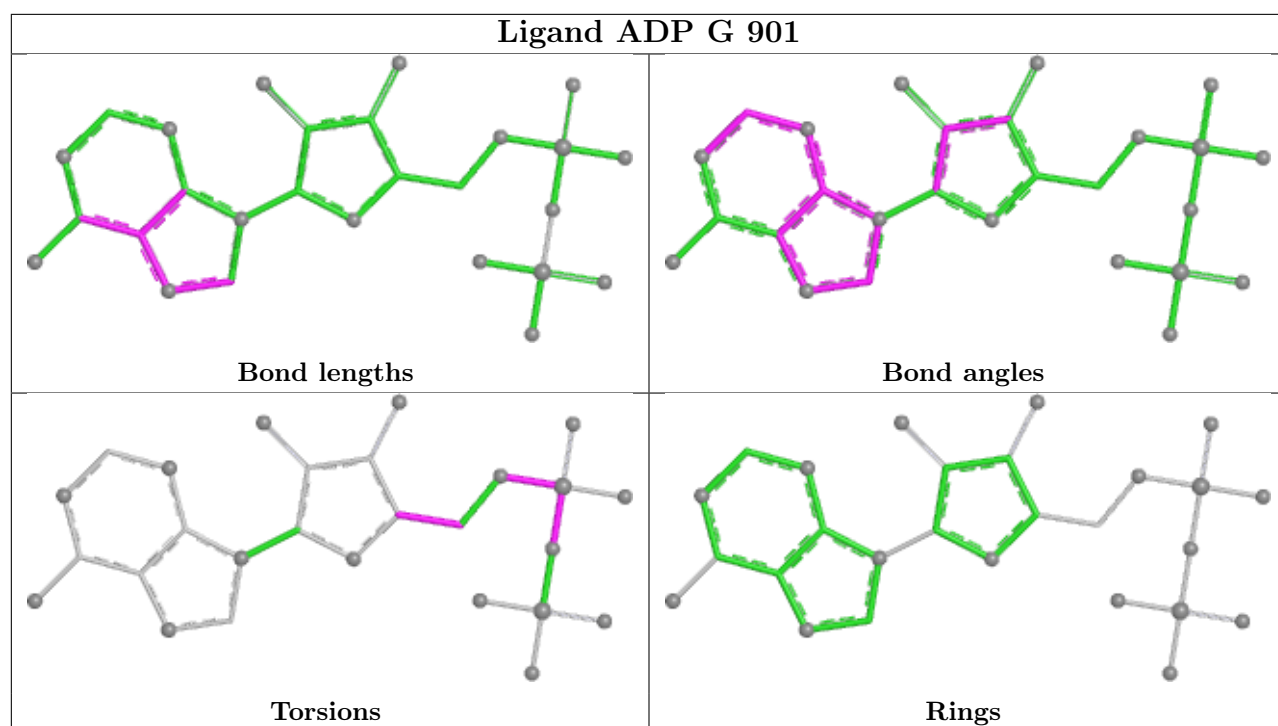
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

