



wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 15, 2016 – 11:36 AM EST

PDB ID : 5TBZ
Title : E. Coli RNA Polymerase complexed with NusG
Authors : Liu, B.; Steitz, T.A.
Deposited on : 2016-09-13
Resolution : 7.00 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 : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
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) : rb-20028442

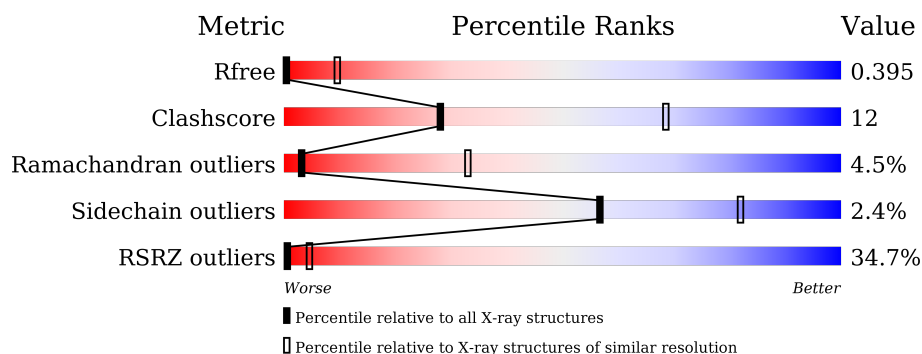
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 7.00 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	1014 (9.50-3.66)
Clashscore	102246	1063 (10.00-3.70)
Ramachandran outliers	100387	1035 (9.50-3.66)
Sidechain outliers	100360	1005 (9.50-3.66)
RSRZ outliers	91569	1013 (9.50-3.66)

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	242	<div> <div>26%</div> <div> <div>73%</div> <div>18%</div> <div>• 7%</div> </div> </div>
1	B	242	<div> <div>47%</div> <div> <div>69%</div> <div>18%</div> <div>• 11%</div> </div> </div>
1	F	242	<div> <div>23%</div> <div> <div>72%</div> <div>20%</div> <div>• 7%</div> </div> </div>
1	G	242	<div> <div>38%</div> <div> <div>71%</div> <div>17%</div> <div>• 11%</div> </div> </div>
2	C	1342	<div> <div>32%</div> <div> <div>77%</div> <div>20%</div> <div>••</div> </div> </div>
2	H	1342	<div> <div>34%</div> <div> <div>75%</div> <div>21%</div> <div>••</div> </div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div></div><div>29%63%26%•7%</div></div>
3	I	1407	<div><div></div><div>35%64%25%•7%</div></div>
4	J	181	<div><div></div><div>27%61%18%•19%</div></div>
4	K	181	<div><div></div><div>33%56%22%••19%</div></div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50147 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	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	B	215	Total	C	N	O	S	0	0	0
			1657	1034	291	326	6			
1	F	225	Total	C	N	O	S	0	0	0
			1740	1082	309	343	6			
1	G	216	Total	C	N	O	S	0	0	0
			1667	1040	294	327	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ALA	-	expression tag	UNP P0A7Z6
A	-5	HIS	-	expression tag	UNP P0A7Z6
A	-4	HIS	-	expression tag	UNP P0A7Z6
A	-3	HIS	-	expression tag	UNP P0A7Z6
A	-2	HIS	-	expression tag	UNP P0A7Z6
A	-1	HIS	-	expression tag	UNP P0A7Z6
A	0	HIS	-	expression tag	UNP P0A7Z6
B	-6	ALA	-	expression tag	UNP P0A7Z6
B	-5	HIS	-	expression tag	UNP P0A7Z6
B	-4	HIS	-	expression tag	UNP P0A7Z6
B	-3	HIS	-	expression tag	UNP P0A7Z6
B	-2	HIS	-	expression tag	UNP P0A7Z6
B	-1	HIS	-	expression tag	UNP P0A7Z6
B	0	HIS	-	expression tag	UNP P0A7Z6
F	-6	ALA	-	expression tag	UNP P0A7Z6
F	-5	HIS	-	expression tag	UNP P0A7Z6
F	-4	HIS	-	expression tag	UNP P0A7Z6
F	-3	HIS	-	expression tag	UNP P0A7Z6
F	-2	HIS	-	expression tag	UNP P0A7Z6
F	-1	HIS	-	expression tag	UNP P0A7Z6
F	0	HIS	-	expression tag	UNP P0A7Z6

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Chain	Residue	Modelled	Actual	Comment	Reference
G	-6	ALA	-	expression tag	UNP P0A7Z6
G	-5	HIS	-	expression tag	UNP P0A7Z6
G	-4	HIS	-	expression tag	UNP P0A7Z6
G	-3	HIS	-	expression tag	UNP P0A7Z6
G	-2	HIS	-	expression tag	UNP P0A7Z6
G	-1	HIS	-	expression tag	UNP P0A7Z6
G	0	HIS	-	expression tag	UNP P0A7Z6

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			
2	H	1319	Total	C	N	O	S	0	1	0
			10401	6524	1814	2020	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1302	Total	C	N	O	S	0	0	0
			10085	6326	1800	1911	48			
3	I	1306	Total	C	N	O	S	0	0	0
			10126	6353	1809	1916	48			

