

wwPDB X-ray Structure Validation Summary Report (i)

Oct 31, 2023 – 12:52 PM EDT

PDB ID	:	3I4M
Title	:	8-oxoguanine containing RNA polymerase II elongation complex D
Authors	:	Damsma, G.E.; Cramer, P.
Deposited on	:	2009-07-02
Resolution	:	3.70 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 (i) 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 (1)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure: $X\text{-}RAY\;DIFFRACTION$

The reported resolution of this entry is 3.70 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.



Motria	Whole archive	Similar resolution
wietric	$(\# {\rm Entries})$	$(\# { m Entries}, { m resolution} { m range}({ m \AA}))$
R _{free}	130704	1049 (3.88-3.52)
Clashscore	141614	1027 (3.86-3.54)
Ramachandran outliers	138981	1069 (3.88-3.52)
Sidechain outliers	138945	1065 (3.88-3.52)
RSRZ outliers	127900	1578 (3.90-3.50)
RNA backbone	3102	1027 (4.40-3.00)

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 <=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	А	1733	16%	53%	13%	•	18%
2	В	1224	17%	58%		16%	• 8%
3	С	324	18%	50%	15%	•	17%
4	D	221	2% 19%	51%	13%	•	15%



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Mol	Chain	Length		Qua	lity of chain		
5	Е	215	.%		66%		16% •
6	F	155	9%	42%	5% •	43%	
7	G	171	28%		60%		11% •
8	Н	146	17%		58%	17%	• 6%
9	Ι	122	18%		59%	17	% • 5%
10	J	70	10%	59%		23%	• 7%
11	K	120	2% 25%	_	59%		12% •
12	L	70	.% • 3	9%	24% •	33%	
13	Т	26		73%		8%	19%
14	N	12	25%		67%		8%
15	Р	16	6% 19%	38%	6%	38%	



2 Entry composition (i)

There are 17 unique types of molecules in this entry. The entry contains 32355 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		Α	toms		ZeroOcc	AltConf	Trace	
1	А	1429	Total 11240	C 7079	N 1966	O 2133	S 62	0	0	0

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

Mol	Chain	Residues		Α	toms		ZeroOcc	AltConf	Trace	
2	В	1125	Total 8942	C 5659	N 1571	O 1657	${ m S}{55}$	0	0	0

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
3	С	270	Total 2125	C 1336	N 353	0 422	S 14	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
С	-5	HIS	-	EXPRESSION TAG	UNP P16370
С	-4	HIS	-	EXPRESSION TAG	UNP P16370
С	-3	HIS	-	EXPRESSION TAG	UNP P16370
С	-2	HIS	-	EXPRESSION TAG	UNP P16370
С	-1	HIS	-	EXPRESSION TAG	UNP P16370
С	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	187	Total 1504	C 930	N 269	O 301	${S \over 4}$	0	0	0

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



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01 1111

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
5	Е	214	Total 1752	C 1111	N 309	O 321	S 11	0	0	0

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

Mol	Chain	Residues		At	oms		ZeroOcc	AltConf	Trace	
6	F	88	Total 712	$\begin{array}{c} \mathrm{C} \\ 455 \end{array}$	N 120	0 134	${ m S} { m 3}$	0	0	0

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

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

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

Mol	Chain	Residues		Atoms					AltConf	Trace
8	Н	137	Total 1101	C 693	N 185	0 218	${f S}{5}$	0	0	0

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

Mol	Chain	Residues		Atoms					AltConf	Trace
9	Ι	116	Total 944	C 581	N 172	O 181	S 10	0	0	0

• 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 532	C 339	N 93	0 94	S 6	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
11	K	116	Total 929	C 596	N 158	0 173	$\begin{array}{c} \mathrm{S} \\ \mathrm{2} \end{array}$	0	0	0

• 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 370	C 228	N 73	O 65	$\frac{S}{4}$	0	0	0

• Molecule 13 is a DNA chain called DNA (5'-D(*AP*G*CP*TP*CP*AP*AP*GP*TP*AP* CP*TP*TP*AP*(80G)P*GP*CP*CP*(BRU)P*GP*GP*TP*CP*AP*TP*T)-3').

