



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 05:28 PM UTC

PDB ID : 1R9T / pdb_00001r9t
Title : RNA POLYMERASE II STRAND SEPARATED ELONGATION COM-
PLEX, MISMATCHED NUCLEOTIDE
Authors : Westover, K.D.; Bushnell, D.A.; Kornberg, R.D.
Deposited on : 2003-10-30
Resolution : 3.50 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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

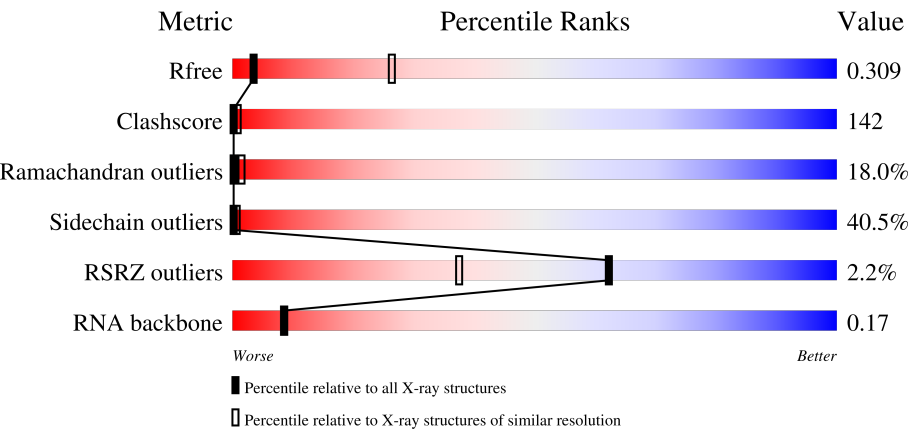
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)
RNA backbone	3983	1010 (3.98-3.02)

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	R	10	90% 50% 50%
2	T	28	68% 50% 43% 7%
3	N	14	50% 79% 21%
4	A	1733	7% 36% 36% 20%

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Mol	Chain	Length	Quality of chain
5	B	1224	
6	C	318	
7	E	215	
8	F	155	
9	H	146	
10	I	122	
11	J	70	
12	K	120	
13	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
15	MG	A	2001	-	-	-	X
15	MG	A	2002	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 29248 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 RNA chain called RNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	R	10	Total	C	N	O	P	0	0	0
			217	98	45	65	9			

- Molecule 2 is a DNA chain called DNA template strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	T	28	Total	C	N	O	P	0	0	0
			566	271	104	164	27			

- Molecule 3 is a DNA chain called DNA nontemplate strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	N	14	Total	C	N	O	P	0	0	0
			284	137	49	85	13			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	A	1395	Total	C	N	O	S	0	0	0
			10969	6917	1923	2068	61			

- Molecule 5 is a protein called DNA-directed RNA polymerase II 140 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	B	1106	Total	C	N	O	S	0	0	0
			8792	5568	1538	1631	55			

- Molecule 6 is a protein called DNA-directed RNA polymerase II 45 kDa polypeptide.

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

- Molecule 7 is a protein called DNA-directed RNA polymerases I, II, and III 27 kDa polypeptide.

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

- Molecule 8 is a protein called DNA-directed RNA polymerases I, II, and III 23 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	F	84	Total	C	N	O	S	0	0	0
			679	434	115	127	3			

- Molecule 9 is a protein called DNA-directed RNA polymerases I, II, and III 14.5 kDa polypeptide.

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

- Molecule 10 is a protein called DNA-directed RNA polymerase II 14.2 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
10	I	119	Total	C	N	O	S	0	0	0
			971	596	179	186	10			

- Molecule 11 is a protein called DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide.

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

- Molecule 12 is a protein called DNA-directed RNA polymerase II 13.6 kDa polypeptide.

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

- Molecule 13 is a protein called DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
13	L	46	Total	C	N	O	S	0	0	0
			363	224	72	63	4			

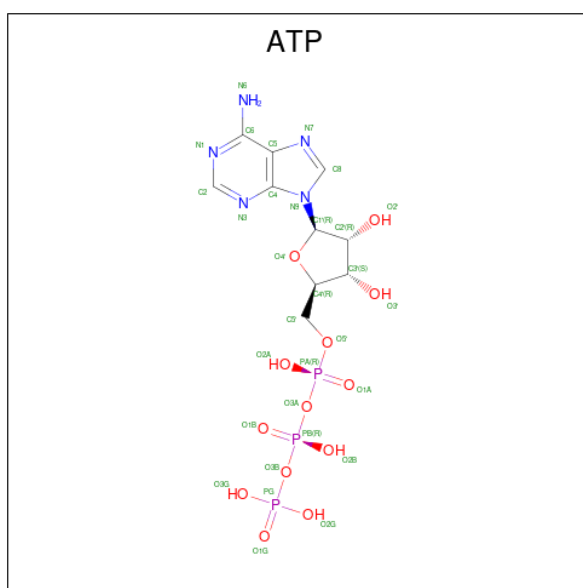
- Molecule 14 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	2	Total	Zn	0	0
			2	2		
14	B	1	Total	Zn	0	0
			1	1		
14	C	1	Total	Zn	0	0
			1	1		
14	I	2	Total	Zn	0	0
			2	2		
14	J	1	Total	Zn	0	0
			1	1		
14	L	1	Total	Zn	0	0
			1	1		

