



## wwPDB EM Validation Summary Report ⓘ

Nov 7, 2022 – 01:14 AM EST

PDB ID : 6C06  
EMDB ID : EMD-7323  
Title : Mycobacterium tuberculosis RNAP Holo/RbpA/Fidaxomicin  
Authors : Darst, S.A.; Campbell, E.A.; Boyaci Selcuk, H.; Chen, J.; Lilic, M.  
Deposited on : 2017-12-27  
Resolution : 5.15 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](mailto: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.dev43  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : **FAILED**  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2



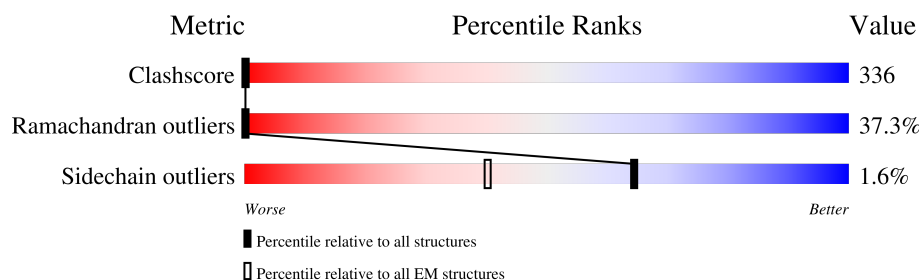
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 5.15 Å.

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



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

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  $\geq 3$ , 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	A	347	37% 28% 35%
1	B	347	48% 19% 32%
2	C	1181	58% 33% 6%
3	D	1324	54% 37% 5%
4	E	110	37% 35% 25%
5	F	531	39% 19% 39%
6	J	111	63% 31%

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 crite-



ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	FI8	D	1404	X	-	-	-



## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 26170 atoms, of which 74 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	226	Total	C	N	O	S	0	0
			1724	1085	297	339	3		
1	B	237	Total	C	N	O	S	0	0
			1775	1120	304	348	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	1111	Total	C	N	O	S	0	0
			8556	5361	1504	1652	39		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1179	LEU	-	expression tag	UNP V9Z879
C	1180	ALA	-	expression tag	UNP V9Z879
C	1181	ARG	-	expression tag	UNP V9Z879
C	1182	HIS	-	expression tag	UNP V9Z879
C	1183	GLY	-	expression tag	UNP V9Z879
C	1184	GLY	-	expression tag	UNP V9Z879
C	1185	SER	-	expression tag	UNP V9Z879
C	1186	GLY	-	expression tag	UNP V9Z879
C	1187	ALA	-	expression tag	UNP V9Z879

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	D	1263	Total	C	N	O	S	0	0
			9857	6175	1791	1850	41		

There are 8 discrepancies between the modelled and reference sequences:



Chain	Residue	Modelled	Actual	Comment	Reference
D	1317	HIS	-	expression tag	UNP A0A045J9E2
D	1318	HIS	-	expression tag	UNP A0A045J9E2
D	1319	HIS	-	expression tag	UNP A0A045J9E2
D	1320	HIS	-	expression tag	UNP A0A045J9E2
D	1321	HIS	-	expression tag	UNP A0A045J9E2
D	1322	HIS	-	expression tag	UNP A0A045J9E2
D	1323	HIS	-	expression tag	UNP A0A045J9E2
D	1324	HIS	-	expression tag	UNP A0A045J9E2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
4	E	83	Total	C	N	O	0	0
			649	414	108	127		

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	1	GLY	-	expression tag	UNP A0A0T9N9K3

- Molecule 5 is a protein called RNA polymerase sigma factor SigA.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	F	326	Total	C	N	O	S	0	0
			2588	1617	467	495	9		

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	-2	GLY	-	expression tag	UNP A0A045HD00
F	-1	PRO	-	expression tag	UNP A0A045HD00
F	0	HIS	-	expression tag	UNP A0A045HD00

- Molecule 6 is a protein called RNA polymerase-binding protein RbpA.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	J	107	Total	C	N	O	S	0	0
			872	539	162	168	3		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

