



wwPDB X-ray Structure Validation Summary Report ⓘ

Sep 11, 2017 – 09:38 AM EDT

PDB ID : 5UAQ
Title : Escherichia coli RNA polymerase RpoB H526Y mutant
Authors : Molodtsov, V.; Scharf, N.T.; Stefan, M.A.; Garcia, G.A.; Murakami, K.S.
Deposited on : unknown
Resolution : 3.60 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

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
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20029824
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
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)	:	rb-20029824

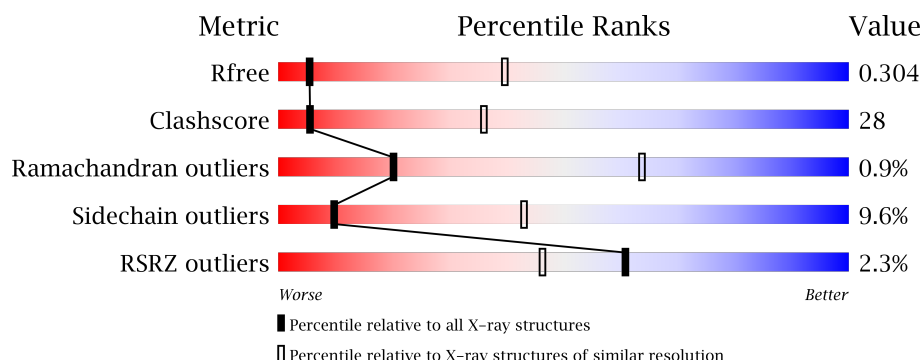
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.60 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}	100719	1026 (3.74-3.46)
Clashscore	112137	1036 (3.70-3.50)
Ramachandran outliers	110173	1030 (3.72-3.48)
Sidechain outliers	110143	1030 (3.72-3.48)
RSRZ outliers	101464	1051 (3.74-3.46)

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	<div> <div>0.1%</div> <div> <div>42%</div> <div>42%</div> <div>9%</div> <div>6%</div> </div> </div>
1	B	329	<div> <div>2%</div> <div> <div>29%</div> <div>33%</div> <div>•</div> <div>34%</div> </div> </div>
1	G	329	<div> <div>0.1%</div> <div> <div>29%</div> <div>31%</div> <div>6%</div> <div>•</div> <div>32%</div> </div> </div>
1	H	329	<div> <div>4%</div> <div> <div>27%</div> <div>35%</div> <div>•</div> <div>•</div> <div>34%</div> </div> </div>
2	C	1342	<div> <div>2%</div> <div> <div>44%</div> <div>47%</div> <div>9%</div> <div>•</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	I	1342	<div><div></div><div>4%</div><div>50%</div><div>44%</div><div>6%</div></div>
3	D	1407	<div><div></div><div>%</div><div>35%</div><div>38%</div><div>9%</div><div>17%</div></div>
3	J	1407	<div><div></div><div>2%</div><div>36%</div><div>38%</div><div>8%</div><div>18%</div></div>
4	E	91	<div><div></div><div>2%</div><div>64%</div><div>31%</div><div>• •</div></div>
4	K	91	<div><div></div><div>15%</div><div>53%</div><div>33%</div><div>•</div><div>13%</div></div>
5	F	613	<div><div></div><div>2%</div><div>40%</div><div>31%</div><div>5%</div><div>24%</div></div>
5	L	613	<div><div></div><div>%</div><div>36%</div><div>34%</div><div>6%</div><div>23%</div></div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 55699 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	309	Total	C	N	O	S	0	0	0
			2403	1505	421	469	8			
1	B	217	Total	C	N	O	S	0	0	0
			1672	1044	295	327	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	217	Total	C	N	O	S	0	0	0
			1667	1041	293	327	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
			10572	6634	1839	2056	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10568	6632	1838	2055	43			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	526	TYR	HIS	engineered mutation	UNP P0A8V2
I	526	TYR	HIS	engineered mutation	UNP P0A8V2

- 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
			9107	5723	1634	1704	46			
3	J	1155	Total	C	N	O	S	0	0	0
			9029	5676	1620	1687	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	467	Total	C	N	O	S	0	0	0
			3806	2385	677	721	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

- 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		

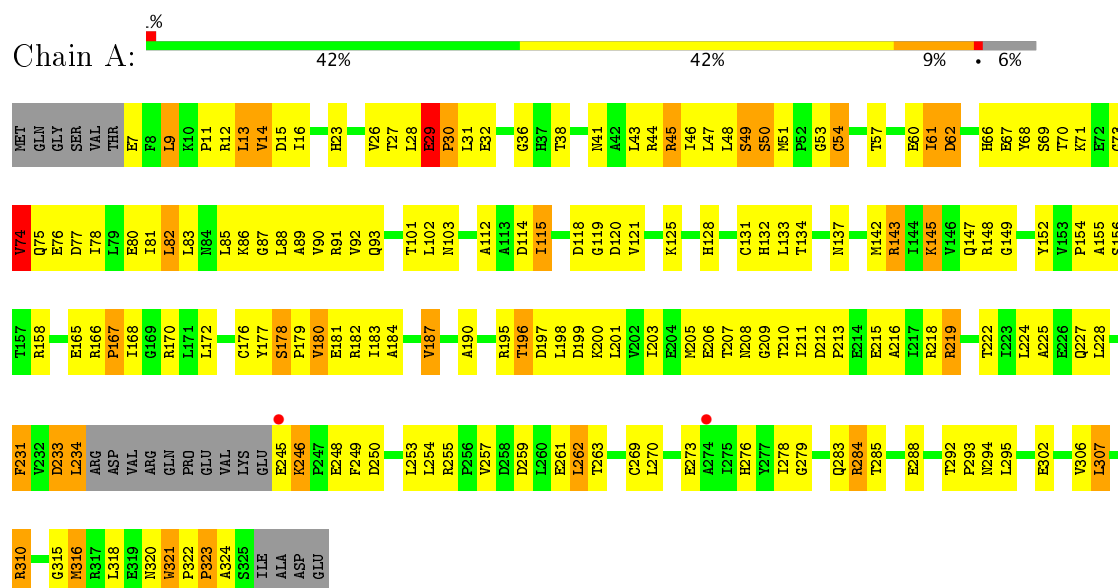
- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