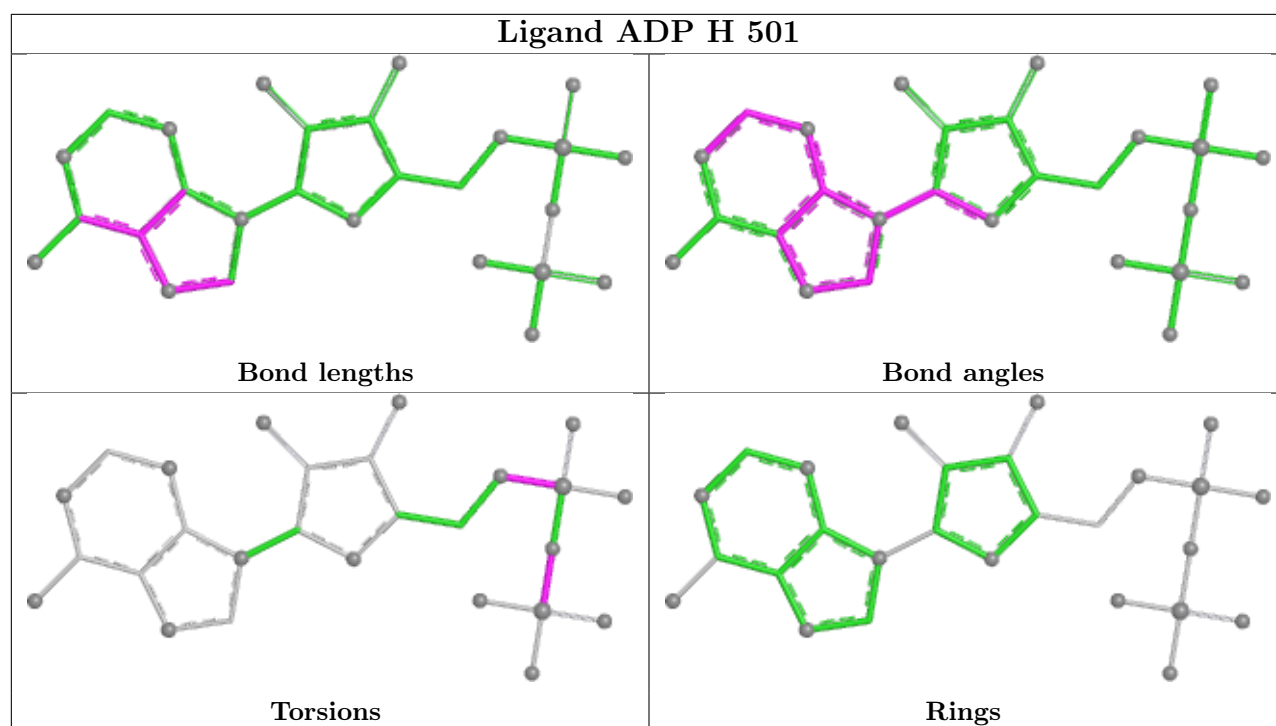
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

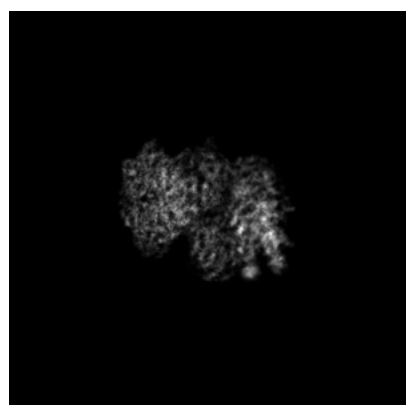
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-44075. These allow visual inspection of the internal detail of the map and identification of artifacts.

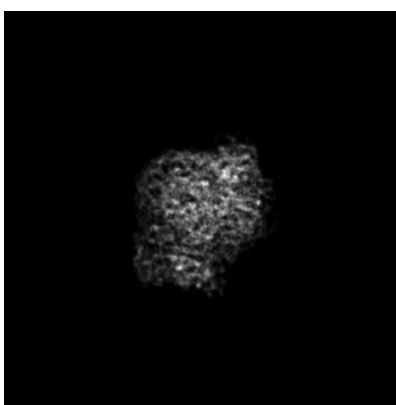
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