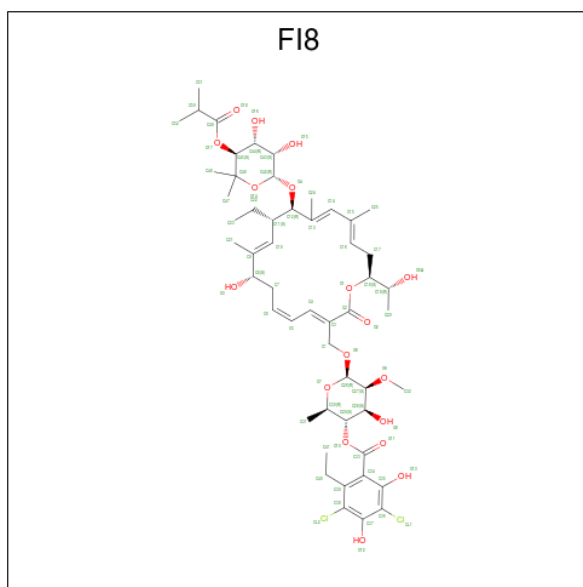


Mol	Chain	Residues	Atoms		AltConf
7	D	2	Total	Zn	0
			2	2	

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
8	D	1	Total	Mg	0
			1	1	

- Molecule 9 is Fidaxomicin (three-letter code: FI8) (formula: C<sub>52</sub>H<sub>74</sub>Cl<sub>2</sub>O<sub>18</sub>).



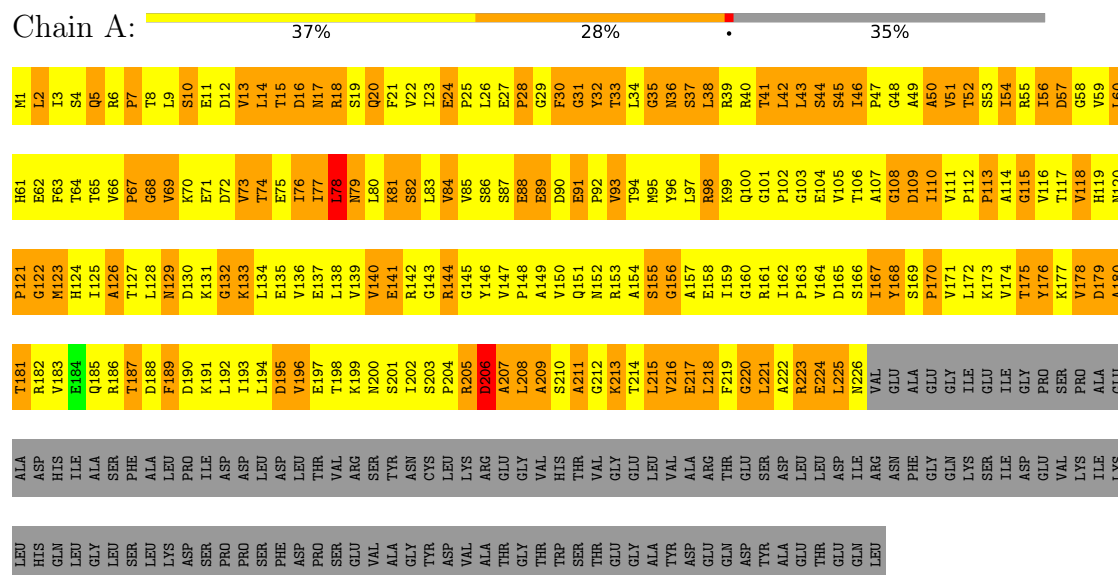
Mol	Chain	Residues	Atoms					AltConf
9	D	1	Total	C	Cl	H	O	0
			146	52	2	74	18	



### 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. 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: DNA-directed RNA polymerase subunit alpha





Chain C: .

