



wwPDB EM Validation Summary Report ⓘ

Apr 24, 2023 – 12:23 PM JST

PDB ID : 8HSR
EMDB ID : EMD-35004
Title : Thermus thermophilus Rho-engaged RNAP elongation complex
Authors : Murayama, Y.; Ehara, H.; Sekine, S.
Deposited on : 2022-12-20
Resolution : 4.00 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 ⓘ 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:

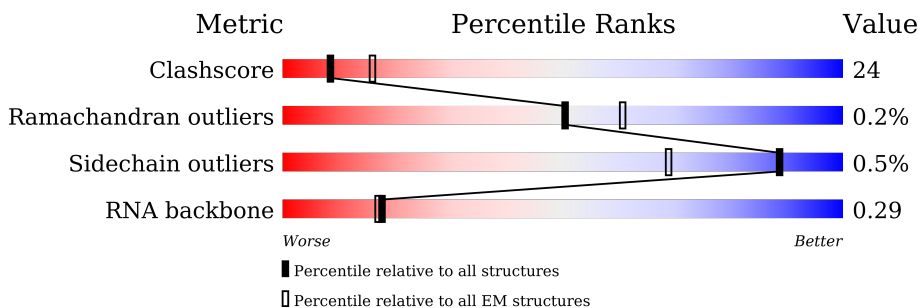
EMDB validation analysis : 0.0.1.dev50
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.32.2

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.00 Å.

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






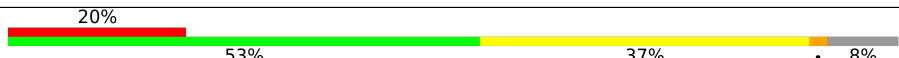
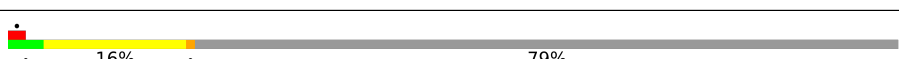
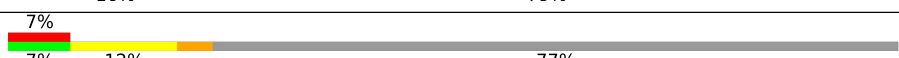

Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826
RNA backbone	4643	859

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	428	<div style="display: flex; justify-content: space-between;"> 6% 36% 48% 16% </div>
1	B	428	<div style="display: flex; justify-content: space-between;"> 10% 39% 45% 16% </div>
1	C	428	<div style="display: flex; justify-content: space-between;"> 9% 39% 46% 14% </div>
1	D	428	<div style="display: flex; justify-content: space-between;"> 9% 42% 42% 16% </div>
1	E	428	<div style="display: flex; justify-content: space-between;"> 6% 38% 45% 16% </div>
1	F	428	<div style="display: flex; justify-content: space-between;"> 7% 39% 44% 16% </div>
2	G	315	<div style="display: flex; justify-content: space-between;"> • 49% 23% 27% </div>

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Mol	Chain	Length	Quality of chain
2	H	315	
3	I	1119	
4	J	1532	
5	K	99	
6	T	184	
7	R	125	
8	N	180	

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
11	BEF	B	502	-	-	X	-
11	BEF	C	1004	-	-	X	-
11	BEF	D	1002	-	-	X	-
11	BEF	F	1002	-	-	X	-

2 Entry composition i

There are 12 unique types of molecules in this entry. The entry contains 42577 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 Transcription termination factor Rho.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	361	2842	1790	517	528	7	0	0
1	B	361	2842	1790	517	528	7	0	0
1	C	367	2882	1814	526	535	7	0	0
1	D	361	2842	1790	517	528	7	0	0
1	E	361	2842	1790	517	528	7	0	0
1	F	361	2842	1790	517	528	7	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q5SJE9
A	0	PRO	-	expression tag	UNP Q5SJE9
B	-1	GLY	-	expression tag	UNP Q5SJE9
B	0	PRO	-	expression tag	UNP Q5SJE9
C	-1	GLY	-	expression tag	UNP Q5SJE9
C	0	PRO	-	expression tag	UNP Q5SJE9
D	-1	GLY	-	expression tag	UNP Q5SJE9
D	0	PRO	-	expression tag	UNP Q5SJE9
E	-1	GLY	-	expression tag	UNP Q5SJE9
E	0	PRO	-	expression tag	UNP Q5SJE9
F	-1	GLY	-	expression tag	UNP Q5SJE9
F	0	PRO	-	expression tag	UNP Q5SJE9

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	229	Total	C	N	O	S	0	0
			1806	1153	313	337	3		
2	H	229	Total	C	N	O	S	0	0
			1806	1153	313	337	3		

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	1119	Total	C	N	O	S	0	0
			8829	5581	1577	1647	24		

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	1303	Total	C	N	O	S	0	0
			10280	6508	1821	1919	32		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1525	ASP	-	expression tag	UNP Q8RQE8
J	1526	TYR	-	expression tag	UNP Q8RQE8
J	1527	LYS	-	expression tag	UNP Q8RQE8
J	1528	ASP	-	expression tag	UNP Q8RQE8
J	1529	ASP	-	expression tag	UNP Q8RQE8
J	1530	ASP	-	expression tag	UNP Q8RQE8
J	1531	ASP	-	expression tag	UNP Q8RQE8
J	1532	LYS	-	expression tag	UNP Q8RQE8

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	91	Total	C	N	O	S	0	0
			735	467	129	135	4		

- Molecule 6 is a DNA chain called DNA (41-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
6	T	38	Total	C	N	O	P	0	0
			786	371	154	223	38		

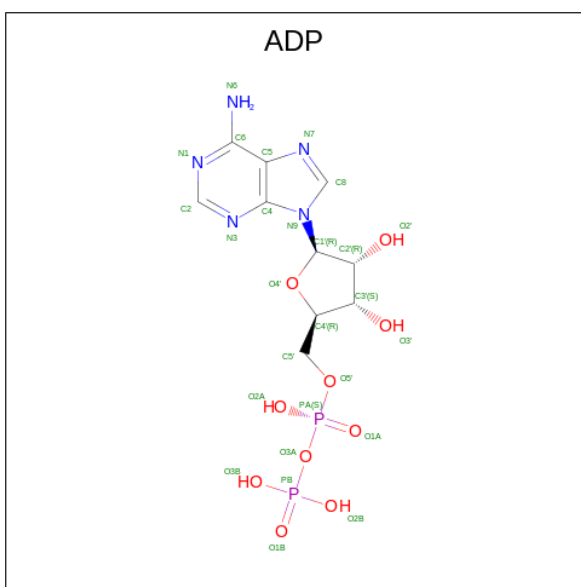
- Molecule 7 is a RNA chain called RNA (29-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
7	R	29	474	208	47	190	29	0	0

- Molecule 8 is a DNA chain called DNA (31-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
8	N	28	574	273	99	174	28	0	0

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

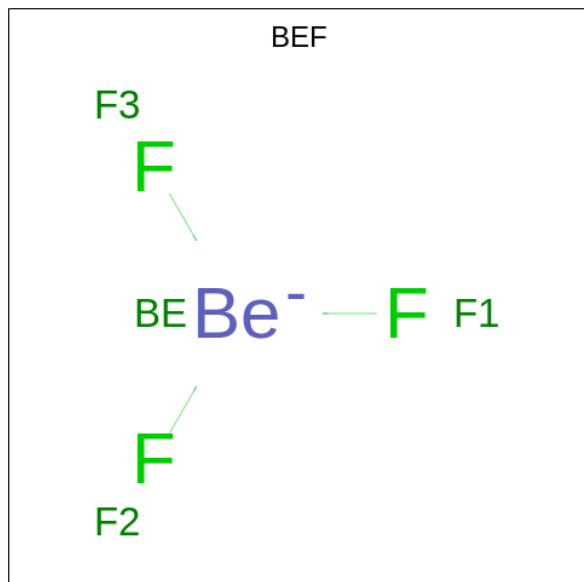


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
9	A	1	27	10	5	10	2	0
9	B	1	27	10	5	10	2	0
9	C	1	27	10	5	10	2	0
9	D	1	27	10	5	10	2	0
9	E	1	27	10	5	10	2	0
9	F	1	27	10	5	10	2	0

- Molecule 10 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
10	A	1	Total Mg 1 1	0
10	C	2	Total Mg 2 2	0
10	D	1	Total Mg 1 1	0
10	E	1	Total Mg 1 1	0
10	F	1	Total Mg 1 1	0
10	J	1	Total Mg 1 1	0

- Molecule 11 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total Be F 4 1 3	0
11	B	1	Total Be F 4 1 3	0
11	C	1	Total Be F 4 1 3	0
11	D	1	Total Be F 4 1 3	0
11	E	1	Total Be F 4 1 3	0
11	F	1	Total Be F 4 1 3	0

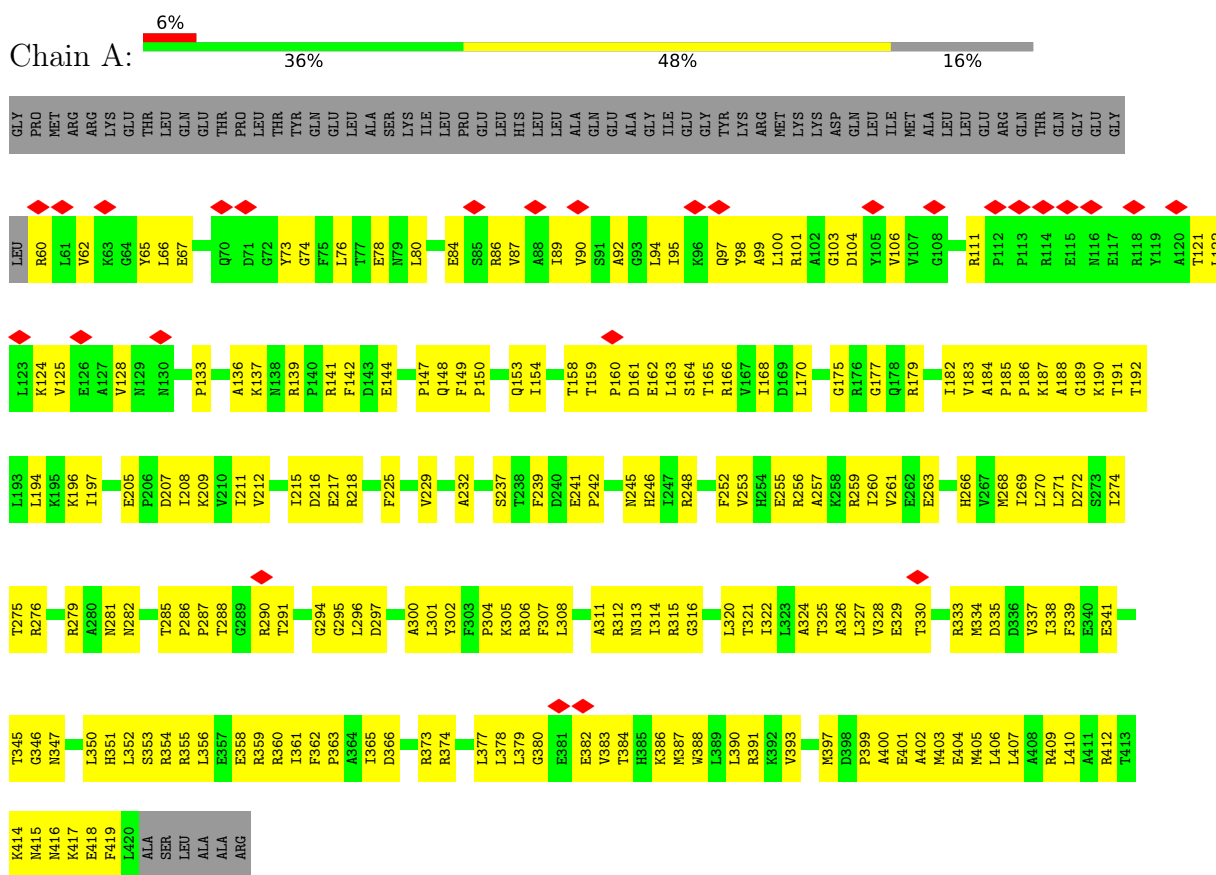
- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
12	J	2	Total 2	Zn 2	0

