



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 8, 2026 – 06:20 AM UTC

PDB ID : 3I4N / pdb_00003i4n
Title : 8-oxoguanine containing RNA polymerase II elongation complex E
Authors : Damsma, G.E.; Cramer, P.
Deposited on : 2009-07-02
Resolution : 3.90 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

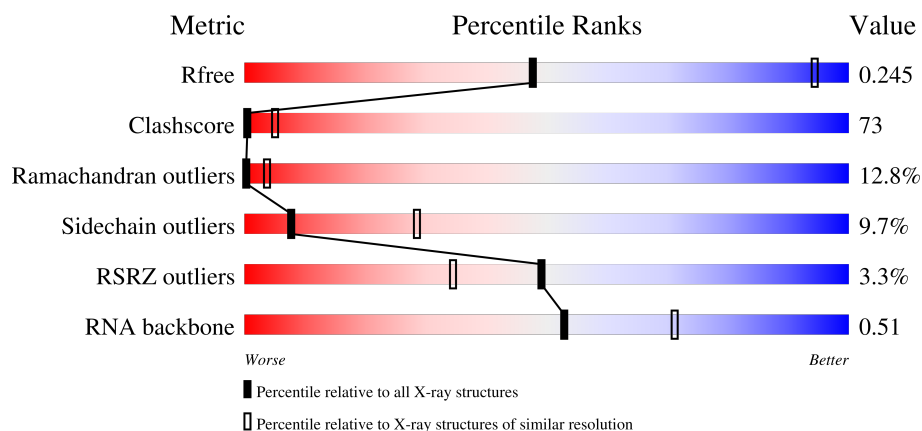
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 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.



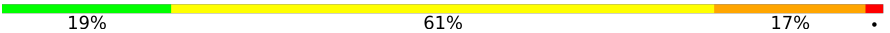
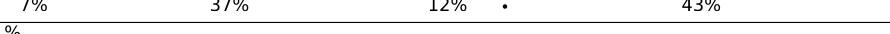
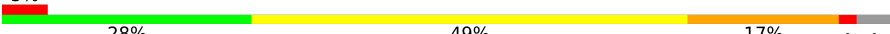
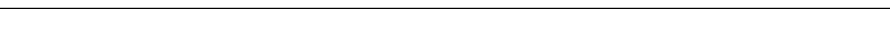
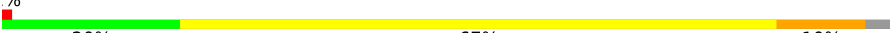
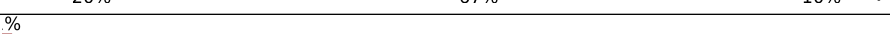
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1270 (4.10-3.70)
Clashscore	190562	1034 (4.08-3.72)
Ramachandran outliers	187476	1251 (4.10-3.70)
Sidechain outliers	187428	1243 (4.10-3.70)
RSRZ outliers	180081	1269 (4.10-3.70)
RNA backbone	3983	1014 (4.70-3.10)

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	1733	14% 51% 16% • 18%
2	B	1224	5% 19% 55% 16% • 8%
3	C	324	17% 50% 15% • 17%
4	D	221	5% 18% 48% 14% • 18%

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Mol	Chain	Length	Quality of chain
5	E	215	
6	F	155	
7	G	171	
8	H	146	
9	I	122	
10	J	70	
11	K	120	
12	L	70	
13	T	26	
14	N	12	
15	P	16	

2 Entry composition

There are 17 unique types of molecules in this entry. The entry contains 32307 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 II subunit RPB1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1429	Total	C	N	O	S	0	0	0
			11240	7079	1966	2133	62			

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1125	Total	C	N	O	S	0	0	0
			8942	5659	1571	1657	55			

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	270	Total	C	N	O	S	0	0	0
			2125	1336	353	422	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-5	HIS	-	expression tag	UNP P16370
C	-4	HIS	-	expression tag	UNP P16370
C	-3	HIS	-	expression tag	UNP P16370
C	-2	HIS	-	expression tag	UNP P16370
C	-1	HIS	-	expression tag	UNP P16370
C	0	HIS	-	expression tag	UNP P16370

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	182	Total	C	N	O	S	0	0	0
			1465	904	262	296	3			

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	214	Total	C	N	O	S	0	0	0
			1752	1111	309	321	11			

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	88	Total	C	N	O	S	0	0	0
			712	455	120	134	3			

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	171	Total	C	N	O	S	0	0	0
			1340	861	222	249	8			

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	137	Total	C	N	O	S	0	0	0
			1101	693	185	218	5			

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
9	I	117	Total	C	N	O	S	0	0	0
			952	586	173	182	11			

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	J	65	Total	C	N	O	S	0	0	0
			532	339	93	94	6			

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total	C	N	O	S	0	0	0
			929	596	158	173	2			

