



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 15, 2026 – 10:02 AM UTC

PDB ID : 4YFX / pdb_00004yfx
Title : Escherichia coli RNA polymerase in complex with Myxopyronin B
Authors : Molodtsov, V.; Fleming, P.R.; Eyermann, C.J.; Ferguson, A.D.; Foulk, M.A.;
McKinney, D.C.; Masse, C.E.; Buurman, E.T.; Murakami, K.S.
Deposited on : 2015-02-25
Resolution : 3.84 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

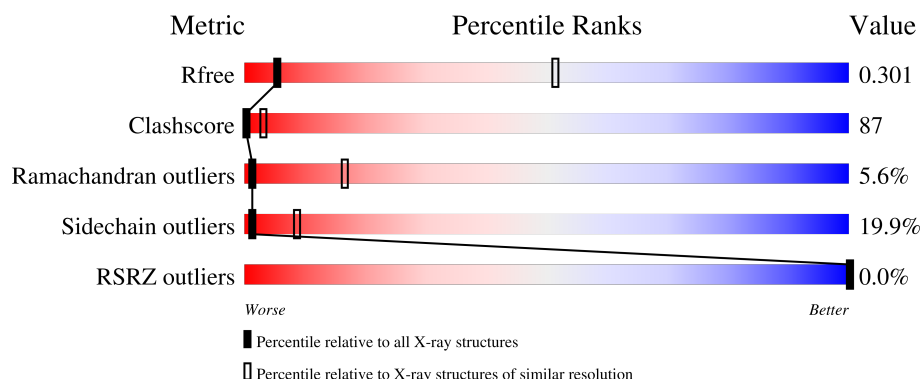
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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	G	329	
1	H	329	
2	C	1342	

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55388 atoms, of which 33 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	229	Total	C	N	O	S	0	0	0
			1779	1108	316	349	6			
1	B	289	Total	C	N	O	S	0	0	0
			2239	1403	393	435	8			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10564	6628	1838	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10552	6621	1835	2053	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9062	5701	1622	1693	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9021	5675	1617	1683	46			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	458	Total	C	N	O	S	0	0	0
			3726	2332	668	703	23			
5	L	458	Total	C	N	O	S	0	0	0
			3640	2282	647	690	21			

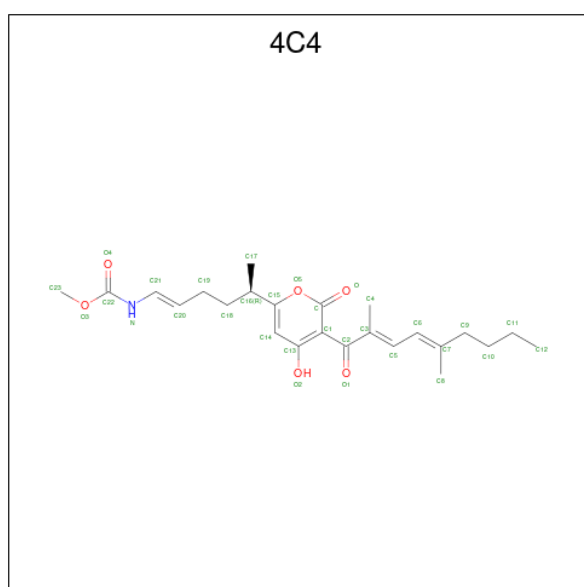
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	1	Total	Mg	0	0
			1	1		
6	J	1	Total	Mg	0	0
			1	1		

- 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	J	2	Total	Zn	0	0
			2	2		

- Molecule 8 is Myxopyronin B (CCD ID: 4C4) (formula: C₂₄H₃₃NO₆).