- Molecule 15 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
15	A	2	Total	Mg	0	0
			2	2		

- Molecule 16 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).

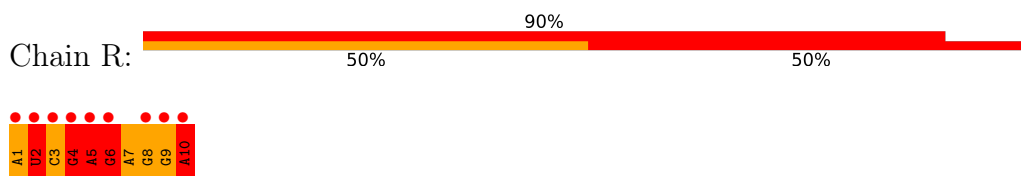


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
16	B	1	31	10	5	13	3	0	0

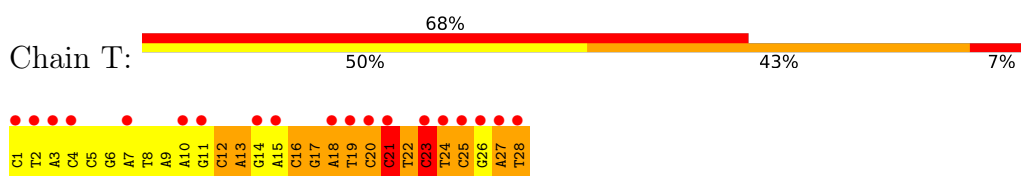
3 Residue-property plots [i](#)

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.