- Molecule 12 is a protein called DNA-directed RNA polymerases I, II, and III subunit RPABC4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
12	L	47	Total	C	N	O	S	0	0	0
			370	228	73	65	4			

- Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
13	T	20	Total	Br	C	N	O	P	0	0	0
			407	1	194	72	121	19			

- Molecule 14 is a DNA chain called DNA (5'-D(*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
14	N	11	Total	C	N	O	P	0	0	0
			224	108	42	64	10			

- Molecule 15 is a RNA chain called RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*AP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	P	10	Total	C	N	O	P	0	0	0
			207	94	35	69	9			

- Molecule 16 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
16	A	1	Total	Mg	0	0
			1	1		

- Molecule 17 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	A	2	Total	Zn	0	0
			2	2		
17	B	1	Total	Zn	0	0
			1	1		
17	C	1	Total	Zn	0	0
			1	1		
17	I	2	Total	Zn	0	0
			2	2		

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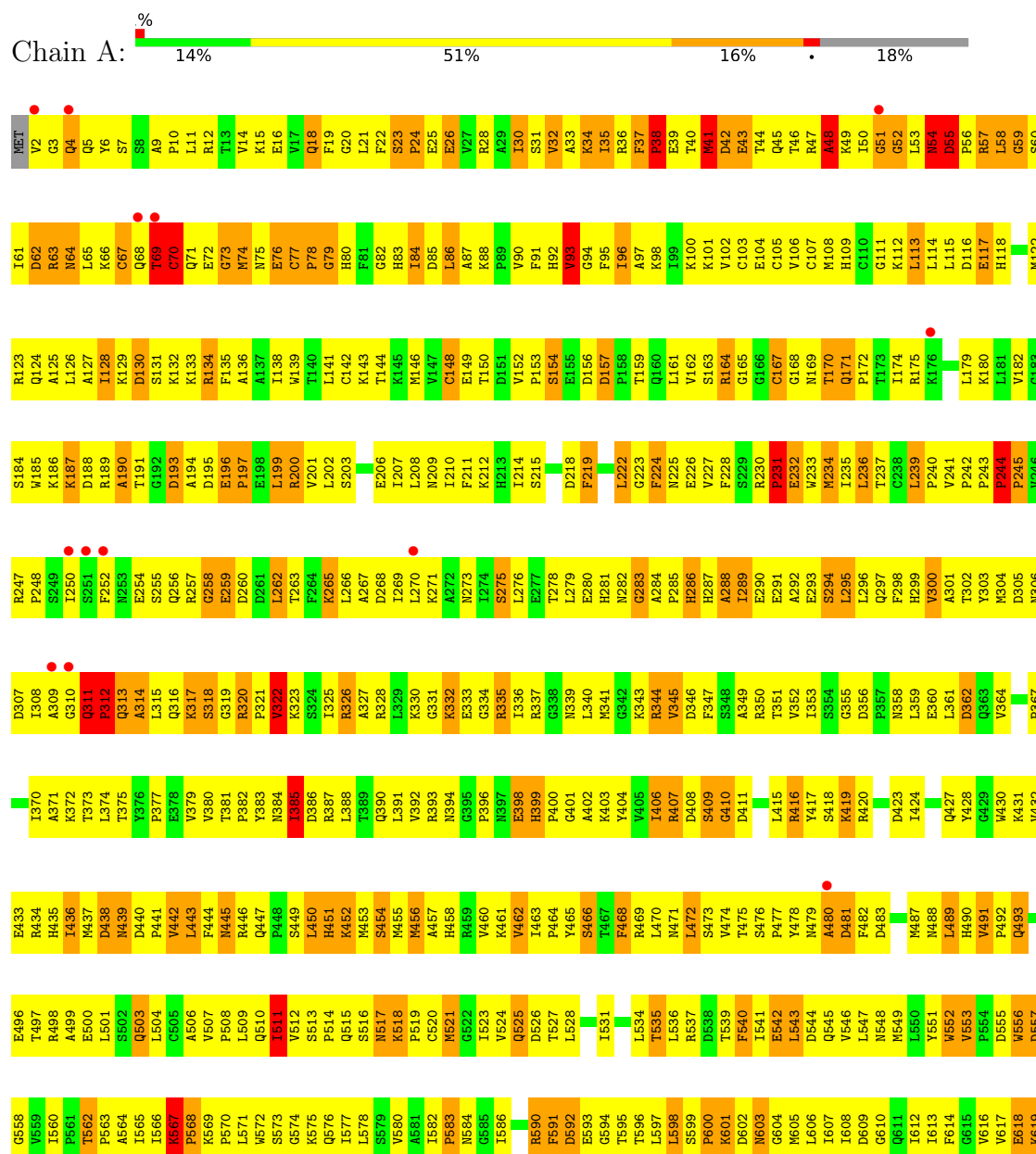
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
17	J	1	Total 1	Zn 1	0	0
17	L	1	Total 1	Zn 1	0	0