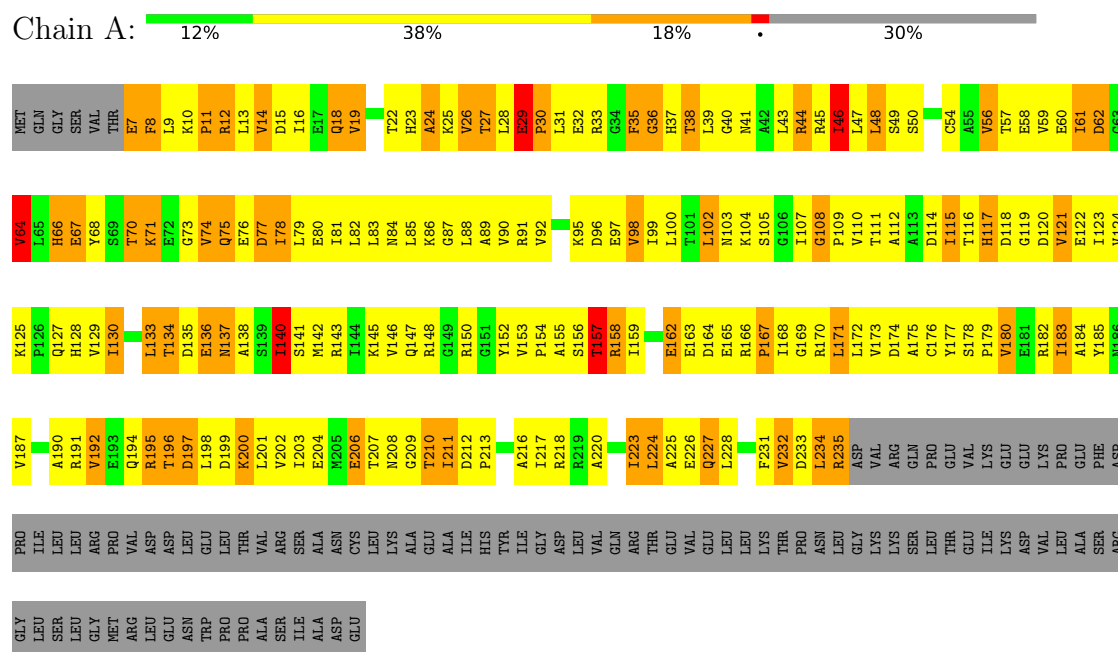


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	H	N	O	0	0
			64	24	33	1	6		

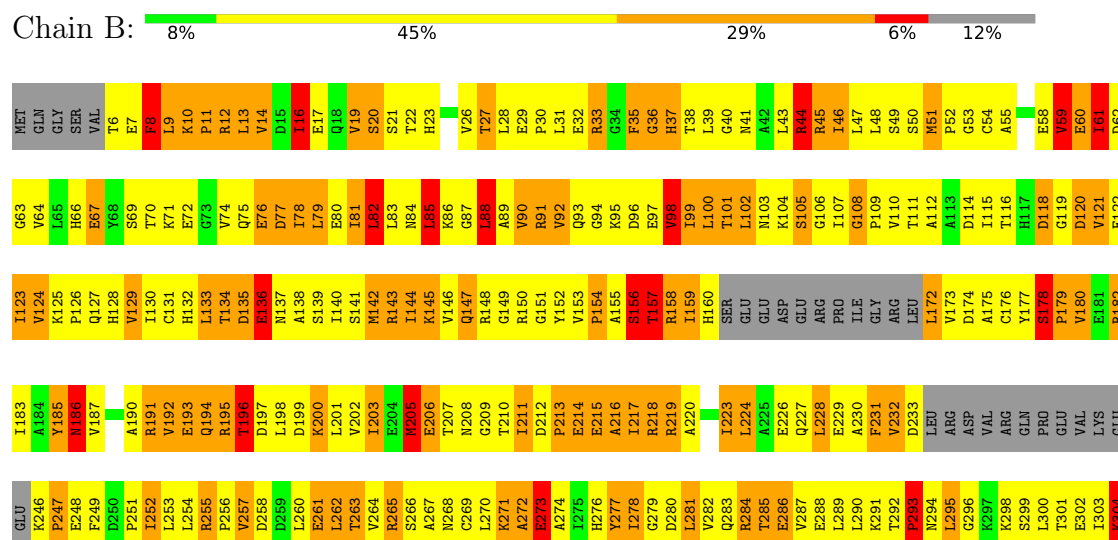
3 Residue-property plots

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 electron 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

