



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:39 PM GMT

PDB ID : 4YFX
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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

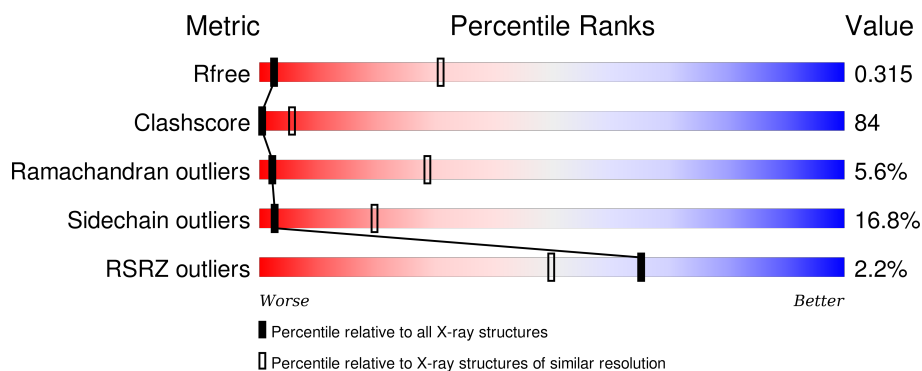
1 Overall quality at a glance

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}	91344	1334 (4.18-3.50)
Clashscore	102246	1036 (4.16-3.52)
Ramachandran outliers	100387	1415 (4.18-3.50)
Sidechain outliers	100360	1410 (4.18-3.50)
RSRZ outliers	91569	1342 (4.18-3.50)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	

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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MG	J	2001	-	-	-	X
8	4C4	D	2004	-	-	-	X

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			

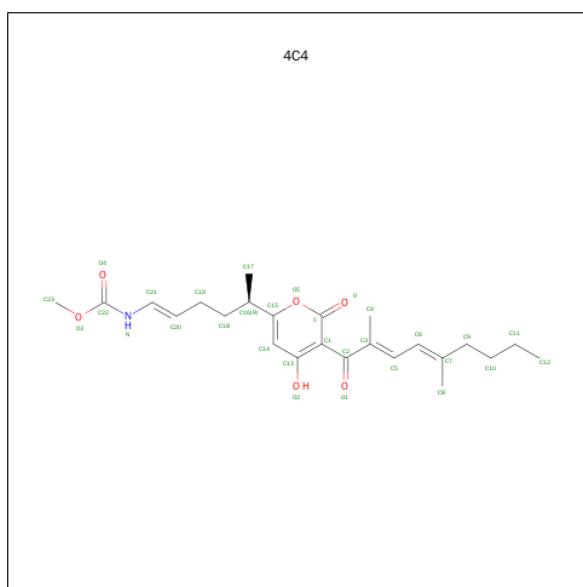
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

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

- Molecule 8 is Myxopyronin B (three-letter code: 4C4) (formula: C₂₄H₃₃NO₆).

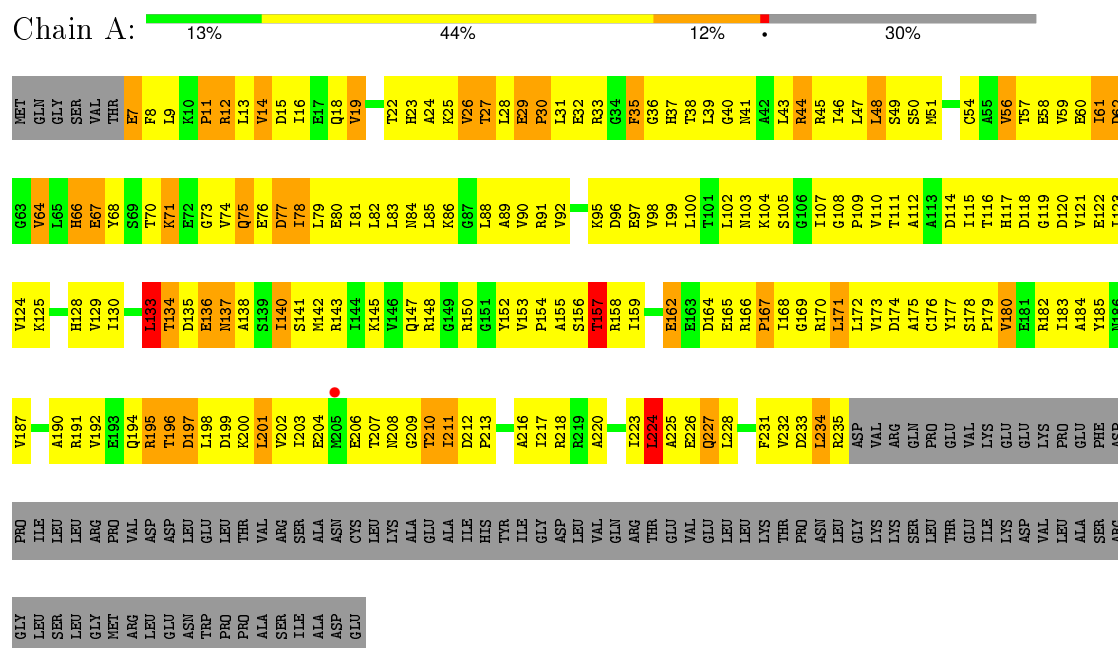


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	D	1	Total	C	H	N	O	0	0
			64	24	33	1	6		

