



wwPDB EM Model Validation Summary Report ⓘ

Mar 15, 2020 – 03:52 PM EDT

PDB ID : 6PSU
EMDB ID : EMD-20464
Title : Escherichia coli RNA polymerase promoter unwinding intermediate (TRPi2)
with TraR and rpsT P2 promoter
Authors : Chen, J.; Chiu, C.E.; Campbell, E.A.; Darst, S.A.
Deposited on : 2019-07-13
Resolution : 3.90 Å(reported)

This is a wwPDB EM Model Validation Summary Report for a publicly released PDB/EMDB 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.0 (224370), CSD as540be (2019)
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.8

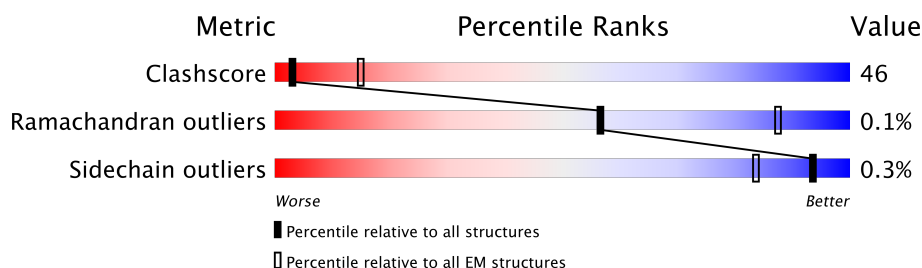
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.90 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	136327	1886
Ramachandran outliers	132723	1663
Sidechain outliers	132532	1531

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 on 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 $\leq 5\%$.

Mol	Chain	Length	Quality of chain
1	N	72	44% 56%
2	G	329	32% 38% 30%
2	H	329	24% 42% 34%
2	M	329	9% 13% 78%
3	I	1342	36% 63% .
4	J	1430	34% 59% 6%
5	K	91	27% 52% 21%
6	L	616	25% 61% 14%
7	O	85	. 46% 51%

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Mol	Chain	Length	Quality of chain
8	P	85	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 32323 atoms, of which 156 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 Protein TraR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	N	72	Total	C	N	O	S	0	0
			571	353	105	108	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	G	230	Total	C	N	O	S	0	0
			1775	1108	314	347	6		
2	H	217	Total	C	N	O	S	0	0
			1668	1043	293	326	6		
2	M	73	Total	C	N	O	S	0	0
			572	362	100	108	2		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	1344	Total	C	N	O	S	0	0
			10433	6556	1856	1971	50		

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	1	VAL	-	expression tag	UNP P0A8T7
J	1408	LEU	-	expression tag	UNP P0A8T7
J	1409	GLU	-	expression tag	UNP P0A8T7
J	1410	LEU	-	expression tag	UNP P0A8T7
J	1411	GLU	-	expression tag	UNP P0A8T7

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Chain	Residue	Modelled	Actual	Comment	Reference
J	1412	VAL	-	expression tag	UNP P0A8T7
J	1413	LEU	-	expression tag	UNP P0A8T7
J	1414	PHE	-	expression tag	UNP P0A8T7
J	1415	GLN	-	expression tag	UNP P0A8T7
J	1416	GLY	-	expression tag	UNP P0A8T7
J	1417	PRO	-	expression tag	UNP P0A8T7
J	1418	SER	-	expression tag	UNP P0A8T7
J	1419	SER	-	expression tag	UNP P0A8T7
J	1420	GLY	-	expression tag	UNP P0A8T7
J	1421	HIS	-	expression tag	UNP P0A8T7
J	1422	HIS	-	expression tag	UNP P0A8T7
J	1423	HIS	-	expression tag	UNP P0A8T7
J	1424	HIS	-	expression tag	UNP P0A8T7
J	1425	HIS	-	expression tag	UNP P0A8T7
J	1426	HIS	-	expression tag	UNP P0A8T7
J	1427	HIS	-	expression tag	UNP P0A8T7
J	1428	HIS	-	expression tag	UNP P0A8T7
J	1429	HIS	-	expression tag	UNP P0A8T7
J	1430	HIS	-	expression tag	UNP P0A8T7

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	K	72	Total	C	N	O	S	0	0
			577	352	110	114	1		

- Molecule 6 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	529	Total	C	N	O	S	0	0
			4277	2677	753	821	26		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	-2	SER	-	expression tag	UNP Q0P6L9
L	-1	GLU	-	expression tag	UNP Q0P6L9
L	0	PHE	-	expression tag	UNP Q0P6L9

