



wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 15, 2023 – 04:18 AM EDT

PDB ID : 1TWA
Title : RNA polymerase II complexed with ATP
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2004-06-30
Resolution : 3.20 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
buster-report : 1.1.7 (2018)
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) : 2.35

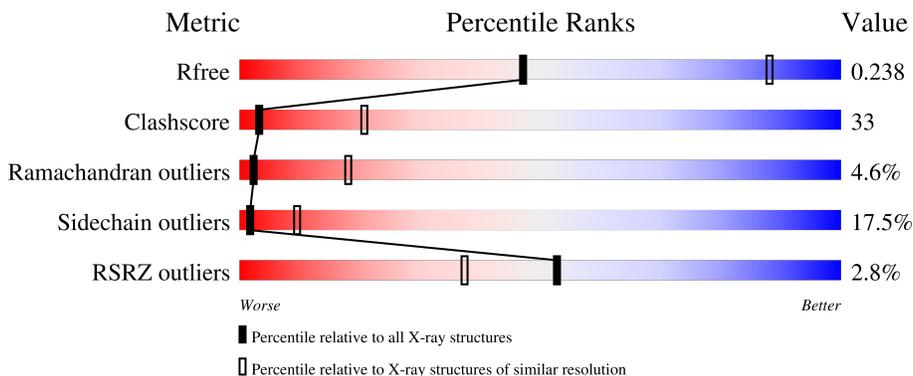
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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.



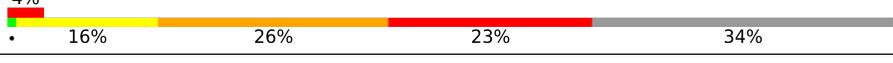
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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	
2	B	1224	
3	C	318	
4	E	215	
5	F	155	

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Mol	Chain	Length	Quality of chain
6	H	146	
7	I	122	
8	J	70	
9	K	120	
10	L	70	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	ZN	C	3002	-	-	X	-
12	ZN	J	3001	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 27757 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 largest subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	1352	10635	6711	1842	2024	58	0	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	1091	8690	5511	1516	1610	53	0	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	266	2095	1317	348	417	13	0	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	E	215	1760	1116	310	322	12	0	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
5	F	83	670	428	114	125	3	0	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
6	H	133	1068	673	180	211	4	0	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
7	I	121	990	610	181	188	11	0	0	0

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
8	J	64	525	334	92	93	6	0	0	0

- Molecule 9 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
9	K	114	919	590	156	171	2	0	0	0

- Molecule 10 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
10	L	46	364	224	72	64	4	0	0	0

- Molecule 11 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	2	Total	Mn	0	0
			2	2		

- Molecule 12 is ZINC ION (three-letter code: ZN) (formula: Zn).

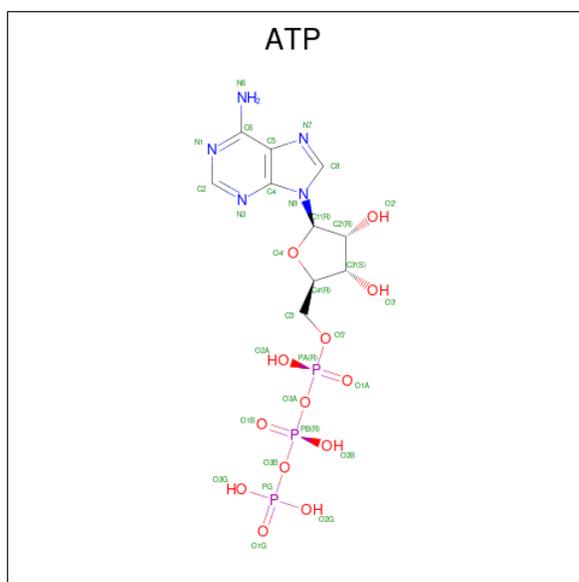
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	2	Total	Zn	0	0
			2	2		
12	B	1	Total	Zn	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	C	1	Total	Zn	0	0
			1	1		
12	I	2	Total	Zn	0	0
			2	2		
12	J	1	Total	Zn	0	0
			1	1		
12	L	1	Total	Zn	0	0
			1	1		

