



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 01:39 PM UTC

PDB ID : 4KMU / pdb_00004kmu
Title : X-ray crystal structure of the Escherichia coli RNA polymerase in complex with Rifampin
Authors : Murakami, K.S.
Deposited on : 2013-05-08
Resolution : 3.85 Å(reported)

This is a wwPDB X-ray Structure 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/XrayValidationReportHelp>

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:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

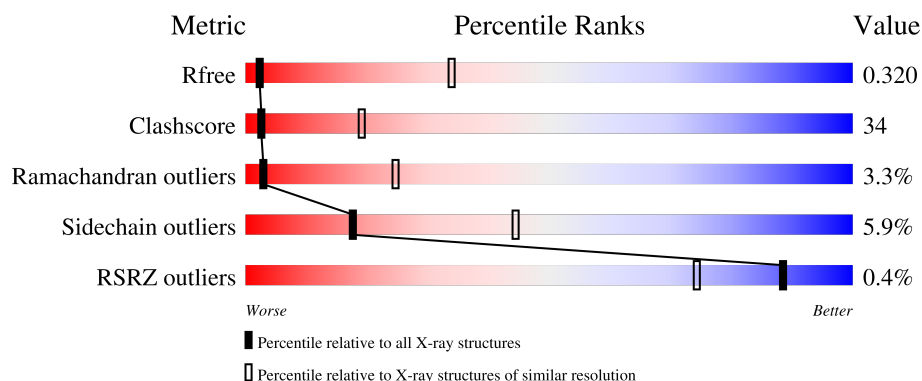
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.85 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1165 (4.02-3.70)
Clashscore	190562	1207 (4.02-3.70)
Ramachandran outliers	187476	1149 (4.02-3.70)
Sidechain outliers	187428	1142 (4.02-3.70)
RSRZ outliers	180081	1164 (4.02-3.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	
1	B	329	
1	F	329	
1	G	329	
2	C	1342	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	H	1342	48% 45% 6% ..
3	D	1407	31% 45% 5% 18%
3	I	1407	34% 43% 5% 18%
4	E	91	51% 43% . ..
4	J	91	% 44% 35% . . 16%
5	X	613	43% 39% . 16%
5	Y	613	36% 36% . 25%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 56315 atoms, of which 116 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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					ZeroOcc	AltConf	Trace
1	A	323	Total	C	N	O	S	0	0	0
			2514	1571	443	492	8			
1	B	221	Total	C	N	O	S	0	0	0
			1706	1065	300	335	6			
1	F	229	Total	C	N	O	S	0	0	0
			1775	1106	313	350	6			
1	G	217	Total	C	N	O	S	0	0	0
			1671	1045	293	327	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			
2	H	1335	Total	C	N	O	S	0	0	0
			10523	6601	1836	2043	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			
3	I	1160	Total	C	N	O	S	0	0	0
			9060	5695	1621	1697	47			

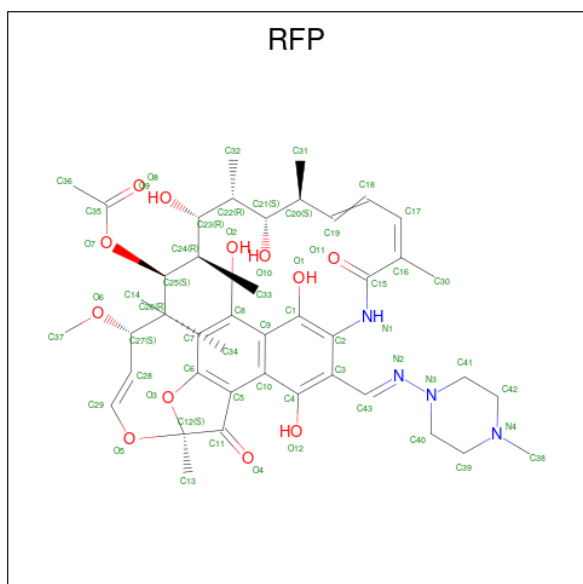
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	90	Total	C	N	O	S	0	0	0
			708	430	136	141	1			
4	J	76	Total	C	N	O	S	0	0	0
			605	368	115	121	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	X	517	Total	C	N	O	S	0	0	0
			4198	2621	745	806	26			
5	Y	458	Total	C	N	O	S	0	0	0
			3732	2335	671	703	23			

- Molecule 6 is RIFAMPICIN (CCD ID: RFP) (formula: $C_{43}H_{58}N_4O_{12}$).



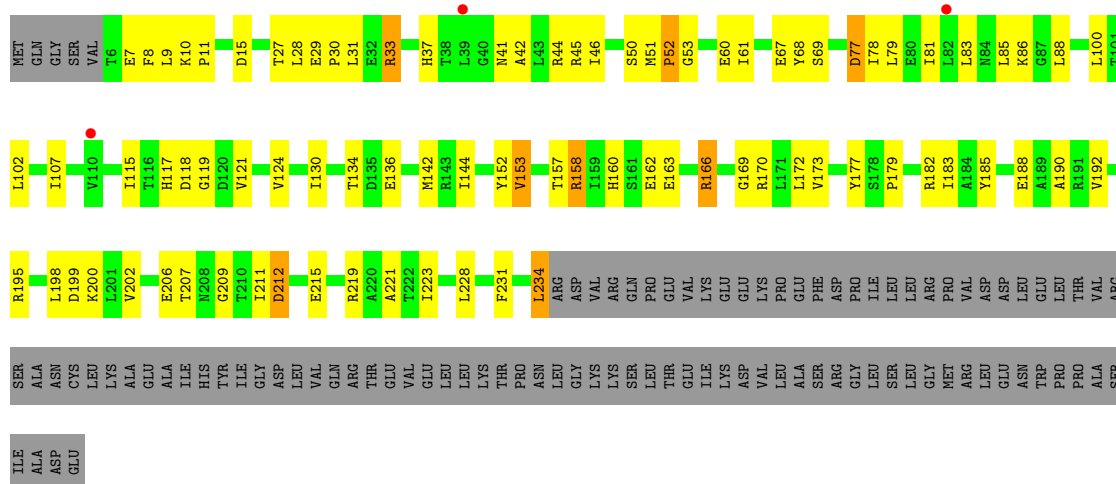
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	N	O	0	0
			117	43	58	4	12		
6	H	1	Total	C	H	N	O	0	0
			117	43	58	4	12		

