



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 22, 2024 – 09:56 PM EDT

PDB ID : 4XLQ  
Title : Crystal structure of T.aquaticus transcription initiation complex containing upstream fork (-11 base-paired) promoter  
Authors : Bae, B.; Darst, S.A.  
Deposited on : 2015-01-13  
Resolution : 4.60 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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

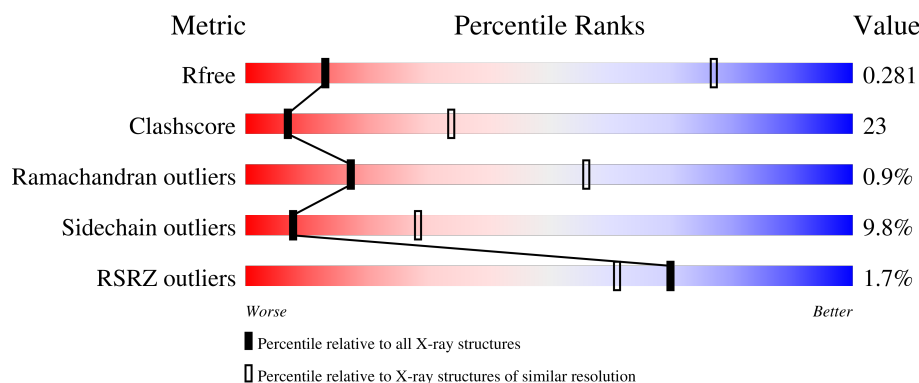
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.60 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))
$R_{free}$	130704	1062 (5.40-3.80)
Clashscore	141614	1130 (5.40-3.80)
Ramachandran outliers	138981	1074 (5.40-3.80)
Sidechain outliers	138945	1055 (5.40-3.80)
RSRZ outliers	127900	1113 (5.50-3.70)

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  $\geq 3$ , 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  $\leq 5\%$ . 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	314	<div> <div>40%</div> <div>28%</div> <div>•</div> <div>28%</div> </div>
1	B	314	<div> <div>33%</div> <div>34%</div> <div>5%</div> <div>28%</div> </div>
1	G	314	<div> <div>5%</div> <div>36%</div> <div>31%</div> <div>5%</div> <div>28%</div> </div>
1	H	314	<div> <div>35%</div> <div>32%</div> <div>5%</div> <div>28%</div> </div>
2	C	1119	<div> <div>2%</div> <div>45%</div> <div>48%</div> <div>6%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	I	1119	
3	D	1524	
3	J	1524	
4	E	99	
4	K	99	
5	F	347	
5	L	347	
6	O	30	
6	R	30	
7	P	26	
7	S	26	

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 56477 atoms, of which 0 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	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	B	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	G	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			
1	H	227	Total	C	N	O	S	0	0	0
			1770	1130	303	334	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			
2	I	1112	Total	C	N	O	S	0	0	0
			8739	5531	1553	1632	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1490	Total	C	N	O	S	0	0	0
			11761	7439	2088	2196	38			
3	J	1367	Total	C	N	O	S	0	0	0
			10779	6810	1923	2010	36			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			
4	K	93	Total	C	N	O	S	0	0	0
			768	490	136	138	4			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			
5	L	345	Total	C	N	O	S	0	0	0
			2787	1758	502	523	4			

- Molecule 6 is a DNA chain called DNA (30-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	O	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			
6	R	30	Total	C	N	O	P	0	0	0
			613	296	109	179	29			

- Molecule 7 is a DNA chain called DNA (26-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	P	25	Total	C	N	O	P	0	0	0
			510	245	91	149	25			
7	S	26	Total	C	N	O	P	0	0	0
			527	255	93	154	25			

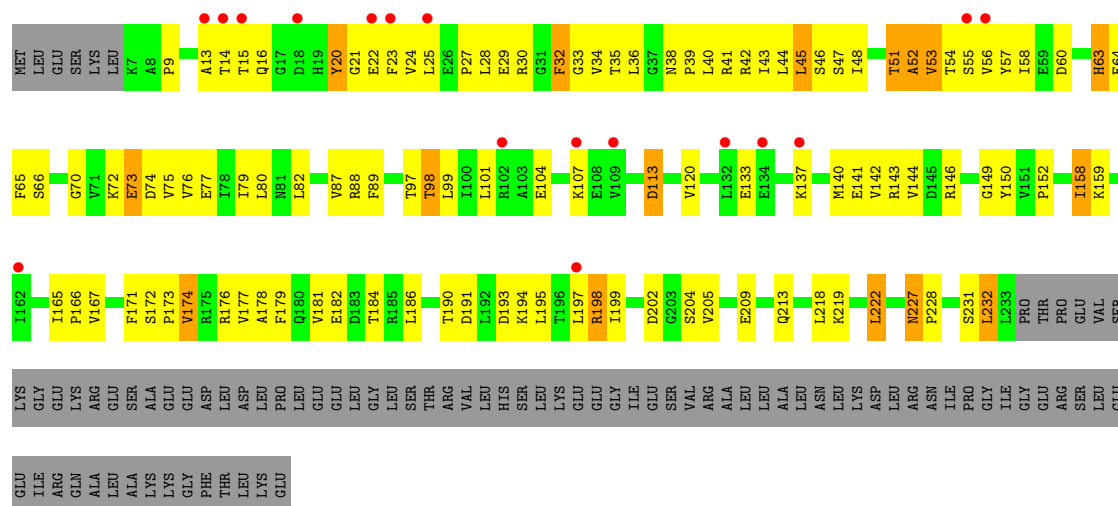
- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

