



wwPDB EM Validation Summary Report ⓘ

Mar 30, 2026 – 03:15 AM UTC

PDB ID : 6Z9T / pdb_00006z9t
EMDB ID : EMD-11091
Title : Transcription termination intermediate complex 5
Authors : Said, N.; Hilal, T.; Loll, B.; Wahl, M.C.
Deposited on : 2020-06-04
Resolution : 4.10 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:

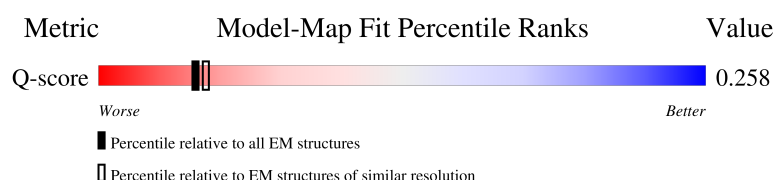
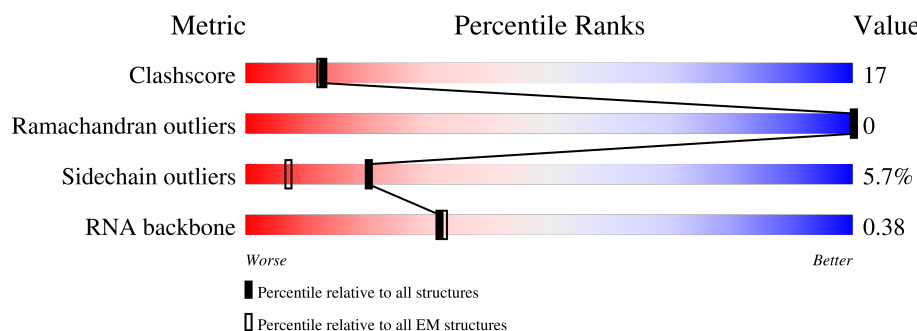
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 4.10 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.



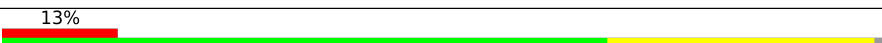
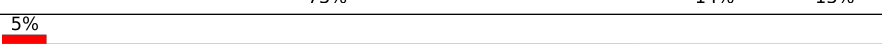
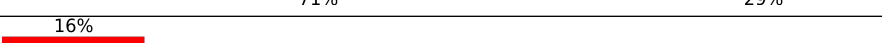
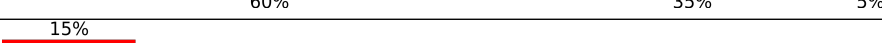
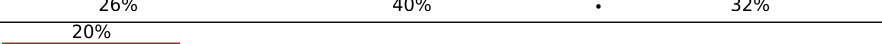
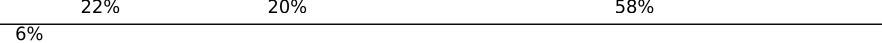
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
RNA backbone	8273	3508	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	8% 56% 37% 6%
1	b	419	5% 58% 36% 6%
1	c	419	58% 35% 6%

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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	L	53	
8	K	50	
9	R	99	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 51415 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
			3850	2395	669	773	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	1343	Total	C	N	O	S	0	0
			10433	6550	1862	1971	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 template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	L	36	Total	C	N	O	P	0	0
			724	345	129	215	35		

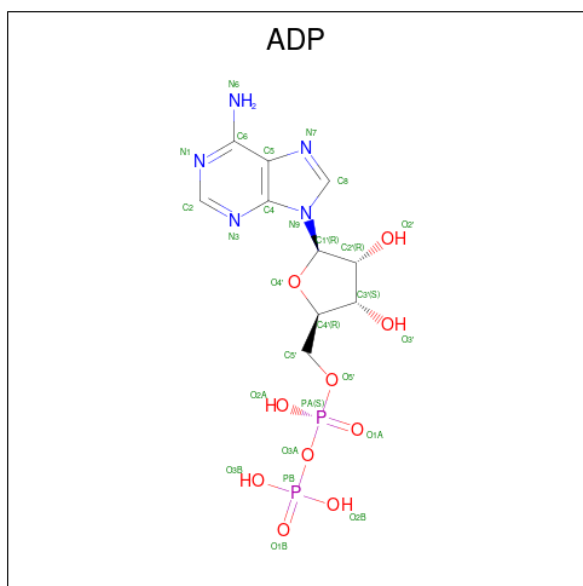
- Molecule 8 is a DNA chain called non template strand.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	K	21	Total	C	N	O	P	0	0
			437	205	86	125	21		

- Molecule 9 is a RNA chain called rut RNA.

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

- 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	C	N	O	P	0
			27	10	5	10	2	
10	b	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	c	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	d	1	Total	C	N	O	P	0
			27	10	5	10	2	
10	e	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

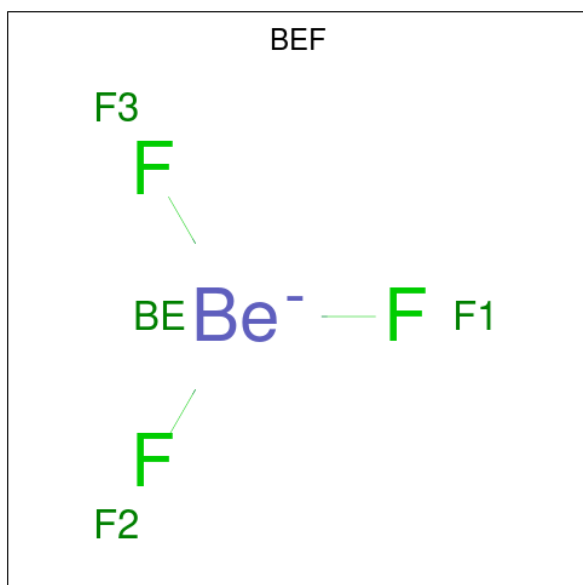
Mol	Chain	Residues	Atoms		AltConf
11	a	1	Total	Mg	0
			1	1	
11	b	1	Total	Mg	0
			1	1	
11	c	1	Total	Mg	0
			1	1	
11	d	1	Total	Mg	0
			1	1	

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

- Molecule 12 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



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

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

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

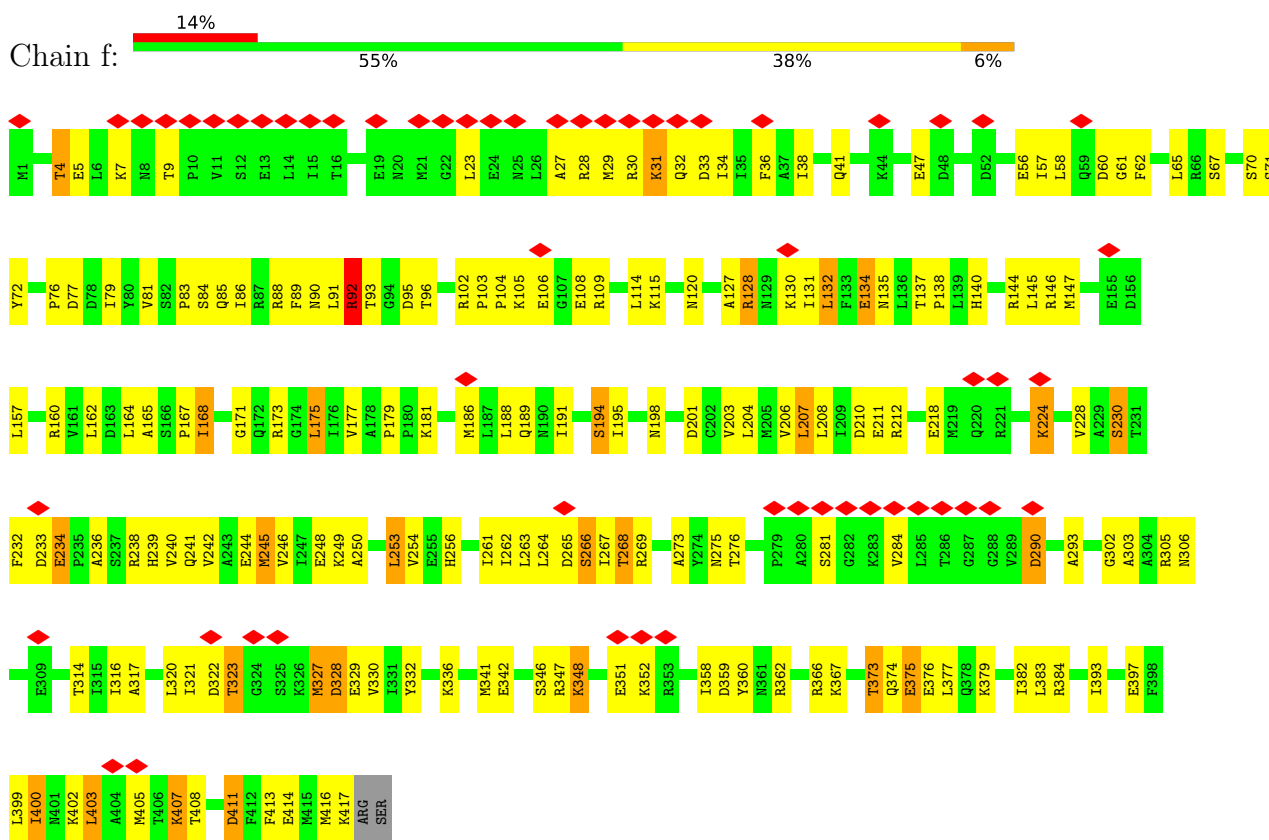
- Molecule 14 is water.

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

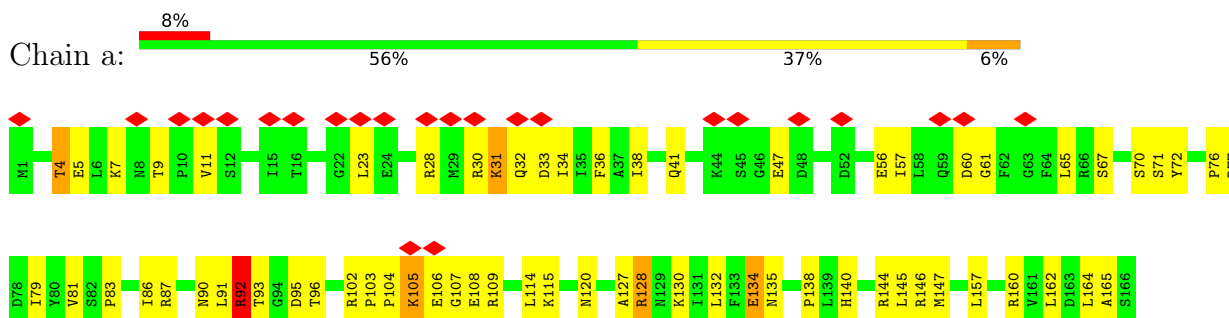
3 Residue-property plots

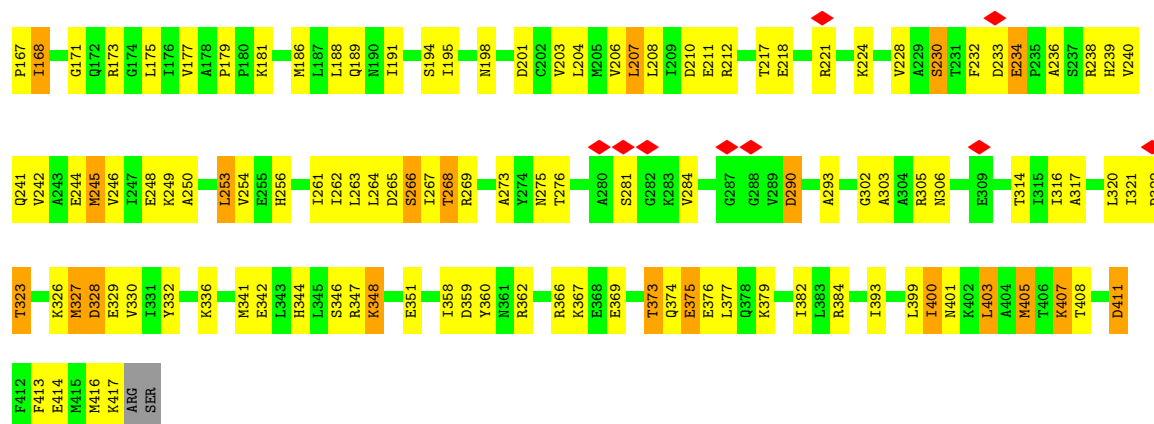
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

