



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 11:31 PM UTC

PDB ID : 5W1T / pdb_00005w1t
Title : X-ray crystal structure of Escherichia coli RNA polymerase and DksA complex
Authors : Murakami, K.S.; Molodtsov, V.
Deposited on : 2017-06-04
Resolution : 4.50 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
Xtriage (Phenix) : 2.0
EDS : 3.0
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

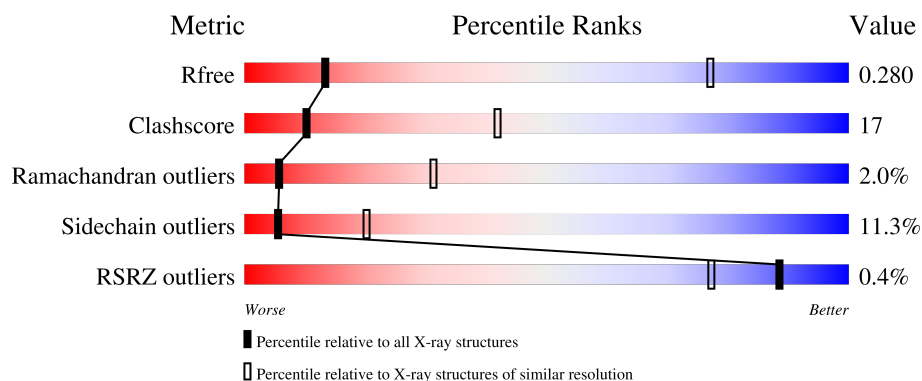
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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.



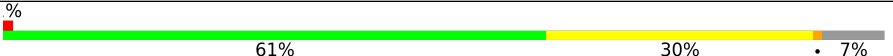
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1127 (5.10-3.90)
Clashscore	190562	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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	 44% 41% 12% . .
1	B	329	 41% 22% . 34%
1	G	329	 % 40% 24% 5% 31%
1	H	329	 43% 21% . 34%
2	C	1342	 57% 37% 5%

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Mol	Chain	Length	Quality of chain
2	I	1342	 58%37%5%
3	D	1407	 %47%31%5%17%
3	J	1407	 46%32%18%
4	E	91	 65%26%7%
4	K	91	 60%20%7%13%
5	F	613	 47%26%24%
5	L	613	 46%27%23%
6	M	151	 %61%30%7%
6	N	151	 57%30%5%7%

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 58066 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	319	Total	C	N	O	S	0	0	0
			2490	1557	439	486	8			
1	B	217	Total	C	N	O	S	0	0	0
			1677	1047	295	329	6			
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
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1171	Total	C	N	O	S	0	0	0
			9085	5712	1626	1701	46			
3	J	1159	Total	C	N	O	S	0	0	0
			9021	5671	1616	1688	46			

- Molecule 4 is a protein called RpoZ.

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	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- Molecule 6 is a protein called RNA polymerase-binding transcription factor DksA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			
6	N	140	Total	C	N	O	S	0	0	0
			1140	703	206	224	7			

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

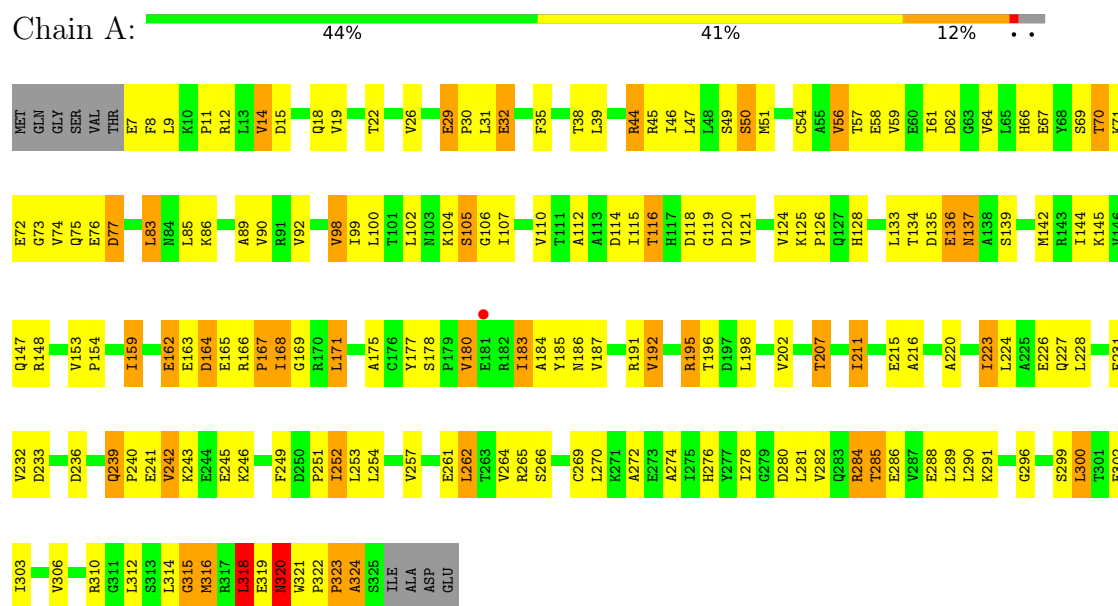
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	D	2	Total	Zn	0	0
			2	2		
8	J	2	Total	Zn	0	0
			2	2		
8	M	1	Total	Zn	0	0
			1	1		
8	N	1	Total	Zn	0	0
			1	1		