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

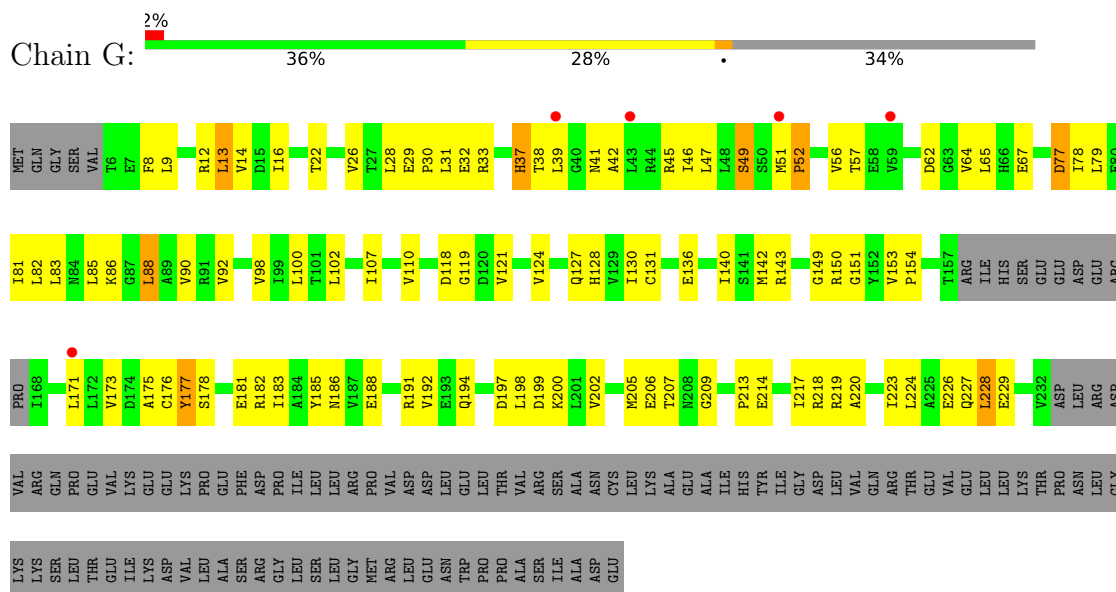
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	I	2	Total	Zn	0	0
			2	2		

- Molecule 8 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

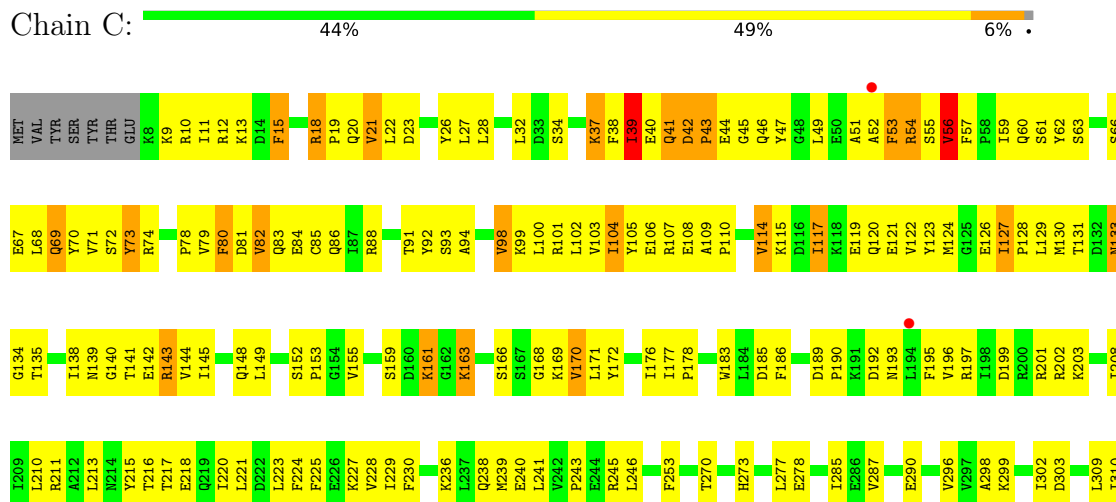
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	1	Total 1	Mg 1	0	0
8	I	1	Total 1	Mg 1	0	0

