



wwPDB EM Validation Summary Report ⓘ

Aug 27, 2026 – 08:00 pm BST

PDB ID : 7ADC / pdb_00007adc
EMDB ID : EMD-11723
Title : Transcription termination intermediate complex 3 delta NusG
Authors : Said, N.; Hilal, T.; Loll, B.; Wahl, C.M.
Deposited on : 2020-09-14
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.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

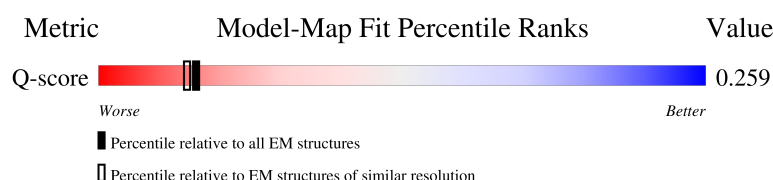
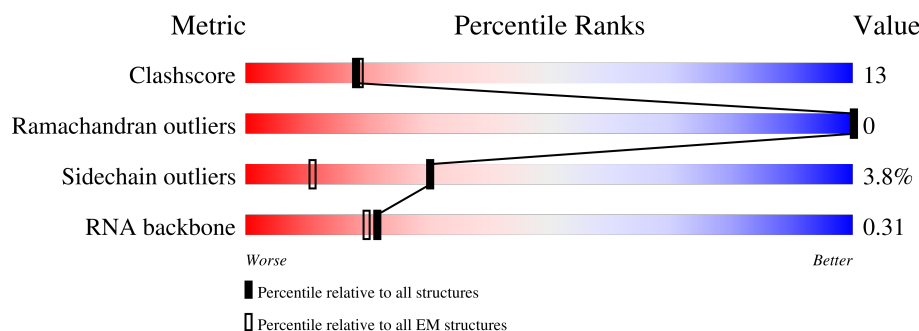
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	7587 (3.50 - 4.50)

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	419	21% 61% 35% .
1	b	419	14% 61% 35% .
1	c	419	11% 62% 34% .

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Mol	Chain	Length	Quality of chain
1	d	419	
1	e	419	
1	f	419	
2	A	497	
3	U	329	
3	V	329	
4	W	91	
5	X	1342	
6	Y	1416	
7	K	50	
8	L	50	
9	R	99	

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
12	BEF	c	503	-	-	X	-

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51565 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
1	f	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	a	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	b	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	c	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	d	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		
1	e	417	Total	C	N	O	S	0	0
			3280	2065	581	617	17		

- Molecule 2 is a protein called Transcription termination/antitermination protein NusA.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	A	495	Total	C	N	O	S	0	0
			3852	2396	669	774	13		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP C3SSN7
A	0	ALA	-	expression tag	UNP C3SSN7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	U	235	Total	C	N	O	S	0	0
			1825	1135	325	359	6		
3	V	321	Total	C	N	O	S	0	0
			2504	1566	441	489	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	W	79	Total	C	N	O	S	0	0
			627	382	118	126	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	X	1340	Total	C	N	O	S	0	0
			10567	6631	1841	2052	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	1358	Total	C	N	O	S	0	0
			10545	6620	1883	1992	50		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
Y	1408	LEU	-	expression tag	UNP C3SIA2
Y	1409	GLU	-	expression tag	UNP C3SIA2
Y	1410	VAL	-	expression tag	UNP C3SIA2
Y	1411	HIS	-	expression tag	UNP C3SIA2
Y	1412	HIS	-	expression tag	UNP C3SIA2
Y	1413	HIS	-	expression tag	UNP C3SIA2
Y	1414	HIS	-	expression tag	UNP C3SIA2
Y	1415	HIS	-	expression tag	UNP C3SIA2
Y	1416	HIS	-	expression tag	UNP C3SIA2

- Molecule 7 is a DNA chain called ntDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	25	Total	C	N	O	P	0	0
			515	244	98	148	25		

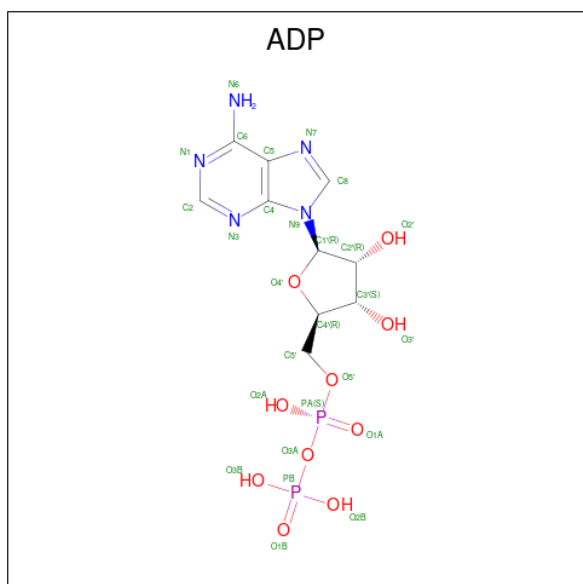
- Molecule 8 is a DNA chain called tDNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	L	34	Total	C	N	O	P	0	0
			682	325	122	202	33		

- Molecule 9 is a RNA chain called rut RNA.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	R	28	Total 590	C 264	N 103	O 195	P 28	0	0

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



Mol	Chain	Residues	Atoms					AltConf
10	a	1	Total 27	C 10	N 5	O 10	P 2	0
10	b	1	Total 27	C 10	N 5	O 10	P 2	0
10	c	1	Total 27	C 10	N 5	O 10	P 2	0
10	d	1	Total 27	C 10	N 5	O 10	P 2	0
10	e	1	Total 27	C 10	N 5	O 10	P 2	0

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

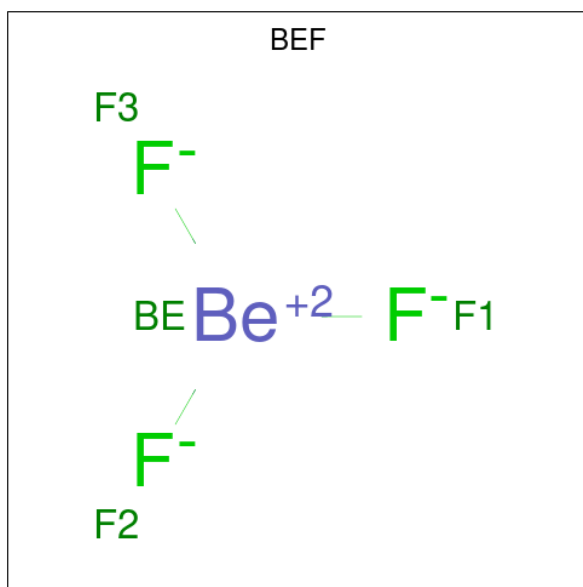
Mol	Chain	Residues	Atoms	AltConf
11	a	1	Total Mg 1 1	0
11	b	1	Total Mg 1 1	0
11	c	1	Total Mg 1 1	0
11	d	1	Total Mg 1 1	0

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Mol	Chain	Residues	Atoms		AltConf
11	e	1	Total 1	Mg 1	0
11	Y	1	Total 1	Mg 1	0

- Molecule 12 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms			AltConf
12	a	1	Total 4	Be 1	F 3	0
12	b	1	Total 4	Be 1	F 3	0
12	c	1	Total 4	Be 1	F 3	0
12	c	1	Total 4	Be 1	F 3	0
12	e	1	Total 4	Be 1	F 3	0

- Molecule 13 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
13	Y	2	Total 2	Zn 2	0

- Molecule 14 is water.

Mol	Chain	Residues	Atoms		AltConf
14	a	3	Total 3	O 3	0
14	b	3	Total 3	O 3	0
14	c	3	Total 3	O 3	0
14	d	3	Total 3	O 3	0
14	e	3	Total 3	O 3	0

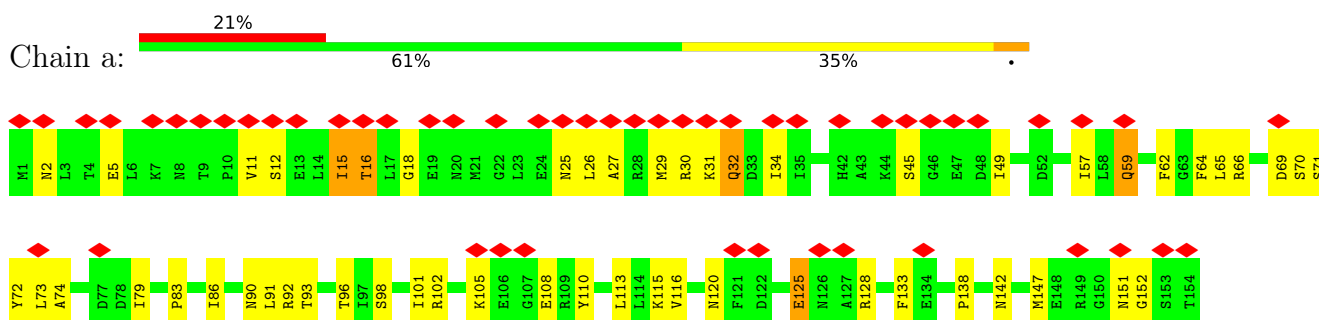
3 Residue-property plots

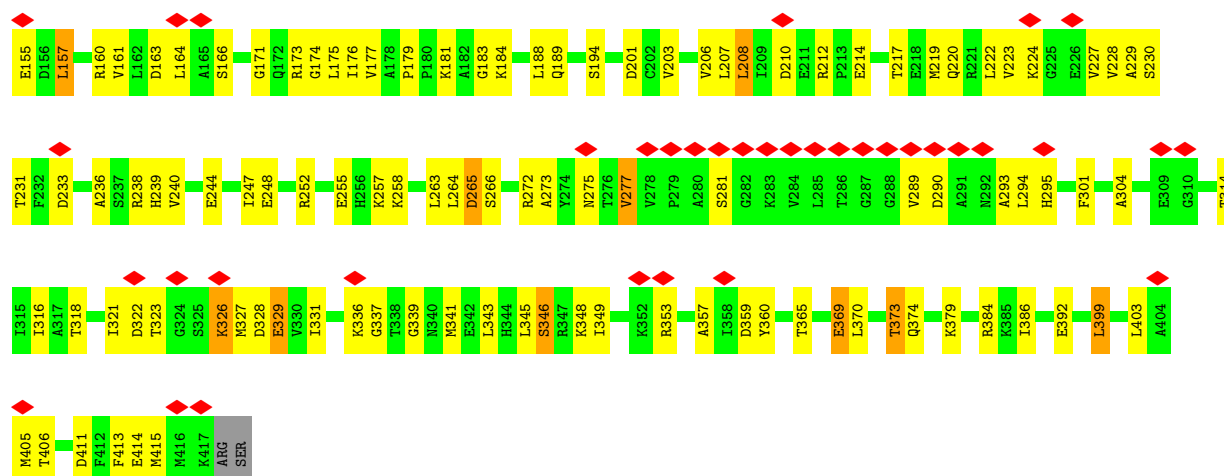
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