- Molecule 7 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	42	Total	C	N	O	P	0	0
			863	411	168	242	42		

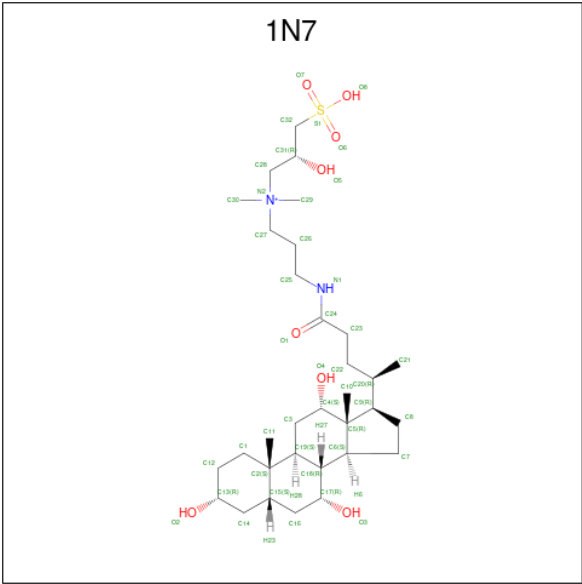
- Molecule 8 is a DNA chain called DNA (85-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	37	Total	C	N	O	P	0	0
			752	363	117	235	37		

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
9	J	2	Total	Zn	0
			2	2	
9	N	1	Total	Zn	0
			1	1	

- Molecule 10 is CHAPSO (three-letter code: 1N7) (formula: C₃₂H₅₉N₂O₈S).



Mol	Chain	Residues	Atoms				AltConf
10	N	1	Total	C	H	O	0
			66	24	39	3	
10	I	1	Total	C	H	O	0
			66	24	39	3	
10	J	1	Total	C	H	O	0
			66	24	39	3	

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Mol	Chain	Residues	Atoms				AltConf
10	L	1	Total	C	H	O	0
			66	24	39	3	

- Molecule 11 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
11	J	1	Total	Mg	0
			1	1	

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA 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. 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. 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.

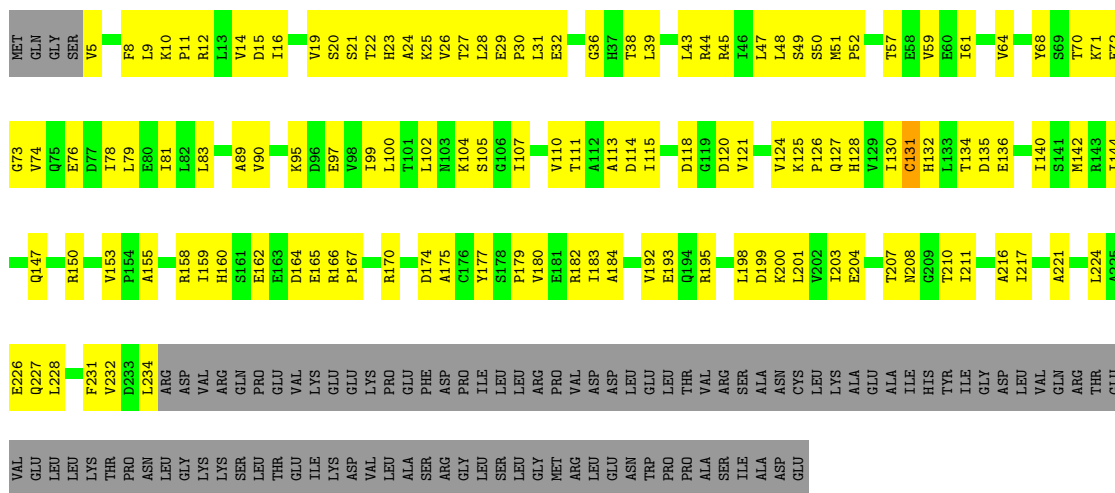
- Molecule 1: Protein TraR

Chain N: 