58%

33%

6%

Y1027	Q967	L907	V847	R787	E727	R667	M607	P547	E487	L427	T387	D307	Q247	F187	M127	S67	ME1
M1028	P968	A908	R848	G788	G728	R668	G608	I548	T488	K428	D388	L308	I248	D188	T128	P88	ALA
Y1029	N969	D909	G849	I789	H729	T669	A609	D549	P489	E429	B389	A309	V249	E189	A129	R89	ASP
I1030	A970	G910	R850	V790	H730	T670	N610	D550	P490	F430	I370	R310	E250	T190	A130	W70	SER
M1031	I971	T911	R851	H791	E731	H671	N611	D551	G491	F431	D371	V311	P251	I191	A131	R71	ARG
K1032	V972	P912	V852	I792	E732	H672	D612	G552	P492	G432	H372	G312	F252	D192	A132	E72	GLN
L1033	S973	V913	R853	G793	D733	R673	R613	R553	R493	T433	F373	R313	G253	K193	L133	S73	SER
H1034	T974	D914	S854	A794	A734	K674	Q614	V554	S494	S434	G374	Y314	P254	S194	F134	A74	LYS
L1035	P975	I915	R855	E795	I735	F675	A615	V555	G495	Q435	N375	R315	S255	T195	V135	A75	THR
L1036	V976	I916	E856	V796	I736	A676	V616	E556	L496	L436	R376	V316	E256	T136	A136	E76	ALA
V1037	F977	L917	D857	H797	I737	R677	P617	P557	I497	S437	R377	N317	I257	K197	A137	R77	ALA
D1038	D978	N918	E858	G798	S738	S678	L618	R558	G498	L438	R378	K318	M258	T198	E138	G78	SER
D1039	G979	T919	D859	H799	H739	R679	V619	V559	S499	F439	R379	K319	R259	L199	F139	D79	PHE
K1040	A980	H920	E860	D800	R740	H680	R620	L580	M440	M440	T380	L320	S260	H200	I140	V80	SER
I1041	E981	G921	L861	I801	L741	G681	S621	V561	D441	D441	V381	G321	T261	S201	N141	N81	PRO
H1042	E982	V922	P862	L802	V742	T682	E622	R562	Q442	Q442	G382	L322	L262	V202	M142	P82	SER
A1043	A983	P923	A863	H803	E743	C683	A623	R563	Y503	N443	E383	K203	E263	K148	V83	ARG	ARG
R1044	E984	R924	G864	G804	E744	A684	P624	K564	A504	N444	L384	V324	K264	V204	T144	G84	PRO
S1045	L985	N925	V865	H805	D745	N685	L625	A565	R505	P445	I385	G325	D265	I205	G145	G85	GLN
T1046	Q986	H926	R866	V806	V746	Q686	V626	G566	V506	L446	Q386	E326	M266	P206	E146	L86	SER
G1047	G987	N927	E867	T807	L747	C687	G627	E567	N507	S447	N387	P327	T267	S207	I147	E87	SER
P1048	L988	I928	L868	P808	T748	P688	T628	V568	P508	G448	Q388	I328	V268	R208	K148	E88	ASN
Y1049	L989	G929	V869	K809	S749	T689	G629	E569	F509	L449	I389	T329	G269	G209	S149	V89	ASN
S1050	S990	Q930	R870	G810	I750	V690	N630	Y570	T450	T450	R390	S330	T270	A210	Q150	L90	N30
M1051	C991	I931	H871	E811	H751	D691	E631	V571	F511	H451	V391	S331	T271	W211	T151	Y91	N30
I1052	T992	L932	H872	T812	I752	A692	L632	P572	I512	K452	G392	T392	E272	L212	V152	E92	V32
L1053	L993	E933	H873	E813	E753	G693	R633	S573	E513	R453	N393	L333	A273	E213	F153	E92	V32
Q1054	P994	T934	A874	L814	E754	D694	A634	S574	T514	R454	S394	T334	L274	F214	M154	S94	G34
Q1055	N995	H935	Q875	H815	H755	R695	A635	E575	P515	L455	R395	E335	L275	G155	G155	P95	G34
P1056	R996	L936	K876	P816	E756	V696	L636	V576	Y516	S456	N396	E336	D276	D156	G156	P96	P36