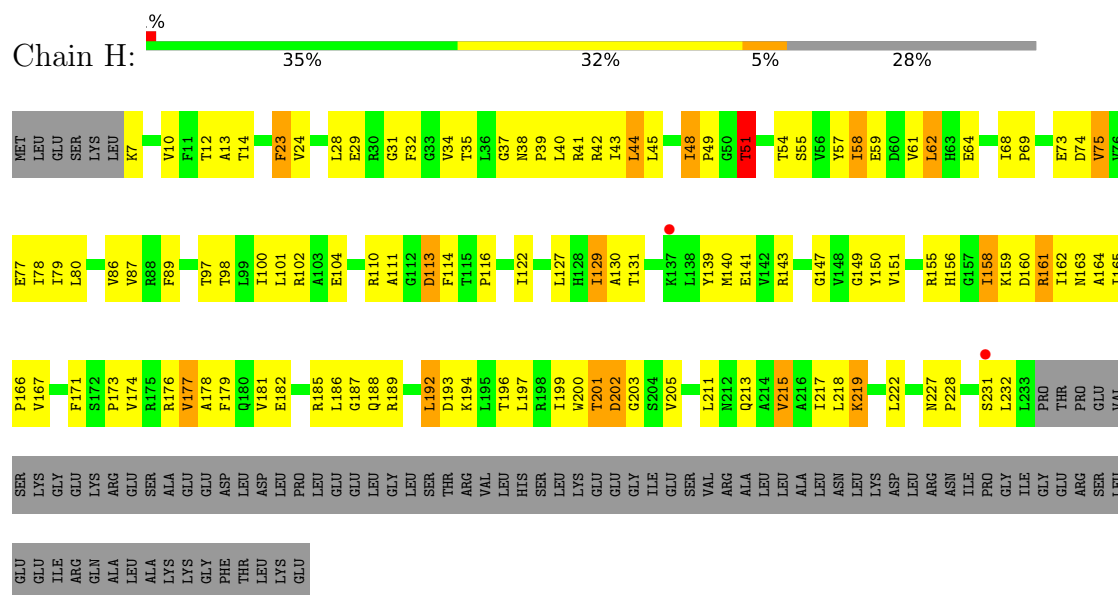
- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