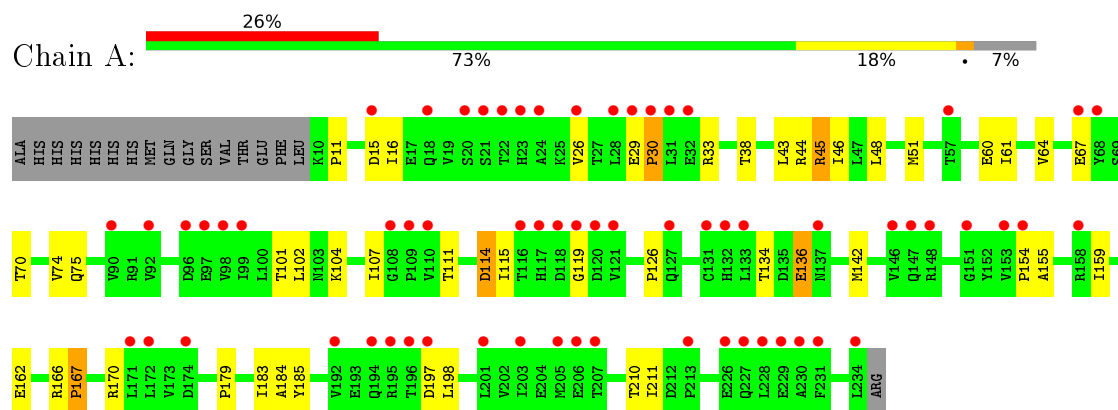
- Molecule 4 is a protein called Transcription termination/antitermination protein NusG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			
4	K	147	Total	C	N	O	S	0	0	0
			1165	740	201	217	7			

3 Residue-property plots [i](#)

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.

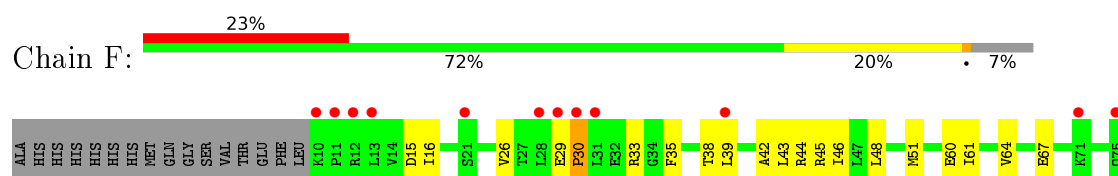
- Molecule 1: DNA-directed RNA polymerase subunit alpha