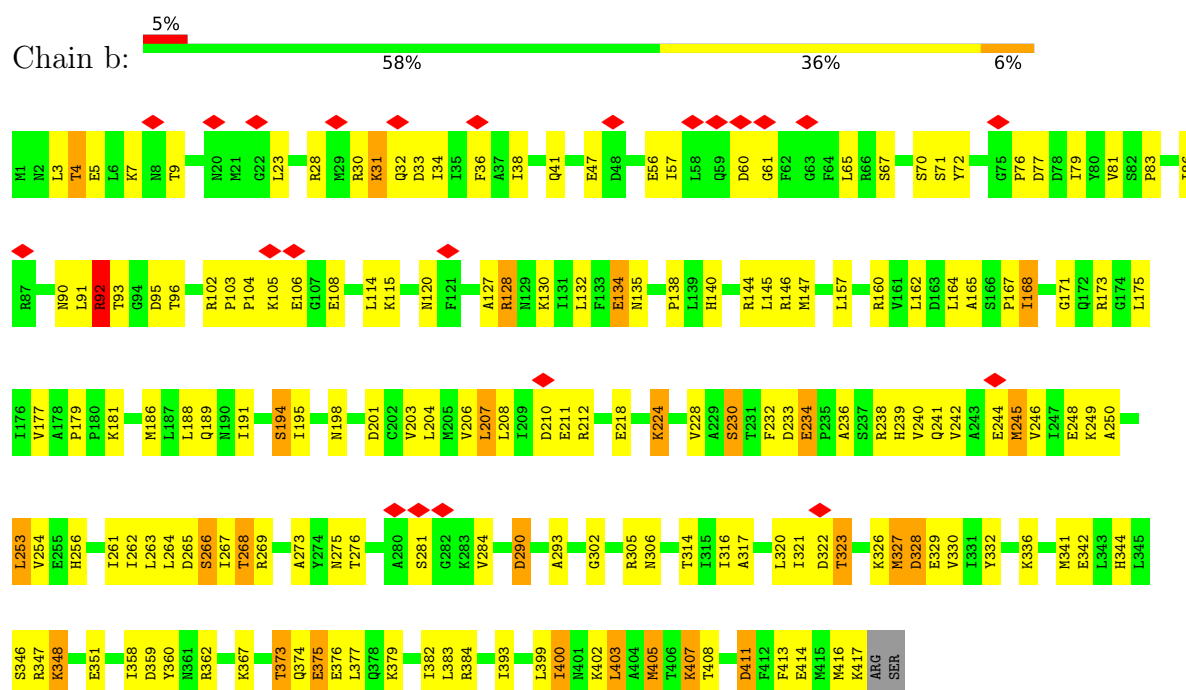


- Molecule 1: Transcription termination factor Rho

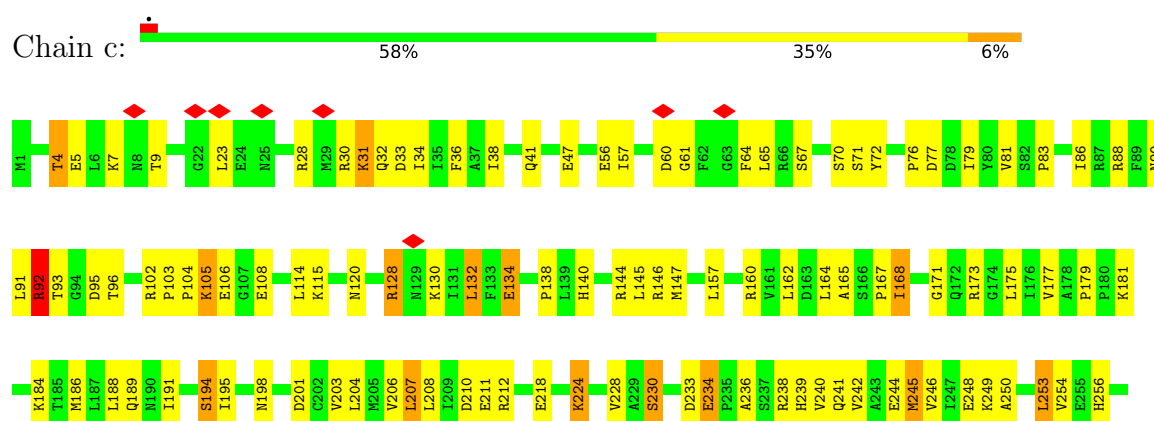


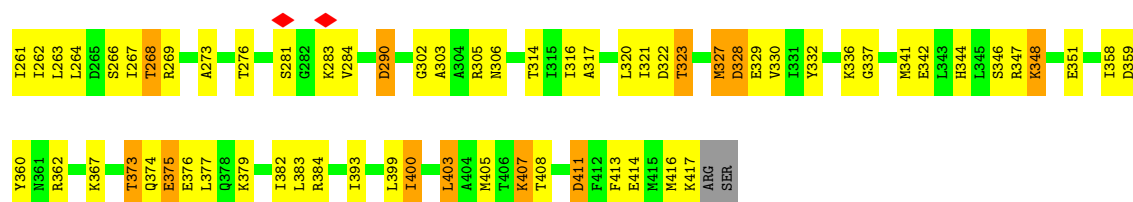


• Molecule 1: Transcription termination factor Rho

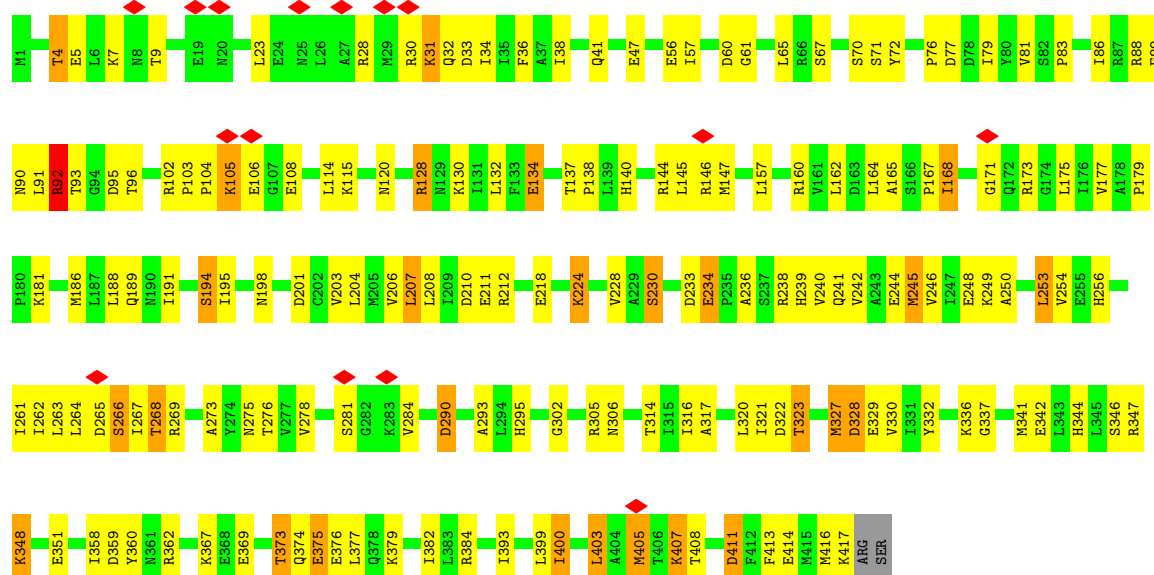


• Molecule 1: Transcription termination factor Rho

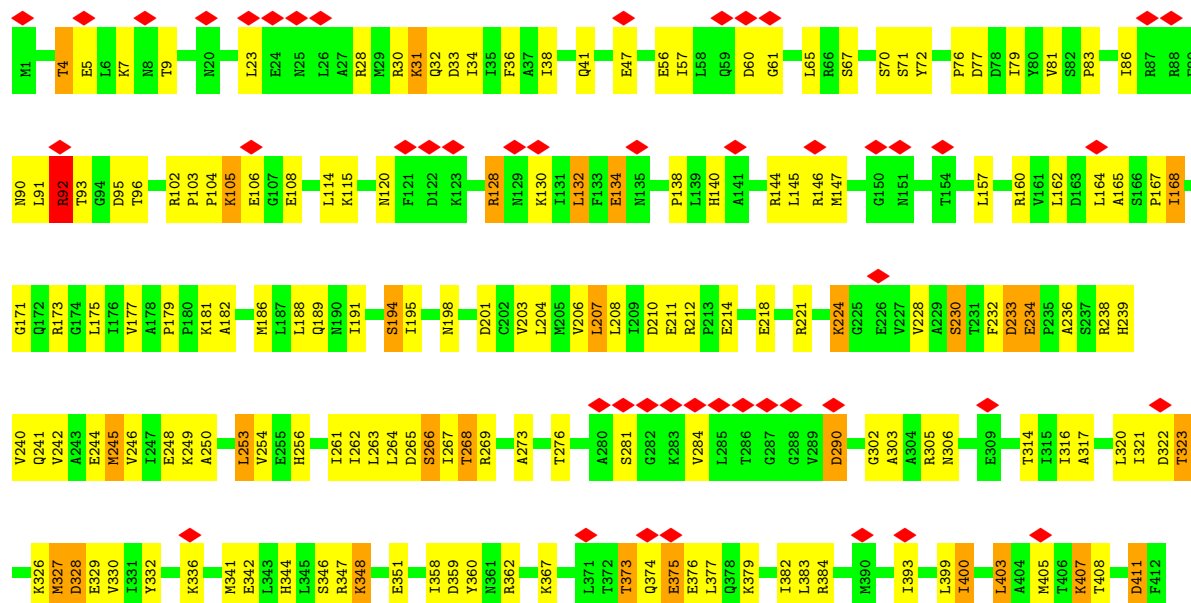


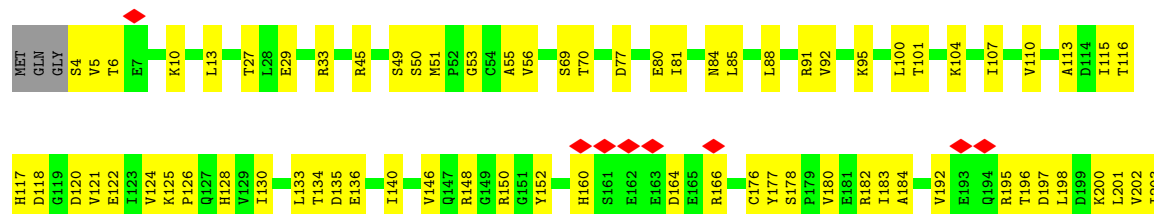


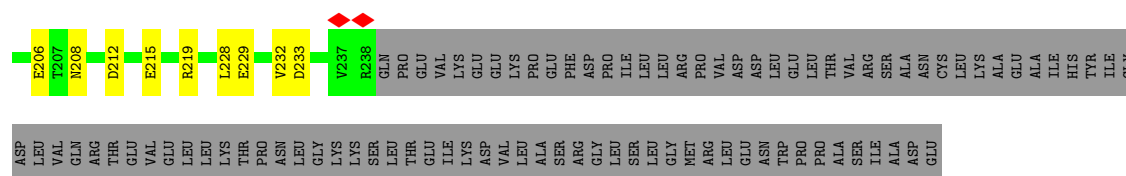
• Molecule 1: Transcription termination factor Rho