6.1.1 Primary map



X



Y

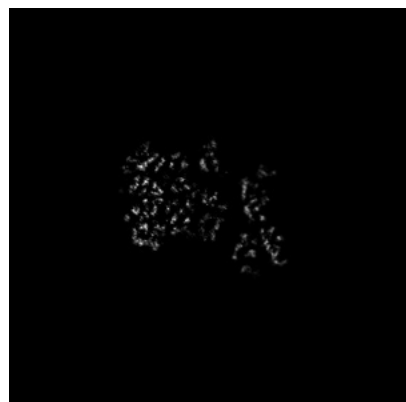


Z

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

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 192



Y Index: 192



Z Index: 192

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: 193



Y Index: 245

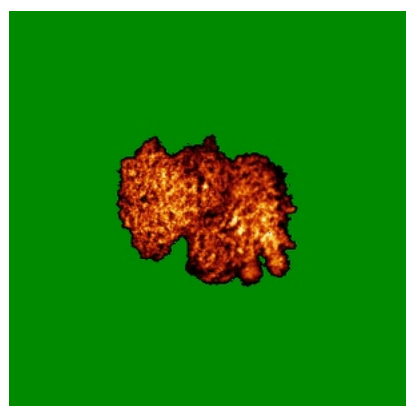


Z Index: 192

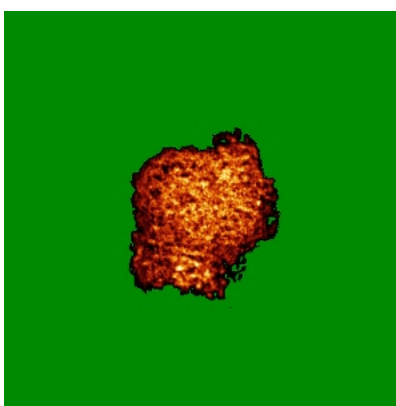
The images above show the largest variance slices of the map in three orthogonal directions.