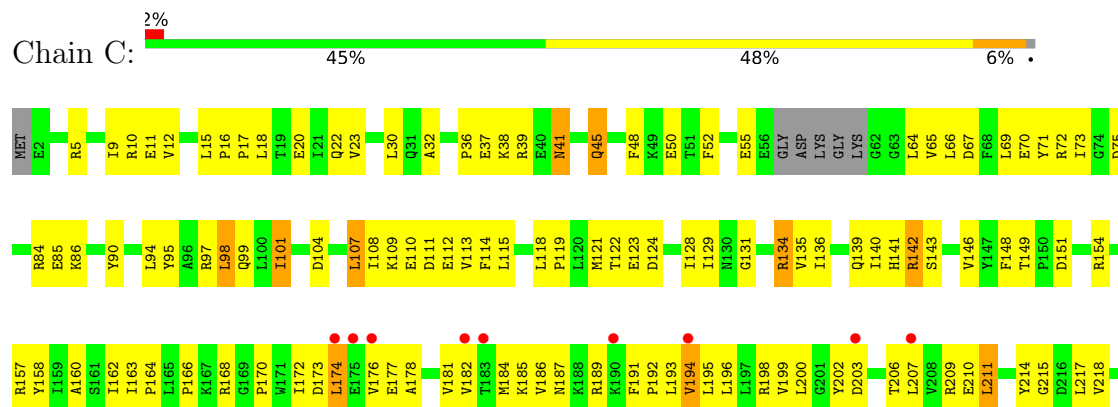


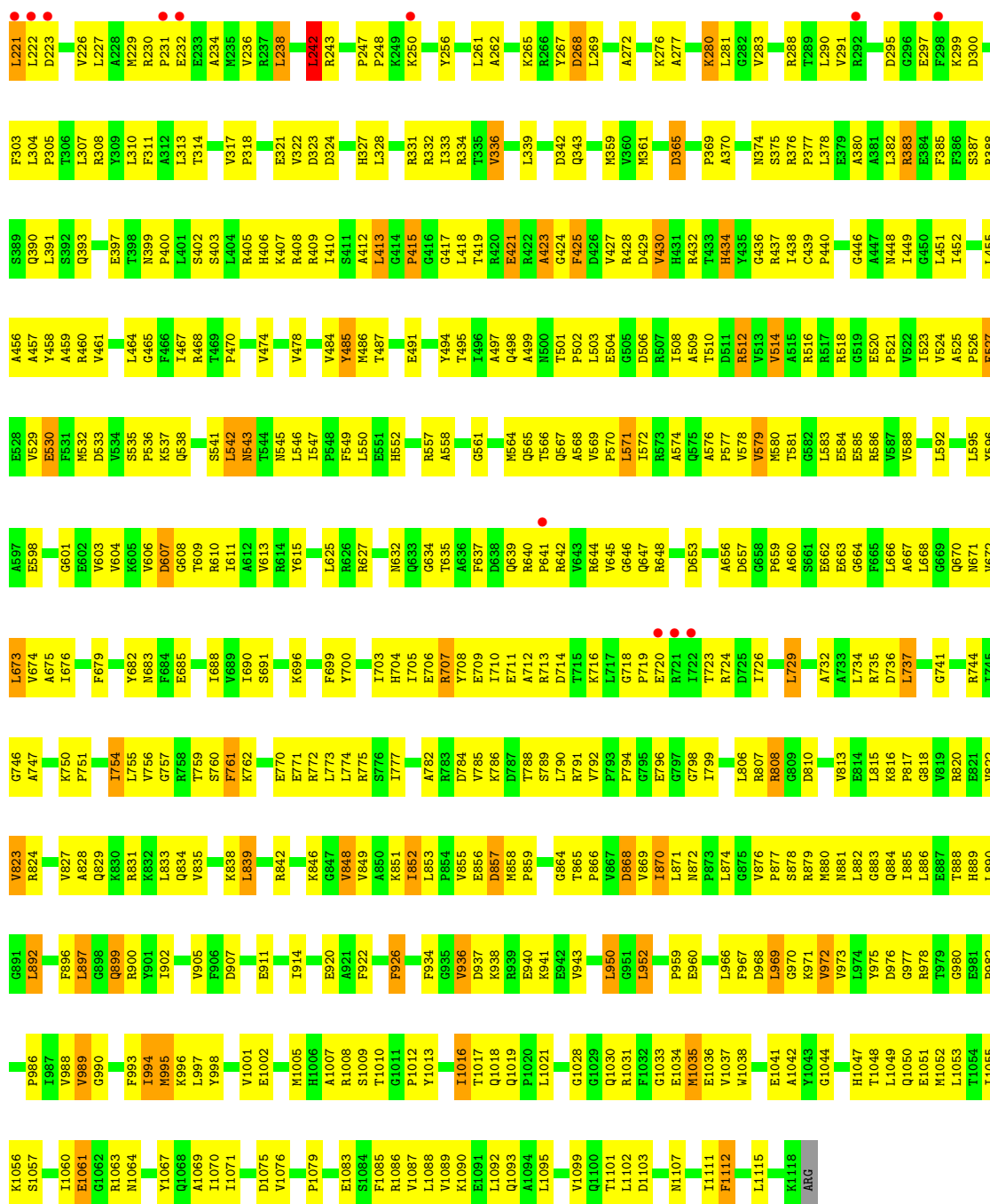


• Molecule 1: DNA-directed RNA polymerase subunit alpha

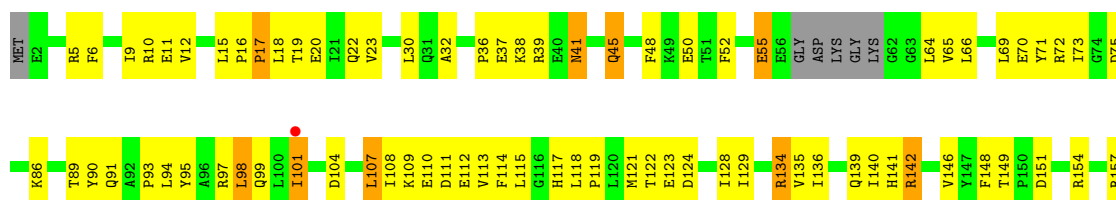