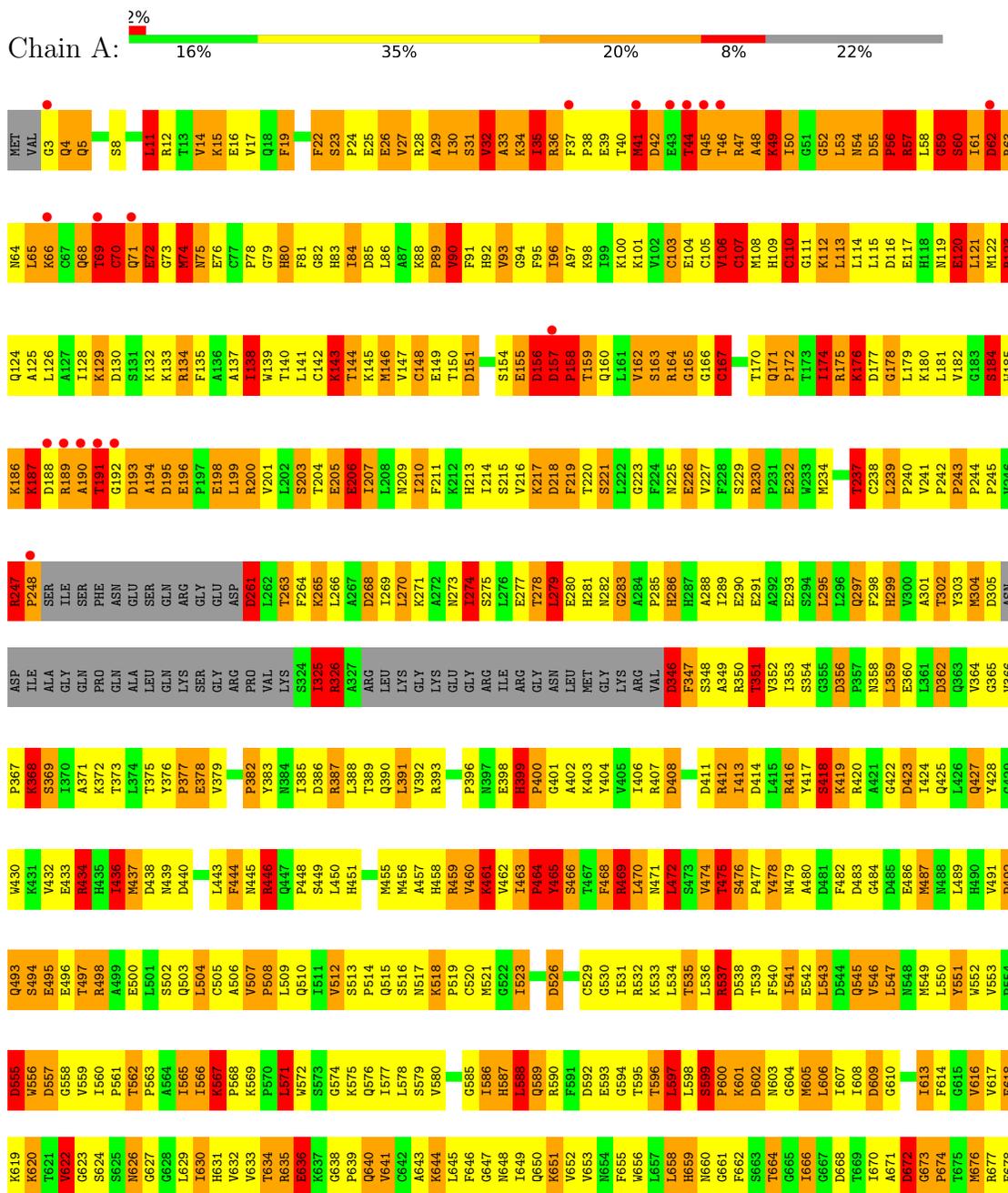
- Molecule 13 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



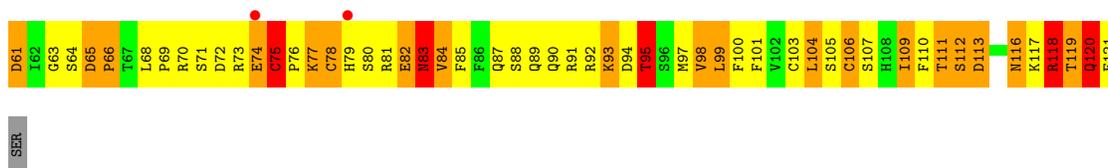
3 Residue-property plots

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.

