



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 01:49 AM UTC

PDB ID : 2VZ9 / pdb_00002vz9
Title : Crystal Structure of Mammalian Fatty Acid Synthase in complex with NADP
Authors : Maier, T.; Leibundgut, M.; Ban, N.
Deposited on : 2008-07-31
Resolution : 3.30 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

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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

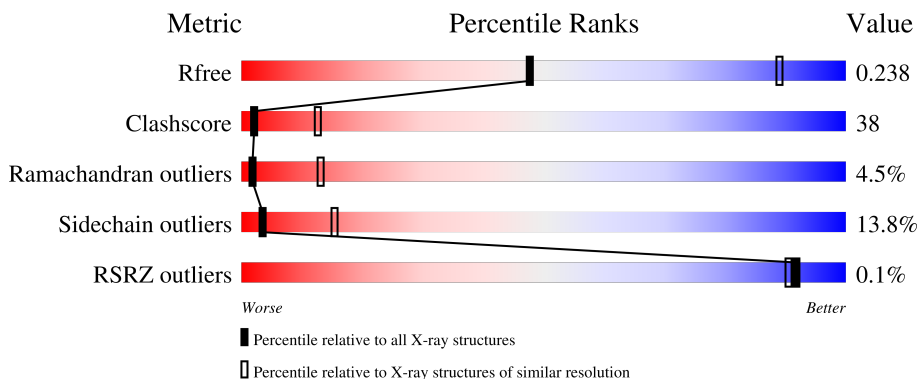
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

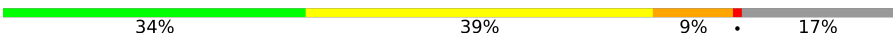
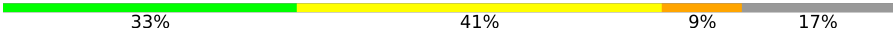
The reported resolution of this entry is 3.30 Å.

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	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	2512	
1	B	2512	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 31949 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.

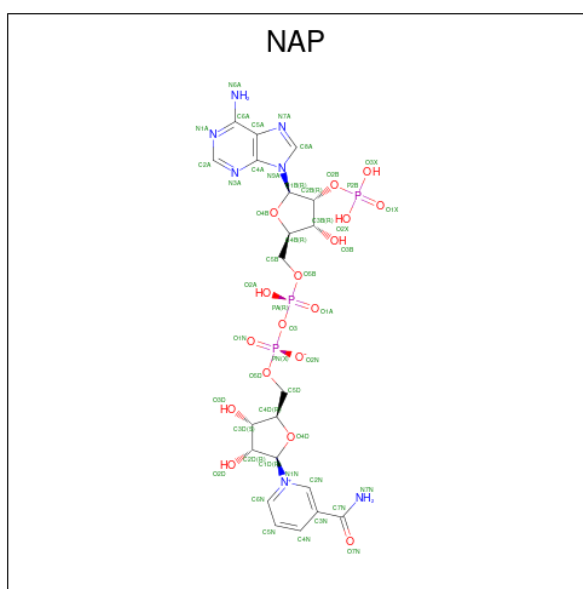
- Molecule 1 is a protein called FATTY ACID SYNTHASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	2081	Total	C	N	O	S	0	0	0
			15858	10015	2786	2973	84			
1	B	2086	Total	C	N	O	S	0	0	0
			15899	10041	2793	2981	84			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	834	ILE	UNK	conflict	UNP A5YV76
B	834	ILE	UNK	conflict	UNP A5YV76

- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NAP) (formula: $C_{21}H_{28}N_7O_{17}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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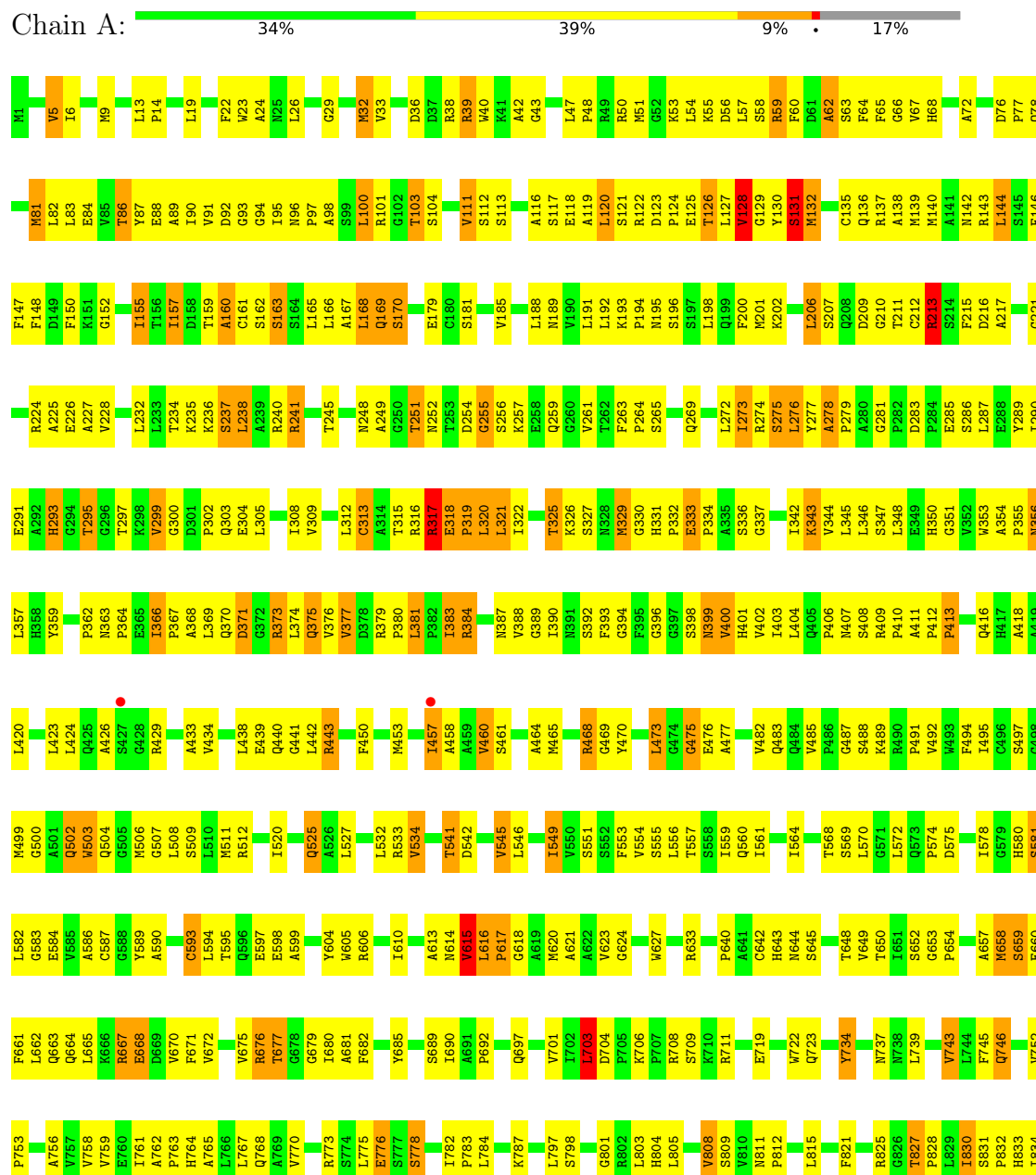
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