Mol	Chain	Residues			Aton	ns			ZeroOcc	AltConf	Trace
13	Т	21	Total 426	Br 1	C 203	N 75	O 127	Р 20	0	0	0

• 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	Ν	11	Total 224	C 108	N 42	O 64	Р 10	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
15	Р	10	Total 205	C 93	N 33	O 70	Р 9	0	0	0

• Molecule 16 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Ato	ms	ZeroOcc	AltConf
16	А	1	Total 1	Mg 1	0	0

• Molecule 17 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
17	А	2	Total Zn 2 2	0	0
17	В	1	Total Zn 1 1	0	0
17	С	1	Total Zn 1 1	0	0
17	Ι	2	Total Zn 2 2	0	0



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



3 Residue-property plots (i)

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



K689	V690	L691 D692	V693	T694 KGGF	E696	409/ 0698	A699	N7 00 L7 01	L702	T703 4704	K705	H7 06	T7 09	L710	к/11 Е712	S713	F714 F715		V718	V719 R720	F721	L722	ET 24	A7 25	R726 D727	KT 28	A7 29 C7 30	R731	L732	E734	V735	N/ 30 L737	K738	D739 1.740	N741	N742 V743	K744	Q745	M7 46 V7 47		S751 K752
G753	S754	F755 T756	N757	1758 4759	0160 1760	8762	A763	C764 V765	G766	0767 0768	S769	V770 E774		R774	L//5 A776	F777	G778 F779	V780	D781	R782 T783	L784	P785	н/80 F787	S788	K789 D790		Р794 Б705	S796	K797	F799	V800	E601 N802	S803	Y804 1.805		L808 Tean	P810	Q811	E812 F813	F814	F815 H816
A817	M818	6819 6820	R821	E822	1825	1827 T827	A828	V829 K830	T831	A832 F833	T834	G835 vo <i>3e</i>	1030 1837	0838 0838	R840	L841	V842 K843	A844	L845	E846 D847	1848	M849	Y852	D853	N854 TREE	1000 T856	R857 NR58	8859	L860	TOOP	1864	4000 F866	1867	Y868 G869	E870	D871	M873	D874	A875 A876	H877	1878 E879
K880	Q881	S882 1.883	D884	T885 T886	G887	6000 8880	D890	A891	E894	K895 R896	7897	R898 Veoo	0060	L901	L902 N903	T904	D905 HQAA	T907	L908	D909 P910	S911	L912	E914	S915	G916 S017	E918	1919	L923	K924	1926 0926	V927	L920 L929	D930	E931 E932	Y933	K934	L936	V937	K938 D939	R940	K941 F942
L943	R944	E945 V946	F947	V948 D949	G950	A952	N953	955 P955	-	V958 N959	0961	R961	1963 1963	1964	1966 N966	A967	0968 0969	1970	F971	H972 1973	D974	H975 T076	19/0	8979	D980 1 081	T982	1983 K084	D985	1986 1986	1988 L988		1994 0994	E995	7997 1997	L998	V999	R1001	G1002	K1003 N1004	E1005	11006 11007
Q1008	N1009	A1010 01011	R1012	D1013 A1014	V1015	L1017	F1018	C1019 C1020	L1021	L1022	R1025	L1026	T1028	R1029	K1030 V1031	L1032	01033 11034	Y1035	R1036	L1037 T1038	K1039	Q1040	F1042	D1043	W1044	L1046	S1047 N1048	11049	E1050	01052 01052	F1053	L1034 R1055	S1056	V1057 V1058	H1059	P1060	E1062	M1063	V1064 G1065	V1066	L1067 A1068