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 II subunit RPB1



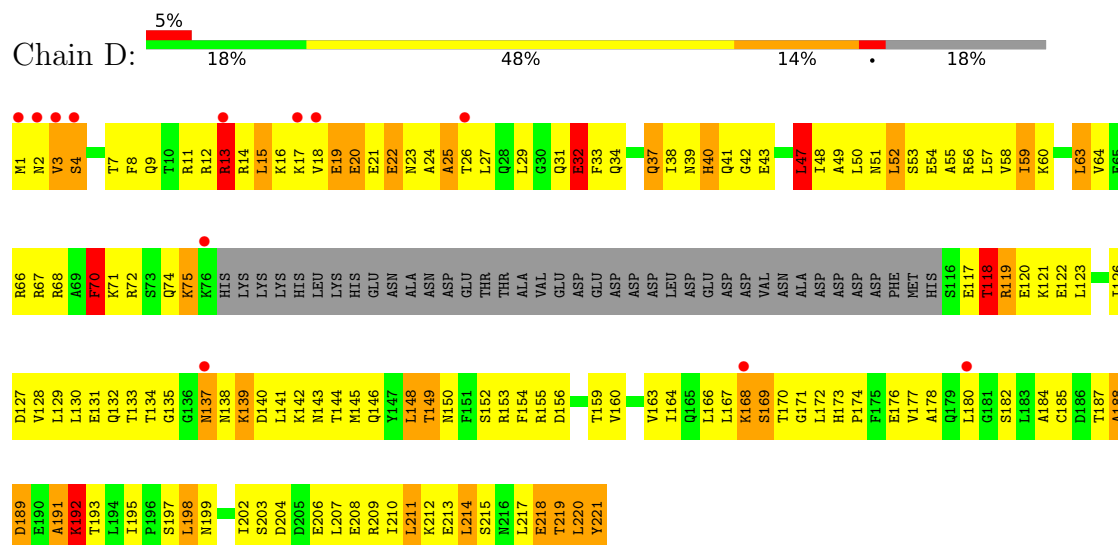
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LEU	L1430	M1368	W1304	T1117	S1056	M996	E932	M746	A686	T621
MET	Q1431	A1369	V1305	D1178	V1057	L997	Y933	M747	K687	V622
PHE	Q1432	L1370	L1306	Y1119	V1058	L998	Y934	M748	K688	G623
SER	M1433	L1371	L1244	H1059	H1059	V999	L936	A749	K689	S624
PRO	A1434	V1372	P1245	E1121	P1060	L1000	V937	G750	G625	G627
LEU	P1435	D1309	GLU	E1122	G1061	R1001	K938	S751	M626	L691
VAL	I1436	GLN	GLN	G1123	E1062	G1002	D939	K752	D692	D692
ASP	G1437	SER	GLN	H1124	M1063	L1003	A874	G753	G628	G628
SER	T1438	PHE	ASP	A1125	V1064	E1005	R940	S754	F694	L694
GLY	G1439	ALA	ASP	A1126	G1065	M1006	F942	F755	K695	I630
SER	A1440	GLU	GLU	Q1187	V1066	L1007	L943	I756	G696	H631
ASN	F1441	THR	THR	D1127	L1067	I1006	R944	M757	A697	G632
ASP	D1442	GLU	GLU	E1128	A1068	Q1008	E945	I758	Q698	V633
ALA	V1316	GLU	GLU	E1129	A1068	Q1008	E945	I758	V633	V633
ALA	M1317	P1190	S1189	Q1130	A1069	M1009	V946	A759	A699	T634
MET	T1318	W1191	P1190	Q1131	Q1070	A1010	F947	Q760	N700	R635
ALA	V1319	L1192	L1192	S1071	S1071	Q1011	V948	Q761	M761	L701
GLY	D1446	D1257	L1193	K1133	I1072	R1012	D949	S762	L702	K637
GLY	E1447	H1258	L1193	K1133	I1072	R1012	D949	S762	L702	K637
PHE	E1448	H1258	L1193	K1133	I1072	R1012	D949	S762	L702	K637
THR	S1449	M1259	L1197	R1135	E1074	M1014	E951	G764	T703	G636
THR	T1325	M1260	D1198	S1136	P1075	L1015	A952	G765	A704	A704
ALA	R1326	K1261	GLU	I1137	A1076	T1016	N953	G766	H706	H706
TYR	T1327	K1262	GLU	I1138	T1077	L1017	W954	Q767	G707	G707
GLY	Y1328	I1263	M1202	E1139	Q1078	F1018	P955	Q768	M708	M708
GLY	S1329	E1264	M1203	H1140	M1079	G1019	L956	E771	T709	T709
ALA	N1330	N1265	D1204	T1141	T1080	C1020	P957	E771	L710	L710
ASP	P1485	T1266	K1205	T1142	ASN	L1021	P958	G772	R711	R711
TYR	G1395	M1267	D1206	L1143	THR	L1022	N959	K773	E712	E712
GLN	A1396	L1268	P1207	K1144	PHE	R1023	R960	R774	S713	S713