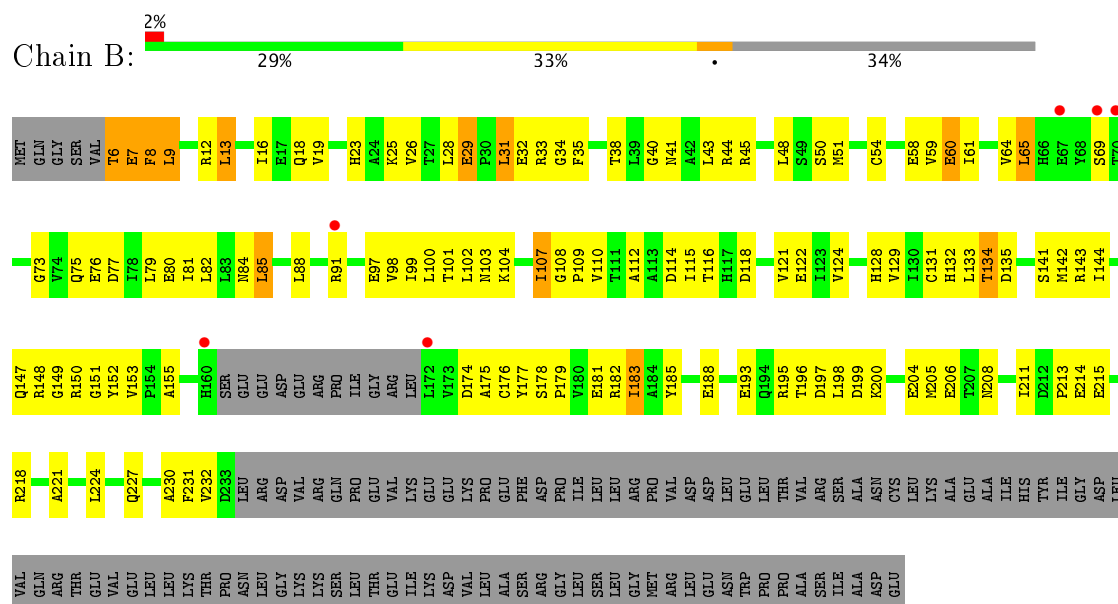
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

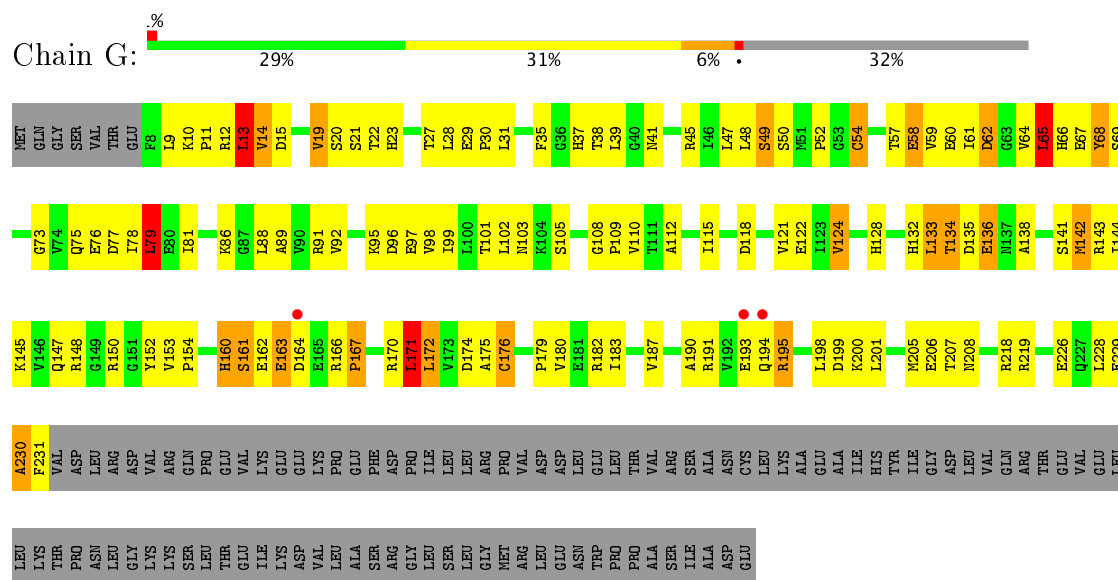
• Molecule 1: DNA-directed RNA polymerase subunit alpha