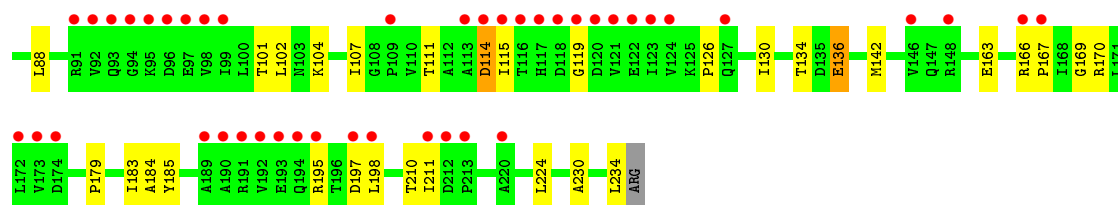


- Molecule 1: DNA-directed RNA polymerase subunit alpha

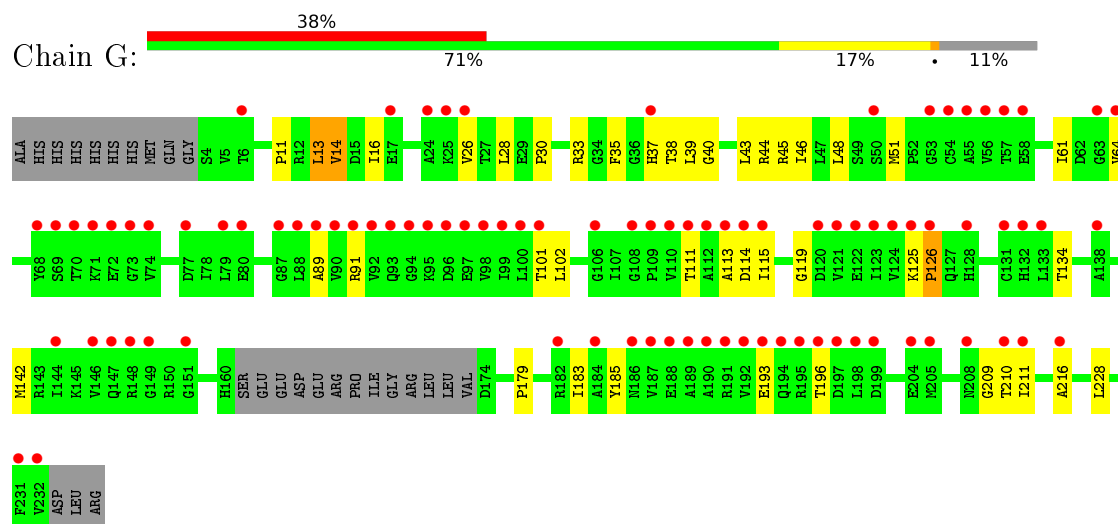


- Molecule 1: DNA-directed RNA polymerase subunit alpha