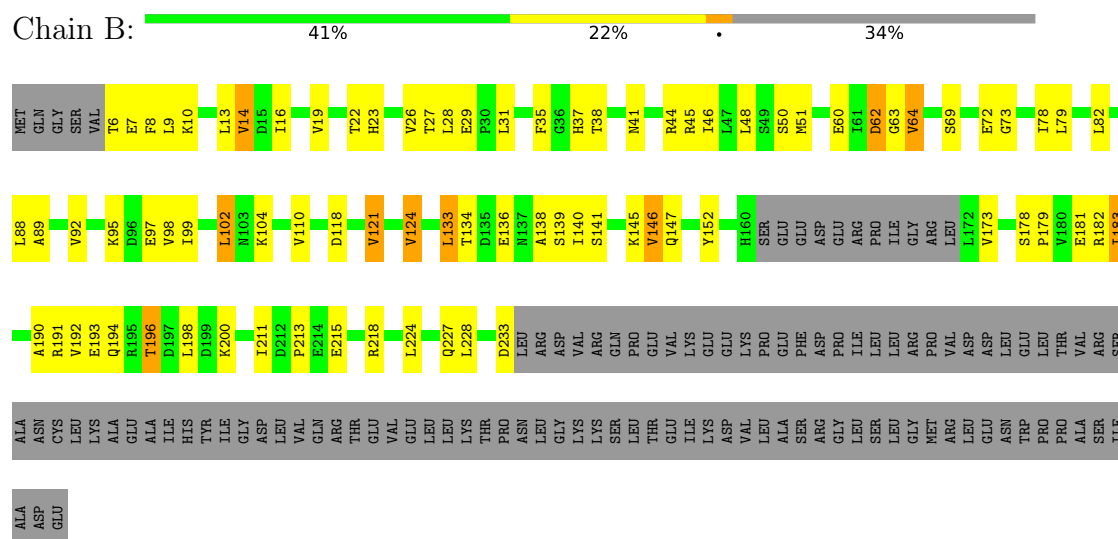
3 Residue-property plots

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

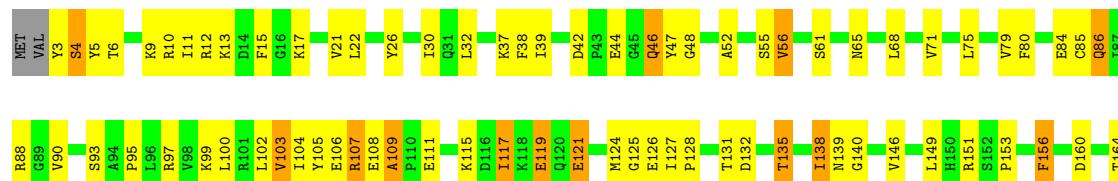


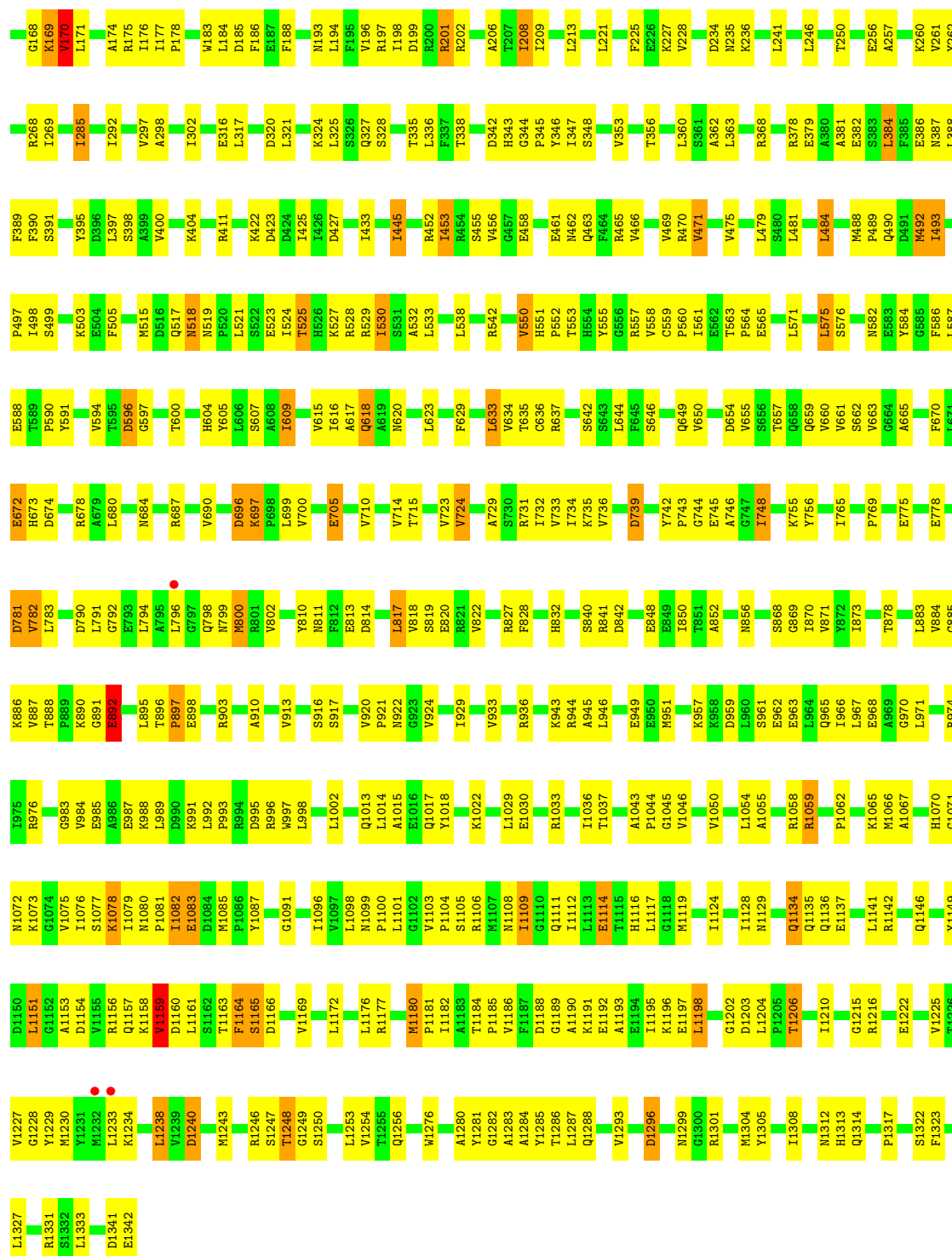
[illegible][illegible]