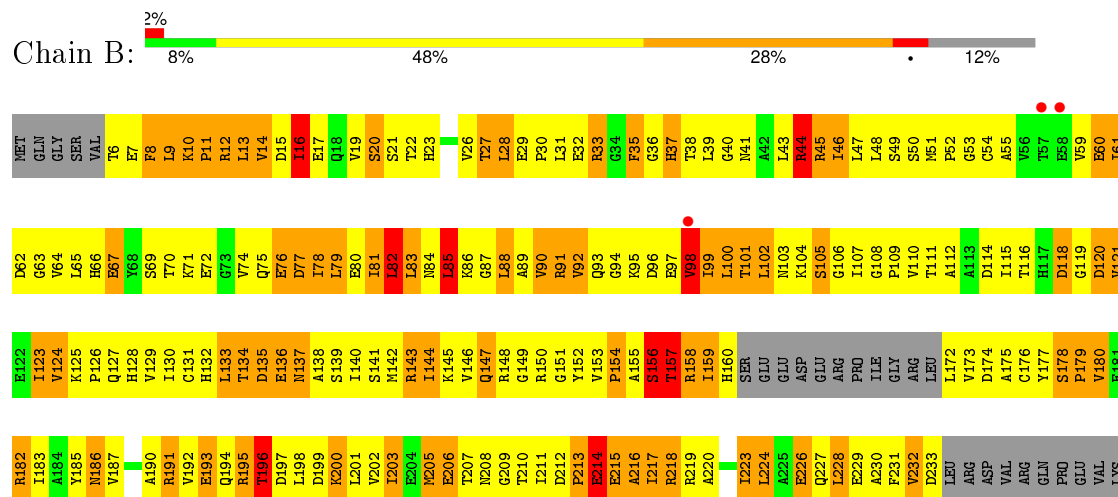
3 Residue-property plots

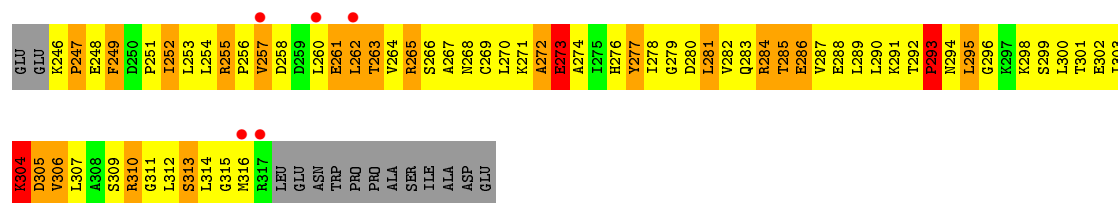
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