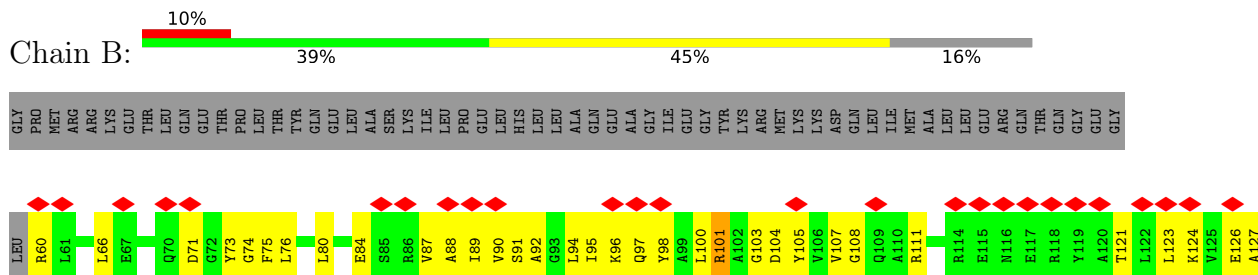
3 Residue-property plots [i](#)

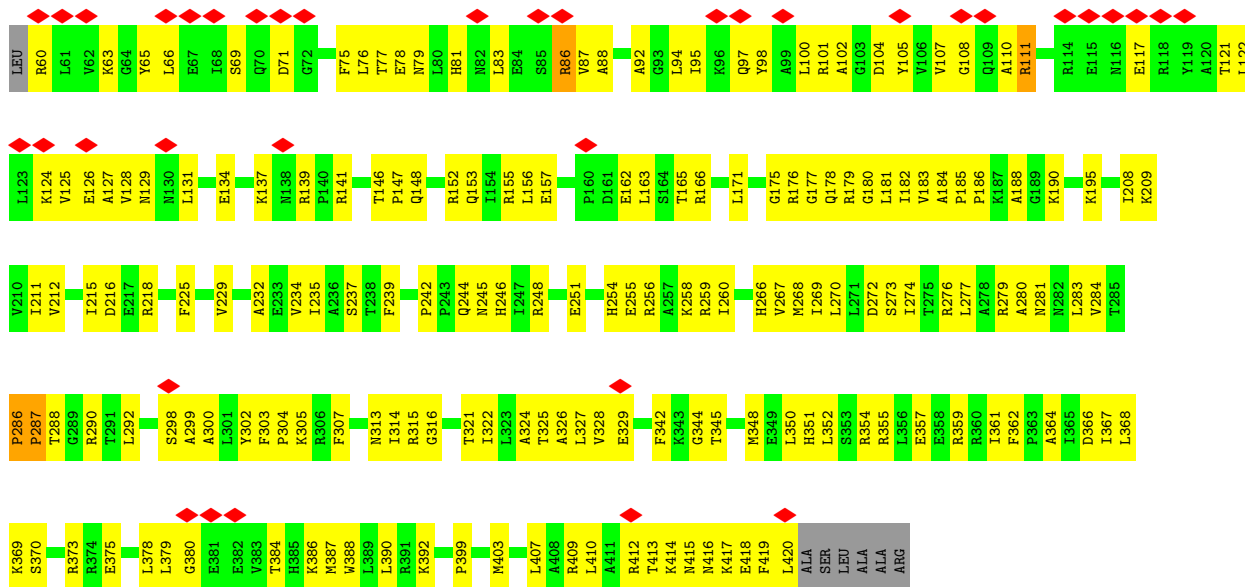
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