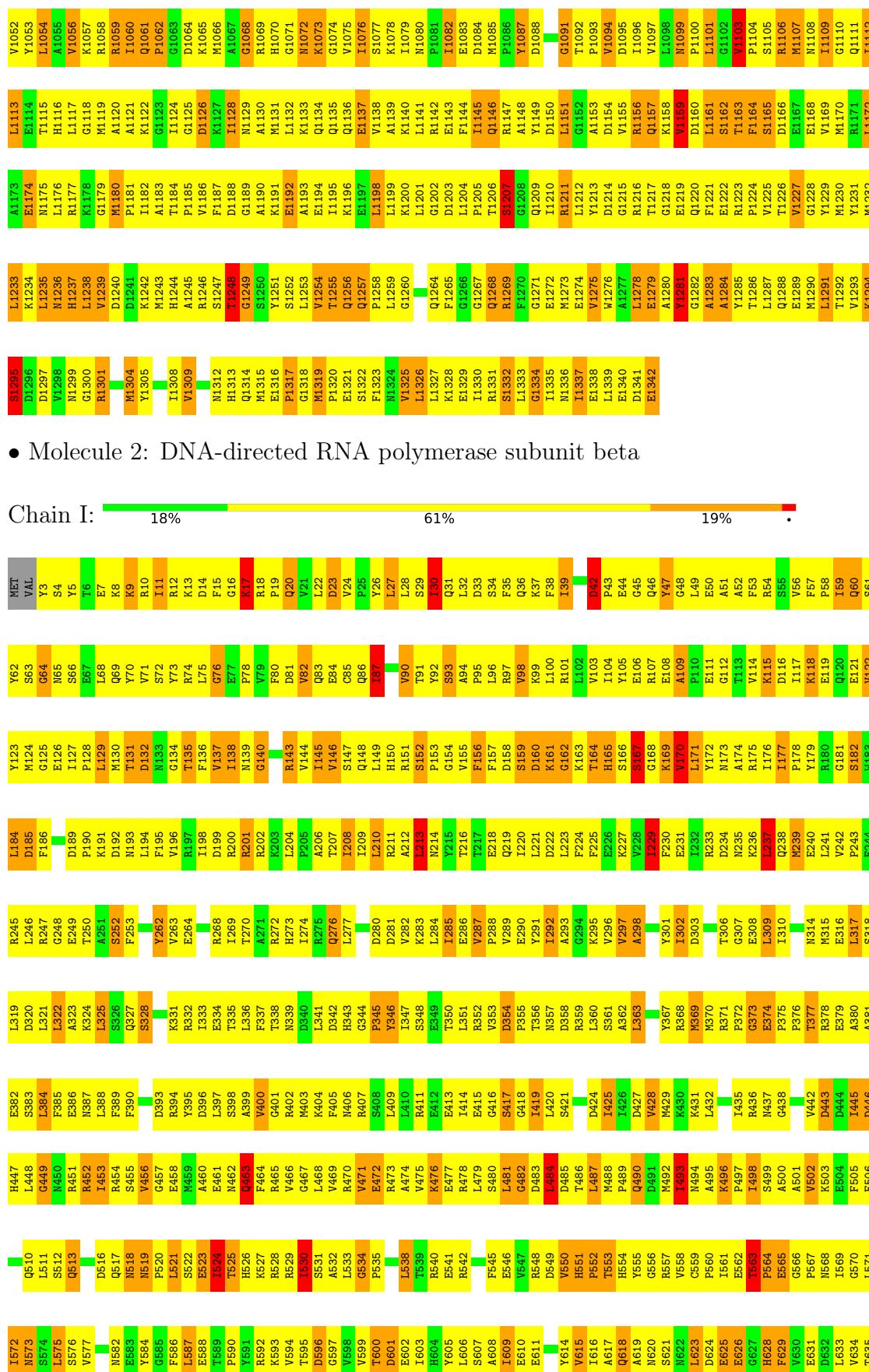
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha









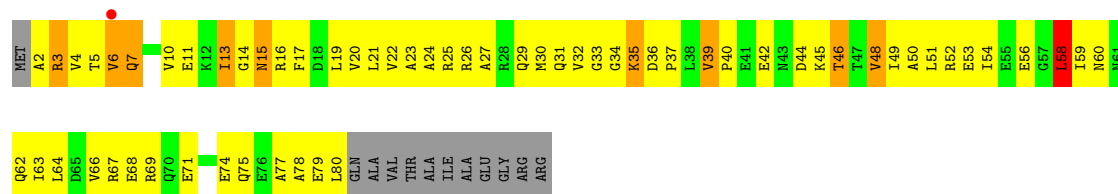


L1223	R1284	R1345	ASP
R1224	V1285	G1346	ASN
G1225	K1286	G1347	GLU
V1226	K1287	K1348	
I1227	L1288	E1349	
H1228	M1289	I1350	
A1228		V1351	
V1229		I1352	
T1230	L1292	I1353	
E1231	E1293	L1354	
Y1232	A1294	G1355	
N1233	N1295	L1356	
G1234	G1296	I1357	
T1235	K1297	L1358	
H1236	V1298	A1359	
V1237	A1300	G1360	
D1238	Q1301	T1361	
T1239	T1302	G1362	
V1240	V1303	I1363	
Y1241	S1304	Y1364	
R1242	R1305	A1365	
L1243	D1306	I1366	
		Q1367	
V1246	L1307	H1368	
K1247	K1308	D1369	
I1248	I1309	M1370	
N1249	T1310	R1371	
D1250	K1311	L1372	
Q1251	A1312	L1373	
Q1259	S1313	A1374	
M1260	R1252	I1375	
L1261	I1253	A1376	
L1262	E1254	GLU	
V1265	V1255	ALA	
V1257	E1317	PRO	
R1258	S1318	ALA	
Q1259	F1319	THR	
M1260	I1320	ALA	
L1261	S1321	PRO	
L1262	A1322	GLN	
K1263	A1323	VAL	
A1264	F1325	THR	
T1265	Q1326	ALA	
I1266	E1327	GLU	
V1267	T1328	ASP	
N1268	T1329	ALA	
A1269	R1330	SER	
G1270	V1331	ALA	
S1271	L1332	SER	
S1272	T1333	LEU	
D1273	E1334	ALA	
F1274	A1335	GLU	
L1275	A1336	LEU	
E1276	V1337	LEU	
G1277	A1338	ASN	
E1278	G1339	ALA	
Q1279	K1340	GLY	
V1280	R1341	LEU	
E1281	D1342	GLY	
Y1282	E1343	GLY	
S1283	L1344	SER	