A1069	Q1070	S1071 11072	G1073	E1074 P1075	A1076	01078 01078	M1079	11080 L1081	ASN	THR PHE	HIS	PHE	GLY	VAL	ALA SER	LYS	K1093 V1094	T1095	S1096	G1097 V1098	P1099	R1100	K1102	E1103	11104 11105	N1106	V1107 A1108	K1109	N1110	K1112	T1113	81114 S1115	L1116	T1117 V1118	Y1119	L1120	P1122	G1123	H1124 A1125	A1126	D1127 Q1128
E1129	Q1130	A1131 K1132	L1133	I1134	11138 1128	H1140	T1141	T1142 L1143	K1144	S1145 V1146	T1147	11148 A1140	S1150	E1151	11152 Y1153	Y1154	D1155 D1156	D1157	P1158	R1159 S1160	T1161	V1162	11103 P1164	E1165	D1166 F1167	E1168	11169 11170		H1173 F1173	511/4 S1175	L1176	D1178	E1179	GLU AT.A	GLU	GLN	DHE	ASP	41187 01188	S1189	P1190 W1191
L1192	L1193	R1194 1.1195	E1196	L1197 D1198	R1199	A1200 A1201		K1205 D1206	L1207	T1208 M1209	G1210	Q1211 V1212	01212 61213	E1214	K1215 11216	K1217	Q1218 T1219	F1220	K1221	N1222 D1223	L1224	F1225	V 1226 11227	W1228	S1229 F1230	D1231	N1232	E1234	K1235	L1230 11237	I1238	C1240	R1241	V1242 V1243	R1244	P1245	SER.	LEU	ASP ALA	GLU	GLU
A1254	E1255	E1256 D1257	H1258	M1259 11260	K1261	11263 II263	E1264	N1265 T1266	M1267	L1268 E1269	N1270	11271 T1270	L1273	R1274	01275 V1276	E1277	N1278 11279	E1280		M1284 M1285		R1289	V1291	P1292	S1293 D1704	T1295	G1296 F1297	Y1298	V1299	DOCTU	E1303	V1305	L1306	E1307 T1308	D1309	G1310 11211	N1312	L1313	S1314 E1315	V1316	M1317 T1318
V1319		11322 D1323	P1324	T1325 B1326	11327	11328 T1329	N1330	51331 F1332	I1333	D1334 11335		V1338	G1340	11341	E1342 A1343	G1344	R1345	L1348	Y1349	K1350 E1351	V1352	Y1353	V1355 V1355	I1356	A1357	Y1362	V1363 N1364	Y1365	R1366	M1368	A1369	L1371	V1372	D1373 V1374	M1375	T1376 T1277	01378		L1381 T1382	S1383	V1384 T1385
R1386	H1387	G1388 F1389	N1390	R1391 S1392	N1393	11394 G1395	A1396	L1397 M1398	R1399	C1400	F1402	E1403	T1405	0 - - -	11408 L1409	F1410	E1411 A1410	G1413	A1414	S1415 41416	E1417	L1418	D1419 D1420	C1421	R1422 C1423	V1424	S1425 F1476	N1427	V1428	L1430	G1431	41432 M1433	A1434	P1435 T1436	G1437	T1438	A1440	F1441	D1442 V1443	M1444	11445 D1446
E1447	E1448	S1449 1.1450	V1451	K1452 V1453	M1454	GLU GLU	GLN	LYS ILE	THR	GLU TLE	GLU	ASP	CLN	ASP	GLY	VAL	THR PRO	TYR	SER	GLII	SER	CLY GLY	VAL	ASN	ALA	LEU	ASP VAT	LYS	ASP	TEU	MET	SER	PRO	LEU VAI.	ASP	SER	SER	ASN	ASP ALA	MET	ALA GLY
GLY	PHE	THR AI.A	TYR	GL Y	ALA	TYR	GLY	GLU ALA	THR	SER	PHE	GLY	TYR	GLY	GLU	PRO	THR	PRO	GLY	PHE CI.Y	VAL	SER	PRO	GLY	PHE	PRO	THR	PRO	THR	SER	PRO	SER	PR.0	ALA TYR	SER	PRO TUD	SER	PRO	TYR	SER	PRO THR
SER	PRO	TYR	SER	PRO THR	SER	SER	TYR	PRO	THR	SER	SER	TYR	PRO	THR	PRO	SER	TYR	PRO	THR	DER	SER	TYR	PRO	THR	SER	SER	TYR SFR	PRO	THR	PRO	SER	I IR SER	PRO	THR	PRO	SER	1 I.R. SER	PRO	THR SER	PRO	SER TYR
SER	PRO	THR	PRO	SER TVR	SER	THR	SER	PRU SER	TYR	SER	THR	SER	SER	TYR	PRO	THR	SER	SER	TYR	DER	THR	SER	ALA	TYR	SER	THR	SER	SER	TYR	PRO	THR	PRO	SER	TYR SER	PRO	THR	PRO	SER	TYR SER	PRO	THR