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: FATTY ACID SYNTHASE



R1841	L1767	G1692	A1619	P1550	S1475	P1413	F1343	V1267	A1205	Q1137	H1064	S988	S904	K835
Y1842	E1768	C1693	E1620	L1551	M1476	L1416	L1344	M1268	Q1206	E1138	R1065	Q989	Q905	W836
A1843	I1769	R1694	G1621	L1552	L1477	L1417	L1345	D1269	R1207	E1139	Q1066	Y993	R906	D837
A1844	G1770	V1695	L1622	Y1553	S1417	L1418	L1346	L1270	R1208	L1140	L1067	K994	L907	H838
Q1845	K1772	F1696	A1623	L1554	T1480	V1419	H1347	Y1271	P1209	G1145	Y1068	T910	T910	S839
H1848	F1772	T1697	A1624	L1555	S1481	E1419	L1348	D1272	L1210	L1146	L1070	P911	P911	W842
L1773	S1695	T1698	S1626	P1556	P1482	D1420	L1349	T1273	L1211	L1147	L1071	V912	V912	D843
L1774	V1626	T1699	L1627	A1557	A1483	T1421	L1350	A1274	C1212	L1150	Q1072	R999	V913	W844
S1775	L1627	S1698	S1628	S1558	A1484	S1422	H1354	T1275	D1213	L1151	D1073	G1000	F914	E915
K1851	L1628	Q1559	M1496	Q1560	E1485	F1423	R1354	D1276	P1215	THR	T1075	Y1001	E915	S846
V1852	L1629	Q1560	M1496	Q1560	E1485	R1424	P1354	L1285	P1216	L1216	Q1076	Y1002	D916	D849
V1853	L1629	Q1560	M1496	Q1560	E1485	R1424	P1354	L1285	P1216	L1216	Q1076	Y1002	D916	F850
Q1855	L1633	R1562	P1498	R1562	H1487	V1425	G1356	A1285	L1217	L1217	G1077	G1004	V917	P851
V1856	W1634	L1563	S1488	L1563	P1488	V1426	G1356	A1285	L1217	L1217	G1077	G1004	V917	F850
R1857	W1634	L1563	S1488	L1563	P1488	V1426	G1356	A1285	L1217	L1217	G1077	G1004	V917	P851
E1858	E1635	S1488	S1488	L1563	S1488	V1426	G1356	A1285	L1217	L1217	G1077	G1004	V917	S852
E1859	F1712	F1712	F1712	S1565	S1490	S1428	M1358	E1290	G1219	VAL	A1078	P1005	L919	S852
E1860	P1713	P1713	P1713	V1566	L1493	L1429	V1359	Q1291	L1220	GLN	F1006	F1006	L924	F1007
E1860	F1713	P1637	P1637	V1566	L1493	L1429	V1359	Q1291	L1220	GLN	F1006	F1006	L924	S853
Q1861	Q1714	Q1714	Q1714	V1567	L1493	K1430	G1360	L1292	L1221	GLY	Q1008	Q1008	L925	S854
Q1862	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	S855
K1877	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1878	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1879	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1880	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1881	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1882	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1883	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1884	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1885	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1886	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1887	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1888	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1889	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1890	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1891	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1892	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1893	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1894	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1895	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1896	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1897	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1898	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1899	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1900	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1901	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1902	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1903	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1904	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1905	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1906	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1907	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1908	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1909	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1910	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1911	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1912	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1913	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1914	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1915	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856
K1916	L1715	L1715	L1715	V1568	V1496	D1431	F1361	H1293	D1222	GLY	L1009	L1009	V931	C856