L1057	D997	G937	R877	E817	I757	E697	D637	D577	R517	A457	E397	D337	I277	D217	F157	E97	N37
G1058	Q998	K978	K878	E818	D758	A698	A638	Y578	K518	L458	R398	V338	Y278	K218	P158	D98	R38
G1059	D999	C939	L879	R819	A759	G699	G639	M579	V519	G459	V339	R339	R279	R219	M159	F99	V39
K1060	L1000	H940	S880	L820	R760	Q700	D640	D580	P460	P460	V400	A340	K280	D220	M160	S100	S40
A1061	L1001	H941	D881	L821	D761	V701	V641	V581	G461	G461	R401	T341	L281	T221	T161	G101	F41
F1062	D1002	S942	G882	R822	T762	I702	V642	S582	G522	G462	E402	I342	R282	V222	E162	S102	A42
D1003	G943	G943	D883	A823	K763	A703	V643	P583	V523	L463	R403	E343	G283	G223	K163	M103	K43
G1064	A1004	V944	K884	T824	L764	D704	A644	B584	V524	S464	M404	Y344	G284	V224	G164	S104	L44
G1065	D1005	K945	L885	F825	G765	G705	E645	Q585	S525	R465	T405	V345	E285	R225	T165	L105	R45
Q1066	G1006	V946	A886	G826	A766	P706	E646	M586	D526	E466	T406	V346	P286	L226	F166	S106	E46
F1067	K1007	D947	G887	E827	E767	C707	G647	V587	E527	R467	Q407	R347	P287	D227	I167	F107	P47
F1068	A1008	A948	R888	K828	E768	T708	G648	S588	I528	A468	D408	L348	T288	R228	I168	S108	L48
G1069	M1009	A949	H889	A829	I769	D709	V649	V589	V529	G469	V409	R349	K289	K229	M169	D109	E49
E1070	L1010	K950	G890	R830	T770	D710	L650	A590	L470	L470	E410	E350	E290	R230	G170	P110	V50
M1071	F1011	G951	N891	E831	R771	G711	E651	T591	L531	E471	A411	G351	S291	R231	T171	R111	P51
O1072	D1012	V952	K892	V832	D772	E712	E652	A592	T532	V472	I412	G352	A292	Q232	E172	F112	G52
C1073	G1013	P953	G893	R833	I773	M713	V653	M593	A533	R473	T413	T353	Q293	P233	R173	D113	L53
V1074	R1014	D954	H894	D834	P774	A714	S654	D534	D534	D474	P414	T354	T294	V174	V174	D114	L54
A1075	S1015	N955	I895	T835	N775	L715	A655	P595	V475	V475	Q415	M355	L295	T235	V175	V115	D55
M1076	G1016	A956	G896	S836	I776	G716	D656	F596	H476	H476	T416	T356	L296	V236	V176	K116	V56
Q1077	E1017	A957	K897	L837	S777	H717	V657	L597	D537	P477	L417	V357	E297	L237	S177	A117	Q57
A1078	P1018	R958	L898	K838	D778	M718	L658	E598	R538	S478	I418	P358	N298	L238	Q178	P118	T58
Y1079	F1019	L959	L899	H839	E779	L719	T659	H599	H479	H479	N419	G359	L299	K239	L179	V119	D59
G1080	P1020	P960	P900	P840	V780	L720	V660	D600	V540	V480	I420	G360	F300	A240	V180	D120	S80
A1081	Y1021	D961	E901	H841	A781	V721	H661	D601	V541	G481	R421	V361	F301	L241	R181	E121	F61
L1082	P1022	E962	E902	G842	A782	H662	H662	A602	A542	H482	P422	E362	K302	G242	S182	C122	E62
Y1083	V1023	L963	D903	E843	D783	I723	D683	M603	Q543	M483	V423	V363	E303	W243	P183	K123	W63
L1084	T1024	R964	R904	S844	L784	M724	N664	A544	C484	C484	V424	P364	R304	T244	G184	D124	L64
L1085	E965	P905	G845	D785	E785	P725	G665	A605	N545	P485	V425	V365	R305	S245	G185	K125	I65
Q1086	G1026	A966	F906	K846	E786	M726	T666	L606	S546	I486	A426	E366	Y306	E246	Y186	D126	G66