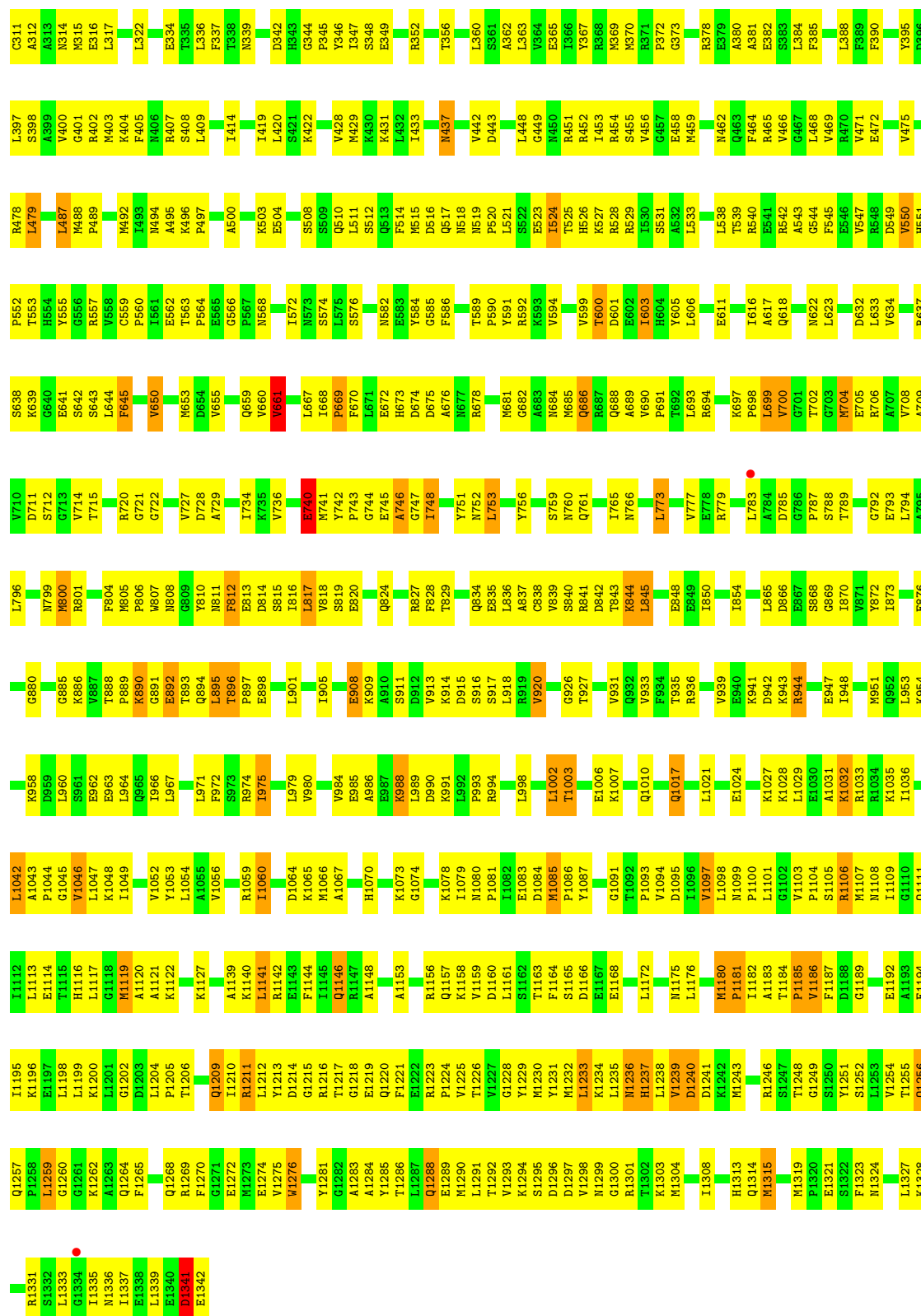


• Molecule 1: DNA-directed RNA polymerase subunit alpha

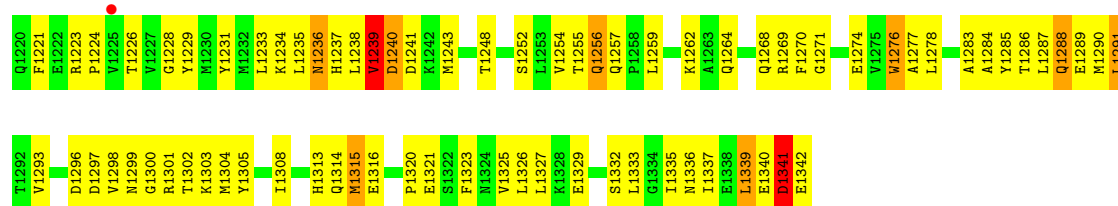


• Molecule 2: DNA-directed RNA polymerase subunit beta



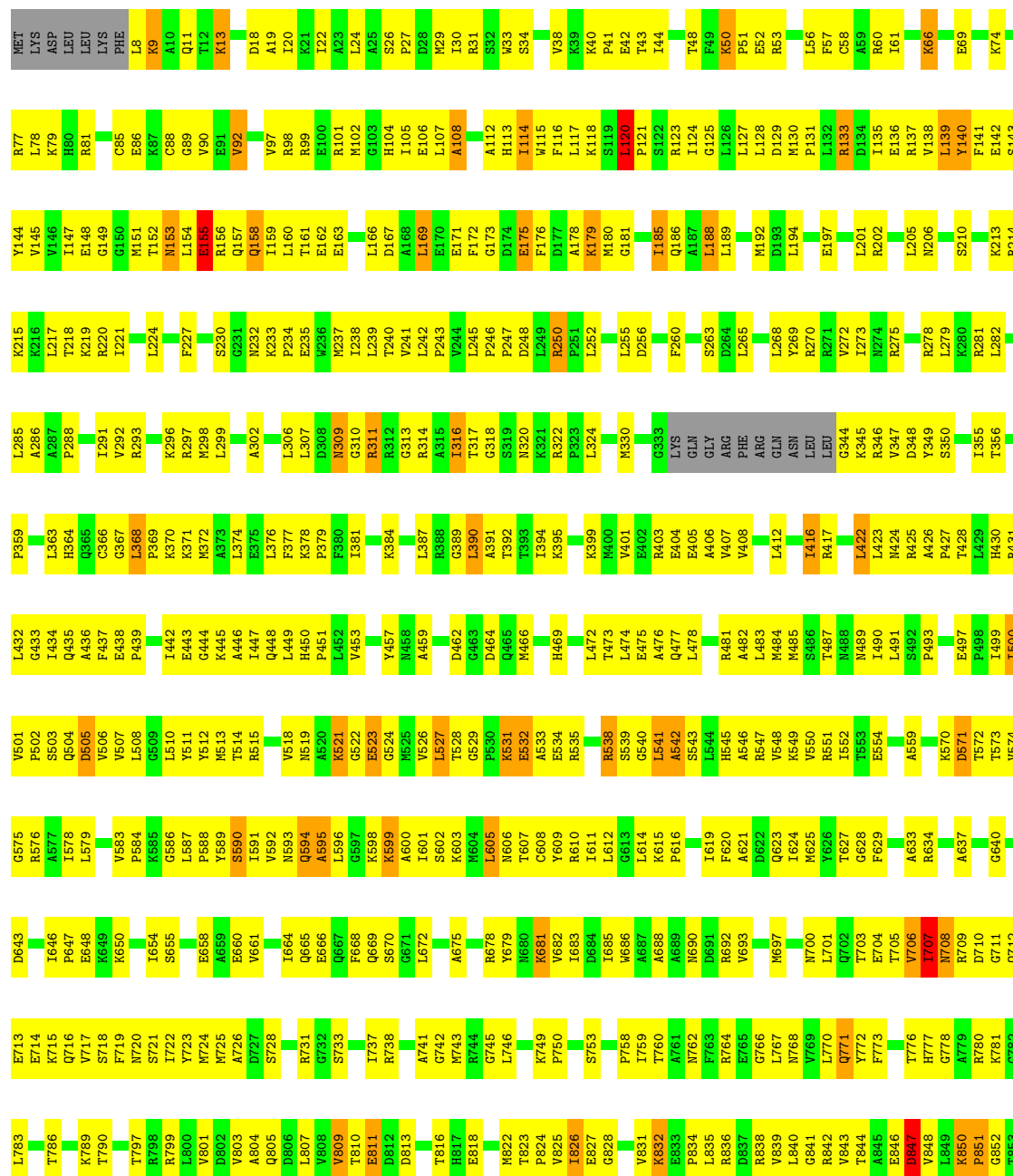


F1144	K1073	V980	L902	T816	Y742	S666	B582	G507	I435	Y346	F136	L68	MET
I1145	G1074	V981	L905	L817	P743	L667	G585	S508	R436	I347	Y137	Q69	VAL
R1146	V1075	V984	V905	S818	A746	T668	G586	L511	R437	L351	I138	V70	TYR
R1147	I1076	E985	I1076	S819	A747	P669	F586	L512	G438	L356	N139	V71	SER
A1148	S1077	A986	E908	P670	I748	F670	L587	Q513	R439	T217	G140	S72	THR
R1156	K1078	K909	K909	L671	I748	L671	E588	F514	Y442	E218	T141	Y73	
Q1157	I1079	K988	A910	E672	D749	E672	T593	F514	D443	Q219	E142	R74	GLU
Q1157	M1080	L989	S911	H673	H673	H673	P590	H615	D443	I220	R143		K8
K1158	P1081	D990	D912	F678	N752	A679	Y591	D516	D446	Y154	V144	P78	K9
V1159	I1082	V913	V913	T829	L753	L753	R592	Q517	H447	I145	V146	F80	R10
D1160	E1083	L992	S916	T830	Y756	L680	G599	N519	L448	L223	V82	D81	R12
T1163	M1085	R934	S917	T831	Y759	H681	T600	P520	L366	F230	Q148	V82	K13
F1164	P1086	D995	L918	I831	S759	D601	E602	L521	R452	K236			D14
S1165	Y1087	R996	R919	C839	N760	N684	G602	E522	R453	R151		Q86	F15
D1166	E1083	W997	V920	S840	I763	Q686	T603	E523	R454	S152		R88	R18
E1167	T1092	L998	S925	S841	T763	Q687	G607	I524	F458	I87			P19
E1168	P1093	G923	G923	D842	I765	Q688	E610	H526	M459	R88		T91	Q20
R1171	V1094	G924	V924	T843	I766	A689	E611	K527	M462	V242		Y92	V21
L1172	V1097	S925	S925	T844	Q767	V690	E611	R528	Q463	R245		S93	L22
A1173	L1098	E1005	G926	L845	Q767	M768	P691	R529	F464	L246		A94	D23
E1174	N1099	E1006	T927	L845	P769	P691	I616	P535	R465	F253		P95	V24
N1175	P1100	G933	V933	E848	C770	K697	A617	P535	V466	D254		R97	P25
L1176	L1101	V933	V933	E849	C770	P698	Q618	L538	Q467	G152		V98	V26
R1177	G1102	V933	V933	T850	S772	L699	A619	I539	L384	K163			L27
A1178	V1103	R936	R936	T850	L773	V700	L623	I539	N387			K99	L28
K1179	P1104	K941	K941	T854	G774	G701	L623	I539	L388	S166		L100	S29
M1180	S1105	D942	D942	E854	E775	T702	H628	A543	R470	S167		R101	I30