GLU	L1397	E1269	T1208	S1145	THR	S1024	R961	I775	K651	K651
ALA	I1335	M1270	M1209	V1146	HIS	R1025	R962	A776	E715	E715
THR	M1336	I1271	G1210	T1147	PHE	L1026	I963	F777	T716	T716
SER	GLU	I1272	Q1211	I1148	ALA	A1027	I964	G778	N717	N717
PRO	I1401	L1273	V1212	A1149	GLY	T1028	Q965	F779	F655	F655
PHE	F1402	R1274	G1213	S1150	VAL	R1029	N966	L841	V719	V719
GLY	E1403	G1275	E1214	E1151	ALA	R1030	Q967	D781	L657	L657
ALA	E1404	V1276	R1215	I1152	SER	V1031	Q968	E782	F721	F721
TYR	T1405	E1277	I1216	Y1153	LYS	L1032	Q969	T783	L722	L722
GLY	V1406	M1278	K1217	Y1154	K1093	Q1033	L913	L784	L658	L658
GLU	E1407	I1279	Q1218	D1155	V1094	E1034	L908	L785	R660	R660
ALA	L1408	E1280	T1219	D1156	T1095	V1035	P910	H786	G661	G661
PRO	VAL	L1409	F1220	D1157	S1096	R1036	H972	F787	F662	F662
THR	THR	M1283	K1221	P1158	G1097	T1037	D974	S788	T664	T664
PRO	PRO	M1284	R1222	R1159	V1098	L1038	H975	K789	G665	G665
PRO	G1413	M1285	D1223	S1160	P1099	K1039	T976	D790	L666	L666
GLY	A1414	L1224	L1224	T1161	R1100	Q1040	K977	G791	G667	G667
PHE	S1415	F1225	F1225	V1162	L1101	A1041	P978	Y792	D672	D672
GLY	A1416	K1290	V1226	I1163	K1102	F1042	S979	S793	L732	L732
VAL	E1417	V1291	I1227	P1164	E1103	D1043	D980	F794	A733	A733
SER	L1418	P1292	V1228	E1165	L1104	V1044	L981	E795	E734	E734
SER	D1419	S1293	S1229	D1166	L1105	V1045	T982	S796	V735	V735
PRO	VAL	T1294	E1230	E1167	M106	L1046	I983	K797	L736	L736
GLY	ASN	T1295	D1231	E1168	S1047	L1047	K984	G798	L737	L737
PHE	ALA	G1296	N1232	I1169	M1048	N1048	D985	F799	K738	K738
SER	ASP	E1297	D1233	I1170	I1049	E1050	I986	V800	E678	E678
PRO	LEU	V1298	Q1171	Q1171	A1051	V987	Q926	L740	L679	L679
THR	ASP	V1299	L1172	L1172	A1051	V987	Q926	E801	T680	T680
SER	VAL	K1300	H1173	H1173	Q1052	L927	V927	N741	E681	E681
PRO	VAL	E1301	T1237	T1237	L1113	L928	L928	S803	T682	T682
THR	ASP	N1427	R1239	S1175	P1114	L933	L933	Y804	L742	L742
THR	ASP	P1302	R1239	S1175	S1115	L1054	Q994	L805	A684	A684