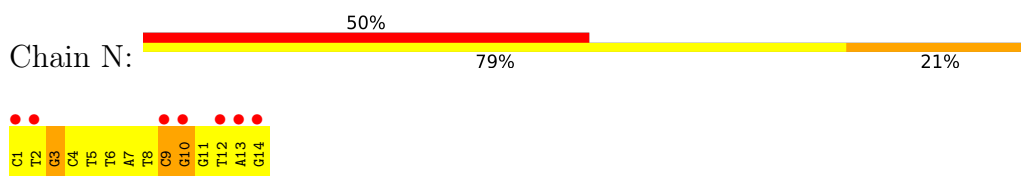
- Molecule 1: RNA strand



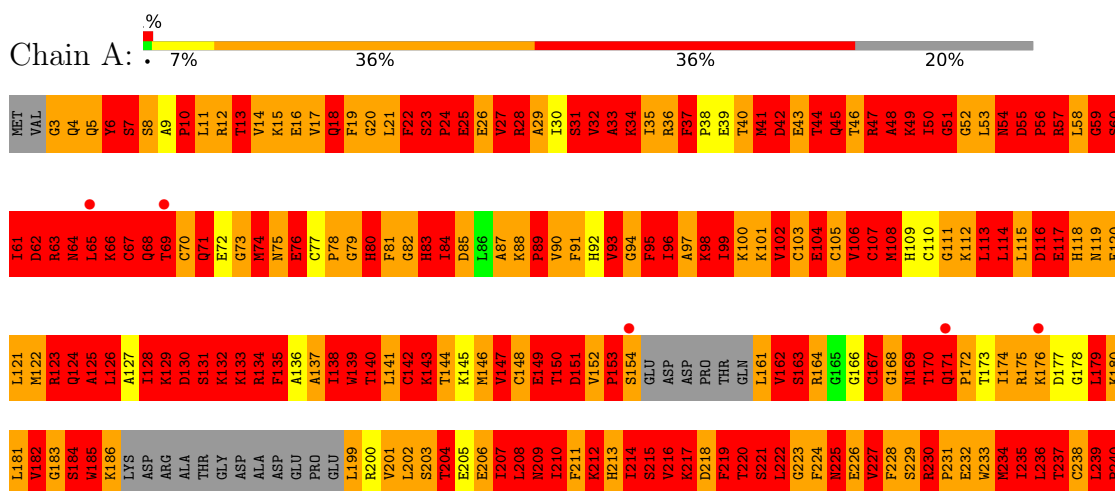
- Molecule 2: DNA template strand



- Molecule 3: DNA nontemplate strand



- Molecule 4: DNA-directed RNA polymerase II largest subunit



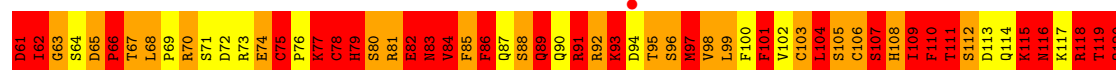
A1201	T1141	L1081	L1021	R961	L901	L841	D781	F721	G661	K601	I541	D481	A421	L361	A301	V241
M1202	T1142	ASN	L1022	R962	L902	V842	R782	L722	F662	D602	E542	F482	G422	D362	T302	P242
N1203	L1143	THR	R1023	R963	X903	K843	T783	R723	S663	N603	L543	F483	D423	D363	X303	P243
K1204	L1144	PHE	S1024	T964	A844	A844	L784	E724	T664	G604	L544	G484	L424	V364	X304	P244
K1205	S1145	HIS	R1025	Q965	D905	L845	R785	A725	G665	M805	Q545	D485	Q425	G365	X305	P245
D1206	V1146	PHE	L1026	N966	H906	E846	H786	R726	T666	L606	Q546	D486	L426	V366	X306	P246
L1207	T1147	ALA	A1027	A967	T907	D847	F787	D727	G667	I607	L547	M487	Q427	P367	D307	R247
T1208	I1148	GLY	T1028	Q968	L908	I848	S788	R728	D668	I608	N548	M488	Y428	K368	L308	P248
M1209	A1149	VAL	R1029	Q969	D909	M849	R789	A729	T669	D609	M549	L489	G429	S369	A309	S249
Q1210	S1150	ALA	R1030	T970	S910	V850	D790	G730	I670	G610	L550	H490	W430	S369	L250	S249
Q1211	E1151	SER	V1031	F971	S911	H851	D791	R731	A671	Q611	L551	H491	W431	A371	Q311	S251
G1212	I1152	K1092	L1032	H972	L912	H852	Y792	L732	D672	I612	N552	P492	V432	K372	P312	P252
G1213	V1153	K1093	Q1033	I973	L913	H853	S793	A733	G673	I613	N553	Q493	E433	K373	Q313	N253
E1214	V1154	V1094	E1034	D974	E914	N854	P794	E734	P674	F614	P554	S494	R434	L374	A314	E254
R1215	D1155	P1095	Y1035	H975	S915	T855	E795	V735	T675	G615	D555	E495	H435	T375	L315	S255
R1216	P1156	S1096	R1036	T976	G916	T856	S796	N736	M676	V616	M556	E496	L436	Y376	L316	Q256
K1217	L1157	G1097	L1037	K977	S917	R857	K797	L737	R677	V617	D557	P497	N437	P377	X317	R257
Q1218	P1158	V1098	R1038	P978	E918	N858	G798	K738	E678	E618	G558	R498	D438	E378	S318	D258
T1219	H1159	P1099	K1039	S979	I919	S859	F799	D739	I679	K619	V559	A499	N439	V379	G319	E259
F1220	S1160	R1100	Q1040	D980	L920	L860	V800	L740	T860	K620	I560	E800	D440	V380	K320	D260
K1221	T1161	L1101	A1041	L981	G921	G861	E801	N741	E681	T621	P561	L501	P441	T381	P321	D261
N1222	V1162	E1102	F1042	T982	D922	N862	N802	N742	T682	V622	T562	S502	V442	P382	V322	L262
D1223	I1163	E1103	D1043	I983	L923	K863	S803	K743	I683	G623	P563	Q503	L443	K383	K323	T263
L1224	P1164	I1104	W1044	K984	K924	I864	Y804	K744	A684	S624	A564	L504	F444	N384	S324	F264
F1225	E1165	L1105	V1045	D985	L925	K865	L805	Q745	E685	S625	I565	C505	N445	I385	I325	K265
V1226	D1166	N1106	L1046	I986	Q926	F866	R806	M746	A686	N626	I566	A506	R446	D386	K326	L266
I1227	E1167	V1107	S1047	V987	V927	R867	G807	V747	K687	G627	K567	V507	Q447	K387	A327	A267
N1228	L1168	A1108	N1048	L988	L928	Y868	L808	M748	K688	G628	P568	P508	P448	K388	K328	D268