P1181	R1106	K943	K943	V857	E775	G703	F629	A543	V471	G168		L102	Q31
N1182	M1107	K943	K943	V857	L783	G703	F629	V547	E472	K169		V103	
A1183	N1108	R944	R944	D866	A784	E705	F629	R546		V287		I104	Q36
T1184	I1109	A945	A945	E867	A785	R706	D632	R546	V475	D393		Y105	K37
P1185	G1110	L946	L946	S868	Q786	A707	L633	R550	R476	L171		Y106	K37
V1186	Q1111	E947	E947	G869	P787	A707	H551	V550	E476	Y172		E107	F38
F1187	I1112	L948	L948	K870	S788		P552	T553	R478	N173		R107	I39
D1188	L1113	E949	E949	V871	S788		T553	P552	L479	A174		E108	
G1189	E1114	E950	E950	Y872	L791	S712	R637	H554	S480	R175		A109	
L1199	D1041	R951	R951	E876	G792	S712	R638	H554	L481	I176		P110	
K1200	L1042	Q952	Q952	E876	G793	G713	K639	H555		I177		V114	
L1201	A1043	L953	L953	V877	L794	V714	R643	G556	L484	P178			
G1202	P1044	P1044	P1044	V877	A795	A716	S643	R557	D485			I117	
D1203	V1045	G959	G959	V884	L796	V717	L644	V568	T486	S132		K118	
L1204	L1047	K958	K958	G885	L796	A718	S646	C559	T487	W183		E119	
P1205	L1054	S961	S961	G886	N799		R647	E562	M488	Q120		E50	
T1206	A1055	E962	E962	V887	R801	Q725	R647	P564	P489	F186		A51	
S1207	V1056	E963	E963	T888	V802	V727	S646	T563	R491	D189		F53	
G1208	K1057	K965	K965	P889	V802	D728	S646	P564	D491	Y123		A52	
Q1209	R1058	Q965	Q965	K890	N805	A729	M653	N568	M492	M124		R54	
I1210	R1059	I966	I966	G891	P806		P654		L493	G125		S55	
R1211	I1060	I967	I967	E892	N807	I732	V655	I573	A494	L194		Y86	
Y1213	Q1134	L971	L971	T893	N808	V733	G658	R572	M494	I128		F57	
D1214	A1139	T895	T895	Q894	G809	L734	Q659	S574	D427	P128		P58	
R1216	K1140	P897	P897	L895	Y810	K735	V660	L576	V428	L129		I59	
T1217	L1141	A977	A977	T896	N811	V736	S662	S576	M429	M130		Y62	
G1218	R1142	V978	V978	P897	F812		S662	V577	K430	T131		S63	
E1219	E1143	L979	L979	E899	E813	D739	V663	Y578	K431	D132		N65	
					D814	E740	G664	Q580	L432	A206		G134	
					S815	M741	A665	T581	D434	I208		T135	



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

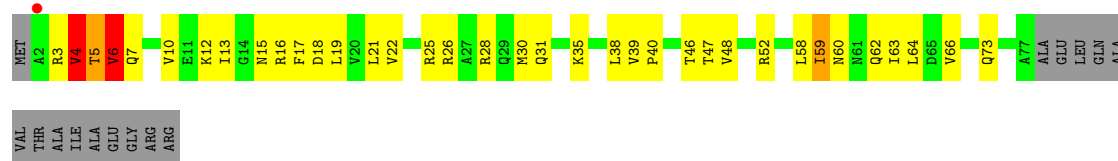
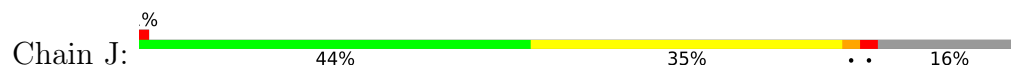
Chain D: 31% 45% 5% 18%