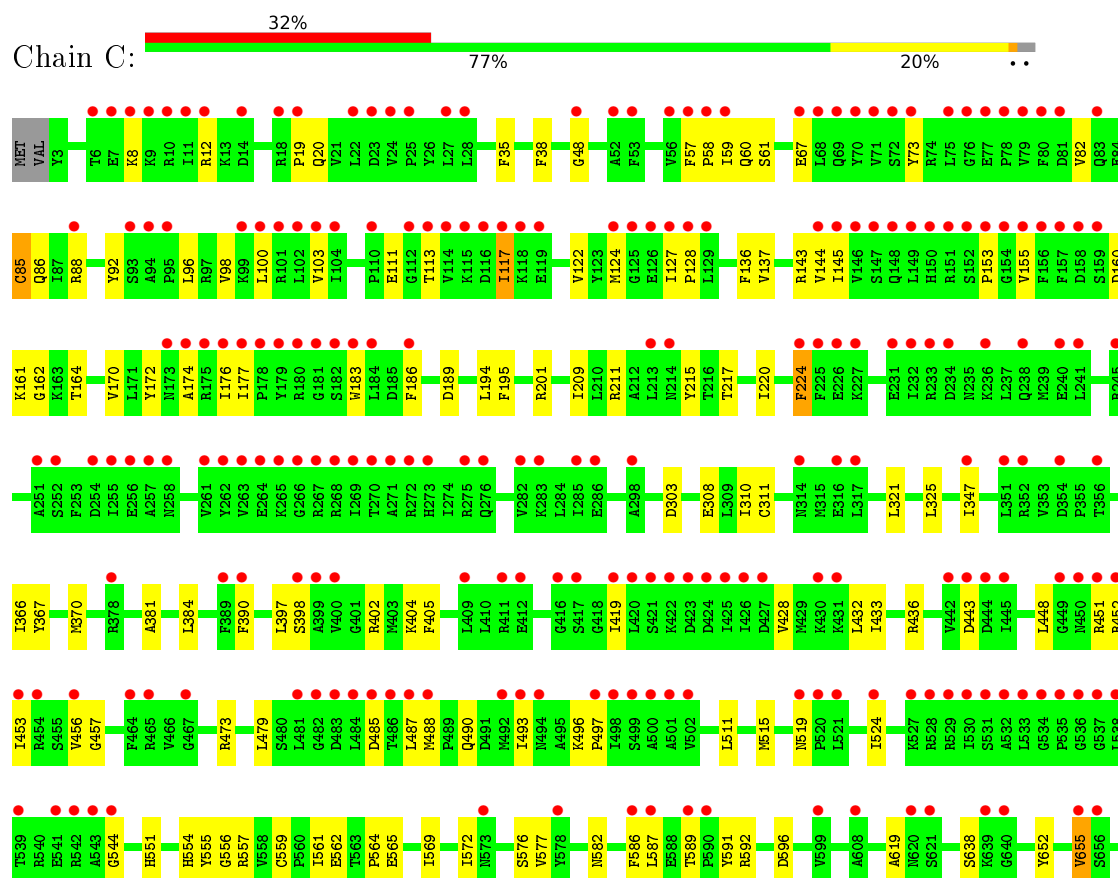


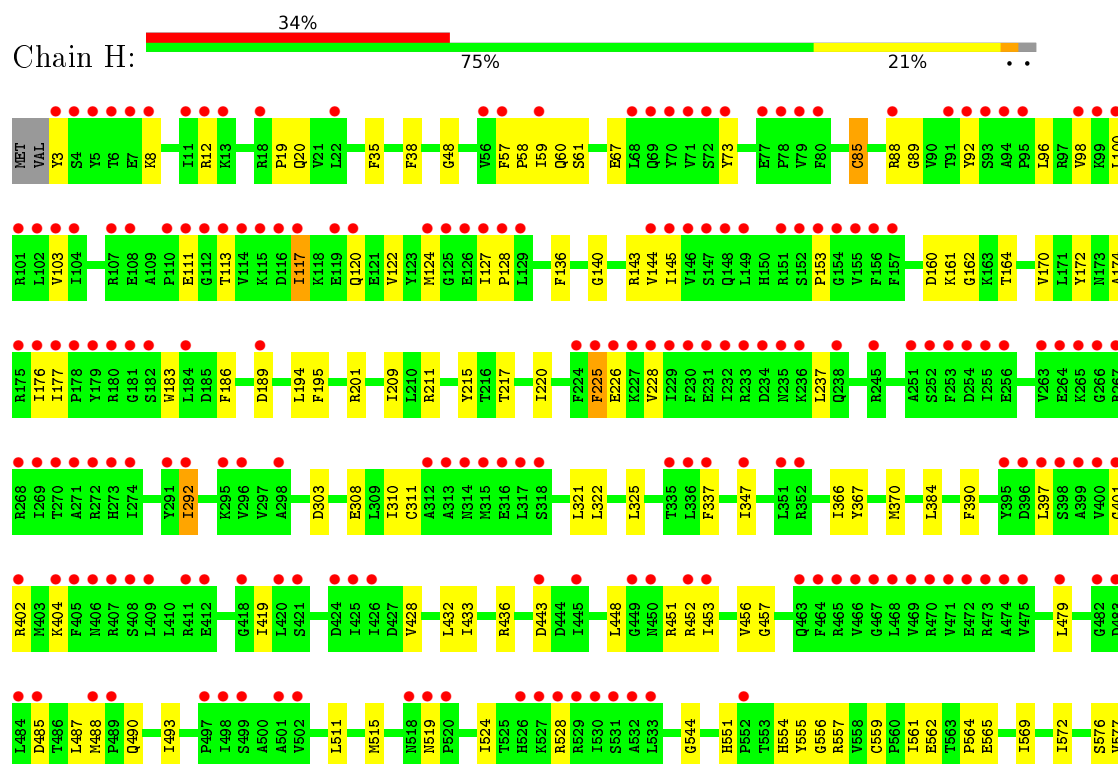


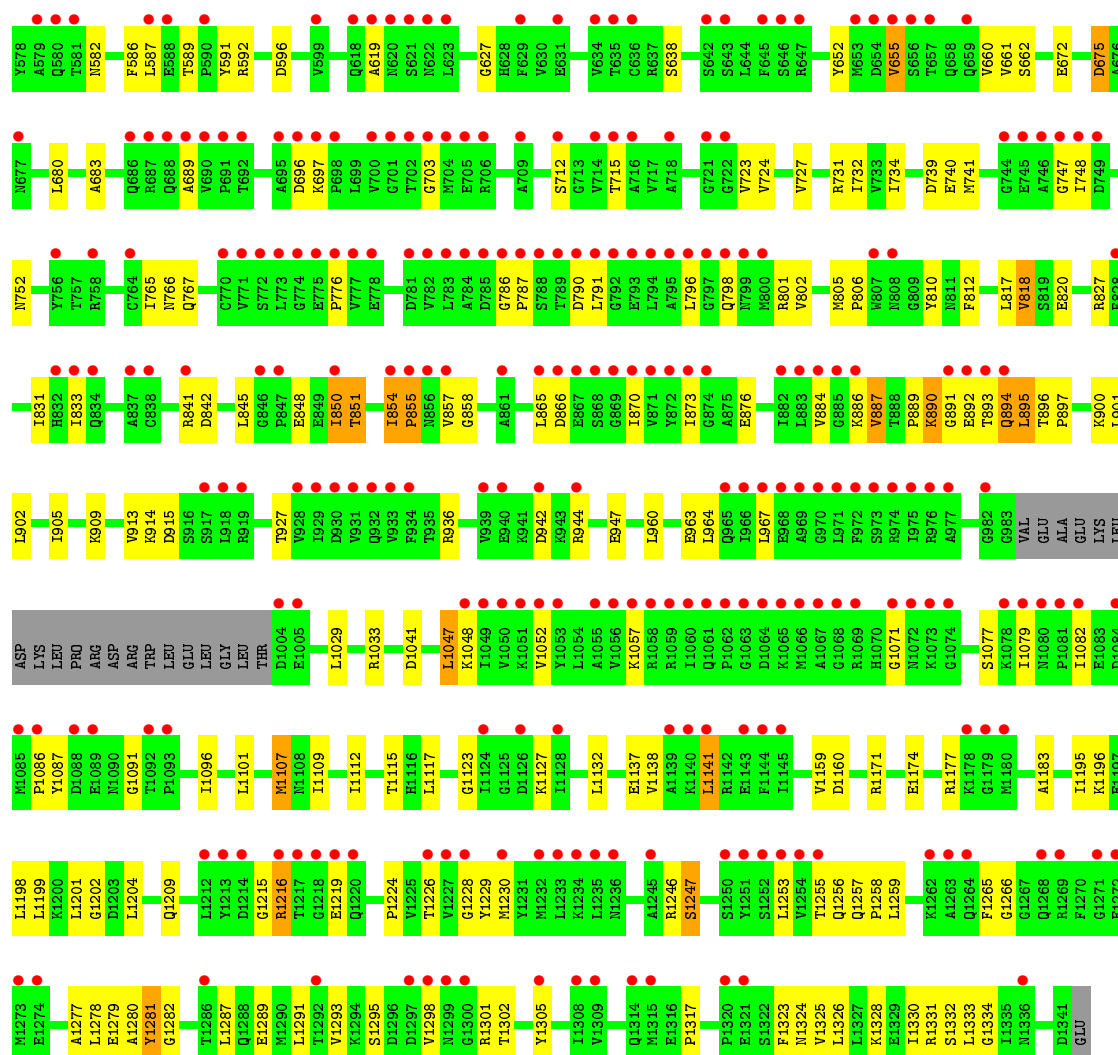
• Molecule 1: DNA-directed RNA polymerase subunit alpha