Chain C:

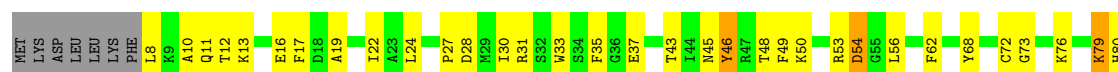
Item	Category	Percentage
S159	MET	100%
K163	MET	100%
T164	MET	100%
G168	MET	100%
K169	MET	100%
V170	MET	100%
L171	MET	100%
Y172	MET	100%
M173	MET	100%
A174	MET	100%
R175	MET	100%
I176	MET	100%
L184	MET	100%
D185	MET	100%
F186	MET	100%
E187	MET	100%
F188	MET	100%
D189	MET	100%
P190	MET	100%
L194	MET	100%
F195	MET	100%
V196	MET	100%
R197	MET	100%
I198	MET	100%
R201	MET	100%
R202	MET	100%
A206	MET	100%
T207	MET	100%
I208	MET	100%
I209	MET	100%
L210	MET	100%
R211	MET	100%
A212	MET	100%
L213	MET	100%
E218	MET	100%
L221	MET	100%
E226	MET	100%
K227	MET	100%
F230	MET	100%
K236	MET	100%
L237	MET	100%
Q238	MET	100%
M239	MET	100%
V242	MET	100%
R245	MET	100%
L246	MET	100%
L247	MET	100%
V90	VAL	100%
T91	VAL	100%
Y92	VAL	100%
S93	VAL	100%
A94	VAL	100%
R97	VAL	100%
V98	VAL	100%
R101	VAL	100%
L102	VAL	100%
V103	VAL	100%
Y105	VAL	100%
E106	VAL	100%
R107	VAL	100%
E108	VAL	100%
A109	VAL	100%
P110	VAL	100%
E111	VAL	100%
G112	VAL	100%
T113	VAL	100%
V114	VAL	100%
K115	VAL	100%
D116	VAL	100%
I117	VAL	100%
K118	VAL	100%
E119	VAL	100%
Q120	VAL	100%
E121	VAL	100%
V122	VAL	100%
G125	VAL	100%
E126	VAL	100%
I127	VAL	100%
P128	VAL	100%
L129	VAL	100%
M130	VAL	100%
T131	VAL	100%
G134	VAL	100%
T135	VAL	100%
I138	VAL	100%
M139	VAL	100%
G140	VAL	100%
R143	VAL	100%
V144	VAL	100%
I145	VAL	100%
V146	VAL	100%
S147	VAL	100%
Q148	VAL	100%
L149	VAL	100%
H150	VAL	100%
R151	VAL	100%
P152	VAL	100%
P153	VAL	100%
D159	VAL	100%
MET	MET	100%
VAL	VAL	100%
S4	VAL	100%
Y5	VAL	100%
T6	VAL	100%
E7	VAL	100%
K8	VAL	100%
K9	VAL	100%
R10	VAL	100%
I11	VAL	100%
D14	VAL	100%
F15	VAL	100%
E16	VAL	100%
K17	VAL	100%
L22	VAL	100%
D23	VAL	100%
Y26	VAL	100%
L27	VAL	100%
L32	VAL	100%
K37	VAL	100%
F38	VAL	100%
I39	VAL	100%
E40	VAL	100%
Q41	VAL	100%
D42	VAL	100%
P43	VAL	100%
E44	VAL	100%
G45	VAL	100%
Q46	VAL	100%
V56	VAL	100%
S61	VAL	100%
Y62	VAL	100%
S63	VAL	100%
G64	VAL	100%
N65	VAL	100%
Q69	VAL	100%
Y73	VAL	100%
R74	VAL	100%
L75	VAL	100%
V79	VAL	100%
F90	VAL	100%
D81	VAL	100%
E84	VAL	100%
C85	VAL	100%
Q86	VAL	100%
I87	VAL	100%
R88	VAL	100%
C89	VAL	100%