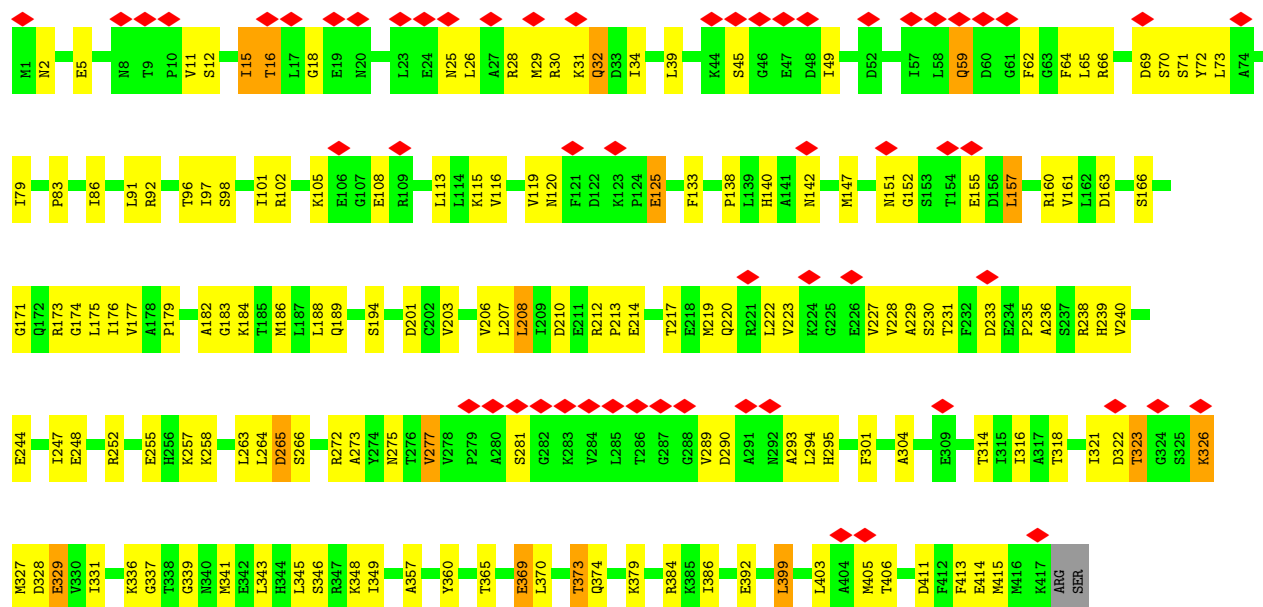


- Molecule 1: Transcription termination factor Rho

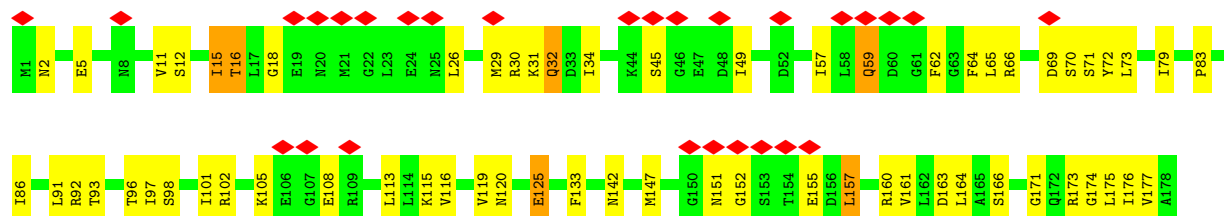


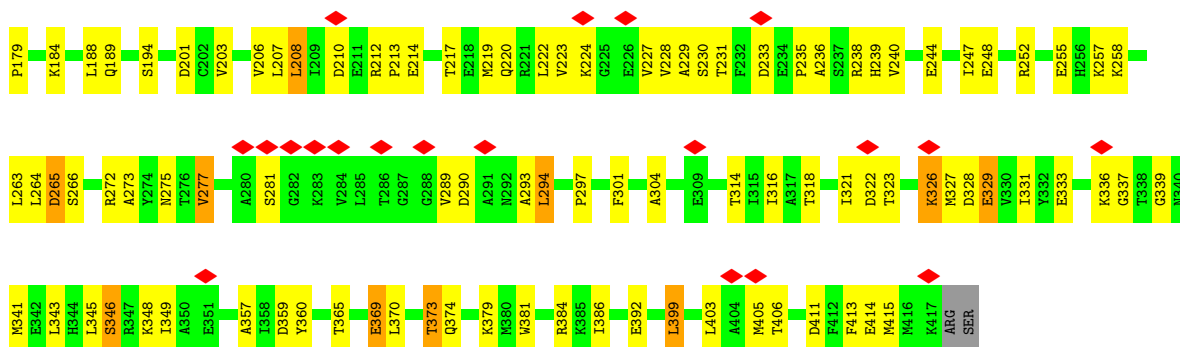


• Molecule 1: Transcription termination factor Rho

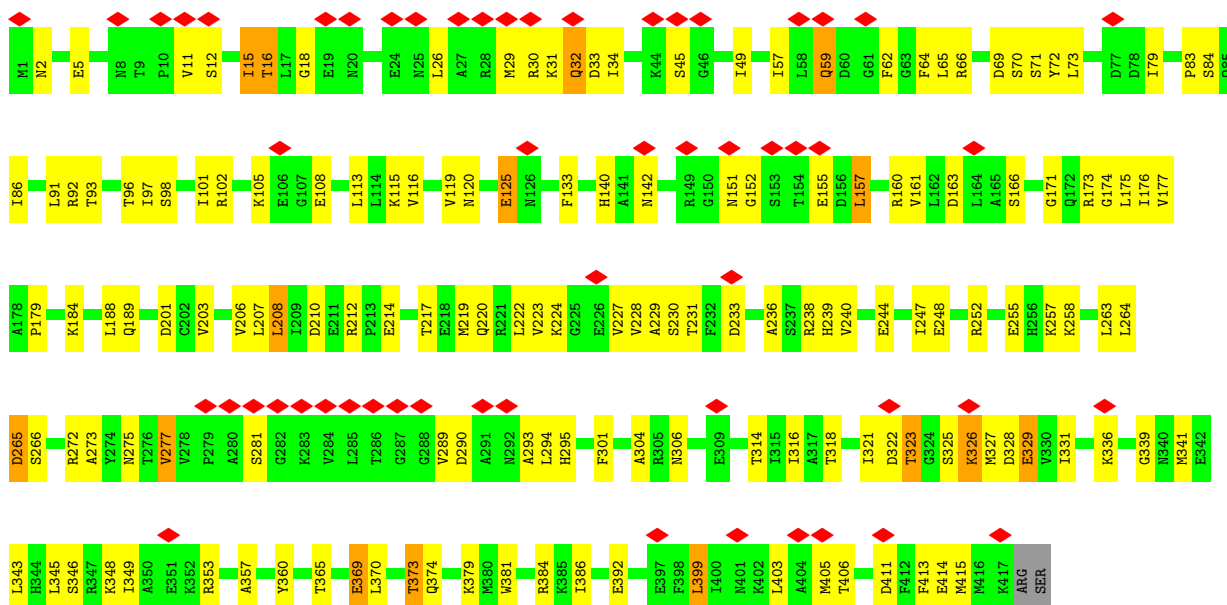


• Molecule 1: Transcription termination factor Rho

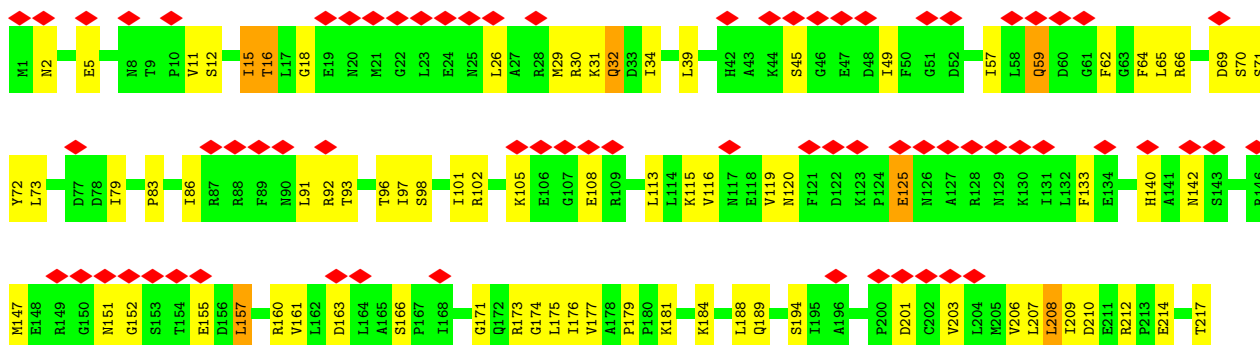


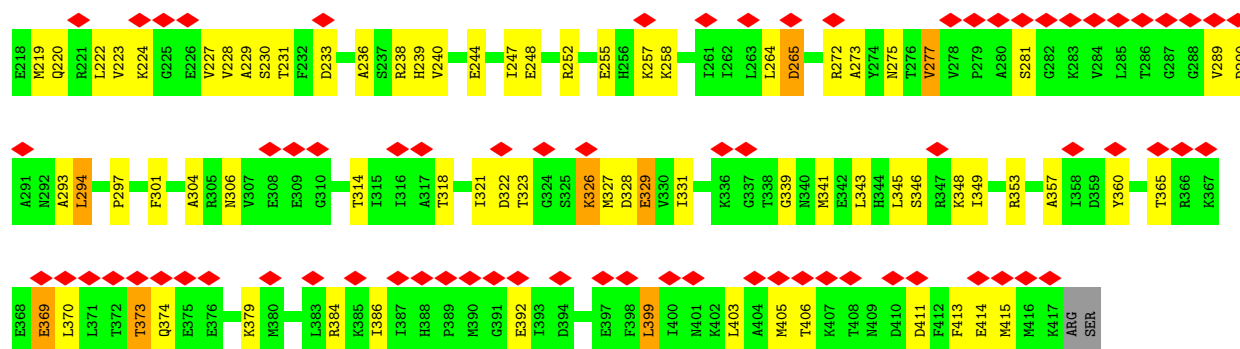


• Molecule 1: Transcription termination factor Rho

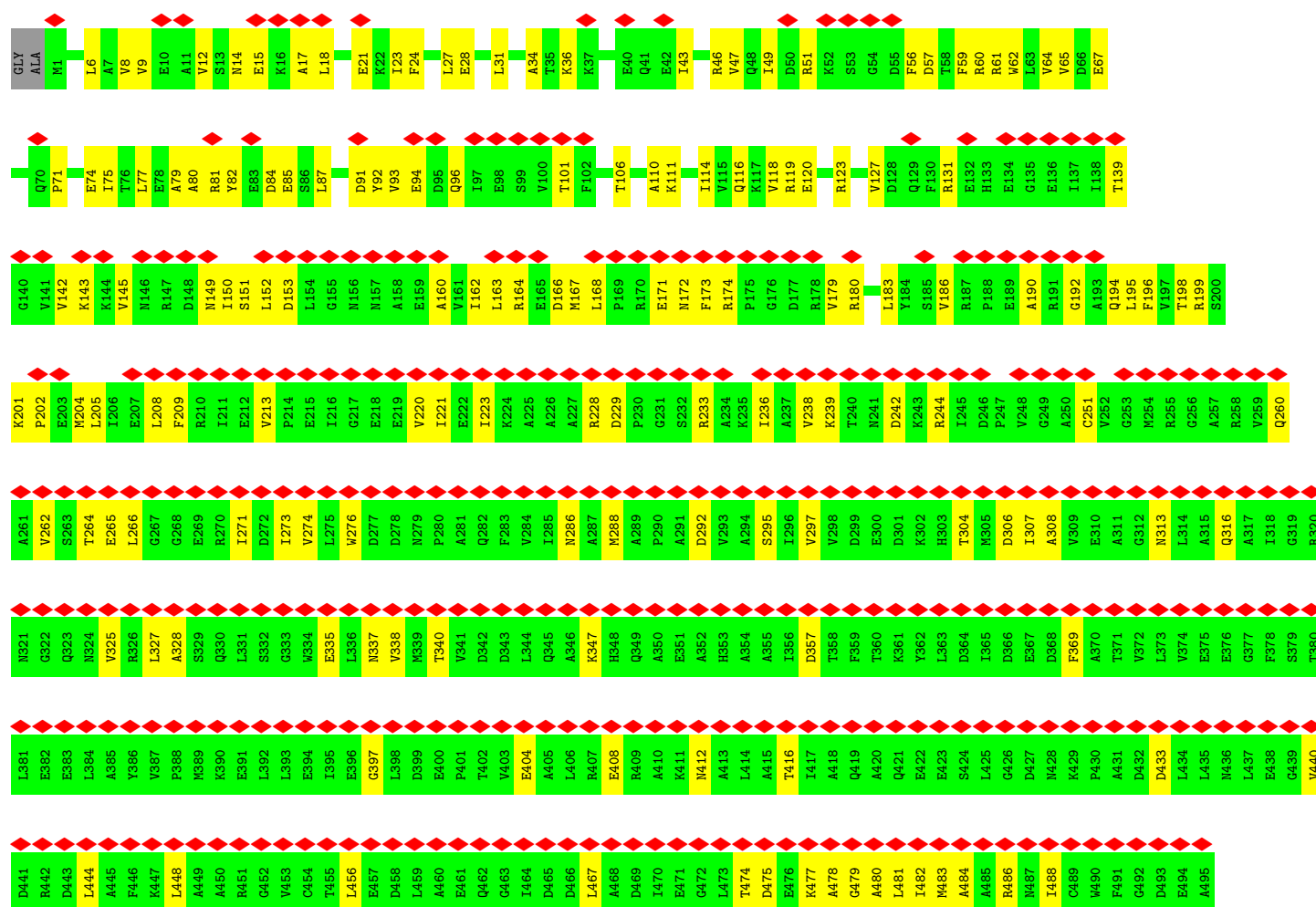
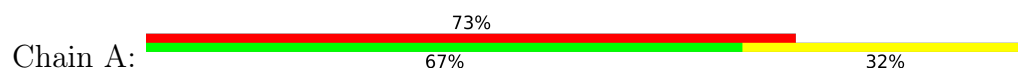