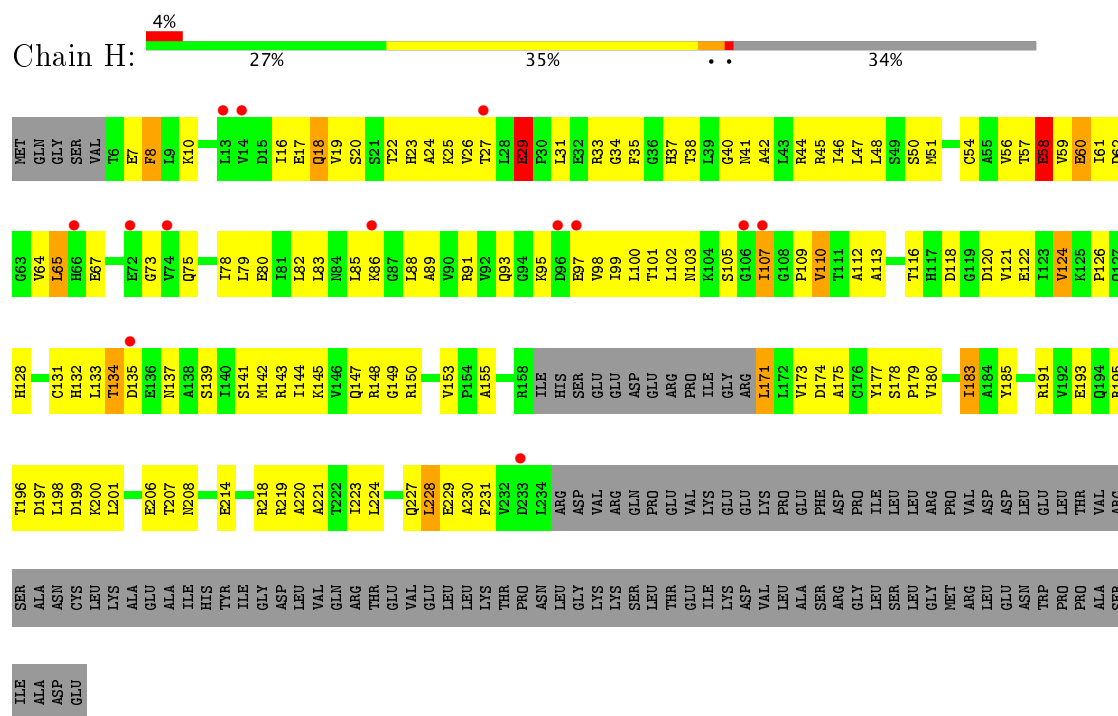
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 1: DNA-directed RNA polymerase subunit alpha



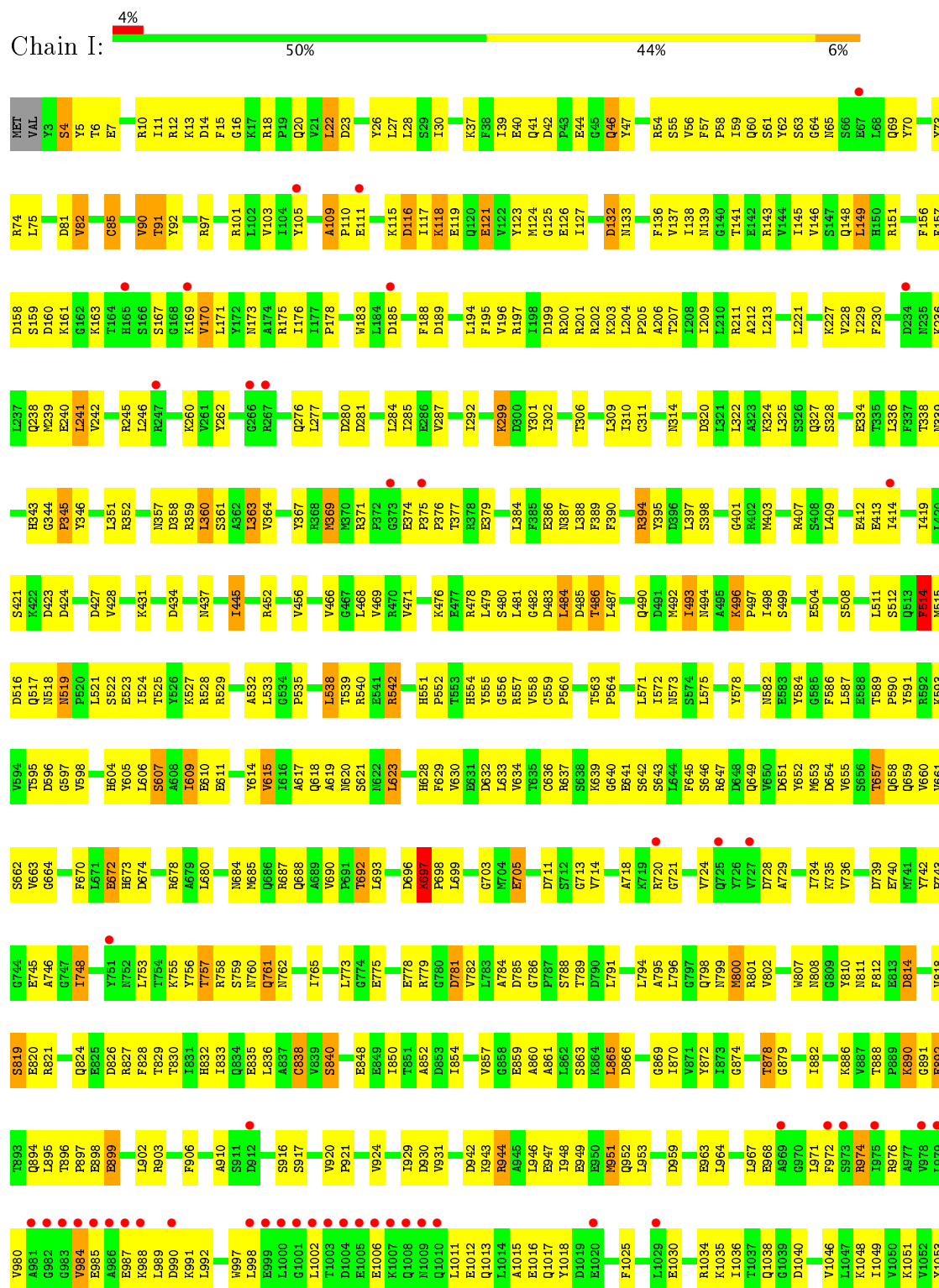
• Molecule 1: DNA-directed RNA polymerase subunit alpha