• Molecule 2: DNA-directed RNA polymerase II subunit RPB2





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



<u>%</u>				
Chain L:	39%	24% •	33%	
	•			
MET SER ARG GLU GLU GLV CLU GLN ILE PRO THR THR THR THR	ASP ALA ALA ALA ALA ALA ALA GLY TTHR SER SER SER CLN ALA ALA ALA ALA ALA ALA ALA ALA ALA K28 K28 K28	Y29 130 C31 A32 E33 E33 E33 E33 C34 S35 S35 S35 S35 L38 S39 S39 S39 S39 S39 S39 S39 S39 S39 S39	841 842 842 842 845 845 845 847 847 847 847 847 847 849 8649 8652 652 652 652 652 853 854 854 852 855 855 855 855 855 855 855 855 855	L57 K58 A59 R60 R60
T61 K62 K63 L64 V65 V65 C68 E68 R70 R70				
• Molecule 13. 1	DNA (5'-D(*AP*G*C)	P*TP*CP*∆P*		TP*TP*AP*(8OG)P
*GP*CP*CP*(H	BRU)P*GP*GP*TP*C	$(P^*AP^*TP^*T)$ -3	(1) (1)	II II /II (000)I
0)	
Chain T:	73%		8% 19%	
DA C7 C7 C7 C9 C9 C15 C12 C12 C15 C15 C15 C15 C15 C15 C15 C15 C15 C15	T17 A18 G19 G20 G20 G224 G224 G224 G225 G225 D4 D1 D1			
• Moleculo 14. I	ΟΝΔ (5' D(*ΔΡ*CΡ*1		TP*CP*AP*CP*CP	*T) 3')
• Wolecule 14. 1				1)-0)
Chain N:	25%	67%	8%	
	2270		0.0	
о				
A1 A1 A1 A1 A1 A1 A1 A1 A1 A1				
• Molecule 15: I	RNA (5'-R(*UP*GP*C	CP*AP*UP*C*U	UP*UP*CP*CP*AP*C	GP*GP*CP*CP*U)-3
,)				
6%				
Chain P:	% 38%	6%	38%	
a a a a a a a a a a a a a a a a a a a				



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants	220.65Å 392.00Å 281.45Å	Deperitor
a, b, c, α , β , γ	90.00° 90.00° 90.00°	Depositor
$\mathbf{P}_{\text{oscolution}}(\mathbf{\hat{A}})$	50.00 - 3.70	Depositor
Resolution (A)	49.00 - 3.70	EDS
% Data completeness	99.6(50.00-3.70)	Depositor
(in resolution range)	$100.0 \ (49.00-3.70)$	EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) > 1$	1.93 (at 3.67 Å)	Xtriage
Refinement program	CNS 1.2	Depositor
D D	0.225 , 0.258	Depositor
Λ, Λ_{free}	0.227 , 0.253	DCC
R_{free} test set	2439 reflections $(1.88%)$	wwPDB-VP
Wilson B-factor $(Å^2)$	114.2	Xtriage
Anisotropy	0.492	Xtriage
Bulk solvent $k_{sol}(e/Å^3), B_{sol}(Å^2)$	0.30 , 97.9	EDS
L-test for twinning ²	$< L > = 0.45, < L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.029 for 1/2 *h-1/2 *k,-3/2 *h-1/2 *k,-1	Xtriage
	0.034 for 1/2 *h + 1/2 *k, 3/2 *h - 1/2 *k, -1	1101100,00
F_o, F_c correlation	0.93	EDS
Total number of atoms	32355	wwPDB-VP
Average B, all atoms (A^2)	89.0	wwPDB-VP

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

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.



¹Intensities estimated from amplitudes.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 80G, BRU

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).

Mal	Chain	Bo	nd lengths	Bo	ond angles
WIOI	Ullalli	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.44	0/11441	0.74	3/15473~(0.0%)
2	В	0.41	0/9116	0.70	0/12291
3	С	0.42	0/2163	0.69	0/2930
4	D	0.38	0/1516	0.63	0/2031
5	Ε	0.39	0/1788	0.64	0/2406
6	F	0.52	0/724	0.82	0/977
7	G	0.44	0/1368	0.72	0/1844
8	Н	0.37	0/1119	0.68	0/1514
9	Ι	0.38	0/962	0.66	0/1295
10	J	0.44	0/541	0.74	0/727
11	Κ	0.46	0/947	0.68	0/1279
12	L	0.39	0/372	0.68	0/495
13	Т	0.56	1/426~(0.2%)	0.87	0/650
14	N	0.41	0/251	0.81	0/386
15	Р	0.42	0/227	0.80	0/351
All	All	0.43	1/32961~(0.0%)	0.71	3/44649~(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	А	0	1
2	В	0	1
All	All	0	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	Т	27	DC	C1'-N1	5.98	1.57	1.49



Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
1	А	567	LYS	C-N-CD	5.82	140.63	128.40
1	А	3	GLY	N-CA-C	-5.75	98.73	113.10
1	А	509	LEU	CA-CB-CG	-5.00	103.79	115.30

All (3) bond angle outliers are listed below:

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1035	TYR	Sidechain
2	В	797	TYR	Sidechain