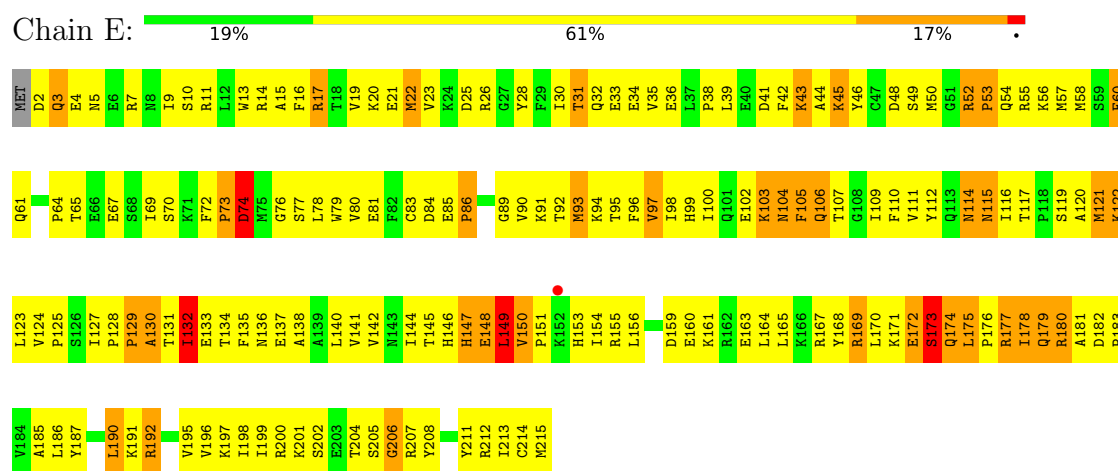


THR
GLY
SER
GLY
TYR
GLY
ASP
ASN
ALA
TRP

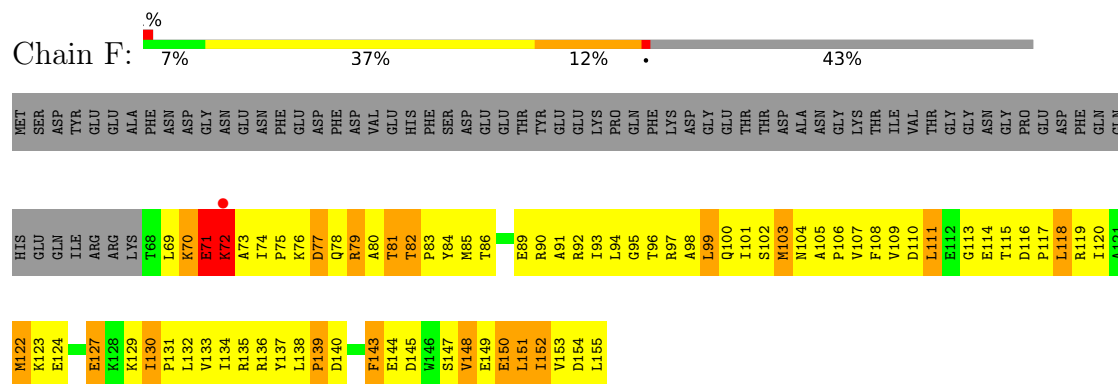
• Molecule 4: DNA-directed RNA polymerase II subunit RPB4



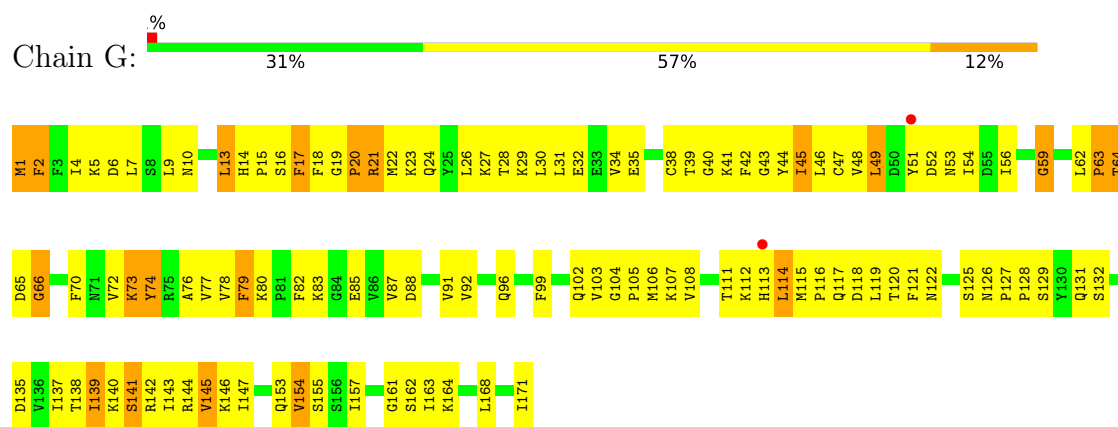
• Molecule 5: DNA-directed RNA polymerases I, II, and III subunit RPABC1



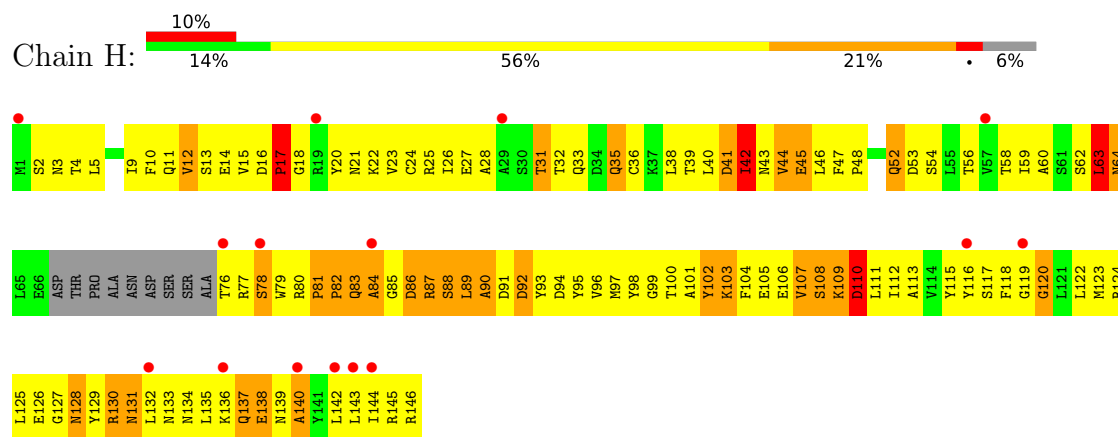
• Molecule 6: DNA-directed RNA polymerases I, II, and III subunit RPABC2