• Molecule 1: Transcription termination factor Rho



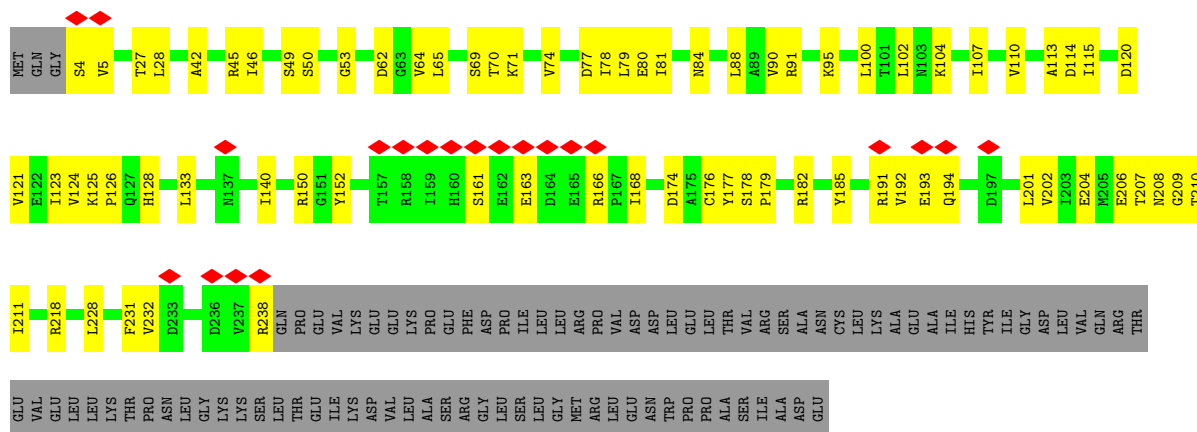


• Molecule 2: Transcription termination/antitermination protein NusA

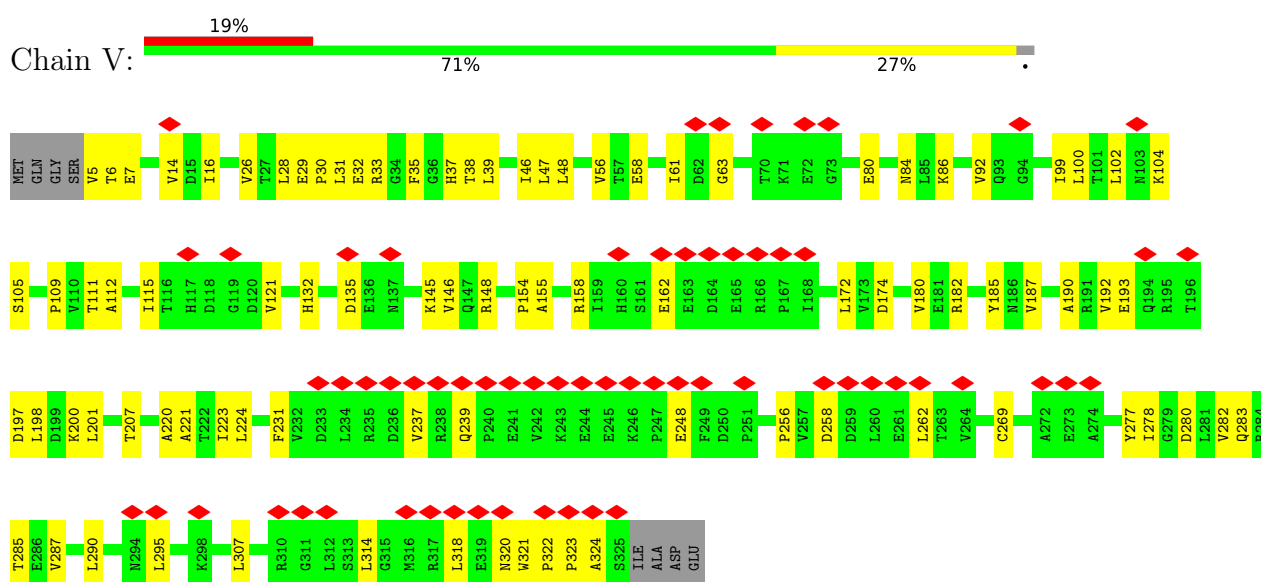


• Molecule 3: DNA-directed RNA polymerase subunit alpha

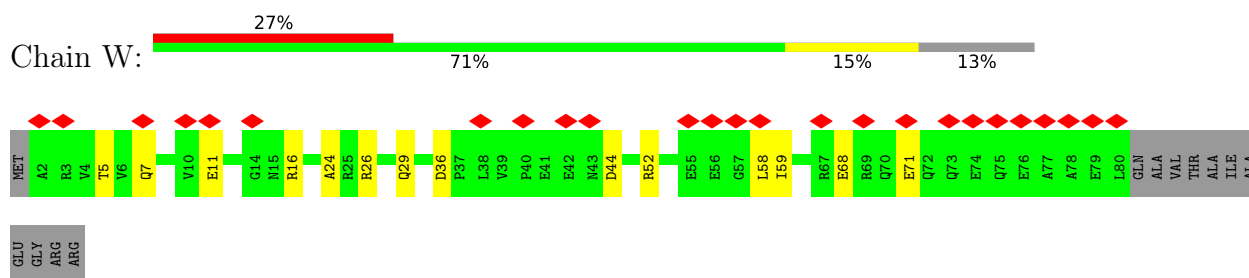




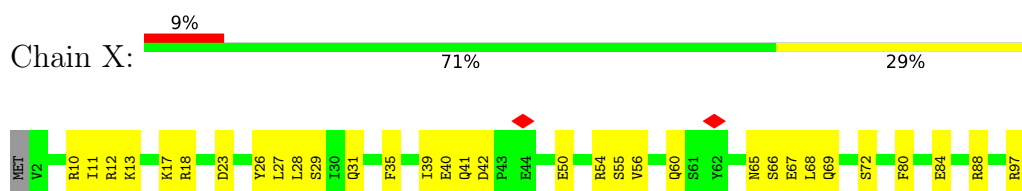
• Molecule 3: DNA-directed RNA polymerase subunit alpha

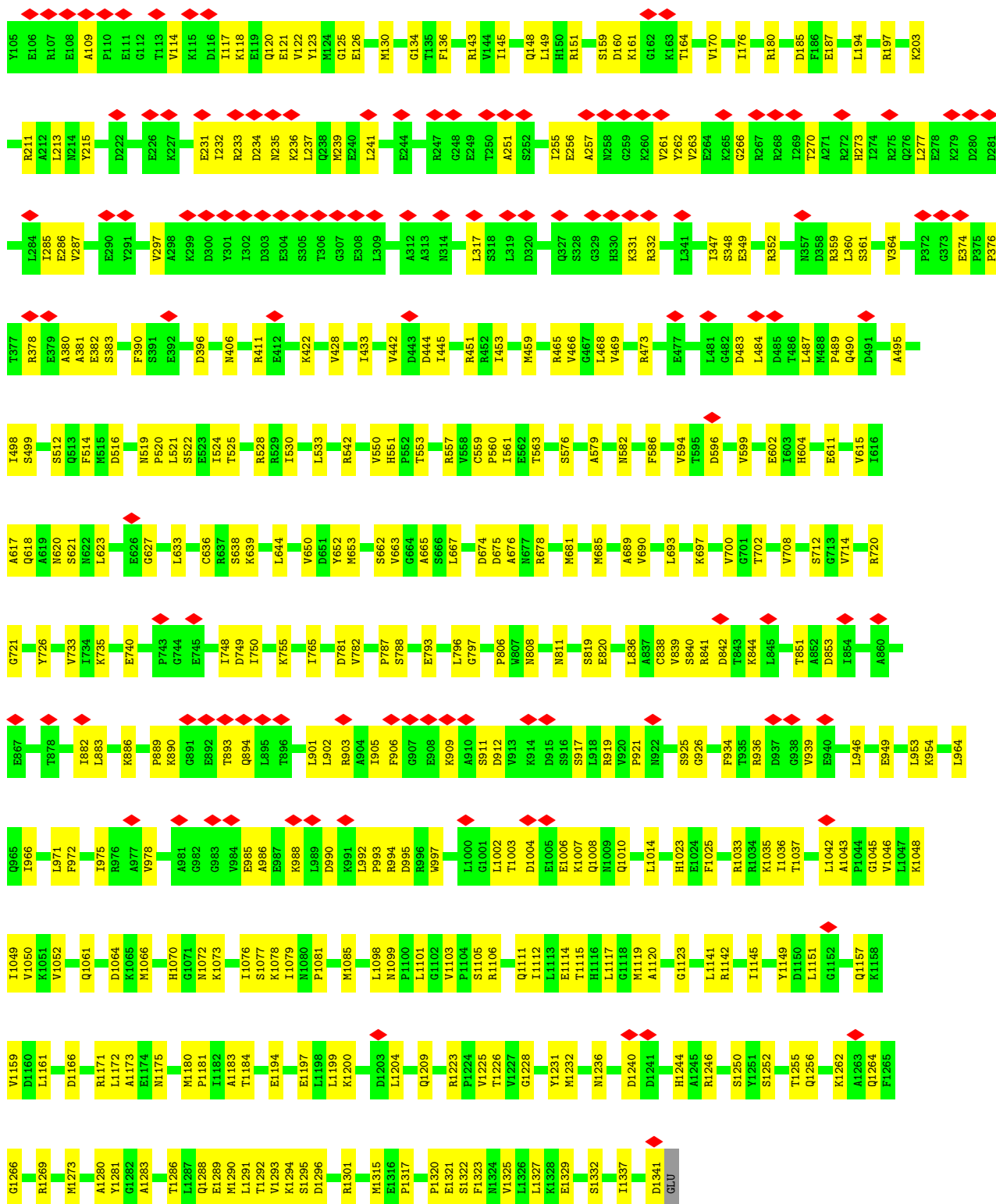


• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: DNA-directed RNA polymerase subunit beta