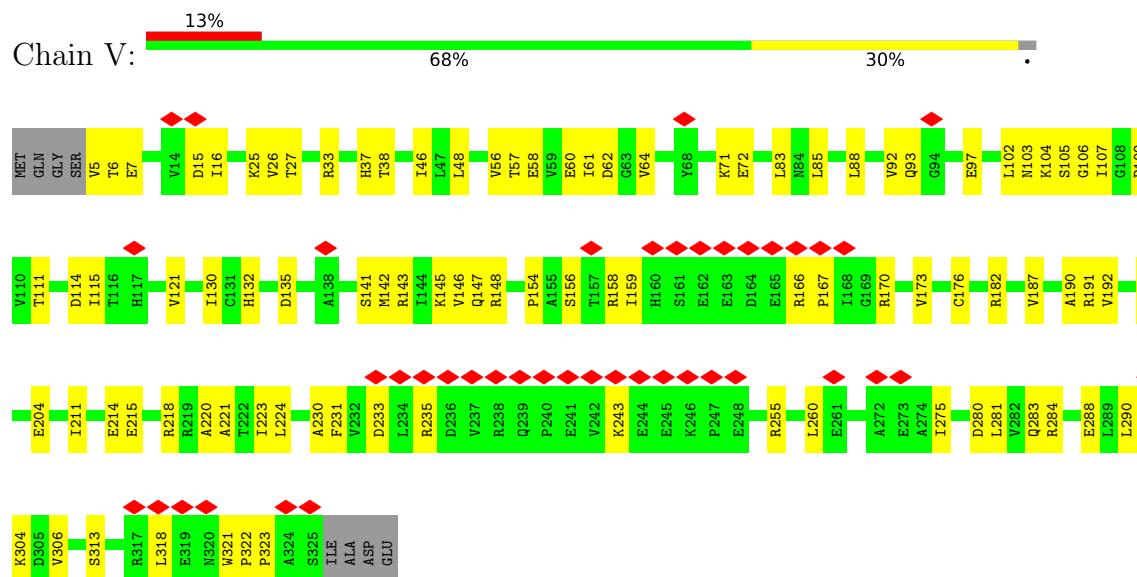
• Molecule 1: Transcription termination factor Rho



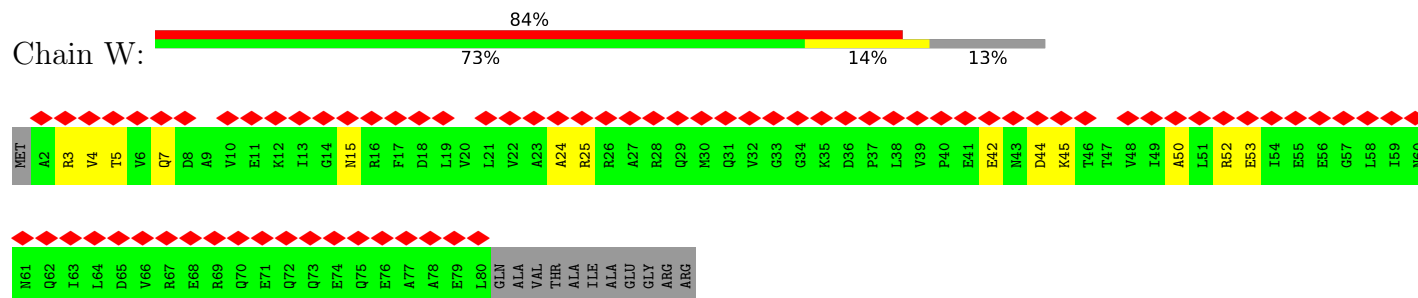




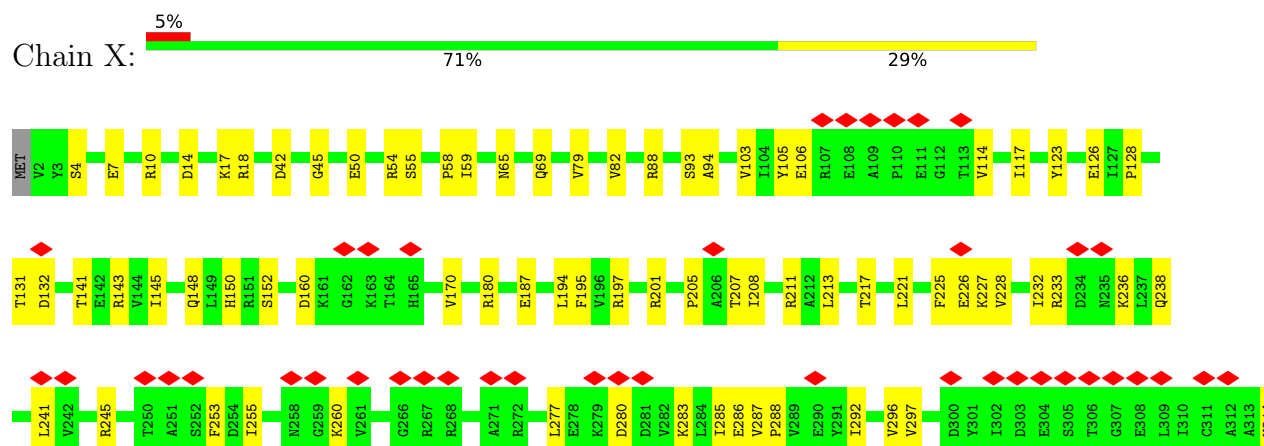
• Molecule 3: DNA-directed RNA polymerase subunit alpha

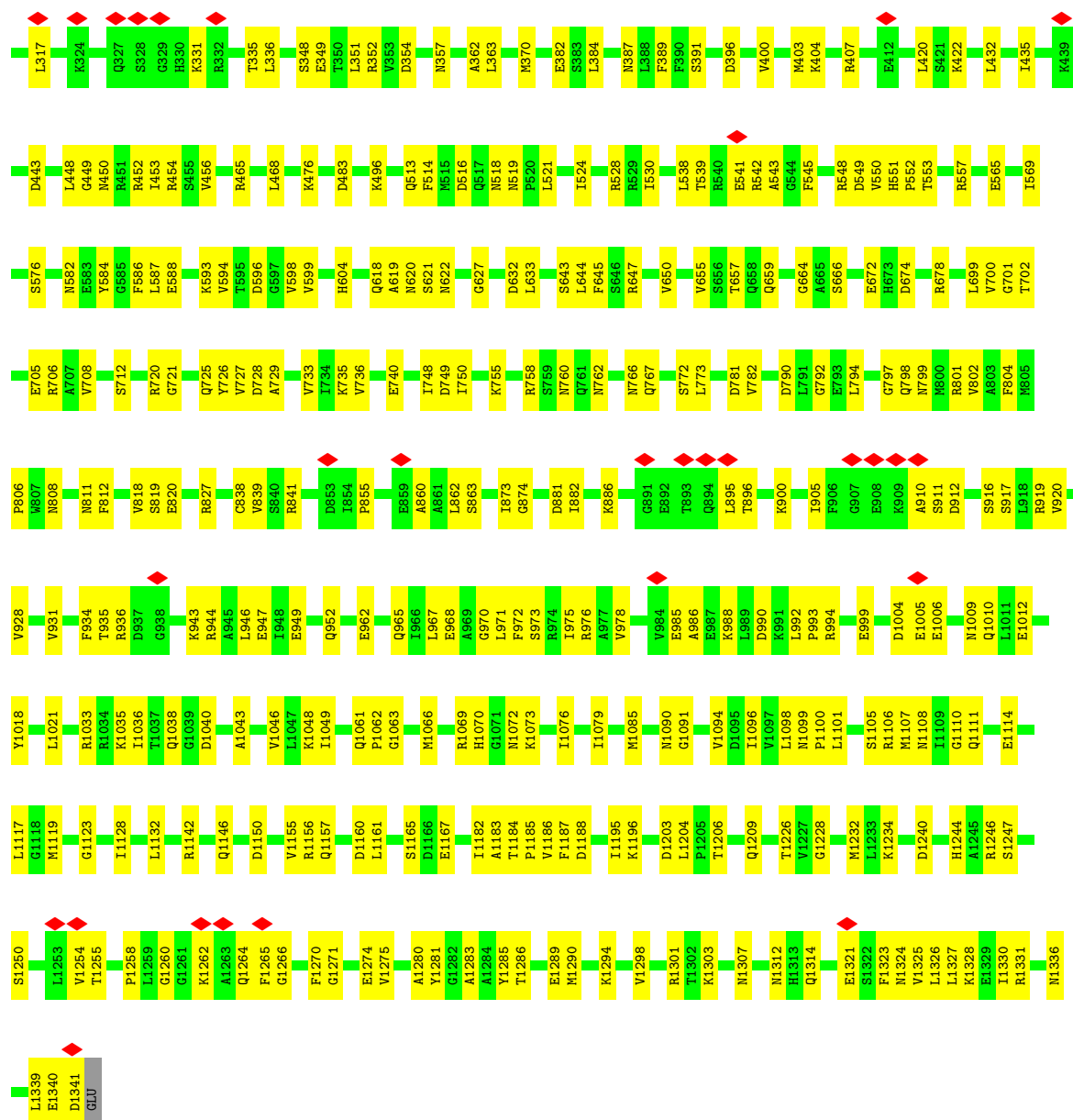


• Molecule 4: DNA-directed RNA polymerase subunit omega

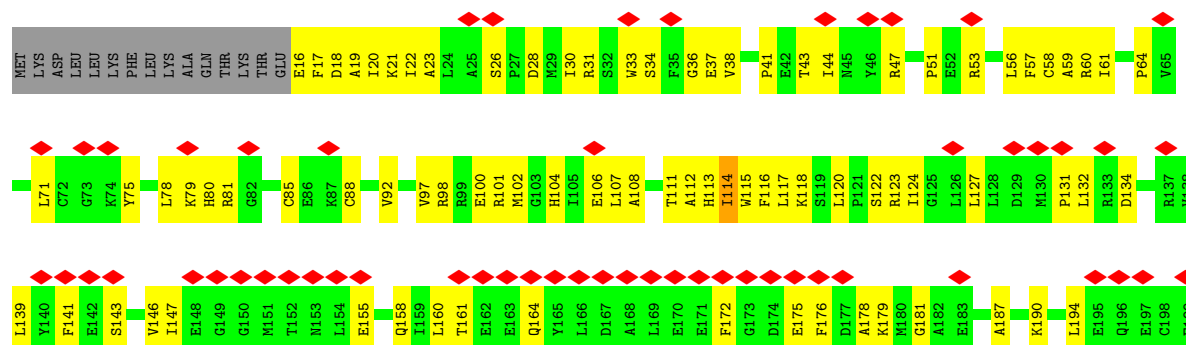


• Molecule 5: DNA-directed RNA polymerase subunit beta





• Molecule 6: DNA-directed RNA polymerase subunit beta'