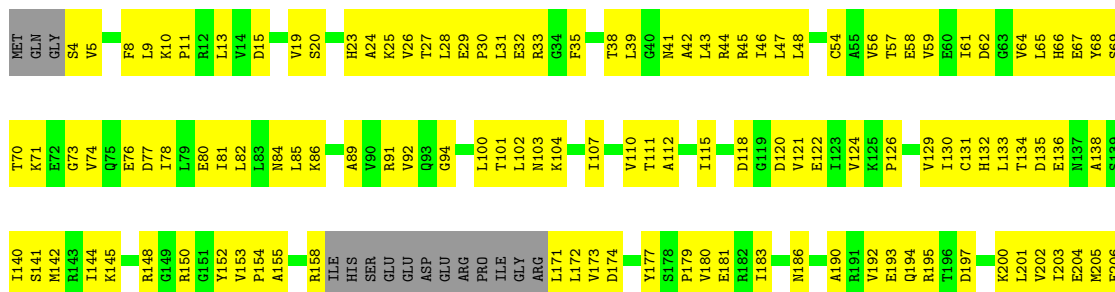
- Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain G: 



- Molecule 2: DNA-directed RNA polymerase subunit alpha

Chain H: 





S1058	V997	E866	L788	V639	V564	S492	R425	G358	P288	D134	C70	VAL
L1059	P998	Q667	N720	V639	A565	N495	A426	P369	D289	I135	L71	LYS
V1060	G1000	W868	I722	G640	K586	N495	P427	Y360	I290	R136	C72	ASP
V1061	G1006	C869	I723	I641	T567	N495	T428	L361	I291	R137	G73	LEU
L1062	A1001	D870	W724	D642	S568	I499	L429	R362	R292	V138	K74	LEU
S1063	V1002	L871	L796	D643	L569	I500	H430	L363	R293	L139	Y75	LEU
S1064	L1003	L872	W725	M644	K570	Y501	R431	H364	N294	Y140	PHE	LEU
A1065	A1004	E873	S726	V645	D571	S502	L432	Q365	E295	F141	L78	LEU
K1066	K1005	R798	S728	I646	T572	S503	F437	C366	K222	K79	K79	LYS
L1067	L1006	S876	R731	P647	V574	V506	P437	G367	L223	H80	H80	ALA
G1071	D1007	W801	G732	P647	V574	V507	P439	L368	E225	I147	V83	GLN
L1072	G1008	D878	S733	I653	G575	L508	V440	P369	E226	E148	R84	THR
D1073	Q1010	A804	A735	E658	R576	G509	L441	K370	F227	K371	C85	LYS
L1074	V1011	Q805	I736	V661	L579	L510	L442	K372	V228	M151	T83	THR
P1075	A1012	W803	I737	V661	W580	Y511	E443	A373	Q229	N153	E86	GLU
P1076	G1013	R883	R738	I664	M581	Y512	E444	L374	K233	L154	K87	F17
A1077	G1014	S884	Q739	I664	T582	M513	L307	E375	P234	C88	C88	D18
L1078	E1015	W885	W740	V583	T514	T514	L376	L376	E235	V90	V90	A19
K1079	T1016	V886	A741	Q667	P584	R515	F377	F377	W236	I159	E91	I20
I1080	V1017	D889	G742	V673	K585	D516	K378	P379	V241	L160	V92	S26
V1081	N1018	T890	G745	V673	G586	C517	H450	V518	T317	T161	T93	S26
D1082	A1019	D891	I746	R678	L587	N519	L452	V518	G318	E163	Q94	M29
N1086	W1020	V894	A747	V679	F588	N519	V453	V244	P243	Q164	T95	I30
D1087	D1021	C895	A748	I680	W589	M525	C454	L245	W244	Y165	R88	W33
V1088	H1022	W825	I749	I680	I591	V526	M458	L385	P246	L166	R99	S34
L1089	T1024	R826	P750	V682	V592	L527	M458	E386	L249	D167	E100	F35
M1095	M1025	W899	D751	I683	V592	P530	A460	L387	R250	E170	M102	G36
P1096	P1026	Q900	G752	D684	A595	E531	F461	R388	L327	E171	G103	E37
A1097	V1027	R901	S753	I686	I601	E532	D462	G389	P251	E172	H104	V38
Q1098	I1028	D902	I754	V686	S602	A533	G463	L390	L252	G173	I105	K39
E1099	T1029	L903	I755	A687	W602	A533	D464	L390	V253	E106	E106	K40
F1100	E1030	A904	E756	A688	M604	L536	Q465	T393	P254	D175	P41	P41
L1101	S1032	R836	T757	A689	L605	L536	M466	I394	R259	F176	E42	E42
A1105	G1033	W839	I758	R692	R606	Y537	A467	G333	F260	D177	T43	T43
I1106	V1035	R842	N762	V693	T607	W538	V468	K334	K334	P110	T111	I44
V1107	R1036	W843	F763	S694	C608	G540	H469	Q335	A261	T111	H112	I44
Q1108	F1037	T844	I764	M697	Y609	L541	V471	G336	T262	A178	A113	M45
L1109	T1038	A845	E765	N697	R610	A542	L472	R338	L265	G181	I114	W115
E1110	D1039	D847	G766	N700	L612	H545	T473	Q340	L267	A182	W115	F116
D1111	M1040	D847	I767	L701	L612	A546	L474	R341	D267	F117	F116	F116
G1112	I1041	I915	W768	E704	K615	R547	E475	L342	L268	L118	K118	P51
V1113	T1042	P851	Q771	T705	P616	V548	A476	L343	Y269	S119	S119	E52
Q1114	G1045	R855	I774	W706	F620	R551	E479	K345	R270	L189	L120	R53
I1115	I1046	D856	S775	I707	A621	T552	A482	R346	R275	D193	P121	D54
S1117	T1047	I856	T776	W708	R622	T553	L483	V347	N276	L194	S122	G55
G1118	R1048	R857	I776	R709	Q623	Y554	E482	D348	E195	E195	R123	L56
Q1049	Q1049	P926	A779	D710	T624	S554	L483	Y349	L279	Q196	I124	C58
T1050	T1050	W858	G711	G711	T624	Y555	M484	S350	K280	E197	G125	A59
D1051	D1051	R859	W780	Q712	M625	E556	M485	G351	R281	C198	L126	R60
E1052	E1052	R860	K781	E713	Y626	K557	S486	R352	L282	E199	L127	I61
L1053	L1053	W861	G782	E714	T627	D558	T487	R353	L283	G200	L128	F62
R1123	E1062	S931	L783	V717	A632	A559	M488	S353	L284	L201	M129	K66
T1124	T1064	T862	L783	W717	A632	A559	M488	V354	D284	L202	M130	D67
Q1125	Q1065	R863	T786	S718	A633	E562	M489	L422	L285	E203	P131	Y68
Q1126	L1056	L864	A787	F719	R634	L563	L491	L423	A286	G204	L132	Y68
GLU	S1057	H865							V357		R133	E69