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

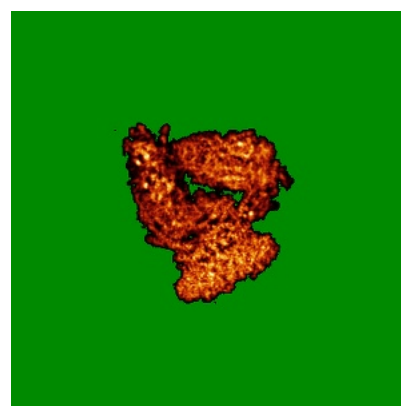
6.4.1 Primary map



X



Y

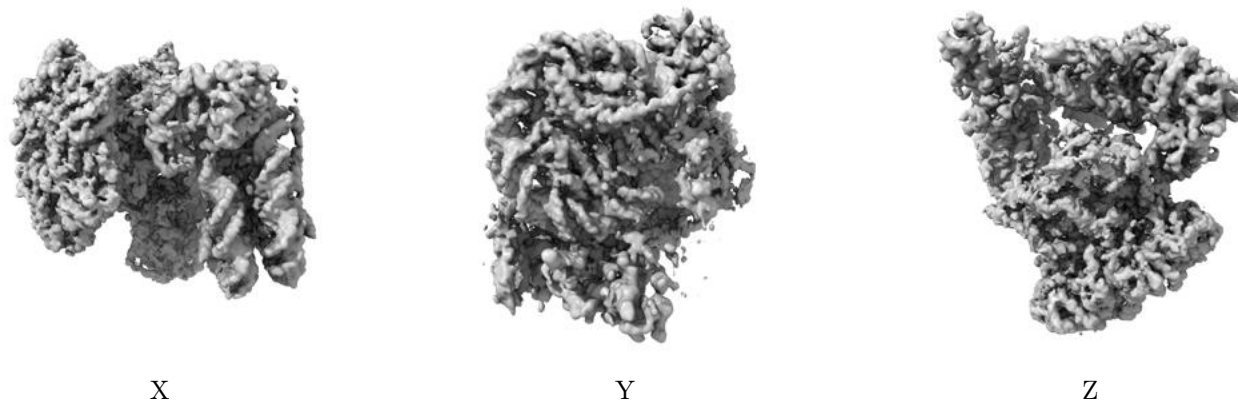


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

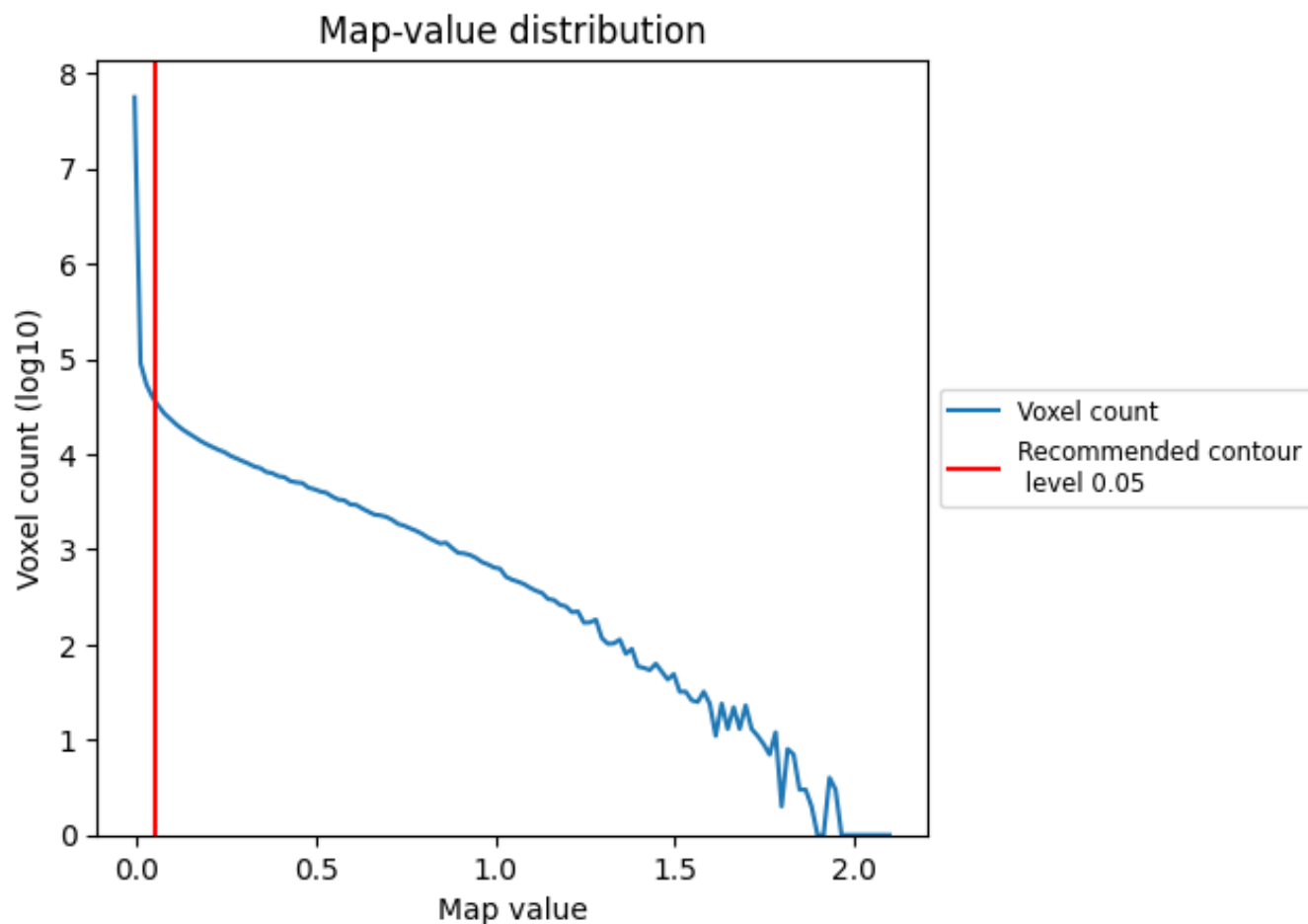
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