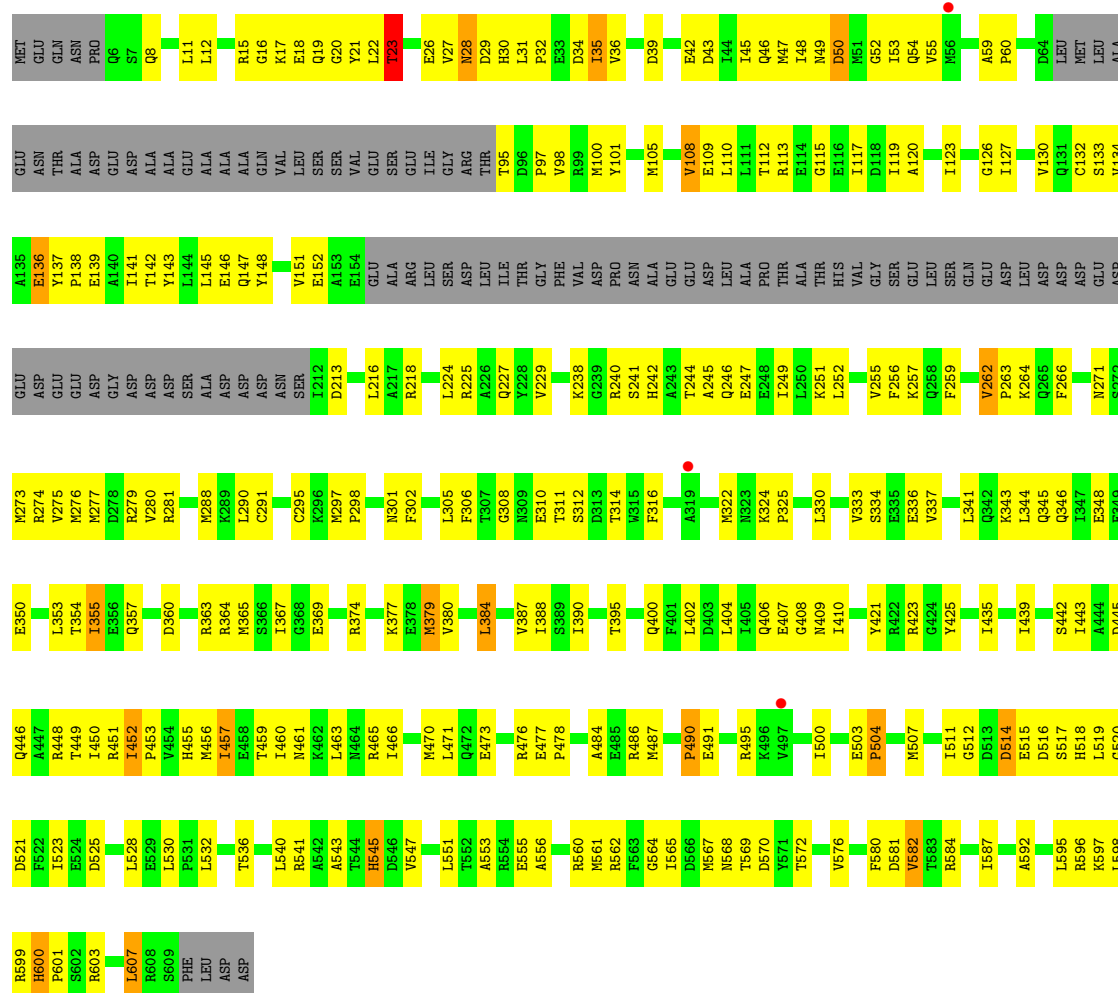




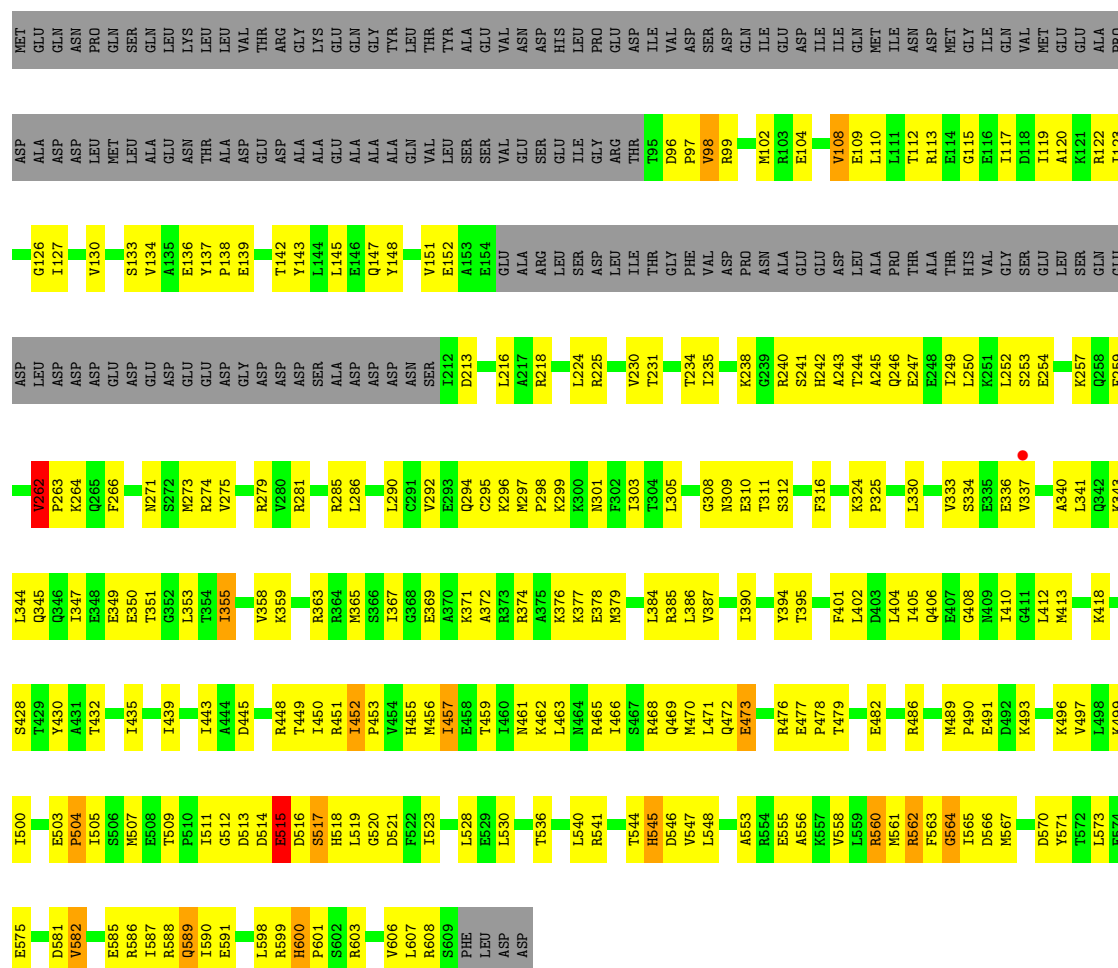
• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 5: RNA polymerase sigma factor RpoD



