



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 07:13 am BST

PDB ID : 2VZ9
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.

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 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

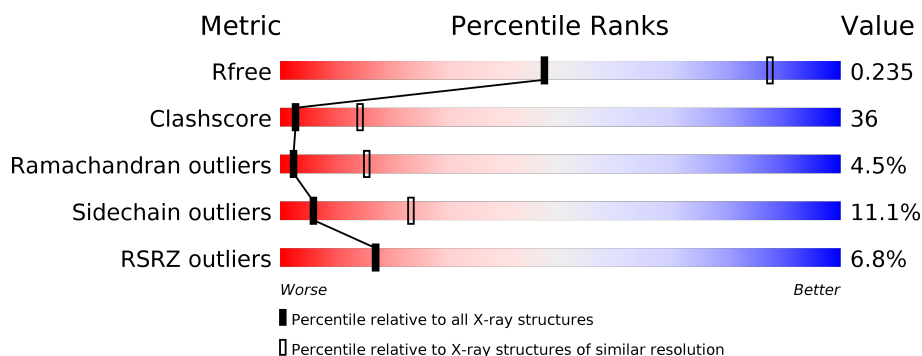
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	130704	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)

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 ≥ 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	<div> <div>5%</div> <div>38%</div> <div>38%</div> <div>7%</div> <div>17%</div> </div>
1	B	2512	<div> <div>6%</div> <div>36%</div> <div>40%</div> <div>7%</div> <div>17%</div> </div>

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.

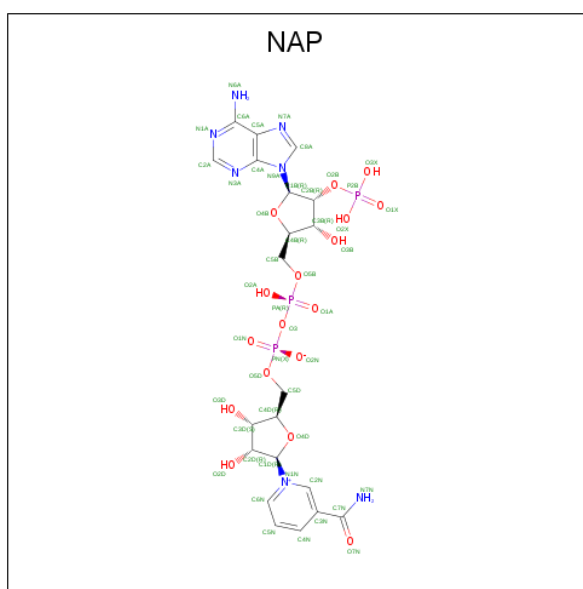
- Molecule 1 is a protein called FATTY ACID SYNTHASE.

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

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 (three-letter code: 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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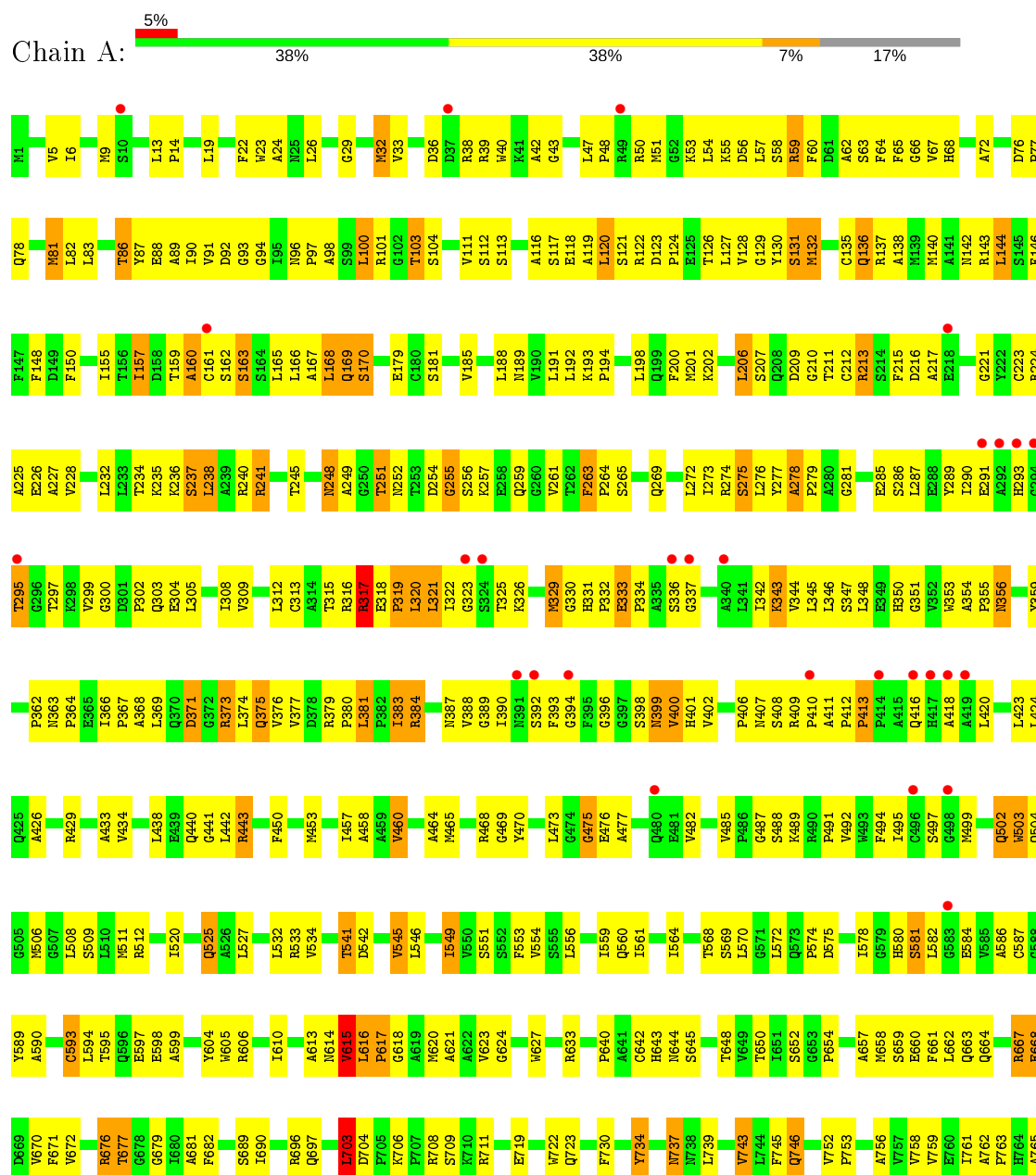
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