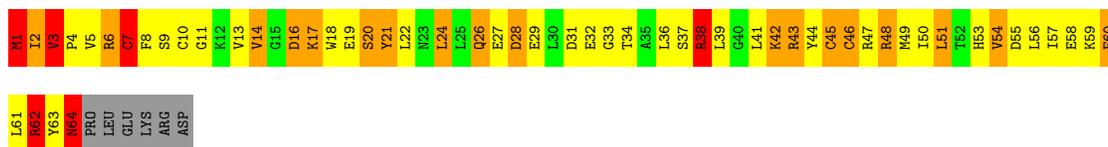
- Molecule 1: DNA-directed RNA polymerase II largest subunit



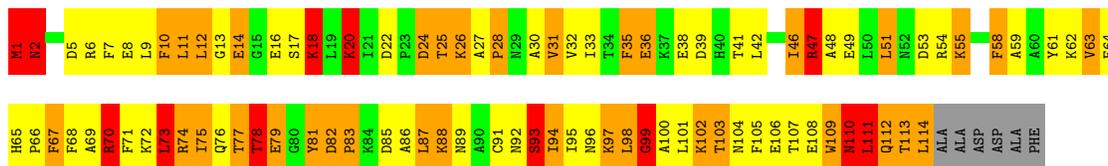
THR	T1376	E1315	R1194	L1134	Y999	V937	D874	G807	V743	E681
SER	T1377	V1316	L1195	R1135	L1000	K938	A875	L808	K744	I682
PRO	G1378	M1317	L1196	A1136	R1001	D930	T809	T809	K745	I683
ASP	G1379	E1256	L1197	A1137	G1002	R940	E879	P810	M746	A684
ALA	G1380	D1257	H1198	E1138	K1003	K941	K880	Q811	M747	A685
TYR	G1381	H1258	R1199	E1139	K1004	F942	Q881	Q812	M748	E686
PRO	L1382	L1260	A1200	H1140	E1005	A1076	S882	F813	A749	K687
THR	G1383	K1261	A1201	T1077	I1006	L943	L883	F814	G750	K688
GLY	V1384	K1262	A1202	Q1078	T1007	R944	D884	F815	S751	K689
GLY	T1385	I1263	M1203	T1080	A1010	E945	D884	F816	K752	K690
PRO	T1386	E1264	L1143	T1081	Q1011	F946	T885	H816	K753	K691
SER	T1387	K1265	K1204	L1081	R1012	F947	T886	H817	K754	K692
ALA	R1326	H1266	K1205	ASN	R1013	V948	I886	H818	K755	K693
TYR	I1327	T1266	V1146	THR	D1014	D949	I887	H819	K756	K694
PRO	Y1328	M1267	L1147	PHE	A1014	G950	E822	E822	K757	K695
THR	T1329	L1268	I1148	HIS	V1015	D890	D890	A759	K758	K696
THR	N1330	E1269	M1209	HIS	T1016	A891	A891	A760	K759	K697
ALA	N1331	E1269	A1149	PHE	T1017	A892	I825	M761	K760	K698
PRO	S1331	L1270	Q1210	ALA	L1017	F893	D826	M762	K761	K699
ASP	F1332	I1271	G1211	GLY	F1018	F894	V829	S762	K762	K700
THR	I1333	T1272	Q1212	VAL	C1019	L956	V829	A763	K763	K701
GLN	D1334	L1273	G1213	VAL	C1020	P957	K830	C764	K764	K702
GLY	D1334	L1273	G1213	ALA	C1020	P957	K830	C765	K765	K703
ILE	I1335	E1274	E1214	SER	R1023	V988	E833	C766	K766	K704
LEU	M1336	G1275	R1215	K1092	S1024	R959	T834	Q767	K767	K705
THR	E1337	V1276	I1216	K1093	S1024	R960	T835	Q768	K768	K706
THR	E1337	E1277	K1217	R1156	R1025	R961	T836	S769	K769	K707
PRO	V1338	E1278	Q1218	T1095	L1026	R962	I837	V770	K708	K708
GLU	L1339	I1278	T1219	T1096	A1027	R963	Q838	V771	K709	K709
ASP	G1340	I1279	R1159	S1096	A1027	R964	Q839	E772	K710	K710
GLY	I1341	E1280	S1160	G1097	R1030	R965	R839	K772	K711	K711
GLY	E1403	R1281	K1221	V1098	R1030	Q965	T904	K773	K712	K712
GLN	E1404	V1282	N1222	P1099	E1034	N966	R906	R774	K713	K713
ASP	T1405	G1344	D1223	R1100	A967	K843	H906	I775	K714	K714