LEU	GLY	ASN	GLY	LEU	GLY	GLY	SER	ASN	ASN	GLU	LEU	GLU	LEU	GLU	VAL	LEU	PHE	GLN	GLY	PRO	SER	SER	GLY	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS	HIS
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• Molecule 5: DNA-directed RNA polymerase subunit omega

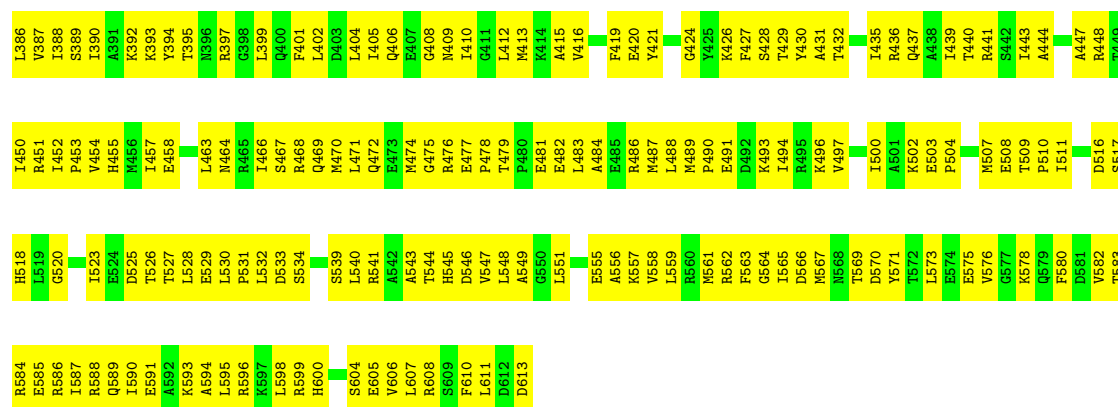
Chain K:  27% 52% 21%

MET	ALA	R3	V4	T5	D8	A9	V10	E11	K12	I13	G14	N15	R16	F17	D18	L19	V20	L21	V22	A23	A24	R25	R26	A27	R28	Q29	M30	D36	P37	L38	V39	P40	N43	D44	K45	V48	I49	R52	E53	I54	E55	E56	G57	L58	I59	N60	Q62	I63	L64	D65	V66	R67	E68																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
E74	GLN	GLU	ALA	ALA	GLU	GLU	LEU	LEU	ALA	VAL	THR	ALA	ILE	ALA	GLU	GLY	ARG	ARG																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																									