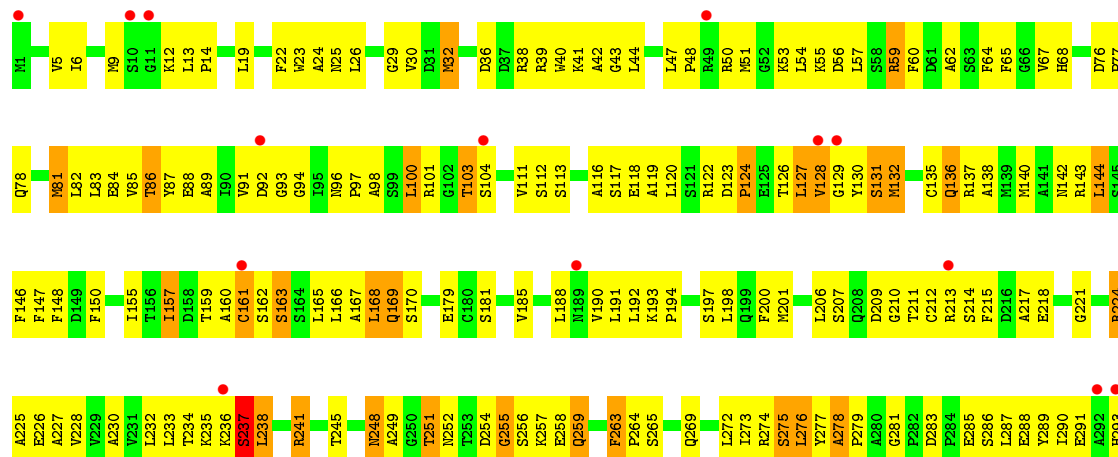
3 Residue-property plots [i](#)

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 ($RSRZ > 2$). 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



E1703	S1695	Y1553	T1421	G1356	L1289	L1221	MTT	M1085	Q1008	T928	P851	L766
R1704	V1626	A1483	S1422	E1357	E1290	D1222	VAL	L1086	L1009	T928	S852	L767
A1705	L1627	P1484	F1423	M1358	Q1291	A1223	VAL	M1087	L1010	V831	G853	Q768
A1706	L1628	P1556	R1424	M1359	L1292	P1224	PRO	T1088	L1011	V831	S854	A769
R1711	L1629	M1486	M1425	G1360	H1293	A1225	GLY	V1089	D1014	E834	S855	V770
F1712	T1633	H1487	V1426	F1361	L1294	L1226	LEU	G1092	L1015	V835	C856	R773
C1719	V1636	D1487	D1427	L1362	T1295	K1227	ASP	G1092	E1016	V836	S857	S774
F1720	V1636	S1488	S1428	T1363	Q1296	A1228	GLY	F1096	L1019	L937	S858	L775
A1721	T1639	S1489	L1429	S1364	Q1297	C1229	ALA	L1097	R1019	S941	A860	E776
R1724	E1644	L1432	T1432	E1366	M1299	D1231	ALA	S1101	L1022	S941	V861	S777
D1725	V1648	A1434	A1434	G1367	D1300	T1232	ARG	S1101	Q1023	F944	V866	S778
T1726	V1649	D1435	D1435	G1369	A1302	L1234	GLU	R1107	V1029	E945	V866	I782
S1727	V1567	A1436	A1436	R1370	M1303	E1235	PRO	F1108	F1031	V945	S867	P783
F1728	T1569	R1437	R1437	H1371	P1304	M1236	ALA	Q1109	S1030	S947	P888	L784
E1729	S1570	S1438	S1438	L1372	A1305	M1237	GLN	E1110	F1031	H873	H873	K787
T1730	Y1652	R1439	R1439	L1373	P1306	G1245	GLN	E1111	L1032	L953	Y874	
F1732	T1683	S1374	G1307	S1375	G1307	P1240	SER	L1112	D1033	L954	L875	
L1733	R1574	Q1376	S1308	Q1376	S1308	K1241	L1180	I1115	A1034	V876	V876	L797
R1734	A1655	D1376	L1309	D1376	L1309	M1242	P1181	I1115	M1035	V876	V876	S798
H1735	G1655	Q1377	G1310	Q1377	G1310	K1243	R1182	K1118	L1036	H878	H878	G801
T1736	S1658	M1444	K1311	M1444	K1311	V1244	L1183	F1119	H1037	W962	W962	R802
K1739	V1661	A1445	A1445	E1379	L1315	V1245	A1185	G1120	M1038	E963	G882	L803
G1740	V1661	G1447	G1447	L1381	V1316	V1247	A1186	F1121	S1039	S964	G882	R804
V1741	R1682	C1448	C1448	F1382	V1317	L1248	A1187	T1122	I1041	P965	R883	L805
L1742	G1663	F1450	F1450	A1385	L1318	D1251	C1188	T1123	L1042	P967	F886	V808
L1743	M1685	S1451	S1451	S1386	C1319	G1252	Q1189	H1124	P1043	F970	P887	S809
M1746	Q1686	G1452	G1452	L1387	A1320	Q1253	L1190	V1125	S1056	F970	G888	
E1750	E1689	V1453	V1453	L1388	L1321	L1254	Q1191	E1126	P1051	A874	T889	P812
L1753	V1670	V1454	V1454	L1389	L1324	L1255	M1193	C1129	F1054	A975	G890	
S1756	L1672	G1455	G1455	V1390	L1324	S1256	G1194	L1130	T1055	V976	R891	L815
V1757	L1673	V1457	V1457	S1395	P1327	I1258	LEU	G1132	I1057	P978	L894	F821
R1758	S1675	M1458	M1458	Y1397	A1330	A1260	LEU	T1134	D1060	D880	W896	R825
C1759	G1678	C1459	C1459	G1398	M1333	L1261	GLU	A1135	P1061	S881	G897	G826
L1760	G1679	R1461	R1461	S1399	M1334	L1262	L1200	L1136	V1062	T982	T898	T827
A1761	V1680	E1463	E1463	V1400	A1335	Q1265	G1201	Q1137	T1063	E983	L899	P828
Q1762	G1681	F1402	F1402	F1402	A1336	P1266	Q1202	E1138	H1064	A984	A984	
H1763	G1682	L1403	L1403	L1403	T1337	V1267	V1203	E1139	R1065	F885	F885	S831
G1764	A1684	C1404	C1404	C1404	L1338	M1268	L1204	L1140	G1066	R886	R886	P832
R1765	A1684	R1466	R1466	R1405	M1339	D1271	Q1206	G1145	L1068	L987	S988	H833
F1766	I1687	H1467	H1467	Q1406	E1340	Y1272	E1207	L1146	Y1069	Q889	Q889	I834
L1767	I1687	I1469	I1469	Q1407	F1343	T1273	R1208	A1147	T1071	Y893	L907	W836
R1768	G1614	R1470	R1470	P1409	L1344	A1274	P1209	L1070	L1071	K894	T910	H838
I1769	G1615	V1472	V1472	D1411	L1345	D1276	L1211	Q1072	D1073	R997	P911	S839
K1771	P1616	L1473	L1473	P1412	L1346	D1276	C1212	THR	T1074	R997	V912	W842
L1774	V1695	S1475	S1475	H1347	L1347	L1282	D1213	LYS	Q1076	Y1001	V913	D843
F1775	E1620	M1476	M1476	T1348	L1349	E1283	D1214	VAL	A1077	D1545	F914	W842
R1776	G1621	L1477	L1477	L1349	L1350	A1284	P1215	ALA	A1078	Y1001	E915	P845
T1777	T1697	S1478	S1478	A1285	L1355	A1285	L1217	GLN	G1004	Y1003	D916	S846
H1778	T1698	V1478	V1478	Q1286	H1353	Q1286	S1218	GLY	P1005	P1005	V917	
H1779	V1699	T1480	T1480	A1287	P1354	A1287	L1219	LEU	D1083	T924	F1006	D849
		D1420	D1420	K1288	L1355	K1288	L1220	LYS	R1084	F1007	L925	F850