E207	T208	K213	R214	T218	I221	L224	E225	A226	F227	V228	Q229	S230	G231	N232	K233	P234	E235	M236	N237	L238	L239	V241	L242	P243	V244	L245	P246	P247	D248	L249	ARG	PRO	LEU	VAL	PRO	LEU	ASP	GLY	GLY	ARG	PHE	ALA	THR	SER	ASP	L265	N266	D267	L268	Y269	R270	R271	V272	I273	
N274	R275	N276	N277	R278	L279	K280	R281	L282	L283	D284	L285	A286	A287	P288	D289	N290	I291	V292	R293	N294	E295	K296	R297	M298	L299	Q300	E301	A302	V303	D304	L307	G310	R311	G312	R313	R314	A315	I316	S319	N320	K321	L324	K325	D329	M330	I331	K332	G333	K334	Q335	G336	R337	F338	R339	
Q340	N341	L342	L343	Y349	S350	S353	V354	V357	L361	R362	L363	H364	Q365	C366	E375	P379	F380	I381	T393	A396	K399	R403	D410	I411	L412	V415	H419	P420	V421	L422	L423	N424	R425	A426	P427	T428	L429	H430	R431	L432	Q435	A436	F437	E438	P439										
V440	E443	H450	R451	L452	D460	T461	D462	V468	H469	E475	R481	A482	M485	N488	N489	I490	L491	P493	A494	N495	G496	E497	I500	S503	Q504	L510	M513	D516	C517	V518	L519	A520	V526	L527	T528	E531	K531	R532	L536	Y537	L541														
L544	H545	A546	R547	V548	K549	V550	T553	E554	D555	G561	E562	G563	T567	D571	T572	T573	V574	L579	I582	K585	G586	L587	A588	I589	A600	I601	S602	K603	C608	Y609	L612	G613	L614	K615	V618	T627	A633	R634	S635	G636	S638	V639	G640												
D643	S655	E658	V661	Q665	Q666	D667	F668	Q669	S670	G671	L672	V673	E677	W686	D699	T703	E704	N708	R709	Q712	E713	E714	W715	Q716	R731	Q736	A741	R744	M747	D751	I755	E756	T757	I759	N762	F763	L767	N768	V769																
L770	Q771	S775	K781	L788	K789	V809	T816	H817	E818	G819	N821	N822	T823	P824	E827	L835	R836	D837	R838	G841	R842	W843	E844	A845	E846	D847	V848	K849	R850	T853	D854	D855	L856	L857	V858	P859	R860	L863	L864	H865	Q867	W868	L872	E873	E874	N875									
D878	A879	V880	K881	V882	R883	S884	V885	D891	V894	V899	R901	D902	N903	A904	R905	G906	H907	I908	N909	N910	G912	E913	T918	Q921	S922	E925	P926	L930	R933	T934	F935	H936	I937	Q938	Q939	A940	S942	R943	A944	A945	A946	E947	S948	S949	V950	Q951	V952								
K953	N954	S957	S961	N962	V963	V966	V967	N968	S969	S970	G971	K972	L973	V974	I975	R978	H979	T980	K983	L984	I985	D986	E987	R990	Y999	G1000	L1003	A1004	K1005	G1006	D1007	Q1010	V1011	G1014	E1015	T1016	V1017	A1018	N1019	W1020	D1021	P1022	H1023	P1026	V1027	I1028	V1031								
S1032	R1036	F1037	T1038	D1039	M1040	I1041	D1042	G1043	Q1044	T1045	I1046	T1047	R1048	Q1049	T1050	D1051	E1052	L1053	T1054	G1055	L1056	S1057	S1058	V1061	L1062	D1063	S1064	A1065	E1066	R1067	A1069	G1070	G1071	K1072	D1073	L1074	R1075	K1079	I1080	V1081	D1082	A1083	Q1084	G1085	N1086	D1087	V1088	L1089	I1090	P1091	G1092	T1093	D1094	M1095	P1096
A1097	Q1098	Y1099	F1100	L1101	P1102	G1103	K1104	A1105	I1106	V1107	Q1108	D1111	Q1114	I1115	S1116	S1117	G1118	D1119	T1120	L1121	A1122	R1123	T1124	P1125	Q1126	E1127	S1128	G1129	G1130	T1131	K1132	I1134	T1135	G1136	G1137	L1138	P1139	F1145	R1149	P1150	K1151	A1154	I1155	E1156	I1159	S1160	G1161	I1162	V1163	S1164	F1165	G1166			
K1167	E1168	T1169	K1170	G1171	L1174	L1175	V1176	L1177	T1178	P1179	V1180	D1181	D1184	P1185	Y1186	E1187	M1188	N1189	K1192	W1193	V1198	F1199	E1202	R1203	V1204	I1210	S1211	D1212	G1213	P1214	D1219	L1220	L1221	R1222	H1227	R1231	Q1244	I1248	I1253	E1254	V1255	I1256	M1260	L1261	N1268										
S1272	D1273	F1274	L1275	E1276	G1277	V1280	R1284	R1290	G1296	T1301	R1304	D1305	L1306	I1309	T1310	K1311	T1316	E1317	S1318	F1319	I1320	E1327	T1328	T1329	R1330	G1331	L1332	T1333	E1334	A1335	A1336	V1337	K1340	R1341	D1342	L1343	L1344	N1350	V1351	I1352	V1353	G1354	R1355	P1358	G1362										

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	38054	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)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.160	Depositor
Minimum map value	-1.113	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.063	Depositor
Recommended contour level	0.35	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: ADP, MG, ZN, 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	0.17	0/3329	0.46	1/4483 (0.0%)
1	b	0.17	0/3329	0.47	1/4483 (0.0%)
1	c	0.17	0/3329	0.46	1/4483 (0.0%)
1	d	0.17	0/3329	0.46	1/4483 (0.0%)
1	e	0.17	0/3329	0.46	1/4483 (0.0%)
1	f	0.17	0/3329	0.46	1/4483 (0.0%)
2	A	0.12	0/3895	0.35	0/5270
3	U	0.10	0/1847	0.27	0/2503
3	V	0.11	0/2538	0.33	0/3441
4	W	0.09	0/629	0.27	0/847
5	X	0.11	0/10736	0.29	0/14487
6	Y	0.12	0/10590	0.32	1/14296 (0.0%)
7	L	0.39	1/807 (0.1%)	0.56	1/1236 (0.1%)
8	K	0.13	0/490	0.27	0/753
9	R	0.13	0/656	0.34	0/1016
All	All	0.15	1/52162 (0.0%)	0.38	8/70747 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	L	21	DC	O3'-P	9.63	1.75	1.61

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	L	22	DG	C2'-C3'-O3'	-8.62	98.57	111.50
6	Y	114	ILE	N-CA-C	-5.66	108.34	113.71
1	e	92	ARG	NE-CZ-NH2	5.07	123.77	119.20
1	b	92	ARG	NE-CZ-NH2	5.06	123.76	119.20
1	c	92	ARG	NE-CZ-NH2	5.05	123.75	119.20

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	3357	156	0
1	b	3280	0	3358	126	0
1	c	3280	0	3359	130	0
1	d	3280	0	3357	128	0
1	e	3280	0	3357	125	0
1	f	3280	0	3359	152	0
2	A	3850	0	3830	121	0
3	U	1825	0	1853	57	0
3	V	2504	0	2558	72	0
4	W	627	0	634	10	0
5	X	10567	0	10585	312	0
6	Y	10433	0	10650	418	0
7	L	724	0	405	66	0
8	K	437	0	236	11	0
9	R	590	0	305	28	0
10	a	27	0	12	2	0
10	b	27	0	12	1	0
10	c	27	0	12	1	0
10	d	27	0	12	0	0
10	e	27	0	12	4	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	1	0
12	b	4	0	0	0	0
12	c	4	0	0	0	0
12	d	4	0	0	0	0
12	e	4	0	0	1	0
13	Y	2	0	0	0	0
14	a	3	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
14	b	3	0	0	1	0
14	c	3	0	0	2	0
14	d	3	0	0	0	0
14	e	3	0	0	0	0
All	All	51415	0	51263	1707	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 17.

The worst 5 of 1707 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:Y:47:ARG:CG	7:L:22:DG:C8	1.75	1.65
6:Y:47:ARG:CG	7:L:22:DG:N7	1.82	1.40
1:a:107:GLY:CA	7:L:38:DT:H73	1.59	1.33
6:Y:47:ARG:HG3	7:L:22:DG:C8	0.79	1.32
1:a:107:GLY:O	7:L:38:DT:C5	1.86	1.28

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	a	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	b	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	c	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	d	415/419 (99%)	401 (97%)	14 (3%)	0	100	100
1	e	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	f	415/419 (99%)	402 (97%)	13 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	A	493/497 (99%)	448 (91%)	45 (9%)	0	100	100
3	U	233/329 (71%)	224 (96%)	9 (4%)	0	100	100
3	V	319/329 (97%)	295 (92%)	24 (8%)	0	100	100
4	W	77/91 (85%)	75 (97%)	2 (3%)	0	100	100
5	X	1338/1342 (100%)	1255 (94%)	83 (6%)	0	100	100
6	Y	1339/1416 (95%)	1257 (94%)	82 (6%)	0	100	100
All	All	6289/6518 (96%)	5965 (95%)	324 (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%)	306 (86%)	51 (14%)	3	16
1	b	357/359 (99%)	306 (86%)	51 (14%)	3	16
1	c	357/359 (99%)	306 (86%)	51 (14%)	3	16
1	d	357/359 (99%)	306 (86%)	51 (14%)	3	16
1	e	357/359 (99%)	306 (86%)	51 (14%)	3	16
1	f	357/359 (99%)	306 (86%)	51 (14%)	3	16
2	A	408/409 (100%)	408 (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	1122/1177 (95%)	1122 (100%)	0	100	100
All	All	5377/5544 (97%)	5071 (94%)	306 (6%)	20	43

5 of 306 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	d	253	LEU
1	e	284	VAL
1	d	327	MET
1	e	67	SER
1	e	399	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
5	X	737	ASN
6	Y	477	GLN
5	X	932	GLN
6	Y	196	GLN
6	Y	910	ASN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
9	R	26/99 (26%)	9 (34%)	2 (7%)

5 of 9 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
9	R	23	U
9	R	24	U
9	R	25	C
9	R	26	C
9	R	84	A

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
9	R	23	U
9	R	90	G

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	28,29,29	1.42	4 (14%)	43,45,45	1.84	9 (20%)
12	BEF	e	1002	-	0,3,3	-	-	-	-	-
10	ADP	e	1000	11	28,29,29	1.41	4 (14%)	43,45,45	1.84	9 (20%)
10	ADP	c	1000	11	28,29,29	1.44	4 (14%)	43,45,45	1.95	9 (20%)
12	BEF	a	1002	-	0,3,3	-	-	-	-	-
10	ADP	d	1000	11	28,29,29	1.43	4 (14%)	43,45,45	1.84	9 (20%)
12	BEF	c	1002	-	0,3,3	-	-	-	-	-
12	BEF	b	1002	-	0,3,3	-	-	-	-	-
10	ADP	a	1000	11	28,29,29	1.44	5 (17%)	43,45,45	1.88	9 (20%)
12	BEF	d	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	-	2/16/32/32	0/3/3/3
10	ADP	e	1000	11	-	2/16/32/32	0/3/3/3
10	ADP	c	1000	11	-	2/16/32/32	0/3/3/3
10	ADP	d	1000	11	-	2/16/32/32	0/3/3/3
10	ADP	a	1000	11	-	2/16/32/32	0/3/3/3

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	c	1000	ADP	C5-C4	4.81	1.47	1.39
10	d	1000	ADP	C5-C4	4.77	1.47	1.39
10	a	1000	ADP	C5-C4	4.74	1.47	1.39
10	e	1000	ADP	C5-C4	4.73	1.47	1.39
10	b	1000	ADP	C5-C4	4.71	1.47	1.39