S1229	I1169	E1109	I1049	G989	D929	G869	T809	A749	K689	L629	K569	L509	S449	T389	L329	T269
E1230	N1170	N1110	E1050	V990	D930	E370	P810	G750	V690	I630	P570	Q510	L450	Q390	K330	L270
D1231	O1171	K1111	A1051	K991	E931	D871	Q811	S751	L691	H631	L571	T511	H451	L391	G331	K271
N1232	L1172	K1112	F1052	D992	E932	G872	E812	K752	D692	V632	M572	V612	K452	V392	K332	A272
D1233	H1173	T1113	F1053	L993	E933	M873	F813	G753	V693	V633	M573	S513	K453	K393	K273	N273
E1234	F1174	P1114	L1054	Q994	K934	D874	F814	S754	T694	T634	G574	P514	N454	K394	G334	L274
K1235	S1175	S1115	R1055	Q995	Q935	A875	F815	V755	K695	R635	K575	Q515	N455	G395	G335	S275
L1236	L1176	L1116	S1056	N996	L936	A876	H816	I756	E696	E636	Q576	S516	N456	P396	I336	L276
I1237	LEU	T1117	V1057	I997	V937	H877	A817	N757	E697	K637	I577	N517	A457	N397	K337	E277
I1238	ASP	V1118	V1058	L998	K938	I878	H818	I758	Q698	G638	L578	K518	H458	E398	G338	L278
R1239	GLU	Y1119	H1059	V999	D939	E379	G819	A759	A699	P639	S579	P519	R459	H399	N339	L279
C1240	GLU	L1120	P1060	L1000	R940	K850	G820	Q760	N700	Q840	V580	C520	V460	P400	L340	E280
R1241	ALA	E1121	G1061	R1001	K941	Q851	R821	M761	L701	V641	A581	M521	K461	G401	K341	N281
V1242	GLU	P1122	E1062	S892	F942	S892	E822	S762	L702	C642	I582	G522	V462	A402	K342	H282
V1243	GLN	G1123	M1063	L893	L943	L893	G823	A763	T703	A643	P583	I523	K463	K403	K343	G283
ARG	SER	H1124	V1064	N1004	R944	D894	L824	C764	A704	K644	N584	I524	P464	Y404	K344	A284
PRO	PHE	A1125	G1065	E1005	E945	T895	I825	V765	K705	L645	G585	Q525	Y465	V405	V345	P285
LYS	ASP	A1126	V1066	I1006	V946	I896	D826	G766	H706	L646	I586	D526	S466	L406	D346	H286
SER	ASP	D1127	L1067	I1007	F947	G897	T827	Q767	G707	G647	I587	T527	T467	R407	F347	H287
LEU	Q1188	Q1128	A1068	N1008	V948	G898	A828	R768	M708	N648	L588	L528	F468	D408	S348	A288
ASP	S1189	E1129	A1069	N1009	D949	S899	V829	S769	T709	I649	Q589	C529	R469	S409	A349	I289
ALA	Q1190	Q1130	Q1070	G950	G950	D890	K830	V770	L710	Q650	B590	G530	L470	G410	R350	E290
GLU	W1191	A1131	Q1071	Q1011	E951	A891	T831	E771	R711	K651	F591	I531	N471	D411	T351	E291
THR	L1192	K1132	I1072	L1012	A952	A892	A832	G772	E712	V652	D592	R412	L472	R412	V352	A292
GLU	L1193	L1133	G1073	D1013	N953	F893	E833	K773	S713	V653	E593	K533	S473	L413	L353	E293
A1254	R1194	E1134	E1074	A1014	W954	E934	T834	R774	F714	N654	G594	L534	V474	D414	S354	S294
E1255	L1195	R1135	P1075	V1015	P955	K895	G835	I775	E715	F655	T595	T535	T475	L415	G355	L295
E1256	E1196	A1136	A1076	L1016	L956	R896	Y836	A776	D716	M656	T596	L536	S476	R416	P356	L296
D1257	L1197	A1137	T1077	L1017	P957	Y897	I837	F777	N717	L657	L597	R537	P477	Y417	P357	Q297
H1258	D1198	T1138	Q1078	F1018	V958	R898	Q838	G778	V718	L658	L598	D538	Y478	S418	N358	F298
R1259	R1199	E1139	M1079	C1019	N959	R899	H659	F779	V719	H659	S599	T539	N479	R419	L359	F299
L1260	A1200	H1140	T1080	C1020	I960	D900	R840	V780	R720	N660	P600	F540	A480	R420	E360	V300