Category	Percentage
Very bad	33%
Bad	41%
Good	9%
Very good	17%



V1453	H1388	G1319	D1251	A1187	V1125	T1055	A979	H896	F821	N738	I651	Q573	M499	A419
V1454	L1389	A1320	G1252	G1168	E1126	S1056	D980	A897	R825	L739	P654	P574	G500	L420
G1455	V1390	L1321	Q1253	Q1189	S1127	I1057	S981	T898	G826	V743	Q655	D575	Q502	L423
R1394	L1391	A1322	L1254	L1190	G1128	D1060	A983	A900	T827	L744	A656	I578	Q503	L424
N1457	L1323	T1323	Y1255	Q1191	C1129	P1061	E984	L903	P828	F745	A657	Q504	Q504	Q425
C1459	L1324	G1325	S1256	L1192	L1130	Y1062	F985	L903	T829	Q746	P658	S581	G506	A426
L1460	G1326	G1326	R1257	N1195	G1132	T1063	F986	S904	L830	V752	S659	L582	M506	R429
G1398	D1327	LEU	A1260	LEU	N1133	H1064	L987	Q905	S831	P753	L662	A586	Q507	A433
V1400	A1328	GLN	L1261	GLN	L1136	Q1065	S988	N906	P832	A756	Q664	L508	S509	V434
L1401	V1329	LEU	L1262	LEU	L1137	Q1066	Q989	L907	H833	A756	L665	L510	M511	L438
F1402	A1330	E1199	M1263	L1200	Q1137	K1067	G990	E908	R834	A756	Q664	Y589	M512	Q439
G1465	F1331	L1200	T1264	L1200	E1138	L1068	D991	E909	K835	A756	L665	A590	R512	Q440
L1463	G1332	V1203	Q1265	V1203	E1140	Y1069	Y992	T910	P836	V759	E668	C593	L438	E439
C1404	M1334	L1204	M1268	L1204	Q1141	T1070	K994	P911	D837	E760	E668	L594	Q440	Q440
R1405	M1334	L1204	L1269	L1204	Q1141	Y993	K994	P911	D837	E760	E668	L594	Q440	Q440
Q1406	T1337	Q1206	L1270	Q1206	C1143	Q1073	R997	V913	H838	A761	D669	R515	Q440	G441
T1407	L1338	E1207	L1271	E1207	R1144	D1073	L998	G914	S839	A762	V670	T595	G441	G441
T1408	K1339	R1208	Y1272	R1208	G1145	T1074	L998	E915	Q840	H764	F671	Q596	L442	L442
P1409	E1340	P1209	T1273	P1209	G1146	T1075	R999	D916	A841	A765	V672	E597	L443	R443
S1412	G1341	A1274	T1274	A1274	L1146	Q1076	G1000	V917	V844	A765	V675	A598	M453	M453
P1413	G1342	L1211	T1275	L1211	A1147	A1077	Y1001	P845	R676	L767	R677	Y604	Q525	Q525
L1416	F1343	C1212	D1276	C1212	Q1148	A1078	D1002	S846	T677	Q768	G678	W605	N455	N455
S1417	L1344	D1213	R1277	D1213	L1150	V1081	Y1003	L925	G679	A769	G679	R606	L527	L527
V1418	L1345	D1214	M1276	D1214	K1153	V1082	F1007	V931	F880	V770	I680	G607	L530	L530
E1419	L1346	P1215	Q1279	P1215	V1154	M1085	Q1008	E934	A681	L775	A681	Y608	G531	A459
D1420	H1347	L1216	Q1280	L1216	ALA	L1086	L1009	E935	C856	E776	F682	C609	L532	V460
T1421	T1348	L1217	A1281	L1217	ALA	N1087	V935	L935	S777	E776	H683	T610	R533	S461
S1422	L1349	S1218	L1282	S1218	GLN	N1087	R936	R936	S777	E776	H683	T610	R533	S461
F1423	L1350	G1219	A1285	G1219	GLN	T1088	L937	L937	S777	E776	H683	T610	R533	S461
R1424	A1351	L1220	A1285	L1220	GLN	V1089	D1014	S941	A860	A782	F686	E612	V463	V463
V1425	G1352	L1221	K1288	L1221	LEU	V1090	L1015	S941	A860	A782	F686	E612	V463	V463
G1426	H1353	D1222	L1289	D1222	LVS	G1092	E1016	F944	E688	L784	M687	M614	S540	S540
D1427	P1354	P1224	E1290	P1224	VAL	F1096	R1019	V946	A691	L793	A621	V615	T541	R468
S1428	G1360	A1225	Q1291	A1225	VAL	L1097	L1022	S947	P692	L797	P692	A622	E544	E544
L1429	F1361	L1226	L1292	L1226	PRO	S1101	Q1023	L963	H873	S798	Q697	V623	V545	L473
K1430	L1362	K1227	H1293	K1227	GLY	S1102	W1028	L963	H873	S798	Q697	V623	V545	L473
D1431	T1363	A1228	V1294	A1228	LEU	V1103	V1029	L963	H873	S798	Q697	V623	V545	L473
L1432	S1364	L1228	T1295	L1228	ASP	V1103	V1029	L963	H873	S798	Q697	V623	V545	L473
V1502	P1365	A1228	Q1296	A1228	GLY	V1103	V1029	L963	H873	S798	Q697	V623	V545	L473
M1503	E1366	T1231	G1297	T1231	ALA	V1103	V1029	L963	H873	S798	Q697	V623	V545	L473
D1435	Q1367	T1232	Q1298	T1232	ALA	V1103	V1029	L963	H873	S798	Q697	V623	V545	L473
A1436	Q1367	A1233	W1299	A1233	ALA	R1106	F1031	L963	H873	S798	Q697	V623	V545	L473
Y1506	R1370	L1234	W1299	L1234	ALA	R1107	L1032	L963	H873	S798	Q697	V623	V545	L473
S1437	H1371	E1235	P1301	E1235	PRO	P1108	L1032	L963	H873	S798	Q697	V623	V545	L473
D1508	L1372	N1236	D1301	N1236	ARG	Q1109	A1034	L963	H873	S798	Q697	V623	V545	L473
R1439	L1372	M1237	A1302	M1237	GLU	E1110	M1035	L963	H873	S798	Q697	V623	V545	L473
G1509	L1373	A1238	M1303	A1238	ALA	E1111	L1036	L963	H873	S798	Q697	V623	V545	L473
A1510	S1374	S1239	P1304	S1239	PRO	H1111	H1037	L963	H873	S798	Q697	V623	V545	L473
W1511	Q1377	P1240	A1305	P1240	GLN	I1115	M1038	L963	H873	S798	Q697	V623	V545	L473
L1443	W1378	K1241	P1306	K1241	GLN	L1116	S1039	L963	H873	S798	Q697	V623	V545	L473
M1444	F1382	M1242	K1311	M1242	SER	E1117	T1040	L963	H873	S798	Q697	V623	V545	L473
G1447	A1383	K1243	A1312	K1243	GLN	L1118	L1041	L963	H873	S798	Q697	V623	V545	L473
R1515	F1384	F1181	A1312	F1181	GLN	G1120	A1042	L963	H873	S798	Q697	V623	V545	L473
H1516	G1384	R1182	L1315	R1182	GLN	C1120	P1043	L963	H873	S798	Q697	V623	V545	L473
F1517	A1385	V1245	V1316	V1245	GLN	F1121	A1043	L963	H873	S798	Q697	V623	V545	L473
S1451	S1386	E1246	G1317	E1246	GLN	T1122	P1051	L963	H873	S798	Q697	V623	V545	L473
E1520	Q1452	V1247	L1248	V1247	GLN	P1123	P1051	L963	H873	S798	Q697	V623	V545	L473
Q1521	L1387	L1248	N1318	L1248	GLN	H1124	F1054	L963	H873	S798	Q697	V623	V545	L473