The worst 5 of 45 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	c	1000	ADP	C5-C4-N3	-6.46	117.82	126.72
10	a	1000	ADP	C5-C4-N3	-5.93	118.56	126.72
10	d	1000	ADP	C5-C4-N3	-5.82	118.70	126.72
10	e	1000	ADP	C5-C4-N3	-5.79	118.75	126.72
10	b	1000	ADP	C5-C4-N3	-5.76	118.79	126.72

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	c	1000	ADP	O4'-C4'-C5'-O5'
10	b	1000	ADP	O4'-C4'-C5'-O5'
10	c	1000	ADP	C3'-C4'-C5'-O5'
10	b	1000	ADP	C3'-C4'-C5'-O5'
10	d	1000	ADP	O4'-C4'-C5'-O5'

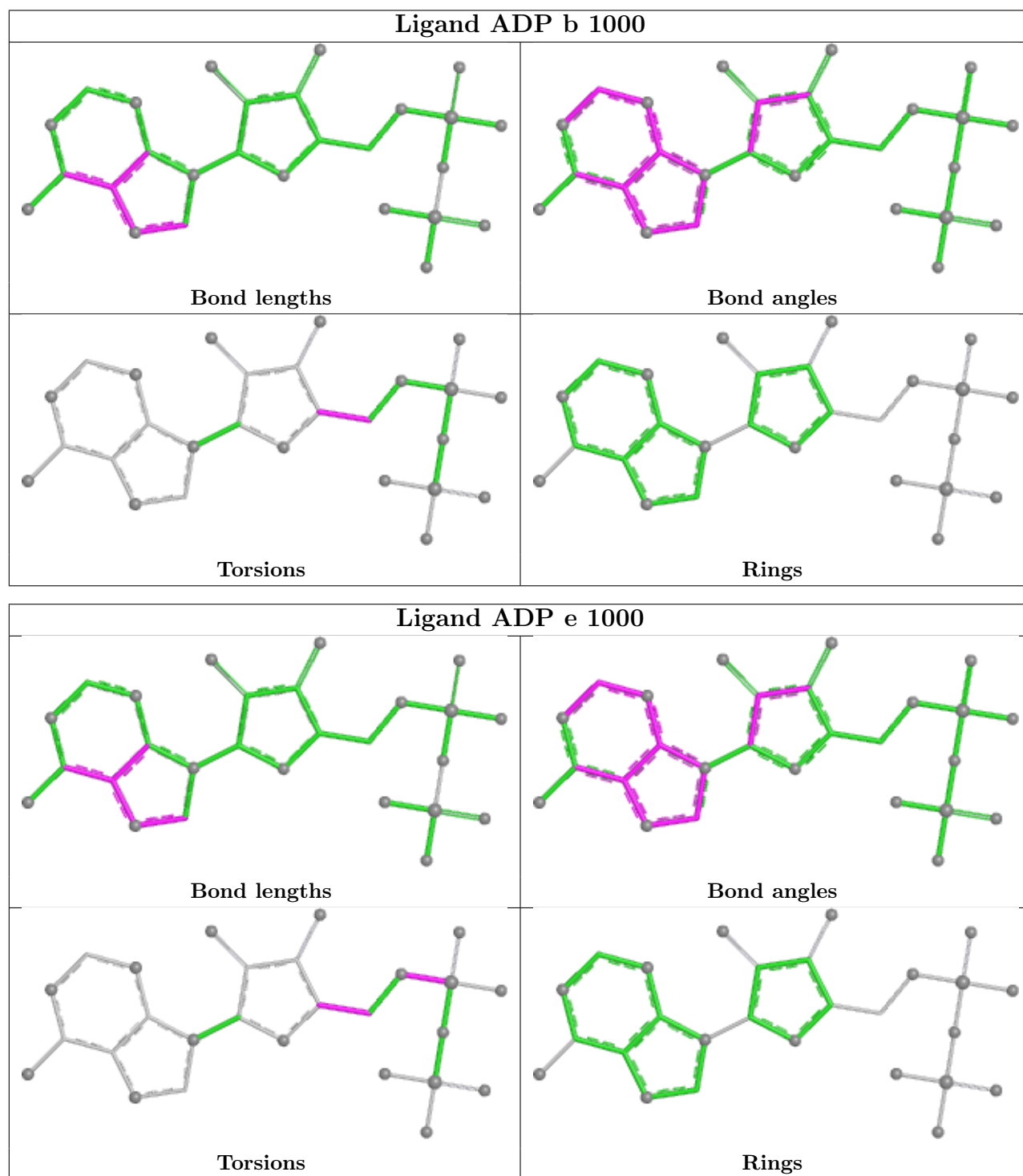
There are no ring outliers.

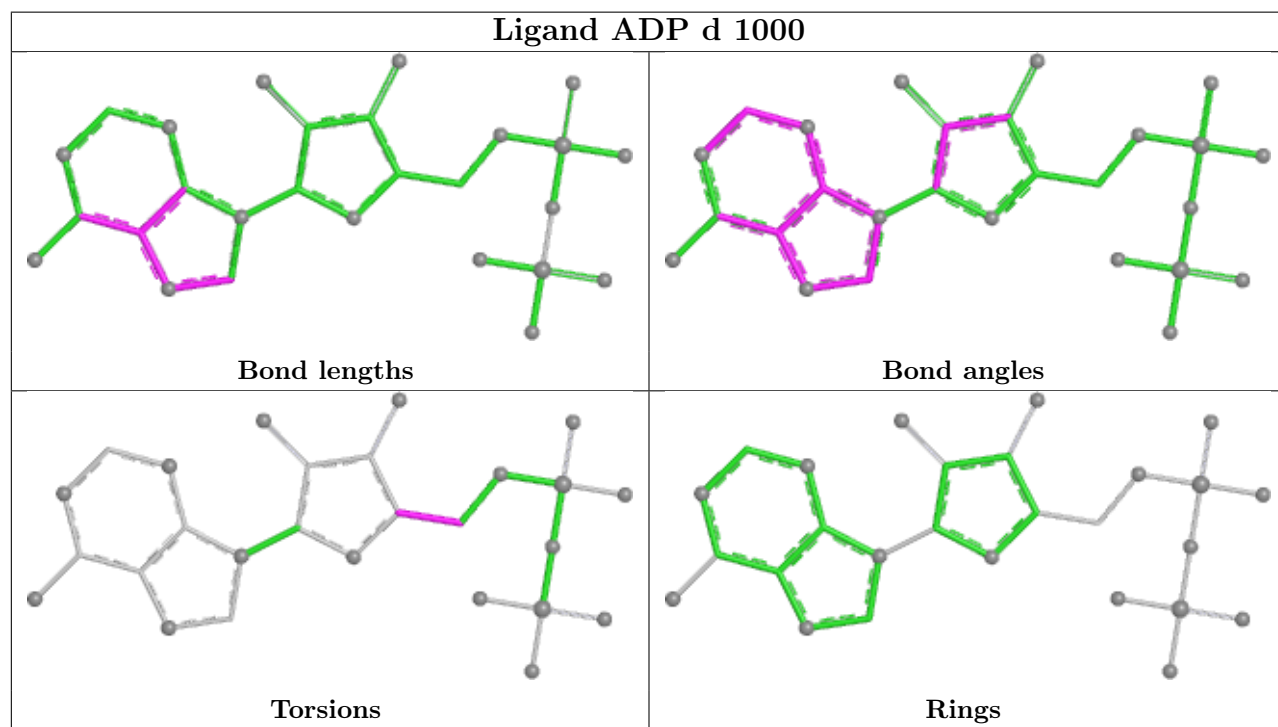
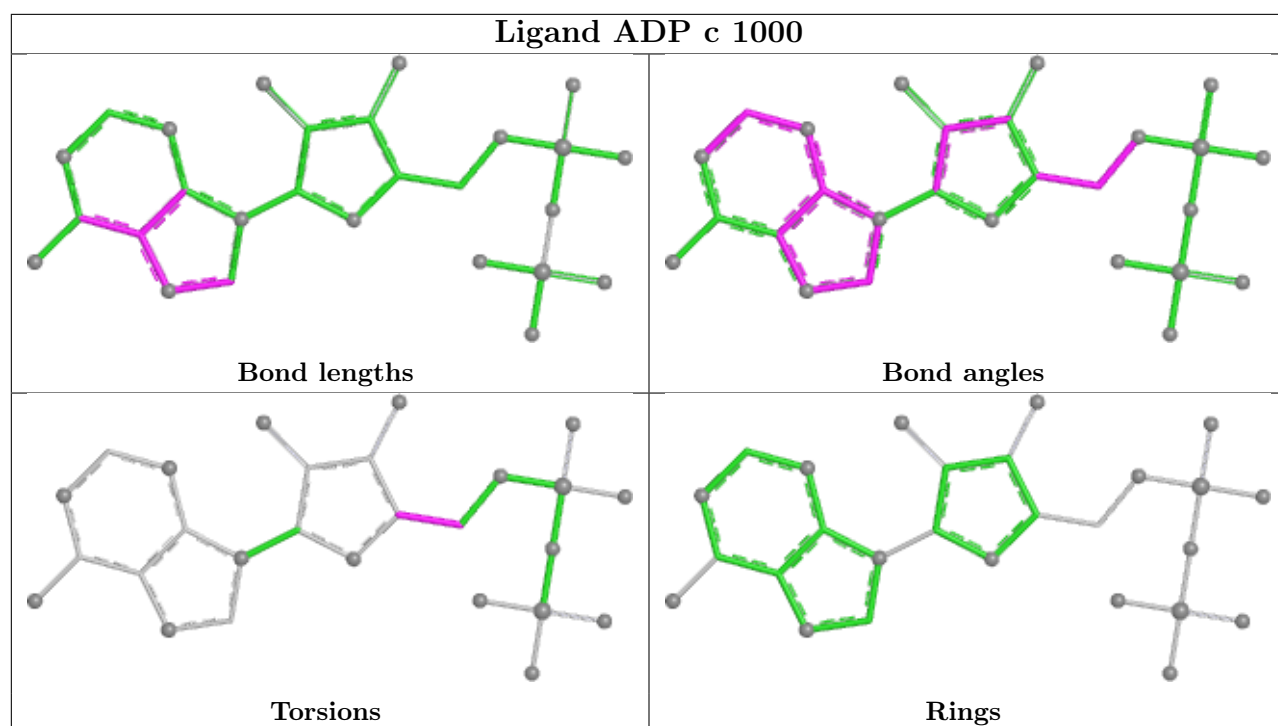
6 monomers are involved in 9 short contacts:

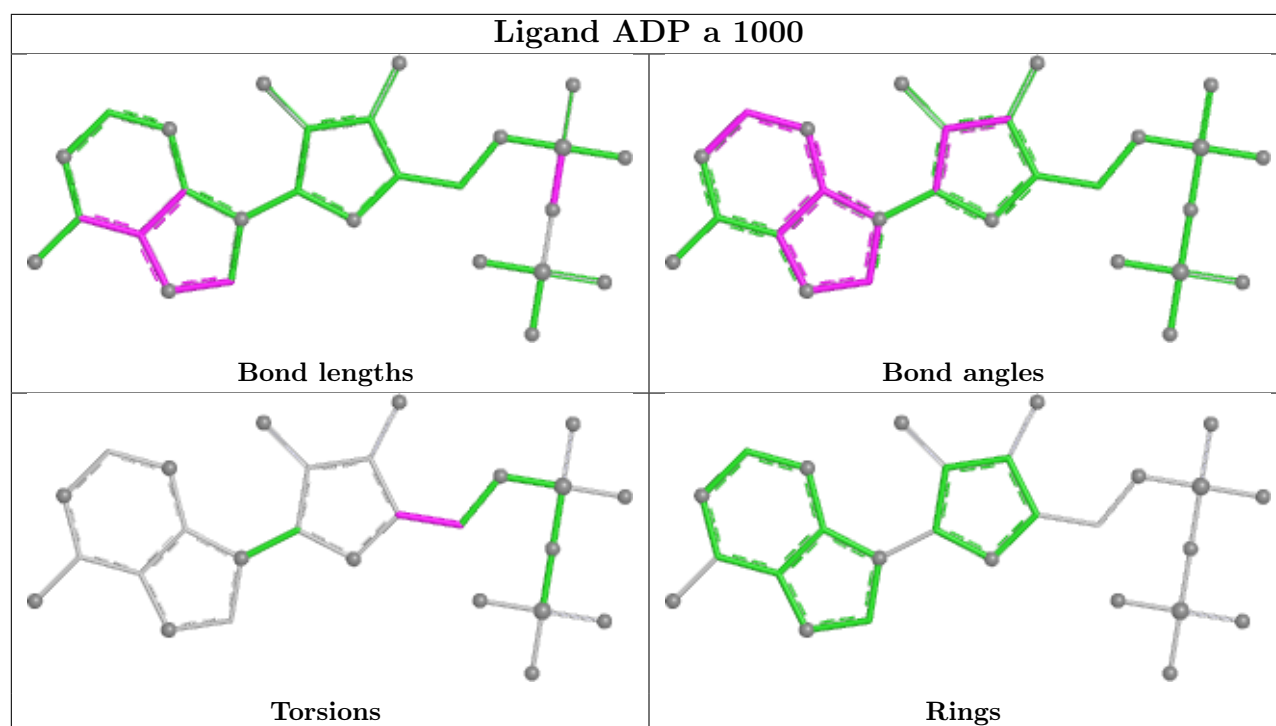
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	b	1000	ADP	1	0
12	e	1002	BEF	1	0
10	e	1000	ADP	4	0
10	c	1000	ADP	1	0
12	a	1002	BEF	1	0
10	a	1000	ADP	2	0

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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
7	L	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	37:DA	O3'	38:DT	P	15.03
1	L	21:DC	O3'	22:DG	P	1.75

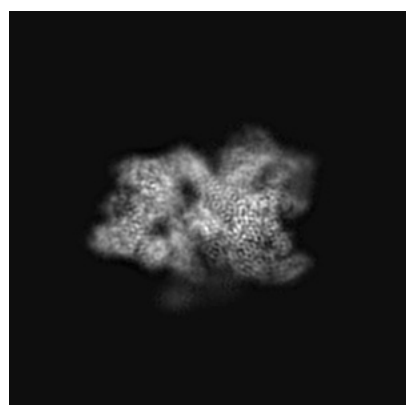
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-11091. These allow visual inspection of the internal detail of the map and identification of artifacts.

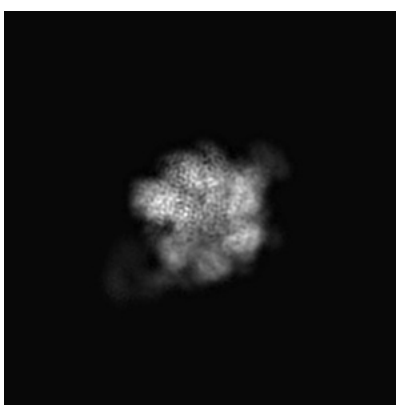
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

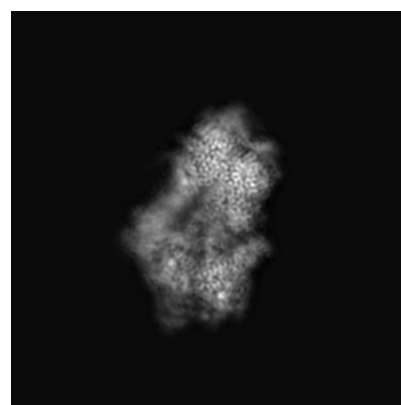
6.1.1 Primary map



X



Y

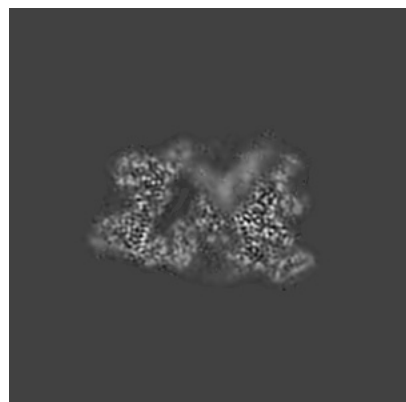


Z

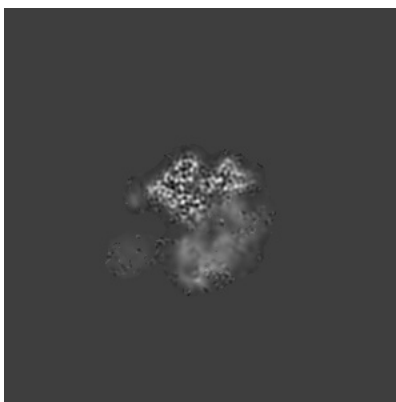
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

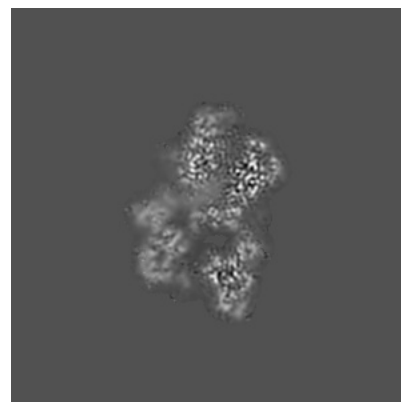
6.2.1 Primary map



X Index: 150



Y Index: 150

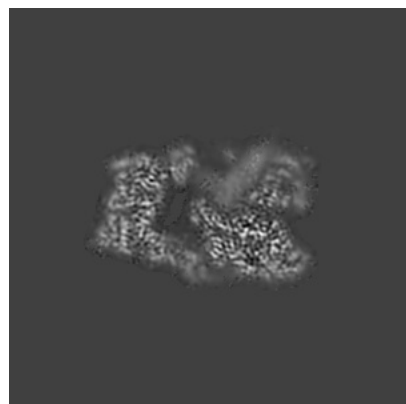


Z Index: 150

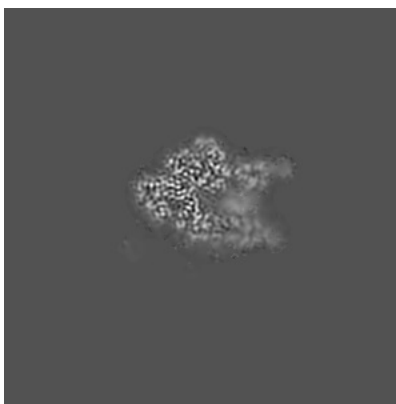
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

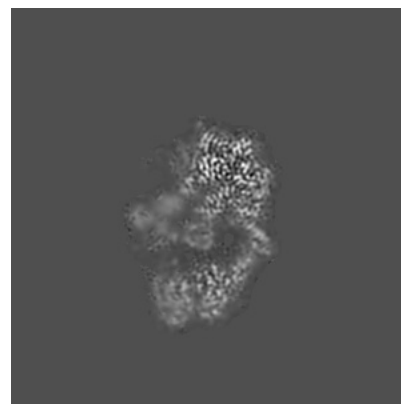
6.3.1 Primary map



X Index: 157



Y Index: 177

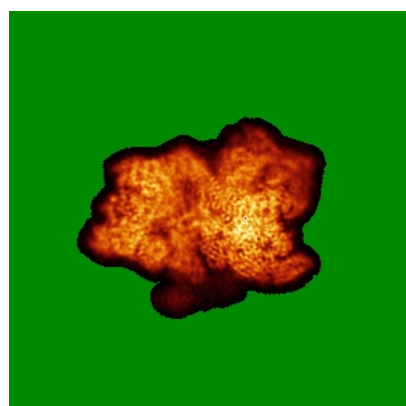


Z Index: 136

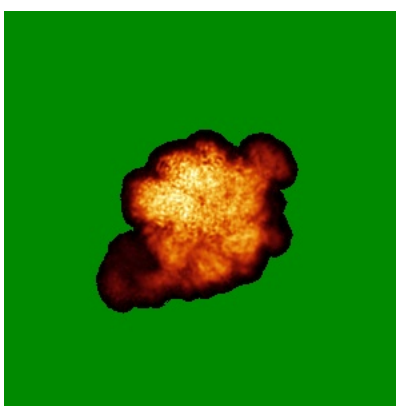
The images above show the largest variance slices of the map in three orthogonal directions.

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

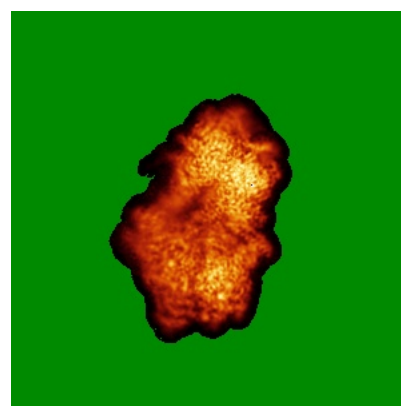
6.4.1 Primary map



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

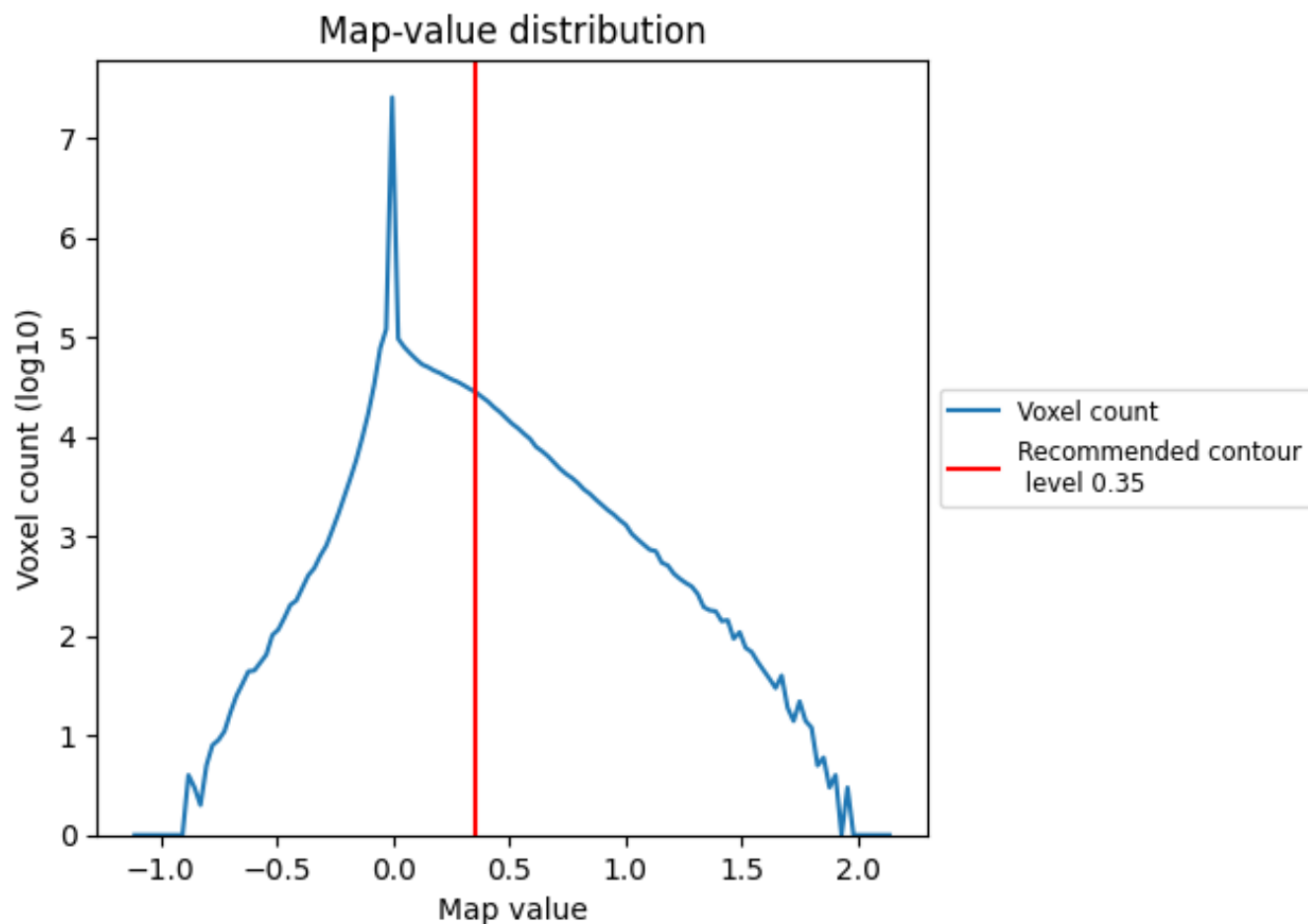
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

