



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 21, 2020 – 05:09 am BST

PDB ID : 1SK6  
Title : Crystal structure of the adenylyl cyclase domain of anthrax edema factor (EF) in complex with calmodulin, 3',5' cyclic AMP (cAMP), and pyrophosphate  
Authors : Guo, Q.; Shen, Y.; Zhukovskaya, N.L.; Tang, W.J.  
Deposited on : 2004-03-04  
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](mailto: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.

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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 : 2.11  
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) : 2.11

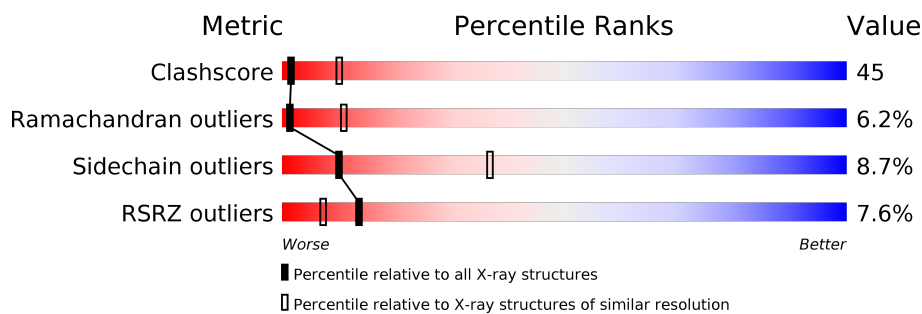
# 1 Overall quality at a glance

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))
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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	510	<div> <div>2%</div> <div>36% 50% 8% • 6%</div> </div>
1	B	510	<div> <div>5%</div> <div>23% 52% 12% • 11%</div> </div>
1	C	510	<div> <div>4%</div> <div>38% 47% 8% • 5%</div> </div>
2	D	148	<div> <div>16%</div> <div>41% 48% 7% • •</div> </div>
2	E	148	<div> <div>28%</div> <div>45% 41% 11% •</div> </div>
2	F	148	<div> <div>16%</div> <div>39% 49% 9% •</div> </div>

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
4	CMP	A	289	X	-	-	-
4	CMP	B	290	X	-	-	-
4	CMP	C	910	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 15050 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 Calmodulin-sensitive adenylyate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3924	2511	668	742	3			
1	B	454	Total	C	N	O	S	0	0	0
			3706	2370	628	705	3			
1	C	483	Total	C	N	O	S	0	0	0
			3937	2519	670	745	3			

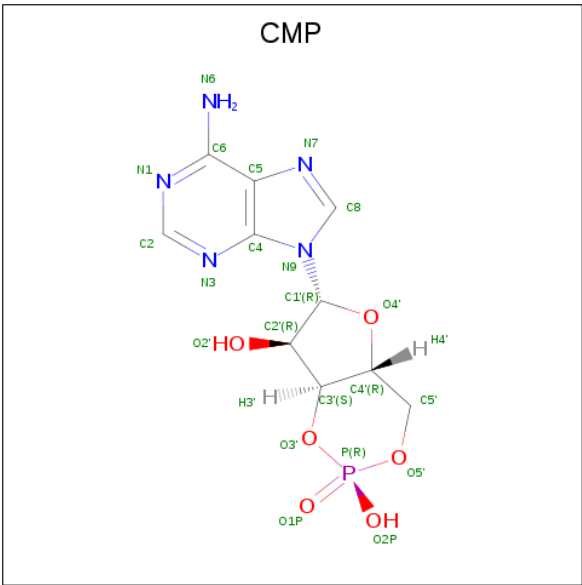
- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	E	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			
2	F	143	Total	C	N	O	S	0	0	0
			1125	690	181	245	9			

- Molecule 3 is YTTERBIUM (III) ION (three-letter code: YB) (formula: Yb).

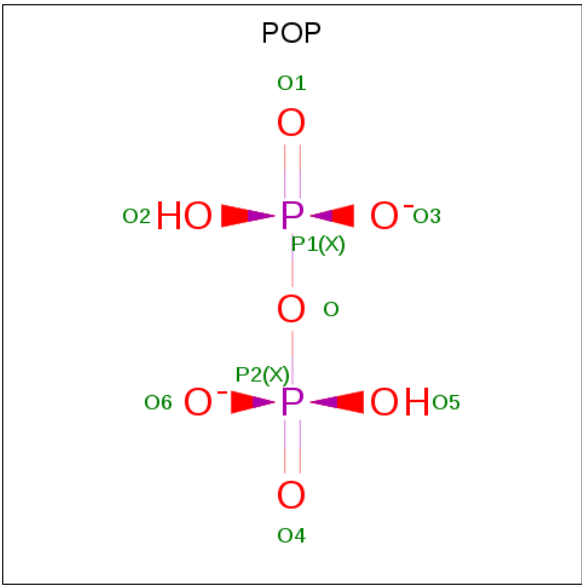
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Yb	0	0
			3	3		
3	A	3	Total	Yb	0	0
			3	3		
3	C	3	Total	Yb	0	0
			3	3		

- Molecule 4 is ADENOSINE-3',5'-CYCLIC-MONOPHOSPHATE (three-letter code: CMP) (formula: C<sub>10</sub>H<sub>12</sub>N<sub>5</sub>O<sub>6</sub>P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	B	1	Total	C	N	O	P	0	0
			22	10	5	6	1		
4	C	1	Total	C	N	O	P	0	0
			22	10	5	6	1		

- Molecule 5 is PYROPHOSPHATE 2- (three-letter code: POP) (formula:  $\text{H}_2\text{O}_7\text{P}_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			9	7	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	O	P	0	0
			9	7	2		
5	C	1	Total	O	P	0	0
			9	7	2		

- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	D	2	Total	Ca	0	0
			2	2		
6	F	2	Total	Ca	0	0
			2	2		
6	E	2	Total	Ca	0	0
			2	2		

These plots are drawn for all protein, RNA and DNA 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 ( $\text{RSRZ} > 2$ ). 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.