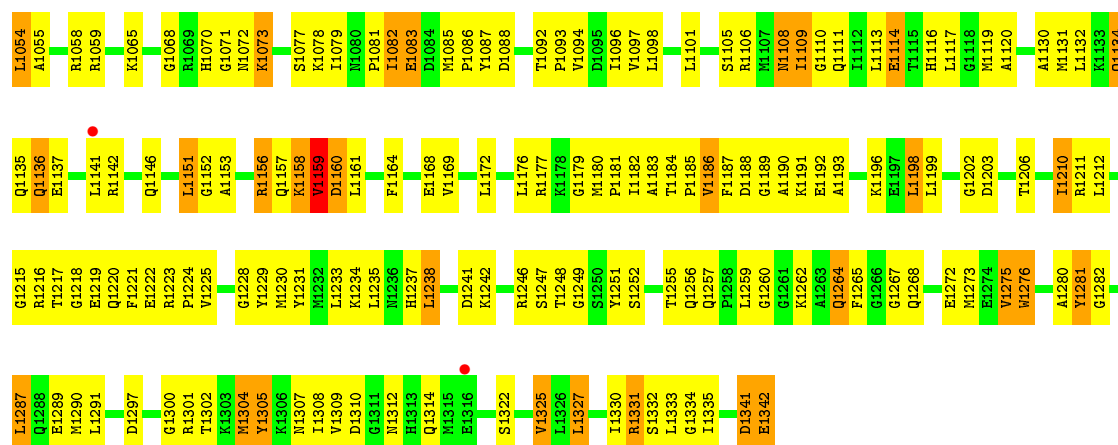


K1262	D1488	M1119	Y984	F812	I732	G664	V598	R529	F464	L366	E286	L210	V137
A1263	G1189	A1120	E985	E813	I732	A665	D601	I530	R465	L367	V287	R211	I138
Q1264	A1190	G1123	E986	D814	V736	S666	E602	G534	G467	R368	V289	A212	N139
G1266	E1192	G1124	R988	S815	E740	L668	I603	L538	L468	R369	L232	R214	T141
Q1268	A1193	R1058	R989	L817	E745	R669	H604	T539	R470	R377	L232	Y215	E142
E1195	E1194	I1060	Q990	V818	E746	R670	Y605	R540	R471	R378	V296	L221	I145
I1195	Q1061	Q1062	R991	S819	A746	L671	L606	E541	E472	R379	V297	F224	V146
E1197	M1131	E898	L992	E872	I748	E672	S607	R542	R473	E380	E298	F225	S147
M1273	E1134	E899	R993	H673	I748	H673	I609	G544	A474	A381	K299	R225	Q148
A1276	K1065	D995	R994	G824	K755	A676	V615	G544	V475	E382	D300	V228	L149
Q1277	M1066	R996	R996	E825	K756	N677	I616	G544	E477	L384	I302	L229	H150
L1278	A1067	R997	R997	D826	Y756	R678	I617	R547	R478	L387	T306	F230	R151
E1279	G1068	L998	L998	R827	T757	A679	Q618	R548	L479	L388	T306	E231	F156
G1280	R1069	R999	R999	F828	R758	L680	A619	H551	S480	L389	L309	L232	F157
Y1281	H1070	L1000	L1000	T829	S759	M681	N620	H552	P552	P552	I310	N235	D158
G1282	N1072	Y913	Y913	T830	N760	G682	S621	T553	L481	P389	C311	K236	S159
A1283	K1073	L1002	L1002	I831	Q761	A683	M622	H554	G482	R394	A312	N235	D160
A1284	G1074	T1003	T1003	H832	N762	M684	G622	H554	L483	T395	E316	P243	K163
I1285	V1075	D1004	D1004	I833	T763	H685	L623	H554	L484	T396	S318	E244	T164
T1286	Q1146	E1005	E1005	Q834	C764	Q686	D624	G556	T485	L397	L319	R245	H165
L1287	S1077	E1006	E1006	R687	C764	Q687	E625	R557	T486	S398	E240	L246	S167
Q1288	K1078	K1007	K1007	L836	M768	G627	G626	V558	L487	E398	L317	R247	L171
E1289	I1079	Q1008	Q1008	L837	P769	T692	G627	C559	M488	E316	E316	T250	Y172
Y1290	N1080	N1009	N1009	C838	C770	L693	H628	P560	P489	V400	H330	A251	H173
G1215	P1081	Q1010	Q1010	R839	L773	A695	P629	I561	Q490	G401	H331	E256	R175
T1217	L1011	L1011	L1011	S840	L773	G696	E631	T563	M492	R404	L325	E256	K169
A1153	E1012	R841	R841	E775	E775	K697	D632	P564	L493	L409	L322	R247	L171
R1156	D1084	Q1013	Q1013	R698	P776	L699	L633	P565	M494	L409	A323	T250	H172
Q1157	M1085	L1014	L1014	L699	R779	V700	P635	G566	A495	E412	K324	A251	N173
K1158	Y1087	E940	E940	V700	G780	G701	C636	N568	R496	E413	L325	E256	R175
E1159	G1091	R941	R941	G857	D781	T702	R637	I569	I498	I177	Q327	A257	I177
L1161	K1022	R943	R943	E858	V782	G703	S638	G570	S499	L419	S328	N258	P178
F1164	H1023	R944	R944	E859	L783	N704	K639	L571	K503	D423	G329	V261	W183
S1165	E1024	R945	R945	L862	A784	E705	G640	I572	E504	F506	H332	V262	L184
E1026	F1025	L946	L946	S863	S788	R706	E641	N573	F506	V428	R331	V263	D185
K1027	E1026	L946	L946	K864	S788	A707	S642	L575	F506	V428	R332	E264	D185
E1030	K1027	P951	P951	L865	L791	A708	F645	Y578	Q510	K431	T335	R267	D189
R1033	E1030	L953	L953	E867	G792	D710	S646	R582	S512	D434	L336	R268	P190
K1035	R1034	R958	R958	I870	E793	S712	R647	R582	Q513	T445	G344	R269	K191
V1103	V1103	D959	D959	V871	A795	G713	Q649	E583	Q513	T446	P345	T270	D192
S1105	S1105	L960	L960	Y872	L796	V714	V650	Y584	D516	R447	Y346	A271	N193
R1106	R1106	S961	S961	I873	G797	V714	D651	G585	Q517	L448	I347	R273	L194
M1107	M1107	Q1038	Q1038	V877	Q798	V717	V652	F586	Q517	L448	I347	R273	F195
N1108	N1108	E963	E963	V877	N799	A718	M653	L587	N518	L448	I347	R273	F195
I1109	I1109	D1040	D1040	T878	N800	K719	D654	L587	N518	L448	I347	R273	V196
G1110	G1110	G1109	G1109	R879	R801	R720	V655	T589	P520	R452	T356	R274	D199
D1041	D1041	L967	L967	G880	V802	G721	S656	P590	L521	L453	N357	R276	R200
L1042	L1042	R974	R974	D881	T657	T657	T657	Y591	S522	R454	R359	Q276	R200
A1043	A1043	R975	R975	I882	M805	Q658	Q658	R592	E523	S455	R359	D280	R201
P1044	P1044	R976	R976	L883	R806	Q659	Q659	K593	I524	V456	S361	D281	R202
V1046	V1046	L1115	L1115	V884	W807	Y726	V660	V594	T525	G457	A362	V282	K203
L1116	L1116	L1116	L1116	G885	Y810	V727	V661	T595	Y526	E461	L363	R283	R202
L1117	L1117	V980	V980	K886	Y810	V728	S662	T595	K527	E461	L363	R283	K203
F1187	F1187	T1049	T1049	V887	N811	A729	V663	G597	R528	E461	L363	R283	K203