K1192	K1193	V1198	F1199	E1200	G1201	E1202	E1205	R1206	G1207	I1210	S1211	D1212	D1219	R1222	L1223	E1236	V1237	Q1238	E1239	V1240	T1241	R1242	V1246	I1247	I1248	H1252	E1253	E1254	V1255	I1256	Q1259	M1260	L1261	R1262	G1270	D1273	L1292	E1293	G1296	K1297	L1306	L1307	G1308	I1309	T1310											
A1105	I1106	V1107	Q1108	L1109	E1110	D1111	G1112	V1113	Q1114	I1115	S1116	S1117	G1118	T1120	L1121	A1122	R1123	P1125	Q1126	E1127	S1128	G1129	G1130	T1131	K1132	I1134	T1135	G1136	I1155	L1156	A1157	G1161	G1166	K1167	E1168	T1169	K1170	G1171	R1174	P1179	V1180	D1181	G1182	S1183	D1184	P1185	Y1186	E1187	E1188	M1189						
Q1044	T1045	I1046	T1047	R1048	Q1049	T1050	D1051	E1052	L1053	T1054	G1055	L1056	S1057	S1058	L1059	V1060	V1061	L1062	D1063	S1064	A1065	E1066	R1067	T1068	A1069	G1070	G1071	K1072	D1073	L1074	R1075	L1078	K1079	I1080	V1081	D1082	A1083	G1085	N1086	D1087	V1088	L1089	I1090	P1091	G1092	T1093	D1094	M1095	P1096	A1097	Q1098	Y1099	F1100	L1101	P1102	K1104
S969	S970	G971	K972	L973	V974	T975	T976	S977	R978	T980	S981	D986	E987	F988	G989	R990	T991	K992	K996	Y999	G1000	A1001	V1002	G1006	D1007	G1008	E1009	Q1010	G1013	G1014	A1018	N1019	W1020	D1021	P1022	H1023	P1026	V1027	I1028	T1029	E1030	V1031	S1032	F1037	T1038	D1039	M1040	I1041	D1042	G1043						
T862	G752	C869	D870	L871	T875	E876	N874	N875	D878	R883	V884	V885	H897	R905	G912	T918	Q921	G924	E925	P926	L930	R933	T934	F935	H936	T937	G938	G939	A940	A941	S942	R943	A944	A945	V952	K953	I1028	N954	K955	K959	L960	S961	N962	V963	K964	S965	V966	N967	N968							
D751	G752	S753	T754	T755	E756	T757	P758	T759	T760	R764	M768	V769	L770	Q771	R780	K789	T797	R798	R799	V803	A804	D805	D806	V809	T816	H822	T823	P824	D830	V831	K832	L835	R836	D837	R838	L849	K850	P851	G852	T853	A854	L857	V858	P859	R860	N861										
A633	R634	S635	G636	A637	S638	V639	G640	D643	M644	P647	S655	E658	A659	E660	V661	E662	E663	S670	G671	L672	K681	D684	T685	V686	M697	M698	Q702	T703	E704	T705	N708	R709	Q712	S718	S721	M724	R731	M743	L746	K749	P750															
K531	R535	R538	L541	H545	V548	K549	V550	E554	D558	A559	N560	G561	K566	T572	T573	R576	A577	M581	V582	V583	G586	L587	P588	V589	N593	L596	T601	C608	L612	G613	L614	K615	F620	Q623	I624	M625	V626	V631	A632																	
R425	A426	P427	T428	L429	H430	R431	T434	P439	V440	E443	H450	V453	C454	Y457	D460	D464	Q465	P471	L472	T473	L474	E475	R481	A482	L483	N488	N489	I490	L491	I499	P502	S503	Q504	M513	T514	R515	D516	N519	E523	L527	P530															
A305	L306	G310	R311	R312	G313	R314	A315	G318	S319	N320	K321	R322	F323	S326	L327	A328	D329	K332	Q335	F338	L342	L343	G344	K345	R346	V347	D348	V354	Y360	L361	R362	Q365	C366	I381	G389	R403	D410	I411	L412	H419	P420	V421	N424													
N209	S210	E211	T212	K213	R214	L217	T221	K222	L223	F227	E235	L239	T240	L245	P246	P247	D248	P251	V253	P254	T255	D256	G257	G258	R259	F260	S263	D267	L268	T269	R270	L285	A286	A287	P288	D289	T290	T291	V292	R293	R297	Q300	E301	A302	V303	D304										
W115	F116	L117	K118	S119	L120	P121	S122	R123	L126	L127	L128	D129	R133	D134	R137	S143	Y144	E148	G149	G150	M151	T152	N153	L154	E155	A156	Q157	L160	T161	E162	E163	Q164	D167	E170	E171	D174	K179	A184	I185	L188	L189	E204	L205	N206	E207	T208										
MET	LYS	ASP	LEU	LEU	LYS	PHE	LEU	LYS	ALA	GLN	THR	LYS	THR	GLU	E16	A19	S34	F35	G36	Y46	R47	T48	F49	R53	D54	C58	A59	R60	I61	G73	K76	K79	E86	V97	R98	R99	E100	R101	M102	G103	H104	L107	A108	T111	A112	H113	I114									

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	64696	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	8000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	31000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.331	Depositor
Minimum map value	-0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.11	Depositor
Map size (Å)	372.0, 372.0, 372.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.24, 1.24, 1.24	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: ZN, ADP, MG, BEF

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	0.14	0/3329	0.38	0/4483
1	b	0.14	0/3329	0.38	0/4483
1	c	0.14	0/3329	0.38	0/4483
1	d	0.14	0/3329	0.38	0/4483
1	e	0.14	0/3329	0.38	0/4483
1	f	0.14	0/3329	0.38	0/4483
2	A	0.10	0/3897	0.31	0/5273
3	U	0.11	0/1847	0.30	0/2503
3	V	0.11	0/2538	0.32	0/3441
4	W	0.10	0/629	0.26	0/847
5	X	0.11	0/10736	0.28	0/14487
6	Y	0.10	0/10706	0.28	0/14456
7	K	0.19	0/577	0.39	0/886
8	L	0.20	0/762	0.40	0/1171
9	R	0.95	1/656 (0.2%)	0.70	2/1016 (0.2%)
All	All	0.16	1/52322 (0.0%)	0.34	2/70978 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	R	24	U	C4'-O4'	24.03	1.81	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	R	24	U	C1'-O4'-C4'	-17.65	92.05	109.70
9	R	24	U	C5'-C4'-O4'	-8.06	97.00	109.10

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	3280	0	3358	116	0
1	b	3280	0	3358	104	0
1	c	3280	0	3357	108	0
1	d	3280	0	3358	108	0
1	e	3280	0	3358	95	0
1	f	3280	0	3359	104	0
2	A	3852	0	3835	115	0
3	U	1825	0	1853	54	0
3	V	2504	0	2558	58	0
4	W	627	0	634	12	0
5	X	10567	0	10585	267	0
6	Y	10545	0	10762	254	0
7	K	515	0	282	11	0
8	L	682	0	382	26	0
9	R	590	0	304	30	0
10	a	27	0	12	3	0
10	b	27	0	12	2	0
10	c	27	0	12	1	0
10	d	27	0	12	0	0
10	e	27	0	12	1	0
11	Y	1	0	0	0	0
11	a	1	0	0	0	0
11	b	1	0	0	0	0
11	c	1	0	0	0	0
11	d	1	0	0	0	0
11	e	1	0	0	0	0
12	a	4	0	0	0	0
12	b	4	0	0	1	0
12	c	8	0	0	2	0
12	e	4	0	0	1	0
13	Y	2	0	0	0	0
14	a	3	0	0	0	0
14	b	3	0	0	0	0
14	c	3	0	0	0	0
14	d	3	0	0	1	0
14	e	3	0	0	0	0
All	All	51565	0	51403	1357	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 13.

The worst 5 of 1357 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:f:108:GLU:HB3	9:R:24:U:O4	1.17	1.28
9:R:24:U:C4'	9:R:24:U:O4'	1.81	1.24
1:f:108:GLU:HB3	9:R:24:U:C4	1.94	1.01
1:a:110:TYR:HH	8:L:21:DC:H5	1.02	0.97
1:f:108:GLU:CB	9:R:24:U:O4	2.13	0.94

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	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	b	415/419 (99%)	403 (97%)	12 (3%)	0	100	100
1	c	415/419 (99%)	403 (97%)	12 (3%)	0	100	100
1	d	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	e	415/419 (99%)	403 (97%)	12 (3%)	0	100	100
1	f	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
2	A	493/497 (99%)	459 (93%)	34 (7%)	0	100	100
3	U	233/329 (71%)	217 (93%)	16 (7%)	0	100	100
3	V	319/329 (97%)	294 (92%)	25 (8%)	0	100	100
4	W	77/91 (85%)	76 (99%)	1 (1%)	0	100	100
5	X	1338/1342 (100%)	1256 (94%)	82 (6%)	0	100	100
6	Y	1356/1416 (96%)	1297 (96%)	59 (4%)	0	100	100
All	All	6306/6518 (97%)	6014 (95%)	292 (5%)	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	357/359 (99%)	323 (90%)	34 (10%)	8	28
1	b	357/359 (99%)	323 (90%)	34 (10%)	8	28
1	c	357/359 (99%)	323 (90%)	34 (10%)	8	28
1	d	357/359 (99%)	323 (90%)	34 (10%)	8	28
1	e	357/359 (99%)	323 (90%)	34 (10%)	8	28
1	f	357/359 (99%)	323 (90%)	34 (10%)	8	28
2	A	409/409 (100%)	409 (100%)	0	100	100
3	U	203/286 (71%)	203 (100%)	0	100	100
3	V	280/286 (98%)	280 (100%)	0	100	100
4	W	67/75 (89%)	67 (100%)	0	100	100
5	X	1155/1157 (100%)	1155 (100%)	0	100	100
6	Y	1134/1177 (96%)	1134 (100%)	0	100	100
All	All	5390/5544 (97%)	5186 (96%)	204 (4%)	30	51

5 of 204 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	c	203	VAL
1	d	98	SER
1	e	386	ILE
1	c	230	SER
1	c	373	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 95 such sidechains are listed below:

Mol	Chain	Res	Type
5	X	41	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
5	X	1013	GLN
5	X	343	HIS
5	X	761	GLN
5	X	1236	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	26/99 (26%)	9 (34%)	0

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	24	U
9	R	25	C
9	R	26	C
9	R	84	A
9	R	86	A

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 8 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
10	ADP	b	1000	11	27,29,29	1.37	4 (14%)	42,45,45	1.97	10 (23%)
10	ADP	a	1000	11	27,29,29	1.36	4 (14%)	42,45,45	2.00	10 (23%)
12	BEF	a	1002	-	0,3,3	-	-	-	-	-
12	BEF	e	1002	-	0,3,3	-	-	-	-	-
10	ADP	d	1000	11	27,29,29	1.36	4 (14%)	42,45,45	2.01	10 (23%)
10	ADP	e	1000	11,1	27,29,29	1.34	4 (14%)	42,45,45	2.00	11 (26%)
12	BEF	c	503	-	0,3,3	-	-	-	-	-
10	ADP	c	501	11,1	27,29,29	1.36	4 (14%)	42,45,45	1.98	11 (26%)
12	BEF	c	504	-	0,3,3	-	-	-	-	-
12	BEF	b	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. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ADP	b	1000	11	-	3/16/32/32	0/3/3/3
10	ADP	a	1000	11	-	5/16/32/32	0/3/3/3
10	ADP	d	1000	11	-	1/16/32/32	0/3/3/3
10	ADP	e	1000	11,1	-	2/16/32/32	0/3/3/3
10	ADP	c	501	11,1	-	4/16/32/32	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)
10	d	1000	ADP	C5-C4	4.59	1.47	1.39
10	b	1000	ADP	C5-C4	4.55	1.47	1.39
10	c	501	ADP	C5-C4	4.53	1.47	1.39
10	a	1000	ADP	C5-C4	4.47	1.47	1.39
10	e	1000	ADP	C5-C4	4.44	1.47	1.39

The worst 5 of 52 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	d	1000	ADP	C5-C4-N3	-6.43	118.36	126.75
10	a	1000	ADP	C5-C4-N3	-6.38	118.42	126.75
10	e	1000	ADP	C5-C4-N3	-6.20	118.67	126.75
10	c	501	ADP	C5-C4-N3	-6.19	118.68	126.75
10	b	1000	ADP	C5-C4-N3	-6.07	118.84	126.75