• Molecule 2: DNA-directed RNA polymerase subunit beta

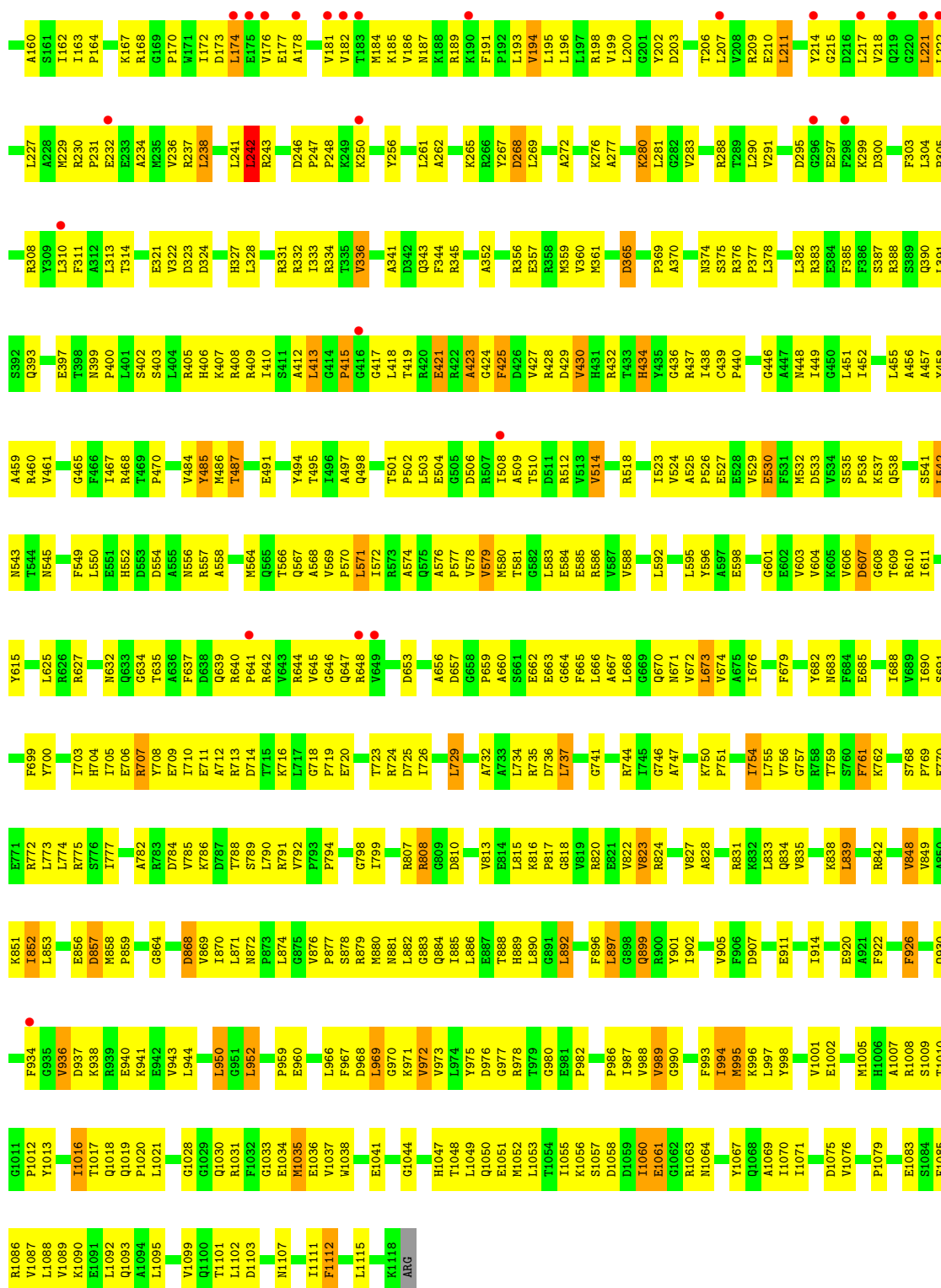




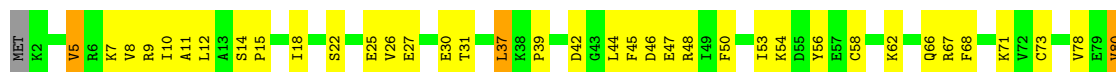
• Molecule 2: DNA-directed RNA polymerase subunit beta