GLY	F1406	R1345	P1164	R1101	Y1085	T907	A844	A776	K715	K715
GLY	V1407	M1284	L1101	K1102	R1036	Q968	L845	A777	K716	K716
VAL	E1407	M1285	E1165	K1103	L1037	Q969	E846	F777	K717	K717
THR	I1408	K1286	V1226	E1103	L1037	T970	E847	F778	K718	K718
THR	L1409	Y1287	I1227	L1104	T1038	P910	D847	F779	K719	K719
PRO	F1410	D1288	W1228	L1105	K1039	S911	I848	F780	K720	K720
PRO	E1411	R1289	S1229	L1106	F1042	L912	M849	D781	K721	K721
SER	E1411	K1290	E1230	R1107	F1043	L913	V850	D782	K722	K722
ASN	E1411	V1291	D1231	A1108	D1043	E914	H851	T783	K723	K723
GLU	A1414	P1292	N1232	K1109	W1044	S915	Y852	L784	K724	K724
GLY	S1415	P1293	D1233	M1110	L1046	G916	P785	L784	K725	K725
SER	A1416	P1294	E1234	M1111	R1047	S917	N854	L785	K726	K726
LEU	E1417	E1234	K1235	M1112	S1047	E918	T855	F787	K727	K727
LEU	L1418	K1235	L1236	K1112	N1048	I919	T856	A724	K728	K728
VAL	D1419	L1237	L1237	L1116	E1049	L981	K788	A725	K729	K729
ASN	D1420	I1237	I1237	L1117	I1049	L981	R857	D727	K730	K730
ASP	C1421	I1238	I1238	T1117	E1050	G921	K888	D727	K731	K731
LEU	R1422	R1239	R1239	Y1118	A1051	D922	S889	D791	K732	K732
ASP	G1423	K1300	C1240	Y1119	Q1052	D922	S889	D791	K733	K733
THR	Y1362	E1301	C1240	Y1119	Q1052	L923	L860	A729	K734	K734
THR	Y1363	P1302	R1241	L1120	D985	K924	G861	Y792	K735	K735
PRO	N1364	E1303	R1242	E1121	I986	L925	N862	S793	K736	K736
PRO	Y1365	W1304	V1243	E1121	R1055	L925	N862	P794	K737	K737
THR	R1366	V1305	ARG	F1122	S1056	Q926	N863	E795	K738	K738
SER	H1367	L1306	PRO	G1123	V1057	V927	I864	E796	K739	K739
LEU	H1367	L1306	PRO	G1123	V1057	V927	I864	E796	K740	K740
LEU	H1367	L1306	PRO	G1123	V1057	V927	I864	E796	K741	K741
MET	A1368	E1307	LYS	A1126	G1061	L929	F866	V736	K742	K742
THR	A1369	T1308	SER	D1127	G1061	D930	F867	V737	K743	K743
PRO	L1370	D1309	LEU	Q1128	E931	E931	Y868	N802	K744	K744
PRO	L1371	G1310	ASP	Q1189	M1063	E932	G869	N802	K745	K745
PRO	L1371	G1310	ASP	Q1189	M1063	E932	G869	N802	K746	K746
LEU	V1372	V1311	ALA	Q1130	V1064	Q933	E870	S803	K747	K747
THR	D1373	M1312	THR	W1191	G1085	K934	E870	S803	K748	K748
THR	L1374	L1313	GLU	W1192	G1085	K934	E870	S803	K749	K749
PRO	M1375	S1314	GLU	L1193	L1067	E935	D871	Y804	K750	K750
SER	M1375	S1314	GLU	L1193	L1067	E935	D871	Y804	K751	K751