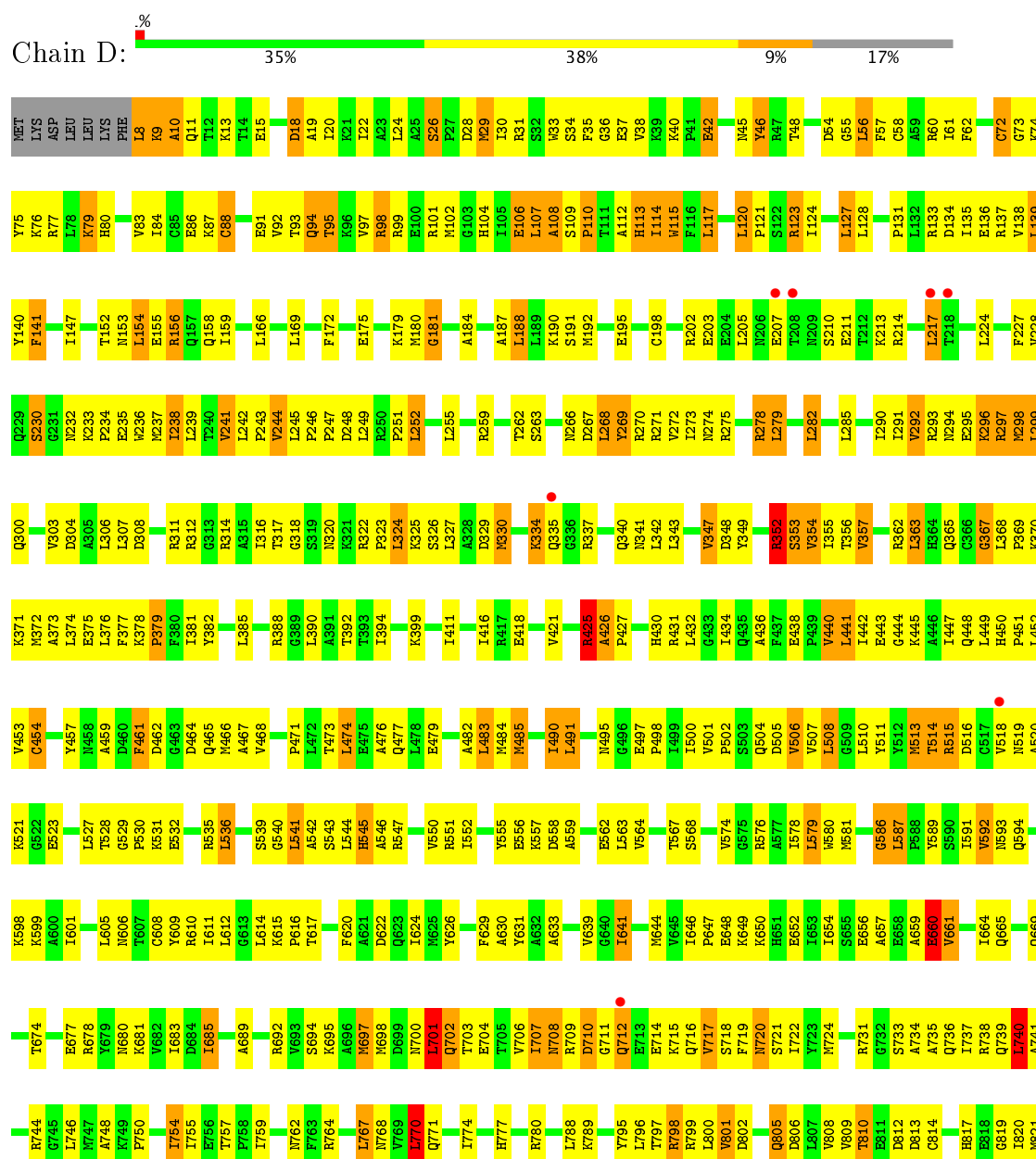
D1341
E1342

• Molecule 2: DNA-directed RNA polymerase subunit beta





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





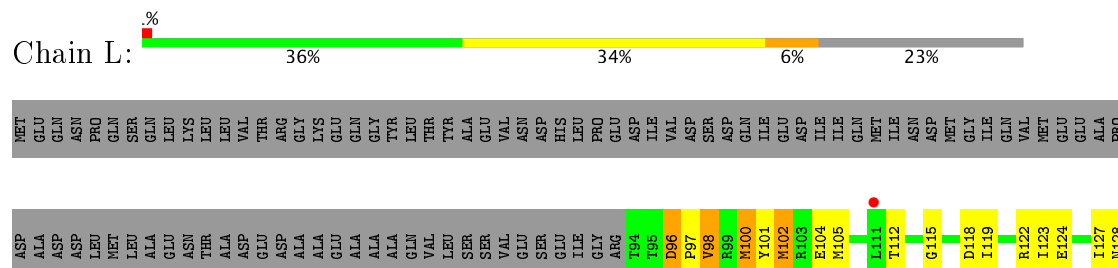
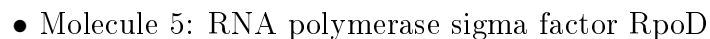
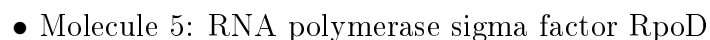
LEU	Q1326	K1247	R1173	GLN	P926	T853	E785	1685	N593	D516	E443
ALA	E1327	I1248	R1174	LEU	L930	A854	L770	5894	Q594	C517	Q448
LEU	T1328	D1250	V1175	ASP	T931	D855	D855	5894	L596	V518	L448
LEU	T1329	K1251	V1176	GLY	ARG	I856	F773	N697	L596	K521	H450
ASN	R1330	H1252	T1177	VAL	THR	L857	L774	N698	K398	G597	P451
ALA	V1331	V1255	T1178	GLN	SER	P859	S775	D898	K399	G522	L452
GLY	L1332	V1256	P1179	ILE	PHE	R860	T776	N700	A600	E523	V453
LEU	T1333	I1255	V1180	LYS	HIS	N861	R780	L701	I601	L527	C454
GLY	E1334	V1257	S1183	SER	LYS	T862	R780	Q702	S802	T528	Y457
GLY	R1258	R1258	D1184	VAL	ARG	L863	L795	T703	K803	G529	N458
SER	V1337	K1259	P1185	PRO	GLY	T863	R796	T703	M604	P530	N458
ASP	A1338	M1260	Y1186	VAL	GLY	H864	L788	E704	M604	K531	A459
ASN	R1341	L1261	E1187	VAL	ALA	H865	K789	T705	L605	E532	D460
GLU	R1342	K1262	P1191	LEU	SER	Q867	T795	V706	G613	A533	F461
	D1342	K1263	K1192	LEU	ARG	W868	L796	N707	L614	E534	D462
	E1343	A1264	V1193	SER	ALA	C969	T797	R709	D462	R535	Q463
	L1344	T1265	W1193	ALA	LYS	L872	R798	D710	T617	L536	D464
	R1345	I1266	R1194	GLY	GLY	L872	R799	G711	F620	Y537	O465
		G1270	V1198	ARG	ASP	V877	L800	Q712	A621	R538	A467
		D1273	F1199	THR	GLY	K881	R801	K715	Q622	S539	
		F1274	E1202	ALA	GLU	V882	D802	Q716	Q623	G540	
		L1275	R1203	GLY	ILE	V883	W803	Q717	I624	A542	