• Molecule 5: RNA polymerase sigma factor RpoD



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.52Å 203.87Å 307.87Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.97 – 3.85 29.97 – 3.85	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.97-3.85) 87.2 (29.97-3.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.54 (at 3.75Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.264 , 0.321 0.265 , 0.320	Depositor DCC
R_{free} test set	5158 reflections (4.51%)	wwPDB-VP
Wilson B-factor (Å ²)	117.3	Xtriage
Anisotropy	0.291	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 68.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	56315	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.68% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.26	0/2548	0.74	5/3454 (0.1%)
1	B	0.26	0/1725	0.75	0/2337
1	F	0.27	0/1797	0.77	4/2436 (0.2%)
1	G	0.25	0/1690	0.75	0/2290
2	C	0.27	0/10690	0.77	12/14423 (0.1%)
2	H	0.27	1/10690 (0.0%)	0.75	16/14423 (0.1%)
3	D	0.26	0/9198	0.77	13/12413 (0.1%)
3	I	0.26	0/9198	0.76	12/12413 (0.1%)
4	E	0.25	0/710	0.71	0/956
4	J	0.25	0/607	0.70	0/817
5	X	0.25	0/4253	0.72	2/5719 (0.0%)
5	Y	0.25	0/3783	0.72	2/5083 (0.0%)
All	All	0.26	1/56889 (0.0%)	0.75	66/76764 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	663	VAL	CA-C	5.63	1.60	1.52

The worst 5 of 66 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	120	LEU	CA-C-N	-8.62	110.39	120.13
3	D	120	LEU	C-N-CA	-8.62	110.39	120.13
2	C	42	ASP	CA-C-N	6.72	128.24	119.84
2	C	42	ASP	C-N-CA	6.72	128.24	119.84
3	I	120	LEU	CA-C-N	-6.65	112.62	120.13

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	2514	0	2566	170	0
1	B	1706	0	1738	108	0
1	F	1775	0	1800	77	0
1	G	1671	0	1706	95	0
2	C	10523	0	10546	834	0
2	H	10523	0	10546	719	0
3	D	9060	0	9257	832	0
3	I	9060	0	9257	769	0
4	E	708	0	719	52	0
4	J	605	0	612	44	0
5	X	4198	0	4250	256	0
5	Y	3732	0	3809	218	0
6	C	59	58	56	8	0
6	H	59	58	56	14	0
7	D	2	0	0	0	0
7	I	2	0	0	0	0
8	D	1	0	0	0	0
8	I	1	0	0	0	0
All	All	56199	116	56918	3861	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 34.

The worst 5 of 3861 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)
2:H:1119:MET:HG2	2:H:1228:GLY:HA2	1.20	1.17
3:D:1173:ARG:HA	3:D:1174:ARG:HB2	1.26	1.14
3:I:610:ARG:HG3	3:I:864:LEU:HD13	1.29	1.14
2:C:700:VAL:HG11	2:C:1114:GLU:HG3	1.30	1.12
3:I:1173:ARG:HA	3:I:1174:ARG:HB2	1.28	1.12

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 X-ray entries followed by that with respect to entries of similar resolution.

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	321/329 (98%)	254 (79%)	52 (16%)	15 (5%)	2	19
1	B	217/329 (66%)	188 (87%)	23 (11%)	6 (3%)	4	27
1	F	227/329 (69%)	194 (86%)	28 (12%)	5 (2%)	5	31
1	G	213/329 (65%)	188 (88%)	20 (9%)	5 (2%)	5	31
2	C	1333/1342 (99%)	1066 (80%)	225 (17%)	42 (3%)	3	25
2	H	1333/1342 (99%)	1065 (80%)	222 (17%)	46 (4%)	3	23
3	D	1154/1407 (82%)	919 (80%)	193 (17%)	42 (4%)	2	23
3	I	1154/1407 (82%)	925 (80%)	192 (17%)	37 (3%)	3	25
4	E	88/91 (97%)	76 (86%)	7 (8%)	5 (6%)	1	16
4	J	74/91 (81%)	64 (86%)	5 (7%)	5 (7%)	1	14
5	X	511/613 (83%)	444 (87%)	54 (11%)	13 (2%)	4	29
5	Y	454/613 (74%)	410 (90%)	33 (7%)	11 (2%)	4	30
All	All	7079/8222 (86%)	5793 (82%)	1054 (15%)	232 (3%)	3	25

5 of 232 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	52	PRO
1	B	20	SER
1	B	52	PRO
2	C	21	VAL
2	C	39	ILE

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 X-ray entries followed by that with respect to entries of similar resolution.

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	281/286 (98%)	270 (96%)	11 (4%)	28	52
1	B	189/286 (66%)	185 (98%)	4 (2%)	47	65
1	F	197/286 (69%)	191 (97%)	6 (3%)	36	57
1	G	185/286 (65%)	180 (97%)	5 (3%)	39	60
2	C	1150/1157 (99%)	1073 (93%)	77 (7%)	15	41
2	H	1150/1157 (99%)	1075 (94%)	75 (6%)	15	42
3	D	971/1168 (83%)	902 (93%)	69 (7%)	13	40
3	I	971/1168 (83%)	904 (93%)	67 (7%)	14	41
4	E	74/75 (99%)	70 (95%)	4 (5%)	20	46
4	J	65/75 (87%)	61 (94%)	4 (6%)	16	43
5	X	460/540 (85%)	443 (96%)	17 (4%)	30	54
5	Y	407/540 (75%)	387 (95%)	20 (5%)	22	48
All	All	6100/7024 (87%)	5741 (94%)	359 (6%)	18	44

5 of 359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	844	LYS
3	I	188	LEU
2	H	971	LEU
2	H	1262	LYS
3	I	531	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 127 such sidechains are listed below:

Mol	Chain	Res	Type
4	E	31	GLN
3	I	504	GLN
5	X	446	GLN
3	I	489	ASN
5	Y	128	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 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	$\# Z > 2$
6	RFP	H	1401	-	63,63,63	2.20	10 (15%)	94,94,94	1.92	26 (27%)
6	RFP	C	1401	-	63,63,63	2.15	11 (17%)	94,94,94	2.28	28 (29%)

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
6	RFP	H	1401	-	-	18/60/85/85	0/5/5/5
6	RFP	C	1401	-	-	39/60/85/85	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	1401	RFP	O3-C6	10.86	1.57	1.37
6	H	1401	RFP	O3-C6	10.74	1.57	1.37
6	H	1401	RFP	C15-N1	6.97	1.50	1.35
6	C	1401	RFP	C15-N1	6.31	1.48	1.35
6	C	1401	RFP	C12-C11	-4.58	1.36	1.54

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	1401	RFP	C2-C3-C43	-8.46	115.01	123.99
6	C	1401	RFP	O7-C35-C36	5.63	121.14	111.09
6	C	1401	RFP	O4-C11-C5	-5.21	122.02	131.63
6	H	1401	RFP	C17-C18-C19	-5.10	112.60	124.43
6	C	1401	RFP	C37-O6-C27	5.01	124.47	112.99

There are no chirality outliers.