57%





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

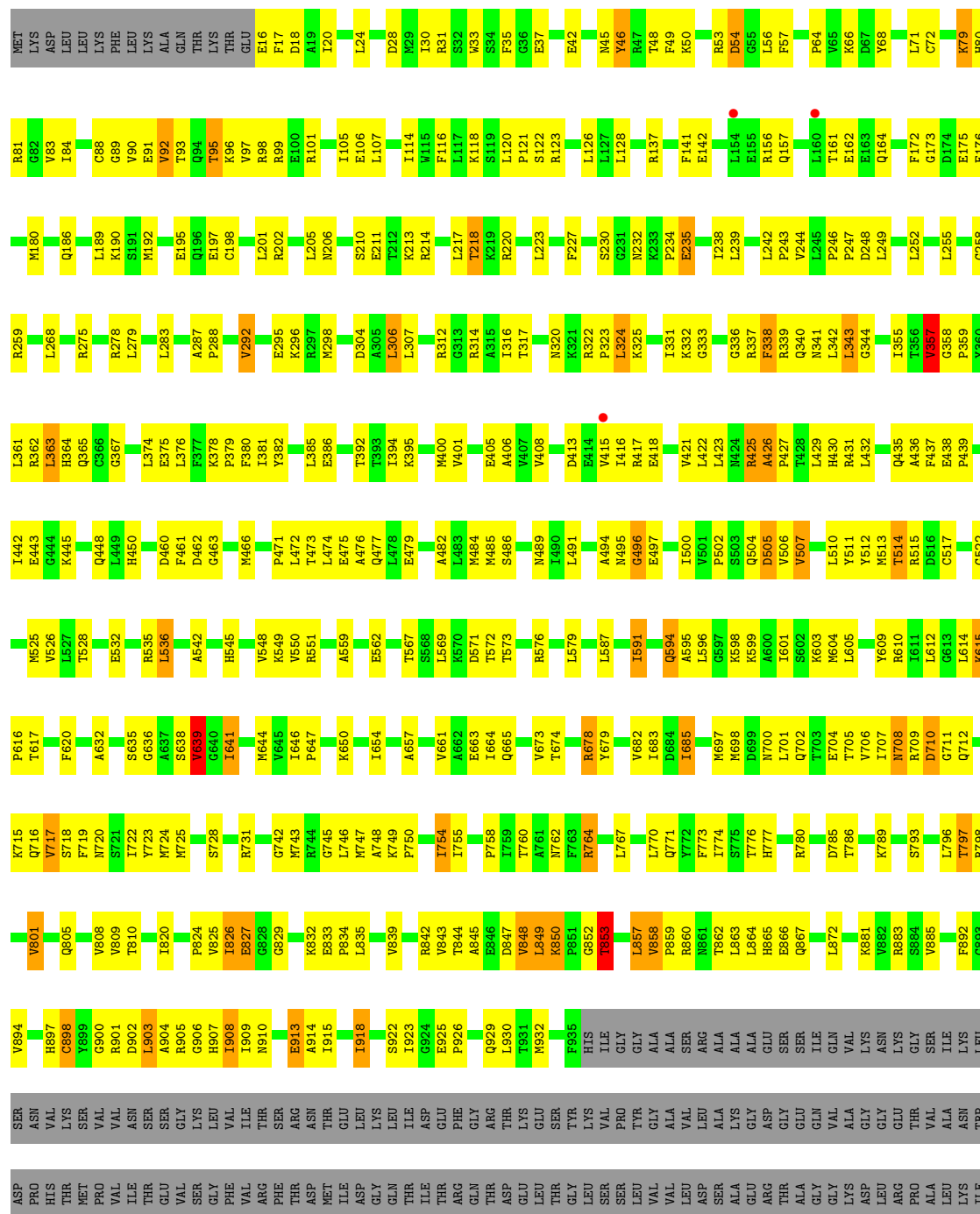


V1229	R1148	ASN	PRO	VAL	V882	Q805	R709	K599	V506	A426	G344	L252	L160	R81
T1230	I1155	ASP	VAL	VAL	R883	V809	D710	K599	V507	P427	K345	V253	T161	G82
Y1231	L1156	LEU	THR	ASN	G884	T810	G711	A600	L508	T428	R346	P254	Q164	V83
I1233	A1157	ILE	GLU	SER	V885	E811	Q712	I601	G509	L429	V347	L255		I84
E1236	E1158	PRO	VAL	GLY	T890	D812	Q716	M604	L510	R430	D348	G258	F172	C88
V1237	I1159	GLY	SER	LYS	G893	D813	V717	Y609	Y512	H431	G173	R259	G173	G89
Q1238	G1161	THR	PHE	VAL	V894	H817	S718	L614	M513	L432	D174	T262	D174	V90
	V1163	PRO	ARG	THR	R901	I820	S721	L614	R515	Q435	E175	G266	F176	E91
	S1164	ALA	PHE	SER	D902	R821	T722	P616	R518	A436	A357	N266	E183	V92
V1246	L1165	GLN	THR	ARG	L903	R822	Y723	R634	M525	F437	L268	D267	E183	T93
K1247	G1166	ASP	ASP	ARG	A904	T823	M724	S638	V526	E438	L268	T269	L188	K96
I1248	K1167	PHE	MET	THR	R905	R824	M725	V639	L527	I442	H964	R270	L189	V97
	E1168	LEU	ILE	GLU	G906	V825	S728	G639	T528	E443	Q366	G358	K190	R98
K1251	T1169	PRO	ASP	LEU	H907	R826	R731	I641	G529	G444	G367	R275	L194	R99
H1252	K1170	GLY	GLY	LYS	I908	G828	G732	G640	G529	E443	G367	R276	L194	E100
	G1171	LYS	GLN	LEU	E913	G829	S733	I641	E532	K445	R372	R277	E197	R101
V1255	H1172	ALA	THR	ILE		D830	S733	P647	A533	Q448	A373	R278	E197	M102
I1256	R1173	ILE	ILE	ASP		V831	Q736	K650	A534	L279	L374	R279	L201	G103
V1257	R1174	VAL	THR	GLU	T918	R832	T737	K650	E534	H450	E375	R280	R202	H104
	L1175	GLN	ARG	PHE		R833	Q738		R535					
M1260	V1176	LEU	GLN	GLY	E925	R834	Q739	A659	L536	A459	F377	V292	L205	L107
R1262	I1177	ASP	THR	ARG	P926	L835	L740	E660	L541	D460	K378	E295	L205	P110
A1263	T1178	GLY	GLU	THR	Q929			E660	A542	F461	P379	K296	S210	T111
A1264	D1181	VAL	LEU	LYS	L930		M743	E663	S543	D462	R297	K296	S210	T111
I1265	G1182	GLN	THR	SER		V839	R744	I664	R543	R462	F380	K297	K213	A112
I1266	S1183	ILE	GLY	TYR	F935	R842	G745	Q665	H545	Q463	I381	M298	K213	H113