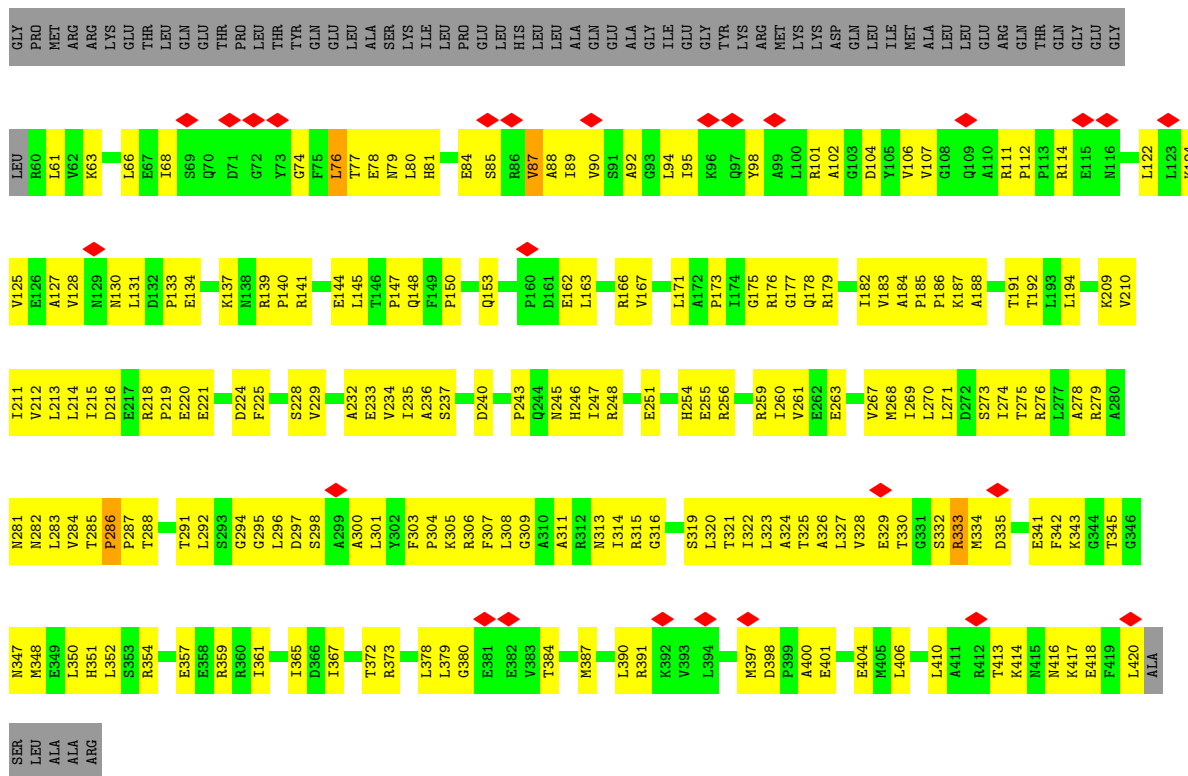


- Molecule 1: Transcription termination factor Rho

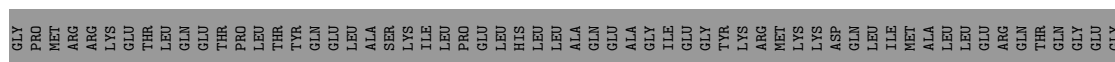


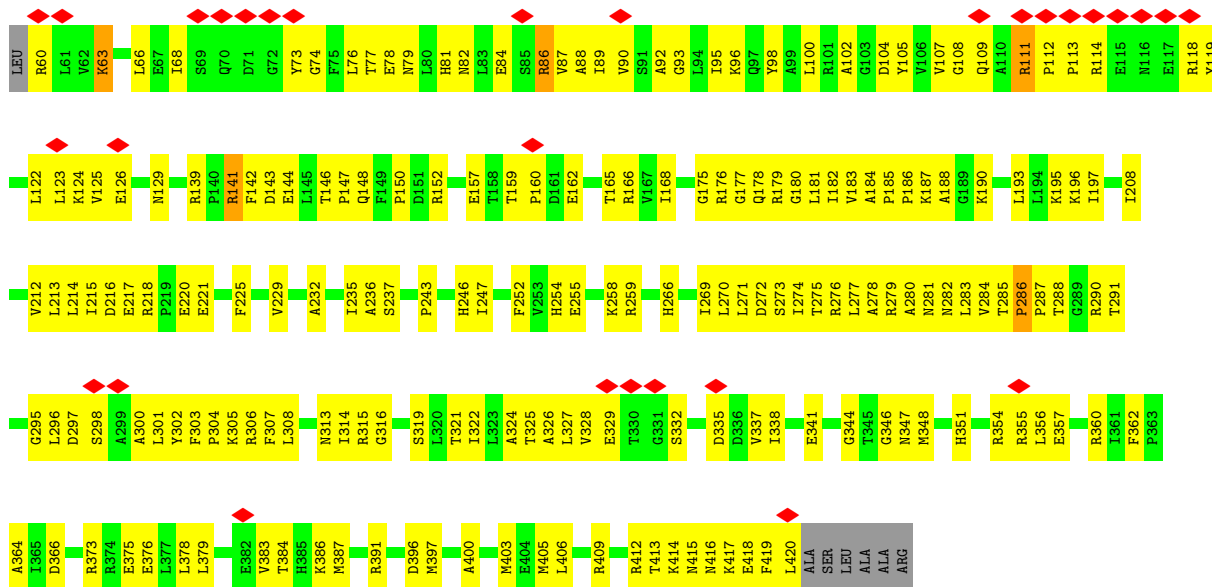


• Molecule 1: Transcription termination factor Rho

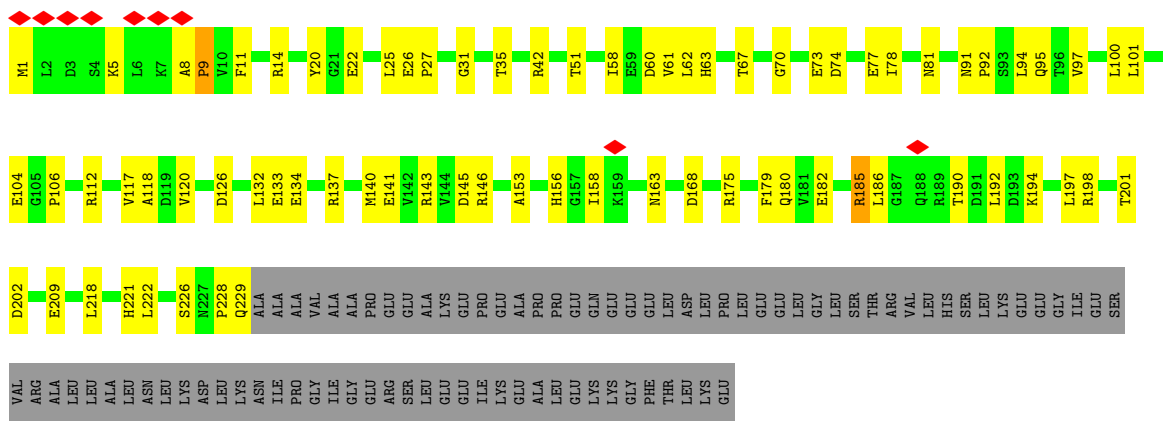


• Molecule 1: Transcription termination factor Rho

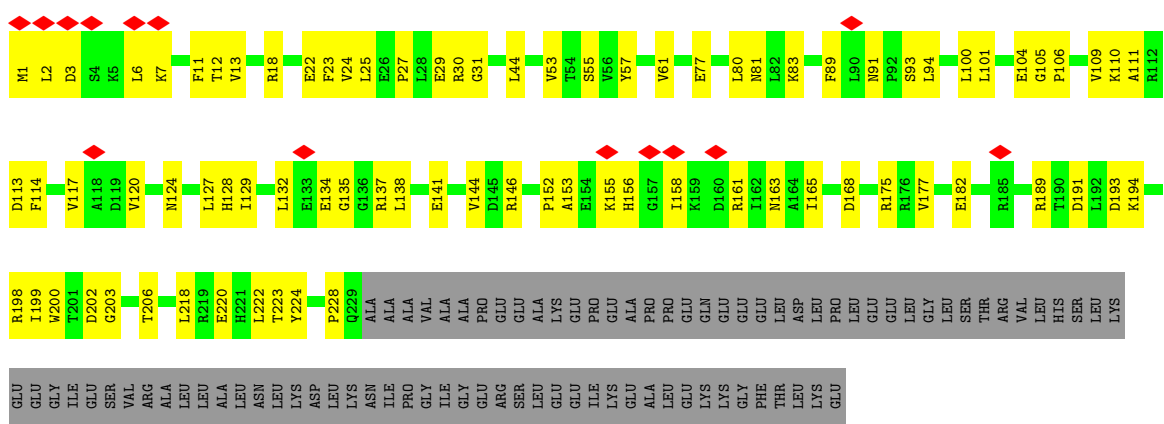




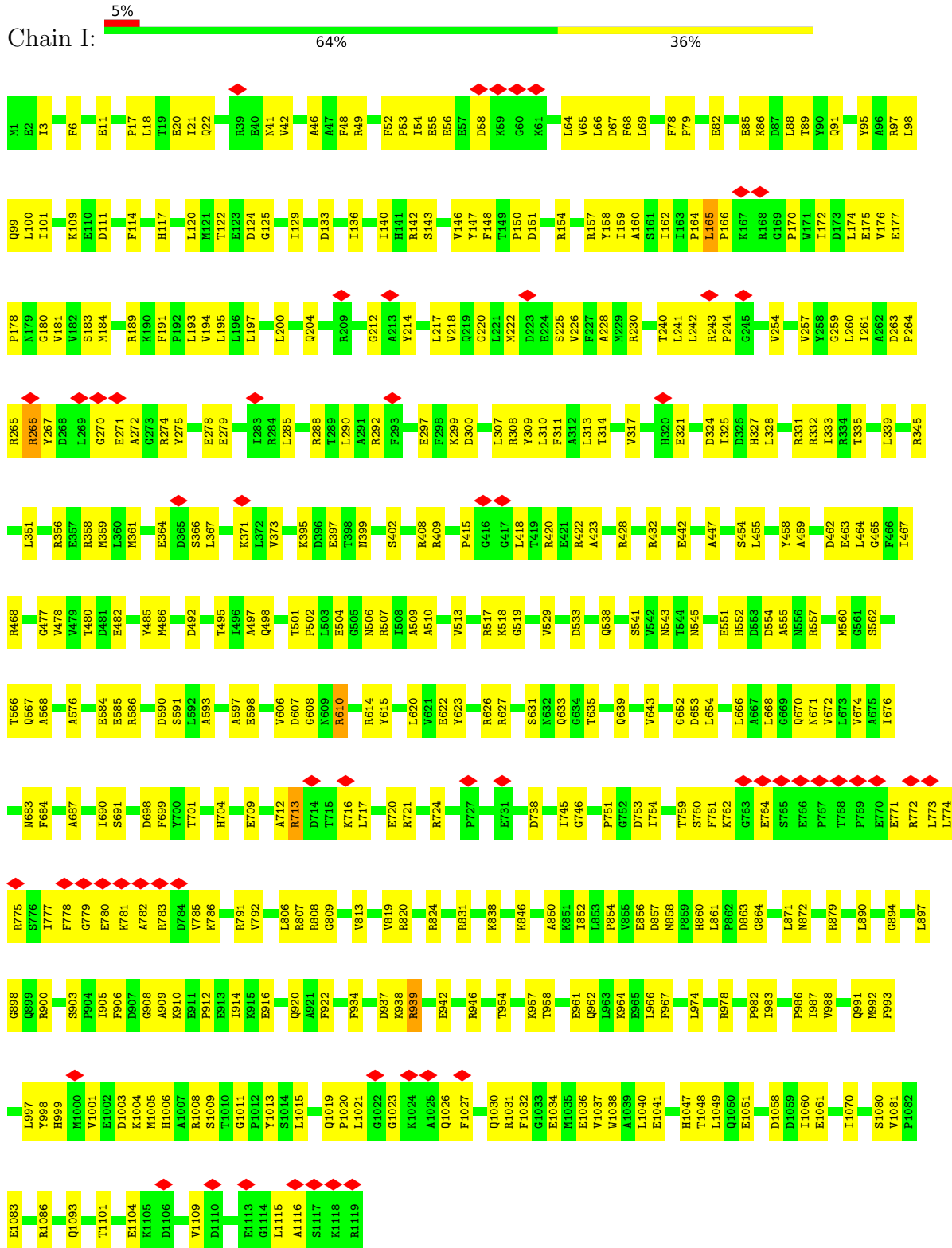
• Molecule 2: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit alpha

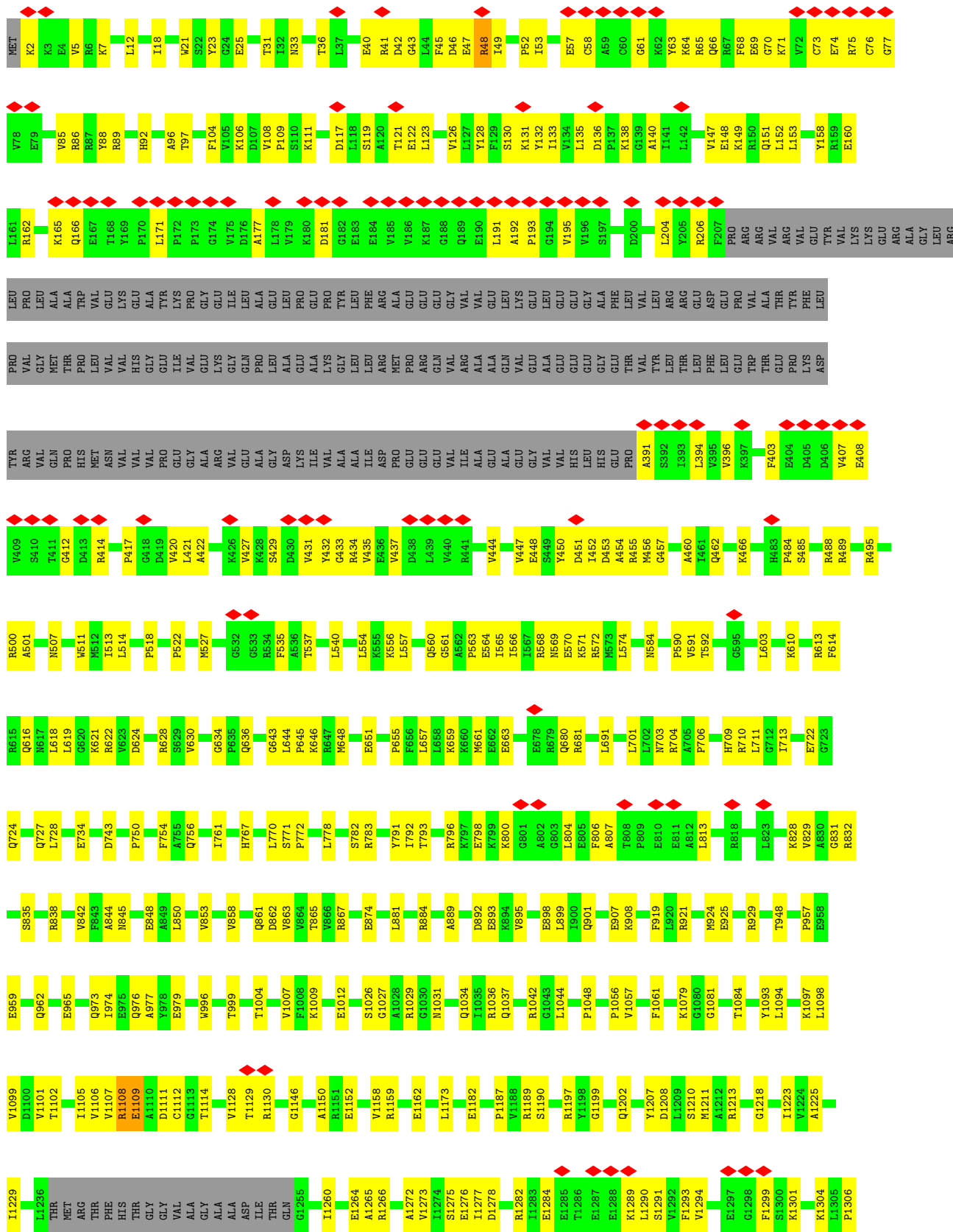


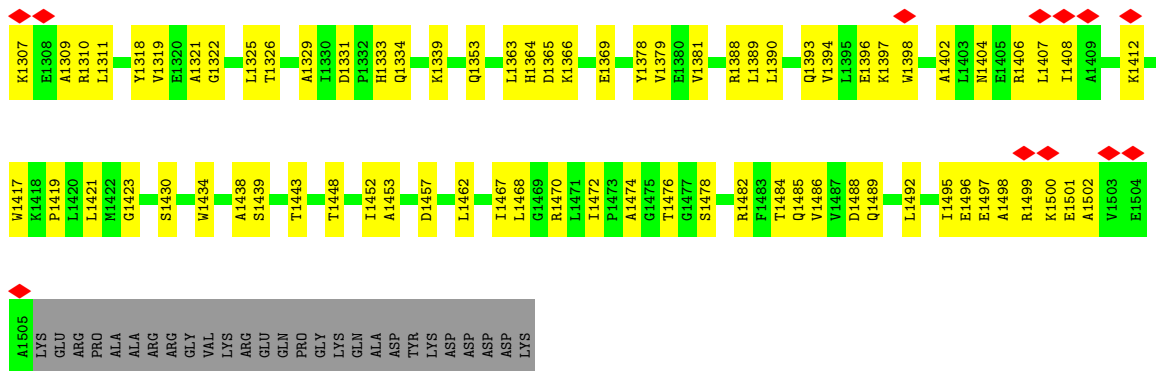
• Molecule 3: DNA-directed RNA polymerase subunit beta



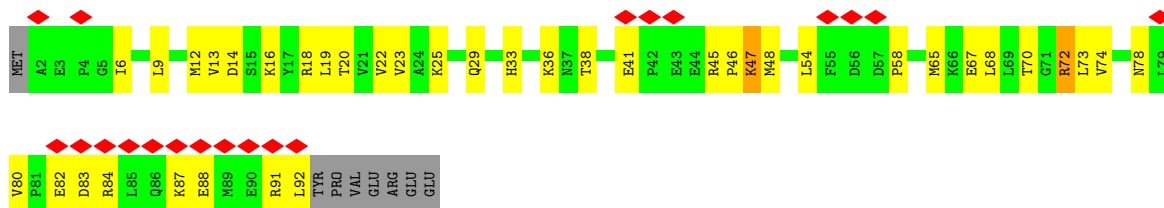
• Molecule 4: DNA-directed RNA polymerase subunit beta'