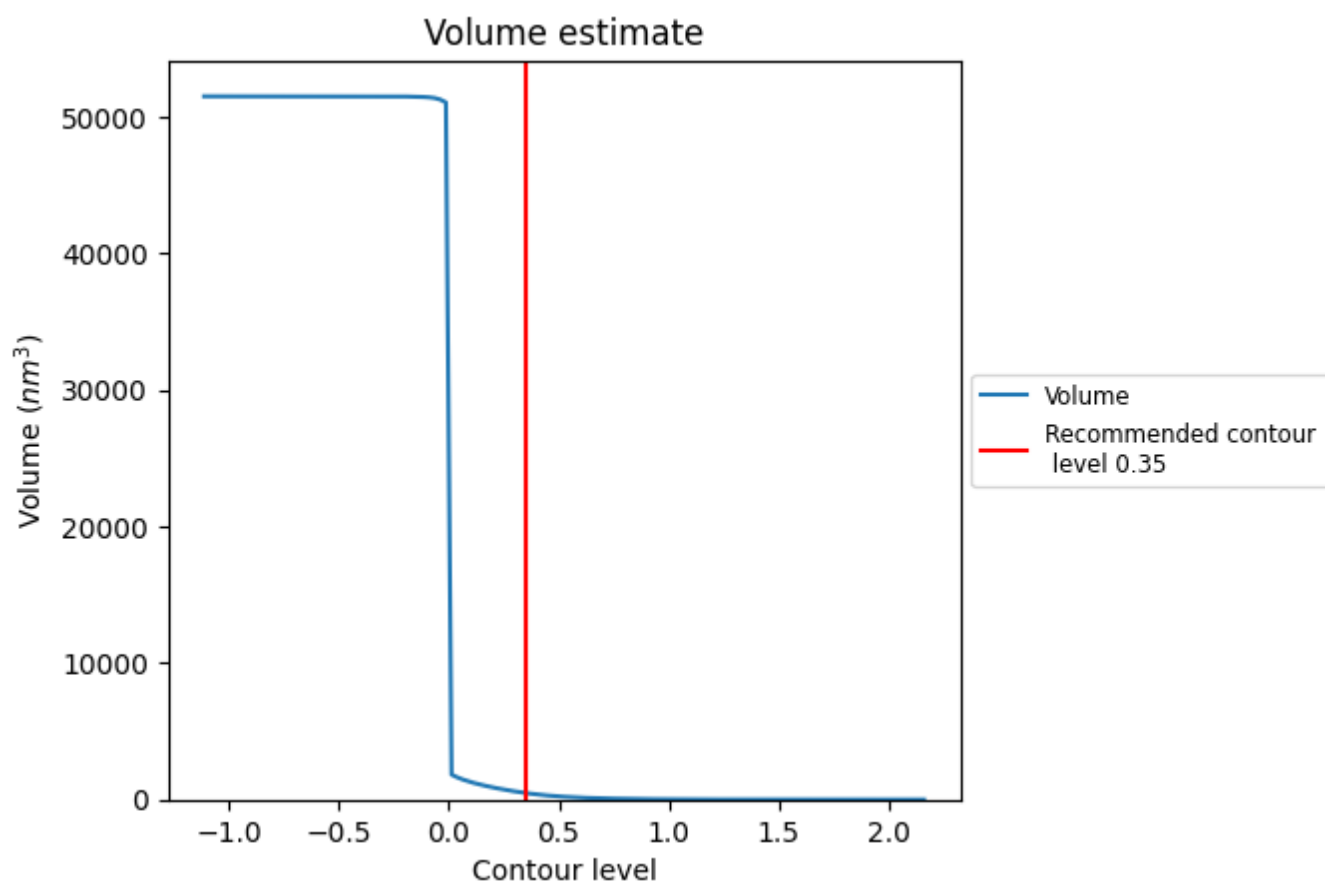
This section contains the results of statistical analysis of the map.

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.

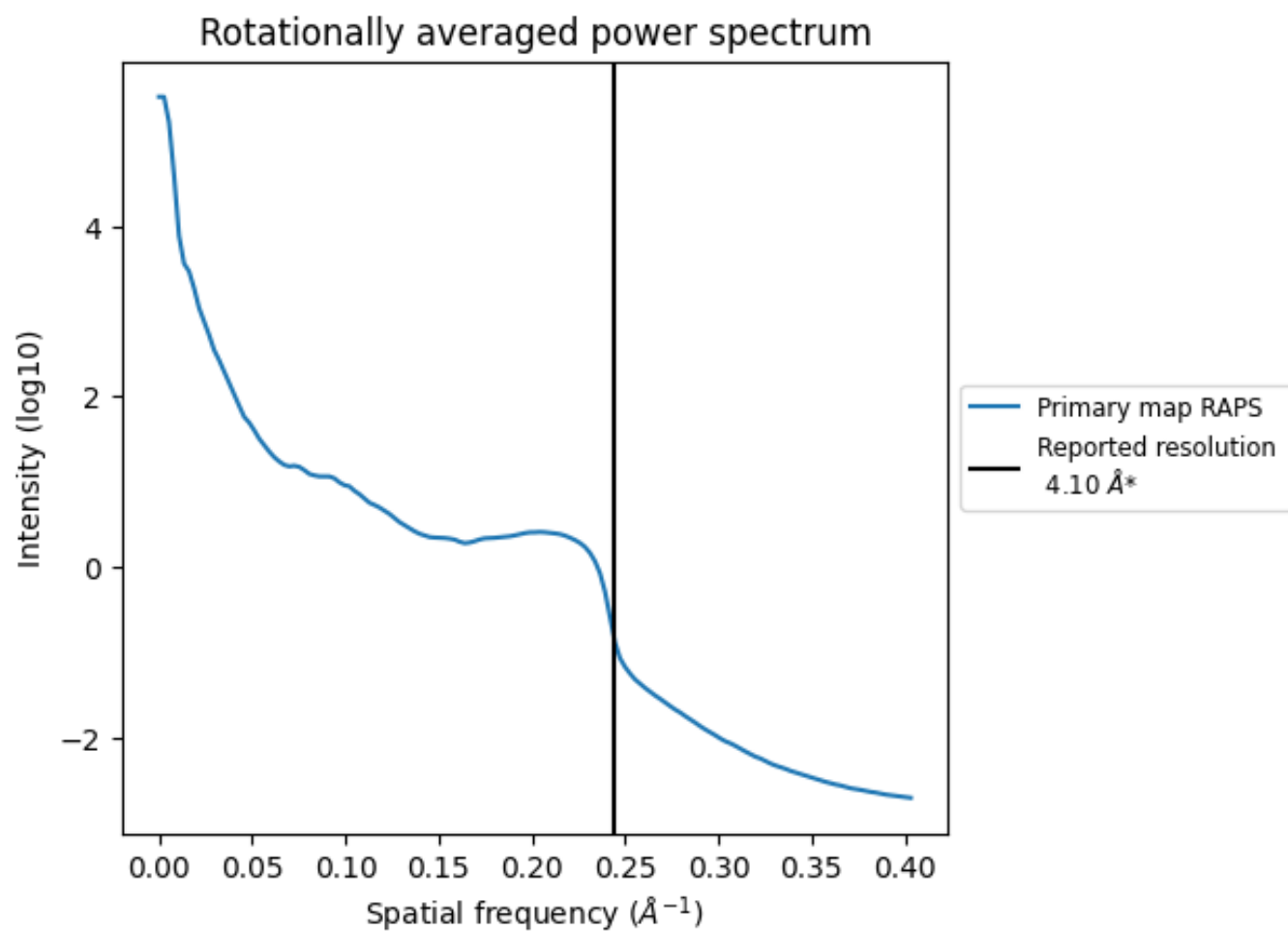
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 477 nm³; this corresponds to an approximate mass of 431 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 ⓘ