- Molecule 10: DNA-directed RNA polymerase II 14.2 kDa polypeptide



PHE
SER

- Molecule 11: DNA-directed RNA polymerases I, II, and III 8.3 kDa polypeptide



L61
R62
Y63
Y64
P65
LEU
GLU
LYS
ARG
ASP

- Molecule 12: DNA-directed RNA polymerase II 13.6 kDa polypeptide



- Molecule 13: DNA-directed RNA polymerases I, II, and III 7.7 kDa polypeptide



T61
K62
R63
L64
V65
Q66
F67
E68
A69
R70

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	168.85Å 222.96Å 193.60Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	40.00 – 3.50 40.00 – 3.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.50) 93.6 (40.00-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 3.48Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.230 , 0.317 0.226 , 0.309	Depositor DCC
R_{free} test set	8862 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	80.5	Xtriage
Anisotropy	0.219	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 114.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29248	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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: MG, ZN, ATP

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	R	2.68	14/244 (5.7%)	2.95	27/380 (7.1%)
2	T	1.69	14/633 (2.2%)	2.50	49/971 (5.0%)
3	N	0.91	2/316 (0.6%)	1.06	4/484 (0.8%)
4	A	4.65	2243/11163 (20.1%)	4.25	3160/15091 (20.9%)
5	B	4.64	1772/8963 (19.8%)	4.25	2551/12086 (21.1%)
6	C	4.38	421/2133 (19.7%)	4.19	575/2891 (19.9%)
7	E	4.87	395/1788 (22.1%)	4.18	508/2406 (21.1%)
8	F	4.60	141/691 (20.4%)	4.30	186/933 (19.9%)
9	H	5.16	264/1086 (24.3%)	4.35	321/1470 (21.8%)
10	I	4.74	212/989 (21.4%)	4.60	310/1331 (23.3%)
11	J	4.17	96/541 (17.7%)	3.92	117/727 (16.1%)
12	K	4.37	196/937 (20.9%)	3.99	247/1265 (19.5%)
13	L	5.37	92/365 (25.2%)	4.48	107/485 (22.1%)
All	All	4.57	5862/29849 (19.6%)	4.18	8162/40520 (20.1%)

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	R	0	1
2	T	1	2
4	A	2	121
5	B	4	114
6	C	1	11
7	E	0	17
8	F	0	5
9	H	0	16
10	I	1	18
11	J	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	K	0	9
13	L	0	5
All	All	9	321

The worst 5 of 5862 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	437	MET	SD-CE	68.53	3.50	1.79
7	E	117	THR	CA-CB	56.95	2.43	1.53
4	A	1285	MET	SD-CE	47.79	2.99	1.79
4	A	820	GLY	C-O	-44.84	0.63	1.23
4	A	1398	MET	SD-CE	44.29	2.90	1.79

The worst 5 of 8162 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	821	ARG	N-CA-C	-50.67	56.86	114.62
5	B	62	ILE	N-CA-C	-27.51	86.57	113.53
7	E	184	VAL	N-CA-C	-26.19	89.04	111.56
4	A	257	ARG	N-CA-C	25.96	148.54	112.45
4	A	325	ILE	CA-C-O	-25.56	88.83	120.78

5 of 9 chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	T	21	DC	C3'
4	A	317	LYS	CA
4	A	324	SER	CA
5	B	636	PRO	CA
5	B	637	LEU	CA

5 of 321 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	A	3	GLY	Mainchain
4	A	6	TYR	Peptide
1	R	10	A	Sidechain
2	T	21	DC	Sidechain
2	T	23	DC	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	R	217	0	110	34	0
2	T	566	0	314	83	4
3	N	284	0	162	44	0
4	A	10969	0	11061	3557	0
5	B	8792	0	8821	2445	0
6	C	2095	0	2051	500	0
7	E	1752	0	1776	548	0
8	F	679	0	701	204	0
9	H	1068	0	1040	390	0
10	I	971	0	929	314	0
11	J	532	0	543	168	0
12	K	919	0	929	268	0
13	L	363	0	387	100	0
14	A	2	0	0	0	0
14	B	1	0	0	0	0
14	C	1	0	0	0	0
14	I	2	0	0	0	0
14	J	1	0	0	0	0
14	L	1	0	0	0	0
15	A	2	0	0	0	0
16	B	31	0	12	7	0
All	All	29248	0	28836	8229	4

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 142.

The worst 5 of 8229 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:N:12:DT:P	7:E:117:THR:HG21	1.32	1.67
4:A:128:ILE:CB	4:A:128:ILE:CA	1.74	1.66
5:B:422:LYS:CB	5:B:422:LYS:CG	1.74	1.65
5:B:866:TYR:CG	5:B:866:TYR:CB	1.80	1.65
4:A:37:PHE:CB	4:A:37:PHE:CG	1.74	1.65

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:T:1:DC:C4'	2:T:1:DC:C4'[2_656]	1.63	0.57
2:T:1:DC:C5'	2:T:1:DC:O4'[2_656]	1.69	0.51
2:T:1:DC:O4'	2:T:1:DC:O4'[2_656]	1.78	0.42
2:T:1:DC:C4'	2:T:1:DC:O4'[2_656]	1.80	0.40