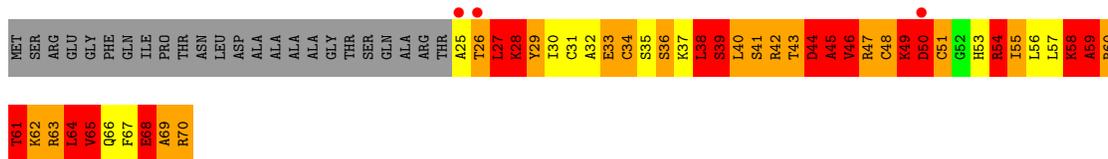
- Molecule 8: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



- Molecule 9: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 10: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	123.00Å 223.00Å 374.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.20 39.69 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.20) 97.5 (39.69-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 3.12Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.227 , 0.246 0.195 , 0.238	Depositor DCC
R_{free} test set	2779 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 42.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	27757	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% 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: ATP, MN, ZN

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	3.53	1385/10822 (12.8%)	2.62	715/14641 (4.9%)
2	B	3.54	1164/8860 (13.1%)	2.56	552/11945 (4.6%)
3	C	3.57	288/2133 (13.5%)	2.62	126/2891 (4.4%)
4	E	3.50	210/1796 (11.7%)	2.40	107/2416 (4.4%)
5	F	3.12	78/682 (11.4%)	2.30	35/922 (3.8%)
6	H	3.37	138/1086 (12.7%)	2.46	68/1470 (4.6%)
7	I	3.73	145/1009 (14.4%)	2.69	86/1357 (6.3%)
8	J	3.41	75/533 (14.1%)	3.10	53/715 (7.4%)
9	K	3.36	117/937 (12.5%)	2.65	61/1265 (4.8%)
10	L	3.99	58/366 (15.8%)	2.90	43/485 (8.9%)
All	All	3.52	3658/28224 (13.0%)	2.59	1846/38107 (4.8%)

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	41
2	B	0	40
3	C	0	13
4	E	1	6
5	F	0	2
6	H	0	12
7	I	0	6
8	J	0	1
9	K	0	1
10	L	0	2
All	All	1	124

The worst 5 of 3658 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	552	MET	CG-SD	26.10	2.49	1.81
1	A	728	LYS	CD-CE	24.04	2.11	1.51
2	B	598	GLU	CG-CD	23.97	1.88	1.51
1	A	771	GLU	CD-OE2	23.53	1.51	1.25
3	C	165	LYS	CE-NZ	23.14	2.06	1.49

The worst 5 of 1846 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	774	ARG	NE-CZ-NH1	34.28	137.44	120.30
1	A	469	ARG	NE-CZ-NH2	-32.36	104.12	120.30
1	A	1366	ARG	NE-CZ-NH1	31.49	136.04	120.30
3	C	35	ARG	NE-CZ-NH2	-28.02	106.29	120.30
3	C	34	ARG	NE-CZ-NH2	-27.97	106.32	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	E	204	THR	CB

5 of 124 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	PRO	Peptide
1	A	165	GLY	Peptide
1	A	44	THR	Peptide
1	A	60	SER	Peptide
1	A	74	MET	Peptide

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	10635	0	10688	689	0
2	B	8690	0	8715	513	0
3	C	2095	0	2053	155	0
4	E	1760	0	1788	130	0
5	F	670	0	689	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	1068	0	1040	164	0
7	I	990	0	949	71	0
8	J	525	0	537	44	0
9	K	919	0	929	73	0
10	L	364	0	388	65	0
11	A	2	0	0	0	0
12	A	2	0	0	1	0
12	B	1	0	0	1	0
12	C	1	0	0	2	0
12	I	2	0	0	0	0
12	J	1	0	0	2	0
12	L	1	0	0	1	0
13	A	31	0	12	0	0
All	All	27757	0	27788	1823	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 33.

The worst 5 of 1823 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:1057:LYS:CE	2:B:1057:LYS:CD	1.75	1.65
1:A:368:LYS:CD	1:A:368:LYS:CE	1.75	1.65
1:A:919:ILE:CD1	1:A:919:ILE:CG1	1.75	1.64
4:E:37:LEU:CD1	4:E:37:LEU:CG	1.75	1.64
1:A:1112:LYS:CD	1:A:1112:LYS:CE	1.74	1.64