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

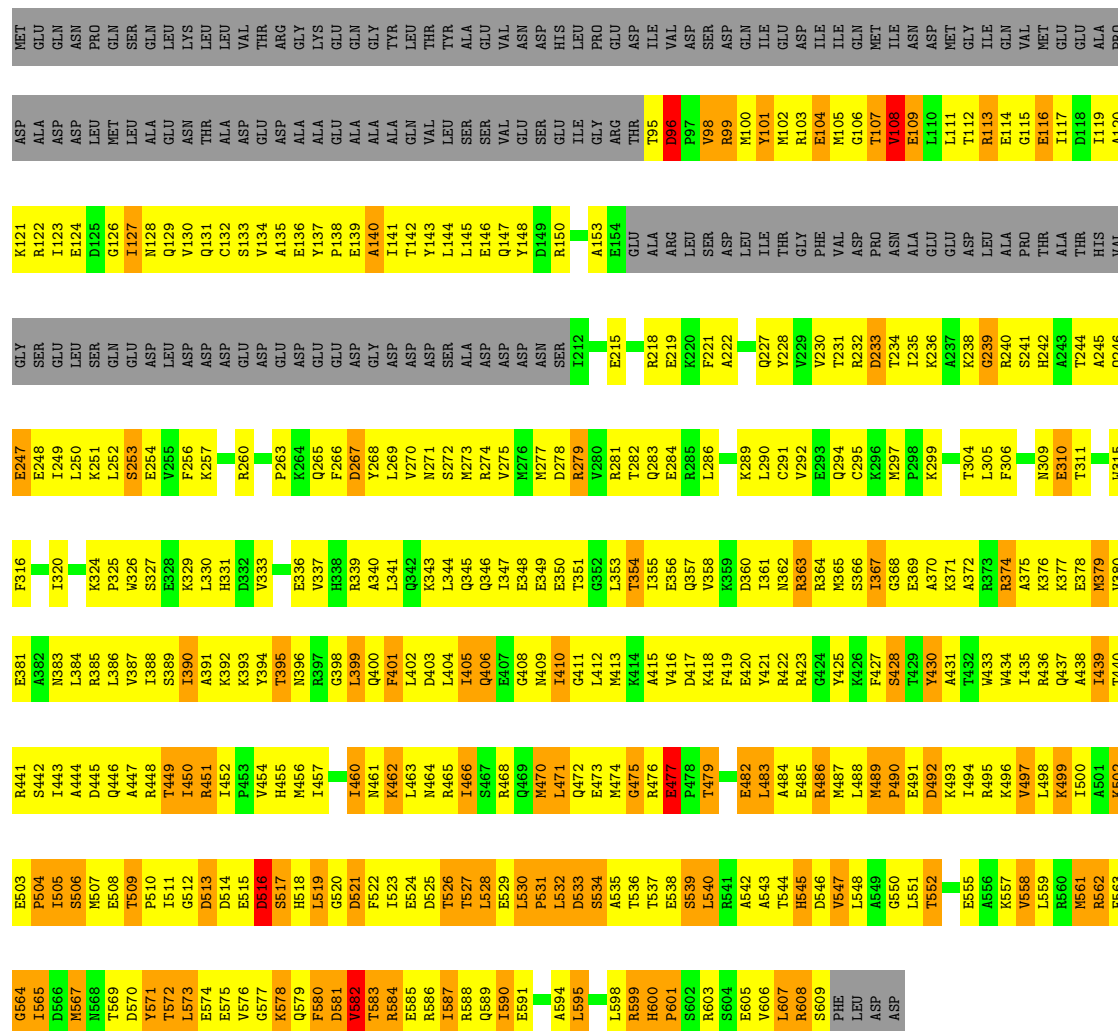
Chain J: 12% 48% 20% 18%

MET	L61	I124	A184	P247	D308	L368	L432	S492	Y555	P616
LYS	F62	G125	I185	D248	N309	P369	G433	F493	E556	T617
ASP	G63	L126	Q186	L249	G310	K370	L434	A494	K557	V618
LEU	P64	L127	A187	R250	R311	K371	Q435	N495	D558	I619
		L128	L188	P251	G312	M372	A436	A496	A559	F620
		L129	L189	L252	G313	A373	F437	E497	N560	A621
		M130	K190	V253	R314	L374	E438	P498	G561	D622
		P131	S191		A315	E375	F439	L499	E562	Q623
		L132	M192	D256	L316	L376	Y440	I500	S563	Q624
		R133	L193	G257	T317	F377	L441	V501	Y564	L624
		L134	L194	G258	G318	K378	L442	P502	A565	M625
		G73	L195	R259	S319	P379	E443	S503	K566	T627
		THR	Q196	F260	G320	F380	G444	O504	T567	G628
		K74	E197	A261	K321	L381	K445	D505	S568	P629
		Y75	C198	T262	R322	Y392	A446	V506	L569	A630
		K76		S263	P323	T447	L447	V507	K570	G631
		H80	L201	D264	K324	Q448	L449	L508	D571	A632
		R81	R202	L265	K325	L449	L450	O509	T572	A633
		G82	E203	M266	S326	L390	H450	L510	T573	R634
		V83	E204	D267	L327	A391	P451	V511	V574	G635
		C85	L205	R269	A328	T392	L452	Y512	G575	S636
		E86	N206	Y270	D329	T393	V453	M513	R576	A637
		K87	E207	R271	M330	I394	C454	T514	A577	S638
		L24		R272	K331	K395	A455	R515	T578	V639
		A25	S210	L273	G332	A396	A456	D516	L579	G640
		S26	E211	L274	G333	A397	Y457	C517	V580	L641
		P27	T212	R275	K334	K398	M458	V518	M581	D642
		D28	L221	K276	Q335	K399	A459	N519	T582	G643
		M29	R214	N276	G336	M400	D460	A520	V583	M644