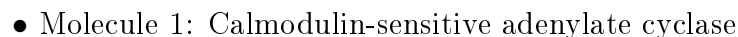
Chain A:

29% 36% 50% 8% 6%

ASN VAL GLY VAL TVR LYS ASP SER GLY ASP LYS ASP PHE TVR LYS LYS GLU SER VAL K695 K696 K697 K698 K699 K700 K634 K635 K636 K704 K705 K706 K707 K708 K709 K710 K711 K712 K713 K714 K715 K716 K717 K718 K719 K720 K721 K722 K723 K724 K725 K726 K727 K728 K729 K730 K731 K732 K733 K734 K735 K736 K737 K738 K739 K740 K741 K742 K743 K744 K745 K746 K747 K748 K749 K750 K751 K752 K753 K754 K755 K756 K757 K758 K759 K760 K761 K762 K763 K764 K765 K766 K767 K768 K769 K770 K771 K772 K773 K774 K775 K776 K777 K778 K779 K780 K781 K782 K783 K784 K785 K786 K787 K788 K789 K790 K791 K792 K793 K794 K795 K796 K797 K798 K799 K800 K801 K802 K803 K804 K805 K806 K807 K808 K809 K810 K811 K812 K813 K814 K815 K816 K817 K818 K819 K820 K821 K822 K823 K824 K825 K826 K827 K828 K829 K830 K831 K832 K833 K834 K835 K836 K837 K838 K839 K840 K841 K842 K843 K844 K845 K846 K847 K848 K849 K850 K851 K852 K853 K854 K855 K856 K857 K858 K859 K860 K861 K862 K863 K864 K865 K866 K867 K868 K869 K870 K871 K872 K873 K874 K875 K876 K877 K878 K879 K880 K881 K882 K883 K884 K885 K886 K887 K888 K889 K890 K891 K892 K893 K894 K895 K896 K897 K898 K899 K900 K901 K902 K903 K904 K905 K906 K907 K908 K909 K910 K911 K912 K913 K914 K915 K916 K917 K918 K919 K920 K921 K922 K923 K924 K925 K926 K927 K928 K929 K930 K931 K932 K933 K934 K935 K936 K937 K938 K939 K940 K941 K942 K943 K944 K945 K946 K947 K948 K949 K950 K951 K952 K953 K954 K955 K956 K957 K958 K959 K960 K961 K962 K963 K964 K965 K966 K967 K968 K969 K970 K971 K972 K973 K974 K975 K976 K977 K978 K979 K980 K981 K982 K983 K984 K985 K986 K987 K988 K989 K990 K991 K992 K993 K994 K995 K996 K997 K998 K999 K1000 K1001 K1002 K1003 K1004 K1005 K1006 K1007 K1008 K1009 K1010 K1011 K1012 K1013 K1014 K1015 K1016 K1017 K1018 K1019 K1020 K1021 K1022 K1023 K1024 K1025 K1026 K1027 K1028 K1029 K1030 K1031 K1032 K1033 K1034 K1035 K1036 K1037 K1038 K1039 K1040 K1041 K1042 K1043 K1044 K1045 K1046 K1047 K1048 K1049 K1050 K1051 K1052 K1053 K1054 K1055 K1056 K1057 K1058 K1059 K1060 K1061 K1062 K1063 K1064 K1065 K1066 K1067 K1068 K1069 K1070 K1071 K1072 K1073 K1074 K1075 K1076 K1077 K1078 K1079 K1080 K1081 K1082 K1083 K1084 K1085 K1086 K1087 K1088 K1089 K1090 K1091 K1092 K1093 K1094 K1095 K1096 K1097 K1098 K1099 K1100 K1101 K1102 K1103 K1104 K1105 K1106 K1107 K1108 K1109 K1110 K1111 K1112 K1113 K1114 K1115 K1116 K1117 K1118 K1119 K1120 K1121 K1122 K1123 K1124 K1125 K1126 K1127 K1128 K1129 K1130 K1131 K1132 K1133 K1134 K1135 K1136 K1137 K1138 K1139 K1140 K1141 K1142 K1143 K1144 K1145 K1146 K1147 K1148 K1149 K1150 K1151 K1152 K1153 K1154 K1155 K1156 K1157 K1158 K1159 K1160 K1161 K1162 K1163 K1164 K1165 K1166 K1167 K1168 K1169 K1170 K1171 K1172 K1173 K1174 K1175 K1176 K1177 K1178 K1179 K1180 K1181 K1182 K1183 K1184 K1185 K1186 K1187 K1188 K1189 K1190 K1191 K1192 K1193 K1194 K1195 K1196 K1197 K1198 K1199 K1200 K1201 K1202 K1203 K1204 K1205 K1206 K1207 K1208 K1209 K1210 K1211 K1212 K1213 K1214 K1215 K1216 K1217 K1218 K1219 K1220 K1221 K1222 K1223 K1224 K1225 K1226 K1227 K1228 K1229 K1230 K1231 K1232 K1233 K1234 K1235 K1236 K1237 K1238 K1239 K1240 K1241 K1242 K1243 K1244 K1245 K1246 K1247 K1248 K1249 K1250 K1251 K1252 K1253 K1254 K1255 K1256 K1257 K1258 K1259 K1260 K1261 K1262 K1263 K1264 K1265 K1266 K1267 K1268 K1269 K1270 K1271 K1272 K1273 K1274 K1275 K1276 K1277 K1278 K1279 K1280 K1281 K1282 K1283 K1284 K1285 K1286 K1287 K1288 K1289 K1290 K1291 K1292 K1293 K1294 K1295 K1296 K1297 K1298 K1299 K1300 K1301 K1302 K1303 K1304 K1305 K1306 K1307 K1308 K1309 K1310 K1311 K1312 K1313 K1314 K1315 K1316 K1317 K1318 K1319 K1320 K1321 K1322 K1323 K1324 K1325 K1326 K1327 K1328 K1329 K1330 K1331 K1332 K1333 K1334 K1335 K1336 K1337 K1338 K1339 K1340 K1341 K1342 K1343 K1344 K1345 K1346 K1347 K1348 K1349 K1350 K1351 K1352 K1353 K1354 K1355 K1356 K1357 K1358 K1359 K1360 K1361 K1362 K1363 K1364 K1365 K1366 K1367 K1368 K1369 K1370 K1371 K1372 K1373 K1374 K1375 K1376 K1377 K1378 K1379 K1380 K1381 K1382 K1383 K1384 K1385 K1386 K1387 K1388 K1389 K1390 K1391 K1392 K1393 K1394 K1395 K1396 K1397 K1398 K1399 K1400 K1401 K1402 K1403 K1404 K1405 K1406 K1407 K1408 K1409 K1410 K1411 K1412 K1413 K1414 K1415 K1416 K1417 K1418 K1419 K1420 K1421 K1422 K1423 K1424 K1425 K1426 K1427 K1428 K1429 K1430 K1431 K1432 K1433 K1434 K1435 K1436 K1437 K1438 K1439 K1440 K1441 K1442 K1443 K1444 K1445 K1446 K1447 K1448 K1449 K1450 K1451 K1452 K1453 K1454 K1455 K1456 K1457 K1458 K1459 K1460 K1461 K1462 K1463 K1464 K1465 K1466 K1467 K1468 K1469 K1470 K1471 K1472 K1473 K1474 K1475 K1476 K1477 K1478 K1479 K1480 K1481 K1482 K1483 K1484 K1485 K1486 K1487 K1488 K1489 K1490 K1491 K1492 K1493 K1494 K1495 K1496 K1497 K1498 K1499 K1500 K1501 K1502 K1503 K1504 K1505 K1506 K1507 K1508 K1509 K1510 K1511 K1512 K1513 K1514 K1515 K1516 K1517 K1518 K1519 K1520 K1521 K152