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

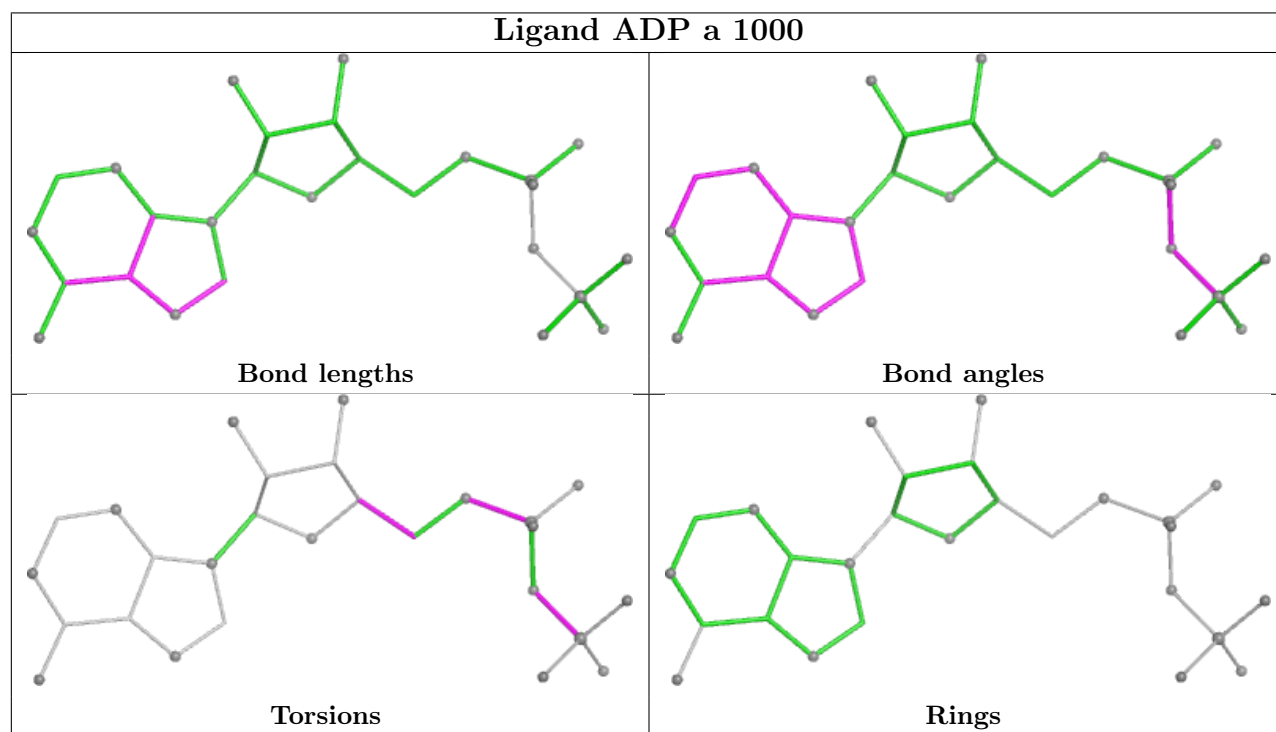
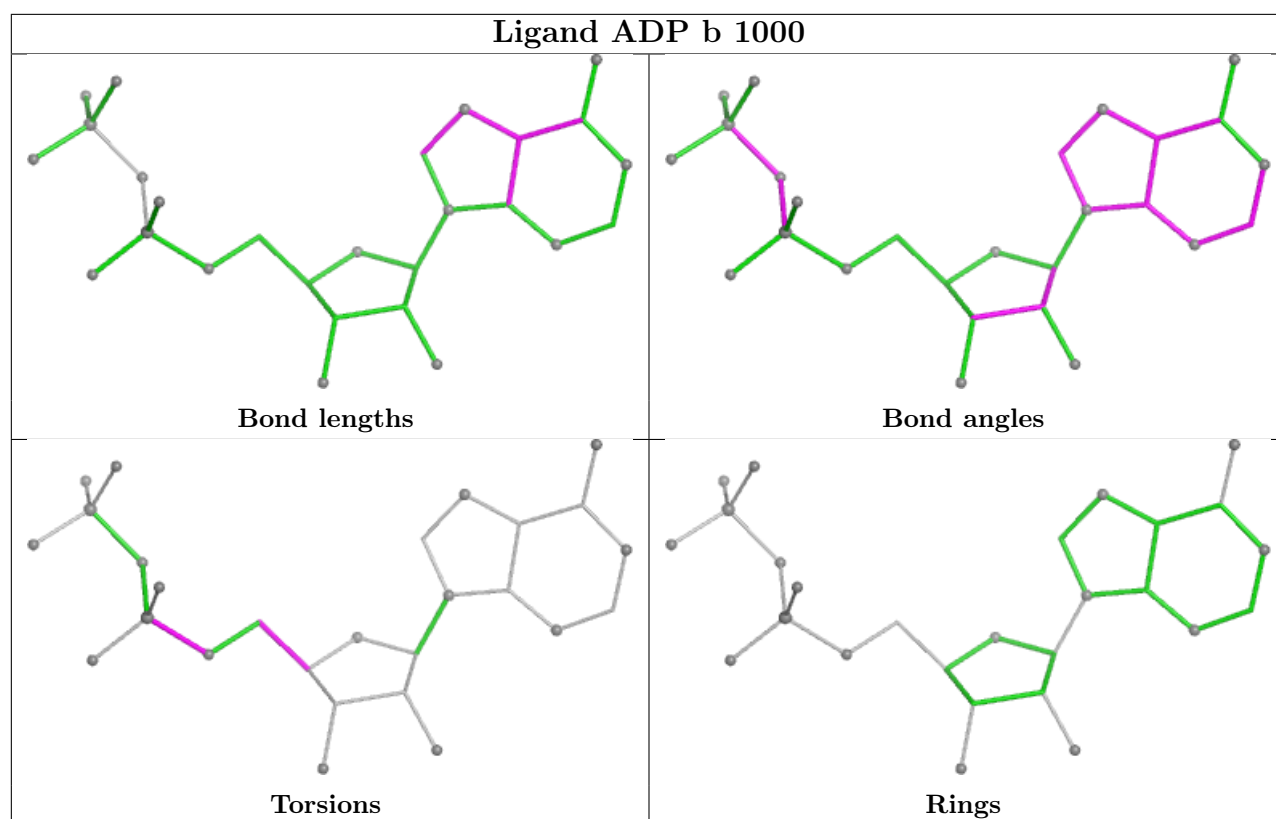
Mol	Chain	Res	Type	Atoms
10	a	1000	ADP	PA-O3A-PB-O3B
10	b	1000	ADP	C5'-O5'-PA-O3A
10	c	501	ADP	O4'-C4'-C5'-O5'
10	c	501	ADP	C3'-C4'-C5'-O5'
10	a	1000	ADP	O4'-C4'-C5'-O5'

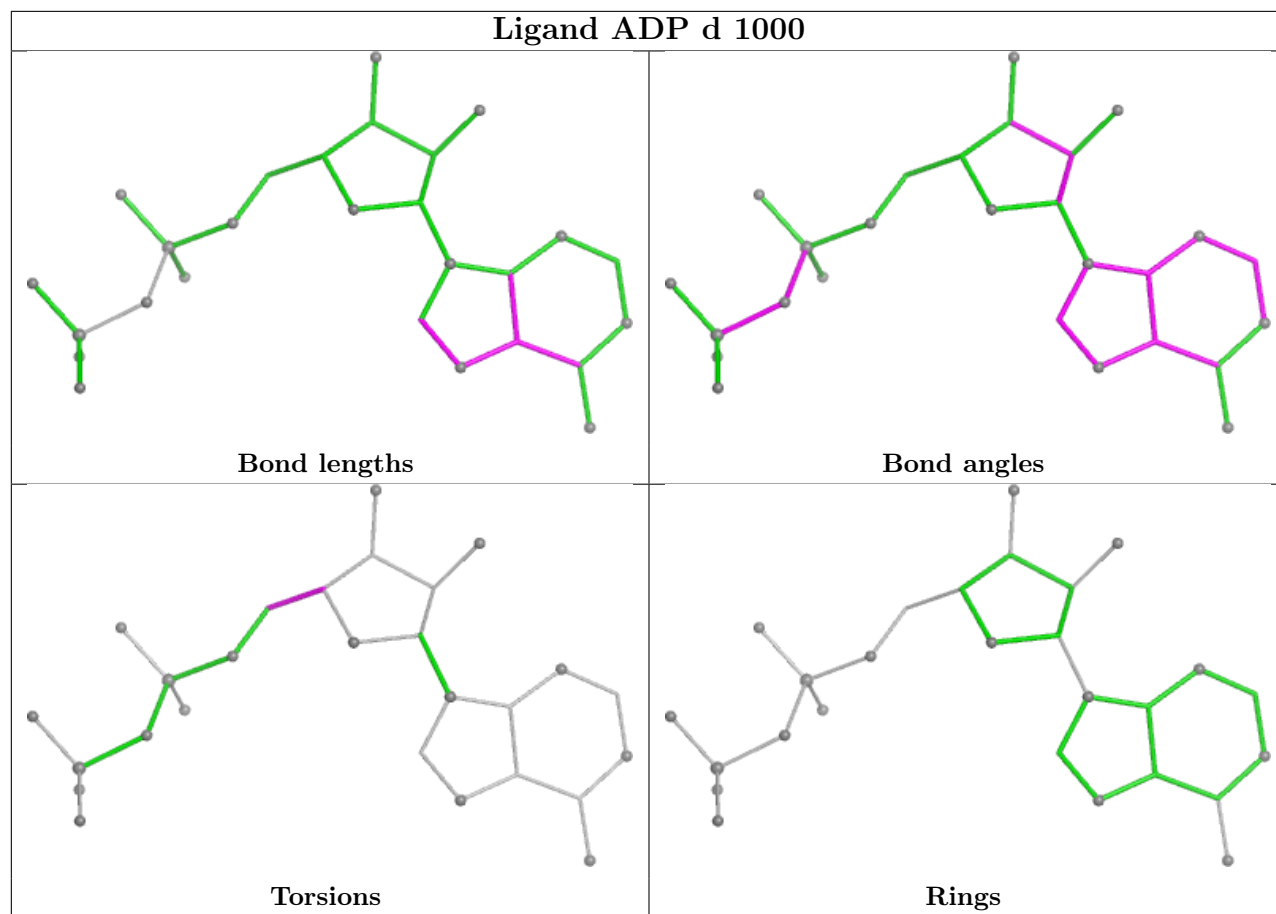
There are no ring outliers.