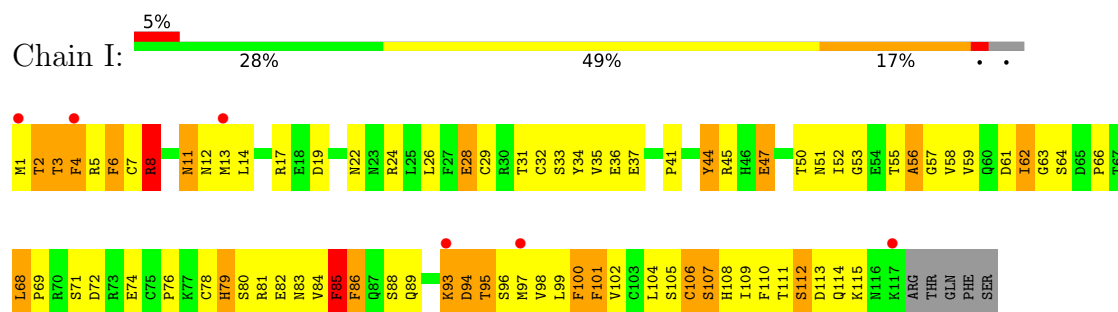
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7



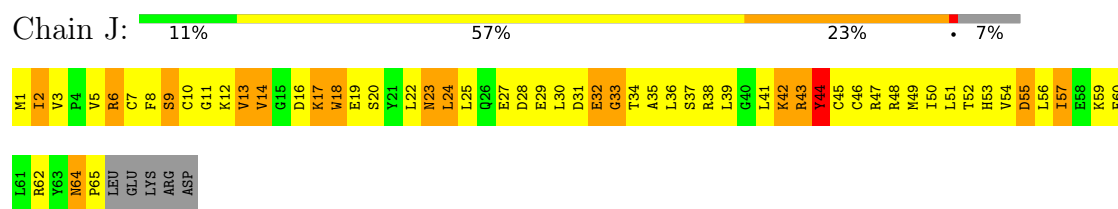
• Molecule 8: DNA-directed RNA polymerases I, II, and III subunit RPABC3



• Molecule 9: DNA-directed RNA polymerase II subunit RPB9

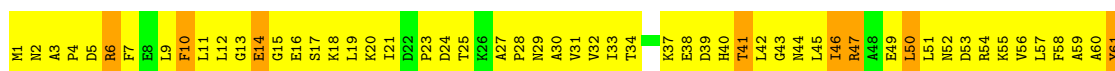


• Molecule 10: DNA-directed RNA polymerases I, II, and III subunit RPABC5

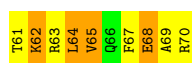
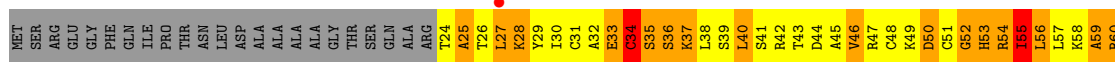


• Molecule 11: DNA-directed RNA polymerase II subunit RPB11





- Molecule 12: DNA-directed RNA polymerases I, II, and III subunit RPABC4



- Molecule 13: DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP*CP*TP*TP*AP*(8OG)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3')



- Molecule 14: DNA (5'-D(*AP*GP*TP*AP*CP*TP*TP*GP*AP*GP*CP*T)-3')