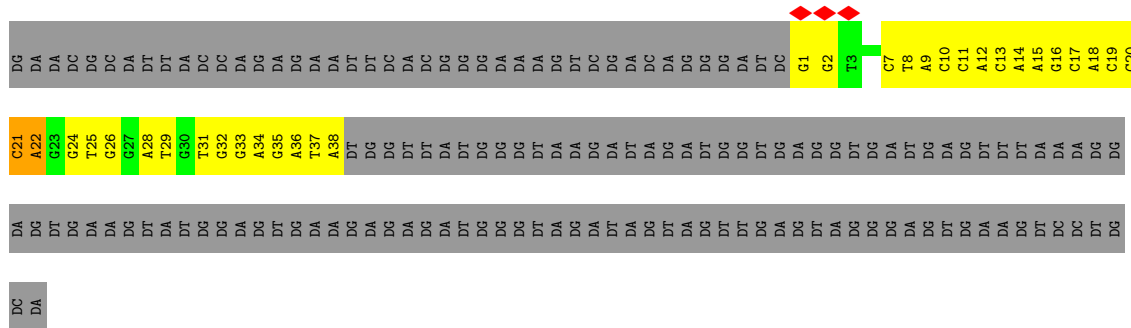




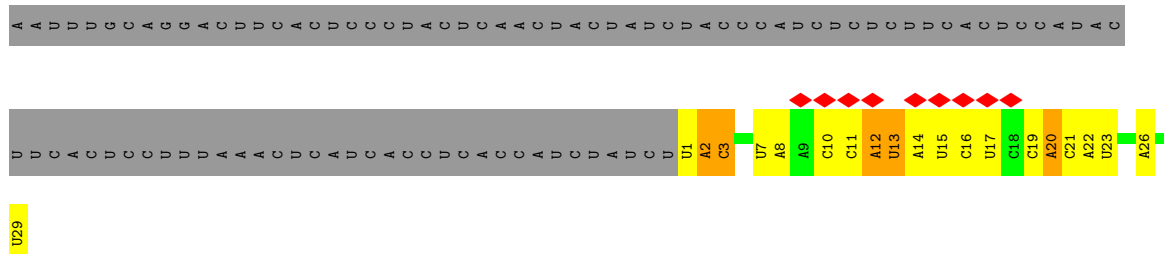
• Molecule 5: DNA-directed RNA polymerase subunit omega



• Molecule 6: DNA (41-MER)



• Molecule 7: RNA (29-MER)



• Molecule 8: DNA (31-MER)

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	43245	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	17.972	Depositor
Minimum map value	-6.489	Depositor
Average map value	-0.012	Depositor
Map value standard deviation	0.925	Depositor
Recommended contour level	4.4	Depositor
Map size (\AA)	339.19998, 339.19998, 339.19998	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.06, 1.06, 1.06	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.29	0/2886	0.59	0/3900
1	B	0.31	0/2886	0.59	0/3900
1	C	0.30	0/2926	0.61	0/3954
1	D	0.29	0/2886	0.58	0/3900
1	E	0.30	0/2886	0.61	2/3900 (0.1%)
1	F	0.28	0/2886	0.58	0/3900
2	G	0.31	0/1838	0.54	0/2498
2	H	0.29	0/1838	0.54	0/2498
3	I	0.32	0/8997	0.56	1/12164 (0.0%)
4	J	0.31	0/10452	0.54	0/14116
5	K	0.30	0/747	0.60	0/1005
6	T	0.74	0/884	1.03	4/1363 (0.3%)
7	R	0.35	0/520	0.85	0/801
8	N	0.60	0/640	1.00	0/984
All	All	0.33	0/43272	0.60	7/58883 (0.0%)

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
2	G	0	1
4	J	0	1
All	All	0	2

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	T	32	DG	O5'-P-OP1	-8.37	98.17	105.70
6	T	31	DT	OP1-P-O3'	7.46	121.61	105.20
1	E	76	LEU	CA-CB-CG	6.44	130.11	115.30
6	T	21	DC	P-O3'-C3'	6.26	127.21	119.70
3	I	165	LEU	CA-CB-CG	5.43	127.79	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	9	PRO	Peptide
4	J	1109	GLU	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2842	0	2924	204	0
1	B	2842	0	2924	198	0
1	C	2882	0	2968	239	0
1	D	2842	0	2924	196	0
1	E	2842	0	2924	209	0
1	F	2842	0	2925	211	0
2	G	1806	0	1861	58	0
2	H	1806	0	1861	68	0
3	I	8829	0	8933	342	0
4	J	10280	0	10509	357	0
5	K	735	0	752	75	0
6	T	786	0	422	78	0
7	R	474	0	246	14	0
8	N	574	0	317	50	0
9	A	27	0	12	8	0
9	B	27	0	12	8	0
9	C	27	0	12	8	0
9	D	27	0	12	5	0
9	E	27	0	11	2	0
9	F	27	0	10	3	0
10	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	C	2	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	J	1	0	0	0	0
11	A	4	0	0	0	0
11	B	4	0	0	4	0
11	C	4	0	0	5	0
11	D	4	0	0	2	0
11	E	4	0	0	1	0
11	F	4	0	0	2	0
12	J	2	0	0	0	0
All	All	42577	0	42559	2039	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 24.

The worst 5 of 2039 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:T:10:DC:N3	8:N:32:DG:N1	1.62	1.46
6:T:10:DC:N4	8:N:32:DG:O6	1.58	1.35
6:T:10:DC:O2	8:N:32:DG:N2	1.57	1.35
1:C:413:THR:OG1	5:K:84:ARG:NH2	1.61	1.34
1:C:412:ARG:HD2	5:K:83:ASP:OD2	1.23	1.31

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	359/428 (84%)	339 (94%)	20 (6%)	0	100	100
1	B	359/428 (84%)	337 (94%)	21 (6%)	1 (0%)	41	75
1	C	365/428 (85%)	345 (94%)	19 (5%)	1 (0%)	41	75
1	D	359/428 (84%)	341 (95%)	16 (4%)	2 (1%)	25	63
1	E	359/428 (84%)	335 (93%)	22 (6%)	2 (1%)	25	63
1	F	359/428 (84%)	339 (94%)	19 (5%)	1 (0%)	41	75
2	G	227/315 (72%)	218 (96%)	9 (4%)	0	100	100
2	H	227/315 (72%)	213 (94%)	14 (6%)	0	100	100
3	I	1117/1119 (100%)	1017 (91%)	99 (9%)	1 (0%)	51	84
4	J	1297/1532 (85%)	1204 (93%)	93 (7%)	0	100	100
5	K	89/99 (90%)	78 (88%)	11 (12%)	0	100	100
All	All	5117/5948 (86%)	4766 (93%)	343 (7%)	8 (0%)	50	79

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	287	PRO
1	C	287	PRO
1	D	287	PRO
1	D	286	PRO
3	I	780	GLU

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/359 (85%)	304 (100%)	0	100	100
1	B	304/359 (85%)	303 (100%)	1 (0%)	92	95
1	C	307/359 (86%)	304 (99%)	3 (1%)	76	86
1	D	304/359 (85%)	302 (99%)	2 (1%)	84	90
1	E	304/359 (85%)	303 (100%)	1 (0%)	92	95

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	304/359 (85%)	300 (99%)	4 (1%)	69	82
2	G	202/273 (74%)	201 (100%)	1 (0%)	88	93
2	H	202/273 (74%)	202 (100%)	0	100	100
3	I	941/941 (100%)	937 (100%)	4 (0%)	91	94
4	J	1100/1287 (86%)	1098 (100%)	2 (0%)	93	96
5	K	80/88 (91%)	77 (96%)	3 (4%)	33	59
All	All	4352/5016 (87%)	4331 (100%)	21 (0%)	89	93

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	713	ARG
4	J	1108	ARG
5	K	78	ASN
5	K	47	LYS
4	J	48	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	180	GLN
4	J	1364	HIS
2	G	229	GLN
4	J	1485	GLN
3	I	1019	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
7	R	28/125 (22%)	12 (42%)	0

5 of 12 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
7	R	2	A
7	R	3	C
7	R	7	U
7	R	8	A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	R	10	C

There are no RNA pucker outliers to report.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 21 ligands modelled in this entry, 9 are monoatomic - leaving 12 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
11	BEF	B	502	1	0,3,3	-	-	-	-	-
9	ADP	E	1000	1,10	24,29,29	0.98	1 (4%)	29,45,45	1.44	4 (13%)
9	ADP	F	1000	1,10	24,29,29	0.98	1 (4%)	29,45,45	1.42	4 (13%)
11	BEF	D	1002	-	0,3,3	-	-	-	-	-
9	ADP	D	1000	1,10	24,29,29	0.98	1 (4%)	29,45,45	1.58	4 (13%)
11	BEF	A	1002	-	0,3,3	-	-	-	-	-
9	ADP	B	501	1,10	24,29,29	0.94	1 (4%)	29,45,45	1.36	3 (10%)
11	BEF	E	1002	-	0,3,3	-	-	-	-	-
11	BEF	C	1004	-	0,3,3	-	-	-	-	-
9	ADP	A	1000	1,10	24,29,29	0.95	1 (4%)	29,45,45	1.35	3 (10%)
9	ADP	C	1002	10	24,29,29	1.04	1 (4%)	29,45,45	1.58	5 (17%)
11	BEF	F	1002	-	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. '2' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	ADP	E	1000	1,10	-	3/12/32/32	0/3/3/3
9	ADP	F	1000	1,10	-	1/12/32/32	0/3/3/3
9	ADP	D	1000	1,10	-	3/12/32/32	0/3/3/3
9	ADP	B	501	1,10	-	7/12/32/32	0/3/3/3
9	ADP	A	1000	1,10	-	10/12/32/32	0/3/3/3
9	ADP	C	1002	10	-	3/12/32/32	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	1002	ADP	C5-C4	2.61	1.47	1.40
9	E	1000	ADP	C5-C4	2.55	1.47	1.40
9	D	1000	ADP	C5-C4	2.55	1.47	1.40
9	F	1000	ADP	C5-C4	2.52	1.47	1.40
9	A	1000	ADP	C5-C4	2.43	1.47	1.40

The worst 5 of 23 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	C	1002	ADP	PA-O3A-PB	-5.24	114.86	132.83
9	D	1000	ADP	PA-O3A-PB	-4.02	119.03	132.83
9	D	1000	ADP	C3'-C2'-C1'	3.85	106.77	100.98
9	E	1000	ADP	C3'-C2'-C1'	3.72	106.57	100.98
9	A	1000	ADP	C3'-C2'-C1'	3.60	106.39	100.98

There are no chirality outliers.