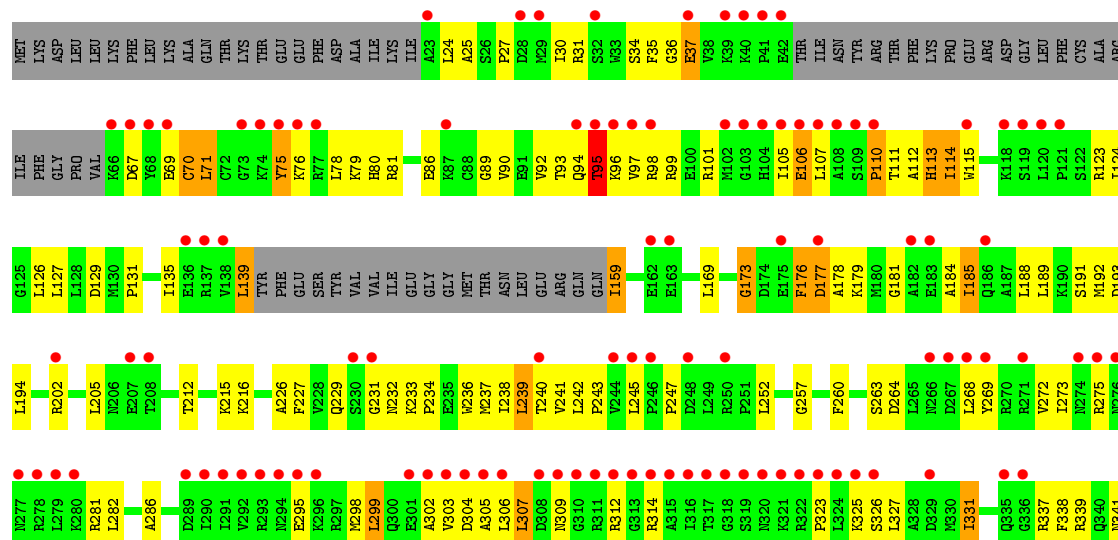
• Molecule 2: DNA-directed RNA polymerase subunit beta