D1251	Q1489	H1124	P1051	A975	L894	P817	Y734	T850	I578	W503	L423	T361	Q294
G1252	L1190	V1125	F1051	V976	L895	P818	W737	I651	G579	Q504	L424	P362	T295
Q1253	Q1191	E1126	F1054	D977	M896	W819	W738	G652	H580	G505	Q425	I363	G296
L1254	L1192	S1127	F1055	P978	T398	E820	L739	G653	S581	M506	A426	P364	T297
V1255	G1128	G1129	S1056	A979	T399	F821	L743	Q654	L582	G507	R429	E365	K298
S1256	Q1193	D980	S1057	D980	L899	W825	W744	Q655	G583	L508	R430	I366	V299
R1257	L1194	L1130	I1057	S981	A900	R826	L745	A656	E584	S509	R431	P367	Q300
	LEU	A1131	D1060	T982	L903	G826	L746	A657	A586	R512	A433	I368	Q301
A1260	GLN	G1132	D1061	A983	L904	T827	W747	W658	A587	R515	V434	L369	P302
L1261	LEU	N1133	V1062	E984	S904	P828	Q746	S659	Y589	R520	L438	Q370	Q303
L1262	E1199	N1133	T1063	F985	Q905	P829	W752	E660	A590	R521	Q440	D371	E304
T1263	L1200	L1136	K1067	L987	L907	S831	P753	L662	C593	D524	R443	R372	L305
Q1264	G1201	Q1137	L1068	S988	T910	P832	A754	Q663	E597	L520	Q441	R373	I308
Q1265	Q1202	E1138	L1069	Q989	T911	H833	W755	Q664	T595	L521	Q442	L374	V309
	V1203	E1139	T1070	S990	P912	R834	A756	L665	A599	D525	R444	Q375	
M1268	L1204	L1142	T1071	D991	V913	H836	W759	K666	Q596	Q526			L312
D1271	Q1205	Q1206	Q1072	V992	V914	D837	E760	E668	E597	A526	W453	R379	
Y1272	R1207	L1146	D1073	Y993	F914	H838	W761	W670	E598	L527	L454	P380	T315
T1273	R1208	A1147	D1074	Y994	E915	S839	W762	W671	E599	L530	W455	R381	R316
A1274	A1148	L1148	T1075	A941	D916	Q840	A763	F671	W604	G531	A458	I383	R317
T1275	A1149	L1150	Q1076	L998	V917	H841	W764	K673	W605	L532	A459	R384	E318
D1276	L1211	L1150	Q1077	L999	V918	A841	W765	K674	R606	R533	W460	G385	P319
R1277	G1212	K1163	A1077	G999	I924	W644	A766	E674	G607	W534	S461	G386	L321
H1278	D1213	V1154	A1078	G1000	L925	P845	L766	W675	Y608		W463	I388	L322
P1279	D1214			Y1001		S846	Q768	W676	C609	L537	P462	I389	I323
Q1280	P1215	ALA	V1081	D1002	T928	D849	L775	T677	I610	L538	W464	G390	S324
A1281	L1216	GLN	V1082	Y1003	G929	F850	W776	E681	A464	L539	W465	I391	T325
L1282	L1217	GLN	D1083	D1003	V931	C856	W777	H682	E612	S540		G392	K326
	S1218	GLY	R1084	F1007	E934		S778	H683	E613	D542	R468	P393	S327
G1219	L1219	LEU	N1085	Q1008	V935			S684	W614	E543	W469	G394	H328
L1220	L1220	LVS	L1086	L1009	R936	V859	W782	W685	M620	A544	W470	F395	R329
L1221	D1222	MET	N1087	V1010	R937	A860	P783	W686	A621	L546	G474	G396	G330
K1288	VAL	VAL	T1088	L1011	L937	H861	W784		G475	G475	G475	G397	H331
L1289	PRO	PRO	V1089	D1014	S941	W866			E476		A477	I398	E333
A1290	GLY	GLY	G1092	L1015		S867	W790	S689	G624	I549		V400	P334
Q1291	LEU	LEU	F1096	E1016	F944	P868	L793	I690	L625	V550		H401	A335
L1292	ASP	ASP	L1097	R1019	E945			A691				V402	S336
H1293	GLY	GLY	S1101	L1022	V946	H873	L797	P692	S626	V554	E481	I403	G337
T1294	ALA	ALA	S1102	Q1023	S947		W798		W627	S555		L404	
Q1296	GLN	GLN	R1106	W1028	L953	V676	W799	Q697	R633	L556	V485	P405	I342
L1297	ALA	ALA	R1107	V1029	I954	D877	W800	L698	C634	T557	P486	P406	K343
A1298	PRQ	PRQ	F1108	S1030		H878	G801	R699	P635	S558	G487	M407	V344
D1300	ALA	ALA	Q1109	F1031	V959	C879	R802		S488	I559	S488	S408	L345
P1301	GLN	GLN	E1110	L1032		I880	L803	L703	P636	Q560	K489	R409	L346
A1302	GLN	GLN	H1111	D1033	W662	D881	H804	S709	G637	I561	R490	P410	S347
N1303	GLN	GLN		A1034	E963	G882	L805	K710	I638	I564	V492	A411	L348
P1304	SER	SER	T1115	M1035	S964	R883		R711	V639		W493	P412	E349
A1305	L1180	L1180	L1116	L1036	P965	W884	W808		P640	T568	L495	P413	H350
P1306	P1181	P1181	E1117	H1037	D966	F886	S809	E719	A641	S569	I495	P414	G351
K1311	R1182	R1182	F1117	H1037	P967	P887	W810		C642	L570	C496	P415	V352
A1312	L1183	L1183	F1118	M1038		G888	R811	W722	H643	L571	C497	Q416	W353
V1245	L1184	L1184	F1119	S1039	F970	T889	P812		N644	G571	S497	H417	A354
E1246	A1185	A1185	G1120	I1040	D971	G890	H813	R728	S645	L572	C498	H418	P355
V1316	A1186	A1186	F1121	L1042	D972	T891	G814		K646	Q573	W499	A419	I356
G1317	L1248	L1248	T1122	A1041	T972	L892	L815	F730	D647	D575	G500	L420	P357
N1318			P1123	P1043	A974	W893	F816		V649			R422	Y359
													H360