5 of 27 torsion outliers are listed below:

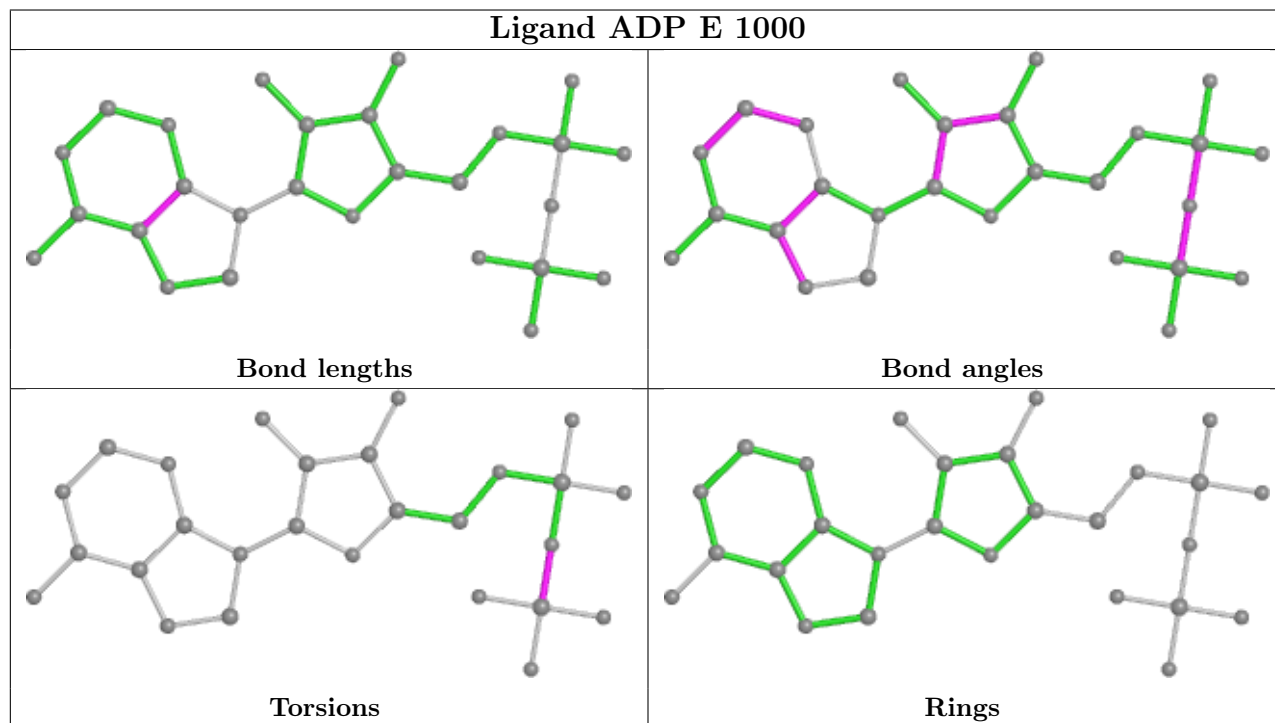
Mol	Chain	Res	Type	Atoms
9	A	1000	ADP	PA-O3A-PB-O3B
9	A	1000	ADP	C5'-O5'-PA-O1A
9	B	501	ADP	PA-O3A-PB-O2B
9	B	501	ADP	PA-O3A-PB-O3B
9	B	501	ADP	C5'-O5'-PA-O3A

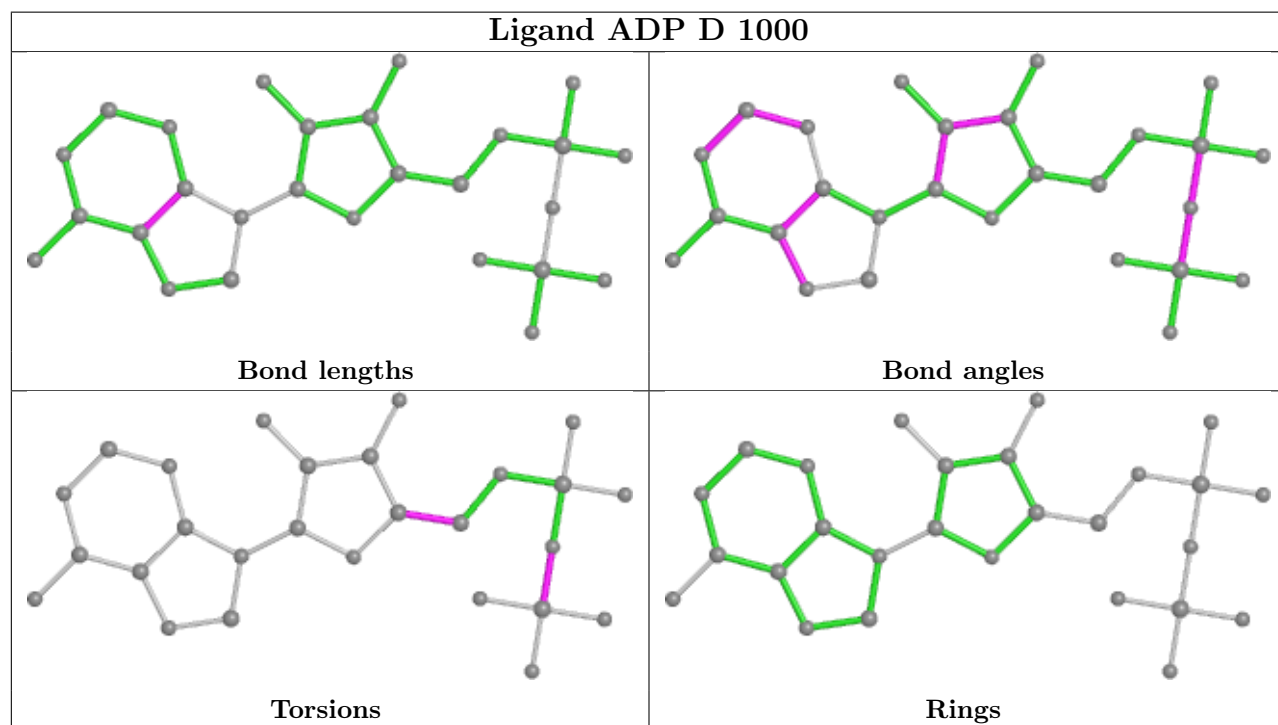
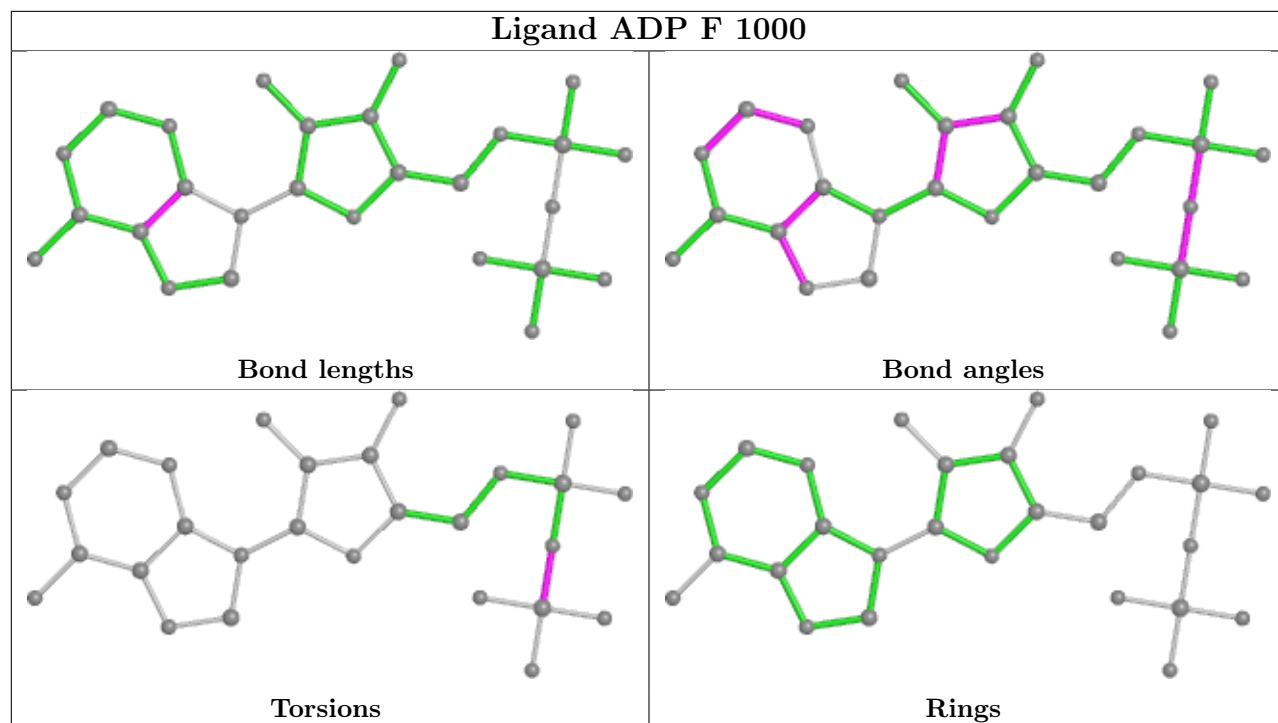
There are no ring outliers.

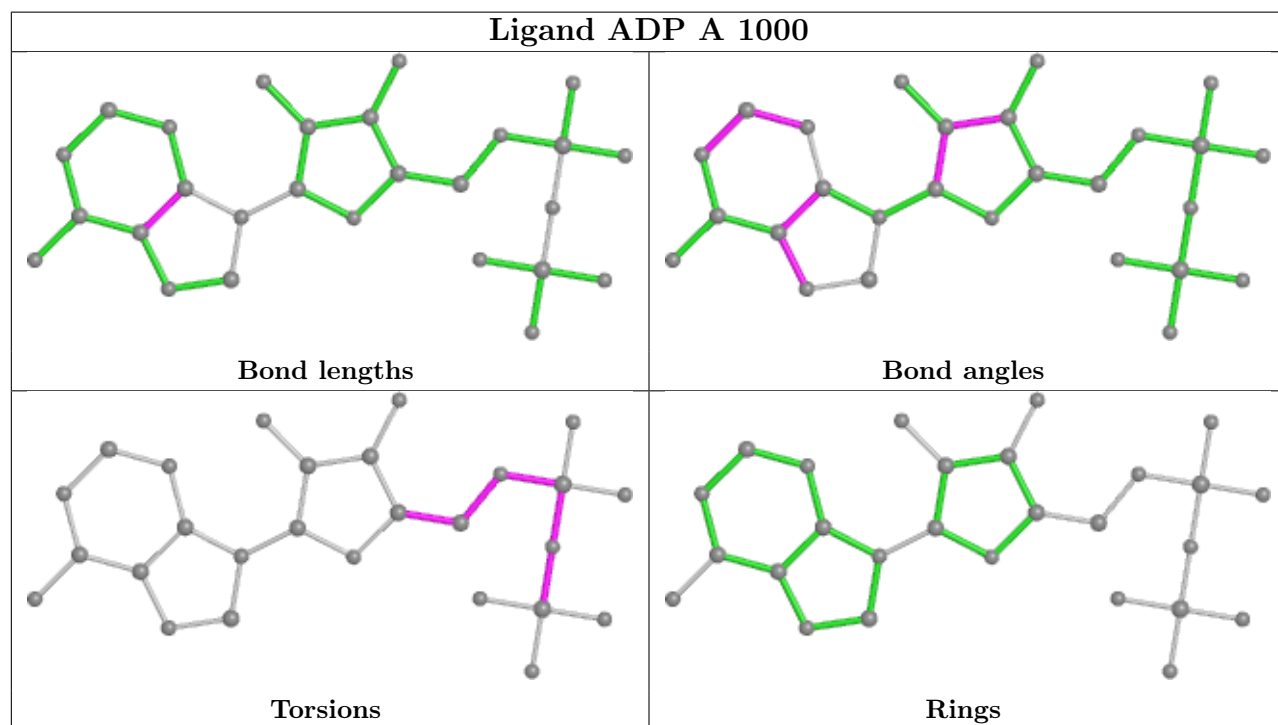
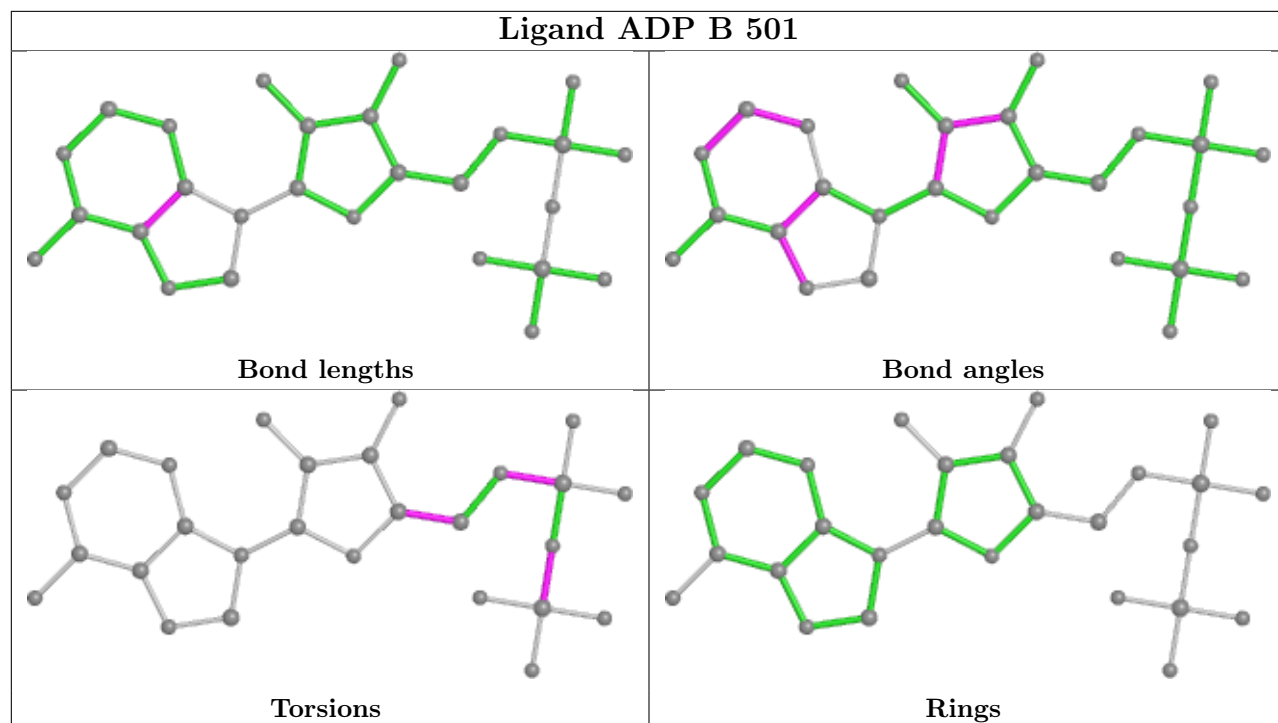
11 monomers are involved in 39 short contacts:

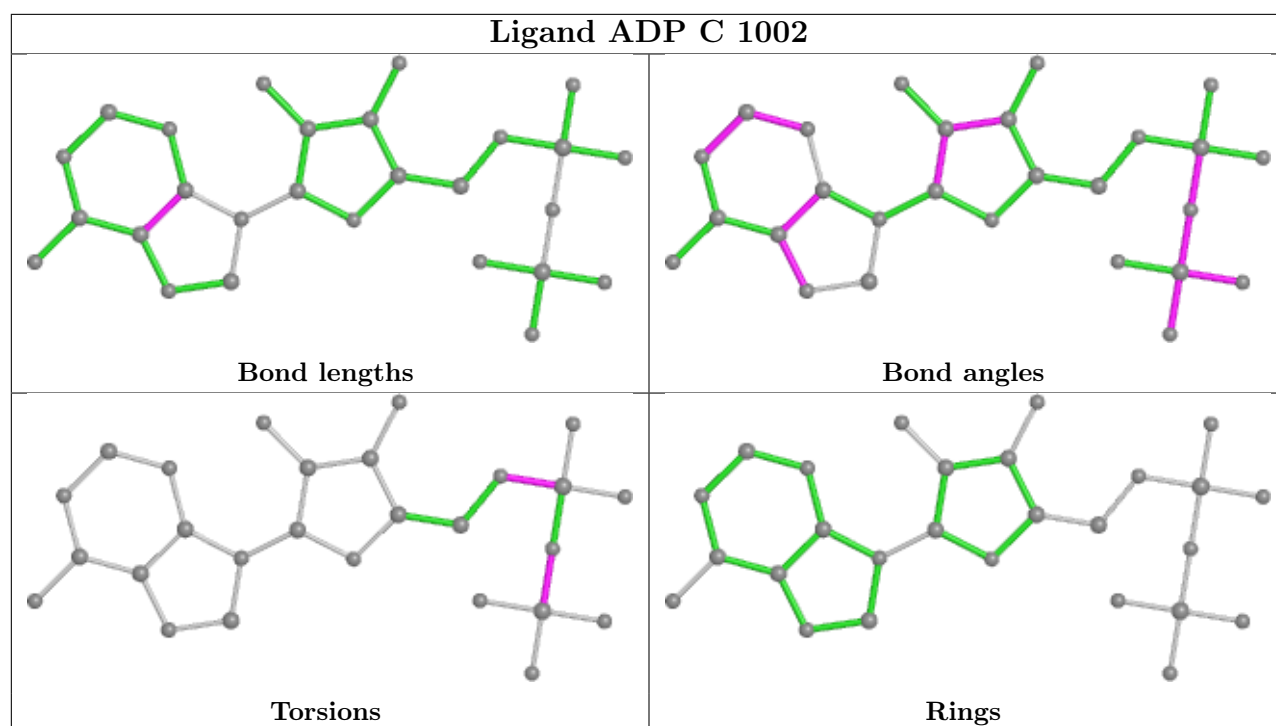
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	502	BEF	4	0
9	E	1000	ADP	2	0
9	F	1000	ADP	3	0
11	D	1002	BEF	2	0
9	D	1000	ADP	5	0
9	B	501	ADP	8	0
11	E	1002	BEF	1	0
11	C	1004	BEF	5	0
9	A	1000	ADP	8	0
9	C	1002	ADP	8	0
11	F	1002	BEF	2	0

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.

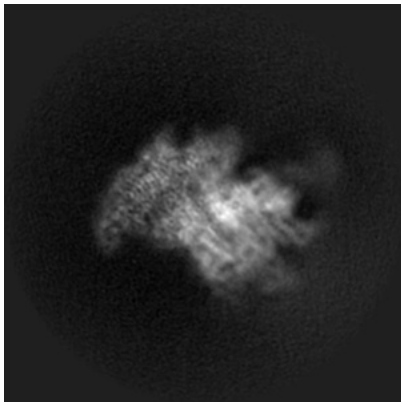
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35004. These allow visual inspection of the internal detail of the map and identification of artifacts.

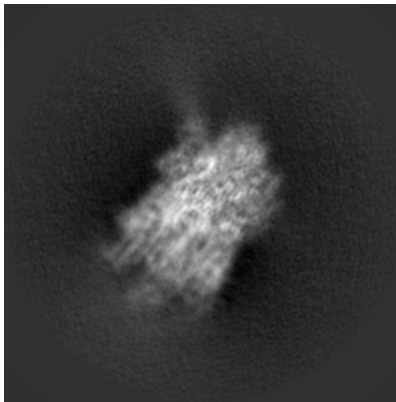
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

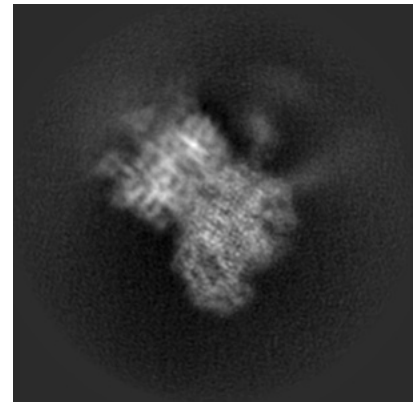
6.1.1 Primary map



X



Y

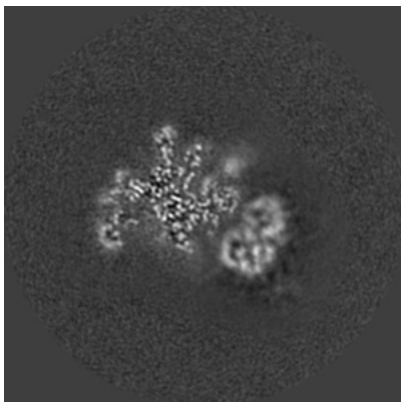


Z

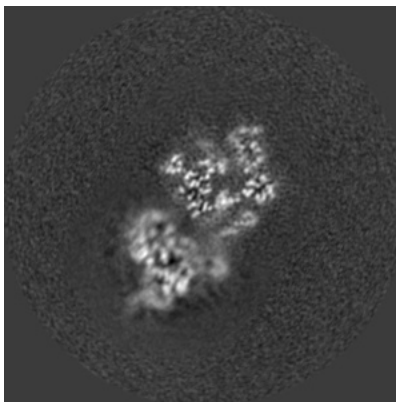
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

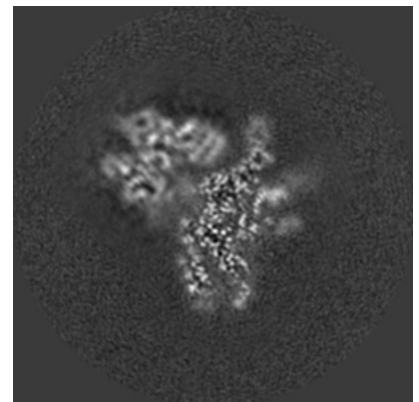
6.2.1 Primary map



X Index: 160



Y Index: 160

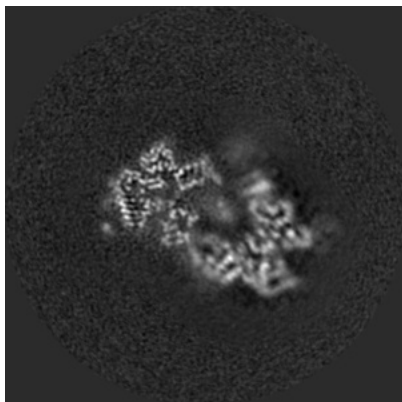


Z Index: 160

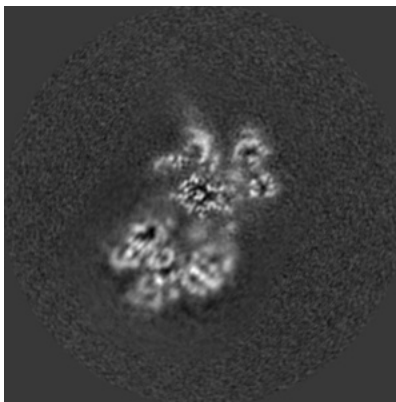
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

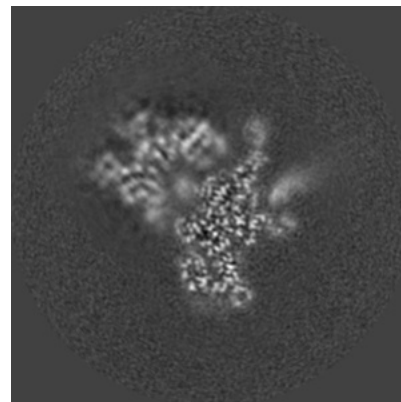
6.3.1 Primary map



X Index: 144



Y Index: 169

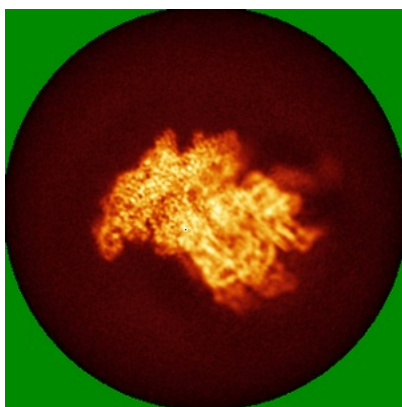


Z Index: 156

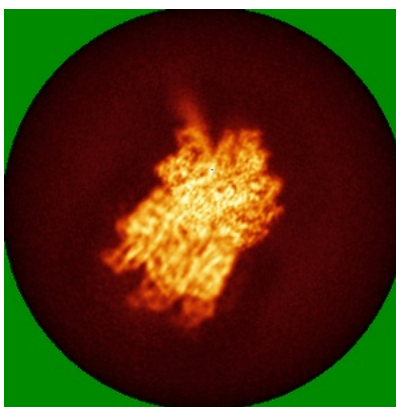
The images above show the largest variance slices of the map in three orthogonal directions.