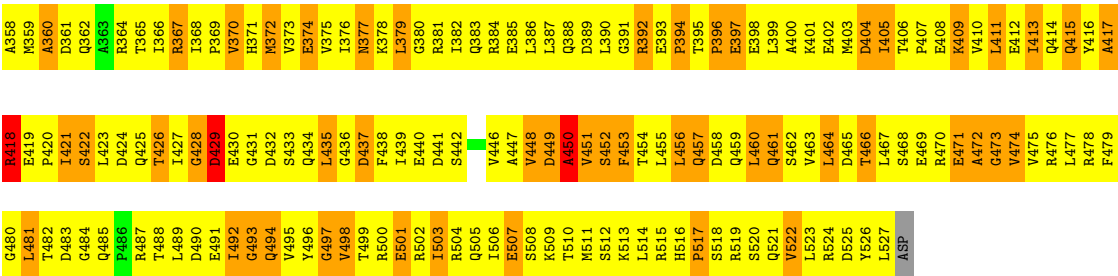
- Molecule 3: DNA-directed RNA polymerase subunit beta'

G843	D783	W723	M683	S603	V543	V483	D423	P363	F302	R242	L181	A121	V61	ME1
	E784	T724	E684	G604	H544	W484	Y424	E364	Q303	E243	L182	P122	C62	LEU
	L845	T725	E685	D605	L545	D485	S425	E365	Q304	L244	E183	K123	C63	ASP
	V846	G726	T686	H606	P546	V486	C426	I366	N307	V245	L184	D124	G64	N4
	L847	S727	T687	P607	L547	L487	R427	V367	N308	D246	E185	L125	V65	V5
	E848	G728	L688	E608	S548	E488	S428	N368	S308	R247	F66	E126	K66	F6
	L849	W729	G689	T609	A549	E489	Y429	N369	P309	Y248	G188	K127	R67	F7
	R789	T730	R679	G610	E550	V490	E490	V429	E370	G249	L128	P128	V68	D8
	E790	V731	E671	V511	A551	L491	A511	Y431	K371	E250	K190	L129	R69	E9
	L851	W732	M672	G612	Q552	A492	V432	V432	R372	N312	E251	L130	F70	L10
G855	H793	G732	M673	S613	A553	E493	C433	K373	V313	F252	D192	F131	K71	R11
	L794	G733	M674	S614	E554	H494	C434	K374	V314	T253	A193	A132	G72	R12
	E795	D735	E675	P615	A555	P495	Q435	Q375	D315	G254	R194	A133	I73	G13
	D796	V736	L676	A516	R556	V496	L436	E376	A316	A255	R195	I134	I74	L14
	R797	L737	L677	E617	L557	L497	R437	S377	V317	K256	K196	V135	C75	A15
	P798	L738	L678	A618	L558	L498	L438	V378	P318	G257	V197	I136	E76	T16
	G799	W739	L679	M559	P559	A499	H439	V379	V319	A258	R198	T137	R77	L17
	L800	P740	G680	M620	L560	E500	Q440	A380	I320	E259	D199	S138	C78	E18
	T801	R741	E681	A621	S561	A501	C441	L381	P321	S260	G200	V139	G79	D19
	D802	G742	P682	A622	S562	P502	C442	F382	P322	I261	G201	D140	V80	I20
G865	H803	T743	E683	D623	N563	T503	L443	K383	E323	Q262	E202	E141	E81	R21
	L804	E744	F684	R624	N564	L504	P444	K384	L324	K263	R203	E142	H82	Q22
	S805	L745	M685	G625	L565	H505	K445	G385	K325	L264	E204	M143	T83	W23
	R806	L746	K686	V626	L566	R506	L446	K386	P326	I265	W205	R144	R84	S24
	A807	D747	Q687	L627	S567	L507	M447	R387	K327	E266	R206	H145	A85	Y25
	E808	H748	P688	S628	P568	G508	A448	G388	V328	I267	Q207	V146	K86	G26
	G809	V749	H689	V629	A569	T509	L449	R389	Q329	F268	I208	E147	V87	E27
	N810	E750	K690	S570	E510	Q510	E450	P390	I330	D269	R209	L348	A88	K28
	F811	E751	K691	A631	G571	A511	L451	V391	D331	I270	R210	S149	R89	K29
	T812	R752	V692	K632	R572	F512	F462	T392	G332	D271	R211	T150	E90	K30
G871	K813	A753	Q693	L633	P573	E513	K453	G393	G333	A272	A212	E151	A91	P31
	L814	D754	E694	K634	L574	P514	P454	P394	R334	E273	Q213	L152	N92	E32
	R815	K755	A695	V635	A575	M515	F455	G395	F335	A274	R214	A153	G93	T33
	T816	V756	L696	R636	M576	L516	V456	G396	A336	E275	E215	E154	H94	I34
	L817	E757	L697	L637	P577	V517	M457	R397	T337	S276	L216	M155	I95	N35
	H818	K758	M698	T638										