		E1276	V1204	LYS	VAL	S884	Q805	S718	A543	S543	
		G1277	E1205	ASP	LYS	V885	D806	F719	L544	L544	
		Q1278	L1206	LEU	ASN	V886	L807	N720	B545	B545	
		Q1279	R1207	ARG	GLY	S887	W808	S721	A546	A546	
		V1280	D1208	THR	THR	C888	R809	I722	R547	R547	
		E1281	V1209	ALA	GLY	D889	T810	I723	V548	V548	
		R1284	L1138	LEU	ILE	T890	E811	N724	K549	K549	
		V1285	P1139	LYS	LYS	D812	D812	N725	V550	V550	
		K1286	R1140	ILE	LEU	D813	D813	I641	R481	R481	
		N1289	L1144	VAL	SER	G893	C814	D642	R482	R482	
		R1290	F1145	ASP	ASN	C895	H817	V645	L483	L483	
		E1293	E1146	GLY	VAL	A896	V825	I646	N484	N484	
		N1295	R1149	THR	SER	H897	I826	K557	L490	L490	
		K1297	P1150	ASN	VAL	C898	E827	K558	S492	S492	
		V1298	K1151	LEU	VAL	Y899	G828	E566	N488	N488	
		G1299	E1152	THR	THR	G900	R901	A665	L491	L491	
		Y1302	P1153	ILE	SER	D902	D830	K566	S492	S492	
		R1303	A1154	GLY	SER	L903	R831	T567	N495	N495	
		D1305	L1155	VAL	LYS	R904	K832	S668	G496	G496	
		E1306	L1156	THR	GLY	R905	R744	E569	E497	E497	
		L1307	E1157	ASP	VAL	G906	R836	K570	P498	P498	
		G1308	E1158	THR	THR	H907	V839	T572	D571	D571	
		T1309	I1159	VAL	THR	I908	V839	T573	T572	T572	
		V1310	S1160	ARG	SER	I909	V839	T573	T572	T572	
		K1311	G1161	ALA	ARG	N910	V839	T573	T572	T572	
		A1312	T1162	THR	ASP	A914	T844	S753	P502	P502	
		S1318	S1163	GLN	ASN	I915	T844	I754	S503	S503	
			F1165	ILE	THR	I915	E846	I754	Q504	Q504	
			T1169	GLY	LEU	I918	D847	P758	D505	D505	
			K1170	LYS	LYS	A919	V848	I759	V506	V506	
			G1171	ALA	GLN	A919	L849	I759	Y512	Y512	
			R1172	THR	THR	G924	R850	N762	M513	M513	
			V1246	VAL	THR	E925	G852	R764	T514	T514	