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	
4	A	1383/1733 (80%)	816 (59%)	306 (22%)	261 (19%)	0	1
5	B	1088/1224 (89%)	708 (65%)	199 (18%)	181 (17%)	0	2
6	C	264/318 (83%)	170 (64%)	58 (22%)	36 (14%)	0	3
7	E	212/215 (99%)	119 (56%)	47 (22%)	46 (22%)	0	1
8	F	82/155 (53%)	45 (55%)	22 (27%)	15 (18%)	0	1
9	H	129/146 (88%)	75 (58%)	28 (22%)	26 (20%)	0	1
10	I	117/122 (96%)	60 (51%)	32 (27%)	25 (21%)	0	1
11	J	63/70 (90%)	41 (65%)	10 (16%)	12 (19%)	0	1
12	K	112/120 (93%)	78 (70%)	18 (16%)	16 (14%)	0	3
13	L	44/70 (63%)	21 (48%)	11 (25%)	12 (27%)	0	0
All	All	3494/4173 (84%)	2133 (61%)	731 (21%)	630 (18%)	0	1

5 of 630 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	A	34	LYS
4	A	44	THR
4	A	48	ALA
4	A	51	GLY

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Mol	Chain	Res	Type
4	A	55	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	
4	A	1218/1520 (80%)	713 (58%)	505 (42%)	0	0
5	B	960/1061 (90%)	585 (61%)	375 (39%)	0	1
6	C	234/274 (85%)	142 (61%)	92 (39%)	0	1
7	E	196/197 (100%)	112 (57%)	84 (43%)	0	0
8	F	74/137 (54%)	42 (57%)	32 (43%)	0	0
9	H	117/128 (91%)	71 (61%)	46 (39%)	0	1
10	I	113/116 (97%)	68 (60%)	45 (40%)	0	1
11	J	60/65 (92%)	36 (60%)	24 (40%)	0	1
12	K	99/102 (97%)	58 (59%)	41 (41%)	0	0
13	L	40/57 (70%)	25 (62%)	15 (38%)	0	1
All	All	3111/3657 (85%)	1852 (60%)	1259 (40%)	0	1

5 of 1259 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	C	125	MET
10	I	24	ARG
6	C	211	ASP
6	C	124	LEU
7	E	182	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 114 such sidechains are listed below:

Mol	Chain	Res	Type
5	B	121	ASN
10	I	120	GLN

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Mol	Chain	Res	Type
5	B	786	ASN
10	I	116	ASN
9	H	83	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	R	10/10 (100%)	4 (40%)	3 (30%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	R	2	U
1	R	5	A
1	R	6	G
1	R	10	A

All (3) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	R	1	A
1	R	4	G
1	R	5	A

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 oligosaccharides 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	$\# Z > 2$
16	ATP	B	1308	-	32,33,33	2.04	9 (28%)	48,52,52	2.77	14 (29%)

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
16	ATP	B	1308	-	-	6/22/38/38	0/3/3/3

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	B	1308	ATP	O5'-C5'	-5.98	1.22	1.44
16	B	1308	ATP	PA-O5'	-4.92	1.40	1.59
16	B	1308	ATP	C1'-N9	3.08	1.54	1.46
16	B	1308	ATP	C5'-C4'	-2.89	1.42	1.51
16	B	1308	ATP	C2-N1	2.81	1.38	1.33

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	B	1308	ATP	O5'-C5'-C4'	10.87	146.02	108.99
16	B	1308	ATP	PA-O5'-C5'	5.78	154.49	121.35
16	B	1308	ATP	N3-C2-N1	-5.62	120.07	128.58
16	B	1308	ATP	C5'-C4'-C3'	-5.52	95.35	115.21
16	B	1308	ATP	C5-C4-N3	-4.70	120.25	126.72

There are no chirality outliers.

5 of 6 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
16	B	1308	ATP	C5'-O5'-PA-O1A
16	B	1308	ATP	C4'-C5'-O5'-PA
16	B	1308	ATP	PB-O3A-PA-O5'
16	B	1308	ATP	C5'-O5'-PA-O3A