GLY	ALA	ILE	LEU	ALA	V2058	L1980	L1893	K1815	V1671	G1597	R1523	M1456	V1390	G1319
ALA	VAL	GLU	SER	VAL	G2059	E1981	G1894	I1818	L1672	M1598	Q1527	V1457	R1394	A1320
CYS	ALA	GLY	SER	ALA	G2060	T1984	G1895	I1818	L1673	L1599	T1528	M1458	R1394	A1321
VAL	ILE	THR	LYS	THR	T1984	P1985	F1896	V1822	H1674	E1602	E1529	C1459	S1395	A1322
PHE	THR	THR	SER	THR	G2065	E1986	G1897	V1823	G1675	F1603	H1530	R1460	F1396	T1323
GLU	VAL	THR	THR	GLY	V2066	F1987	L1898	Q1824	S1677	R1606	A1531	R1461	V1397	L1324
MET	PHE	ILE	ASP	ILE	F1988	F1988	Q1899	P1825	G1678	R1606	F1532	K1462	G1398	G1325
HIS	ALA	ARG	ALA	ARG	V2069	V1991	W1903	R1833	G1679	R1606	V1533	E1463	S1399	D1326
GLY	ASP	ASP	PRO	ASP	L2070	V1991	L1904	R1833	R1680	R1611	N1534	G1465	V1400	P1327
LEU	PRO	VAL	VAL	VAL	E2071	L1904	L1905	V1836	G1681	R1612	F1402	G1466	F1402	A1330
ALA	ALA	ALA	ALA	ALA	T2072	P1994	R1905	V1836	G1682	Q1613	L1403	H1467	V1331	V1331
GLN	THR	SER	THR	SER	N2073	K1995	L1906	A1837	A1684	M1614	C1404	G1468	G1332	G1332
ALA	LYS	ILE	PRO	ILE	G2074	Y1996	A1838	Q1762	A1684	G1615	R1538	I1469	N1333	N1333
LEU	LEU	THR	THR	THR	T2075	T1999	A1839	H1763	G1685	G1616	G1539	I1468	Q1407	M1334
LEU	LEU	THR	THR	THR	N2076	T1999	F1840	G1764	A1686	M1617	D1540	R1470	Q1407	Q1407
ASP	ASP	ASP	PRO	ASP	D2077	V1913	R1841	R1765	G1687	P1618	S1542	T1472	P1408	T1408
GLY	GLY	GLY	GLY	GLY	T2078	L1914	V1914	R1765	L1687	L1622	S1543	L1473	P1409	L1338
SER	SER	SER	SER	SER	V2079	L2002	G1915	F1766	S1690	L1622	I1544	V1474	Q1410	L1339
THR	THR	THR	THR	THR	D2003	D2003	T1915	L1767	R1691	A1623	R1546	S1475	D1411	E1340
LEU	LEU	LEU	LEU	LEU	T2006	T2006	S1916	E1768	G1692	A1623	W1546	M1476	S1412	G1342
VAL	VAL	VAL	VAL	VAL	R2007	R2007	R1917	I1769	G1693	T1624	R1546	L1477	P1413	F1342
ASP	ASP	ASP	VAL	ASP	E2008	E2008	S1918	G1770	R1694	V1626	S1549	T1480	L1416	L1344
GLN	GLY	GLY	GLN	GLY	A2009	C2010	R1921	K1771	V1695	L1627	T1549	T1481	L1416	L1344
THR	THR	THR	THR	THR	L2088	L2088	T1922	L1774	F1696	L1628	A1554	L1481	L1416	L1344
LEU	LEU	LEU	LEU	LEU	L2089	L2089	G1923	S1775	T1697	L1628	L1555	L1345	L1417	L1345
ASP	ASP	ASP	THR	ASP	G2100	G2100	Q1924	M1776	T1698	A1631	P1556	L1346	L1418	L1346
GLY	GLY	GLY	THR	GLY	Q2101	Q2101	Y1924	H1777	V1699	H1631	A1557	P1484	E1419	H1347
ALA	ALA	ALA	THR	ALA	E1931	E1931	Q1925	A1832	T1699	A1632	S1557	E1485	D1420	T1348
THR	THR	THR	THR	THR	S2021	S2021	R1930	H1778	T1699	T1633	S1558	M1486	T1421	L1349
ILE	ILE	ILE	LEU	ILE	G2023	G2023	W1932	H1785	T1699	T1633	C1559	H1487	S1422	L1350
GLN	GLN	GLN	VAL	GLN	C2024	C2024	V1937	F1785	F1712	T1633	Q1560	P1488	R1423	A1351
LEU	LEU	LEU	ASN	LEU	G2025	G2025	Y1937	L1786	E1703	V1636	D1581	L1493	R1424	G1382
LEU	LEU	LEU	ASN	LEU	R2026	R2026	V1937	L1786	K1704	E1643	S1565	L1494	W1425	H1383
GLY	GLY	GLY	GLY	GLY	G2027	G2027	V1941	K1787	K1704	E1644	V1566	V1496	W1426	P1354
THR	THR	THR	GLY	THR	Q2031	Q2031	Y1944	M1788	C1719	E1644	Y1567	G1499	S1427	G1360
GLN	GLN	GLN	GLY	GLN	A2032	A2032	S1944	T1789	F1720	S1647	T1569	D1500	D1427	F1361
VAL	VAL	VAL	THR	VAL	N2033	N2033	G1954	F1791	A1721	V1648	T1569	L1501	S1428	L1362
THR	THR	THR	THR	THR	Y2034	Y2034	L1955	H1792	S1723	P1649	T1569	M1502	L1429	L1362
ARG	ARG	ARG	LEU	ARG	G2035	G2035	I1956	G1793	D1725	T1649	L1570	V1503	K1430	T1363
VAL	VAL	VAL	LEU	VAL	I1957	I1957	L1956	L1794	D1725	T1649	L1570	M1503	D1431	S1364
ALA	ALA	ALA	LEU	ALA	F2036	F2036	T1957	L1795	T1726	V1651	R1574	Y1506	L1433	P1365
LEU	LEU	LEU	LEU	LEU	A2037	A2037	G1958	L1796	S1727	T1653	M1577	N1504	S1437	E1366
ASN	ASN	ASN	ASN	ASN	N2038	N2038	T1957	D1797	E1729	T1653	M1577	N1504	S1437	Q1367
VAL	VAL	VAL	VAL	VAL	S2039	S2039	G1967	S1798	E1729	T1653	M1577	N1504	S1437	Q1367
GLN	GLN	GLN	VAL	GLN	V1968	V1968	L1968	L1799	E1729	T1653	M1577	N1504	S1437	Q1367
PRO	PRO	PRO	VAL	PRO	A2040	A2040	G1968	L1799	E1729	T1653	M1577	N1504	S1437	Q1367
GLY	GLY	GLY	GLN	GLY	M2041	M2041	F1969	G1875	E1729	T1653	M1577	N1504	S1437	Q1367
CYS	CYS	CYS	VAL	CYS	E2042	E2042	H1970	L1876	T1728	T1653	M1577	N1504	S1437	Q1367
GLY	GLY	GLY	ALA	GLY	R2043	R2043	G1970	L1876	E1729	T1653	M1577	N1504	S1437	Q1367
PRO	PRO	PRO	GLY	PRO	G2043	G2043	L1971	E1801	V1732	T1653	M1577	N1504	S1437	Q1367
ALA	ALA	ALA	GLY	ALA	R2046	R2046	A1972	E1802	L1733	T1653	M1577	N1504	S1437	Q1367
GLU	GLU	GLU	THR	GLU	K2047	K2047	G1973	G1803	H1734	T1653	M1577	N1504	S1437	Q1367
ALA	ALA	ALA	PRO	ALA	L2048	L2048	V1974	Q1804	R1735	T1653	M1577	N1504	S1437	Q1367
LYS	LYS	LYS	LEU	LYS	R2048	R2048	L1975	V1810	T1736	T1653	M1577	N1504	S1437	Q1367
ASP	ASP	ASP	PHE	ASP	G1976	G1976	L1976	S1811	K1739	T1653	M1577	N1504	S1437	Q1367
LEU	LEU	LEU	LEU	LEU	A1977	A1977	V1887	S1811	G1740	T1653	M1577	N1504	S1437	Q1367
VAL	VAL	VAL	VAL	VAL	D1978	D1978	V1888	L1812	V1741	T1653	M1577	N1504	S1437	Q1367
HIS	HIS	HIS	HIS	HIS	L2054	L2054	A1978	L1813	D1742	T1653	M1577	N1504	S1437	Q1367
THR	THR	THR	THR	THR	LYS	LYS	V1887	L1814	L1743	T1653	M1577	N1504	S1437	Q1367