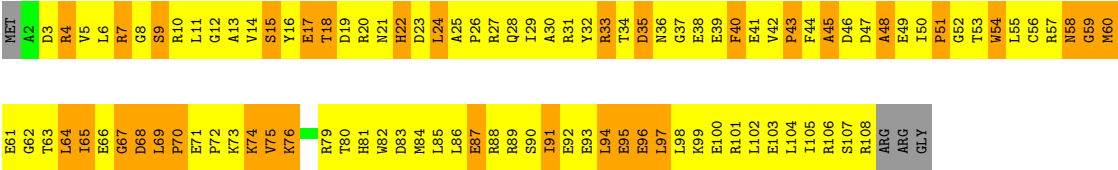
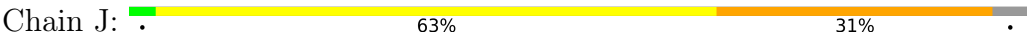








● Molecule 6: RNA polymerase-binding protein RbpA





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171547	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	6.7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	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: FI8, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.51	0/1750	0.70	1/2380 (0.0%)
1	B	0.49	0/1802	0.69	0/2454
2	C	0.56	1/8714 (0.0%)	0.73	12/11824 (0.1%)
3	D	0.55	0/10021	0.73	11/13549 (0.1%)
4	E	0.53	0/662	0.71	0/901
5	F	0.46	0/2622	0.62	1/3538 (0.0%)
6	J	0.48	0/888	0.63	0/1199
All	All	0.54	1/26459 (0.0%)	0.71	25/35845 (0.1%)

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
1	A	0	3
1	B	0	2
2	C	0	32
3	D	0	36
4	E	0	4
5	F	0	5
6	J	0	1
All	All	0	83

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	723	ILE	C-N	-5.45	1.21	1.34

The worst 5 of 25 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	723	ILE	C-N-CA	-11.72	92.40	121.70
3	D	114	LEU	CA-CB-CG	-7.88	97.17	115.30
2	C	237	LEU	CA-CB-CG	-7.35	98.40	115.30
3	D	374	LEU	CA-CB-CG	-7.30	98.52	115.30
1	A	78	LEU	CA-CB-CG	-7.17	98.81	115.30

There are no chirality outliers.

5 of 83 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	220	GLY	Peptide
1	A	42	LEU	Peptide
1	A	69	VAL	Peptide
1	B	204	PRO	Peptide
1	B	214	THR	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	A	1724	0	1768	1333	0
1	B	1775	0	1809	1380	0
2	C	8556	0	8459	5988	0
3	D	9857	0	9923	7031	0
4	E	649	0	645	424	0
5	F	2588	0	2602	1573	0
6	J	872	0	852	560	0
7	D	2	0	0	0	0
8	D	1	0	0	0	0
9	D	72	74	0	16	0
All	All	26096	74	26058	17506	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 336.