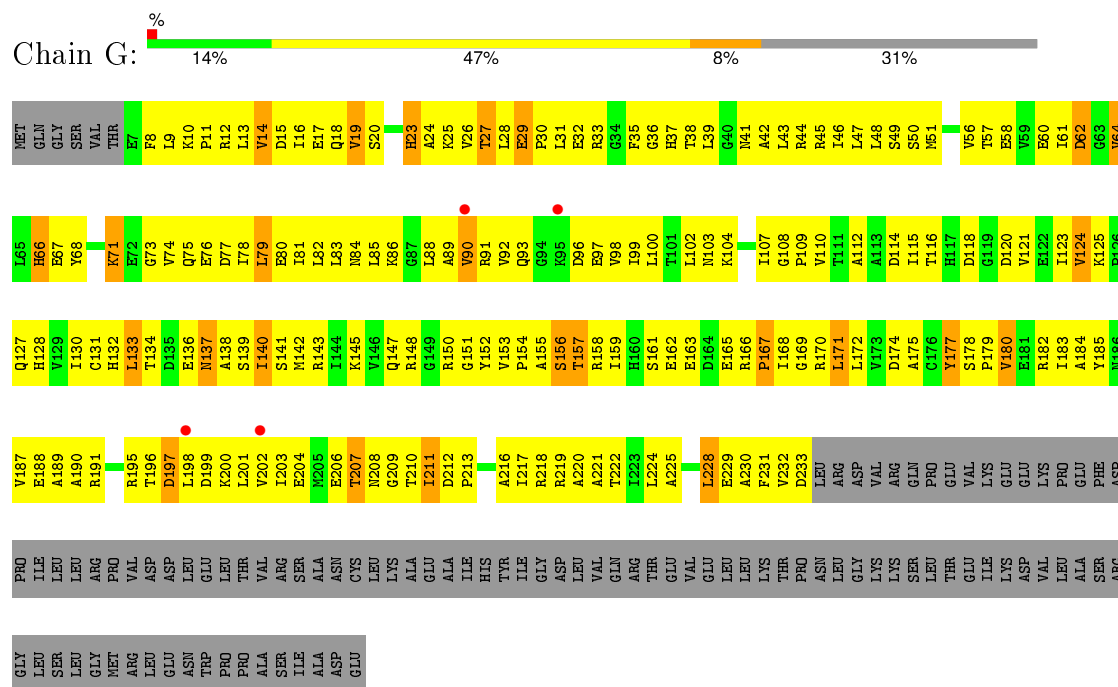


• Molecule 1: DNA-directed RNA polymerase subunit alpha

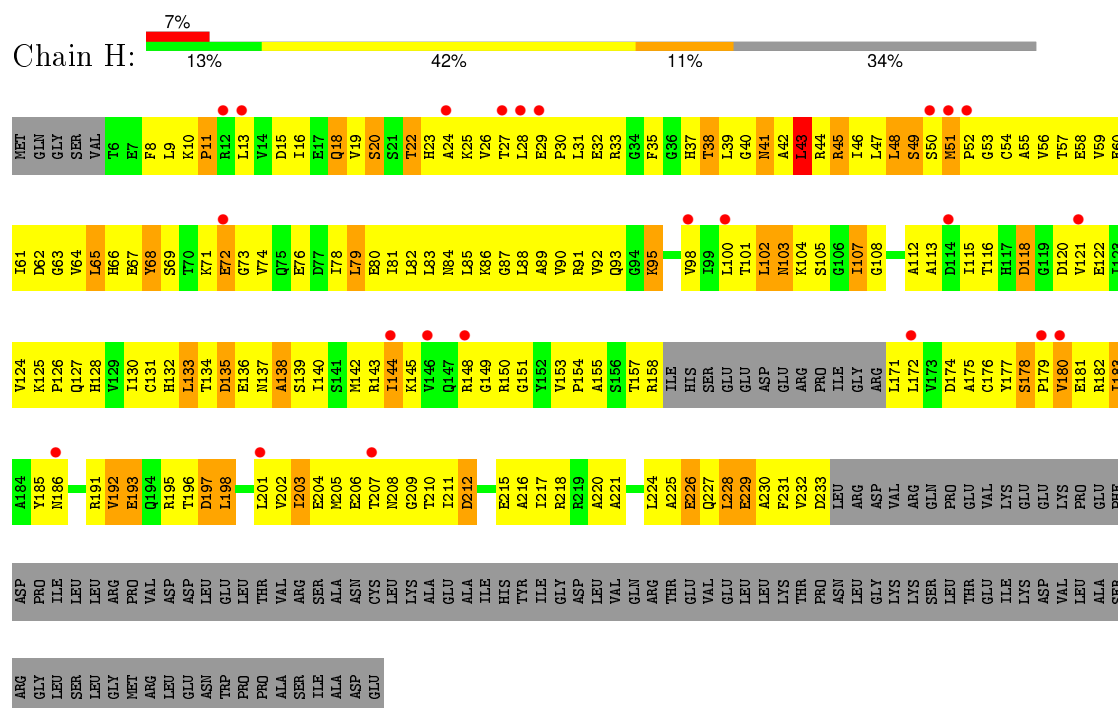




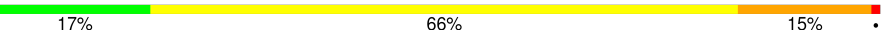
• Molecule 1: DNA-directed RNA polymerase subunit alpha



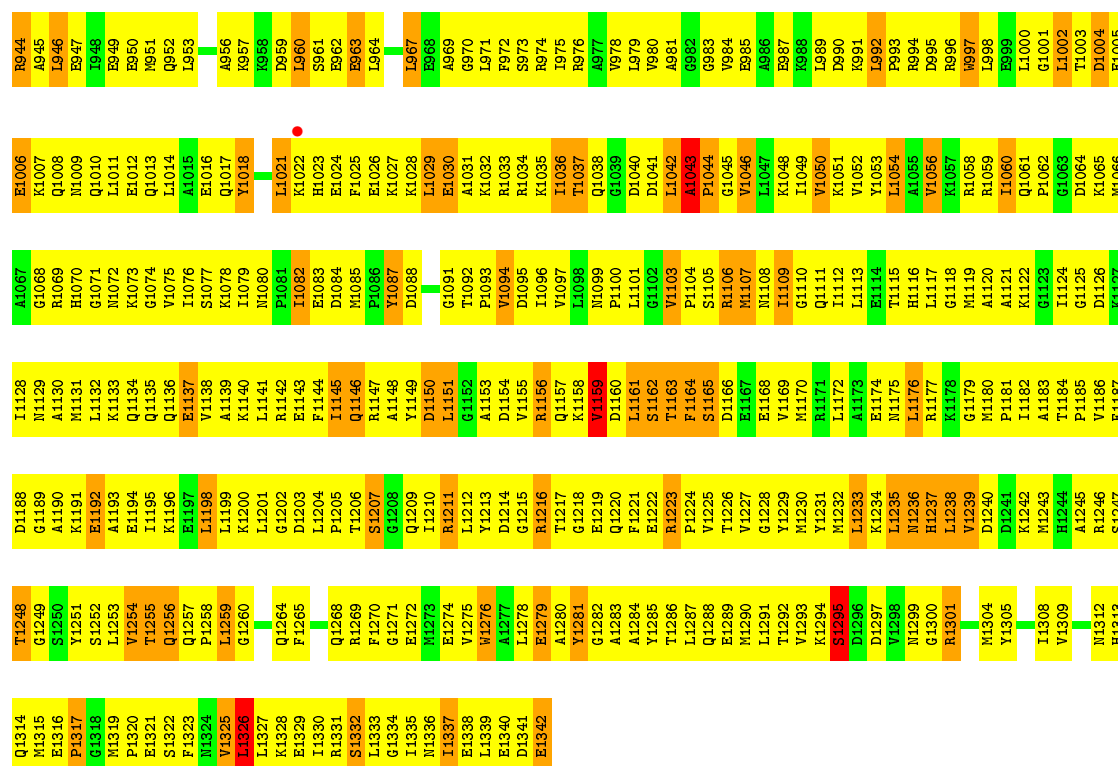
• Molecule 1: DNA-directed RNA polymerase subunit alpha