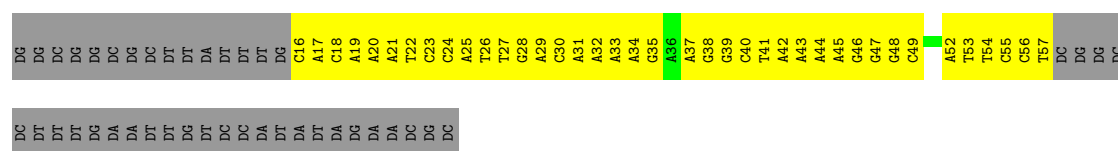
• Molecule 6: RNA polymerase sigma factor RpoD

Chain L:  25% 61% 14%

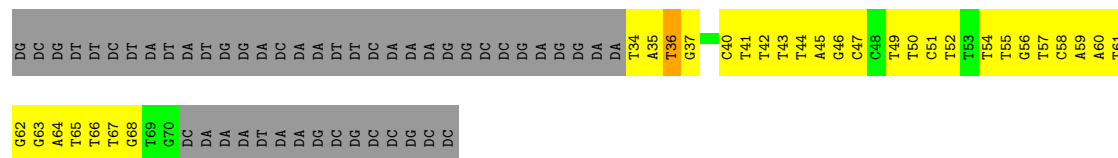
F256	K323	K324	P325	W326	S327	E328	K329	L330	V333	S334	E335	E336	V337	H338	R339	A340	L341	Q342	K343	L344	Q345	Q346	T347	E348	E349	E350	T351	L355	E356	Q357	V358	K359	D360	I361	N362	C363	R364	M365	S366	I367	G368	E369	A370	K371	A372	R373	R374	K375	K376	K377	E378	W379	V380	E381	A382	K383	L384	R385	
ASP	ASP	ASP	ASP	GLU	ASP	GLU	ASP	GLU	ASP	GLY	ASP	ASP	ASP	ASP	SER	ALA	ASP	ASP	ASP	ASN	SER	T212	E215	L216	K217	R218	E219	F220	K221	F222	K223	E224	E225	Y228	T231	T234	T235	K236	ALA	LYS	GLY	ARG	SER	H242	A243	T244	A245	E248	T249	L250	K251	L252	S253	E254	V255				
Q129	V130	C131	C132	S133	V134	A135	E136	Y137	E138	E139	A140	T141	T142	Y143	L144	A145	O146	O147	Y148	D149	R150	V151	A152	E153	E154	E155	A156	R157	L158	S159	D160	L161	P97	V98	R99	M100	Y101	M102	R103	E104	M105	L111	T112	R113	E114	G115	E116	I117	D118	I119	A120	K121	R122	I123	E124	D125	G126	I127	M128
ASP	LEU	MET	LEU	ALA	GLU	ASN	THR	ALA	ASP	GLY	A76	A79	A80	A81	O82	V83	L84	S85	G86	G87	SER	GLU	E152	A153	E154	E155	A156	R157	L158	S159	D160	L161	P97	V98	R99	M100	Y101	M102	R103	E104	M105	L111	T112	R113	E114	G115	E116	I117	D118	I119	A120	K121	R122	I123	E124	D125	G126	I127	M128
GLU	PHE	MET	LEU	ALA	GLU	GLN	ASN	PRO	PRO	PRO	GLN	S7	Q8	L9	K10	L11	L12	V13	T14	R15	G16	K17	E18	L22	T23	E26	V27	N28	D29	H30	L31	PRO	GLU	ASP	ILE	VAL	ASP	SER	D39	Q40	I41	I44	I45	T48	M51	G52	I53	R54	V55	M56	E57	E58	ALA	PRO	ASP	ASP	ALA	M128	



- Molecule 7: DNA (85-MER)



- Molecule 8: DNA (85-MER)



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	46553	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	80	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 1N7, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	N	0.37	0/581	0.50	0/785
2	G	0.40	0/1797	0.53	0/2437
2	H	0.37	0/1687	0.54	0/2287
2	M	0.26	0/579	0.54	0/784
3	I	0.44	0/10736	0.55	1/14487 (0.0%)
4	J	0.41	0/10592	0.54	0/14308
5	K	0.32	0/579	0.49	0/779
6	L	0.29	0/4329	0.47	1/5820 (0.0%)
7	O	0.63	0/971	0.92	0/1495
8	P	0.59	0/837	1.06	1/1290 (0.1%)
All	All	0.41	0/32688	0.57	3/44472 (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
3	I	0	4
4	J	0	1
All	All	0	5