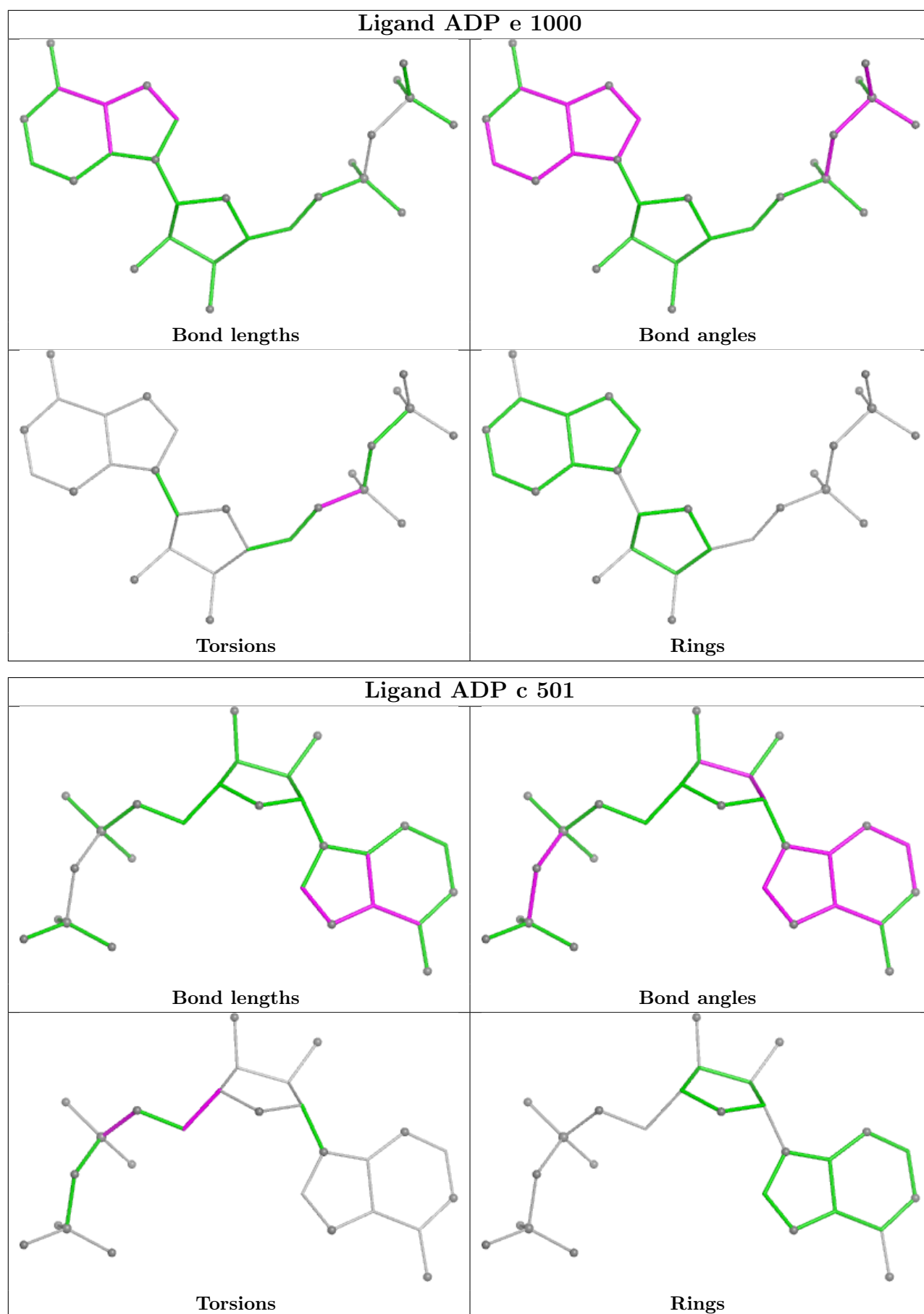
7 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	b	1000	ADP	2	0
10	a	1000	ADP	3	0
12	e	1002	BEF	1	0
10	e	1000	ADP	1	0
12	c	503	BEF	2	0
10	c	501	ADP	1	0
12	b	1002	BEF	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

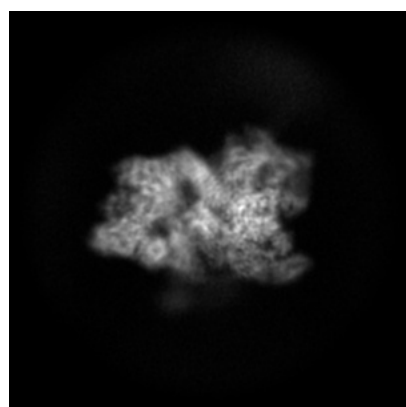
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11723. These allow visual inspection of the internal detail of the map and identification of artifacts.

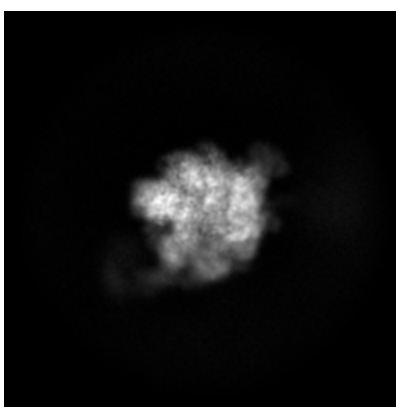
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

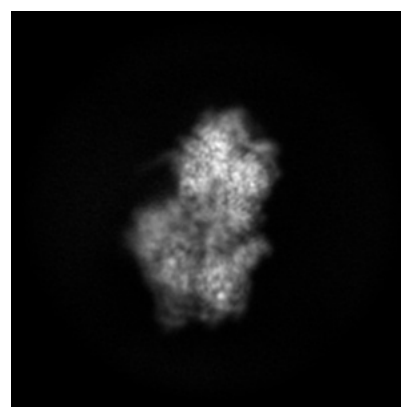
6.1.1 Primary map



X



Y

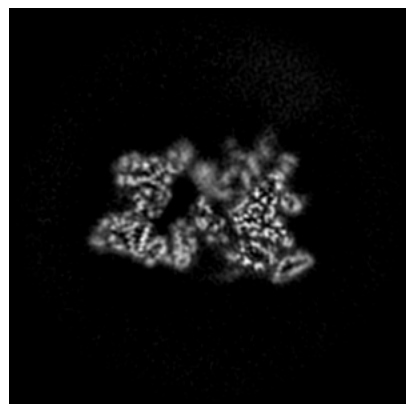


Z

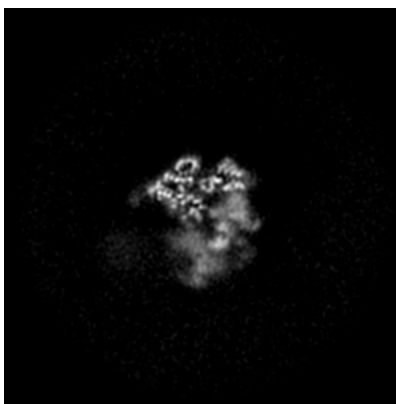
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

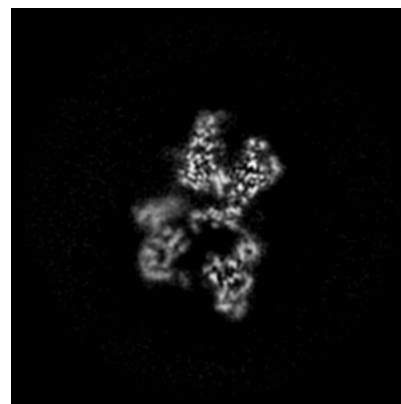
6.2.1 Primary map



X Index: 150



Y Index: 150

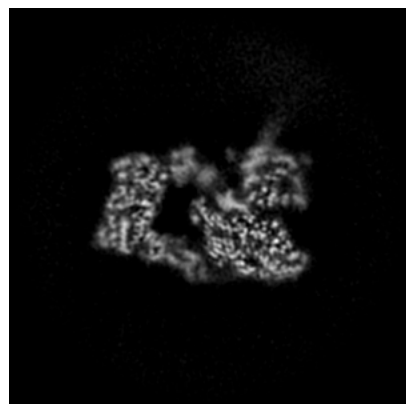


Z Index: 150

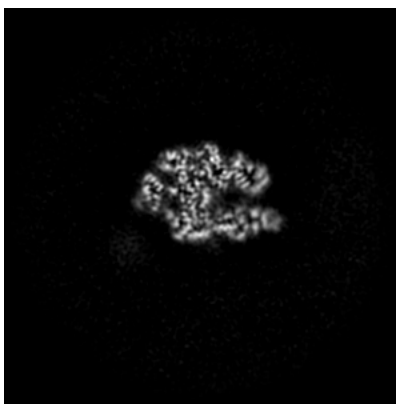
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

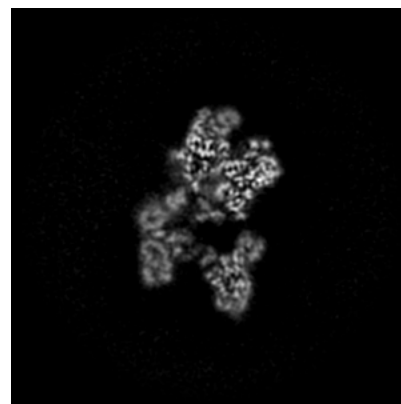
6.3.1 Primary map



X Index: 157



Y Index: 170

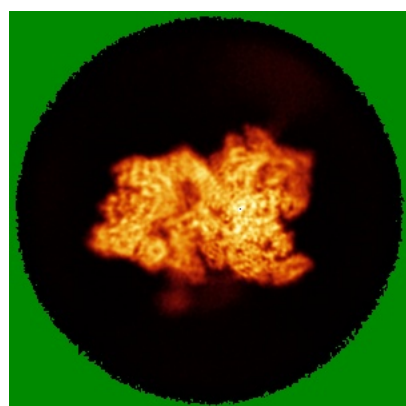


Z Index: 156

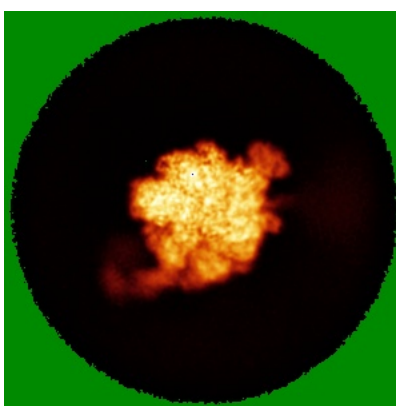
The images above show the largest variance slices of the map in three orthogonal directions.