		T93	K215	K277	R337	V401	F461	K521	P584	V645
		Q94	K216	R278	F338	E402	D462	G522	L587	T646
		R95	L217	L279	R339	R403	C463	E523	P588	P647
		K96	E155	K280	Q340	E404	D464	G524	F589	E648
		V97	Q157	L281	N341	E405	Q465	M525	Y589	K649
		R98	Q158	L282	L342	A406	M466	V526	S590	K650
		R99	I159	L283	L343	V407	A467	L527	I591	H651
		E37	L160	D284	G344	V408	V468	T528	V592	E652
		V98	T161	L285	K345	V409	H469		R593	T653
		K39	M102	E162	R346	D410	V470	K531	Q594	L654
		K40	G103	E163	Y347	L411	L471	E532	A595	S655
		P41	H104	Y165	D348	D413	L472		L596	E656
		E42	I105	D228	Y349	D414	T473		G597	A657
		T43	E106	V229	S350	E414	L474	L536	K598	
		I44	L107	Q230	G351	V415	E475	Y537	R598	S659
		M45	A108	G231	R352	L416	A476	B538	A600	V661
		Y46	S109	N232	R353	R417	Q477	G540	I601	A662
		T48	P110	K233	N294	E418	L478	L541	S602	E663
		F49	T111	P234	E295	H419	E479	A542	K603	T664
		K50	A112	E235	K296	T356	A480	S543	M604	Q665
		H113	H113	W236	P297	V421	B481	L544	L605	E666
		I114	M115	M237	G358	L422	A482	H545	M606	Q667
		E52	F116	L238	L299	L423	L483	A546	T607	F668
		R53	F176	L239	Q300	N424	M484	R547	C608	Q669
		D54	L117	T240	E301	R425	M485	V609	S670	
		G55	K118	V241	A302	R362	A426	K549	R610	G671
		L56	S119	L242	V303	L363	T487	V550	L672	L673
		F57	L120	P243	D304	H364	T428	R551	L612	T674
		C58	P121	V244	A305	Q365	L429	M552	G613	
		A59	S122	L245	L306	C366	T490	T553	L614	A675
		R60	R123	E183	P246	G367	L491	E554	K615	Q676



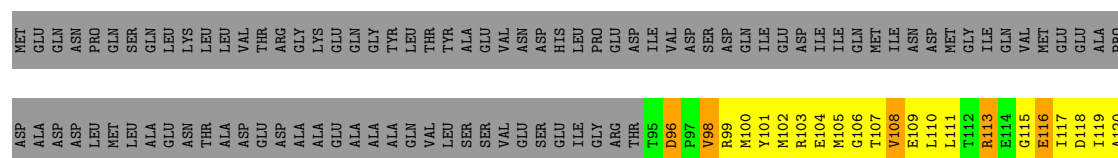
• Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 15% 44% 15% 25%



• Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 15% 49% 11% 25%



R560	R561	R562	F563	G564	I565	D566	R567		Y571	T572	L573	E574	E575	V576	G577	K578		D581	V582	T583	R584	E585	R586	I587	R588	Q589	T590	E591	A592	K593	A594	L595	R596	R597	L598	R599	H600	P601	S602	R603	S604	E605	V606	L607	R608	S609	PHE	LEU	ASP	ASP											
K499	I500	A501	K502	E503	P504	T505	S506	M507	E508	T509	P510	I511	G512	D513	D514	E515	D516	S517	H518	L519	G520	D521	F522	I523	E524	D525	T526	T527	L528	E529	L530	P531	L532	D533		T536	T537	E538	S539	L540	R541	A542	A543	T544	H545	D546	V547	L548	A549	G550	L551	T552	A553	R554	E555	A556	R557	V558	L559		
A438	I439	R440	R441	S442	I443	A444	D445	L446	A447	R448	T449	I450	R451	I452	P453	V454	H455	M456	I457	E458	T459	I460	N461	K462	L463	M464	R465	I466	S467	R468	Q469	M470	L471	Q472	E473	M474	G475	R476	E477	P478	T479		E482	L483	A484	E485	R486	M487	L488	M489	P490	E491	D492	A493	I494	R495	K496	V497	L498		
K376	K377	E378	K379	V380	E381	A382	N383	L384	R385	L386	V387	I388	S389	E390	A391	K392	H393	Y394	T395	N396	K397	G398	L399	Q400	F401	L402	D403	L404	I405	S406	Q407	G408	M409	I410	Q411	L412	M413	K414	A415	E356	D417	K418	F419	E420	Y421	R422	R423		F427	S428	T429	Y430	A431	E369	T432	W433	W434	I435	R436	Q437	
E310	T311	S312	D313	T314	W315	F316		M322	N323	K324	P325	W326	S327	E328	K329	L330	H331	I332	V333	S334	E335	E336		R339	A340	K341	Q342	K343	L344	Q345	Q346	I347	E348	E349	E350		L353	T354	I355	E356	Q357	V358	K359	D360	I361	N362	R363	R364	M365	S366	I367	G368	E369	A370	K371	A372	R373	R374	A375		
Q246	E247	E248	I249	L250	K251	L252	S253	V254	V255	F256	K257	Q258	F259	R260	L261	V262	P263	K264	Q265	F266	D267	Y268	L269	V270	N271	S272	M273	R274	V275	M276	M277	D278	R279	V280	R281	T282	Q283		L286	I287	M288	K289	L290	C291	V292		C295	K296	M297	F298	K299		F302	I303	T304	L305	F306	T307			
SER	GLU	LEU	SER	GLN	GLU	ASP	LEU	ASP	ASP	ASP	GLU	ASP	GLU	ASP	ASP	GLU	ASP	GLY	ASP	ASP	ASP	ASP	ALA	ASP	ASP	ASP	ASN	SER	I212	D213	P214	E215	L216	A217	R218		E223	L224	R225	A226	Q227	GLY	PHE	VAL	ASP	PRO	PRO	ASN	ALA	GLU	GLU	ASP	LEU	ALA	PRO	THR	ALA	THR	HIS	VAL	GLY

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	188.52Å 205.18Å 310.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.95 – 3.84 29.95 – 3.84	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.95-3.84) 79.1 (29.95-3.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.08 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.236 , 0.300 0.243 , 0.301	Depositor DCC
R_{free} test set	1859 reflections (1.62%)	wwPDB-VP
Wilson B-factor (Å ²)	136.1	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 140.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	55388	wwPDB-VP
Average B, all atoms (Å ²)	170.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.12% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 4C4, 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	0.95	0/1801	1.55	28/2440 (1.1%)
1	B	0.67	1/2265 (0.0%)	1.29	21/3066 (0.7%)
1	G	0.65	0/1777	1.30	14/2408 (0.6%)
1	H	0.67	0/1681	1.34	21/2278 (0.9%)
2	C	0.96	4/10733 (0.0%)	1.56	199/14482 (1.4%)
2	I	0.78	0/10721	1.41	129/14468 (0.9%)
3	D	0.93	4/9202 (0.0%)	1.56	164/12424 (1.3%)
3	J	0.77	0/9161	1.45	136/12366 (1.1%)
4	E	0.83	1/693 (0.1%)	1.47	13/935 (1.4%)
4	K	0.47	0/629	1.12	5/847 (0.6%)
5	F	0.72	0/3777	1.31	32/5076 (0.6%)
5	L	0.60	0/3689	1.22	25/4969 (0.5%)
All	All	0.82	10/56129 (0.0%)	1.45	787/75759 (1.0%)

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
1	B	0	1
2	C	0	3
2	I	0	3
3	D	0	5
3	J	0	2
All	All	0	14

The worst 5 of 10 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	127	ILE	CA-CB	-8.73	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	127	ILE	CA-C	-6.21	1.47	1.52
3	D	115	TRP	CA-C	-5.54	1.45	1.52
4	E	17	PHE	CA-C	-5.39	1.48	1.53
3	D	457	TYR	CA-C	-5.25	1.45	1.52

The worst 5 of 787 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	354	ASP	CA-C-N	13.28	132.97	119.56
2	I	354	ASP	C-N-CA	13.28	132.97	119.56
3	D	358	GLY	CA-C-N	-12.99	103.61	119.84
3	D	358	GLY	C-N-CA	-12.99	103.61	119.84
2	C	534	GLY	CA-C-N	12.90	133.77	119.83

There are no chirality outliers.

5 of 14 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	196	THR	Peptide
2	C	236	LYS	Peptide
2	C	600	THR	Peptide
2	C	658	GLN	Peptide
3	D	14	THR	Peptide

5.2 Too-close contacts [i](#)

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	1779	0	1806	354	0
1	B	2239	0	2300	505	0
1	G	1755	0	1773	338	0
1	H	1662	0	1687	295	0
2	C	10564	0	10571	1912	1
2	I	10552	0	10548	1844	0
3	D	9062	0	9227	1861	1
3	J	9021	0	9213	1842	1
4	E	691	0	695	97	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	107	0
5	F	3726	0	3798	660	1
5	L	3640	0	3650	595	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	31	33	32	16	0
All	All	55355	33	55934	9716	2

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 87.