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	1167	GLU	N-CA-C	5.85	126.79	111.00
6	L	149	ASP	CB-CG-OD2	5.24	123.01	118.30
8	P	36	DT	O4'-C4'-C3'	-5.22	102.41	104.50

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	I	1165	SER	Peptide
3	I	1166	ASP	Peptide
3	I	1240	ASP	Peptide
3	I	247	ARG	Peptide
4	J	47	ARG	Peptide

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	N	571	0	556	50	0
2	G	1775	0	1803	131	0
2	H	1668	0	1702	175	0
2	M	572	0	602	61	0
3	I	10567	0	10585	1020	0
4	J	10433	0	10625	1022	0
5	K	577	0	588	53	0
6	L	4277	0	4325	530	0
7	O	863	0	471	74	0
8	P	752	0	426	74	0
9	J	2	0	0	0	0
9	N	1	0	0	0	0
10	I	27	39	39	7	0
10	J	27	39	38	4	0
10	L	27	39	37	3	0
10	N	27	39	38	4	0
11	J	1	0	0	0	0
All	All	32167	156	31835	2955	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 46.

The worst 5 of 2955 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)
10:L:701:1N7:C3	10:L:701:1N7:C19	1.83	1.57
10:I:1401:1N7:C19	10:I:1401:1N7:C3	1.82	1.51
10:N:102:1N7:C19	10:N:102:1N7:C3	1.83	1.51
10:J:1504:1N7:C3	10:J:1504:1N7:C19	1.83	1.50
6:L:284:GLU:HA	6:L:287:ILE:HB	1.36	1.07

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	N	70/72 (97%)	67 (96%)	3 (4%)	0	100	100
2	G	228/329 (69%)	193 (85%)	35 (15%)	0	100	100
2	H	213/329 (65%)	169 (79%)	43 (20%)	1 (0%)	31	71
2	M	71/329 (22%)	68 (96%)	3 (4%)	0	100	100
3	I	1338/1342 (100%)	1156 (86%)	182 (14%)	0	100	100
4	J	1338/1430 (94%)	1187 (89%)	150 (11%)	1 (0%)	53	86
5	K	70/91 (77%)	59 (84%)	11 (16%)	0	100	100
6	L	517/616 (84%)	464 (90%)	53 (10%)	0	100	100
All	All	3845/4538 (85%)	3363 (88%)	480 (12%)	2 (0%)	56	86

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	J	859	PRO
2	H	94	GLY

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	N	61/61 (100%)	61 (100%)	0	100	100
2	G	196/286 (68%)	195 (100%)	1 (0%)	90	95
2	H	185/286 (65%)	185 (100%)	0	100	100
2	M	65/286 (23%)	65 (100%)	0	100	100
3	I	1155/1157 (100%)	1151 (100%)	4 (0%)	93	96
4	J	1122/1189 (94%)	1117 (100%)	5 (0%)	92	96
5	K	63/75 (84%)	63 (100%)	0	100	100
6	L	467/543 (86%)	467 (100%)	0	100	100
All	All	3314/3883 (85%)	3304 (100%)	10 (0%)	93	96

5 of 10 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	I	1216	ARG
4	J	137	ARG
4	J	338	PHE
3	I	699	LEU
4	J	304	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
4	J	294	ASN
4	J	489	ASN
6	L	469	GLN
4	J	365	GLN
4	J	450	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	1N7	I	1401	-	30,30,46	4.77	15 (50%)	47,48,72	2.24	16 (34%)
10	1N7	J	1504	-	30,30,46	4.90	14 (46%)	47,48,72	2.10	14 (29%)
10	1N7	L	701	-	30,30,46	4.97	16 (53%)	47,48,72	2.16	14 (29%)
10	1N7	N	102	-	30,30,46	4.90	14 (46%)	47,48,72	2.24	16 (34%)

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	1N7	I	1401	-	-	0/7/72/92	0/4/4/4
10	1N7	J	1504	-	-	1/7/72/92	0/4/4/4
10	1N7	L	701	-	-	5/7/72/92	0/4/4/4
10	1N7	N	102	-	-	7/7/72/92	0/4/4/4

The worst 5 of 59 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	L	701	1N7	C3-C19	17.96	1.83	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	J	1504	1N7	C3-C19	17.68	1.83	1.53
10	N	102	1N7	C3-C19	17.57	1.83	1.53
10	I	1401	1N7	C3-C19	17.15	1.82	1.53
10	N	102	1N7	C3-C4	11.39	1.73	1.53

The worst 5 of 60 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	N	102	1N7	C7-C6-C18	-7.21	108.23	118.32
10	I	1401	1N7	C7-C6-C18	-6.07	109.83	118.32
10	J	1504	1N7	C7-C6-C18	-5.83	110.17	118.32
10	L	701	1N7	C9-C5-C4	-5.47	112.65	117.68
10	L	701	1N7	C7-C6-C18	-5.33	110.86	118.32

There are no chirality outliers.