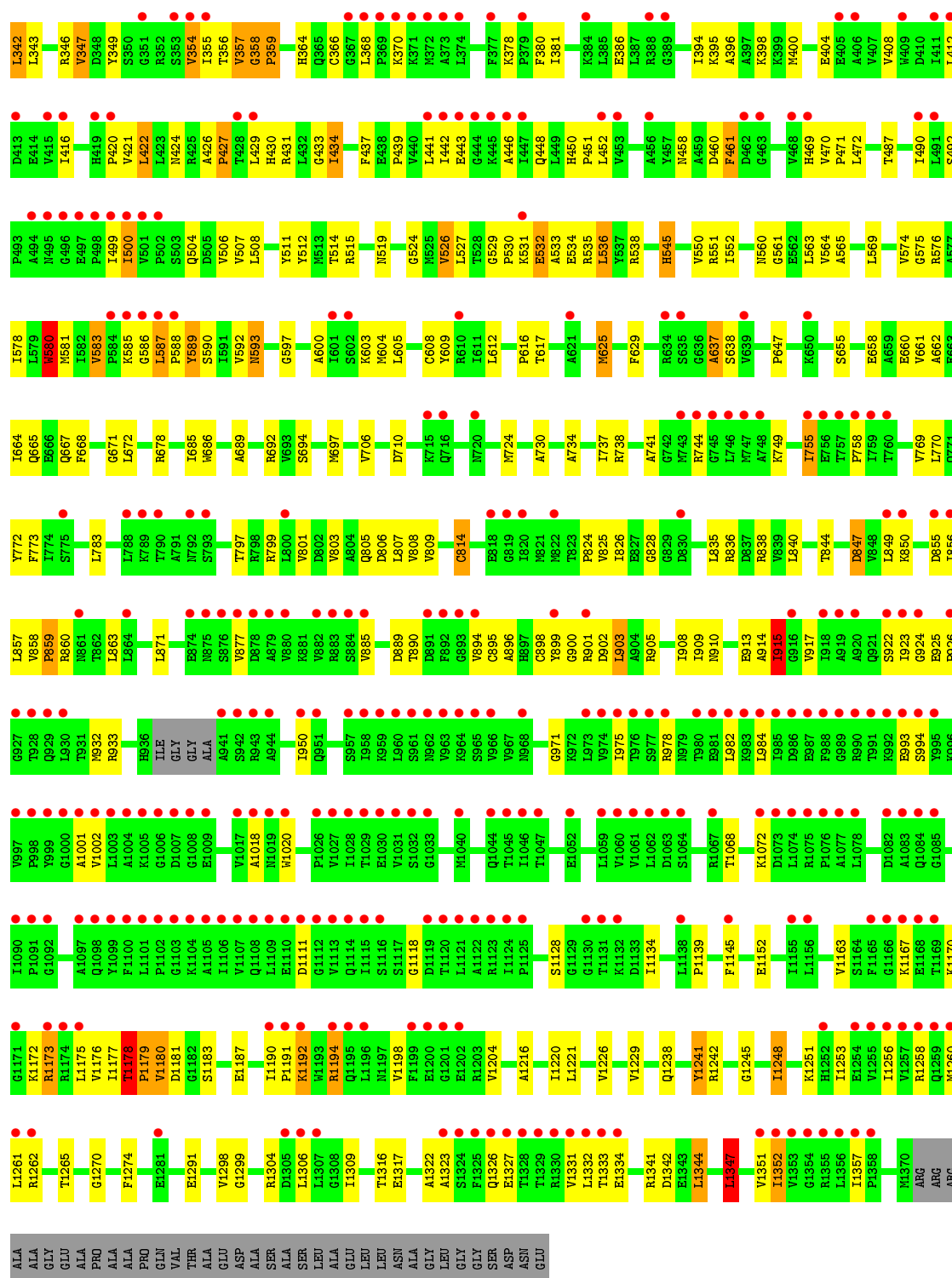




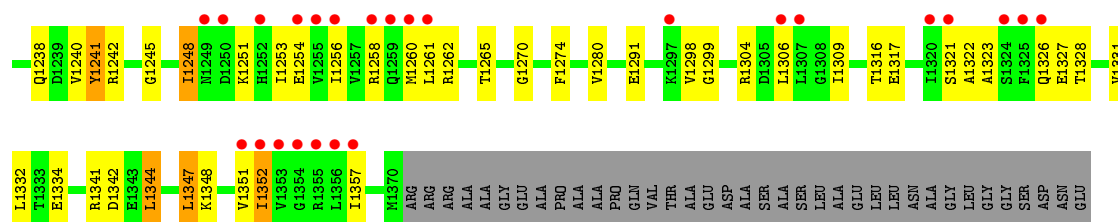


• Molecule 3: DNA-directed RNA polymerase subunit beta'