The worst 5 of 9716 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:88:LEU:HD12	1:B:89:ALA:H	1.07	1.18
2:I:280:ASP:HB3	2:I:282:VAL:HG23	1.24	1.18
3:D:850:LYS:HG2	3:D:857:LEU:HD11	1.24	1.18
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.04	1.17
3:D:1372:ARG:HH21	3:J:854:ALA:HB3	1.07	1.15

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:170:GLU:OE1	3:J:165:TYR:OH[3_444]	2.04	0.16
2:C:44:GLU:OE1	5:F:599:ARG:NE[4_445]	2.09	0.11

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	227/329 (69%)	179 (79%)	35 (15%)	13 (6%)	1	16
1	B	283/329 (86%)	167 (59%)	60 (21%)	56 (20%)	0	1
1	G	225/329 (68%)	177 (79%)	40 (18%)	8 (4%)	2	23
1	H	212/329 (64%)	170 (80%)	35 (16%)	7 (3%)	3	24
2	C	1338/1342 (100%)	1019 (76%)	256 (19%)	63 (5%)	2	19
2	I	1338/1342 (100%)	1031 (77%)	261 (20%)	46 (3%)	3	24
3	D	1162/1407 (83%)	850 (73%)	234 (20%)	78 (7%)	1	14
3	J	1151/1407 (82%)	851 (74%)	232 (20%)	68 (6%)	1	16
4	E	87/91 (96%)	69 (79%)	14 (16%)	4 (5%)	2	19
4	K	77/91 (85%)	61 (79%)	13 (17%)	3 (4%)	2	21
5	F	454/613 (74%)	342 (75%)	89 (20%)	23 (5%)	1	18
5	L	454/613 (74%)	336 (74%)	94 (21%)	24 (5%)	1	17
All	All	7008/8222 (85%)	5252 (75%)	1363 (19%)	393 (6%)	1	16

5 of 393 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	136	GLU
1	A	162	GLU
1	B	11	PRO
1	B	12	ARG
1	B	44	ARG

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 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	197/286 (69%)	154 (78%)	43 (22%)	1	6
1	B	250/286 (87%)	167 (67%)	83 (33%)	0	1
1	G	193/286 (68%)	164 (85%)	29 (15%)	3	16
1	H	183/286 (64%)	148 (81%)	35 (19%)	1	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1154/1157 (100%)	933 (81%)	221 (19%)	1	9
2	I	1151/1157 (100%)	956 (83%)	195 (17%)	2	13
3	D	963/1168 (82%)	728 (76%)	235 (24%)	1	4
3	J	965/1168 (83%)	749 (78%)	216 (22%)	1	5
4	E	72/75 (96%)	59 (82%)	13 (18%)	2	11
4	K	67/75 (89%)	60 (90%)	7 (10%)	7	26
5	F	406/540 (75%)	340 (84%)	66 (16%)	2	14
5	L	385/540 (71%)	334 (87%)	51 (13%)	4	19
All	All	5986/7024 (85%)	4792 (80%)	1194 (20%)	1	9

5 of 1194 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	47	ARG
5	L	136	GLU
3	J	242	LEU
3	J	46	TYR
3	J	682	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 125 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	345	GLN
3	J	1244	GLN
2	I	510	GLN
3	J	1218	HIS
5	L	309	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 6 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	$\# Z > 2$
8	4C4	D	2004	-	31,31,31	0.57	0	32,40,40	0.95	2 (6%)

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
8	4C4	D	2004	-	-	12/30/31/31	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	2004	4C4	O5-C15-C16	3.01	113.99	111.35
8	D	2004	4C4	C4-C3-C2	2.21	119.22	115.68

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	2004	4C4	C13-C1-C2-C3
8	D	2004	4C4	O5-C15-C16-C18
8	D	2004	4C4	O5-C15-C16-C17
8	D	2004	4C4	C14-C15-C16-C17