5 of 13 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
10	N	102	1N7	C21-C20-C22-C23
10	N	102	1N7	C9-C20-C22-C23
10	L	701	1N7	C22-C20-C9-C5
10	L	701	1N7	C20-C22-C23-C24
10	L	701	1N7	C21-C20-C9-C8

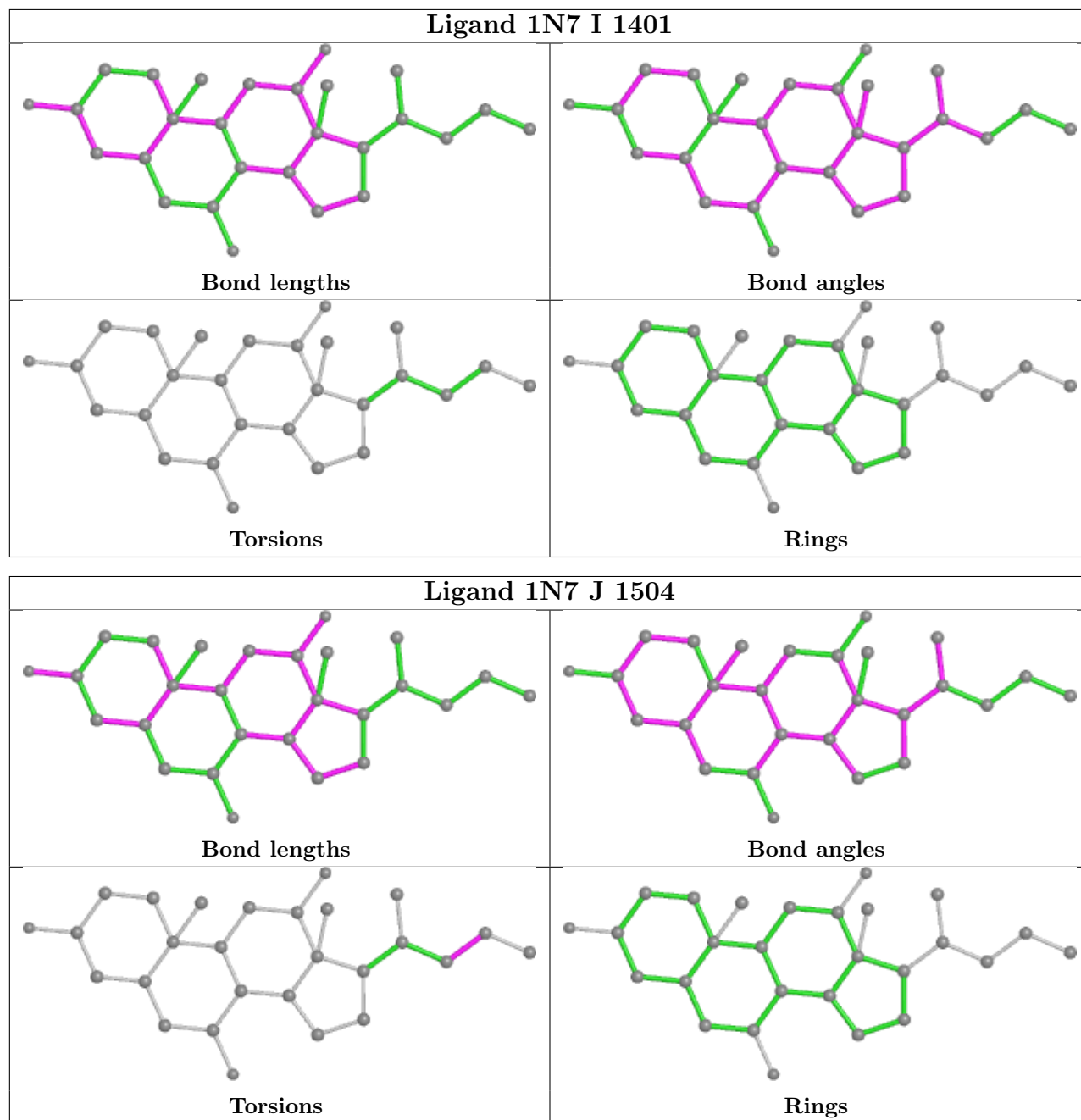
There are no ring outliers.