	D1184	SER	LEU	LYS	HIS	V843	L746	Q667		L472	Y382	D304	K215	I114
P1185	P1185	VAL	VAL	VAL	ILE	T844	M747	Q667	V548	T473	E386	A305	K216	F116
D1273	Y1186	GLY	SER	PRO	GLY	R847	A748	F668	K549	L474	T392	L306	K216	F116
F1274	E1187	ASP	LEU	TYR	GLY	V848	K749	Q669	R551	A476	T393	L307	L217	L117
L1275	E1188	THR	VAL	GLY	ALA	D847	P750			E475	I394	D308	T218	K118
E1276		LEU	VAL	ALA	ALA	L849		L672	L569	Q477	K395	N309	K221	S119
G1277	K1192	ALA	VAL	SER	SER	K850	I754	V673	K570	L478	M400	G310	L223	L120
E1278	V1193	ARG	LEU	ARG	ARG	P851		T674	D571	E479		R311	L224	P121
Q1279	R1194	ILE	ALA	ALA	ALA	G852	P758	A675	A559	A482	V407	R312	L230	S122
V1280		PRO	SER	LYS	ALA	T853		G676		L483	V408	G313	E226	R123
E1281	V1198	GLN	ALA	LYS	ALA	A854	N762	E677	E562	R403	L412	R321	E226	L126
R1284	F1199	GLU	ARG	ASP	GLU	D855	F763	R678	M560	E404	D413	R322	E226	L126
V1285	E1200	SER	THR	GLY	GLU	T856	R764	Y679	L569	A405	E414	P323	A226	L127
K1286	G1201	GLY	ALA	SER	SER	L857		K680	K570	M485	A406	L324	V227	L128
I1287	E1202	GLY	GLY	GLU	ILE	V858	L770	K681	D571	M489	V407	K325	V228	L128
A1288		THR	GLY	GLN	VAL	P859	T776	V682	T572	I490	V408	M320	V229	R133
N1289	G1207	ASP	ASP	GLY	VAL	N861	H777		T573	L491		R321	P234	R137
	I1210	LEU	GLY	GLY	GLY	T862	T766	I685	L579	S492	L412	R322	E235	Y140
L1292		ARG	GLU	GLU	LYS	L863		N690	M580	P493	D413	P323	E235	F141
E1293	E1215	PRO	THR	THR	GLY	L864		M697	M581	A494	E414	L324	E235	E142
	D1219	ALA	VAL	VAL	SER	H865	K789	M698	G586	G496	E417	K330	V241	I147
V1298	P1139	LEU	ALA	ALA	ILE	E866	T790		L587	E497	R417	M330	L242	P243
G1299	L1138	LYS	LYS	ASN	LYS		S793	L701	Y588	E418	E418	Q335	V244	N153
L1221	R1140	ILE	TRP	LEU	LEU	L872			Y589	V501	V421	Q335	L244	L154
R1222	D1143	ASP	ASP	SER	SER	V877	T797	T705	Y589	P502	L422	R337	P246	Q157
H1227	E1146	VAL	THR	ASN	VAL	D878	V801	V705	Q594	S503	L423	L342	P247	Q158
A1228	A1147	LYS	THR	LYS	LYS	A879		N708	L596	Q504	R425		D248	I159
		SER	MET	SER	SER									