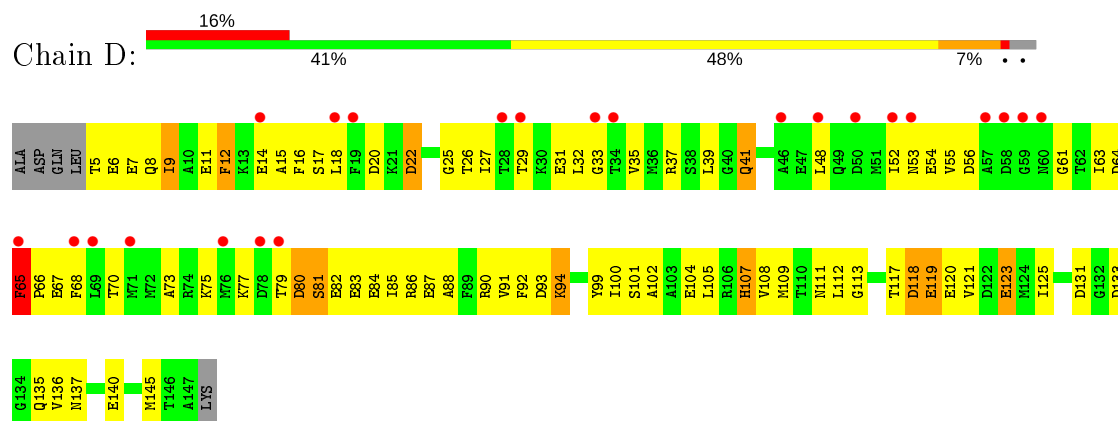
**Chain B:**

Category	Percentage
ASP	5%
ARG	23%
ILE	52%
D294	12%
V295	•
L286	11%
A301	
L302	
G306	
L307	
F309	
E310	
H311	
A312	
D313	
A314	
F315	
K316	
K317	
I318	
A319	
E321	
L322	
N323	
T324	
Y325	
I326	
L327	
F328	
R329	
P330	
V331	
M332	
K333	
L334	
A335	
T336	
N337	
L338	
I339	
K340	
S341	
G342	
V343	
A344	
T345	
K346	
G347	
L348	
I349	
V350	
H351	
G352	
P359	
P360	