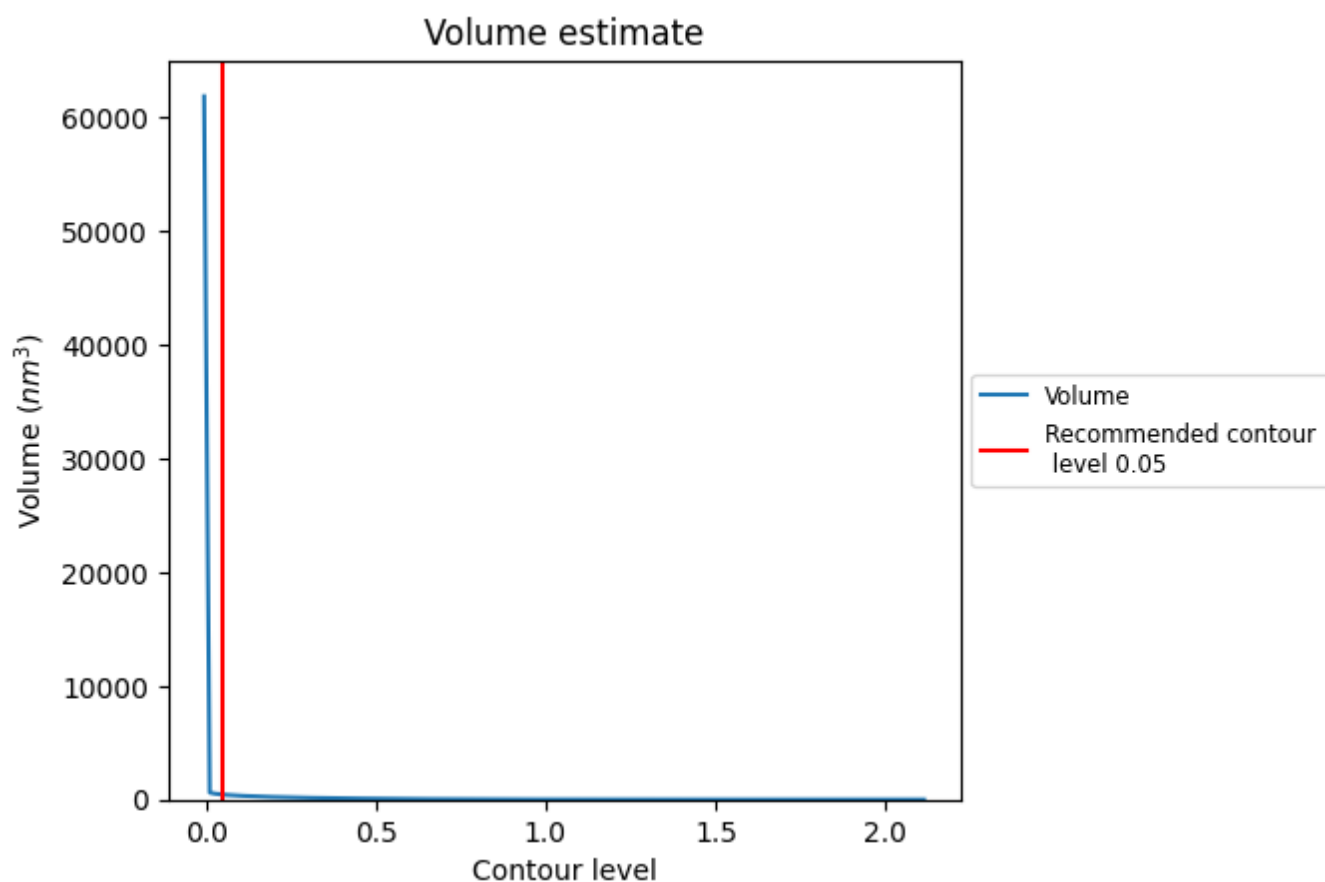
This section contains the results of statistical analysis of the map.

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.