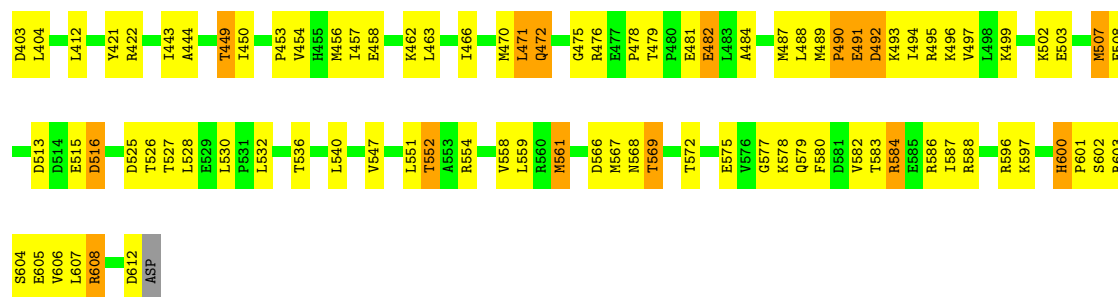


• Molecule 3: DNA-directed RNA polymerase subunit beta'

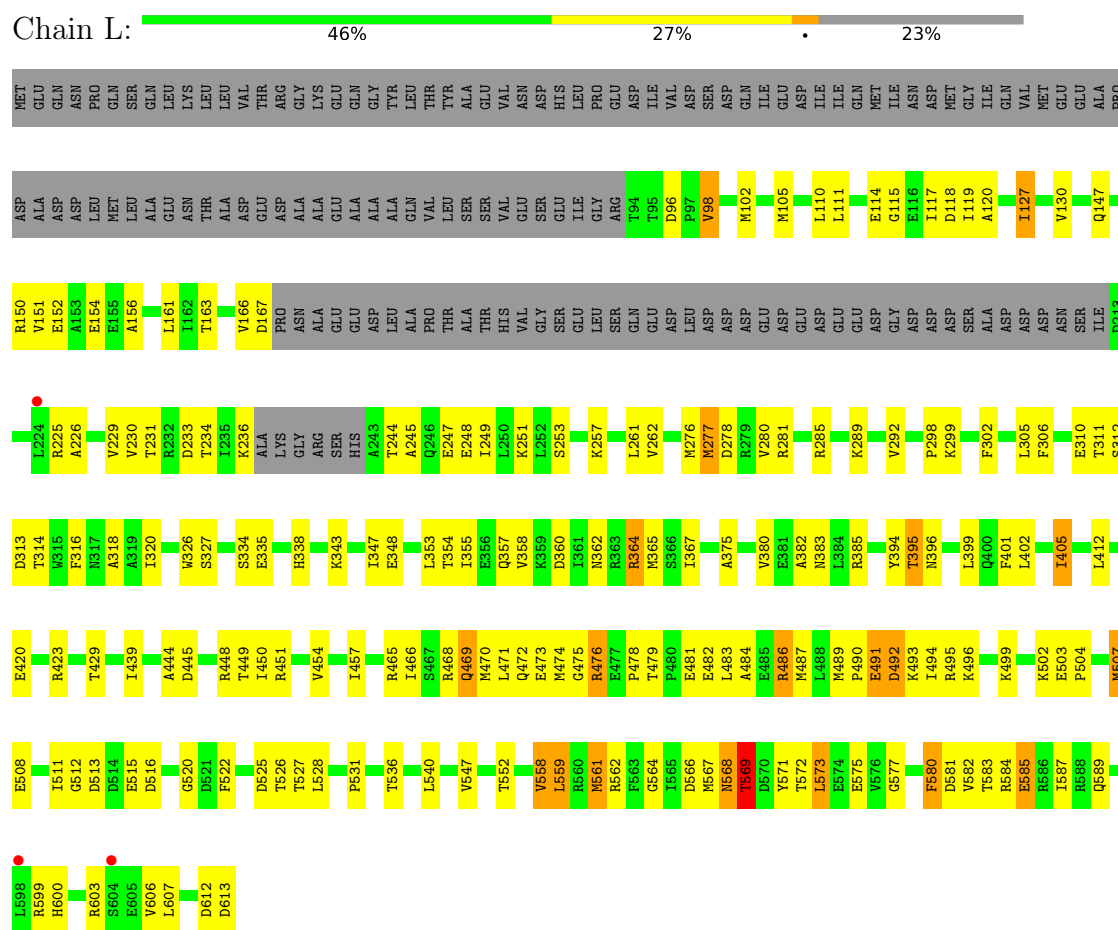
Chain J: 46% 32% 18%



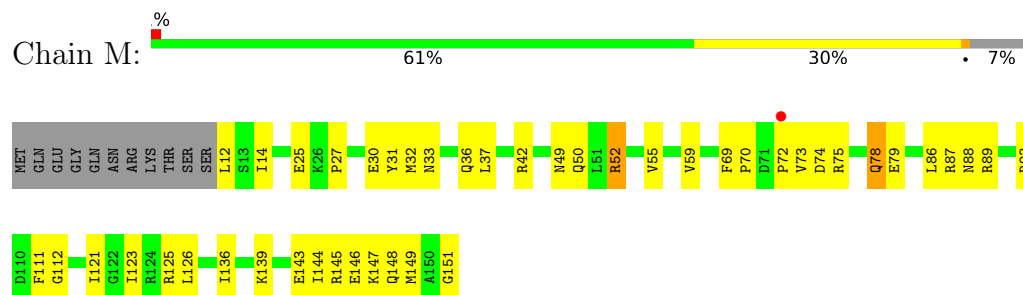




- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 6: RNA polymerase-binding transcription factor DksA



- Molecule 6: RNA polymerase-binding transcription factor DksA



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	184.00Å 204.89Å 314.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.08 – 4.50 47.08 – 4.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.08-4.50) 88.5 (47.08-4.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.95 (at 4.45Å)	Xtriage
Refinement program	PHENIX (1.11.1 _2575: ???)	Depositor
R, R_{free}	0.220 , 0.276 0.225 , 0.280	Depositor DCC
R_{free} test set	2000 reflections (2.81%)	wwPDB-VP
Wilson B-factor (Å ²)	198.5	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 272.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	58066	wwPDB-VP
Average B, all atoms (Å ²)	291.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.60% 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: 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	0.30	0/2524	0.77	2/3421 (0.1%)
1	B	0.27	0/1697	0.73	1/2300 (0.0%)
1	G	0.26	0/1777	0.64	0/2408
1	H	0.23	0/1681	0.66	0/2278
2	C	0.30	0/10739	0.69	0/14489
2	I	0.26	0/10735	0.64	2/14484 (0.0%)
3	D	0.34	0/9225	0.76	1/12458 (0.0%)
3	J	0.30	0/9160	0.71	0/12369
4	E	0.29	0/693	0.64	0/935
4	K	0.21	0/629	0.62	0/847