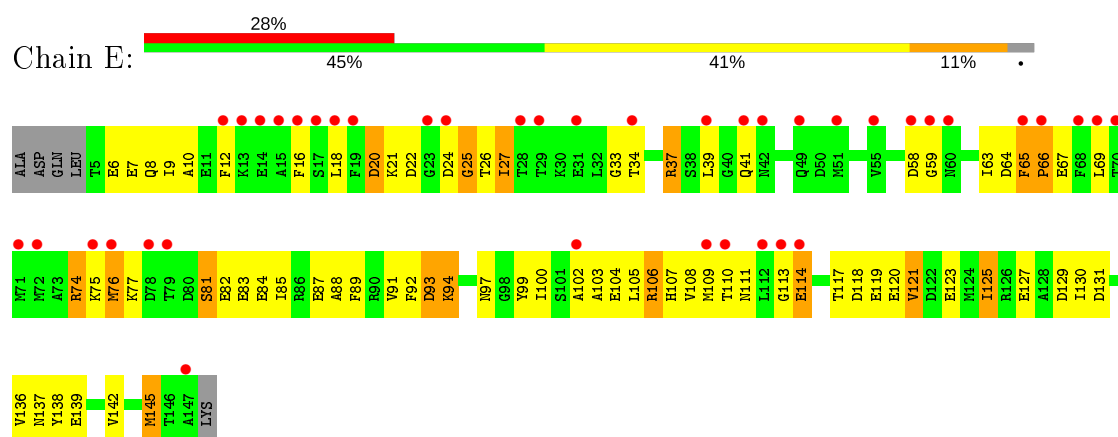




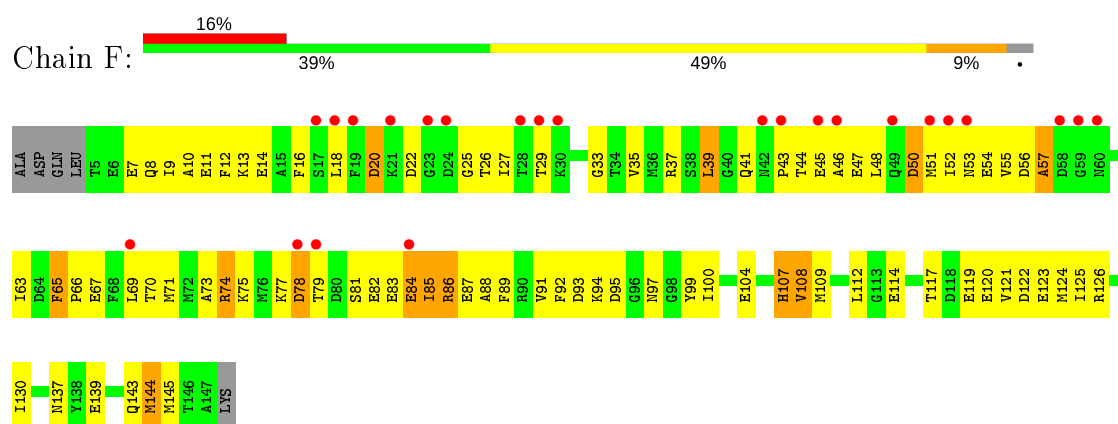
## ● Molecule 2: Calmodulin



## ● Molecule 2: Calmodulin



## ● Molecule 2: Calmodulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	116.87Å 166.45Å 342.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 43.11 – 3.29	Depositor EDS
% Data completeness (in resolution range)	96.2 (50.00-3.20) 95.7 (43.11-3.29)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.13	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.75 (at 3.32Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.250 , 0.307 0.260 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	71.0	Xtriage
Anisotropy	0.216	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	15050	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.31% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, YB, POP, CMP

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	0.57	5/3999 (0.1%)	0.91	25/5382 (0.5%)
1	B	0.64	5/3778 (0.1%)	0.97	22/5088 (0.4%)
1	C	0.84	8/4012 (0.2%)	1.30	36/5400 (0.7%)
2	D	0.39	0/1137	0.56	0/1527
2	E	0.36	0/1137	0.54	0/1527
2	F	0.45	1/1137 (0.1%)	0.62	0/1527
All	All	0.64	19/15200 (0.1%)	0.99	83/20451 (0.4%)

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	2
1	B	0	1
1	C	1	5
All	All	1	8

The worst 5 of 19 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	PRO	N-CD	20.86	1.77	1.47
1	C	773	PHE	C-N	20.19	1.80	1.34
1	C	632	TYR	N-CA	19.71	1.85	1.46
1	C	741	ILE	N-CA	15.98	1.78	1.46
1	C	521	ASN	N-CA	14.19	1.74	1.46

The worst 5 of 83 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	773	PHE	O-C-N	-46.13	48.88	122.70
1	C	773	PHE	CB-CA-C	22.71	155.82	110.40
1	C	773	PHE	N-CA-C	-22.63	49.90	111.00
1	C	520	PRO	CA-N-CD	-18.66	85.37	111.50
1	B	730	ASN	N-CA-CB	-17.00	80.00	110.60

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	773	PHE	CA

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	LYS	Peptide
1	A	773	PHE	Peptide
1	B	729	TYR	Peptide
1	C	427	ASP	Peptide
1	C	510	GLN	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	3924	0	3967	345	0
1	B	3706	0	3728	472	0
1	C	3937	0	3980	329	0
2	D	1125	0	1049	82	0
2	E	1125	0	1049	92	0
2	F	1125	0	1048	103	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
4	A	22	0	10	6	0
4	B	22	0	10	5	0
4	C	22	0	10	3	0
5	A	9	0	0	3	0
5	B	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	9	0	0	1	0
6	D	2	0	0	0	0
6	E	2	0	0	0	0
6	F	2	0	0	1	0
All	All	15050	0	14851	1357	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 45.