- Molecule 15: RNA (5'-R(*UP*GP*CP*AP*UP*C*UP*UP*CP*CP*AP*GP*GP*CP*AP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	221.17Å 394.15Å 282.34Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.90 50.00 – 3.90	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-3.90) 99.9 (50.00-3.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.80 (at 3.88Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.228 , 0.266 0.208 , 0.245	Depositor DCC
R_{free} test set	4364 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	128.1	Xtriage
Anisotropy	0.540	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 99.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.017 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.019 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	32307	wwPDB-VP
Average B, all atoms (Å ²)	145.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.79% 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: BRU, ZN, 8OG, 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	0.53	0/11441	1.10	92/15473 (0.6%)
2	B	0.49	0/9116	1.02	53/12291 (0.4%)
3	C	0.52	0/2163	1.11	17/2930 (0.6%)
4	D	0.46	0/1475	1.01	6/1976 (0.3%)
5	E	0.46	0/1788	1.04	12/2406 (0.5%)
6	F	0.60	0/724	1.28	9/977 (0.9%)
7	G	0.50	0/1368	0.99	5/1844 (0.3%)
8	H	0.45	0/1119	1.06	10/1514 (0.7%)
9	I	0.42	0/970	0.97	6/1305 (0.5%)
10	J	0.50	0/541	0.93	1/727 (0.1%)
11	K	0.50	0/947	1.04	5/1279 (0.4%)
12	L	0.54	0/372	1.06	3/495 (0.6%)
13	T	0.39	0/405	0.91	4/618 (0.6%)
14	N	0.43	0/251	0.84	0/386
15	P	0.41	0/230	0.78	0/356
All	All	0.50	0/32910	1.06	223/44577 (0.5%)

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	B	0	1

There are no bond length outliers.

The worst 5 of 223 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1185	CYS	N-CA-C	-11.56	98.89	113.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	454	SER	N-CA-C	-11.08	98.72	114.12
3	C	148	ARG	N-CA-C	10.98	117.78	108.78
1	A	950	GLY	N-CA-C	-10.28	102.58	113.58
1	A	3	GLY	N-CA-C	-10.15	100.82	115.64

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	797	TYR	Sidechain

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	11240	0	11313	1848	0
2	B	8942	0	8987	1396	0
3	C	2125	0	2090	346	0
4	D	1465	0	1489	222	0
5	E	1752	0	1776	243	0
6	F	712	0	738	137	0
7	G	1340	0	1357	176	0
8	H	1101	0	1075	220	0
9	I	952	0	913	145	0
10	J	532	0	542	121	0
11	K	929	0	939	142	0
12	L	370	0	394	92	0
13	T	407	0	225	43	0
14	N	224	0	126	11	0
15	P	207	0	109	9	0
16	A	1	0	0	0	0
17	A	2	0	0	0	0
17	B	1	0	0	0	0
17	C	1	0	0	0	0
17	I	2	0	0	0	0
17	J	1	0	0	0	0
17	L	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	32307	0	32073	4724	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 73.

The worst 5 of 4724 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:B:577:ALA:HB1	2:B:589:VAL:HG11	1.19	1.14
1:A:320:ARG:HB2	1:A:320:ARG:HH11	1.07	1.14
8:H:33:GLN:HE21	8:H:35:GLN:HB2	1.12	1.13
1:A:899:VAL:HB	1:A:929:LEU:HD11	1.25	1.12
1:A:590:ARG:HH21	1:A:620:LYS:HB3	1.06	1.12

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	1421/1733 (82%)	929 (65%)	311 (22%)	181 (13%)	0	4
2	B	1111/1224 (91%)	712 (64%)	251 (23%)	148 (13%)	0	3
3	C	268/324 (83%)	165 (62%)	69 (26%)	34 (13%)	0	4
4	D	178/221 (80%)	125 (70%)	29 (16%)	24 (14%)	0	3
5	E	212/215 (99%)	145 (68%)	42 (20%)	25 (12%)	0	5
6	F	86/155 (56%)	60 (70%)	21 (24%)	5 (6%)	1	16
7	G	169/171 (99%)	133 (79%)	25 (15%)	11 (6%)	1	15
8	H	133/146 (91%)	78 (59%)	26 (20%)	29 (22%)	0	1
9	I	115/122 (94%)	72 (63%)	29 (25%)	14 (12%)	0	4

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	J	63/70 (90%)	35 (56%)	14 (22%)	14 (22%)	0	1
11	K	114/120 (95%)	80 (70%)	31 (27%)	3 (3%)	4	28
12	L	45/70 (64%)	18 (40%)	13 (29%)	14 (31%)	0	0
All	All	3915/4571 (86%)	2552 (65%)	861 (22%)	502 (13%)	0	4

5 of 502 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	4	GLN
1	A	41	MET
1	A	43	GLU
1	A	48	ALA
1	A	54	ASN

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	1249/1520 (82%)	1125 (90%)	124 (10%)	7	28
2	B	974/1061 (92%)	880 (90%)	94 (10%)	8	28
3	C	238/280 (85%)	217 (91%)	21 (9%)	9	32
4	D	164/200 (82%)	143 (87%)	21 (13%)	4	20
5	E	196/197 (100%)	178 (91%)	18 (9%)	8	30
6	F	78/137 (57%)	68 (87%)	10 (13%)	4	20
7	G	152/152 (100%)	142 (93%)	10 (7%)	15	41
8	H	121/128 (94%)	112 (93%)	9 (7%)	13	38
9	I	111/116 (96%)	103 (93%)	8 (7%)	13	39
10	J	60/65 (92%)	55 (92%)	5 (8%)	10	34
11	K	99/102 (97%)	89 (90%)	10 (10%)	7	27
12	L	41/57 (72%)	33 (80%)	8 (20%)	1	9
All	All	3483/4015 (87%)	3145 (90%)	338 (10%)	8	28