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	1335/1733 (77%)	1187 (89%)	91 (7%)	57 (4%)	2	20
2	B	1071/1224 (88%)	924 (86%)	104 (10%)	43 (4%)	3	21
3	C	264/318 (83%)	231 (88%)	23 (9%)	10 (4%)	3	22
4	E	213/215 (99%)	183 (86%)	16 (8%)	14 (7%)	1	9
5	F	81/155 (52%)	73 (90%)	6 (7%)	2 (2%)	5	32
6	H	129/146 (88%)	89 (69%)	19 (15%)	21 (16%)	0	0
7	I	119/122 (98%)	110 (92%)	8 (7%)	1 (1%)	19	58
8	J	62/70 (89%)	58 (94%)	4 (6%)	0	100	100
9	K	112/120 (93%)	98 (88%)	12 (11%)	2 (2%)	8	41
10	L	44/70 (63%)	24 (54%)	13 (30%)	7 (16%)	0	0
All	All	3430/4173 (82%)	2977 (87%)	296 (9%)	157 (5%)	2	18

5 of 157 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	ILE
1	A	45	GLN
1	A	47	ARG
1	A	59	GLY
1	A	60	SER

5.3.2 Protein sidechains [i](#)

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	1184/1520 (78%)	998 (84%)	186 (16%)	2	12
2	B	947/1061 (89%)	806 (85%)	141 (15%)	3	14
3	C	234/274 (85%)	194 (83%)	40 (17%)	2	10
4	E	197/197 (100%)	152 (77%)	45 (23%)	1	4
5	F	73/137 (53%)	64 (88%)	9 (12%)	4	21
6	H	117/128 (91%)	73 (62%)	44 (38%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	I	115/116 (99%)	91 (79%)	24 (21%)	1	6
8	J	59/65 (91%)	49 (83%)	10 (17%)	2	10
9	K	99/102 (97%)	80 (81%)	19 (19%)	1	8
10	L	40/57 (70%)	21 (52%)	19 (48%)	0	0
All	All	3065/3657 (84%)	2528 (82%)	537 (18%)	2	9

5 of 537 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	H	144	ILE
7	I	61	ASP
6	H	137	GLN
10	L	33	GLU
2	B	89	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 71 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	167	HIS
3	C	252	GLN
7	I	46	HIS
1	A	1364	ASN
1	A	1173	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 10 are monoatomic - leaving 1 for Mogul analysis.

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	ATP	A	3011	11	26,33,33	1.14	2 (7%)	31,52,52	1.57	4 (12%)

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	ATP	A	3011	11	-	2/18/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	A	3011	ATP	C2-N3	4.13	1.38	1.32
13	A	3011	ATP	C2-N1	2.67	1.38	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	A	3011	ATP	N3-C2-N1	-5.48	120.11	128.68
13	A	3011	ATP	PB-O3B-PG	-3.45	120.99	132.83
13	A	3011	ATP	PA-O3A-PB	-3.40	121.17	132.83
13	A	3011	ATP	C3'-C2'-C1'	2.89	105.32	100.98

There are no chirality outliers.