The worst 5 of 1357 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)
4:B:290:CMP:H2	4:B:290:CMP:C2	0.97	1.49
4:A:289:CMP:H2	4:A:289:CMP:C2	0.97	1.48
4:C:910:CMP:C2	4:C:910:CMP:H2	0.97	1.47
1:B:730:ASN:CA	1:B:730:ASN:N	1.73	1.46
1:C:741:ILE:CA	1:C:741:ILE:N	1.78	1.46

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	475/510 (93%)	371 (78%)	83 (18%)	21 (4%)	2	19
1	B	448/510 (88%)	308 (69%)	116 (26%)	24 (5%)	2	14
1	C	477/510 (94%)	358 (75%)	98 (20%)	21 (4%)	2	19
2	D	141/148 (95%)	85 (60%)	43 (30%)	13 (9%)	1	3
2	E	141/148 (95%)	87 (62%)	37 (26%)	17 (12%)	0	2
2	F	141/148 (95%)	88 (62%)	36 (26%)	17 (12%)	0	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1823/1974 (92%)	1297 (71%)	413 (23%)	113 (6%)	<b>1</b> <b>11</b>

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	368	GLN
1	A	521	ASN
1	A	539	GLU
1	A	669	SER
2	D	81	SER

### 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	429/455 (94%)	395 (92%)	34 (8%)	<b>12</b> 43
1	B	405/455 (89%)	350 (86%)	55 (14%)	<b>3</b> 17
1	C	431/455 (95%)	397 (92%)	34 (8%)	<b>12</b> 43
2	D	121/126 (96%)	112 (93%)	9 (7%)	<b>13</b> 46
2	E	121/126 (96%)	114 (94%)	7 (6%)	<b>20</b> 55
2	F	121/126 (96%)	119 (98%)	2 (2%)	60 <b>83</b>
All	All	1628/1743 (93%)	1487 (91%)	141 (9%)	<b>10</b> 37

5 of 141 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	440	GLN
1	B	552	TRP
1	C	632	TYR
1	B	450	ASN
1	B	533	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 69 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	470	ASN
1	B	709	ASN
1	C	759	GLN
1	B	518	ASN
1	B	555	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

### 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 5.6 Ligand geometry ⓘ

Of 21 ligands modelled in this entry, 15 are monoatomic - leaving 6 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	$\# Z  > 2$
4	CMP	C	910	3	22,25,25	1.91	4 (18%)	24,39,39	3.58	15 (62%)
4	CMP	B	290	3	22,25,25	1.82	6 (27%)	24,39,39	3.62	12 (50%)
4	CMP	A	289	3	22,25,25	1.92	7 (31%)	24,39,39	3.80	13 (54%)
5	POP	C	895	3	6,8,8	1.37	1 (16%)	13,13,13	1.39	3 (23%)
5	POP	B	894	3	6,8,8	1.54	2 (33%)	13,13,13	1.39	2 (15%)
5	POP	A	893	3	6,8,8	1.64	1 (16%)	13,13,13	1.32	2 (15%)

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
4	CMP	C	910	3	1/1/5/5	0/0/31/31	0/4/4/4
4	CMP	B	290	3	1/1/5/5	0/0/31/31	0/4/4/4
4	CMP	A	289	3	1/1/5/5	0/0/31/31	0/4/4/4
5	POP	C	895	3	-	0/6/6/6	-
5	POP	B	894	3	-	2/6/6/6	-
5	POP	A	893	3	-	1/6/6/6	-

The worst 5 of 21 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	910	CMP	P-O5'	-6.33	1.50	1.57
4	B	290	CMP	P-O5'	-4.82	1.52	1.57
4	A	289	CMP	P-O3'	-4.44	1.50	1.57
4	A	289	CMP	P-O5'	-3.97	1.53	1.57
4	B	290	CMP	C2'-C1'	3.38	1.58	1.53

The worst 5 of 47 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	910	CMP	O3'-C3'-C2'	10.72	126.11	115.61
4	B	290	CMP	O3'-C3'-C2'	9.85	125.27	115.61
4	A	289	CMP	C1'-N9-C4	9.85	143.94	126.64
4	A	289	CMP	O3'-C3'-C2'	9.71	125.13	115.61
4	B	290	CMP	C1'-N9-C4	8.21	141.07	126.64

All (3) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	289	CMP	C1'
4	C	910	CMP	C1'
4	B	290	CMP	C1'

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	894	POP	P1-O-P2-O5
5	B	894	POP	P1-O-P2-O6
5	A	893	POP	P2-O-P1-O2