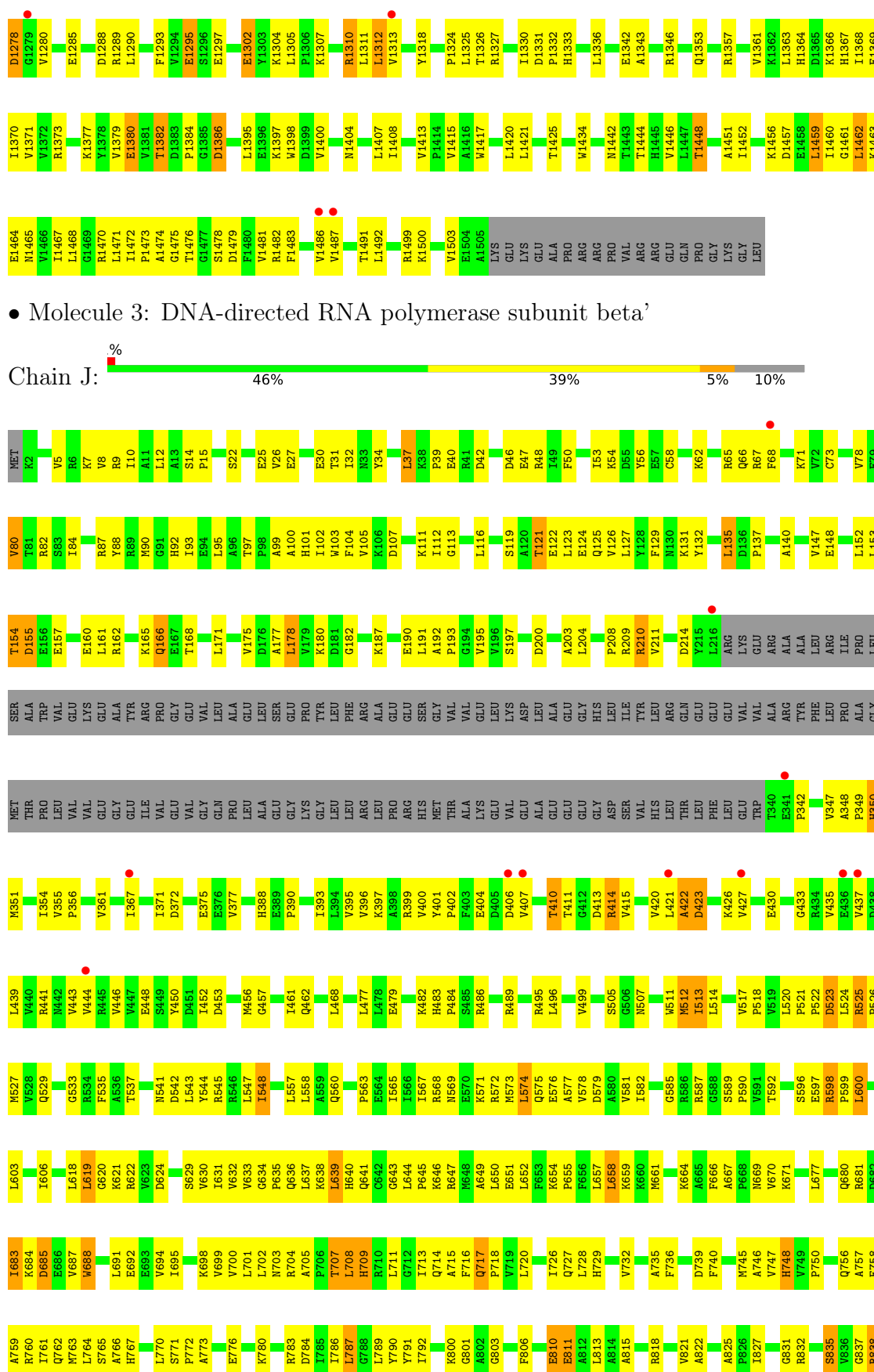




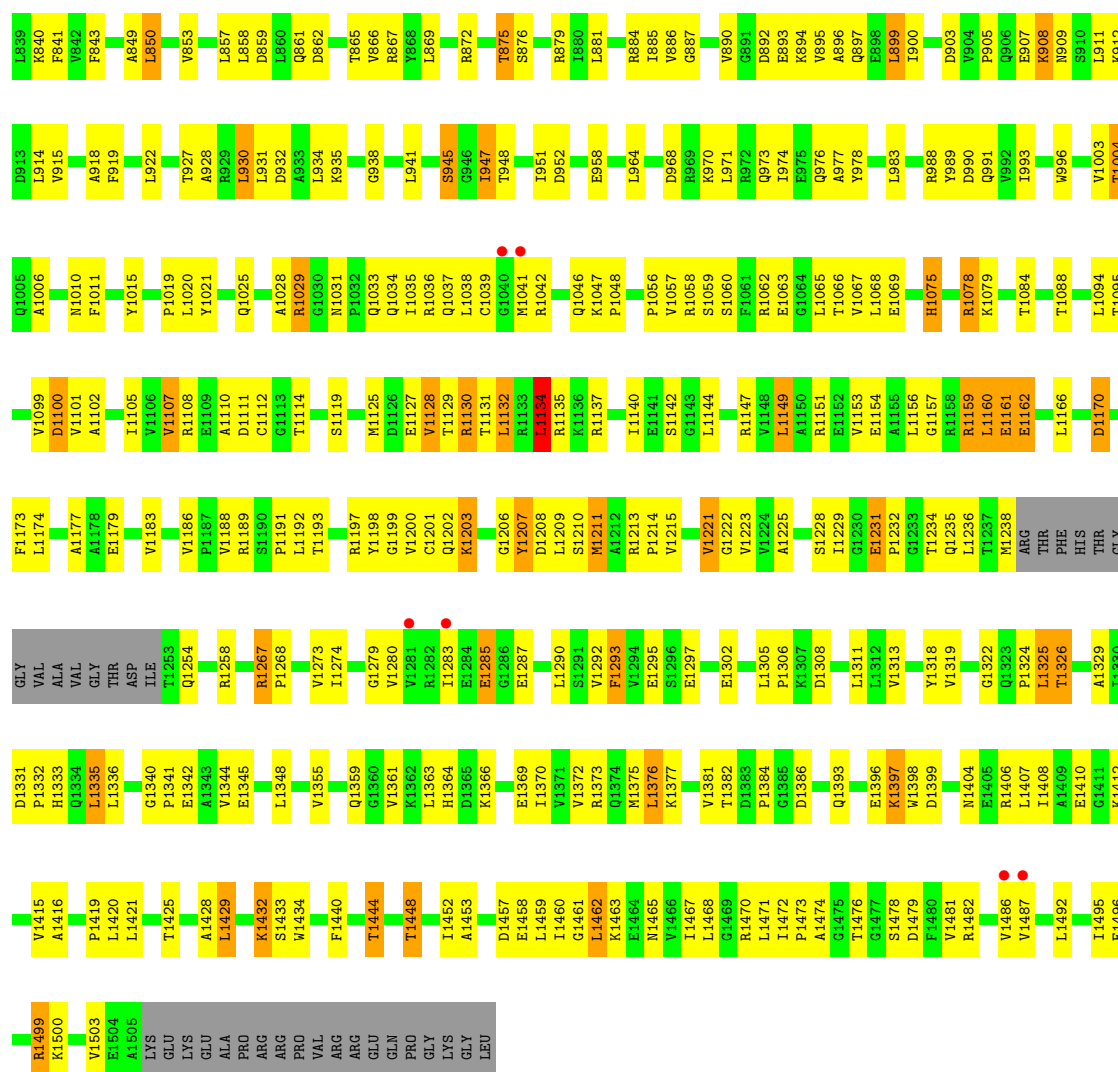
• Molecule 3: DNA-directed RNA polymerase subunit beta'