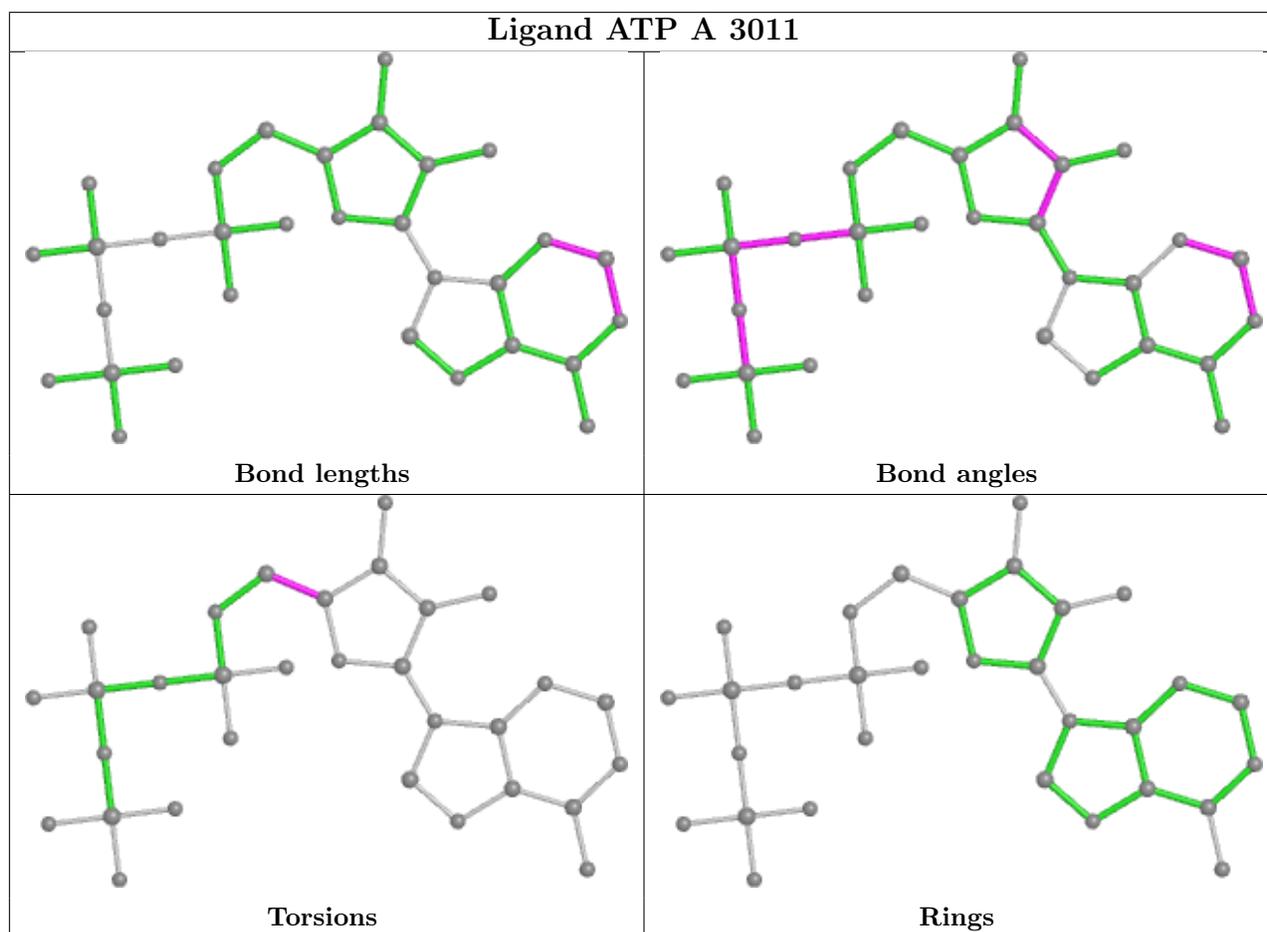
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
13	A	3011	ATP	O4'-C4'-C5'-O5'
13	A	3011	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	5
2	B	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	686:ALA	C	687:LYS	N	1.20
1	A	1064:VAL	C	1065:GLY	N	1.20
1	B	632:ARG	C	633:VAL	N	1.20
1	A	366:VAL	C	367:PRO	N	1.19
1	A	1195:LEU	C	1196:GLU	N	1.19

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	1352/1733 (78%)	-0.36	27 (1%) 65 51	9, 38, 105, 151	0
2	B	1091/1224 (89%)	-0.26	50 (4%) 32 20	10, 36, 111, 138	0
3	C	266/318 (83%)	-0.45	2 (0%) 86 78	21, 42, 72, 123	0
4	E	215/215 (100%)	-0.25	5 (2%) 60 47	13, 51, 102, 134	0
5	F	83/155 (53%)	-0.37	2 (2%) 59 44	18, 36, 64, 73	0
6	H	133/146 (91%)	0.21	6 (4%) 33 21	41, 79, 121, 132	0
7	I	121/122 (99%)	-0.21	2 (1%) 70 57	23, 44, 78, 108	0
8	J	64/70 (91%)	-0.55	0 100 100	21, 35, 61, 76	0
9	K	114/120 (95%)	-0.30	0 100 100	21, 50, 72, 81	0
10	L	46/70 (65%)	0.26	3 (6%) 18 11	39, 89, 118, 121	0
All	All	3485/4173 (83%)	-0.30	97 (2%) 53 37	9, 41, 107, 151	0

The worst 5 of 97 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	1109	GLY	9.4
1	A	69	THR	7.7
2	B	1110	PRO	7.4
1	A	248	PRO	7.1
6	H	85	GLY	6.8

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](#)