5 of 57 torsion outliers are listed below:

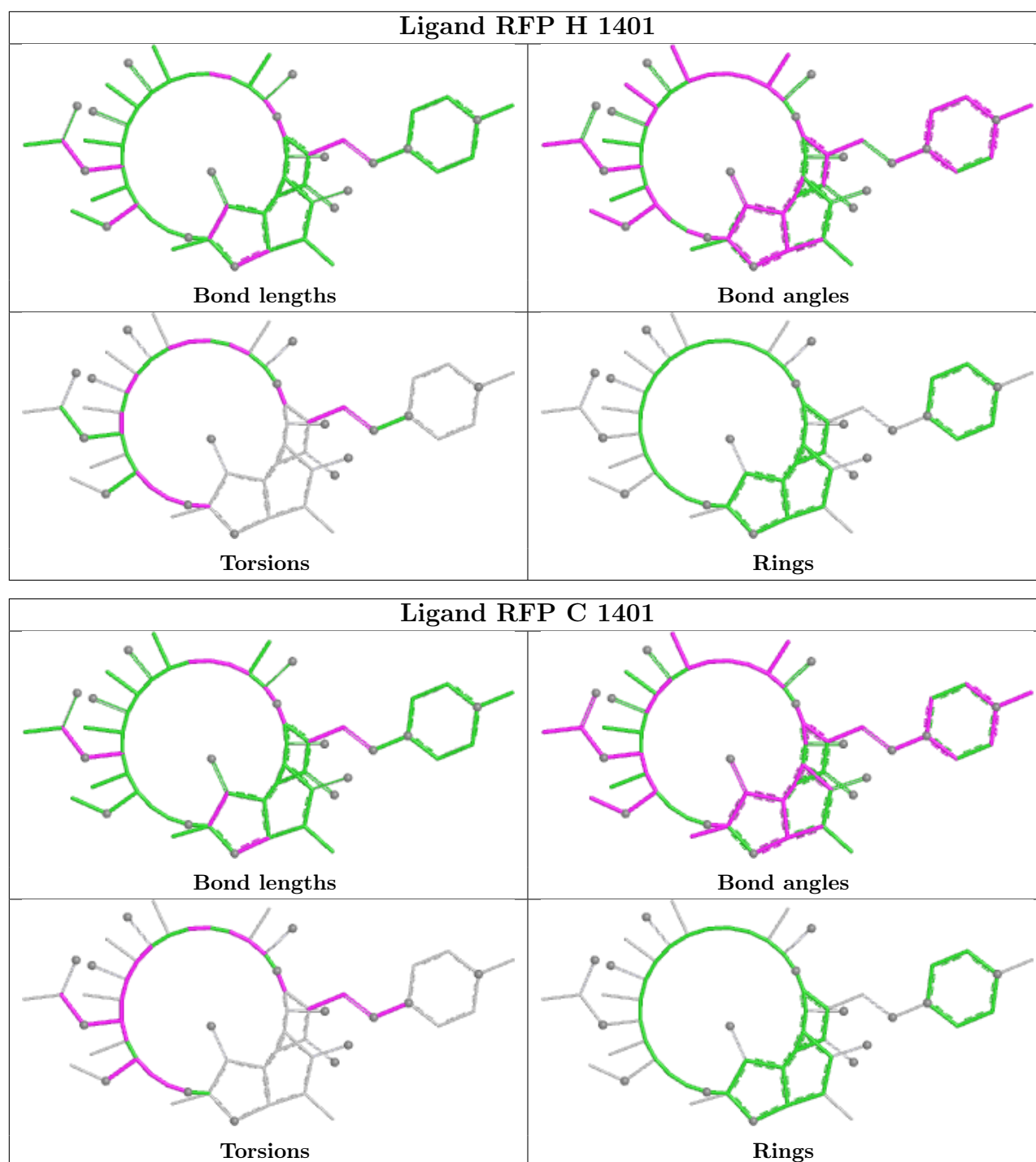
Mol	Chain	Res	Type	Atoms
6	C	1401	RFP	C4-C3-C43-N2
6	C	1401	RFP	C17-C18-C19-C20
6	C	1401	RFP	C23-C24-C25-C26
6	C	1401	RFP	C23-C24-C25-O7
6	C	1401	RFP	C33-C24-C25-C26

There are no ring outliers.

2 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	1401	RFP	14	0
6	C	1401	RFP	8	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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	323/329 (98%)	-0.56	1 (0%) 90 77	0, 73, 165, 263	0
1	B	221/329 (67%)	-0.32	1 (0%) 87 71	3, 97, 189, 266	0
1	F	229/329 (69%)	-0.33	3 (1%) 75 53	16, 121, 201, 266	0
1	G	217/329 (65%)	-0.37	5 (2%) 61 43	39, 111, 186, 215	0
2	C	1335/1342 (99%)	-0.49	4 (0%) 90 77	0, 48, 166, 284	0
2	H	1335/1342 (99%)	-0.51	2 (0%) 92 87	1, 86, 201, 341	0
3	D	1160/1407 (82%)	-0.50	1 (0%) 92 87	0, 40, 157, 284	0
3	I	1160/1407 (82%)	-0.47	4 (0%) 90 77	1, 52, 180, 322	0
4	E	90/91 (98%)	-0.62	0 100 100	0, 40, 109, 159	0
4	J	76/91 (83%)	-0.54	1 (1%) 75 53	5, 76, 155, 167	0
5	X	517/613 (84%)	-0.51	3 (0%) 85 68	3, 99, 228, 365	0
5	Y	458/613 (74%)	-0.50	1 (0%) 91 81	2, 102, 219, 328	0
All	All	7121/8222 (86%)	-0.49	26 (0%) 88 74	0, 70, 190, 365	0

The worst 5 of 26 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	59	VAL	4.5
5	Y	337	VAL	4.0
3	I	637	ALA	3.5
1	G	39	LEU	3.4
5	X	56	MET	3.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