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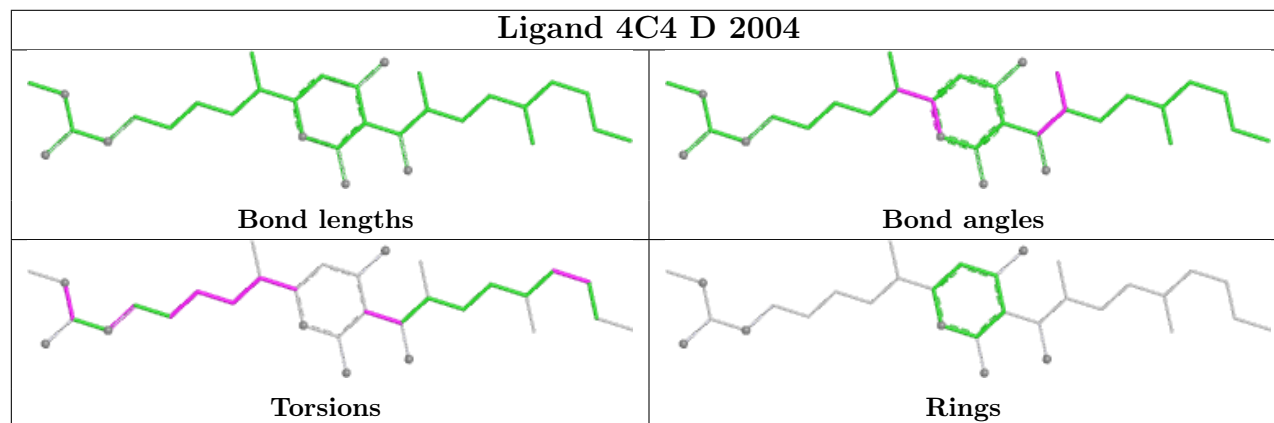
Mol	Chain	Res	Type	Atoms
8	D	2004	4C4	C17-C16-C18-C19

There are no ring outliers.

1 monomer is involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C4	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 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	229/329 (69%)	-0.55	0 100 100	85, 130, 177, 246	0
1	B	289/329 (87%)	-0.53	0 100 100	100, 194, 249, 268	0
1	G	227/329 (68%)	-0.49	0 100 100	184, 217, 237, 248	0
1	H	216/329 (65%)	-0.35	1 (0%) 87 71	179, 244, 274, 286	0
2	C	1340/1342 (99%)	-0.54	0 100 100	75, 125, 228, 303	0
2	I	1340/1342 (99%)	-0.55	1 (0%) 92 87	124, 163, 252, 431	0
3	D	1166/1407 (82%)	-0.52	0 100 100	84, 126, 211, 261	0
3	J	1155/1407 (82%)	-0.51	0 100 100	122, 169, 233, 316	0
4	E	89/91 (97%)	-0.64	0 100 100	118, 140, 168, 177	0
4	K	79/91 (86%)	-0.31	1 (1%) 75 53	223, 285, 342, 352	0
5	F	458/613 (74%)	-0.46	0 100 100	115, 176, 321, 349	0
5	L	458/613 (74%)	-0.42	0 100 100	153, 197, 350, 376	0
All	All	7046/8222 (85%)	-0.51	3 (0%) 100 100	75, 159, 278, 431	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	733	VAL	2.5
4	K	6	VAL	2.3
1	H	24	ALA	2.0

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

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](#)

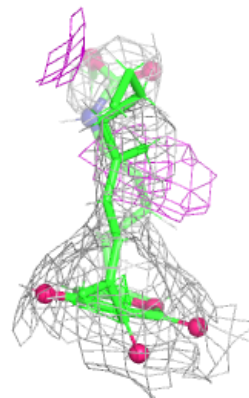
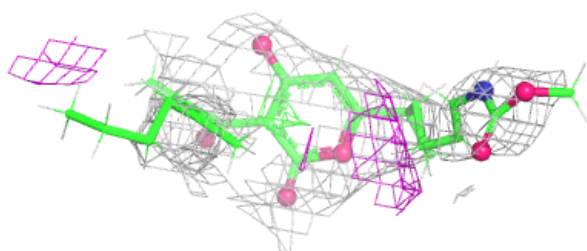
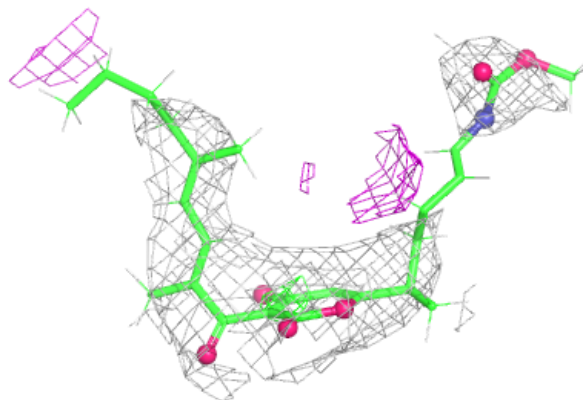
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	MG	D	2001	1/1	0.93	0.09	126,126,126,126	0
8	4C4	D	2004	31/31	0.95	0.15	128,154,155,155	0
7	ZN	J	2003	1/1	0.97	0.06	130,130,130,130	0
6	MG	J	2001	1/1	0.97	0.05	127,127,127,127	0
7	ZN	D	2003	1/1	0.99	0.02	125,125,125,125	0
7	ZN	J	2002	1/1	0.99	0.06	143,143,143,143	0
7	ZN	D	2002	1/1	1.00	0.02	126,126,126,126	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 4C4 D 2004:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.