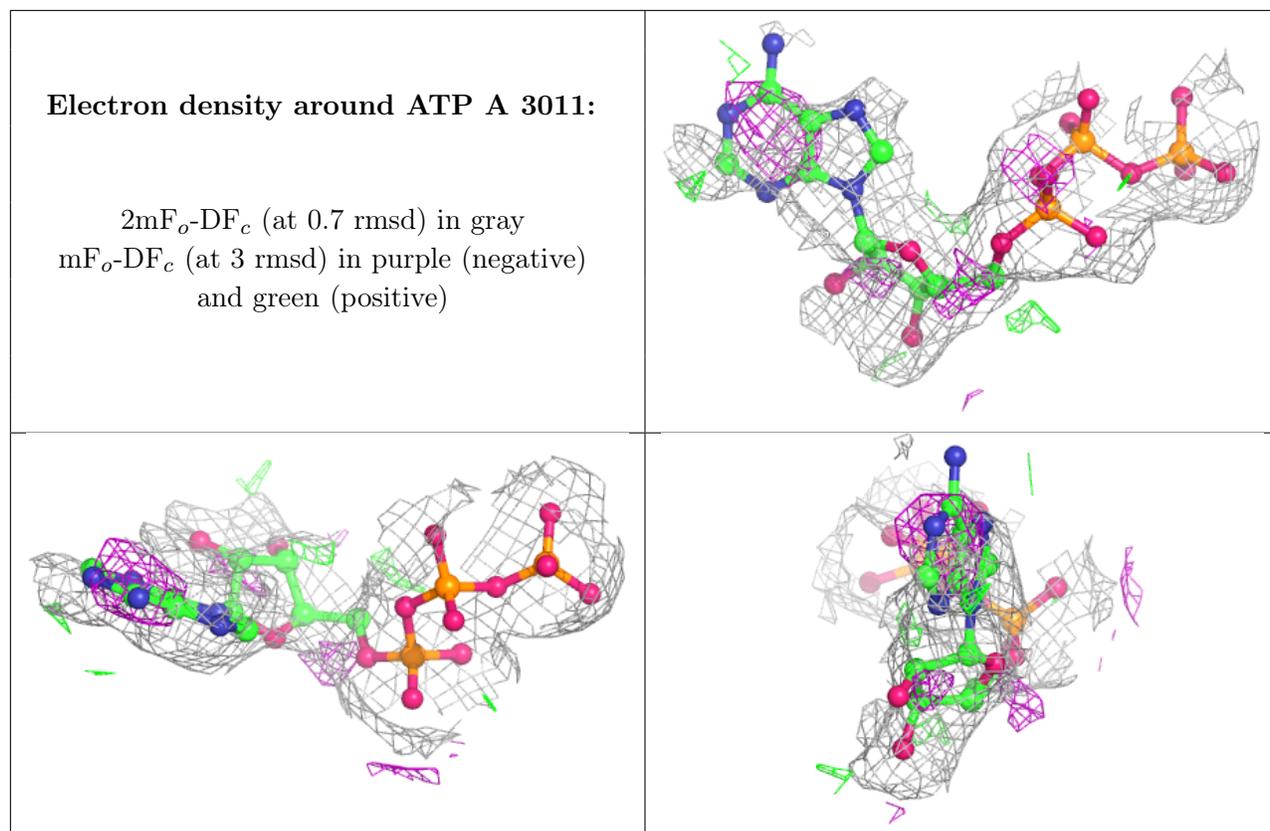
There are no monosaccharides in this entry.

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, 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
12	ZN	L	3005	1/1	0.69	0.06	139,139,139,139	0
12	ZN	I	3003	1/1	0.87	0.06	144,144,144,144	0
13	ATP	A	3011	31/31	0.89	0.23	69,74,83,83	0
12	ZN	B	3007	1/1	0.93	0.06	108,108,108,108	0
12	ZN	A	3006	1/1	0.96	0.04	124,124,124,124	0
12	ZN	I	3004	1/1	0.97	0.05	144,144,144,144	0
11	MN	A	3010	1/1	0.97	0.12	29,29,29,29	0
12	ZN	A	3008	1/1	0.97	0.03	96,96,96,96	0
11	MN	A	3009	1/1	0.98	0.12	24,24,24,24	0
12	ZN	C	3002	1/1	0.98	0.06	78,78,78,78	0
12	ZN	J	3001	1/1	0.99	0.08	84,84,84,84	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



6.5 Other polymers [i](#)

There are no such residues in this entry.