The worst 5 of 17506 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)
5:F:279:ARG:O	5:F:283:TRP:HB3	1.25	1.34
1:B:39:ARG:O	1:B:43:LEU:HB3	1.26	1.33
2:C:1099:ARG:O	2:C:1103:TYR:HB2	1.25	1.32
3:D:162:VAL:O	3:D:166:ARG:HB2	1.28	1.31
2:C:424:VAL:O	2:C:428:LYS:HB3	1.30	1.27

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	224/347 (65%)	80 (36%)	52 (23%)	92 (41%)	0	0
1	B	235/347 (68%)	98 (42%)	68 (29%)	69 (29%)	0	0
2	C	1109/1181 (94%)	394 (36%)	323 (29%)	392 (35%)	0	0
3	D	1257/1324 (95%)	396 (32%)	355 (28%)	506 (40%)	0	0
4	E	81/110 (74%)	14 (17%)	25 (31%)	42 (52%)	0	0
5	F	324/531 (61%)	109 (34%)	104 (32%)	111 (34%)	0	0
6	J	105/111 (95%)	45 (43%)	29 (28%)	31 (30%)	0	0
All	All	3335/3951 (84%)	1136 (34%)	956 (29%)	1243 (37%)	0	0

5 of 1243 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	5	GLN
1	A	16	ASP
1	A	17	ASN
1	A	20	GLN



### 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	195/297 (66%)	190 (97%)	5 (3%)	46	66
1	B	197/297 (66%)	195 (99%)	2 (1%)	76	86
2	C	924/997 (93%)	910 (98%)	14 (2%)	65	80
3	D	1041/1103 (94%)	1026 (99%)	15 (1%)	67	80
4	E	69/89 (78%)	67 (97%)	2 (3%)	42	64
5	F	272/429 (63%)	269 (99%)	3 (1%)	73	84
6	J	93/97 (96%)	90 (97%)	3 (3%)	39	61
All	All	2791/3309 (84%)	2747 (98%)	44 (2%)	64	79

5 of 44 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	500	ARG
3	D	1268	ARG
3	D	733	MET
3	D	1085	ARG
4	E	65	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 64 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	234	GLN
5	F	325	ASN
2	C	751	HIS
2	C	729	HIS
5	F	353	GLN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 3 are monoatomic - leaving 1 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	$\# Z  > 2$
9	FI8	D	1404	-	74,75,75	1.90	19 (25%)	88,109,109	2.08	24 (27%)

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
9	FI8	D	1404	-	2/2/29/29	34/75/118/118	0/3/4/4

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	1404	FI8	C1-C3	5.59	1.57	1.50
9	D	1404	FI8	C14-C15	4.48	1.54	1.45
9	D	1404	FI8	O1-C18	-3.96	1.39	1.46
9	D	1404	FI8	C14-C13	3.88	1.39	1.33
9	D	1404	FI8	O17-C49	3.83	1.43	1.34

The worst 5 of 24 bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	1404	FI8	C5-C4-C3	-7.51	117.97	127.00
9	D	1404	FI8	C29-O10-C33	-5.38	108.61	117.21
9	D	1404	FI8	C26-C27-C28	4.91	118.83	110.38
9	D	1404	FI8	C7-C6-C5	-4.62	119.45	125.41
9	D	1404	FI8	C31-C30-C29	-4.58	106.42	113.41

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	D	1404	FI8	C19
9	D	1404	FI8	C27

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	D	1404	FI8	C9-C10-C11-C12
9	D	1404	FI8	C9-C10-C11-C22
9	D	1404	FI8	C15-C16-C17-C18
9	D	1404	FI8	C16-C17-C18-C19
9	D	1404	FI8	C17-C18-C19-O5A