5	F	0.28	0/3864	0.67	0/5194
5	L	0.25	0/3872	0.62	0/5205
6	M	0.27	0/1155	0.80	2/1549 (0.1%)
6	N	0.28	0/1155	0.90	4/1549 (0.3%)
All	All	0.29	0/58906	0.70	12/79486 (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
1	H	0	1
2	C	0	2
2	I	0	2
3	D	0	2
3	J	0	2
4	K	0	1
All	All	0	10

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(°)
1	A	323	PRO	CA-C-N	5.43	131.48	121.70
1	A	323	PRO	C-N-CA	5.43	131.48	121.70
6	N	109	GLU	CA-C-N	5.42	131.90	121.54
6	N	109	GLU	C-N-CA	5.42	131.90	121.54
6	M	31	TYR	CA-C-N	-5.26	114.19	122.76

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
3	D	1184	ASP	Peptide
3	D	901	ARG	Peptide
1	H	171	LEU	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	2490	0	2542	120	0
1	B	1677	0	1703	53	1
1	G	1755	0	1773	62	1
1	H	1662	0	1687	49	0
2	C	10570	0	10582	401	2
2	I	10566	0	10576	384	0
3	D	9085	0	9218	397	1
3	J	9021	0	9175	391	0
4	E	691	0	695	21	0
4	K	627	0	634	16	0
5	F	3813	0	3880	124	1
5	L	3821	0	3884	116	0
6	M	1140	0	1119	36	0
6	N	1140	0	1119	55	0
7	D	1	0	0	0	0
7	J	1	0	0	0	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
8	M	1	0	0	0	0
8	N	1	0	0	0	0
All	All	58066	0	58587	1996	3

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 17.

The worst 5 of 1996 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:525:THR:HG21	2:C:687:ARG:HD2	1.39	1.04
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.45	0.98
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.43	0.97
1:A:45:ARG:HG2	1:B:38:THR:HB	1.48	0.95
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.49	0.94