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.15Å 244.89Å 135.37Å 90.00° 101.84° 90.00°	Depositor
Resolution (Å)	30.00 – 3.30 30.00 – 3.34	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 90.1 (30.00-3.34)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.244 0.187 , 0.238	Depositor DCC
R_{free} test set	4016 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	117.6	Xtriage
Anisotropy	0.271	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 104.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	31949	wwPDB-VP
Average B, all atoms (Å ²)	151.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.98% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NAP

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	1/16199 (0.0%)	1.00	66/22016 (0.3%)
1	B	0.54	0/16240	0.98	56/22070 (0.3%)
All	All	0.56	1/32439 (0.0%)	0.99	122/44086 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1769	ILE	CA-CB	-5.20	1.47	1.54

The worst 5 of 122 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	886	PHE	CA-C-N	10.78	131.47	119.93
1	A	886	PHE	C-N-CA	10.78	131.47	119.93
1	B	886	PHE	CA-C-N	9.62	130.22	119.93
1	B	886	PHE	C-N-CA	9.62	130.22	119.93
1	B	1223	ALA	CA-C-N	8.75	130.78	119.84

There are no chirality outliers.

There are no planarity outliers.

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	A	15858	0	15834	1200	0
1	B	15899	0	15882	1249	0
2	A	96	0	50	12	0
2	B	96	0	50	4	0
All	All	31949	0	31816	2395	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 38.

The worst 5 of 2395 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)
1:B:333:GLU:HB2	1:B:334:PRO:HD3	1.26	1.17
1:A:333:GLU:HB2	1:A:334:PRO:HD3	1.28	1.13
1:B:1585:PRO:HB3	1:B:1598:MET:HE1	1.29	1.12
1:A:616:LEU:HD23	1:A:617:PRO:HD2	1.32	1.10
1:A:123:ASP:HB3	1:A:126:THR:HB	1.18	1.10

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	2075/2512 (83%)	1683 (81%)	296 (14%)	96 (5%)	2	13
1	B	2080/2512 (83%)	1713 (82%)	276 (13%)	91 (4%)	2	13
All	All	4155/5024 (83%)	3396 (82%)	572 (14%)	187 (4%)	2	13

5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ALA

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Mol	Chain	Res	Type
1	A	317	ARG
1	A	333	GLU
1	A	614	ASN
1	A	854	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	1717/2072 (83%)	1471 (86%)	246 (14%)	3	14
1	B	1722/2072 (83%)	1492 (87%)	230 (13%)	4	16
All	All	3439/4144 (83%)	2963 (86%)	476 (14%)	3	15

5 of 476 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1980	LEU
1	B	1856	VAL
1	B	371	ASP
1	B	1797	ASP
1	B	2088	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 108 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	199	GLN
1	B	614	ASN
1	B	1763	HIS
1	B	259	GLN
1	B	399	ASN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NAP	B	3002	-	50,52,52	1.36	6 (12%)	71,80,80	1.82	14 (19%)
2	NAP	B	3001	-	50,52,52	1.31	3 (6%)	71,80,80	1.72	13 (18%)
2	NAP	A	3001	-	50,52,52	1.38	5 (10%)	71,80,80	1.71	13 (18%)
2	NAP	A	3002	-	50,52,52	1.22	5 (10%)	71,80,80	1.64	10 (14%)

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
2	NAP	B	3002	-	-	9/35/67/67	0/5/5/5
2	NAP	B	3001	-	-	2/35/67/67	0/5/5/5
2	NAP	A	3001	-	-	12/35/67/67	0/5/5/5
2	NAP	A	3002	-	-	10/35/67/67	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	NAP	C2N-N1N	5.62	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3001	NAP	C2N-N1N	5.49	1.41	1.35
2	A	3002	NAP	C2N-N1N	5.17	1.40	1.35
2	A	3001	NAP	C2N-N1N	4.86	1.40	1.35
2	A	3001	NAP	C2A-N3A	3.53	1.40	1.33

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	N3A-C2A-N1A	-6.08	119.37	128.58
2	A	3002	NAP	N3A-C2A-N1A	-5.54	120.20	128.58
2	B	3001	NAP	N3A-C2A-N1A	-5.41	120.39	128.58
2	A	3001	NAP	C2B-C1B-N9A	-5.37	104.91	113.75
2	A	3002	NAP	C2B-C1B-N9A	-5.19	105.21	113.75

There are no chirality outliers.

5 of 33 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	3001	NAP	O4D-C1D-N1N-C6N
2	A	3002	NAP	C5B-O5B-PA-O2A
2	A	3002	NAP	C5B-O5B-PA-O3
2	A	3002	NAP	O4D-C4D-C5D-O5D
2	B	3002	NAP	C5B-O5B-PA-O3