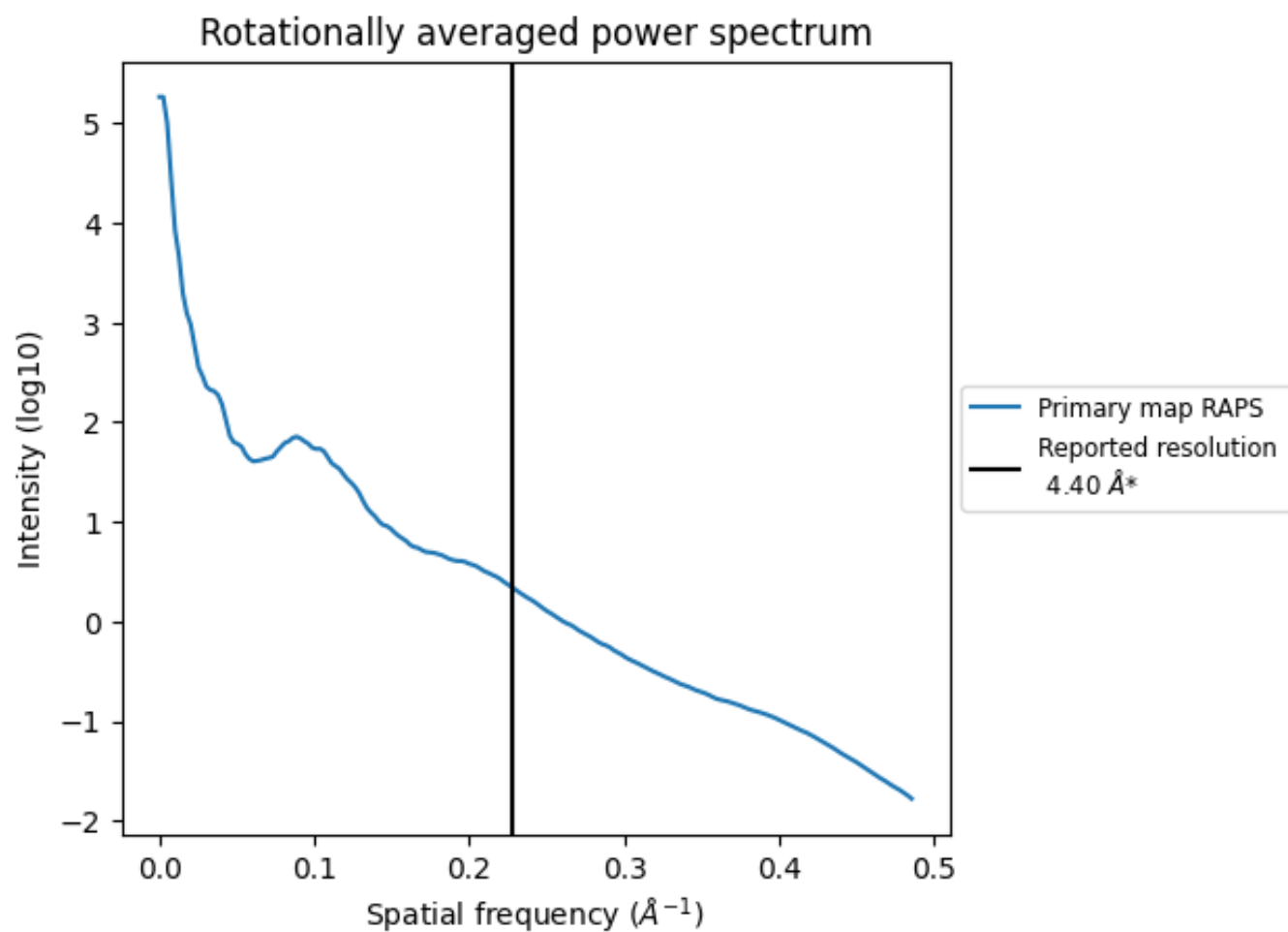
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 440 nm³; this corresponds to an approximate mass of 398 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 0.227 Å⁻¹

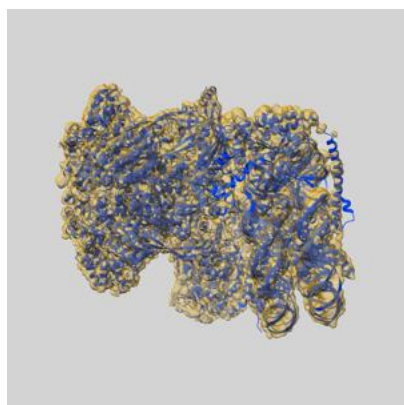
8 Fourier-Shell correlation

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

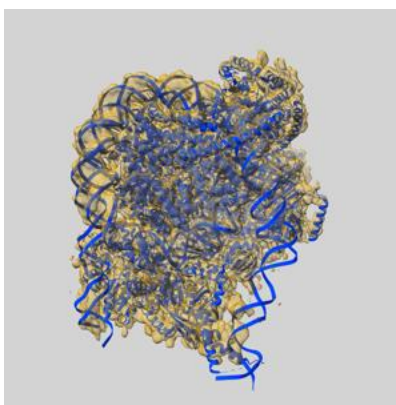
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-44075 and PDB model 9B1E. Per-residue inclusion information can be found in section [3](#) on page [9](#).

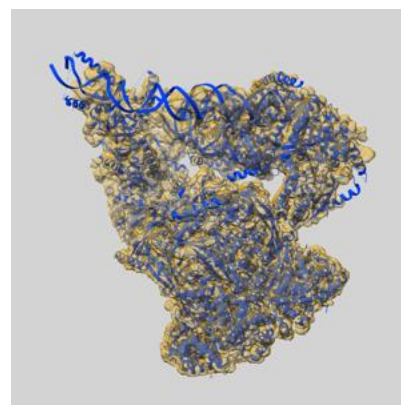
9.1 Map-model overlay [i](#)