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

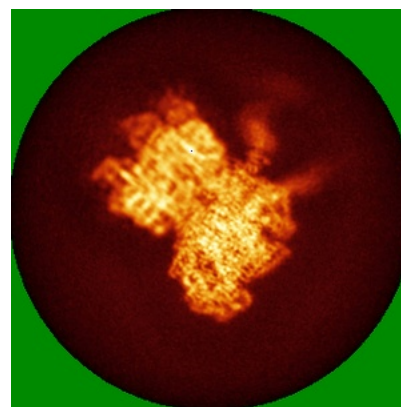
6.4.1 Primary map



X



Y

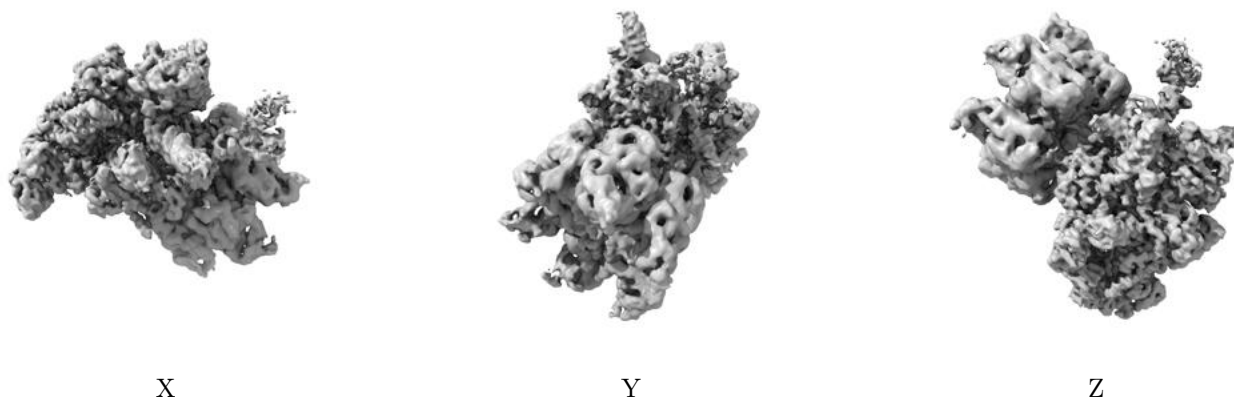


Z

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



The images above show the 3D surface view of the map at the recommended contour level 4.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

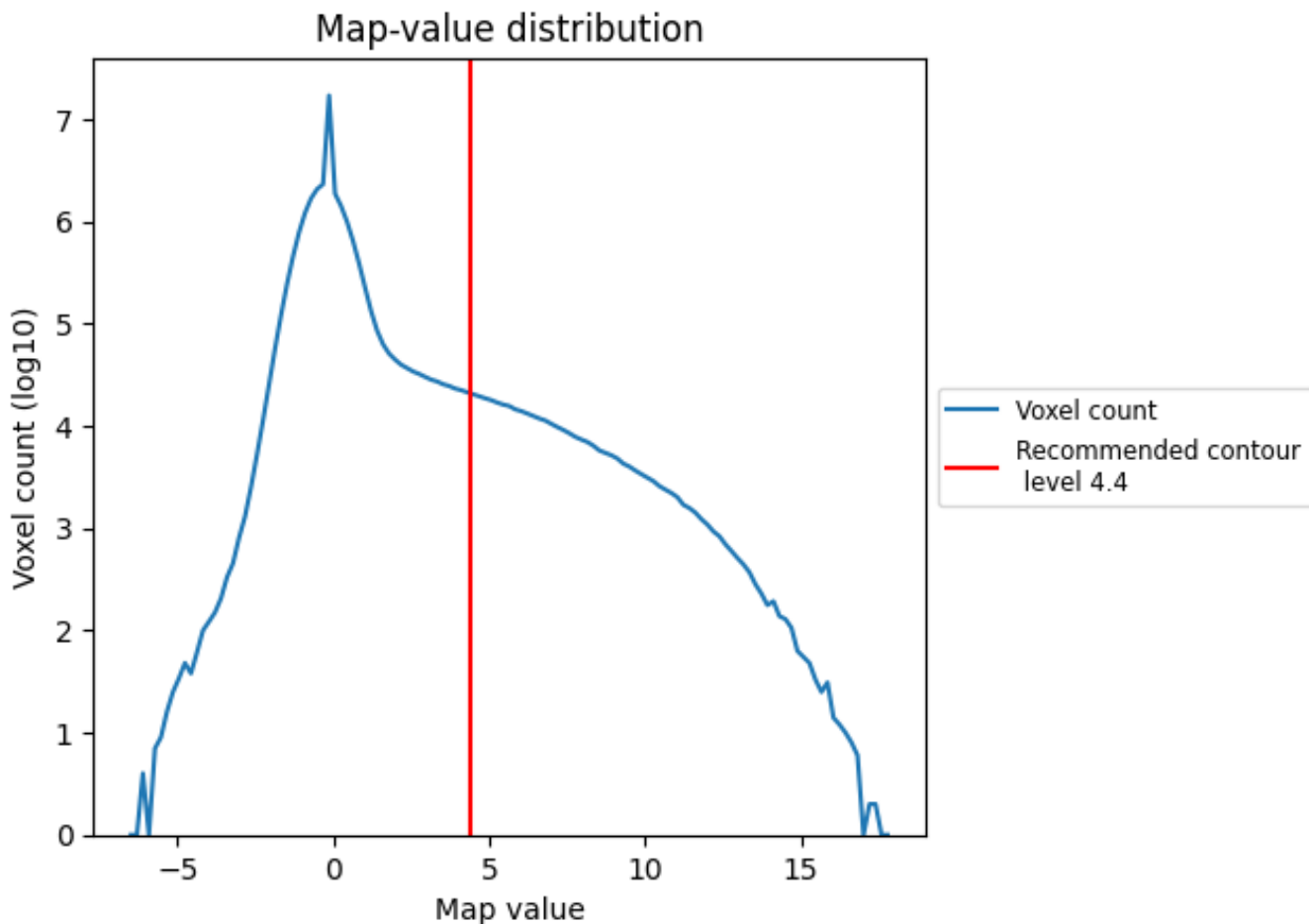
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

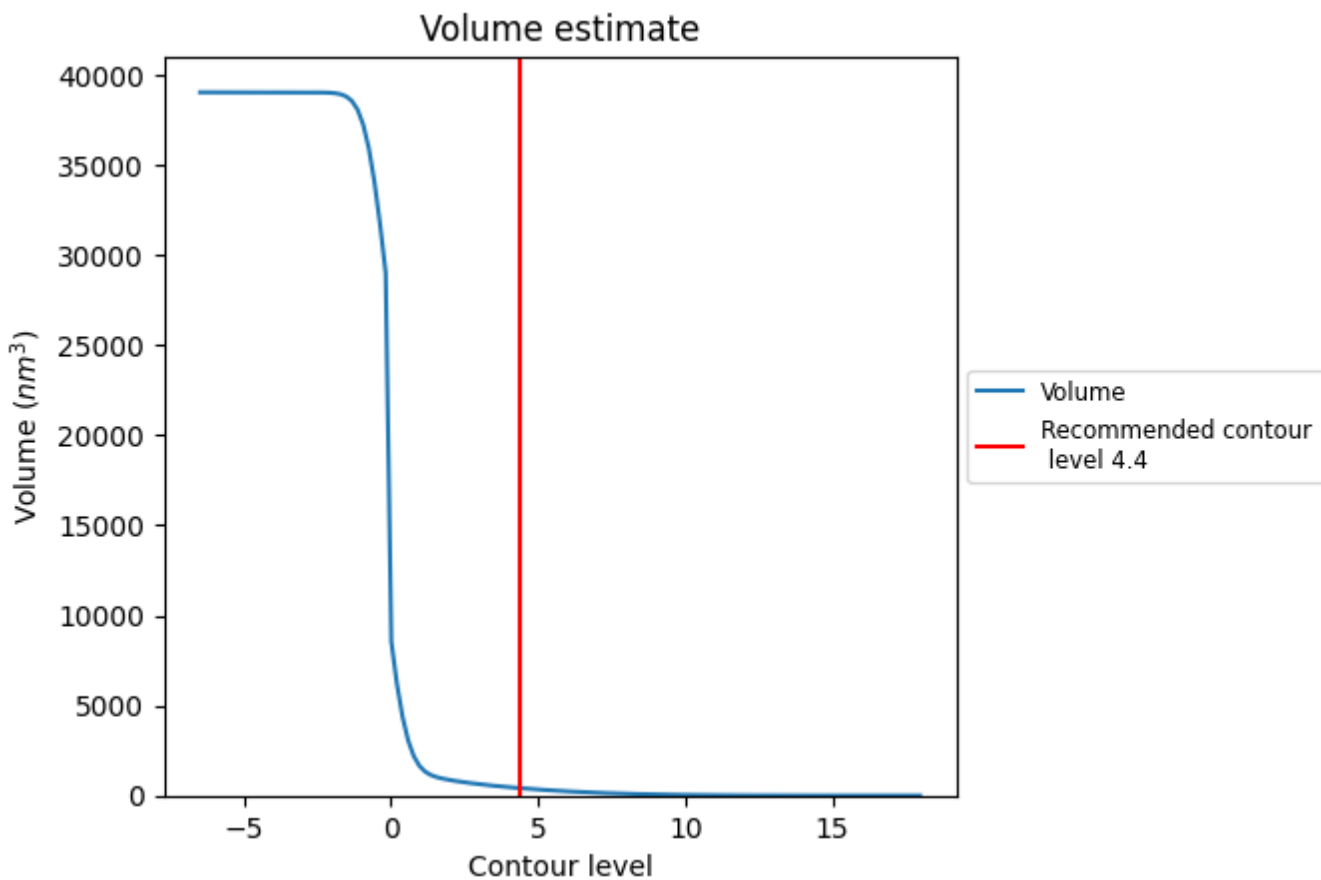
This section contains the results of statistical analysis of the map.

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.