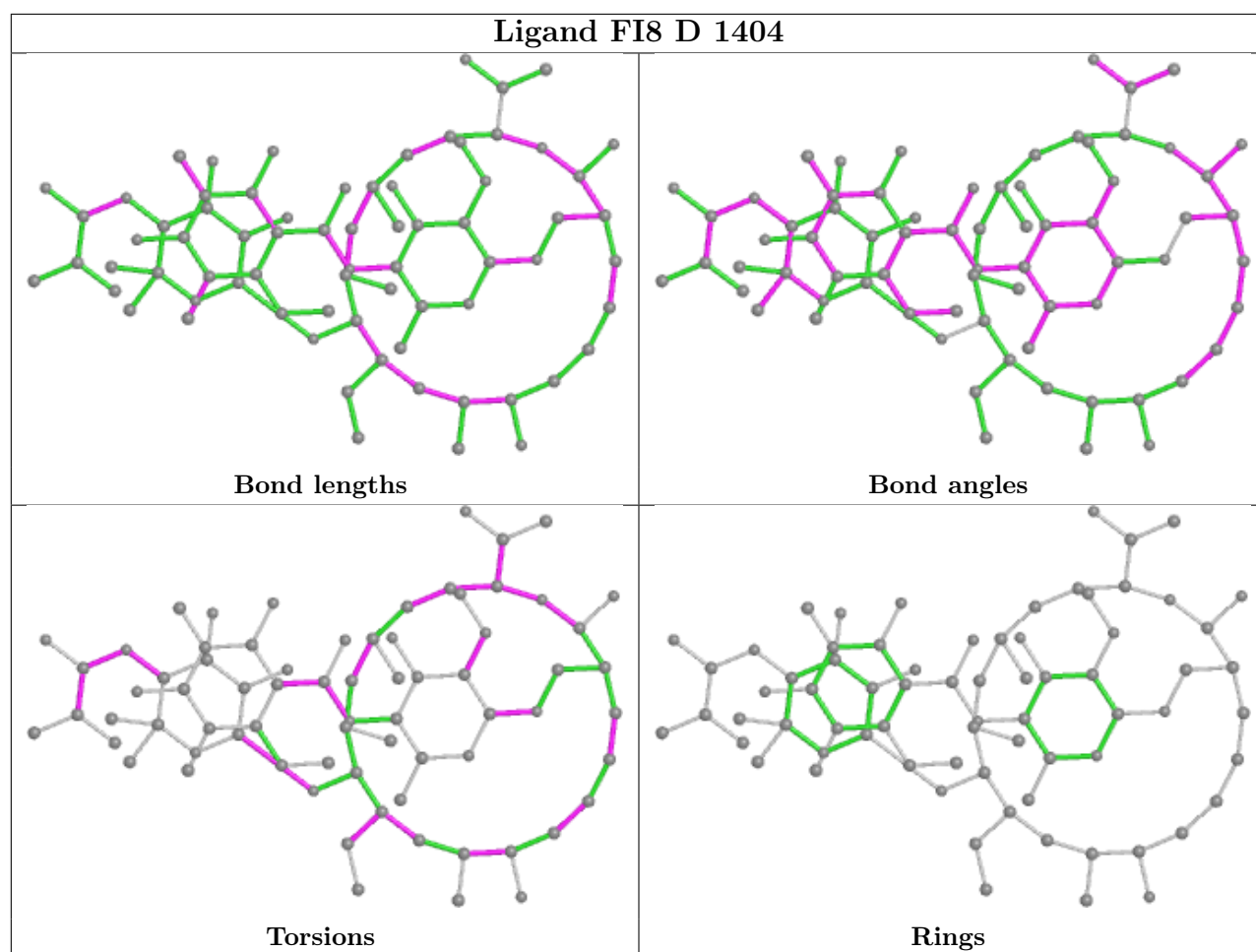
There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	1404	FI8	16	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

This section contains visualisations of the EMDB entry EMD-7323. 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

This section was not generated.

### 6.2 Central slices

This section was not generated.

### 6.3 Largest variance slices

This section was not generated.

### 6.4 Orthogonal surface views

This section was not generated.

### 6.5 Mask visualisation

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



## 7 Map analysis ⓘ

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

### 7.1 Map-value distribution ⓘ

This section was not generated.

### 7.2 Volume estimate versus contour level ⓘ

This section was not generated.

### 7.3 Rotationally averaged power spectrum ⓘ

This section was not generated. The rotationally averaged power spectrum had issues being displayed.



## 8 Fourier-Shell correlation

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



## 9 Map-model fit

This section was not generated.