X



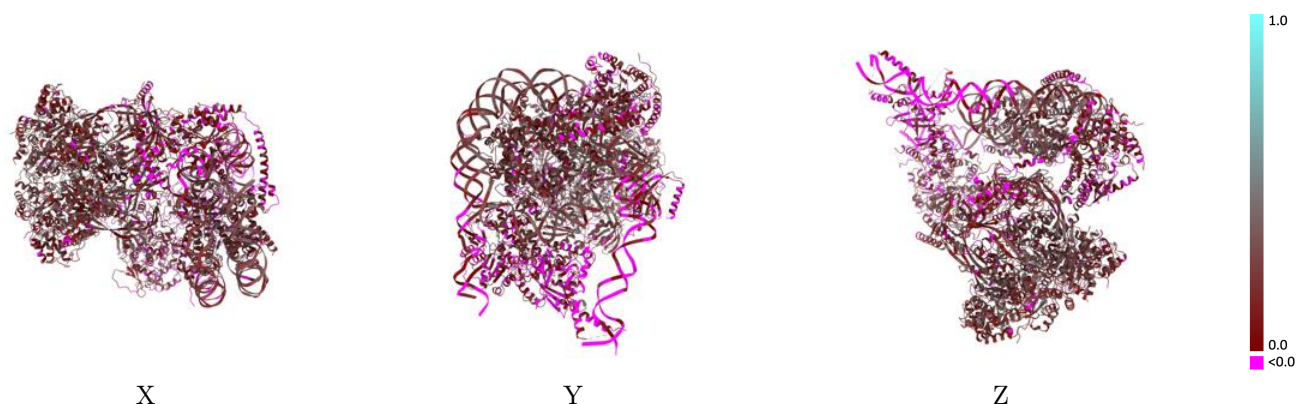
Y



Z

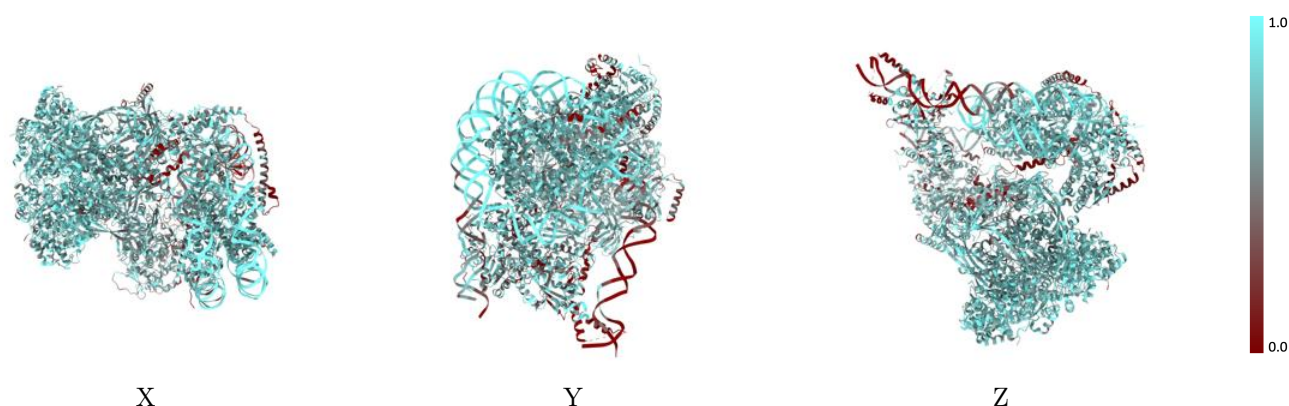
The images above show the 3D surface view of the map at the recommended contour level 0.05 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