PHE	ALA	LEU
PHE	GLU	GLU
VAL	ASN	SER
GLN	TYR	ILE
GLN	TRP	LEU
PHE	PRO	SER
THR	GLN	ILE
ASP	ALA	ILE
MET	THR	HIS
GLU	TYR	SER
GLN	HIS	CYS
GLY	GLY	LEU
LYS	ASN	ALA
VAL	VAL	GLU
LEU	THR	PRO
GLU	LEU	ARG
ALA	LEU	VAL
LEU	ARG	SER
ILE	ALA	VAL
PRO	LYS	ARG
LEU	THR	GLU
GLN	GLY	GLY
GLY	ALA	TYR
LEU	LEU	GLY
ALA	TYR	GLY
GLU	GLY	GLU
ALA	GLU	ARG
VAL	ASP	VAL
ALA	LEU	LEU
ALA	GLY	ALA
THR	ALA	ALA
VAL	ASP	ASP
ASP	TYR	TYR
LEU	ASN	ASN
ILE	LEU	ILE
THR	SER	SER
GLN	GLN	GLN
SER	VAL	VAL
HIS	CYS	CYS
ALA	ASP	ASP
GLY	GLY	GLY
LEU	LYS	LYS
ASP	VAL	VAL
ARG	SER	SER
HIS	VAL	VAL
ALA	HIS	HIS
LEU	VAL	VAL
SER	ILE	ILE
PHE	GLU	GLU
ALA	GLY	GLY
ALA	ASP	ASP
ALA	HIS	HIS
ARG	ARG	ARG
SER	SER	SER
PHE	THR	THR
TYR	LEU	LEU
GLN	LEU	LEU
LYS	GLU	GLU
LEU	GLY	GLY
ARG	SER	SER
ALA	GLY	GLY

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 29.97 – 3.34	Depositor EDS
% Data completeness (in resolution range)	84.1 (30.00-3.30) 90.2 (29.97-3.34)	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 0.184 , 0.235	Depositor DCC
R_{free} test set	4016 reflections (5.02%)	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)	0.28 , 87.4	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	0.44	0/16199	0.64	3/22016 (0.0%)
1	B	0.41	0/16240	0.61	1/22070 (0.0%)
All	All	0.43	0/32439	0.62	4/44086 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1216	LEU	CA-CB-CG	5.89	128.85	115.30
1	B	1216	LEU	CA-CB-CG	5.63	128.25	115.30
1	A	703	LEU	N-CA-C	-5.16	97.08	111.00
1	A	321	LEU	CA-CB-CG	5.01	126.82	115.30

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	1137	0
1	B	15899	0	15882	1193	0
2	A	96	0	50	12	0
2	B	96	0	50	3	0
All	All	31949	0	31816	2282	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 36.

The worst 5 of 2282 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: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
1:A:1477:LEU:HD11	1:A:2043:ARG:HD2	1.36	1.06

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	15
1	B	2080/2512 (83%)	1713 (82%)	276 (13%)	91 (4%)	2	16
All	All	4155/5024 (83%)	3396 (82%)	572 (14%)	187 (4%)	2	15

5 of 187 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	278	ALA
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%)	1522 (89%)	195 (11%)	5	22
1	B	1722/2072 (83%)	1534 (89%)	188 (11%)	6	24
All	All	3439/4144 (83%)	3056 (89%)	383 (11%)	6	23

5 of 383 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1899	GLN
1	B	179	GLU
1	B	1823	VAL
1	A	1930	ARG
1	A	2111	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 98 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2076	ASN
1	B	350	HIS
1	B	1763	HIS
1	A	2086	GLN
1	B	142	ASN

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 [i](#)

There are no carbohydrates 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	-	45,52,52	1.37	4 (8%)	56,80,80	1.23	4 (7%)
2	NAP	B	3001	-	45,52,52	1.32	3 (6%)	56,80,80	1.41	5 (8%)
2	NAP	A	3002	-	45,52,52	1.24	3 (6%)	56,80,80	1.14	3 (5%)
2	NAP	A	3001	-	45,52,52	1.38	3 (6%)	56,80,80	1.22	3 (5%)

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	-	-	8/31/67/67	0/5/5/5
2	NAP	B	3001	-	-	2/31/67/67	0/5/5/5
2	NAP	A	3002	-	-	8/31/67/67	0/5/5/5
2	NAP	A	3001	-	-	11/31/67/67	0/5/5/5