All (3) 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)
1:B:62:ASP:O	1:G:101:THR:OG1[4_545]	1.98	0.22
2:C:44:GLU:OE2	5:F:596:ARG:NH1[4_555]	2.17	0.03
2:C:1006:GLU:OE1	3:D:68:TYR:OH[4_555]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	317/329 (96%)	248 (78%)	52 (16%)	17 (5%)	1 15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	213/329 (65%)	195 (92%)	14 (7%)	4 (2%)	6	32
1	G	225/329 (68%)	202 (90%)	18 (8%)	5 (2%)	5	29
1	H	212/329 (64%)	197 (93%)	11 (5%)	4 (2%)	6	32
2	C	1338/1342 (100%)	1202 (90%)	118 (9%)	18 (1%)	9	41
2	I	1338/1342 (100%)	1197 (90%)	120 (9%)	21 (2%)	7	37
3	D	1167/1407 (83%)	1037 (89%)	103 (9%)	27 (2%)	5	28
3	J	1155/1407 (82%)	1029 (89%)	100 (9%)	26 (2%)	5	28
4	E	87/91 (96%)	80 (92%)	5 (6%)	2 (2%)	5	28
4	K	77/91 (85%)	69 (90%)	4 (5%)	4 (5%)	1	15
5	F	462/613 (75%)	426 (92%)	28 (6%)	8 (2%)	7	35
5	L	463/613 (76%)	425 (92%)	31 (7%)	7 (2%)	8	38
6	M	138/151 (91%)	128 (93%)	8 (6%)	2 (1%)	9	39
6	N	138/151 (91%)	129 (94%)	6 (4%)	3 (2%)	5	29
All	All	7330/8524 (86%)	6564 (90%)	618 (8%)	148 (2%)	6	31

5 of 148 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	14	VAL
1	A	107	ILE
1	A	136	GLU
1	A	162	GLU
1	A	167	PRO

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	278/286 (97%)	222 (80%)	56 (20%)	1	8
1	B	186/286 (65%)	163 (88%)	23 (12%)	4	18
1	G	193/286 (68%)	162 (84%)	31 (16%)	2	12

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	H	183/286 (64%)	168 (92%)	15 (8%)	10	31
2	C	1155/1157 (100%)	1024 (89%)	131 (11%)	5	20
2	I	1154/1157 (100%)	1031 (89%)	123 (11%)	6	22
3	D	962/1168 (82%)	860 (89%)	102 (11%)	6	22
3	J	960/1168 (82%)	859 (90%)	101 (10%)	6	22
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	17
4	K	67/75 (89%)	60 (90%)	7 (10%)	7	22
5	F	417/540 (77%)	375 (90%)	42 (10%)	7	23
5	L	418/540 (77%)	373 (89%)	45 (11%)	6	22
6	M	121/131 (92%)	110 (91%)	11 (9%)	9	28
6	N	121/131 (92%)	109 (90%)	12 (10%)	7	24
All	All	6287/7286 (86%)	5579 (89%)	708 (11%)	5	20

5 of 708 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	I	575	LEU
3	J	514	THR
2	I	705	GLU
2	I	561	ILE
2	I	1238	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 96 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	618	GLN
2	I	1336	ASN
2	I	673	HIS
2	I	1116	HIS
3	J	206	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 8 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 [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	319/329 (96%)	-0.38	1 (0%) 90 80	230, 295, 400, 420	0
1	B	217/329 (65%)	-0.35	0 100 100	243, 301, 356, 388	0
1	G	227/329 (68%)	-0.23	3 (1%) 75 60	270, 312, 357, 389	0
1	H	216/329 (65%)	-0.26	0 100 100	287, 356, 409, 427	0
2	C	1340/1342 (99%)	-0.37	5 (0%) 88 77	166, 255, 352, 403	0
2	I	1340/1342 (99%)	-0.45	3 (0%) 91 83	203, 302, 382, 423	0
3	D	1171/1407 (83%)	-0.30	11 (0%) 81 67	169, 238, 355, 404	0
3	J	1159/1407 (82%)	-0.41	3 (0%) 90 80	183, 262, 356, 405	0
4	E	89/91 (97%)	-0.43	0 100 100	225, 281, 318, 330	0
4	K	79/91 (86%)	-0.34	0 100 100	320, 426, 502, 516	0
5	F	468/613 (76%)	-0.41	1 (0%) 91 83	199, 288, 436, 472	0
5	L	469/613 (76%)	-0.42	3 (0%) 85 73	212, 309, 420, 437	0
6	M	140/151 (92%)	-0.20	1 (0%) 84 71	374, 435, 492, 503	0
6	N	140/151 (92%)	-0.13	0 100 100	417, 439, 458, 465	0
All	All	7374/8524 (86%)	-0.37	31 (0%) 88 77	166, 283, 416, 516	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	GLU	3.8
3	D	502	PRO	3.7
3	D	508	LEU	3.5
3	D	877	VAL	3.3
2	I	796	LEU	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
7	MG	J	2001	1/1	0.71	0.14	335,335,335,335	0
7	MG	D	2001	1/1	0.76	0.14	268,268,268,268	0
8	ZN	M	200	1/1	0.91	0.08	512,512,512,512	0
8	ZN	N	200	1/1	0.93	0.05	506,506,506,506	0
8	ZN	D	2003	1/1	0.99	0.08	245,245,245,245	0
8	ZN	J	2003	1/1	0.99	0.05	211,211,211,211	0
8	ZN	J	2002	1/1	1.00	0.02	269,269,269,269	0
8	ZN	D	2002	1/1	1.00	0.06	271,271,271,271	0

6.5 Other polymers [i](#)

There are no such residues in this entry.