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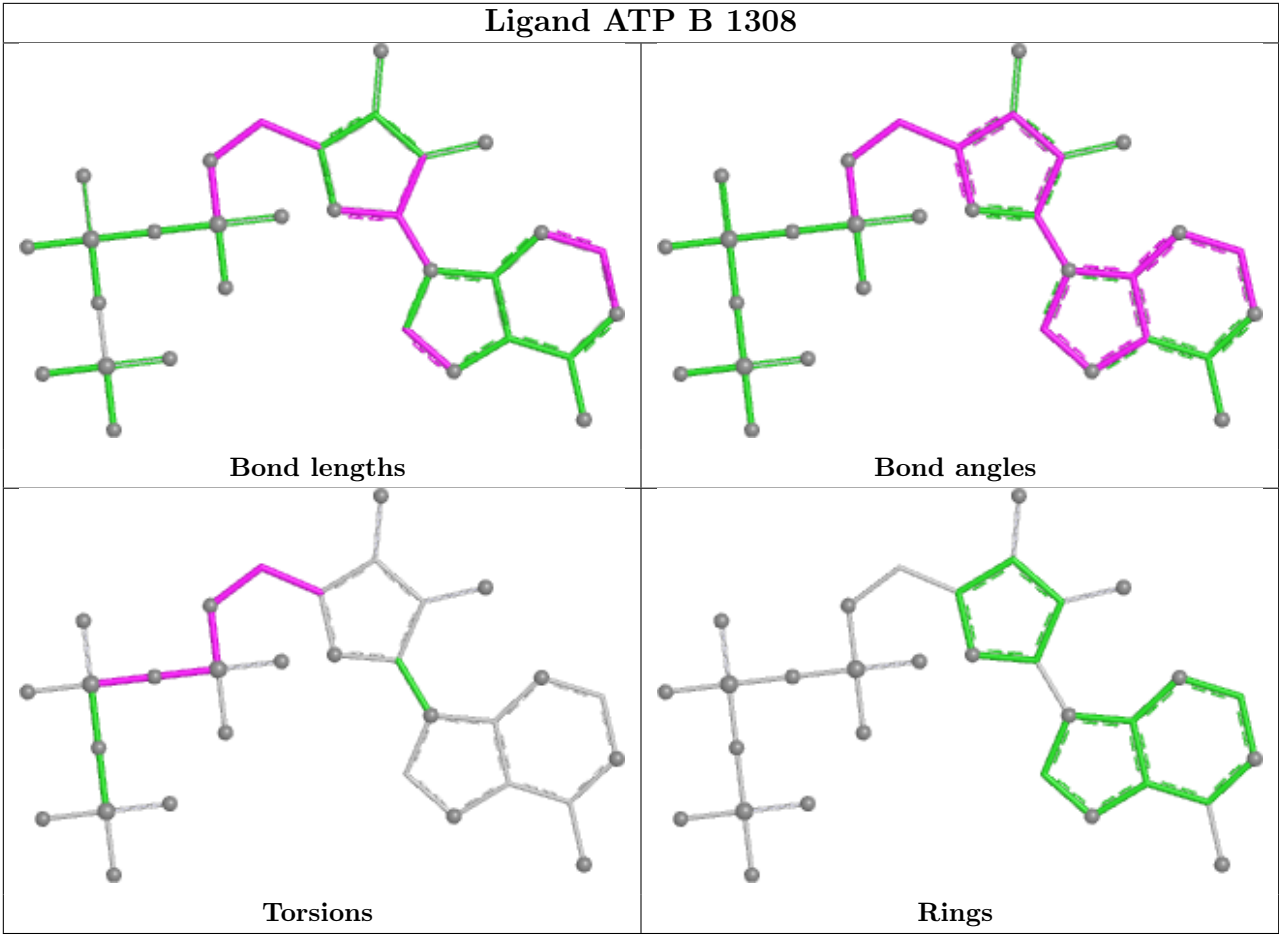
Mol	Chain	Res	Type	Atoms
16	B	1308	ATP	C3'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
16	B	1308	ATP	7	0

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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	T	2
4	A	2
3	N	1
1	R	1

The worst 5 of 6 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	T	15:DA	O3'	16:DC	P	2.98
1	N	2:DT	O3'	3:DG	P	2.67

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	320:ARG	C	321:PRO	N	1.75
1	A	820:GLY	C	821:ARG	N	1.68
1	T	21:DC	O3'	22:DT	P	1.39

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	R	10/10 (100%)	2.58	9 (90%) 0 0	70, 83, 159, 164	0
2	T	28/28 (100%)	2.53	19 (67%) 0 0	84, 188, 200, 200	0
3	N	14/14 (100%)	2.17	7 (50%) 0 1	185, 198, 200, 200	0
4	A	1395/1733 (80%)	-0.07	16 (1%) 78 54	1, 51, 137, 186	0
5	B	1106/1224 (90%)	-0.10	16 (1%) 73 48	1, 43, 119, 194	0
6	C	266/318 (83%)	-0.28	0 100 100	6, 44, 95, 151	0
7	E	214/215 (99%)	0.11	3 (1%) 73 48	13, 79, 141, 165	0
8	F	84/155 (54%)	-0.26	0 100 100	17, 58, 105, 114	0
9	H	133/146 (91%)	0.30	4 (3%) 52 30	19, 74, 132, 154	0
10	I	119/122 (97%)	0.03	1 (0%) 82 60	4, 56, 105, 146	0
11	J	65/70 (92%)	-0.30	0 100 100	11, 40, 92, 116	0
12	K	114/120 (95%)	-0.39	0 100 100	8, 43, 88, 131	0
13	L	46/70 (65%)	0.36	4 (8%) 16 10	17, 84, 143, 163	0
All	All	3594/4225 (85%)	-0.04	79 (2%) 62 37	1, 50, 133, 200	0