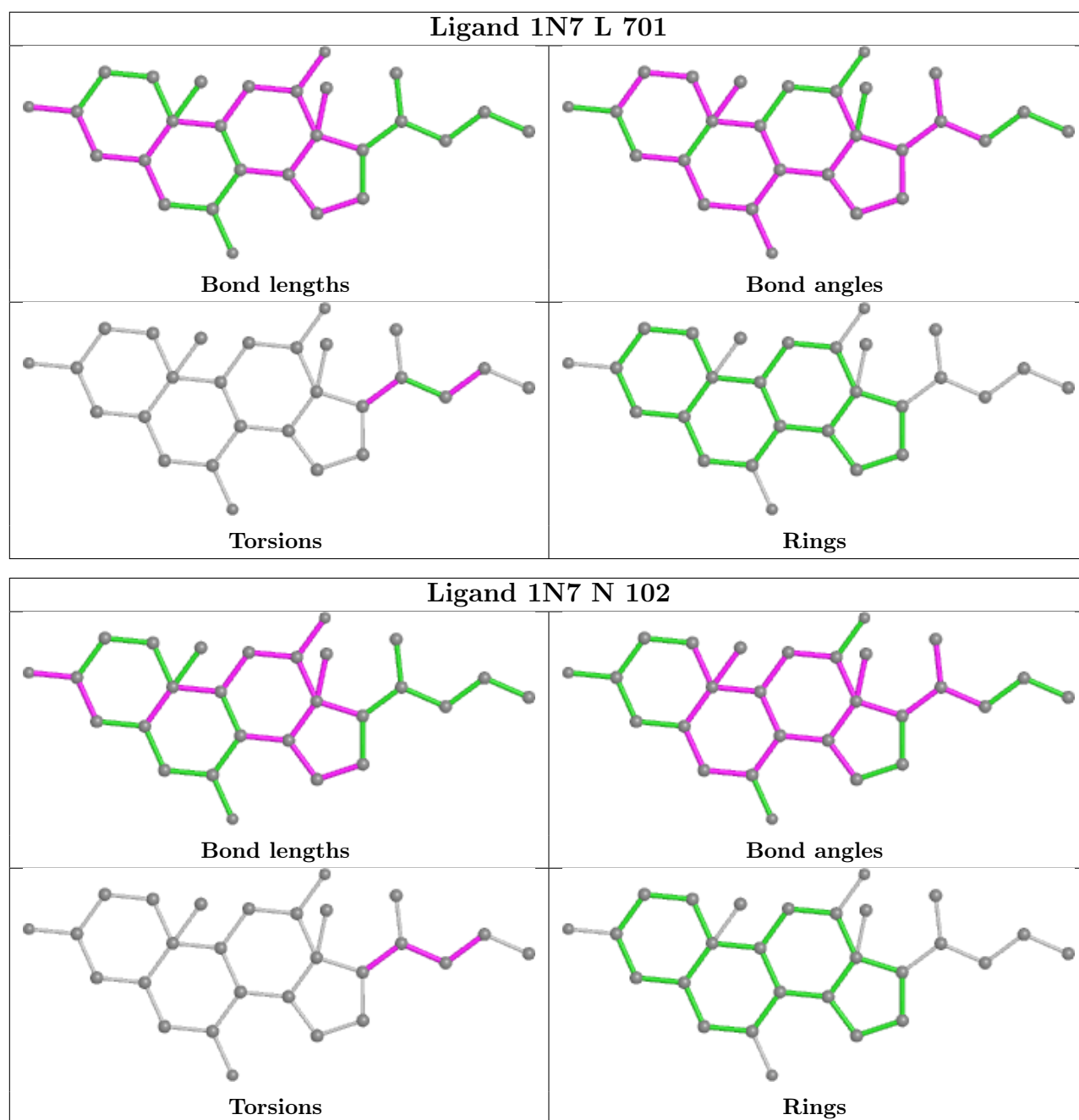
4 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	I	1401	1N7	7	0
10	J	1504	1N7	4	0
10	L	701	1N7	3	0
10	N	102	1N7	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.