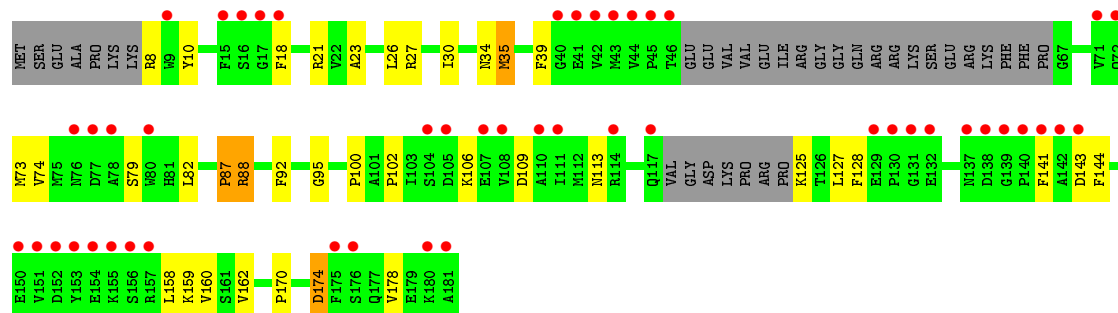




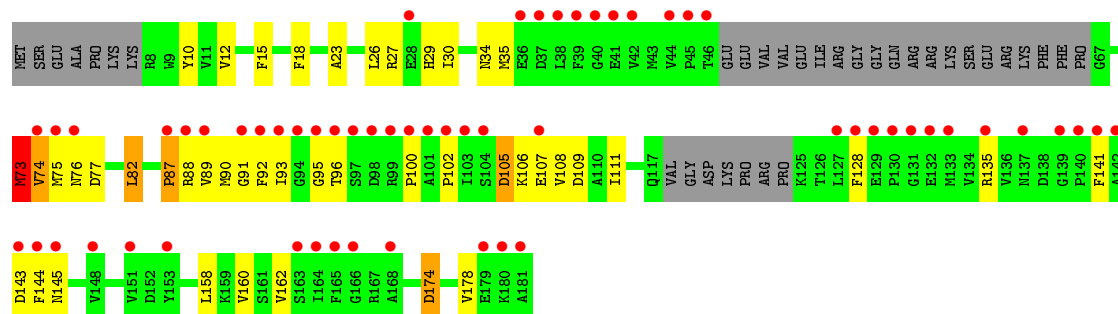
A1157	A1158	V1163	S1164	F1165	G1166	K1167	T1169	K1172	R1173	R1174	L1175	V1176	L1177	T1178	V1179	V1180	D1181	E1187	E1188	M1189	I1190	K1191	K1192	R1193	R1194	Q1195	L1196	M1197	F1198	V1199	E1200	G1201	V1204	S1211	D1212	G1213	P1214	E1215	A1216	P1217	H1218	D1219	L1220	L1221	F1222	L1223	R1224	G1225	V1226	V1229	V1234				
Q1084	G1085	M1086	D1087	V1088	A1089	I1090	P1091	K1092	T1093	F1094	M1095	P1096	A1097	Q1098	V1099	Q1100	G1101	P1102	G1103	K1104	A1105	I1106	V1107	Q1108	V1109	I1110	D1111	G1112	V1113	G1118	D1119	T1120	L1121	A1122	R1123	I1124	P1125	Q1126	E1127	L1128	G1129	G1130	T1131	K1132	I1133	I1134	P1139	F1145	R1149	P1150	P1153	A1154	I1155	A1083	
V997	P998	V999	G1000	A1001	V1002	L1003	A1004	K1005	T1006	D1007	G1008	E1009	Q1010	V1011	A1012	G1013	V1017	A1018	R1019	W1020	P1026	V1027	I1028	T1029	E1030	S1031	F1034	V1035	R1036	F1037	L1038	D1039	M1040	T1045	I1046	L1047	L1048	L1049	V1050	V1061	S1064	R1067	D1073	L1074	R1075	P1076	A1077	L1078	K1079	I1080	D1081	I1082	A1083		
L949	K950	D955	L956	L957	V958	P959	R960	T961	L963	L964	H965	E966	D970	L971	M975	S976	V977	D978	A979	V980	K981	V982	V983	V984	V985	V986	V987	C993	Y999	G900	R901	D902	L903	A904	R905	G906	H907	I908	N909	N910	E913	A914	I915	G916	V917	S922	I923	G924							
E925	F926	G927	D928	Q929	K932	R933	H936	I1E	G1E	G1E	ALA	A941	S942	I950	Q951	V952	K953	R954	R955	I1106	G956	G957	I958	R959	E1109	L960	S961	G962	V963	K964	S965	V966	V967	G971	T974	T975	T976	S977	R978	H979	T980	E981	L982	K983	L984	T985	D986	F988	Q989	R990	T991	K992	E993	S994	G994
I759	T760	A761	V769	L770	Q771	Y772	F773	K781	W792	S793	T797	R798	R799	L800	V801	V802	V803	A804	Q805	D806	L807	V808	V809	C814	H817	E818	G819	I820	M821	M822	Y823	T824	P824	V825	I826	E827	G828	G829	D830	L835	R836	D837	R838	R839	L840	G841	R842	V843	T844	A845	E846	D847	V848		
G575	R576	A577	L578	L579	V580	V583	G586	L587	P588	V589	S590	Y591	V592	L593	G597	A600	M603	M604	L605	C608	V609	L612	P616	T617	A621	M626	F629	A637	S638	V639	G640	G642	M644	V645	I646	P647	B648	B649	B650	V660	V661	A662	B663	B664	B665	B666									
Q667	F668	Q669	S670	G671	L672	A675	R678	L685	W686	H690	M697	Q702	T705	V706	I707	D710	E713	E714	R715	W716	V717	S718	T719	W720	S721	W722	Y723	M724	A734	I737	L740	A741	G742	M743	R744	G745	L746	W747	K748	P750	V754	I755	E756	T757	P758										
P493	A494	P498	I499	I500	V501	S502	Q503	Q504	D505	V506	V507	Y511	Y512	T514	R515	V518	N519	E523	G524	M525	V526	T527	R528	G529	P530	K531	E532	A533	E534	R535	L536	V537	R538	H545	A546	R547	V548	I549	V550	I552	V560	G561	V564	A565	L569	K570	D571	V574							
D413	I416	P420	L422	L423	M424	A426	P427	T428	L429	R430	R431	L432	G433	A434	P437	E438	P439	K370	K371	H372	A373	L374	K375	L376	P377	K378	F379	F380	L381	P382	A383	K384	L385	E386	L387	R388	G389	L390	T393	I394	K395	A396	A397	M400	E404	V408	W409	D410	I411	L412					
R281	L282	L283	L284	L285	N206	N209	S210	E211	K212	L213	K216	A226	F227	V228	W232	K233	P234	E235	W236	T240	V241	L242	P243	V244	L245	P246	P247	R250	P251	L252	G257	G258	R259	F260	S263	D264	L265	N266	D267	L268	E183	Y269	R270	K271	V272	I273	N274	R275	N276	N277	L278	L279	K280		
L126	L127	L128	D129	D134	L135	E136	L139	T139	P139	GLU	SER	TYR	VAL	VAL	ILE	GLU	GLY	GLY	THR	ASN	LEU	GLU	ARG	GLN	GLN	ILE	L160	K96	V97	R98	R101	G103	H104	E106	L107	A108	S109	T111	G181	A182	E183	A184	I185	F116	L117	K118	S119	M120	P121	S122	I123	G125			



• Molecule 4: Transcription termination/antitermination protein NusG



• Molecule 4: Transcription termination/antitermination protein NusG



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	248.16Å 313.78Å 162.79Å 90.00° 130.23° 90.00°	Depositor
Resolution (Å)	162.19 – 7.00 49.91 – 7.00	Depositor EDS
% Data completeness (in resolution range)	96.0 (162.19-7.00) 93.3 (49.91-7.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.04 (at 6.68Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.330 , 0.395 0.330 , 0.395	Depositor DCC
R_{free} test set	707 reflections (5.15%)	DCC
Wilson B-factor (Å ²)	314.0	Xtriage
Anisotropy	0.296	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 500.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.18$	Xtriage
Estimated twinning fraction	0.185 for -h-2*k,l	Xtriage
F_o, F_c correlation	0.78	EDS
Total number of atoms	50147	wwPDB-VP
Average B, all atoms (Å ²)	330.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.98% 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

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	0.45	0/1761	0.72	0/2387
1	B	0.46	0/1676	0.71	0/2271
1	F	0.45	0/1761	0.74	0/2387
1	G	0.47	0/1687	0.70	0/2286
2	C	0.43	0/10569	0.67	0/14258
2	H	0.43	0/10569	0.67	0/14258
3	D	0.44	0/10233	0.76	5/13816 (0.0%)
3	I	0.44	0/10277	0.74	1/13877 (0.0%)
4	J	0.50	0/1188	0.70	0/1603
4	K	0.50	0/1188	0.74	1/1603 (0.1%)
All	All	0.44	0/50909	0.71	7/68746 (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	2
2	H	0	2
3	D	0	1
3	I	0	1
4	K	0	1
All	All	0	7