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

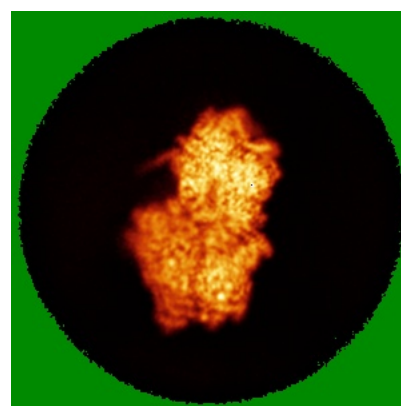
6.4.1 Primary map



X



Y

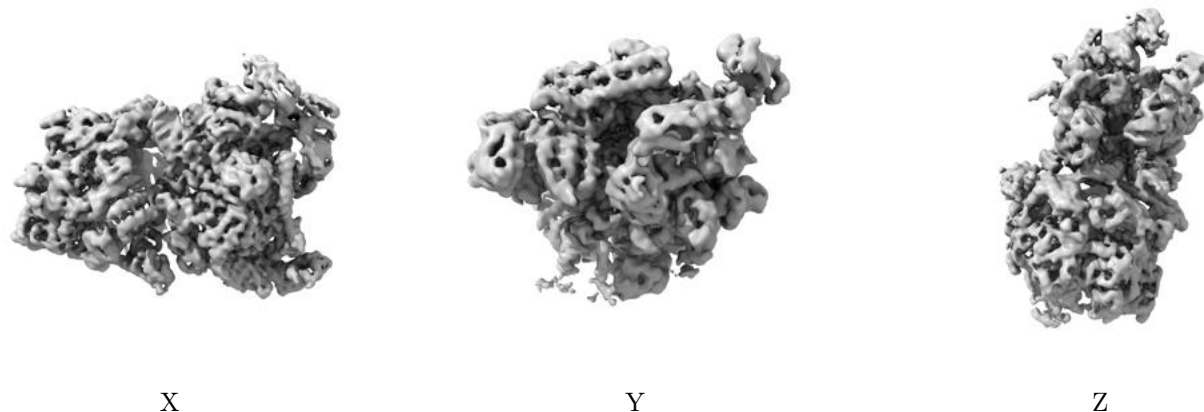


Z

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

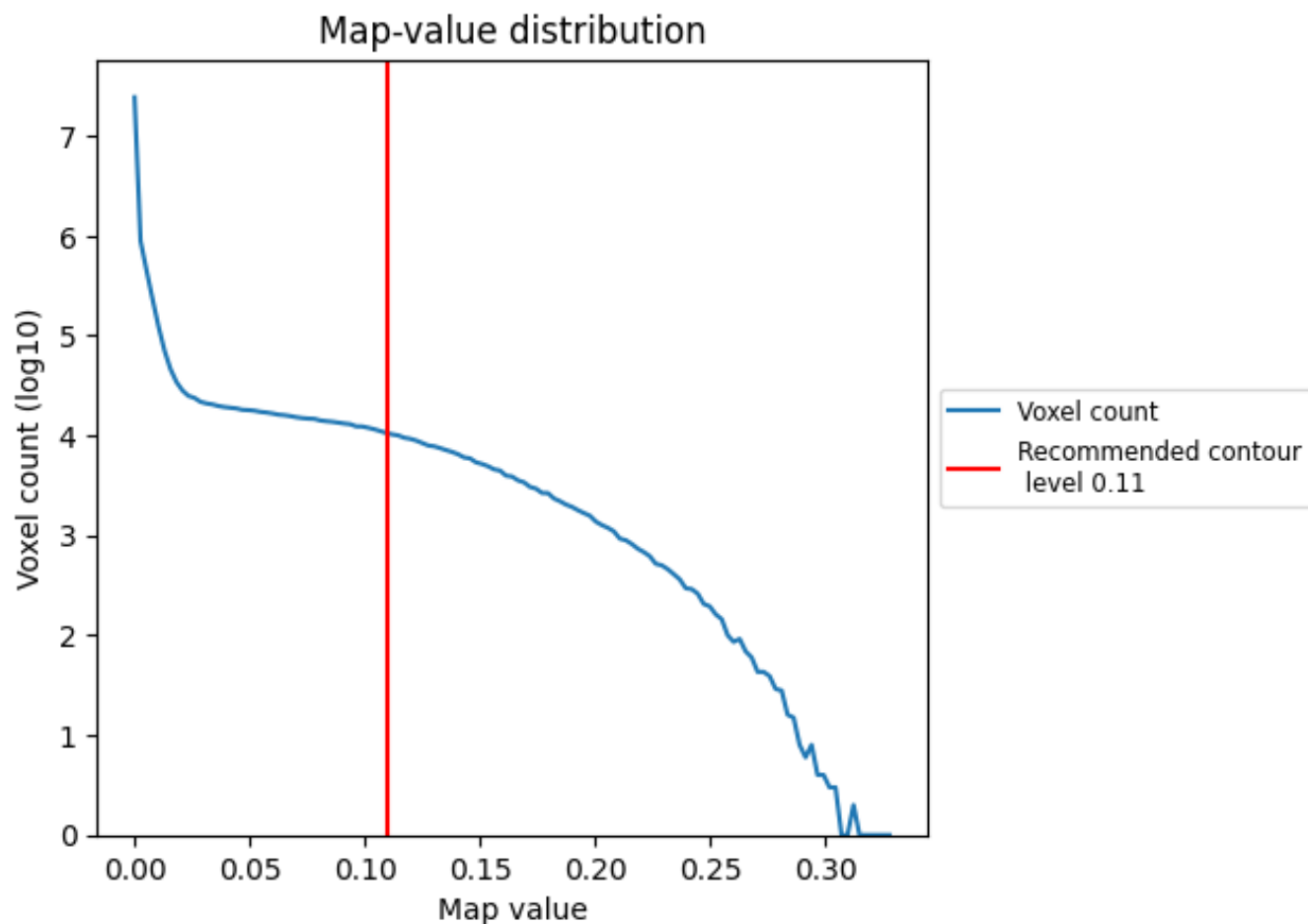
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

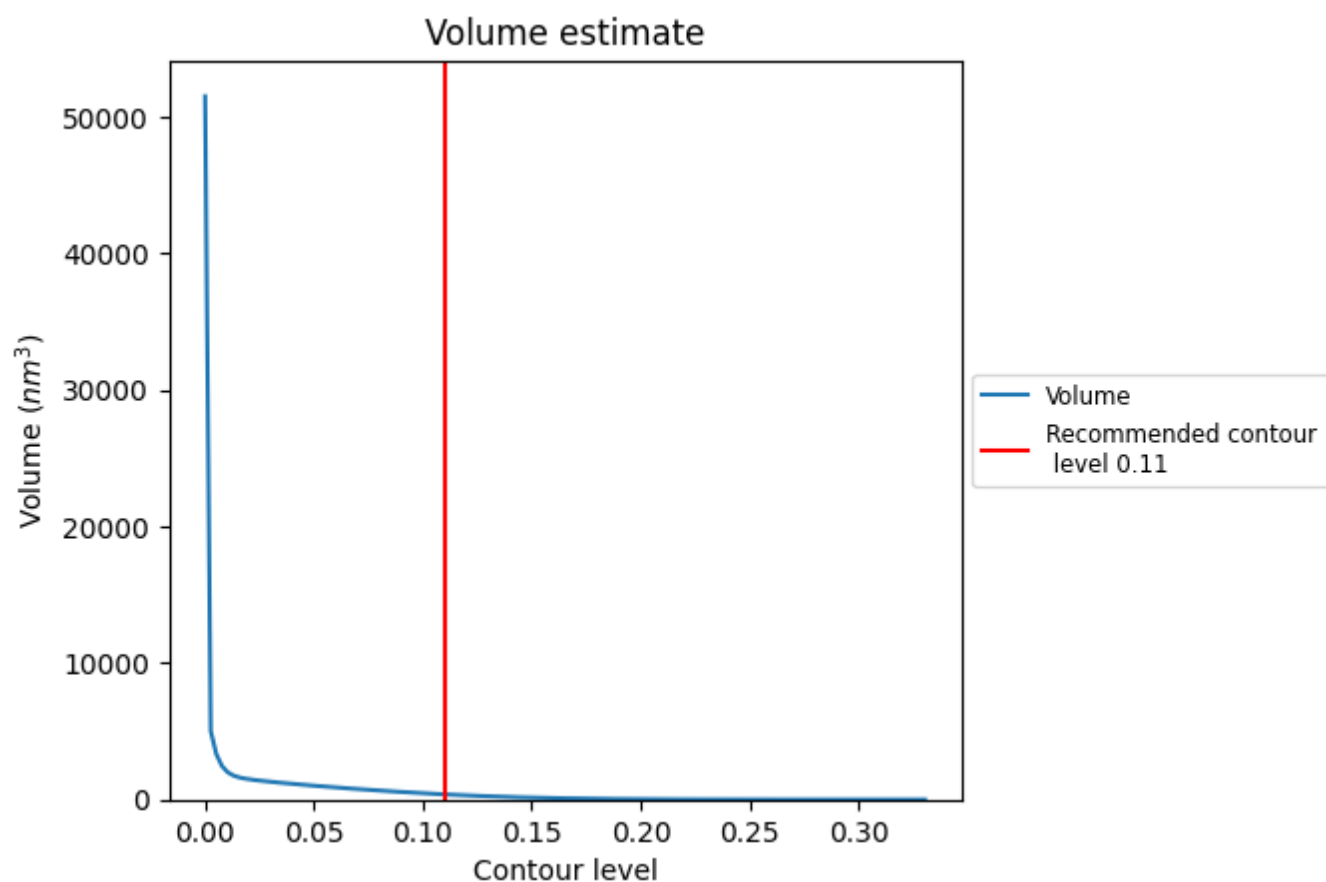
This section contains the results of statistical analysis of the map.

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.

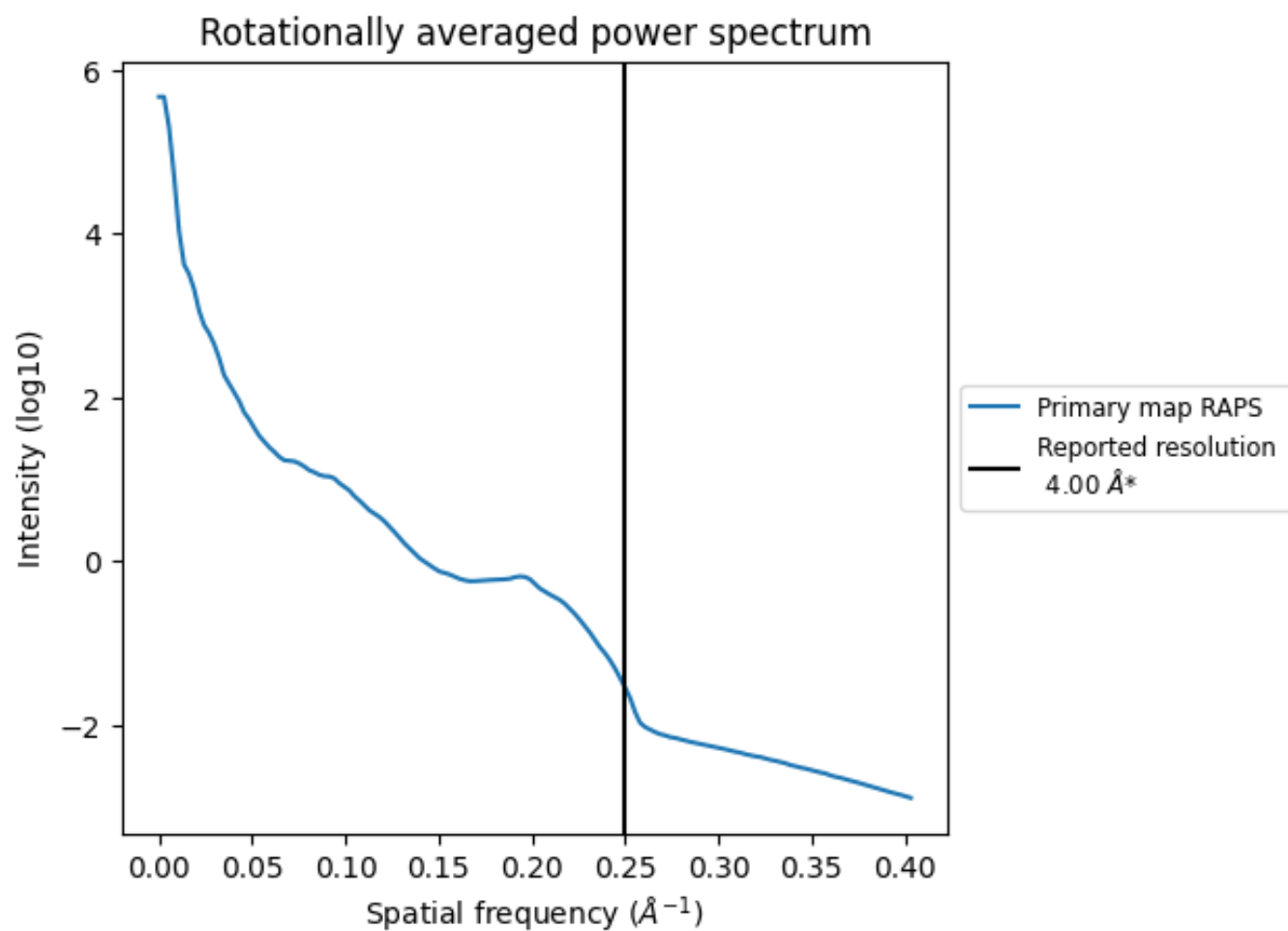
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 378 nm³; this corresponds to an approximate mass of 342 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 ⓘ