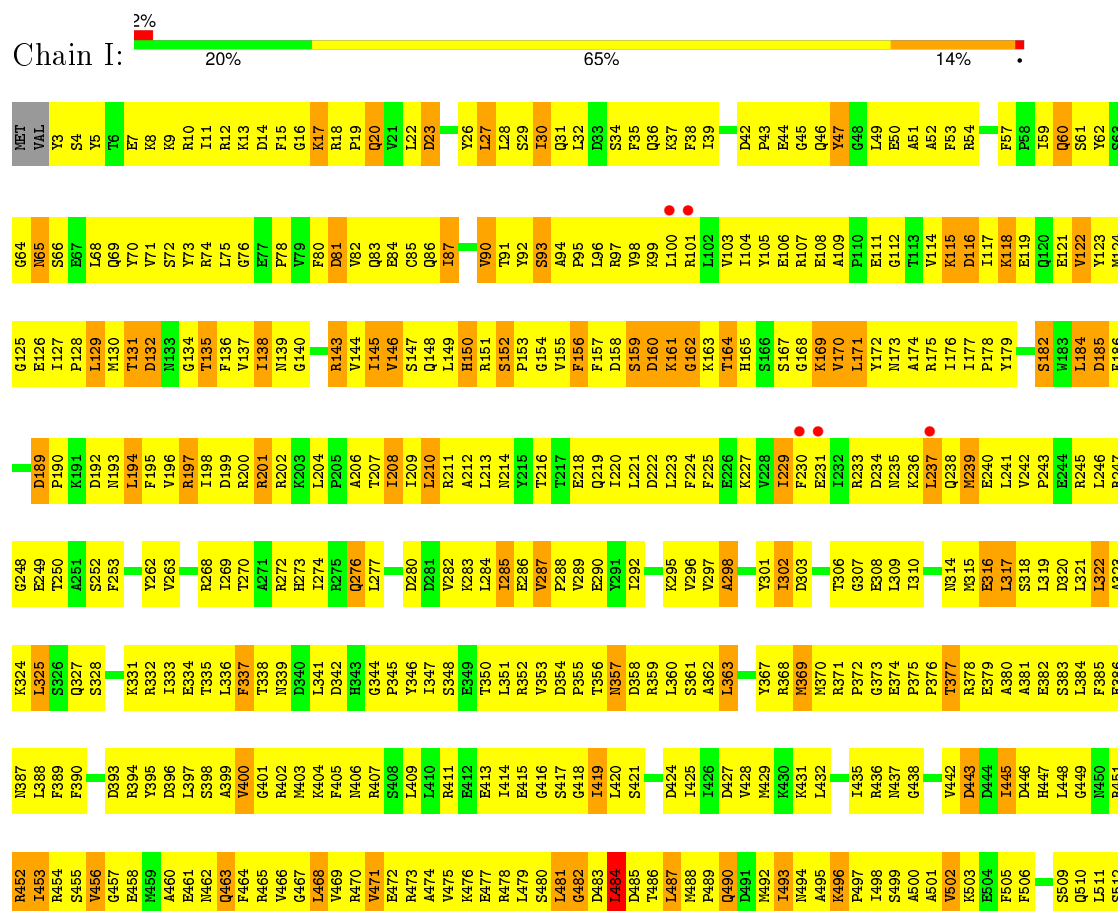
• Molecule 2: DNA-directed RNA polymerase subunit beta

Chain C:  17% 66% 15%

NET	VAL	Y3	S4	Y5	T6	E7	K8	R9	R10	R11	R12	R13	R14	R15	G16	R17	R18	R19	Q20	Y21	D22	D23	Y26	L27	S28	S29	I30	Q31	L32	F35	Q36	K37	F38	I39	E40	Q41	D42	P43	R44	Q45	Q46	Y47	Q48	L49	E50	A51	A52	P53	R54	S55	V56	F57	P58	I59	Q60	S61	Y62																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																															