The worst 5 of 79 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	B	468	GLU	5.3
4	A	307	ASP	5.2
5	B	643	ASP	4.8
2	T	20	DC	4.4
5	B	709	ASP	4.4

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 ⓘ

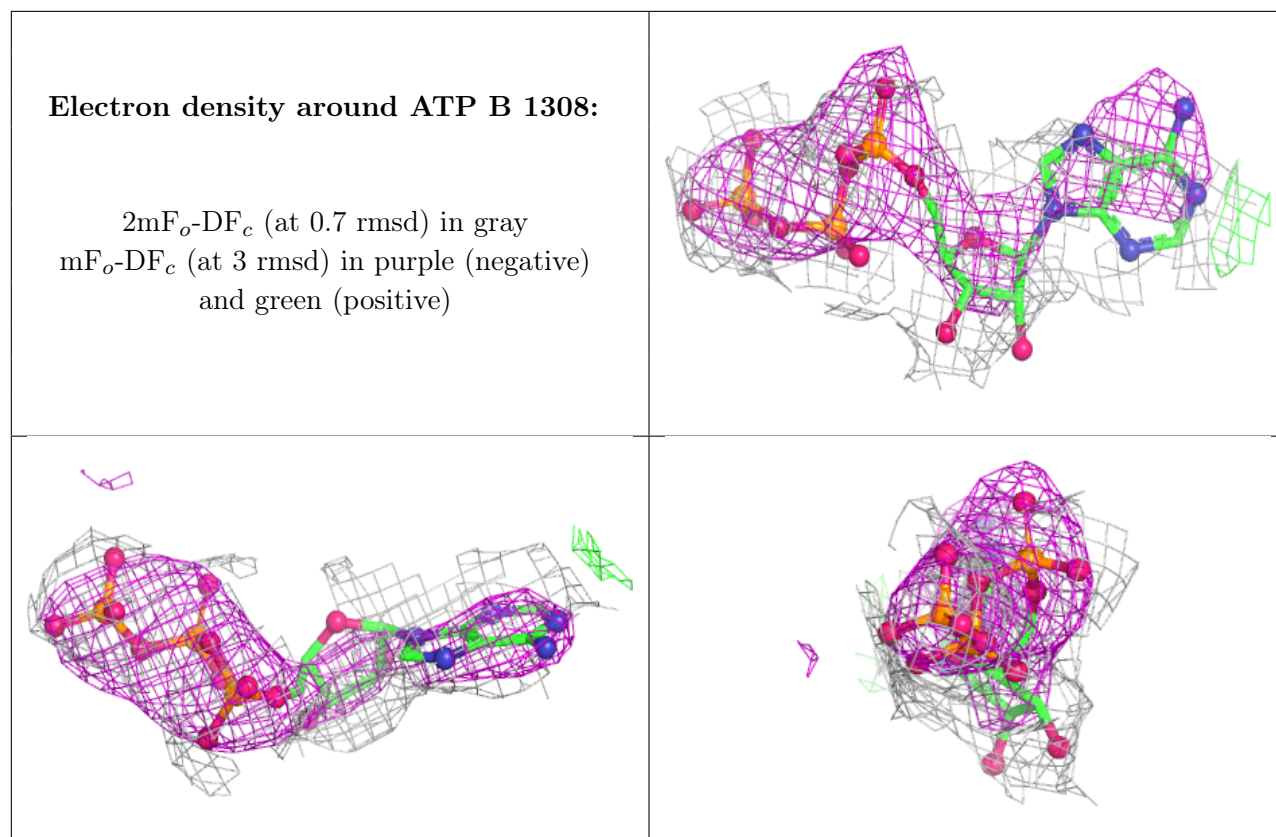
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
16	ATP	B	1308	31/31	0.53	0.17	64,71,77,78	0
15	MG	A	2002	1/1	0.54	0.74	63,63,63,63	0
15	MG	A	2001	1/1	0.55	0.46	55,55,55,55	0
14	ZN	A	1734	1/1	0.95	0.05	115,115,115,115	0
14	ZN	I	204	1/1	0.99	0.03	31,31,31,31	0
14	ZN	J	101	1/1	0.99	0.04	39,39,39,39	0
14	ZN	L	105	1/1	0.99	0.03	76,76,76,76	0
14	ZN	A	1735	1/1	0.99	0.04	75,75,75,75	0
14	ZN	B	1307	1/1	0.99	0.02	80,80,80,80	0
14	ZN	I	203	1/1	0.99	0.04	98,98,98,98	0
14	ZN	C	319	1/1	1.00	0.05	31,31,31,31	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.