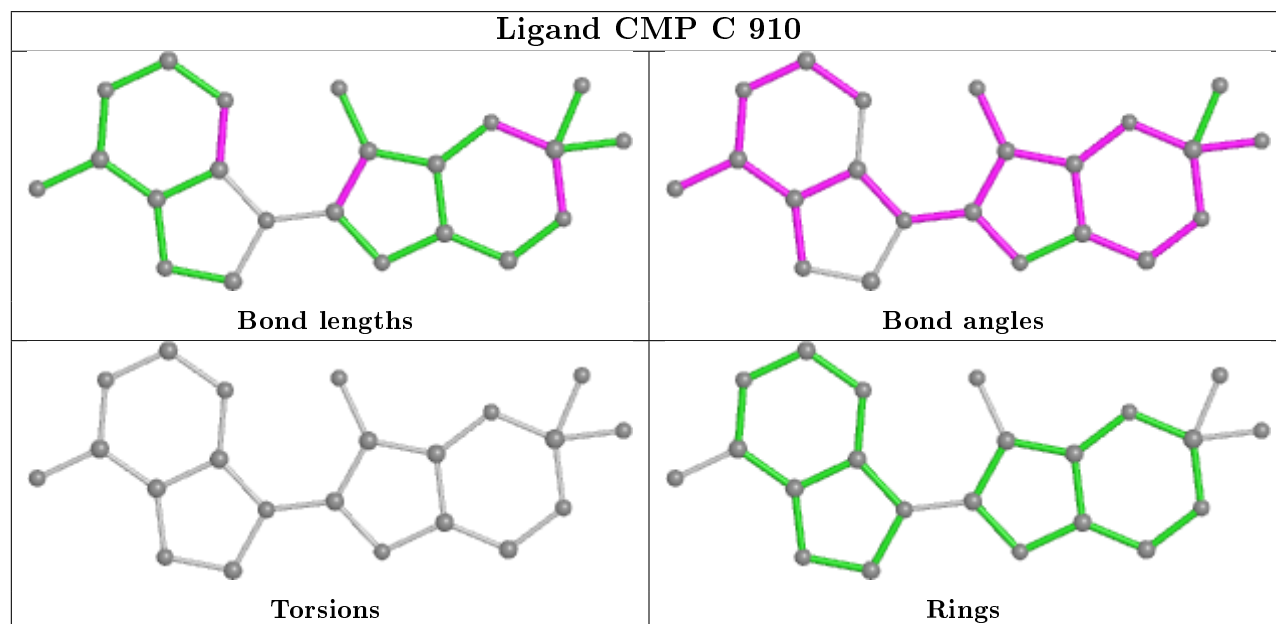


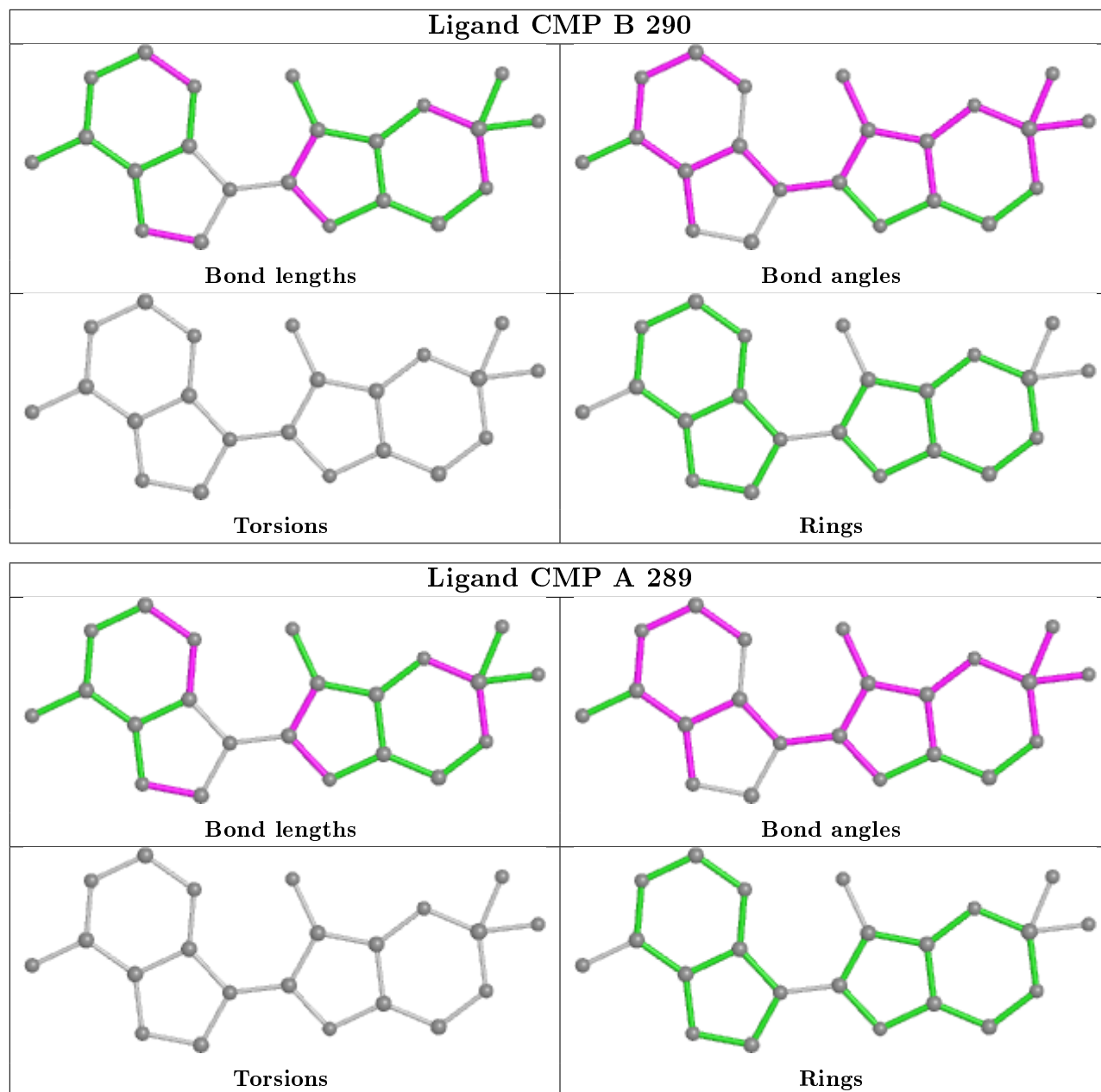
There are no ring outliers.