The worst 5 of 13 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	NAP	C2N-N1N	5.09	1.41	1.35
2	A	3001	NAP	C2A-N3A	5.03	1.40	1.32
2	B	3001	NAP	C2N-N1N	4.97	1.41	1.35
2	A	3002	NAP	C2N-N1N	4.68	1.40	1.35
2	B	3002	NAP	C2A-N3A	4.46	1.39	1.32

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	3001	NAP	N3A-C2A-N1A	-5.95	119.37	128.68
2	A	3002	NAP	N3A-C2A-N1A	-5.42	120.20	128.68
2	B	3001	NAP	N3A-C2A-N1A	-5.30	120.39	128.68
2	B	3002	NAP	N3A-C2A-N1A	-5.02	120.84	128.68
2	B	3001	NAP	C3N-C7N-N7N	-4.36	112.52	117.75

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

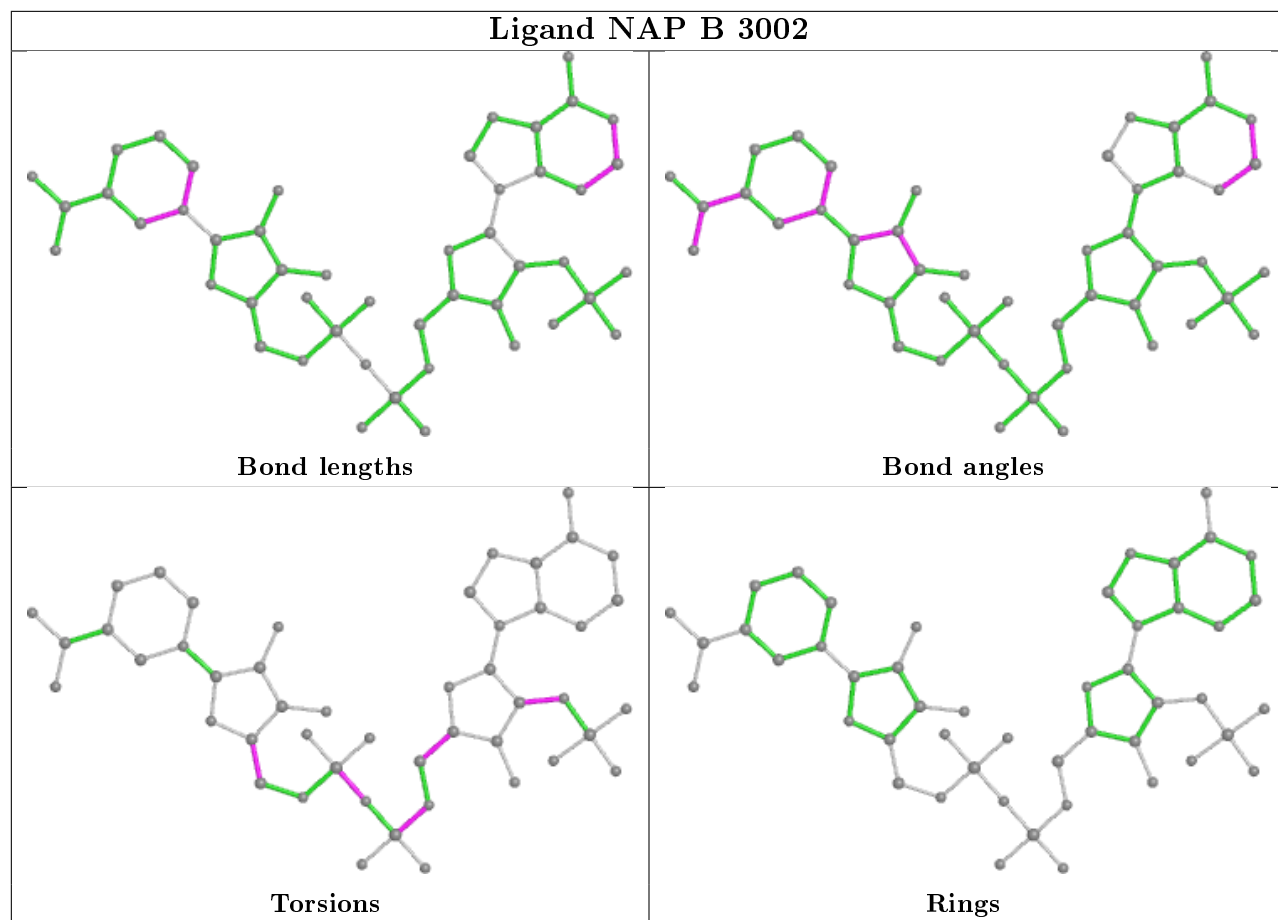
Mol	Chain	Res	Type	Atoms
2	B	3002	NAP	C3B-C4B-C5B-O5B
2	B	3002	NAP	C3B-C2B-O2B-P2B
2	A	3002	NAP	C5B-O5B-PA-O3
2	A	3002	NAP	C3B-C4B-C5B-O5B
2	A	3002	NAP	O4D-C4D-C5D-O5D