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	А	11240	0	11311	1819	0
2	В	8942	0	8986	1481	0
3	С	2125	0	2090	340	0
4	D	1504	0	1518	205	0
5	Е	1752	0	1776	286	0
6	F	712	0	738	138	0
7	G	1340	0	1357	217	0
8	Н	1101	0	1075	206	0
9	Ι	944	0	901	162	0
10	J	532	0	542	129	0
11	Κ	929	0	939	135	0
12	L	370	0	394	90	0
13	Т	426	0	236	37	0
14	N	224	0	126	11	0
15	Р	205	0	109	8	0
16	А	1	0	0	0	0
17	А	2	0	0	0	0
17	В	1	0	0	0	0
17	С	1	0	0	0	0
17	Ι	2	0	0	0	0
17	J	1	0	0	0	0



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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
17	L	1	0	0	0	0
All	All	32355	0	32098	4821	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 75.

The worst 5 of 4821 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:69:LEU:HD13	2:B:429:PHE:CD1	1.39	1.55
2:B:69:LEU:HD13	2:B:429:PHE:CE1	1.66	1.30
2:B:577:ALA:HB1	2:B:589:VAL:HG11	1.24	1.17
2:B:806:THR:HG22	2:B:808:ALA:H	1.08	1.16
2:B:340:ALA:HB3	2:B:343:ILE:HG12	1.29	1.15

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	Perce	entiles
1	А	1421/1733 (82%)	909 (64%)	310 (22%)	202 (14%)	0	3
2	В	1111/1224 (91%)	694 (62%)	257 (23%)	160 (14%)	0	3
3	С	268/324~(83%)	164 (61%)	66 (25%)	38 (14%)	0	3
4	D	183/221~(83%)	108 (59%)	49 (27%)	26 (14%)	0	3
5	Е	212/215~(99%)	134 (63%)	49 (23%)	29 (14%)	0	3
6	F	86/155~(56%)	60 (70%)	20 (23%)	6 (7%)	1	15
7	G	169/171 (99%)	127 (75%)	32 (19%)	10 (6%)	1	18
8	Н	133/146 (91%)	72 (54%)	37 (28%)	24 (18%)	0	1



Mol	Chain	Analysed	Favoured	Allowed	Outliers	Perce	entiles
9	Ι	114/122~(93%)	73~(64%)	26~(23%)	15~(13%)	0	4
10	J	63/70~(90%)	34~(54%)	13~(21%)	16 (25%)	0	0
11	Κ	114/120~(95%)	79~(69%)	26~(23%)	9~(8%)	1	12
12	L	45/70~(64%)	19 (42%)	11 (24%)	15 (33%)	0	0
All	All	3919/4571~(86%)	2473 (63%)	896 (23%)	550 (14%)	0	3

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 $5~{\rm of}~550$ Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	А	4	GLN
1	А	41	MET
1	А	43	GLU
1	А	48	ALA
1	А	58	LEU

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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 side chain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Pe	erce	entiles
1	А	1249/1520~(82%)	1135 (91%)	114 (9%)		9	36
2	В	974/1061~(92%)	879~(90%)	95 (10%)		8	33
3	С	238/280~(85%)	215 (90%)	23 (10%)		8	33
4	D	167/200~(84%)	145 (87%)	22~(13%)		4	22
5	Е	196/197~(100%)	179 (91%)	17 (9%)		10	38
6	F	78/137~(57%)	69~(88%)	9~(12%)		5	27
7	G	152/152~(100%)	138 (91%)	14 (9%)		9	36
8	Н	121/128~(94%)	112 (93%)	9~(7%)		13	44
9	Ι	110/116~(95%)	98~(89%)	12 (11%)		6	29
10	J	60/65~(92%)	55~(92%)	5 (8%)		11	40
11	K	99/102~(97%)	87 (88%)	12 (12%)		5	24
12	L	41/57~(72%)	35~(85%)	6 (15%)		3	18



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Mol	Chain	Analysed Rotameric Outliers		Percentiles	
All	All	3485/4015~(87%)	3147~(90%)	338 (10%)	8 33

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

Mol	Chain	Res	Type
3	С	245	VAL
7	G	73	LYS
4	D	43	GLU
5	Е	74	ASP
8	Н	91	ASP

Sometimes side chains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 130 such side chains are listed below:

Mol	Chain	Res	Type
8	Н	33	GLN
8	Н	139	ASN
1	А	1354	ASN
1	А	1278	ASN
9	Ι	90	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
15	Р	9/16~(56%)	1 (11%)	0

All (1) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
15	Р	11	U

There are no RNA pucker outliers to report.