• Molecule 2: DNA-directed RNA polymerase subunit beta

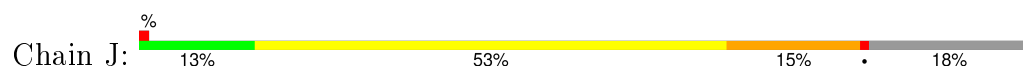




WORLDWIDE
PDB
PROTEIN DATA BANK

M1350	M1351	I1352	V1353	G1354	R1355	L1356	I1357	P1358	A1359	G1360	T1361	G1362	V1363	H1364	D1365	L1366	L1367	P1368	R1369	M1370	R1371	R1372	R1373	A1374	A1375	G1376	GLU	ALA	ALA	PRO	GLN	VAL	THR	ALA	F1325	L1326	K1327	T1328	T1329	R1330	V1331	L1332	T1333	E1334	A1335	V1336	A1337	G1338	K1339	L1340	R1341	D1342	E1343	L1344	ASP	E1345	R1346	L1347	E1348	E1349
I1287	A1288	P1289	E1290	A1294		K1297	V1298	G1299	L1300	T1301	F1302	S1303	R1304	D1305	L1306	L1307	G1308	I1309	T1310	K1311	A1312	S1313	L1314	A1315	T1316	F1317	P1318	G1319	L1320	P1321	A1322	A1323	S1324	F1325	L1326	K1327	T1328	T1329	R1330	V1331	L1332	T1333	E1334	A1335	V1336	A1337	G1338	K1339	L1340	R1341	D1342	E1343	L1344	ASP	E1345	R1346	L1347	E1348	E1349	
V1226	H1227	A1228	V1229	T1230	R1231	V1232	T1233	V1234	E1235	V1237	Q1238	D1239	V1240	V1241	R1242	L1243		V1246	K1247	L1248	M1249	D1250	K1251	H1252	L1253	V1254	V1255	L1256	V1257	R1258	Q1259	T1260	L1266	V1267	M1268	E1269	G1270	S1271	S1272	D1273	F1274	L1275	E1276	G1277	L1278	Q1279	V1280	E1281	L1282	S1283	L1284	R1285	V1286							
G1166	K1167	A1168	T1169	K1170	G1171	K1172	A1173	R1174	L1175	V1176	T1177	P1178	V1179	G1180	D1181	G1182	S1183	D1184	P1185	T1186	E1187	E1188	M1189	T1190	P1191	K1192	A1193	E1194	G1195	L1196	N1197	F1198	E1199	L1200	G1201	E1202	R1203	V1204	E1205	R1206	G1207	N1208	V1209	I1210	S1211	D1212	G1213	P1214	L1215	E1216	P1217	D1218	E1219	E1220	L1221	A1222	L1223	S1224	G1225	
ILE	VAL	GLN	LEU	GLU	ASP	GLY	VAL	GLN	ILE	SER	GLY	ASP	THR	LEU	ALA	ARG	ILE	PRO	GLN	GLU	SER	GLY	GLY	THR	LYS	ASP	ILE	T1135	G1136	G1137	L1138	P1139	R1140	V1141	A1142	D1143	L1144	F1145	E1146	A1147	R1148	R1149	P1150	K1151	P1152	P1153	A1154	I1155	L1156	A1157	E1158	D1159	E1160	S1160	I1162	V1163	V1164	S1165		