6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	910	CMP	3	0
4	B	290	CMP	5	0
4	A	289	CMP	6	0
5	C	895	POP	1	0
5	B	894	POP	1	0
5	A	893	POP	3	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	C	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	C	773:PHE	C	774:LYS	N	1.80

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	481/510 (94%)	-0.09	8 (1%) 70 57	10, 43, 95, 99	0
1	B	454/510 (89%)	0.15	27 (5%) 22 13	10, 51, 95, 98	0
1	C	483/510 (94%)	-0.06	18 (3%) 41 26	10, 43, 95, 97	0
2	D	143/148 (96%)	0.80	23 (16%) 1 1	18, 95, 95, 98	0
2	E	143/148 (96%)	1.29	41 (28%) 0 0	39, 95, 96, 98	0
2	F	143/148 (96%)	0.78	24 (16%) 1 1	17, 95, 95, 97	0
All	All	1847/1974 (93%)	0.22	141 (7%) 13 7	10, 55, 95, 99	0

The worst 5 of 141 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	79	THR	8.9
2	E	59	GLY	7.6
2	E	79	THR	7.1
1	B	740	GLN	7.1
2	E	71	MET	6.9

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

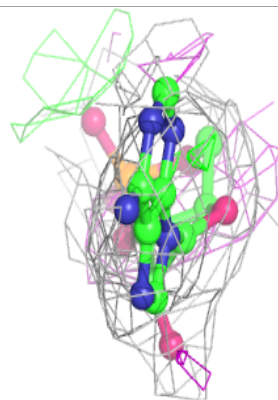
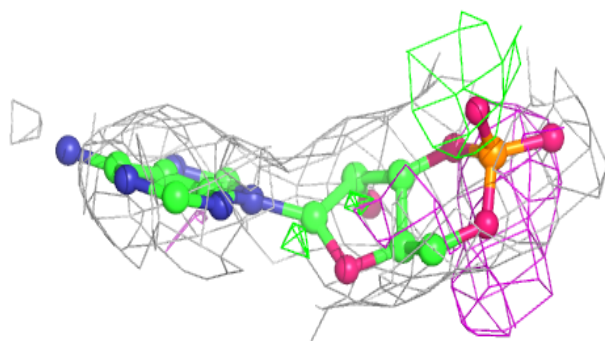
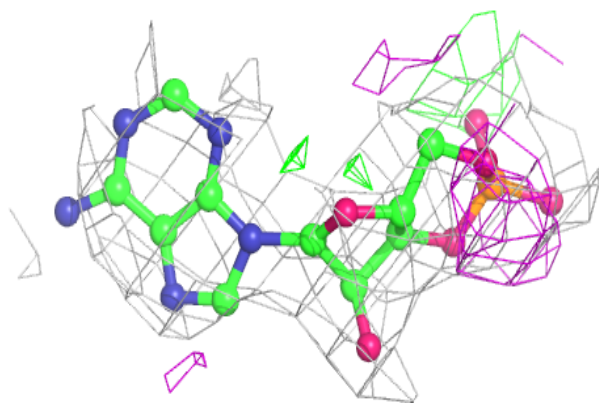
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	CMP	C	910	22/22	0.87	0.28	15,22,44,45	0
5	POP	C	895	9/9	0.88	0.30	50,52,61,62	0
4	CMP	A	289	22/22	0.91	0.25	11,18,39,43	0
4	CMP	B	290	22/22	0.92	0.24	16,25,44,46	0
3	YB	C	909	1/1	0.93	0.42	72,72,72,72	1
5	POP	B	894	9/9	0.93	0.26	51,52,54,55	0
5	POP	A	893	9/9	0.94	0.29	96,101,104,105	0
3	YB	B	908	1/1	0.95	0.36	49,49,49,49	1
3	YB	A	907	1/1	0.95	0.36	49,49,49,49	1
3	YB	A	904	1/1	0.95	0.37	42,42,42,42	1
6	CA	E	802	1/1	0.96	0.04	43,43,43,43	0
6	CA	F	805	1/1	0.96	0.33	21,21,21,21	0
3	YB	C	906	1/1	0.97	0.41	31,31,31,31	1
3	YB	C	903	1/1	0.97	0.45	72,72,72,72	1
3	YB	A	901	1/1	0.97	0.27	50,50,50,50	1
6	CA	D	800	1/1	0.97	0.15	11,11,11,11	0
3	YB	B	902	1/1	0.98	0.34	107,107,107,107	1
3	YB	B	905	1/1	0.98	0.35	31,31,31,31	1
6	CA	D	801	1/1	0.98	0.35	13,13,13,13	0
6	CA	F	804	1/1	0.99	0.11	26,26,26,26	0
6	CA	E	803	1/1	0.99	0.32	23,23,23,23	0