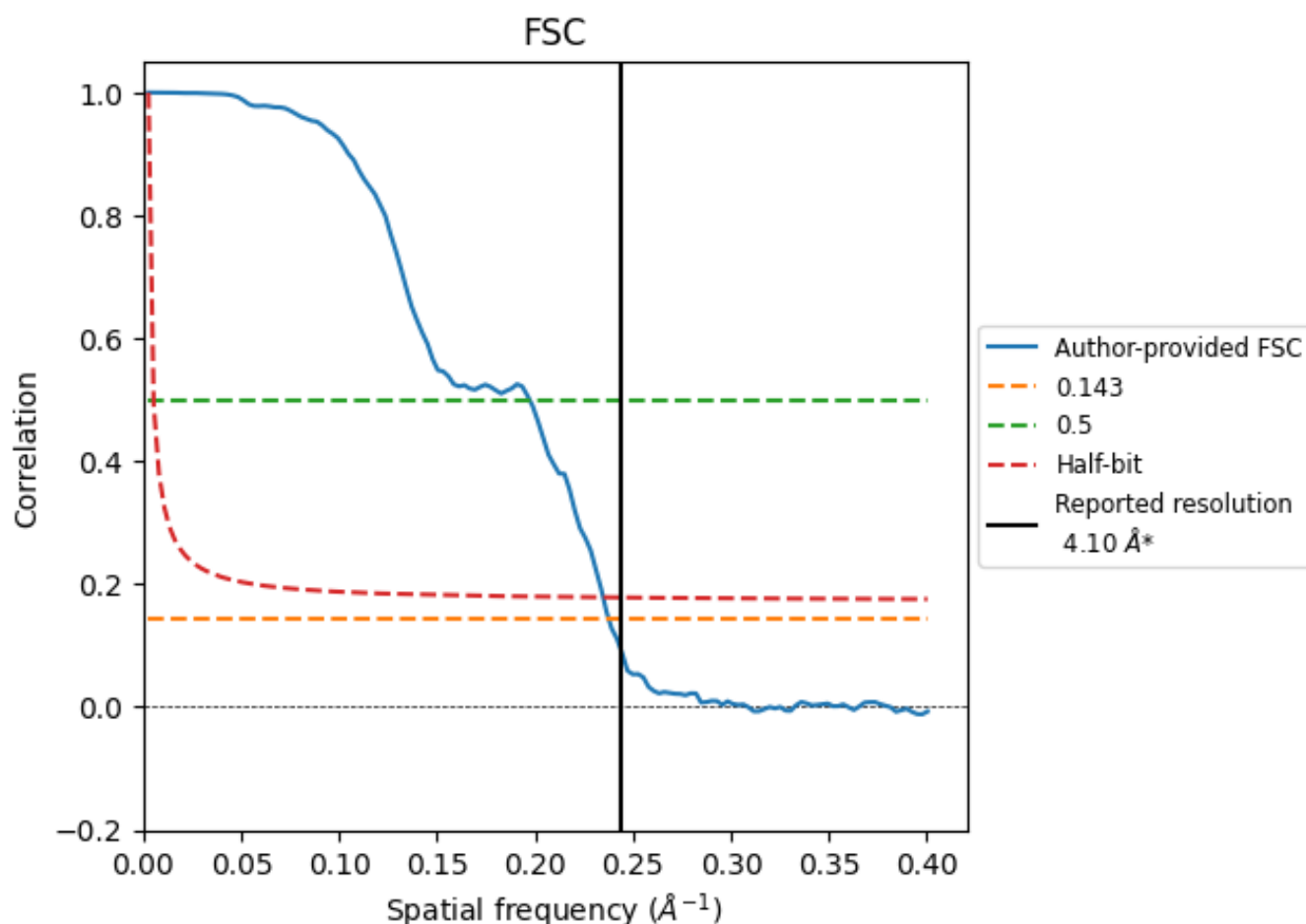


*Reported resolution corresponds to spatial frequency of 0.244 Å⁻¹

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 0.244 Å⁻¹

8.2 Resolution estimates [i](#)

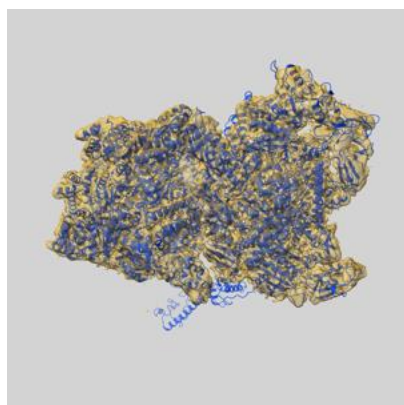
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.10	-	-
Author-provided FSC curve	4.21	5.07	4.26
Unmasked-calculated*	-	-	-

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

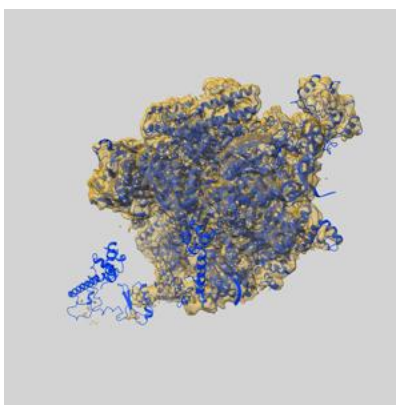
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-11091 and PDB model 6Z9T. Per-residue inclusion information can be found in section [3](#) on page [9](#).

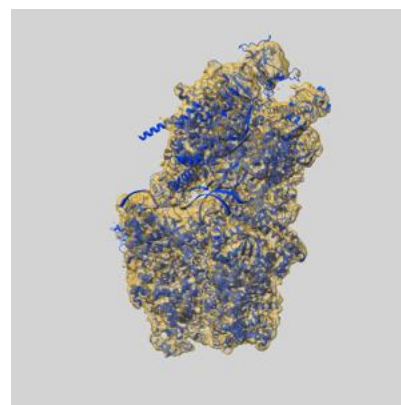
9.1 Map-model overlay [i](#)



X



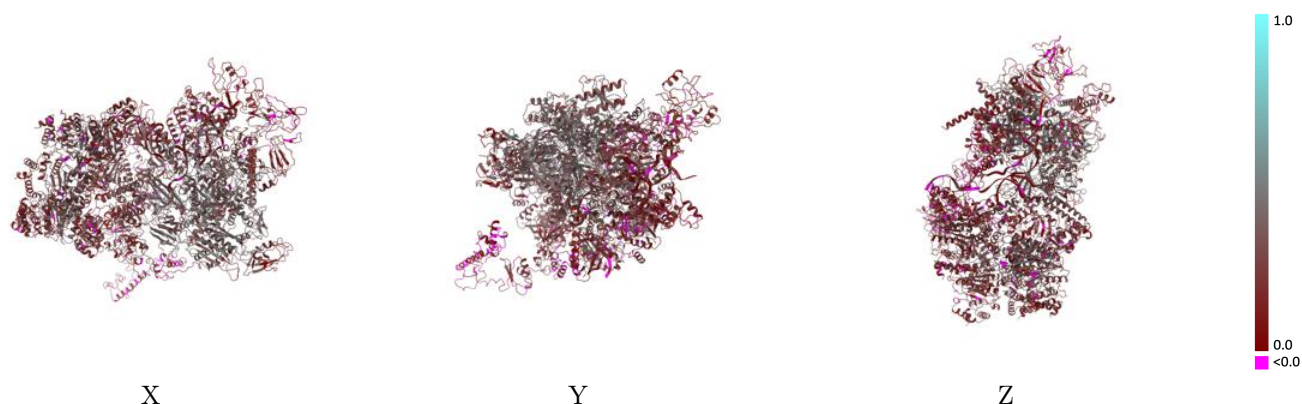
Y



Z

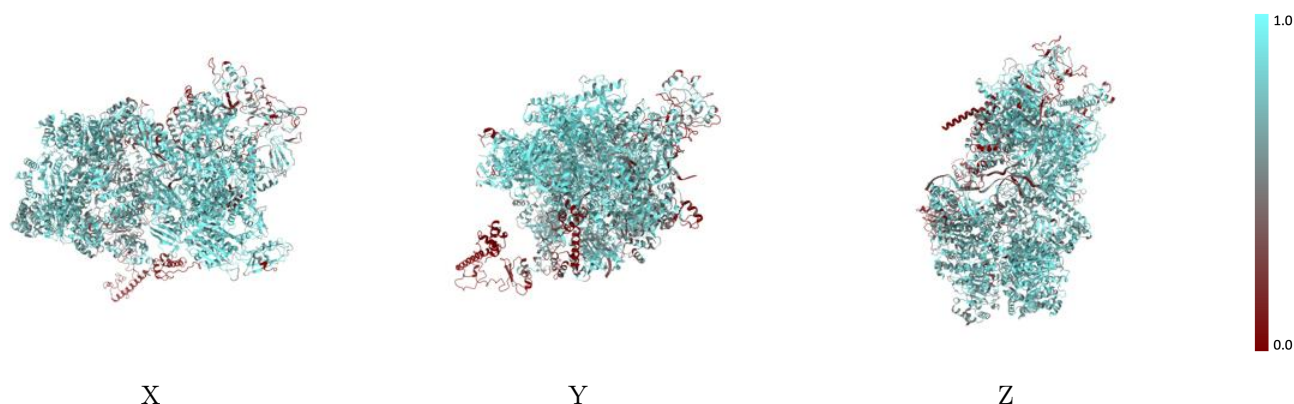
The images above show the 3D surface view of the map at the recommended contour level 0.35 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



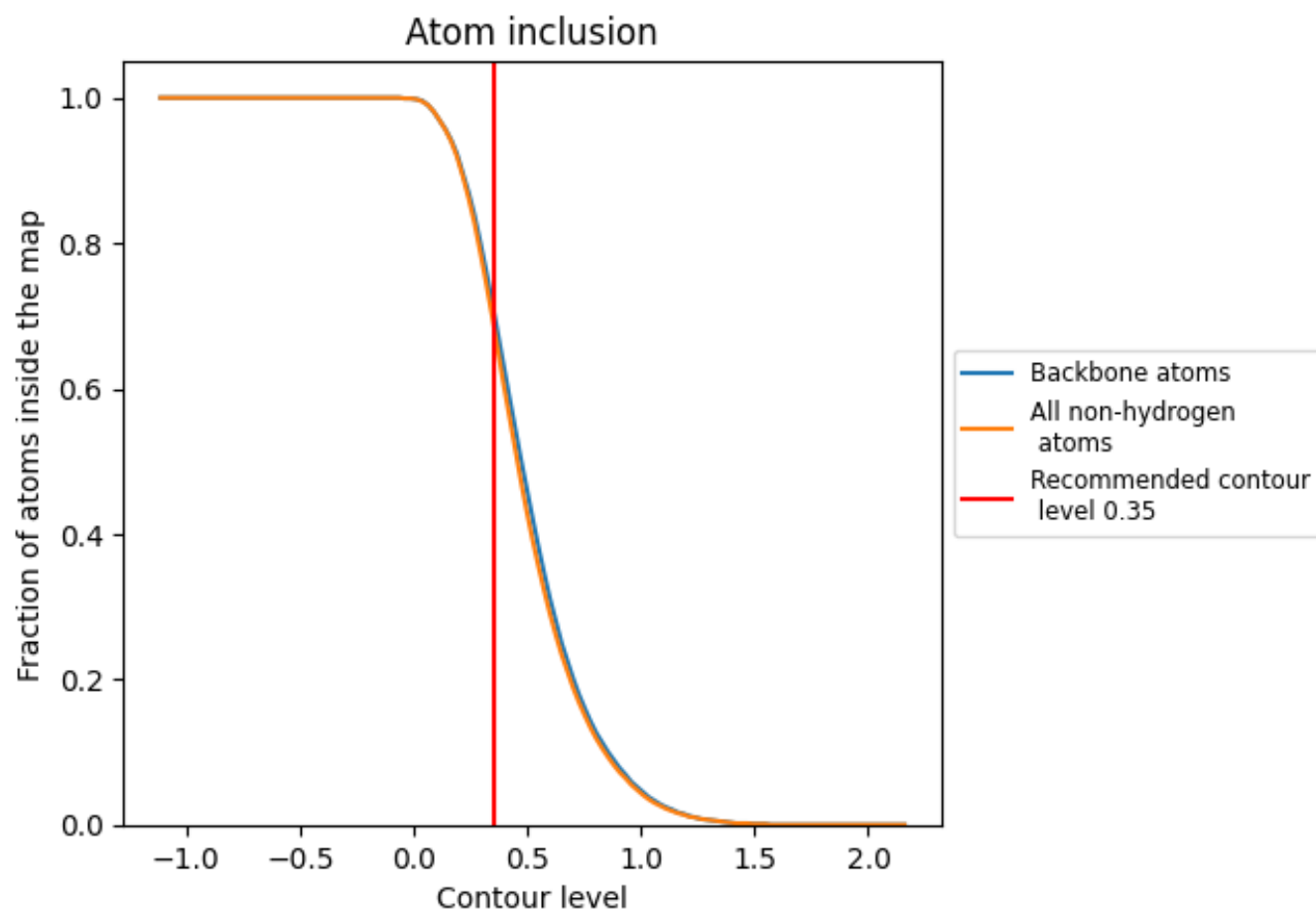
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.35).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 69% 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 (0.35) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6920	 0.2580
A	 0.3530	 0.1520
K	 0.4800	 0.0860
L	 0.6020	 0.1170
R	 0.7200	 0.1680
U	 0.8260	 0.3720
V	 0.7110	 0.2800
W	 0.0750	 0.2110
X	 0.7920	 0.3320
Y	 0.6960	 0.2630
a	 0.7330	 0.2320
b	 0.7620	 0.2670
c	 0.7880	 0.2820
d	 0.7610	 0.2600
e	 0.6690	 0.2000
f	 0.6680	 0.1820