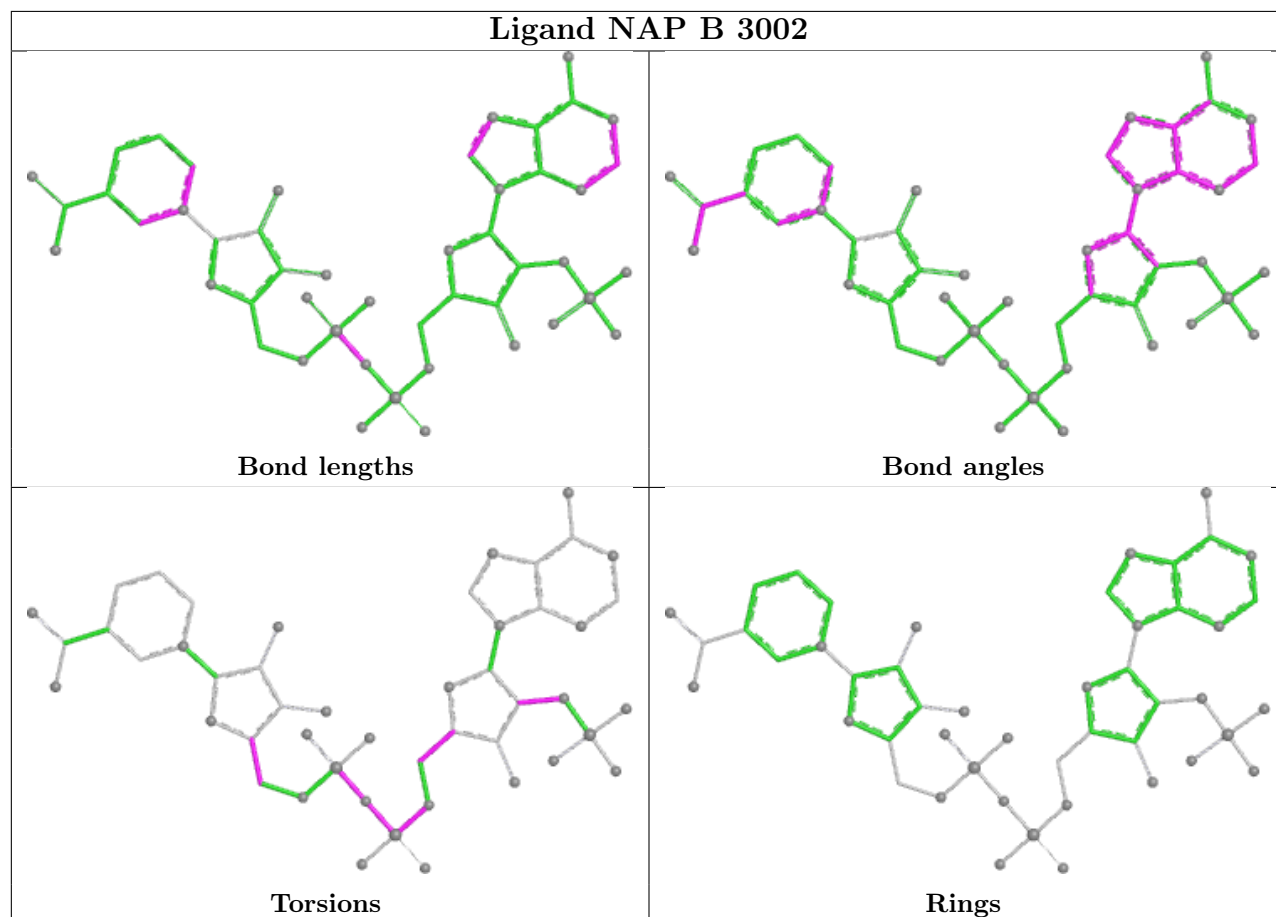
There are no ring outliers.

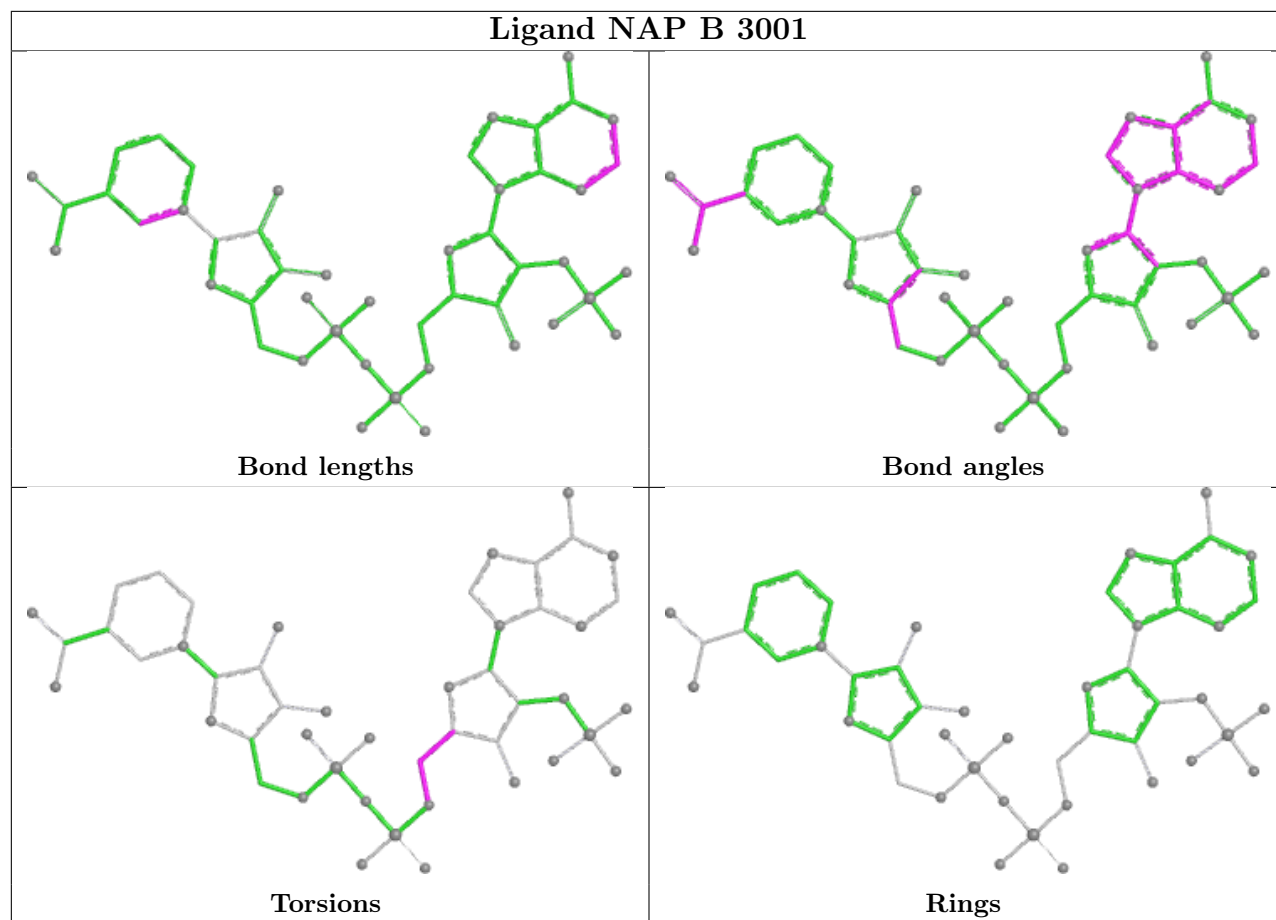
4 monomers are involved in 16 short contacts:

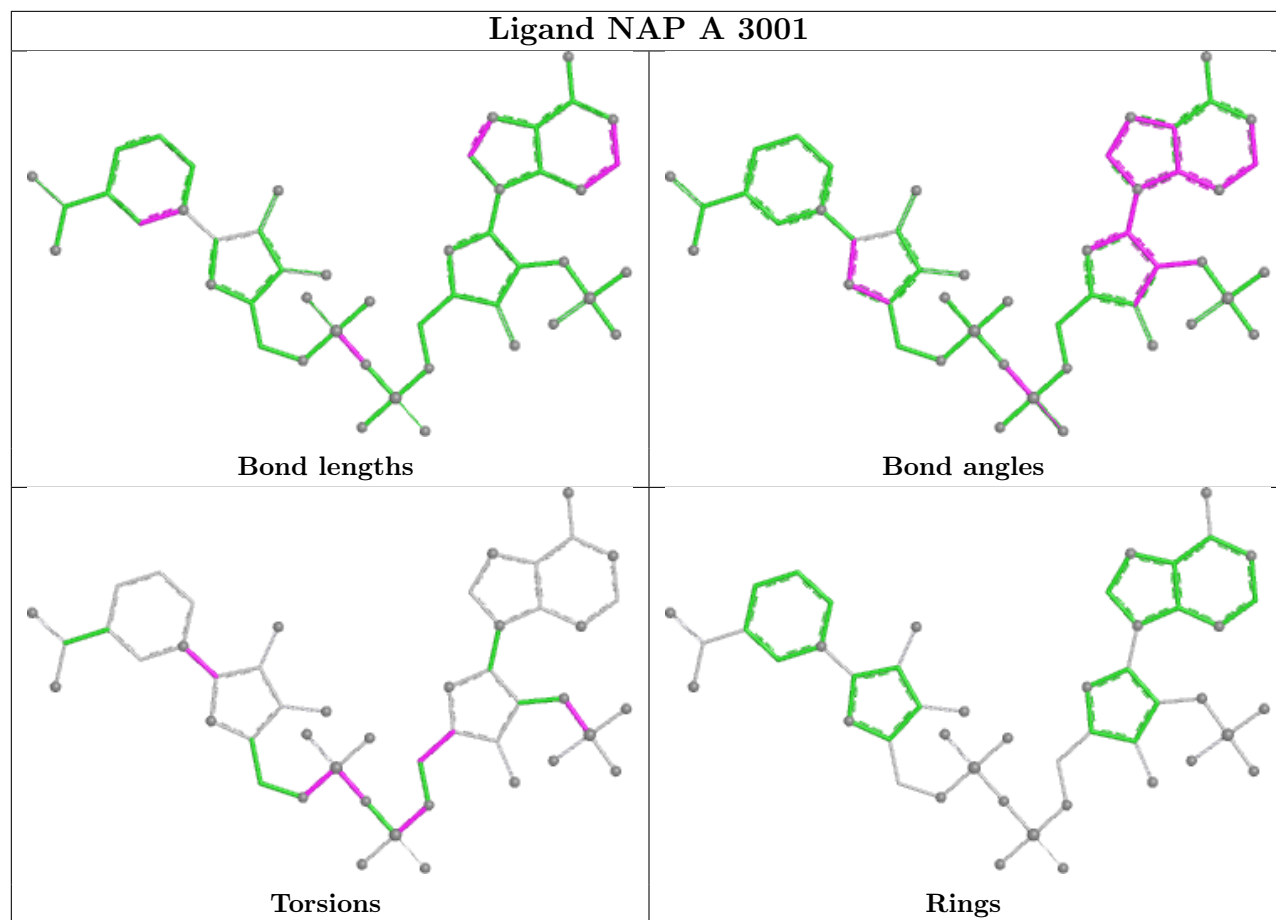
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3002	NAP	2	0
2	B	3001	NAP	2	0
2	A	3001	NAP	8	0
2	A	3002	NAP	4	0

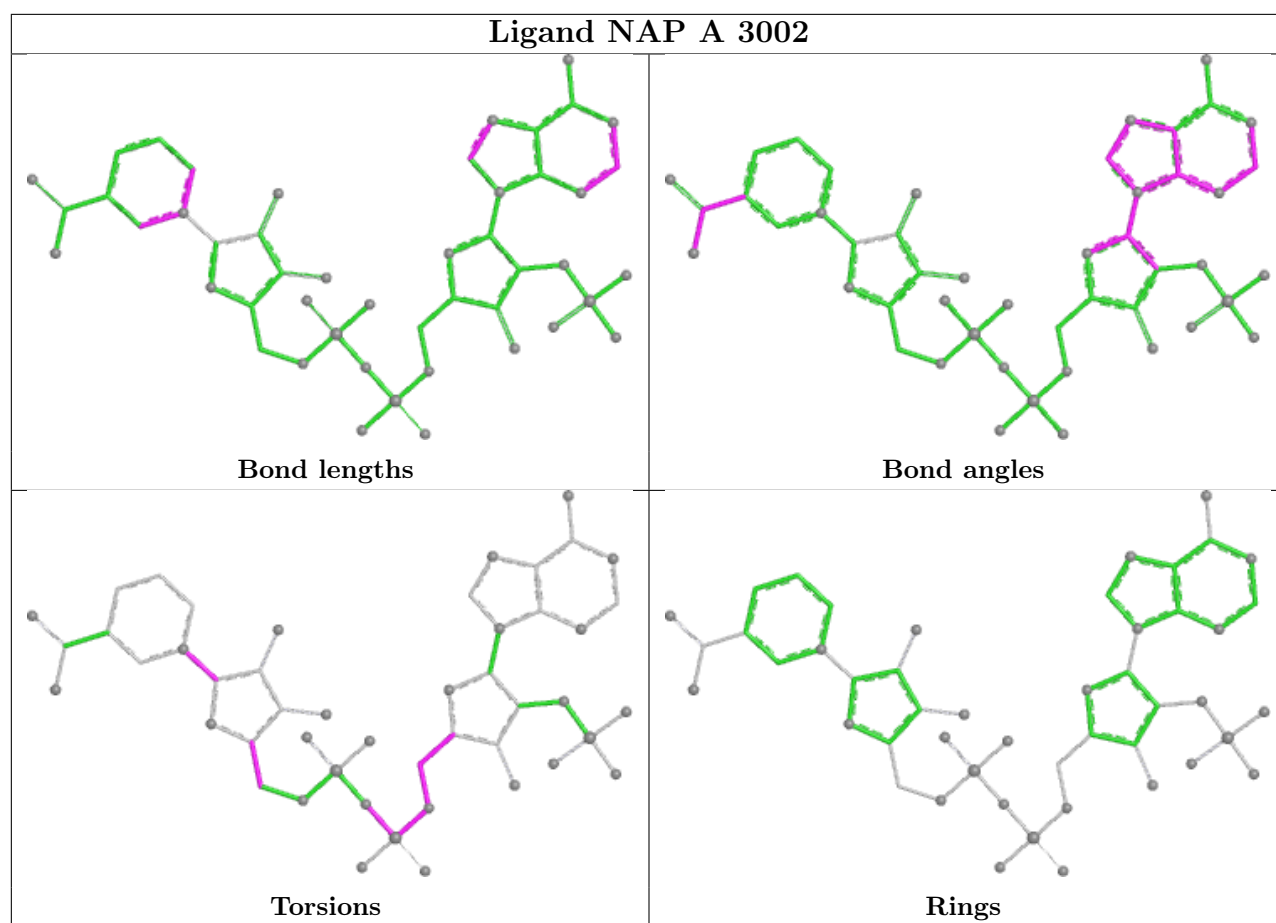
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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](#)