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

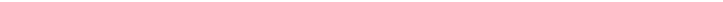


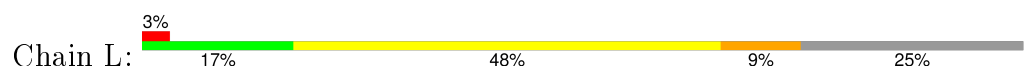
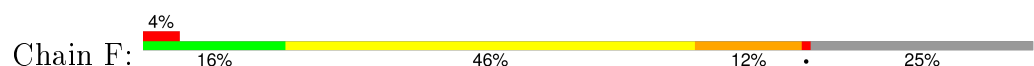
D588	A494	G433	P669	N309	P247	I185	I124	I61	MET
A559	M495	I434	K370	G310	D248	Q186	G125	F62	
N560	G496	Q435	K371	R311	L249	A187	G126	G63	ASP
E497	A497	A436	K372	R312	R251	L188	L127	L64	
E562	G498	F437	A373	G313	R251	L189	L128	LEU	
L563	I499	E438	L374	R314	L282	K190	D129	D67	LYS
V564	I500	P439	E375	A315	V253	S191	M130	Y68	PHE
A565	V501	V440	L376	L316		M192	P131	E69	LEU
E566	S502	L441	F377	T317		D193	L132	C70	LYS
F503	F503	I442	K378	G318		L194	R133	L71	ALA
S504	O504	E443	P379	S319		E195	D134	C72	GLN
D505	D505	G444	F380	N320	F260	Q196	D135	G73	THR
L506	V506	K445	L381	R321	A261	E197	E136	K74	LYS
D571	V507	V446	Y382	P322	T262	C198	R137	Y75	THR
T572	L508	I447		P323	S263		V138	K76	GLU
T573	G509	Q448		L324	D264		L139		E16
V574	L510	L449	L385	K325	L265		Y140	H80	F17
G575	Y511	H450	L390	S326		E203	F141	R81	D18
R576	Y512	P451	A391	S326	V266		E148	G82	A19
L577	M513	L452	T392	L327	D267	E204	E143	I20	
I578	T514	K453	T393	A328	L268	L205	S142	V83	K21
L579	R515	G454	L394	D329	Y269	N206	Y144	I84	
M580	D516	C454	L395	M330	R270	E207	V145	G85	I22
C517	C517		K395	L331	R271	T208	V146	E86	A23
			A396	K332		D209	I147	K87	L24
				G333		S210	E148	C88	A25
				K334		E211	G149	G89	S26
				Q335		T212	G150	V90	P27
				G336		K213	M151	E91	D28
				V401		R214	T152	V92	K29
				D462		K277	K215	T93	I30
				G463		F338	K216	Q94	R31
				Q463		R339	E155	S32	K33
				Q465		Q340	L156	K96	W33
				M466		R281	R157	V97	F35
				A467		L342	Q157	E37	G36
				V468		L343	T158	E100	R99
				H469		G344	L160	K39	
				V470		R345	T161	R101	V38
				A409		C346	L224	M102	K40
				D410		V347	E225	G103	P41
				L411		L287	A226	H104	E42
				L412		P288	V228	I105	T43
				D413		D289	L86	E106	L44
				E414		S350	V228	N45	
				E475		G351	Q229	S109	Y46
				Q476		R352	D229	P110	R47
				S339		G352	Q229	T111	T48
				G540		L416	A168	A112	F49
				Q477		V292	D174	E113	K50
				R478		L239	E175	I114	P51
				L473		R353	M237	H113	L56
				E479		V354	G231	L189	F57
				A481		E418	G231	A108	L120
				L480		L355	N294	E170	C58
				H419		I356	E295	K233	P121
				F420		T356	F172	P110	S49
				R481		V357	E171	T111	E62
				A482		R297	G173	A112	
				L483		V421	E235	E113	
				L484		L422	W236	H113	
				M485		L233	D175	I114	
				L486		R361	E176	W115	
				L487		L362	D177	F116	
				M488		R362	F177	L117	
				L489		R363	A178	K118	
				L490		L364	E179	S119	
				L491		R365	M180	L56	
				L492		L429	G181	L120	
				L493		H430	A182	P121	
				L494		R431	E183	L245	
				L495		A426	G367	S122	
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				L608		L538	L358		
				L609		L539	L359		
				L610		L540	L360		
				L611		L541	L361		
				L612		L542	L362		
				L613		L543	L363		
				L614		L544	L364		
				L615		L545	L365		
				L616		L546	L366		
				L617		L547	L367		
				L618		L548	L368		
				L619		L549	L369		
				L620		L550	L370		
				L621		L551	L371		
				L622		L552	L372		
				L623		L553	L373		
				L624		L554	L374		
				L625		L555	L375		
				L626		L556	L376		
				L627		L557	L377		
				L628		L558	L378		
				L629		L559			

- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  22% 67% 9%

E68	R69	Q70	E71	E74	E75	E76	A77	A78	E79	Q80	Q81	A82	V83	T84	A85	I86	A87	E88	G89	R90	ARG	V6	Q7	D8	A9	V10	E11	M15	R16	F17	D18	L19	V20	L21	A24	R25	R26	A27	R28	Q29	M30	Q31	V32	G33	G34	R35	D36	P37	L38	V39	P40	E41	E42	M43	D44	K45	T46	L47	V48	I49	A50	L51	R52	E53	I54	E55	E56	G57	L58	I59	I63	L64	P67
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- Chain K: 