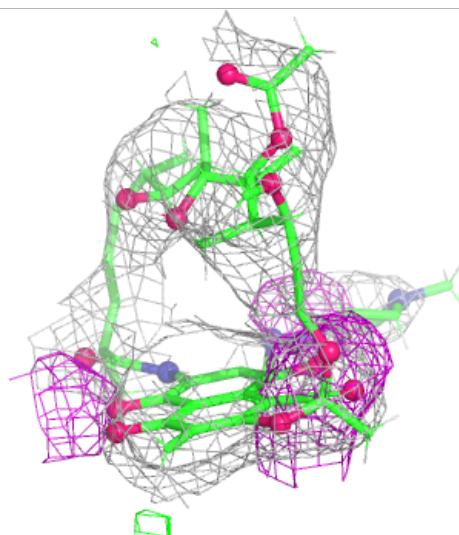
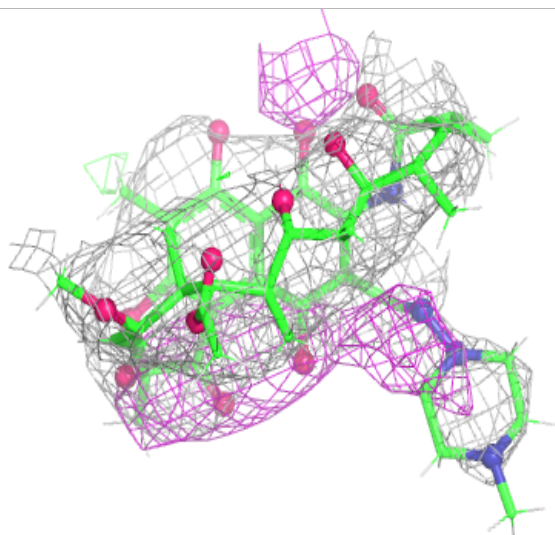
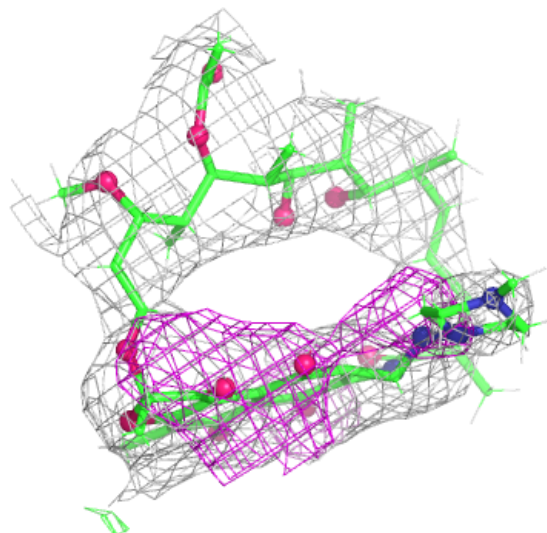
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	RFP	C	1401	59/59	0.82	0.09	20,20,20,20	0
6	RFP	H	1401	59/59	0.84	0.09	20,20,20,20	0
8	MG	I	1503	1/1	0.92	0.18	20,20,20,20	0
8	MG	D	1503	1/1	0.97	0.05	24,24,24,24	0
7	ZN	I	1502	1/1	0.98	0.08	49,49,49,49	0
7	ZN	I	1501	1/1	0.99	0.02	60,60,60,60	0
7	ZN	D	1501	1/1	1.00	0.02	54,54,54,54	0
7	ZN	D	1502	1/1	1.00	0.04	8,8,8,8	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

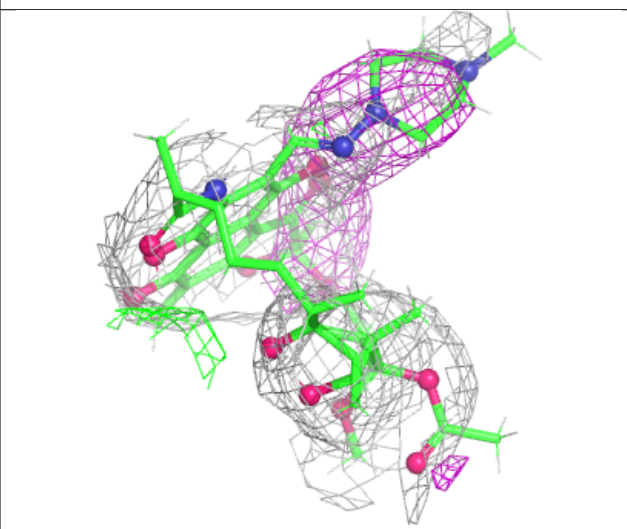
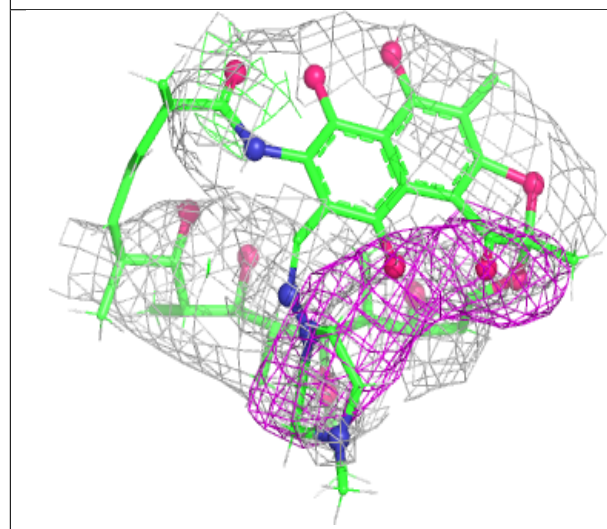
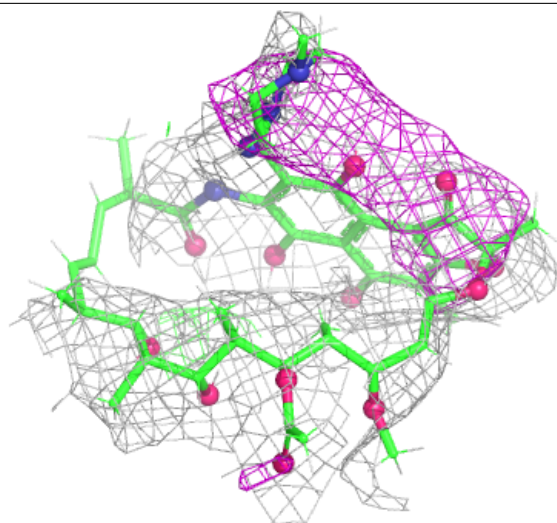
Electron density around RFP C 1401:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around RFP H 1401:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.