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	1194	ARG	NE-CZ-NH2	-6.82	116.89	120.30
3	D	239	LEU	CA-CB-CG	5.33	127.56	115.30
3	D	173	GLY	N-CA-C	5.30	126.36	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	117	LEU	CA-CB-CG	5.29	127.46	115.30
4	K	73	MET	C-N-CA	5.27	134.87	121.70

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	57	PHE	Peptide
2	C	855	PRO	Peptide
3	D	1178	THR	Peptide
2	H	57	PHE	Peptide
2	H	855	PRO	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	1740	0	1767	40	0
1	B	1657	0	1686	40	0
1	F	1740	0	1767	38	0
1	G	1667	0	1693	35	0
2	C	10401	0	10414	216	0
2	H	10401	0	10414	232	0
3	D	10085	0	10303	380	2
3	I	10126	0	10341	316	0
4	J	1165	0	1145	26	0
4	K	1165	0	1145	30	0
All	All	50147	0	50675	1182	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 12.

The worst 5 of 1182 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)
3:I:1001:ALA:HA	3:I:1020:TRP:HE1	1.12	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:29:HIS:HB3	4:K:82:LEU:HG	1.35	1.06
3:D:226:ALA:HB1	3:D:227:PHE:HA	1.31	1.06
3:D:1001:ALA:HA	3:D:1020:TRP:HE1	1.12	1.06
3:D:247:PRO:HB3	3:I:53:ARG:HH12	1.18	1.06

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:184:ALA:O	3:D:191:SER:OG[2_957]	2.03	0.17
3:D:1183:SER:OG	3:D:1183:SER:OG[2_957]	2.12	0.08

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	223/242 (92%)	182 (82%)	29 (13%)	12 (5%)	2	29
1	B	211/242 (87%)	175 (83%)	27 (13%)	9 (4%)	3	34
1	F	223/242 (92%)	183 (82%)	28 (13%)	12 (5%)	2	29
1	G	212/242 (88%)	177 (84%)	26 (12%)	9 (4%)	3	34
2	C	1316/1342 (98%)	1108 (84%)	172 (13%)	36 (3%)	6	45
2	H	1316/1342 (98%)	1110 (84%)	168 (13%)	38 (3%)	6	43
3	D	1294/1407 (92%)	1023 (79%)	190 (15%)	81 (6%)	2	25
3	I	1300/1407 (92%)	1024 (79%)	197 (15%)	79 (6%)	2	26
4	J	141/181 (78%)	123 (87%)	15 (11%)	3 (2%)	9	50
4	K	141/181 (78%)	117 (83%)	18 (13%)	6 (4%)	3	34
All	All	6377/6828 (93%)	5222 (82%)	870 (14%)	285 (4%)	3	33

5 of 285 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	ASP
1	A	67	GLU
1	A	114	ASP
1	A	155	ALA
1	B	114	ASP

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	193/208 (93%)	191 (99%)	2 (1%)	82	92
1	B	184/208 (88%)	182 (99%)	2 (1%)	80	91
1	F	193/208 (93%)	192 (100%)	1 (0%)	92	96
1	G	185/208 (89%)	183 (99%)	2 (1%)	80	91
2	C	1137/1157 (98%)	1121 (99%)	16 (1%)	74	89
2	H	1137/1157 (98%)	1120 (98%)	17 (2%)	72	88
3	D	1087/1168 (93%)	1048 (96%)	39 (4%)	42	74
3	I	1091/1168 (93%)	1054 (97%)	37 (3%)	44	75
4	J	128/158 (81%)	122 (95%)	6 (5%)	32	68
4	K	128/158 (81%)	121 (94%)	7 (6%)	27	63
All	All	5463/5798 (94%)	5334 (98%)	129 (2%)	57	82

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	D	1347	LEU
2	H	1041	ASP
4	J	109	ASP
1	G	14	VAL
2	H	443	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 61 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	777	HIS
1	G	41	ASN
3	I	495	ASN
3	D	1249	ASN
3	D	1366	HIS

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	225/242 (92%)	1.34	64 (28%) 1 5	267, 330, 380, 416	0
1	B	215/242 (88%)	2.69	114 (53%) 0 3	266, 335, 388, 430	0
1	F	225/242 (92%)	1.26	55 (24%) 1 6	248, 320, 383, 403	0
1	G	216/242 (89%)	2.10	91 (42%) 0 4	279, 337, 380, 412	0
2	C	1319/1342 (98%)	1.62	431 (32%) 1 5	232, 313, 384, 510	0
2	H	1319/1342 (98%)	1.75	450 (34%) 0 4	231, 315, 383, 482	0
3	D	1302/1407 (92%)	1.65	415 (31%) 1 5	230, 326, 424, 473	0
3	I	1306/1407 (92%)	2.06	498 (38%) 0 4	231, 332, 431, 492	0
4	J	147/181 (81%)	1.64	49 (33%) 0 5	300, 384, 446, 483	0
4	K	147/181 (81%)	2.13	59 (40%) 0 4	324, 413, 469, 491	0
All	All	6421/6828 (94%)	1.78	2226 (34%) 0 4	230, 324, 419, 510	0

The worst 5 of 2226 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	314	ARG	18.1
3	I	989	GLY	17.0
2	H	788	SER	16.3
3	I	315	ALA	15.7
3	D	315	ALA	15.4

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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.