K557	R495	W434	A372	T311	E247	GLY	K121	ASP	MET
V558	K496	I435	R373	S312	E246	SER	R122	ALA	GLU
L559	V497	R436	R374	D313	L249	LEU	E123	ASP	GLN
	L498	Q437	A375	T314	L250	LEU	E124	ASP	ASN
	K499	A438	K376	W315	K251	SER		LEU	PRO
	I500	I439	K377	F316	L252	GLN	I127	MET	GLN
	A501	T440	E378	R317	S253	GLU	M128	LEU	SER
	R502	R441	R379	A318	E254	ASP	Q129	ALA	GLN
	E503	S442	V380	A319	V255	LEU	V130	GLU	LEU
	P504	I443	E381	I320	F256	ASP	Q131	ASN	LYS
	I505	A444	A382	A321	K257	ASP	C132	THR	LEU
	S506	D445	N383	K322	Q258	ASP	S133	ALA	LEU
	M507	Q446	L384	R323	F259	GLU	V134	VAL	VAL
	E508	A447	R385	K324	R260	ASP	A135	GLU	THR
	T509	R448	L386	P325	L261	GLU	E136	ASP	ARG
	P510	T449	V387	W326	V262	ASP	Y137	ALA	GLY
	I511	I450	I388	S327	F263	GLU	A138	ALA	LYS
	G512	R451	S389	E328	K264	GLU	E139	GLU	GLU
	D513	I452	I390	K329	Q265	ASP	A140	ALA	GLN
	D514	P453	A391	L330	F266	GLY	I141	ALA	GLY
		V454	K392	R331	D267	ASP	T142	ALA	TYR
		H455	K393	D332	Y268	ASP	Y143	GLN	LEU
		M456	Y394	V333	L269	ASP	L144	VAL	THR
		I457	T395	S334	V270	SER	L145	THR	TYR
		E458	N396	E335	N271	ALA	E146	SER	ALA
		T459	R397	E336	S272	ASP	Q147	SER	GLU
		I460	G398	V337	R273	ASP	Y148	VAL	VAL
		M461	L399	R338	R274	GLU	D149	GLN	ASN
		K462	Q400	R339	V275	ASN	R150	SER	ASP
		L463	F401	A340	K276	SER	V151	GLU	HIS
		M464	L402	L341	N277		E152	ILE	LEU
		R465	D403	Q342	D278		A153	GLY	PRO
		L466	L404	K343	R279		E154	ARG	GLU
		S467	I405	L344	V280		GLU	THR	ASP
		R468	Q406	Q345			T95	ILE	ILE
		Q469	E407	Q346			D96	VAL	VAL
		M470	G408	L347	E283		ARG	ASP	ASP
		L471	M409	E348	R285		LEU	SER	SER
		Q472	I410	E349	L286		R99	ASP	ASP
		M473	G411	E350	L287		LEU	LEU	GLN
		T474	L412		M288		ILE	ILE	ILE
		Q475	M413	L353	K289		THR	M102	GLU
		R476	K414	T354	L290		GLY	R103	GLU
		E477	A415	I355	C291		PHE	E104	ILE
		P478	V416	E356	V292		VAL	M105	ILE
		T479	D417	Q357	E293		ASP	G106	ASP
		E482	K418	V358	Q294		PRO	T107	GLN
		L483	F419	K359	C295		ASN	V108	ILE
		A484	E420	D360	K296		ALA	E109	ASN
		E485	Y421	I361	N297		GLU	L110	ASP
		R486	R422	N362	F298		GLU	L111	MET
		M487	R423	R363	K299		ASP	T112	GLY
		L488	F427	R364	C239		LEU	R113	ILE
		M489	S428	N365	R240		ALA	E114	GLN
		P490	T429	S366	S241		PRO	G115	VAL
		E491	Y430	I367	R242		THR	E116	MET
		D492	A431	G368	L305		ALA	I117	GLU
		K493	T432	E369	T307		THR	D118	ALA
		I494	W433	A370	K371		VAL	I119	ALA
								A120	PRO

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 44.64 – 3.84	Depositor EDS
% Data completeness (in resolution range)	92.4 (29.95-3.84) 79.3 (44.64-3.84)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.86 (at 3.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.236 , 0.300 0.259 , 0.315	Depositor DCC
R_{free} test set	1857 reflections (2.08%)	DCC
Wilson B-factor (Å ²)	138.5	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 117.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 106189 reflections	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 2.13% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, MG, 4C4

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	0.75	0/1801	1.11	5/2440 (0.2%)
1	B	0.52	0/2265	0.90	3/3066 (0.1%)
1	G	0.49	0/1777	0.88	0/2408
1	H	0.49	0/1681	0.93	4/2278 (0.2%)
2	C	0.79	4/10733 (0.0%)	1.13	39/14482 (0.3%)
2	I	0.63	0/10721	0.98	23/14468 (0.2%)
3	D	0.77	3/9202 (0.0%)	1.15	45/12424 (0.4%)
3	J	0.62	1/9161 (0.0%)	1.02	17/12366 (0.1%)
4	E	0.67	0/693	1.01	0/935
4	K	0.36	0/629	0.72	0/847
5	F	0.57	0/3777	0.93	6/5076 (0.1%)
5	L	0.48	0/3689	0.83	4/4969 (0.1%)
All	All	0.67	8/56129 (0.0%)	1.03	146/75759 (0.2%)

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 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	377	PHE	CE1-CZ	6.64	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1276	TRP	CB-CG	-6.57	1.38	1.50
2	C	1270	PHE	CE1-CZ	6.17	1.49	1.37
3	D	1319	PHE	CE2-CZ	6.01	1.48	1.37
3	J	686	TRP	CB-CG	-5.50	1.40	1.50

The worst 5 of 146 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	540	LEU	CA-CB-CG	-9.96	92.38	115.30
2	C	32	LEU	CA-CB-CG	-9.67	93.07	115.30
2	I	575	LEU	CA-CB-CG	-9.22	94.10	115.30
2	C	1161	LEU	CA-CB-CG	-9.16	94.23	115.30
3	D	788	LEU	CA-CB-CG	-9.10	94.38	115.30

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

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	347	0
1	B	2239	0	2300	482	0
1	G	1755	0	1773	325	0
1	H	1662	0	1687	285	0
2	C	10564	0	10571	1842	1
2	I	10552	0	10548	1775	0
3	D	9062	0	9227	1784	1
3	J	9021	0	9213	1774	1
4	E	691	0	695	88	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	104	0
5	F	3726	0	3798	623	1
5	L	3640	0	3650	576	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	17	0
All	All	55355	33	55934	9319	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 84.