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

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



3I4M

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).

Mal	Turne	Chain	noin Pog		Bo	ond leng	$_{\rm sths}$	B	ond ang	les
WIOI	туре	Unain	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z >2
13	80G	Т	19	15,13	22,25,26	1.01	1 (4%)	30,37,40	1.55	4 (13%)
13	BRU	Т	23	15,13	18,21,22	<mark>3.91</mark>	1 (5%)	26,30,33	0.97	2 (7%)

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	80G	Т	19	15,13	-	0/7/21/22	0/3/3/3
13	BRU	Т	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)	$\mathrm{Ideal}(\mathrm{\AA})$
13	Т	23	BRU	BR-C5	-16.52	1.49	1.88
13	Т	19	80G	C8-N7	-3.70	1.31	1.38

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
13	Т	19	80G	N7-C8-N9	5.47	113.07	106.58
13	Т	19	80G	C5-N7-C8	-3.45	104.51	109.47
13	Т	19	80G	C2'-C1'-N9	2.75	119.27	116.01
13	Т	23	BRU	C6-C5-C4	-2.59	118.04	120.67
13	Т	19	80G	C4-C5-N7	2.42	110.73	106.08

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	Т	23	BRU	C2'-C1'-N1-C2

There are no ring outliers.

1 monomer is involved in 1 short contact:



Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	Т	23	BRU	1	0

5.5 Carbohydrates (i)

There are no monosaccharides 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 (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, 95^{th} 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	$\mathbf{OWAB}(\mathbf{\AA}^2)$	Q<0.9
1	А	1429/1733~(82%)	-0.31	1 (0%) 95 94	15, 72, 135, 195	0
2	В	1125/1224 (91%)	-0.15	14 (1%) 79 69	11, 88, 154, 194	0
3	С	270/324~(83%)	-0.29	1 (0%) 92 88	34, 73, 131, 174	0
4	D	187/221 (84%)	-0.15	4 (2%) 63 52	58, 98, 152, 197	0
5	Е	214/215~(99%)	-0.26	2 (0%) 84 76	42, 112, 155, 161	0
6	F	88/155~(56%)	-0.47	0 100 100	24, 48, 91, 122	0
7	G	$171/171 \ (100\%)$	-0.23	0 100 100	48, 74, 117, 128	0
8	Н	137/146~(93%)	0.16	3 (2%) 62 50	91, 125, 152, 157	0
9	Ι	116/122~(95%)	-0.13	3 (2%) 56 43	65, 121, 152, 153	0
10	J	65/70~(92%)	-0.42	0 100 100	48, 67, 106, 121	0
11	К	116/120~(96%)	-0.32	2 (1%) 70 59	32, 79, 108, 160	0
12	L	47/70~(67%)	-0.05	1 (2%) 63 52	73, 124, 147, 159	0
13	Т	19/26~(73%)	0.44	0 100 100	128, 194, 200, 200	0
14	Ν	11/12 (91%)	0.88	1 (9%) 9 7	186, 198, 200, 200	0
15	Р	10/16~(62%)	0.33	1 (10%) 7 5	177, 193, 199, 200	0
All	All	4005/4625 (86%)	-0.22	33 (0%) 86 78	11, 83, 152, 200	0

The worst 5 of 33 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	В	471	LYS	6.2
2	В	883	LEU	3.8
11	Κ	116	ALA	3.4
2	В	504	ARG	3.3
2	В	722	ASP	3.2



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, 95^{th} 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	Т	23	20/21	0.68	0.27	153,162,167,170	0
13	80G	Т	19	23/24	0.89	0.17	$131,\!141,\!154,\!155$	0

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
17	ZN	Ι	1122	1/1	0.92	0.04	134,134,134,134	0
16	MG	А	2458	1/1	0.95	0.09	69,69,69,69	0
17	ZN	А	2456	1/1	0.96	0.07	96,96,96,96	0
17	ZN	L	1071	1/1	0.97	0.06	111,111,111,111	0
17	ZN	В	2225	1/1	0.99	0.21	43,43,43,43	0
17	ZN	J	1066	1/1	0.99	0.23	47,47,47,47	0
17	ZN	Ι	1121	1/1	0.99	0.12	70,70,70,70	0
17	ZN	А	2457	1/1	1.00	0.14	38,38,38,38	0
17	ZN	С	1269	1/1	1.00	0.12	39,39,39,39	0

6.5 Other polymers (i)

There are no such residues in this entry.