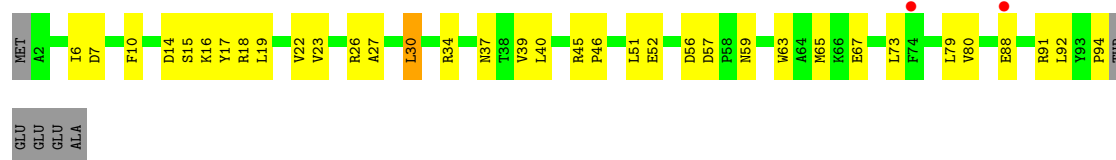
R1213	P1214	S1215	I1216	I1217	V1221	G1222	V1223	V1224	A1225	S1228	I1229	G1230	E1231	G1232	G1233	T1234	G1235	T1236	T1237	M1238	ARG	THR	PHE	HIS	THR	GLY	GLY	VAL	ALA	VAL	GLY	THR	ASP	ILE	T1253	Q1254	G1255	L1256	P1257	R1258	V1259	I1260	E1261	L1262	F1263	E1264	R1267	P1268	K1269	A1270	K1271	A1272	V1273	I1274	I1277						
D1139	I1140	E1141	S1059	S1060	F1061	R1062	E1063	G1064	L1065	T1066	V1067	L1068	E1069	H1075	R1078	K1079	E1161	E1162	G1163	R1164	L1165	S1166	L1167	L1168	E1169	D1170	I1171	L1172	E1173	K1174	E1175	L1176	E1177	A1178	L1179	I1180	T1181	E1182	V1183	P1187	R1188	R1189	L1192	T1193	R1197	Y1198	G1199	V1200	C1201	Q1202	K1203	C1204	Y1205	D1208	L1209	S1210	M1211	A1212	V1213	I1214	I1217
V1057	R1058	S1059	S1060	F1061	R1062	E1063	G1064	L1065	T1066	V1067	L1068	E1069	H1075	R1078	K1079	E1161	E1162	G1163	R1164	L1165	S1166	L1167	L1168	E1169	D1170	I1171	L1172	E1173	K1174	E1175	L1176	E1177	A1178	L1179	I1180	T1181	E1182	V1183	P1187	R1188	R1189	L1192	T1193	R1197	Y1198	G1199	V1200	C1201	Q1202	K1203	C1204	Y1205	D1208	L1209	S1210	M1211	A1212	V1213	I1214	I1217	
L964	P968	R969	K970	L971	R972	Q973	R974	Q975	Q976	A977	Y978	L983	R988	Y989	D990	Q991	Y992	Y993	N996	V1003	T1004	Q1005	A1006	N1010	F1011	Y1015	P1019	L1020	Y1021	Q1025	A1028	R1029	Q1033	Q1034	I1035	R1036	Q1037	L1038	C1039	G1040	M1041	R1042	Q1046	K1047	P1048	P1056															
L881	R884	I885	V886	G887	V890	G891	D892	E893	R894	V895	A896	R897	E898	A899	I900	D903	V904	P905	Q906	E907	K908	N909	S910	G911	K912	D913	L914	V915	A918	F919	L922	T927	A928	R929	L930	L931	D932	A933	L934	K935	G938	L941	S945	I947	T948	R951	D952	P1056													
G801	A802	G803	F806	E810	E811	A812	L813	A814	A815	R818	V821	A822	A825	P826	L827	G831	R832	S835	V836	G837	R838	L839	K840	F841	H842	F843	A849	L850	V853	L857	L858	D859	Q861	D862	T865	V866	R867	Y868	L869	R872	T875	S876	R879	I880																	
V719	L720	I726	Q727	L728	H729	V732	A735	D739	F740	M745	A746	V747	H748	P749	Q756	A757	E758	A759	R760	I761	Q762	M763	L764	S765	A766	H767	L770	S771	P772	A773	S774	E775	E776	K780	R783	D784	I785	I786	L787	G788	L789	Y790	Y791	I792	T793	Q794	V795	K800													
K646	R647	M648	A649	E650	L652	F653	K654	P655	F656	L657	L658	K659	M661	F666	A667	P668	N669	V670	K671	Q680	R681	D682	I683	K684	D685	E686	H687	H688	L691	V694	I695	K698	V699	V700	L701	L702	M703	R704	A705	P706	T707	L708	H709	R710	L711	G712	H640	Q641	C642	G643	Q644	Q645									
R572	M573	L574	Q575	E576	A577	V578	D579	E580	A589	M511	M512	I513	L514	E515	A516	V517	P518	V519	L520	P521	P522	D523	L524	A525	R526	E527	S528	A535	T537	S538	D539	L540	Y544	R545	R546	L547	I548	N551	N552	R553	L554	K555	K556	L557	P563	E564	R565	E566	N569	E570	L571	P578									
V384	H388	E389	P390	A391	S392	I393	L394	V395	V396	K397	D406	V407	R408	V409	R414	L421	A422	D423	K426	S429	G433	L439	N442	V443	V444	R445	V446	V447	E448	S449	Y450	D461	L462	L464	A471	E474	R475	E476	L477	L478	K571																				
V300	G301	L304	P390	A391	S392	I393	L394	V395	V396	K397	D406	V407	R408	V409	R414	L421	A422	D423	K426	S429	G433	L439	N442	V443	V444	R445	V446	V447	E448	S449	Y450	D461	L462	L464	A471	E474	R475	E476	L477	L478	K571																				
K233	E234	A235	Y236	R237	P238	V241	L242	A243	E244	L245	S246	E247	L250	E251	R252	A253	E254	E255	G257	V258	E259	L260	H268	L269	E270	Y271	Q274	E277	V278	V279	A280	R281	Y282	L284	P285	A286	G287	M288	V293	E294	G295	E296	I297	V298	E299																
T81	R82	S83	I84	R87	Y88	H92	I93	E94	L95	A96	D176	A177	V178	L179	D181	E184	K187	E190	L191	A192	P193	L116	G117	L118	S119	A120	T121	E122	L123	E124	Q125	V126	L127	Y128	F129	N130	K131	Y132	L135	D136	P137	K218	F219	R220	R224	I225	L152	T153	D155	E156	V230	E232									