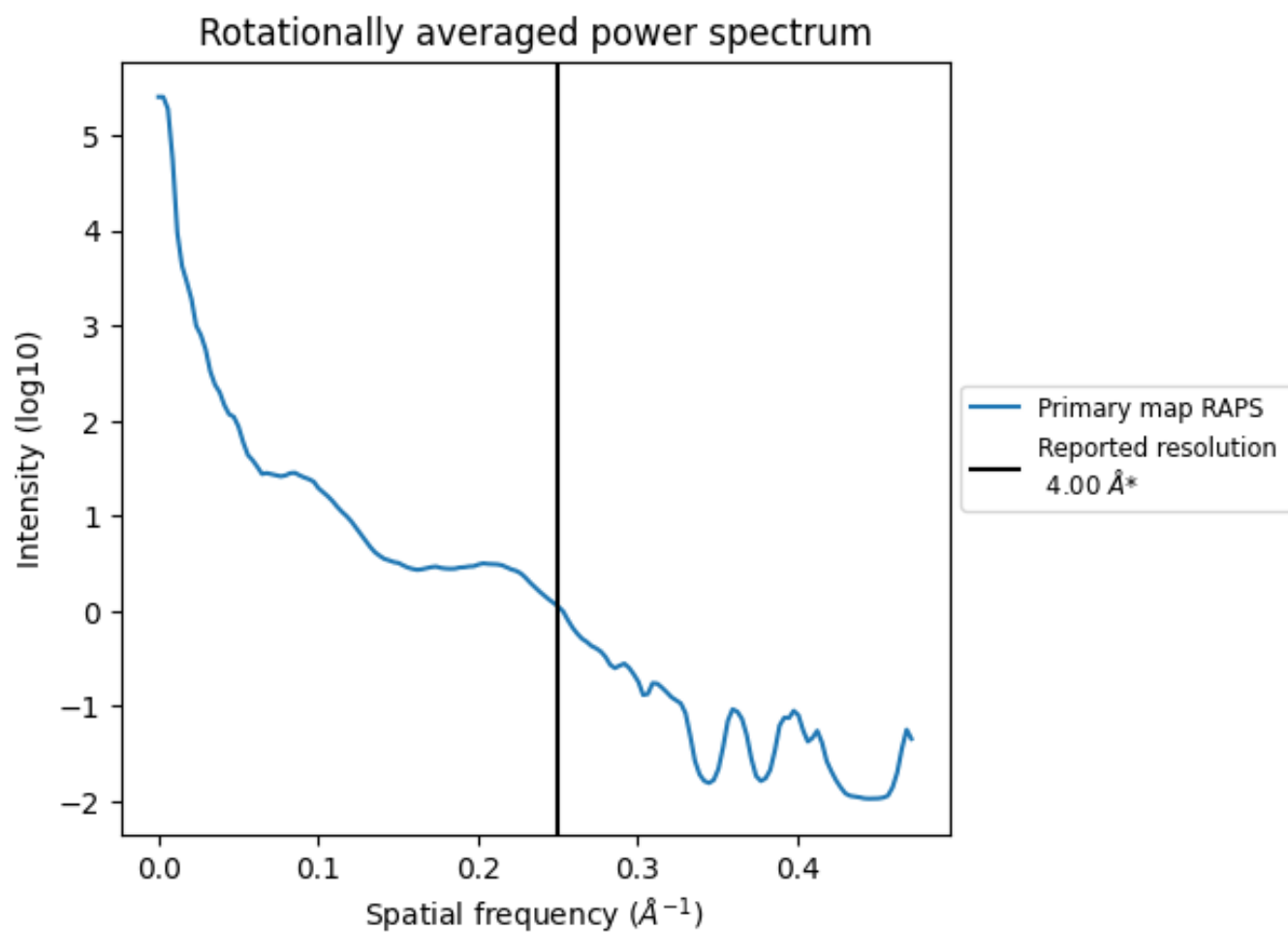
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 410 nm³; this corresponds to an approximate mass of 370 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 0.250\AA^{-1}

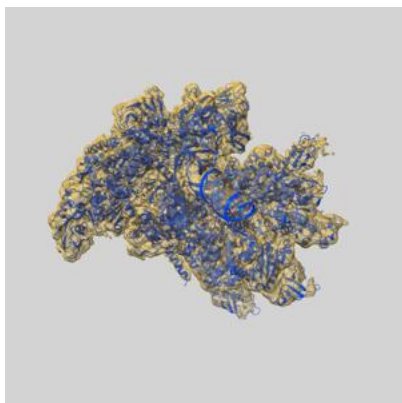
8 Fourier-Shell correlation

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

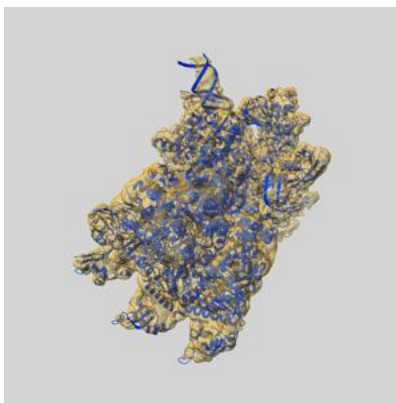
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-35004 and PDB model 8HSR. Per-residue inclusion information can be found in section 3 on page 9.

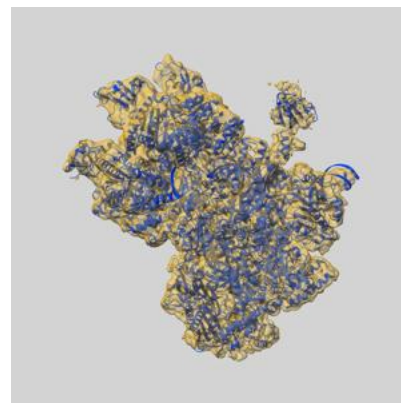
9.1 Map-model overlay [i](#)



X



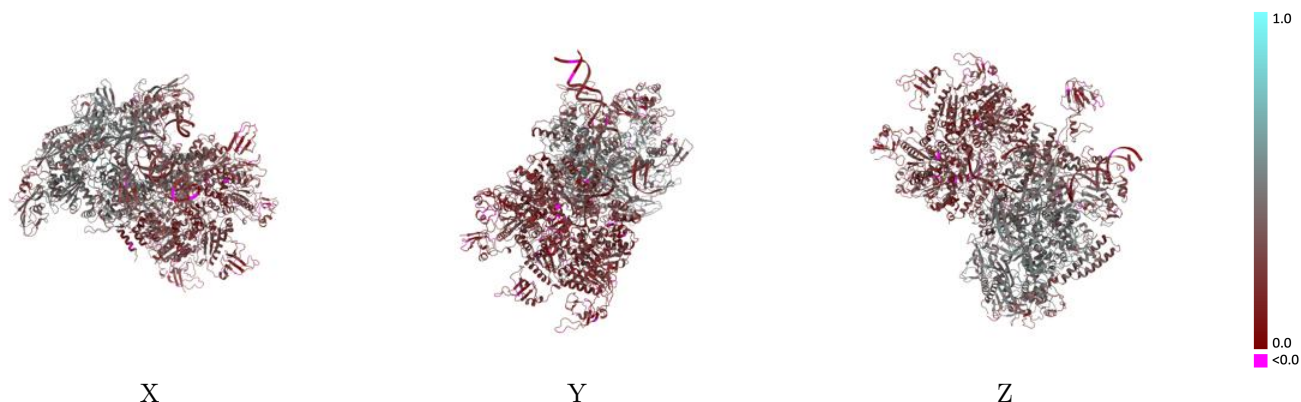
Y



Z

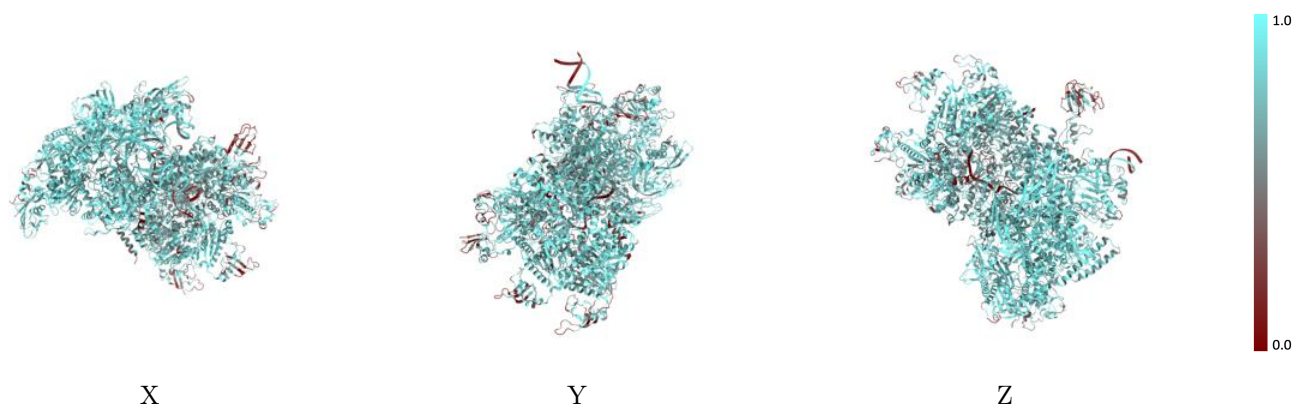
The images above show the 3D surface view of the map at the recommended contour level 4.4 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



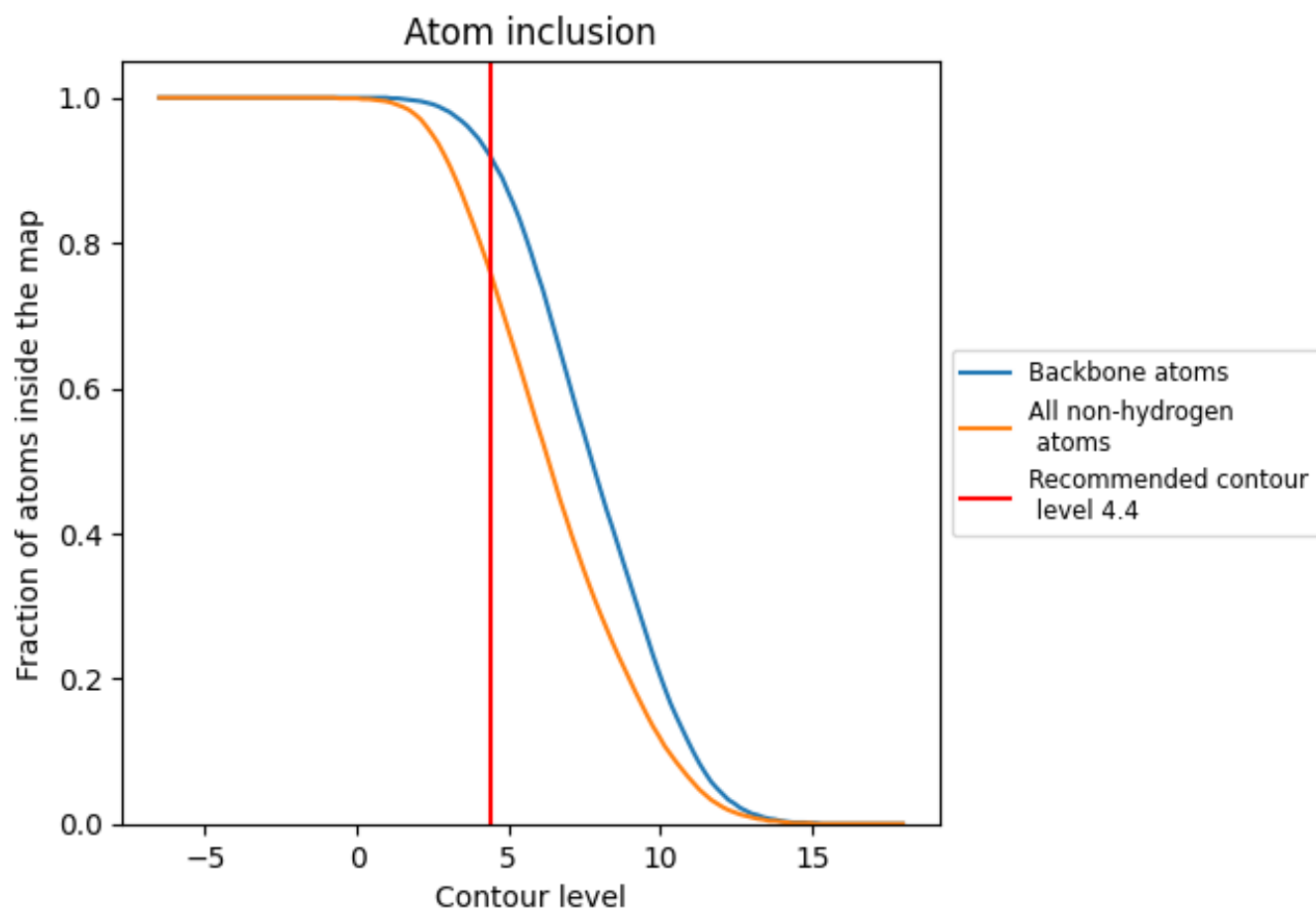
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (4.4).































9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 76% 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 (4.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7590	 0.3170
A	 0.7530	 0.2180
B	 0.7350	 0.2180
C	 0.7230	 0.2190
D	 0.7390	 0.2160
E	 0.7570	 0.2060
F	 0.7710	 0.2150
G	 0.8000	 0.4340
H	 0.7640	 0.3940
I	 0.7960	 0.4130
J	 0.7530	 0.3880
K	 0.6250	 0.2810
N	 0.6810	 0.1600
R	 0.6650	 0.2630
T	 0.8300	 0.2970