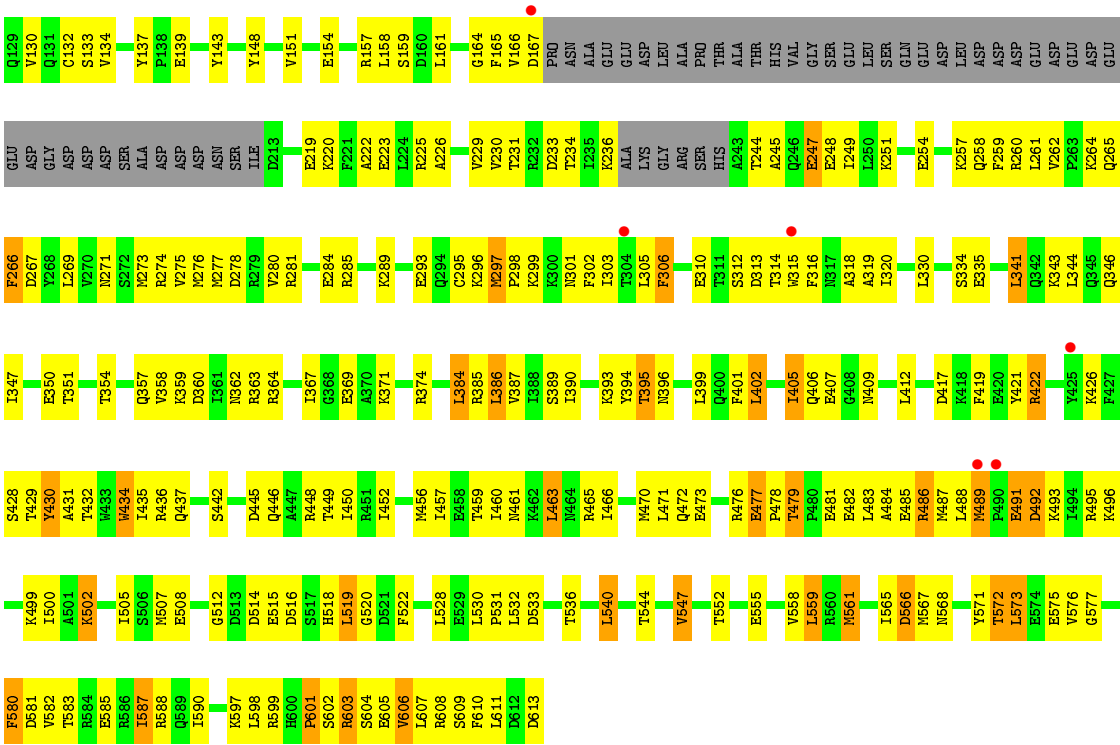
• Molecule 4: DNA-directed RNA polymerase subunit omega



MET	A2	V10	E11	K12	T13	N15	R16	R25	R28	V32	G33	G34	V39	P40	K45	T46	A50	L51	R52	E53	F54	L58	T59	I60	R61	Q62	T63	L64	D65	V66	R69	Q70	E71	V83	T86	R90	ARG
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- Chain K:





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.36Å 206.28Å 308.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.90 – 3.60 29.90 – 3.60	Depositor EDS
% Data completeness (in resolution range)	93.7 (29.90-3.60) 93.7 (29.90-3.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 3.56Å)	Xtriage
Refinement program	PHENIX (1.10.1 _2155: ???)	Depositor
R, R_{free}	0.246 , 0.305 0.245 , 0.304	Depositor DCC
R_{free} test set	1937 reflections (1.51%)	DCC
Wilson B-factor (Å ²)	142.2	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 91.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55699	wwPDB-VP
Average B, all atoms (Å ²)	157.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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	0.84	4/2435 (0.2%)	1.07	12/3300 (0.4%)
1	B	0.75	1/1692 (0.1%)	1.01	5/2293 (0.2%)
1	G	0.58	0/1751	1.05	9/2373 (0.4%)
1	H	0.59	0/1686	0.91	4/2285 (0.2%)
2	C	1.17	37/10741 (0.3%)	1.21	65/14492 (0.4%)
2	I	0.80	7/10737 (0.1%)	0.97	15/14487 (0.1%)
3	D	1.21	60/9246 (0.6%)	1.24	74/12478 (0.6%)
3	J	1.02	27/9168 (0.3%)	1.13	52/12374 (0.4%)
4	E	0.65	0/693	0.83	0/935
4	K	0.38	0/629	0.61	0/847
5	F	0.82	2/3857 (0.1%)	1.05	10/5184 (0.2%)
5	L	0.77	3/3872 (0.1%)	0.99	12/5205 (0.2%)
All	All	0.98	141/56507 (0.2%)	1.10	258/76253 (0.3%)

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	A	0	2
1	G	0	1
2	C	0	11
2	I	0	2
3	D	0	12
3	J	0	9
5	F	0	1
5	L	0	1
All	All	0	39

The worst 5 of 141 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	811	ASN	CB-CG	-9.14	1.30	1.51
1	A	131	CYS	CB-SG	-8.93	1.67	1.82
3	J	145	VAL	CB-CG2	-8.81	1.34	1.52
2	C	636	CYS	CB-SG	-8.52	1.67	1.82
3	J	72	CYS	CB-SG	-7.87	1.68	1.82

The worst 5 of 258 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1287	LEU	CB-CG-CD2	-14.16	86.92	111.00
3	D	376	LEU	CB-CG-CD2	-10.83	92.59	111.00
3	D	114	ILE	CG1-CB-CG2	-10.71	87.84	111.40
2	C	796	LEU	CB-CG-CD2	-9.94	94.10	111.00
3	D	188	LEU	CB-CG-CD2	-9.88	94.20	111.00

There are no chirality outliers.