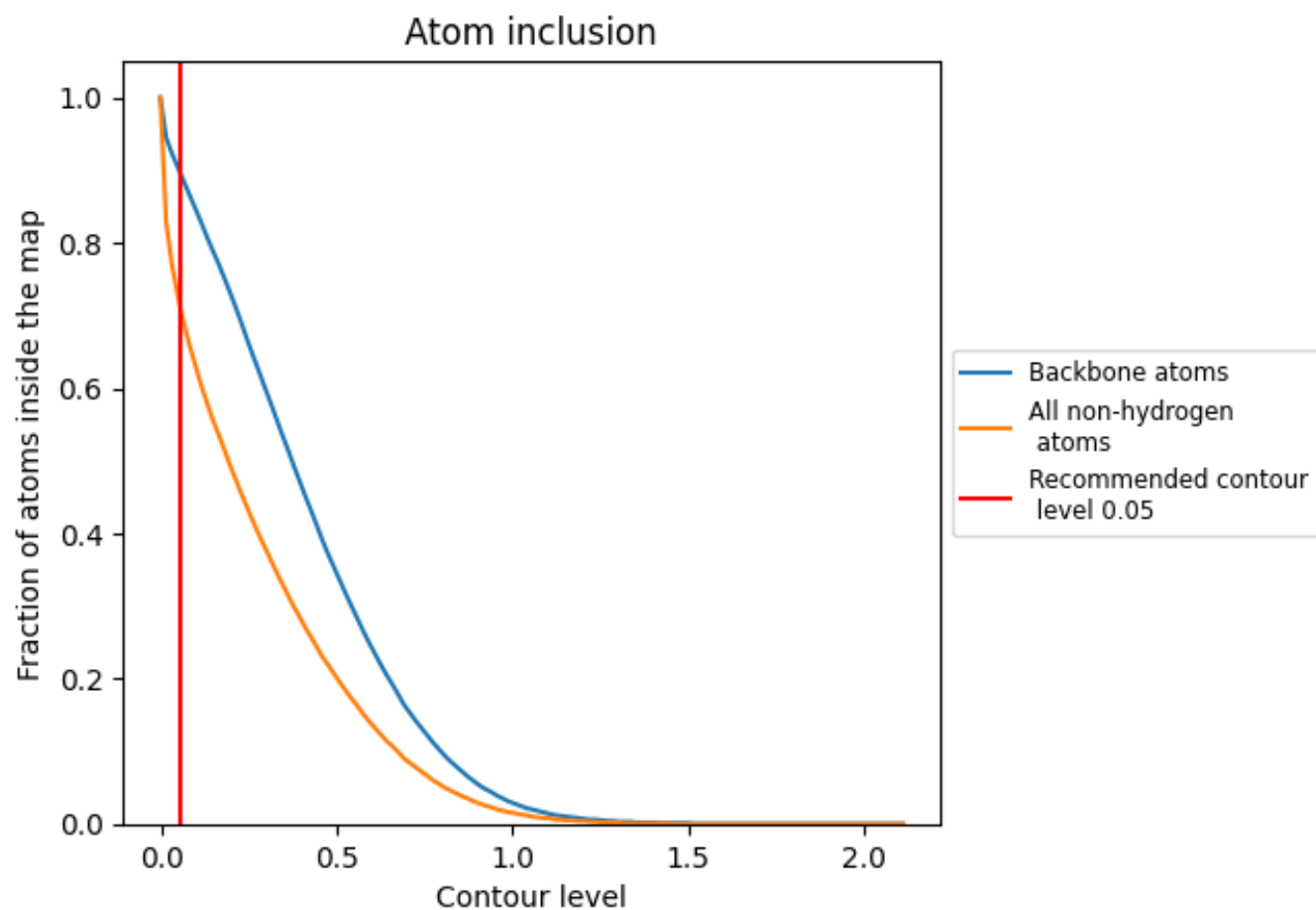
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.05).

9.4 Atom inclusion ⓘ



At the recommended contour level, 90% of all backbone atoms, 71% 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 (0.05) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7140	 0.1910
A	 0.6760	 0.1640
B	 0.5070	 0.0720
C	 0.6910	 0.1560
D	 0.5820	 0.1300
E	 0.7770	 0.2490
F	 0.7610	 0.2370
G	 0.7410	 0.2120
H	 0.7580	 0.2410
I	 0.7550	 0.2340
J	 0.7420	 0.2280
K	 0.5800	 0.0380
Q	 0.7520	 0.2250
R	 0.7920	 0.2290
S	 0.7890	 0.2520
T	 0.7830	 0.2370
U	 0.7280	 0.2130
V	 0.7810	 0.2410
W	 0.7580	 0.2130
X	 0.8060	 0.2570
Y	 0.7520	 0.1870
Z	 0.7350	 0.1840