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, 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	2081/2512 (82%)	-0.68	4 (0%) 91 86	73, 131, 230, 299	0
1	B	2086/2512 (83%)	-0.62	2 (0%) 92 90	72, 166, 228, 299	0
All	All	4167/5024 (82%)	-0.65	6 (0%) 92 90	72, 145, 229, 299	0

The worst 5 of 6 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1191	GLN	3.2
1	A	457	ILE	2.6
1	A	977	ASP	2.3
1	B	1475	SER	2.2
1	A	1312	ALA	2.2

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](#)

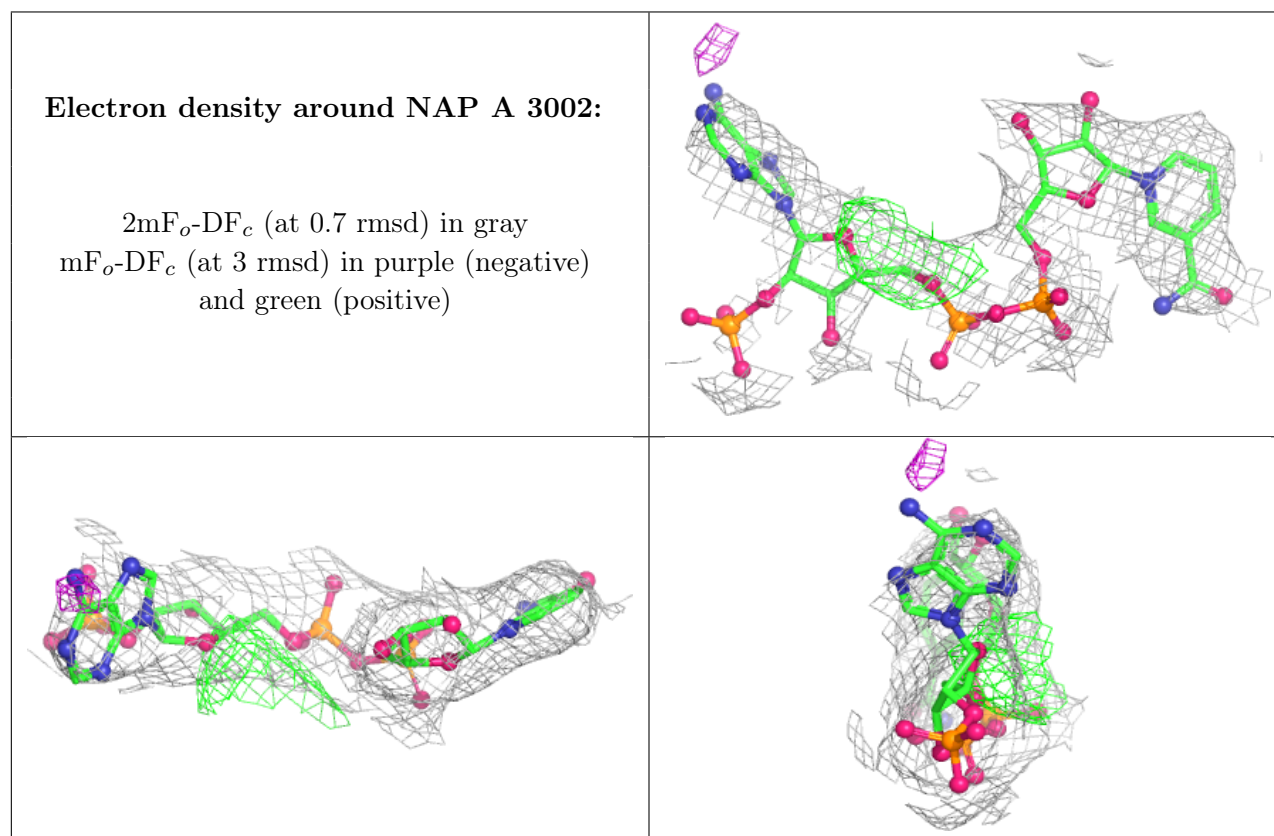
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