5 of 39 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	321	TRP	Peptide
1	A	49	SER	Mainchain
2	C	109	ALA	Peptide
2	C	236	LYS	Peptide
2	C	473	ARG	Mainchain

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	2403	0	2453	197	0
1	B	1672	0	1693	112	0
1	G	1730	0	1756	145	0
1	H	1667	0	1689	123	1
2	C	10572	0	10584	657	3
2	I	10568	0	10578	602	0
3	D	9107	0	9308	612	0
3	J	9029	0	9225	587	0
4	E	691	0	695	22	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	K	627	0	634	26	0
5	F	3806	0	3873	199	2
5	L	3821	0	3884	190	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
All	All	55699	0	56372	3190	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 28.

The worst 5 of 3190 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:A:27:THR:O	1:A:28:LEU:HD12	1.10	1.23
2:I:27:LEU:O	2:I:528:ARG:NH1	1.78	1.17
1:A:27:THR:O	1:A:28:LEU:CD1	1.93	1.17
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.16	1.08
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.36	1.08

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)
2:C:33:ASP:OD1	5:F:554:ARG:NH2[4_455]	1.99	0.21
2:C:44:GLU:OE1	5:F:596:ARG:NH1[4_455]	2.05	0.15
2:C:940:GLU:OE1	1:H:139:SER:OG[4_455]	2.05	0.15

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	305/329 (93%)	271 (89%)	25 (8%)	9 (3%)	5	40
1	B	213/329 (65%)	191 (90%)	20 (9%)	2 (1%)	20	64
1	G	222/329 (68%)	182 (82%)	28 (13%)	12 (5%)	2	24
1	H	213/329 (65%)	193 (91%)	20 (9%)	0	100	100
2	C	1338/1342 (100%)	1225 (92%)	103 (8%)	10 (1%)	25	68
2	I	1338/1342 (100%)	1226 (92%)	100 (8%)	12 (1%)	20	64
3	D	1162/1407 (83%)	1074 (92%)	79 (7%)	9 (1%)	22	65
3	J	1151/1407 (82%)	1064 (92%)	82 (7%)	5 (0%)	38	77
4	E	87/91 (96%)	79 (91%)	8 (9%)	0	100	100
4	K	77/91 (85%)	74 (96%)	3 (4%)	0	100	100
5	F	461/613 (75%)	422 (92%)	37 (8%)	2 (0%)	38	77
5	L	463/613 (76%)	423 (91%)	39 (8%)	1 (0%)	51	85
All	All	7030/8222 (86%)	6424 (91%)	544 (8%)	62 (1%)	20	64

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	GLU
1	A	30	PRO
1	A	324	ALA
1	B	232	VAL
2	C	345	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	268/286 (94%)	249 (93%)	19 (7%)	17	55
1	B	184/286 (64%)	166 (90%)	18 (10%)	9	42
1	G	191/286 (67%)	179 (94%)	12 (6%)	21	60
1	H	183/286 (64%)	165 (90%)	18 (10%)	9	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	1155/1157 (100%)	1046 (91%)	109 (9%)	10	44
2	I	1154/1157 (100%)	1046 (91%)	108 (9%)	10	44
3	D	975/1168 (84%)	875 (90%)	100 (10%)	8	40
3	J	967/1168 (83%)	869 (90%)	98 (10%)	9	40
4	E	72/75 (96%)	64 (89%)	8 (11%)	7	37
4	K	67/75 (89%)	63 (94%)	4 (6%)	22	62
5	F	416/540 (77%)	373 (90%)	43 (10%)	8	40
5	L	418/540 (77%)	372 (89%)	46 (11%)	7	37
All	All	6050/7024 (86%)	5467 (90%)	583 (10%)	10	43

5 of 583 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
5	F	335	GLU
1	H	193	GLU
5	L	100	MET
5	F	445	ASP
5	F	606	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 78 such sidechains are listed below:

Mol	Chain	Res	Type
5	F	396	ASN
2	I	343	HIS
5	L	129	GLN
5	F	406	GLN
5	F	518	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	309/329 (93%)	-0.32	2 (0%) 89 81	99, 147, 225, 245	0
1	B	217/329 (65%)	-0.02	6 (2%) 53 40	112, 194, 254, 272	0
1	G	224/329 (68%)	-0.07	3 (1%) 77 64	163, 206, 241, 270	0
1	H	217/329 (65%)	0.07	13 (5%) 23 16	146, 213, 252, 285	0
2	C	1340/1342 (99%)	-0.35	21 (1%) 72 59	74, 121, 234, 285	0
2	I	1340/1342 (99%)	-0.16	50 (3%) 42 31	86, 159, 261, 388	0
3	D	1166/1407 (82%)	-0.30	14 (1%) 79 66	72, 112, 215, 264	0
3	J	1155/1407 (82%)	-0.22	22 (1%) 67 53	86, 138, 229, 274	0
4	E	89/91 (97%)	-0.02	2 (2%) 62 48	147, 183, 216, 241	0
4	K	79/91 (86%)	0.78	14 (17%) 2 2	202, 277, 319, 350	0
5	F	467/613 (76%)	-0.23	12 (2%) 56 42	93, 165, 290, 340	0
5	L	469/613 (76%)	-0.30	7 (1%) 74 61	116, 178, 288, 353	0
All	All	7072/8222 (86%)	-0.22	166 (2%) 61 46	72, 147, 251, 388	0

The worst 5 of 166 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	I	982	GLY	8.9
3	D	335	GLN	6.3
2	I	1001	GLY	5.3
1	B	160	HIS	5.1
2	I	1000	LEU	4.9

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
7	ZN	D	1502	1/1	0.81	0.13	-0.94	134,134,134,134	0
7	ZN	D	1503	1/1	0.99	0.06	-0.97	51,51,51,51	0
7	ZN	J	1503	1/1	0.95	0.09	-1.43	97,97,97,97	0
7	ZN	J	1502	1/1	0.97	0.02	-1.80	131,131,131,131	0
6	MG	D	1501	1/1	0.94	0.54	-	87,87,87,87	0
6	MG	J	1501	1/1	0.92	0.35	-	94,94,94,94	0

6.5 Other polymers [i](#)

There are no such residues in this entry.