The worst 5 of 9319 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%)	2	28
1	B	283/329 (86%)	167 (59%)	60 (21%)	56 (20%)	0	2
1	G	225/329 (68%)	177 (79%)	40 (18%)	8 (4%)	4	41
1	H	212/329 (64%)	170 (80%)	35 (16%)	7 (3%)	5	43
2	C	1338/1342 (100%)	1019 (76%)	256 (19%)	63 (5%)	3	33
2	I	1338/1342 (100%)	1031 (77%)	261 (20%)	46 (3%)	5	43
3	D	1162/1407 (83%)	850 (73%)	234 (20%)	78 (7%)	1	24
3	J	1151/1407 (82%)	851 (74%)	232 (20%)	68 (6%)	2	27
4	E	87/91 (96%)	69 (79%)	14 (16%)	4 (5%)	3	33
4	K	77/91 (85%)	61 (79%)	13 (17%)	3 (4%)	4	38
5	F	454/613 (74%)	342 (75%)	89 (20%)	23 (5%)	2	31
5	L	454/613 (74%)	336 (74%)	94 (21%)	24 (5%)	2	29
All	All	7008/8222 (85%)	5252 (75%)	1363 (19%)	393 (6%)	2	29

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%)	164 (83%)	33 (17%)	2	20
1	B	250/286 (87%)	169 (68%)	81 (32%)	0	3
1	G	193/286 (68%)	171 (89%)	22 (11%)	7	37
1	H	183/286 (64%)	149 (81%)	34 (19%)	2	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1154/1157 (100%)	982 (85%)	172 (15%)	4	26
2	I	1151/1157 (100%)	987 (86%)	164 (14%)	4	29
3	D	963/1168 (82%)	768 (80%)	195 (20%)	1	12
3	J	965/1168 (83%)	780 (81%)	185 (19%)	2	13
4	E	72/75 (96%)	65 (90%)	7 (10%)	10	44
4	K	67/75 (89%)	60 (90%)	7 (10%)	9	42
5	F	406/540 (75%)	346 (85%)	60 (15%)	4	26
5	L	385/540 (71%)	339 (88%)	46 (12%)	6	35
All	All	5986/7024 (85%)	4980 (83%)	1006 (17%)	2	20

5 of 1006 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1194	ARG
1	G	157	THR
3	J	1242	ARG
3	D	1278	GLU
5	F	448	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	317	ASN
2	I	357	ASN
3	J	1366	HIS
5	F	345	GLN
1	G	84	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 carbohydrates 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	-	26,31,31	1.39	2 (7%)	30,40,40	1.13	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	-	-	2/27/31/31	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C4	C1-C2	-5.60	1.39	1.50
8	D	2004	4C4	O5-C15	2.36	1.38	1.35

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	2004	4C4	C19-C20-C21	-2.37	117.17	125.06
8	D	2004	4C4	O5-C15-C14	2.86	122.29	119.72

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	D	2004	4C4	C23-O3-C22-O4
8	D	2004	4C4	C23-O3-C22-N

There are no ring outliers.

1 monomer is involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C4	17	0

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%)	-0.30	1 (0%) 93 88	85, 130, 177, 246	0
1	B	289/329 (87%)	-0.17	8 (2%) 56 40	100, 194, 249, 268	0
1	G	227/329 (68%)	-0.16	4 (1%) 71 56	184, 217, 237, 248	0
1	H	216/329 (65%)	0.45	23 (10%) 8 5	179, 244, 274, 286	0
2	C	1340/1342 (99%)	-0.28	4 (0%) 94 89	75, 125, 228, 303	0
2	I	1340/1342 (99%)	-0.18	33 (2%) 61 44	124, 163, 252, 431	0
3	D	1166/1407 (82%)	-0.28	7 (0%) 90 82	84, 126, 211, 261	0
3	J	1155/1407 (82%)	-0.20	20 (1%) 73 58	122, 169, 233, 316	0
4	E	89/91 (97%)	-0.26	0 100 100	118, 140, 168, 177	0
4	K	79/91 (86%)	0.53	8 (10%) 9 6	223, 285, 342, 352	0
5	F	458/613 (74%)	-0.06	24 (5%) 31 21	115, 176, 321, 349	0
5	L	458/613 (74%)	-0.00	21 (4%) 36 24	153, 197, 350, 376	0
All	All	7046/8222 (85%)	-0.18	153 (2%) 65 50	75, 159, 278, 431	0

The worst 5 of 153 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	319	ALA	7.4
5	L	315	TRP	6.8
5	F	305	LEU	6.2
5	F	304	THR	6.1
1	H	24	ALA	6.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
6	MG	J	2001	1/1	0.95	0.26	3.48	127,127,127,127	0
8	4C4	D	2004	31/31	0.89	0.43	2.97	128,154,155,155	0
7	ZN	D	2003	1/1	0.99	0.23	-0.86	125,125,125,125	0
7	ZN	J	2003	1/1	0.92	0.14	-1.05	130,130,130,130	0
7	ZN	D	2002	1/1	0.99	0.08	-1.15	126,126,126,126	0
7	ZN	J	2002	1/1	0.99	0.04	-1.41	143,143,143,143	0
6	MG	D	2001	1/1	0.98	0.42	-	126,126,126,126	0

6.5 Other polymers [i](#)

There are no such residues in this entry.