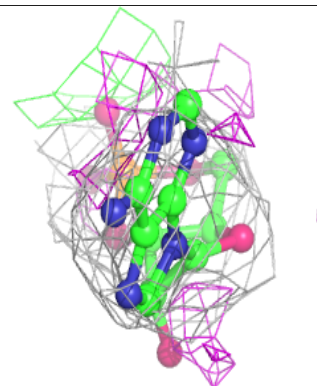
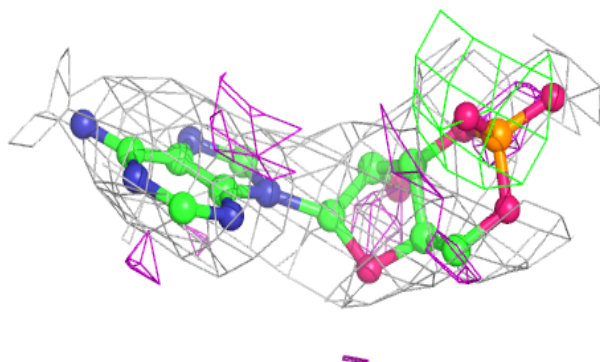
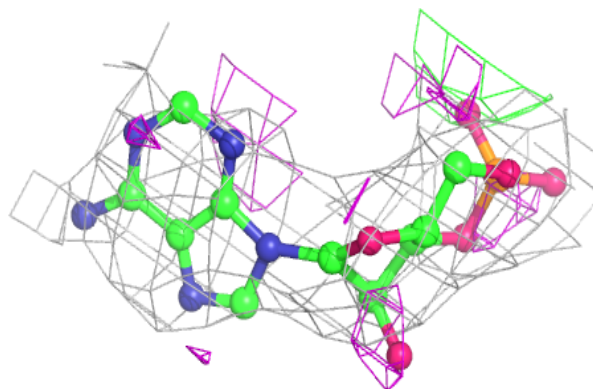
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

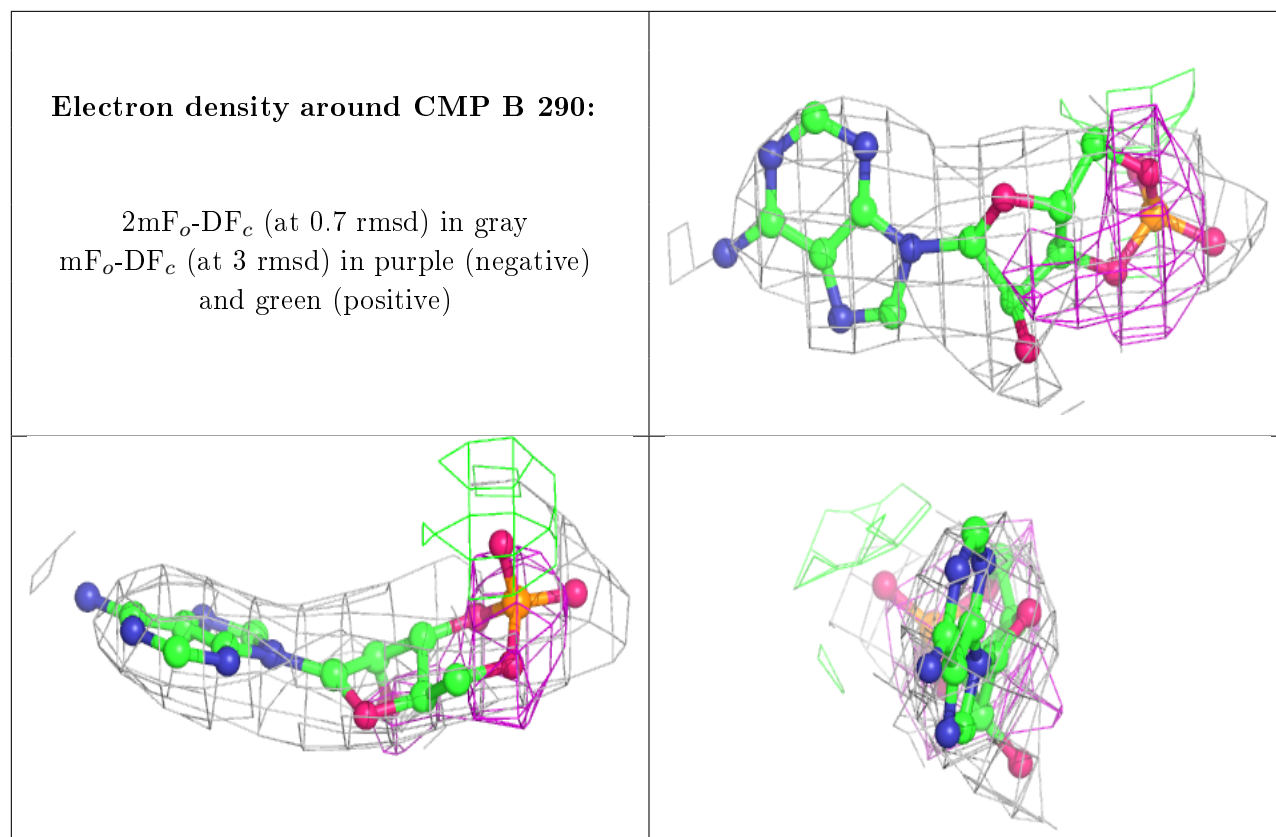
**Electron density around CMP C 910:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around CMP A 289:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.