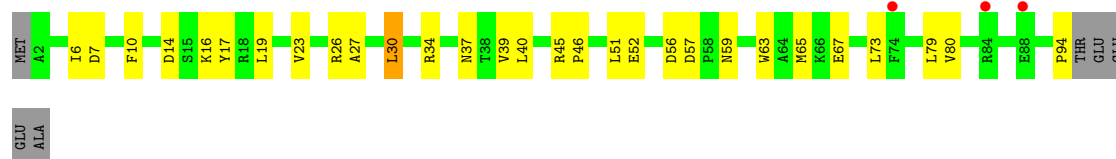
• Molecule 3: DNA-directed RNA polymerase subunit beta'



• Molecule 4: DNA-directed RNA polymerase subunit omega



• Molecule 4: DNA-directed RNA polymerase subunit omega





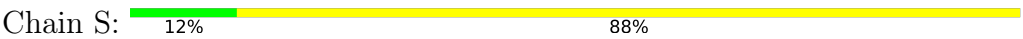
G1	T2	T3	G4	A5	C6	A7	A8	A9	A10	G11	T12	G13	T14	T15	A16	A17	A18	T19	T20	G21	T22	G23	C24	T25	A26	T27	A28	C29	T30
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● Molecule 7: DNA (26-MER)



DT	A2	G3	C4	A5	C6	A7	A8	T9	T10	T11	A12	A13	C14	A15	C16	T17	T18	T19	T20	G21	T22	G23	A24	A25	G26
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● Molecule 7: DNA (26-MER)



T1	A2	G3	A4	A5	C6	A7	A8	T9	T10	T11	A12	A13	C14	A15	C16	T17	T18	T19	T20	G21	T22	G23	A24	A25	G26
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## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	288.23Å 288.23Å 535.25Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.81 – 4.60 49.81 – 4.60	Depositor EDS
% Data completeness (in resolution range)	98.6 (49.81-4.60) 98.6 (49.81-4.60)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.21 (at 4.64Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1839)	Depositor
R, $R_{free}$	0.245 , 0.281 0.245 , 0.281	Depositor DCC
$R_{free}$ test set	6224 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	154.6	Xtriage
Anisotropy	0.027	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 174.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.33$ , $\langle L^2 \rangle = 0.17$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	56477	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	175.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, 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	0.31	0/1804	0.64	1/2455 (0.0%)
1	B	0.30	0/1804	0.61	0/2455
1	G	0.31	0/1804	0.64	1/2455 (0.0%)
1	H	0.30	0/1804	0.61	0/2455
2	C	0.27	0/8905	0.55	2/12040 (0.0%)
2	I	0.27	0/8905	0.55	2/12040 (0.0%)
3	D	0.28	0/11963	0.55	3/16165 (0.0%)
3	J	0.28	0/10959	0.57	1/14802 (0.0%)
4	E	0.25	0/783	0.54	0/1054
4	K	0.25	0/783	0.53	0/1054
5	F	0.27	0/2829	0.55	1/3804 (0.0%)
5	L	0.27	0/2829	0.55	1/3804 (0.0%)
6	O	0.50	0/687	0.92	0/1059
6	R	0.50	0/687	0.91	0/1059
7	P	0.54	0/571	0.93	0/878
7	S	0.54	0/590	0.93	0/908
All	All	0.29	0/57707	0.59	12/78487 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
2	C	0	3
2	I	0	3
3	D	0	1
3	J	0	1
All	All	0	8

There are no bond length outliers.



The worst 5 of 12 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	311	LEU	CA-CB-CG	7.45	132.43	115.30
3	D	1134	LEU	CA-CB-CG	6.98	131.36	115.30
2	I	417	GLY	N-CA-C	6.42	129.14	113.10
2	C	417	GLY	N-CA-C	6.40	129.09	113.10
3	J	1134	LEU	CA-CB-CG	5.63	128.26	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	415	PRO	Peptide
2	C	423	ALA	Peptide
2	C	737	LEU	Peptide
3	D	1208	ASP	Peptide
2	I	415	PRO	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	1770	0	1799	89	0
1	B	1770	0	1799	101	0
1	G	1770	0	1799	103	0
1	H	1770	0	1799	95	0
2	C	8739	0	8841	499	0
2	I	8739	0	8841	485	0
3	D	11761	0	11976	585	0
3	J	10779	0	10993	503	0
4	E	768	0	784	37	0
4	K	768	0	784	29	0
5	F	2787	0	2866	120	0
5	L	2787	0	2866	133	0
6	O	613	0	343	28	0
6	R	613	0	343	26	0
7	P	510	0	284	27	0
7	S	527	0	297	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	J	2	0	0	0	0
9	D	1	0	0	0	0
9	J	1	0	0	0	0
All	All	56477	0	56414	2598	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 23.