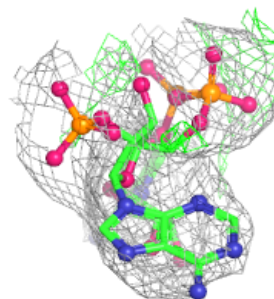
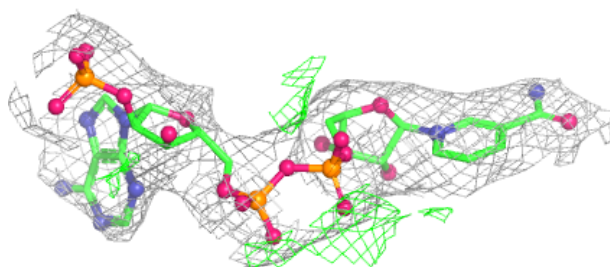
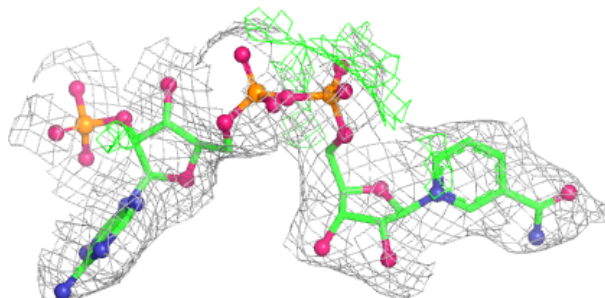
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAP	A	3002	48/48	0.95	0.07	96,135,161,194	0
2	NAP	A	3001	48/48	0.96	0.07	100,122,179,189	0
2	NAP	B	3001	48/48	0.96	0.06	99,123,160,163	0
2	NAP	B	3002	48/48	0.96	0.07	99,122,153,198	0

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.

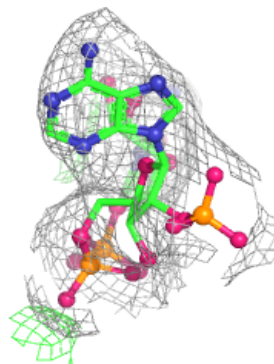
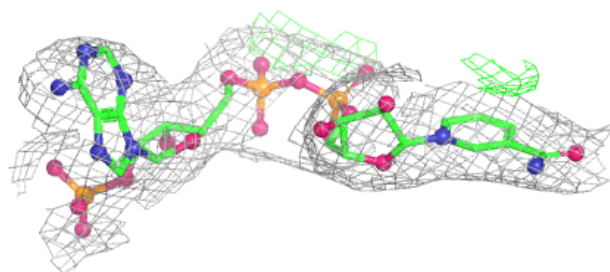
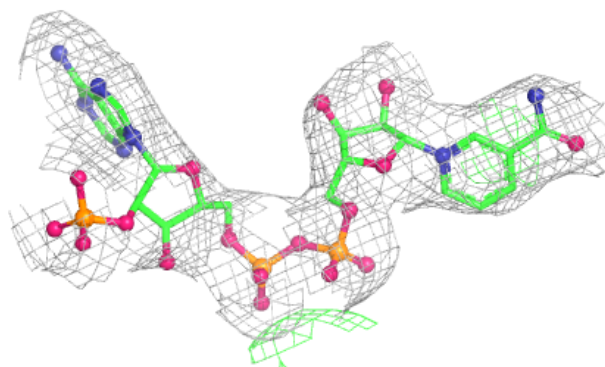


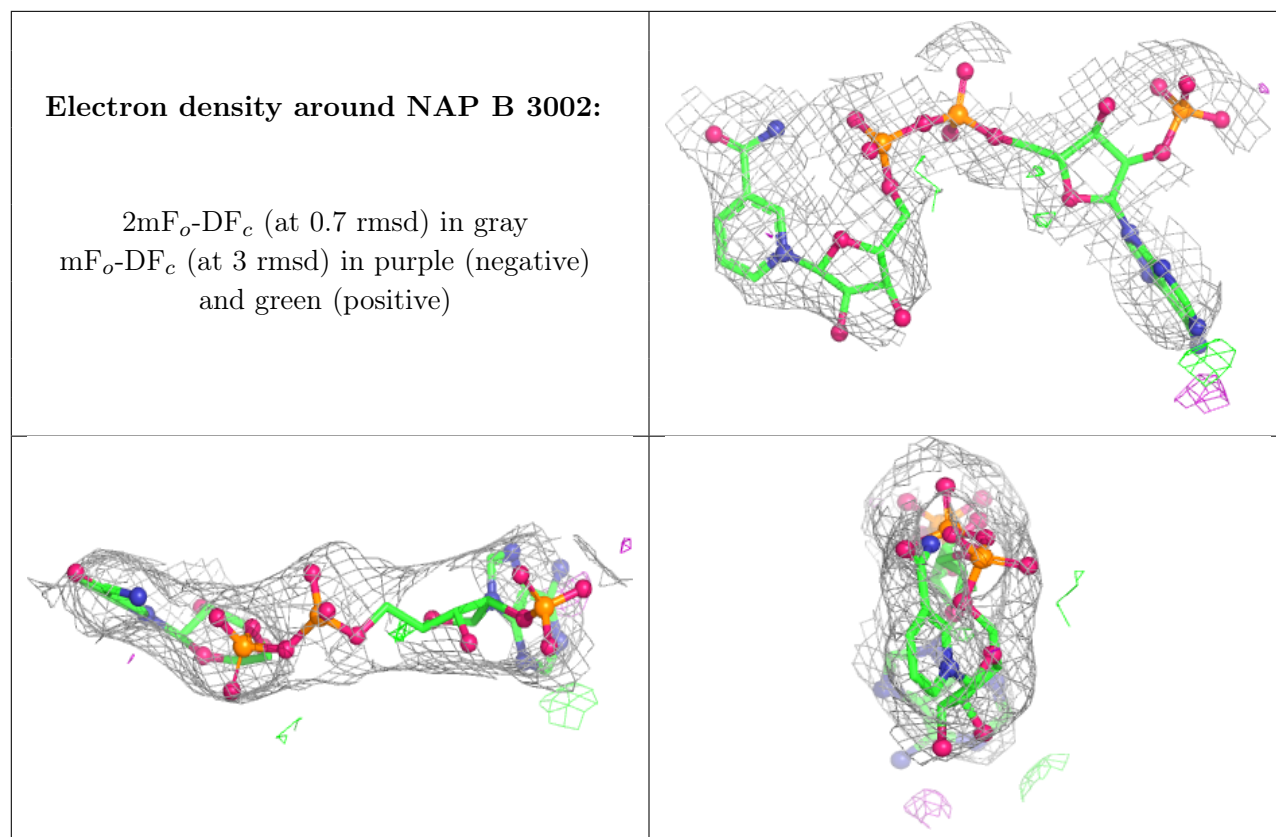
Electron density around NAP A 3001:

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

**Electron density around NAP B 3001:**

$2mF_o-DF_c$ (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.