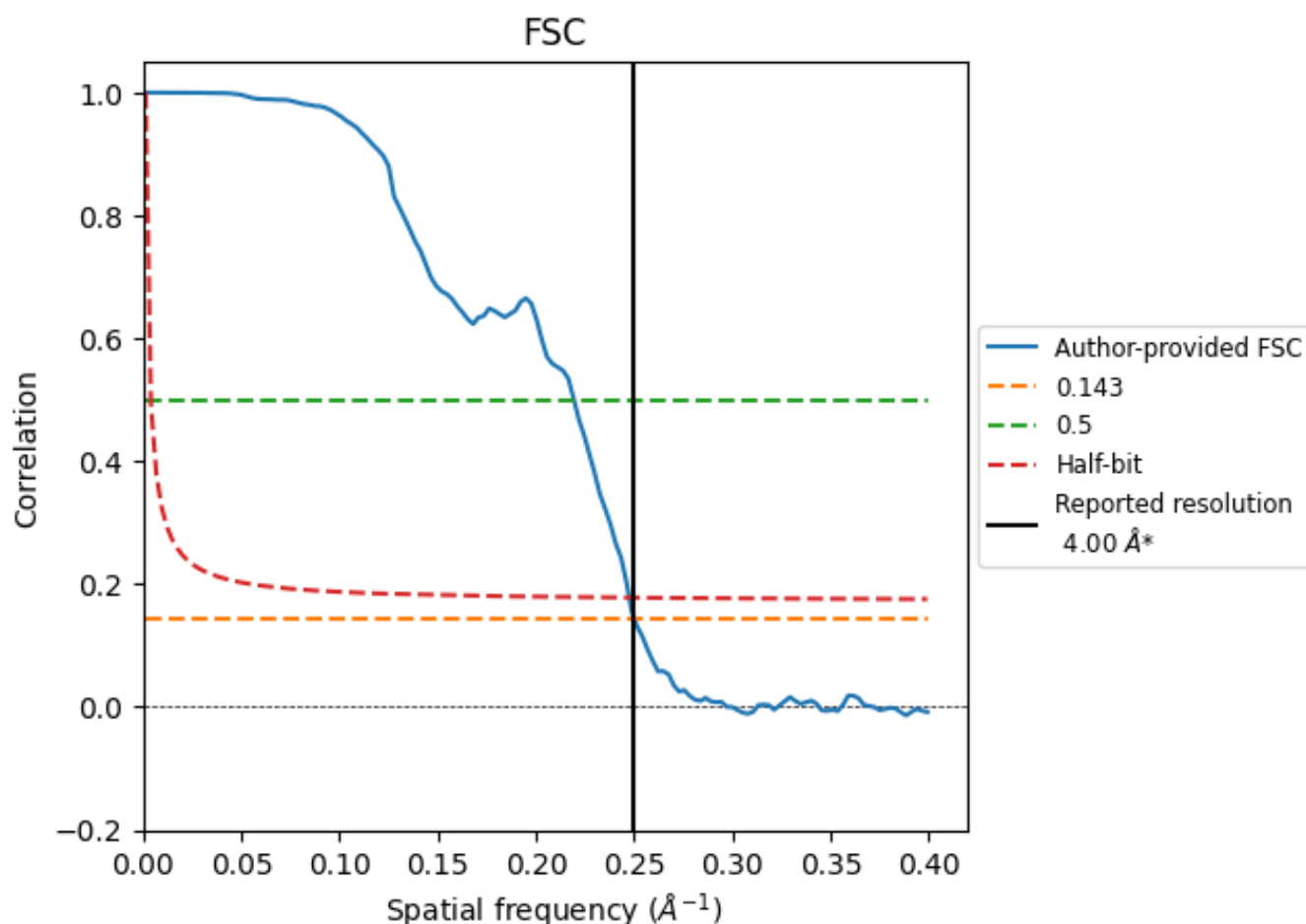


*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8.2 Resolution estimates [i](#)

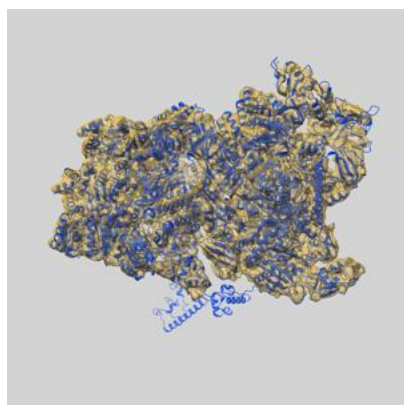
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	4.56	4.04
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

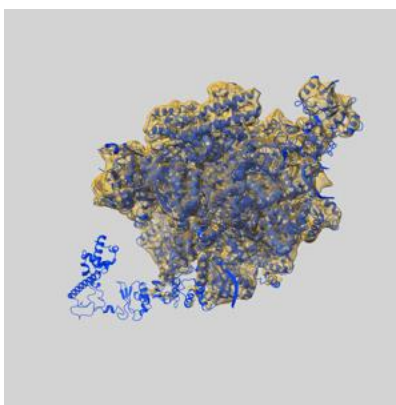
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11723 and PDB model 7ADC. Per-residue inclusion information can be found in [section 3](#) on [page 9](#).

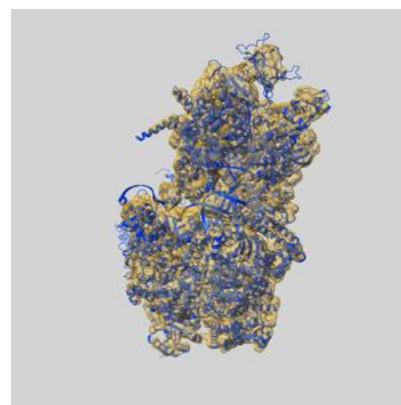
9.1 Map-model overlay [i](#)



X



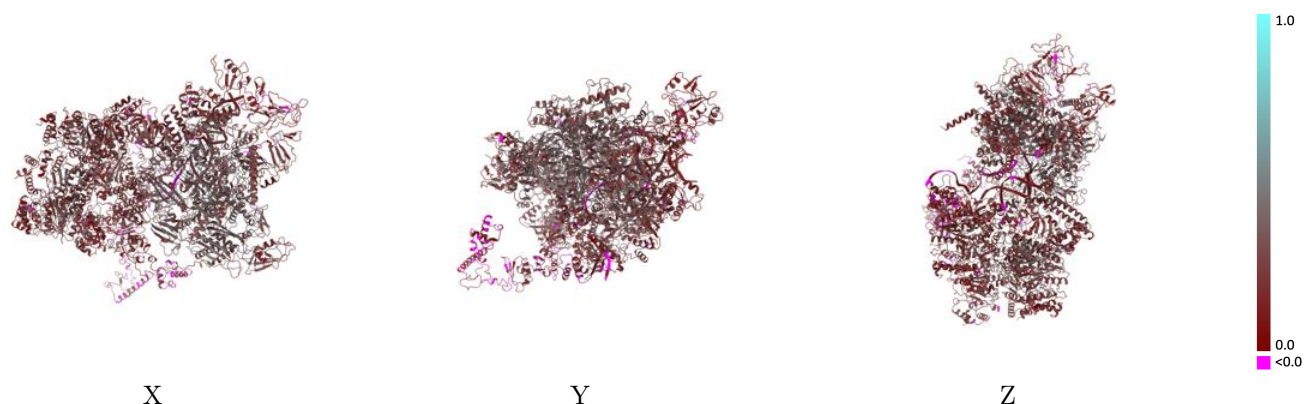
Y



Z

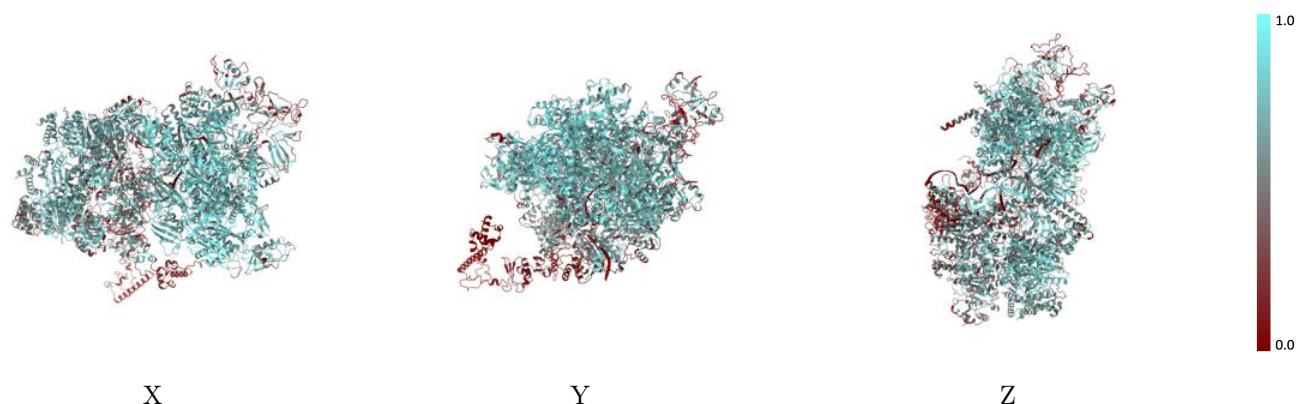
The images above show the 3D surface view of the map at the recommended contour level 0.11 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



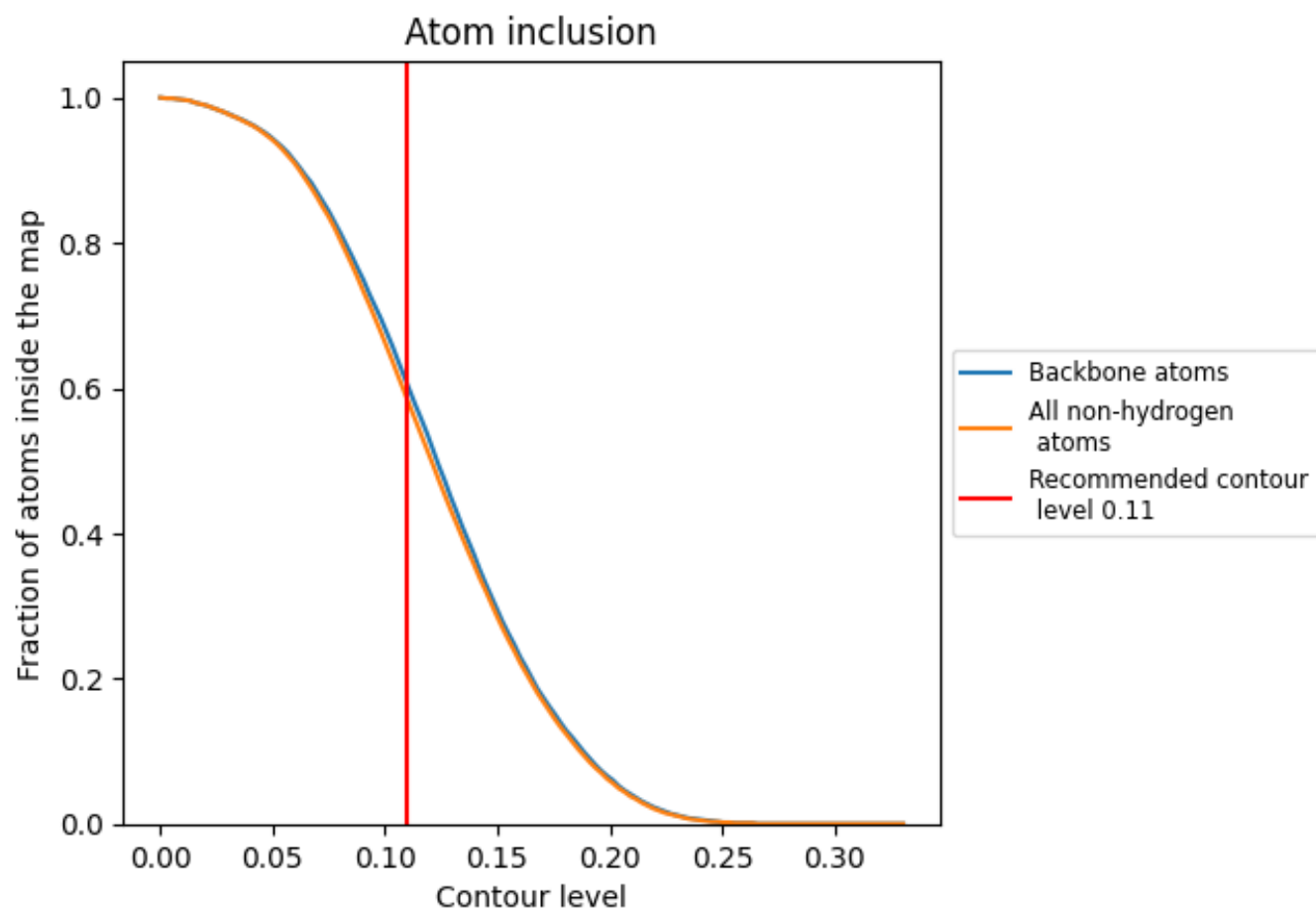
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.11).

9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 58% 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 (0.11) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5840	 0.2590
A	 0.2070	 0.1330
K	 0.5670	 0.1290
L	 0.7840	 0.2270
R	 0.2750	 0.1100
U	 0.7170	 0.3490
V	 0.6010	 0.2770
W	 0.5010	 0.2810
X	 0.7010	 0.3220
Y	 0.6550	 0.2900
a	 0.5760	 0.2160
b	 0.6410	 0.2530
c	 0.6610	 0.2680
d	 0.6420	 0.2620
e	 0.4860	 0.2050
f	 0.4170	 0.1780