5 of 338 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	193	TYR
6	F	151	LEU
3	C	269	LYS
5	E	17	ARG
8	H	63	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 132 such sidechains are listed below:

Mol	Chain	Res	Type
8	H	131	ASN
9	I	79	HIS
11	K	110	ASN
2	B	178	ASN
2	B	60	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	P	9/16 (56%)	2 (22%)	0

All (2) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	P	10	A
15	P	11	U

There are no RNA pucker outliers to report.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
13	8OG	T	19	15,13	22,25,26	1.08	1 (4%)	26,37,40	1.59	3 (11%)
13	BRU	T	23	15,13	18,21,22	3.95	1 (5%)	25,30,33	0.99	2 (8%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	8OG	T	19	15,13	-	2/7/21/22	0/3/3/3
13	BRU	T	23	15,13	-	1/7/21/22	0/2/2/2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	T	23	BRU	BR-C5	-16.71	1.49	1.88
13	T	19	8OG	C8-N7	-4.16	1.30	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	T	19	8OG	N7-C8-N9	5.90	113.18	106.61
13	T	19	8OG	C5-N7-C8	-3.83	104.19	109.47
13	T	19	8OG	C4-C5-N7	2.60	110.81	106.06
13	T	23	BRU	C6-C5-C4	-2.58	118.05	120.67
13	T	23	BRU	O3'-C3'-C2'	-2.22	103.15	110.88

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	T	19	8OG	O4'-C4'-C5'-O5'
13	T	19	8OG	C3'-C4'-C5'-O5'
13	T	23	BRU	C2'-C1'-N1-C2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	19	8OG	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	T	23	BRU	2	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 9 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, 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	1429/1733 (82%)	0.13	24 (1%) 69 48	73, 132, 187, 200	0
2	B	1125/1224 (91%)	0.36	60 (5%) 32 25	79, 146, 196, 200	0
3	C	270/324 (83%)	0.11	1 (0%) 88 74	92, 133, 183, 200	0
4	D	182/221 (82%)	0.37	12 (6%) 24 21	122, 160, 195, 200	0
5	E	214/215 (99%)	0.16	1 (0%) 87 72	111, 170, 198, 200	0
6	F	88/155 (56%)	0.04	1 (1%) 78 57	77, 110, 145, 175	0
7	G	171/171 (100%)	0.19	2 (1%) 76 55	113, 140, 176, 182	0
8	H	137/146 (93%)	0.70	15 (10%) 10 13	147, 178, 198, 200	0
9	I	117/122 (95%)	0.40	6 (5%) 33 26	126, 178, 197, 200	0
10	J	65/70 (92%)	0.17	0 100 100	112, 129, 171, 180	0
11	K	116/120 (96%)	-0.00	1 (0%) 81 62	96, 135, 160, 199	0
12	L	47/70 (67%)	0.55	1 (2%) 63 44	128, 169, 190, 200	0
13	T	18/26 (69%)	1.22	2 (11%) 10 13	182, 200, 200, 200	0
14	N	11/12 (91%)	1.53	3 (27%) 1 3	196, 200, 200, 200	0
15	P	10/16 (62%)	1.10	2 (20%) 3 5	199, 200, 200, 200	0
All	All	4000/4625 (86%)	0.25	131 (3%) 49 34	73, 142, 196, 200	0

The worst 5 of 131 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	1	MET	5.5
2	B	510	LYS	5.1
9	I	1	MET	4.8
2	B	310	MET	4.5
2	B	70	ILE	4.5

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
13	BRU	T	23	20/21	0.70	0.16	198,199,200,200	0
13	8OG	T	19	23/24	0.91	0.10	186,193,198,199	0

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(Å ²)	Q<0.9
16	MG	A	2458	1/1	0.92	0.09	200,200,200,200	0
17	ZN	I	1122	1/1	0.98	0.04	198,198,198,198	0
17	ZN	A	2456	1/1	0.99	0.03	150,150,150,150	0
17	ZN	J	1066	1/1	0.99	0.05	135,135,135,135	0
17	ZN	L	1071	1/1	0.99	0.02	158,158,158,158	0
17	ZN	I	1121	1/1	1.00	0.03	140,140,140,140	0
17	ZN	A	2457	1/1	1.00	0.04	107,107,107,107	0
17	ZN	B	2225	1/1	1.00	0.05	106,106,106,106	0
17	ZN	C	1269	1/1	1.00	0.05	101,101,101,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.