The worst 5 of 2598 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:C:707:ARG:HE	2:C:824:ARG:HE	1.17	0.90
6:R:24:DC:H42	7:S:3:DG:H1	1.18	0.90
3:D:105:VAL:HA	3:D:112:ILE:HD11	1.55	0.88
4:E:30:LEU:HD12	4:E:37:ASN:HD21	1.39	0.88
4:K:30:LEU:HD12	4:K:37:ASN:HD21	1.39	0.87

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	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	17	56
1	B	225/314 (72%)	200 (89%)	20 (9%)	5 (2%)	6	37
1	G	225/314 (72%)	200 (89%)	23 (10%)	2 (1%)	17	56
1	H	225/314 (72%)	201 (89%)	18 (8%)	6 (3%)	5	34
2	C	1108/1119 (99%)	958 (86%)	139 (12%)	11 (1%)	15	54
2	I	1108/1119 (99%)	956 (86%)	140 (13%)	12 (1%)	14	52

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	1486/1524 (98%)	1315 (88%)	162 (11%)	9 (1%)	25	65
3	J	1361/1524 (89%)	1201 (88%)	150 (11%)	10 (1%)	22	62
4	E	91/99 (92%)	75 (82%)	16 (18%)	0	100	100
4	K	91/99 (92%)	75 (82%)	16 (18%)	0	100	100
5	F	343/347 (99%)	299 (87%)	42 (12%)	2 (1%)	25	65
5	L	343/347 (99%)	302 (88%)	40 (12%)	1 (0%)	41	76
All	All	6831/7434 (92%)	5982 (88%)	789 (12%)	60 (1%)	17	56

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	VAL
3	D	1128	VAL
3	D	1209	LEU
1	G	53	VAL
3	J	1128	VAL

### 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	194/270 (72%)	179 (92%)	15 (8%)	13	39
1	B	194/270 (72%)	172 (89%)	22 (11%)	6	24
1	G	194/270 (72%)	178 (92%)	16 (8%)	11	36
1	H	194/270 (72%)	171 (88%)	23 (12%)	5	22
2	C	931/936 (100%)	840 (90%)	91 (10%)	8	28
2	I	931/936 (100%)	840 (90%)	91 (10%)	8	28
3	D	1252/1281 (98%)	1114 (89%)	138 (11%)	6	25
3	J	1150/1281 (90%)	1028 (89%)	122 (11%)	6	26
4	E	83/88 (94%)	79 (95%)	4 (5%)	25	52
4	K	83/88 (94%)	79 (95%)	4 (5%)	25	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	F	296/299 (99%)	276 (93%)	20 (7%)	16	42
5	L	296/299 (99%)	276 (93%)	20 (7%)	16	42
All	All	5798/6288 (92%)	5232 (90%)	566 (10%)	8	28

5 of 566 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	J	685	ASP
3	J	811	GLU
3	J	683	ILE
3	J	1238	MET
3	D	762	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 85 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	498	GLN
3	J	703	ASN
2	I	567	GLN
2	I	962	GLN
3	J	897	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/314 (72%)	0.08	2 (0%) 84 77	107, 189, 236, 264	0
1	B	227/314 (72%)	-0.23	0 100 100	94, 161, 214, 264	0
1	G	227/314 (72%)	0.39	17 (7%) 14 12	116, 199, 240, 276	0
1	H	227/314 (72%)	-0.13	2 (0%) 84 77	116, 173, 216, 267	0
2	C	1112/1119 (99%)	-0.03	21 (1%) 66 58	90, 179, 243, 314	0
2	I	1112/1119 (99%)	0.01	26 (2%) 60 51	94, 185, 244, 315	0
3	D	1490/1524 (97%)	-0.13	13 (0%) 84 77	64, 149, 204, 259	0
3	J	1367/1524 (89%)	-0.08	17 (1%) 79 70	79, 159, 217, 264	0
4	E	93/99 (93%)	0.06	2 (2%) 62 53	100, 159, 205, 238	0
4	K	93/99 (93%)	0.03	3 (3%) 47 38	112, 168, 216, 253	0
5	F	345/347 (99%)	-0.10	1 (0%) 94 90	115, 185, 255, 300	0
5	L	345/347 (99%)	-0.10	7 (2%) 65 56	121, 188, 252, 300	0
6	O	30/30 (100%)	0.70	4 (13%) 3 4	154, 221, 293, 311	0
6	R	30/30 (100%)	0.21	0 100 100	164, 221, 257, 267	0
7	P	25/26 (96%)	0.83	5 (20%) 1 1	172, 235, 306, 326	0
7	S	26/26 (100%)	0.06	0 100 100	184, 224, 263, 283	0
All	All	6976/7546 (92%)	-0.04	120 (1%) 70 61	64, 171, 235, 326	0

The worst 5 of 120 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	176	VAL	5.1
2	I	175	GLU	4.5
2	C	221	LEU	4.4
1	G	13	ALA	4.0
2	C	175	GLU	3.7

## 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 monosaccharides 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, 95<sup>th</sup> 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
9	MG	D	2003	1/1	0.82	0.45	286,286,286,286	0
9	MG	J	2003	1/1	0.84	0.41	331,331,331,331	0
8	ZN	J	2002	1/1	0.93	0.07	147,147,147,147	0
8	ZN	D	2002	1/1	0.96	0.16	182,182,182,182	0
8	ZN	J	2001	1/1	0.97	0.12	166,166,166,166	0
8	ZN	D	2001	1/1	0.99	0.13	107,107,107,107	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.