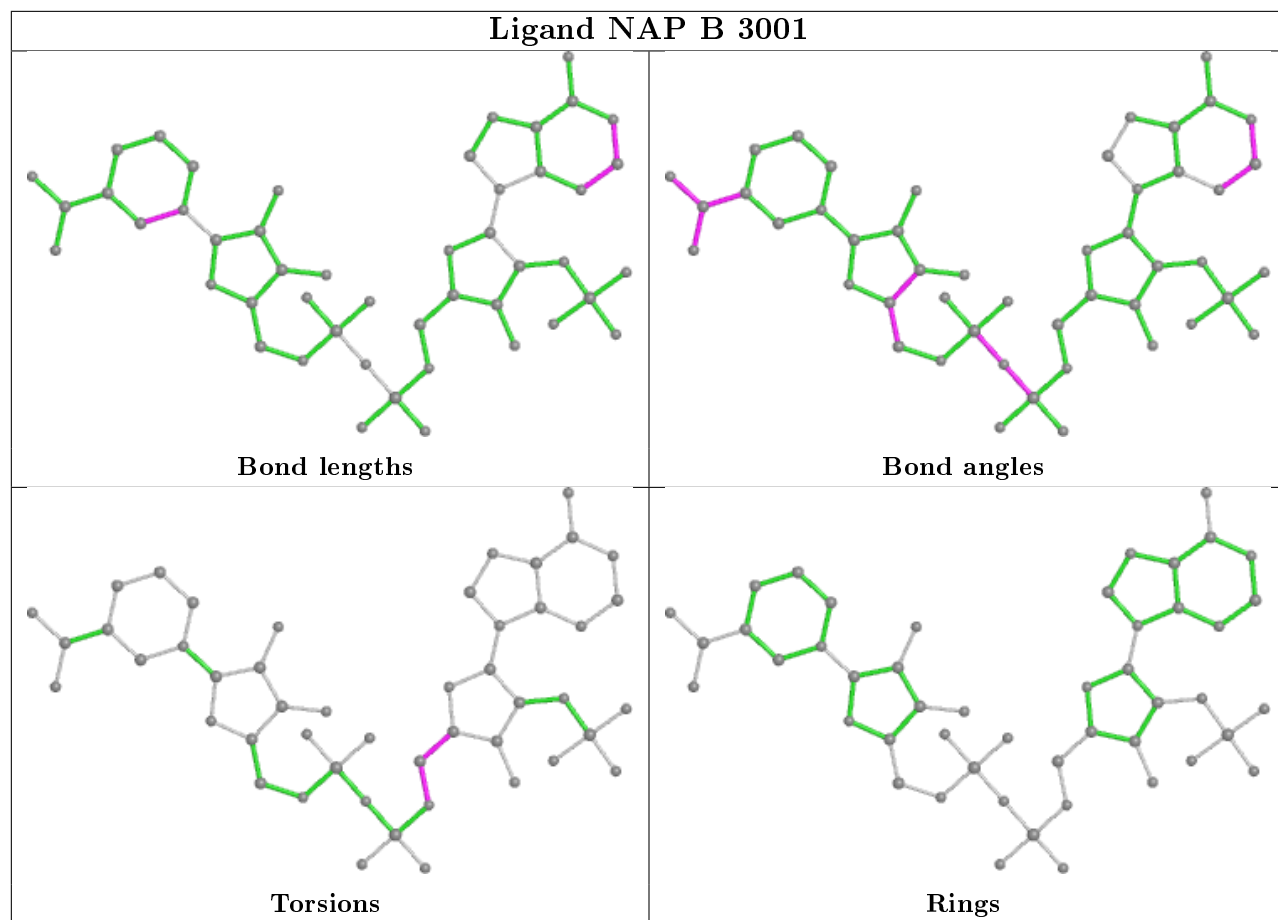
There are no ring outliers.

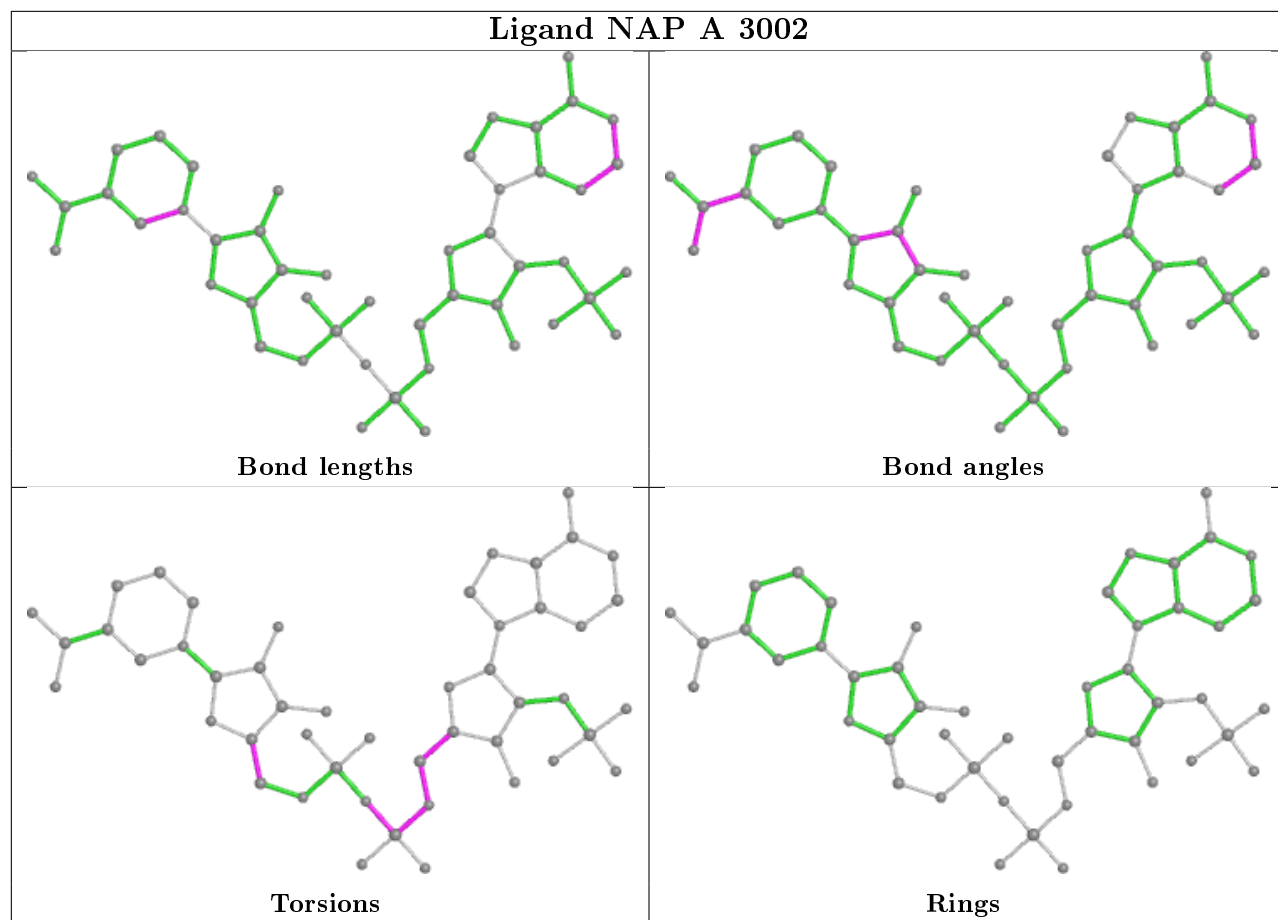
4 monomers are involved in 15 short contacts:

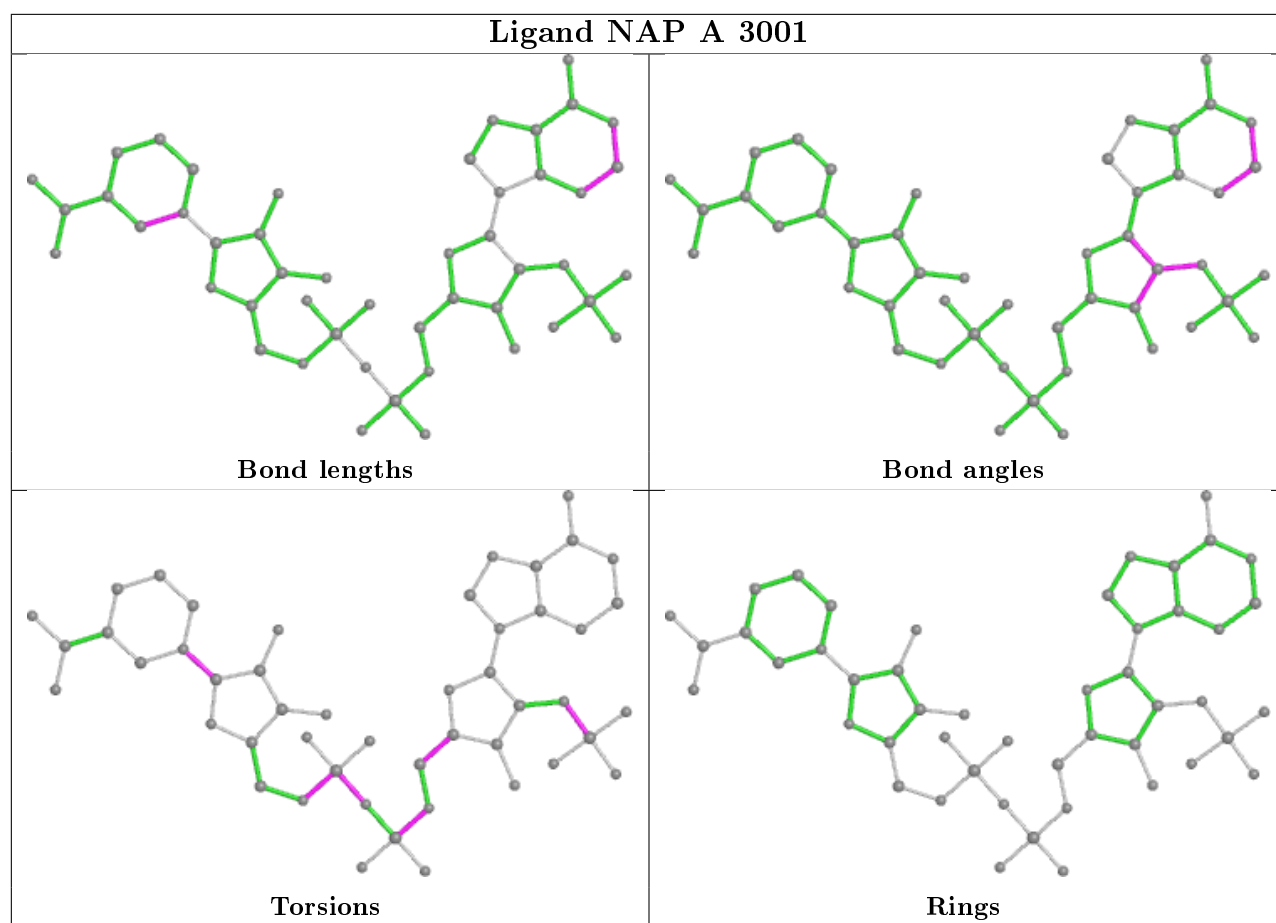
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	3002	NAP	2	0
2	B	3001	NAP	1	0
2	A	3002	NAP	4	0
2	A	3001	NAP	8	0

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%)	0.04	129 (6%)	20 20	73, 131, 230, 299	0
1	B	2086/2512 (83%)	0.22	155 (7%)	14 14	72, 166, 228, 299	0
All	All	4167/5024 (82%)	0.13	284 (6%)	17 17	72, 145, 229, 299	0

The worst 5 of 284 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	416	GLN	9.6
1	A	977	ASP	9.3
1	A	976	VAL	9.0
1	A	1297	GLY	7.1
1	B	672	VAL	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](#)

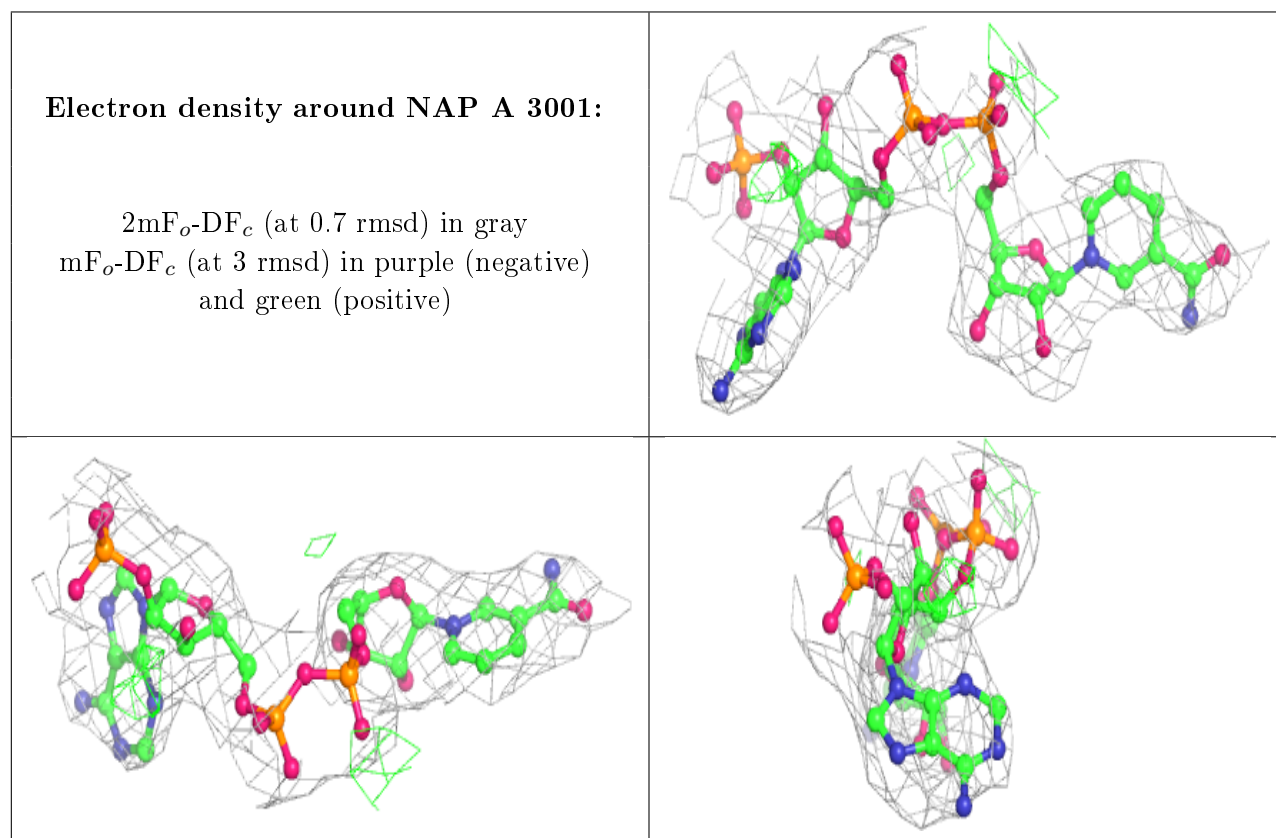
There are no carbohydrates in this entry.

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.

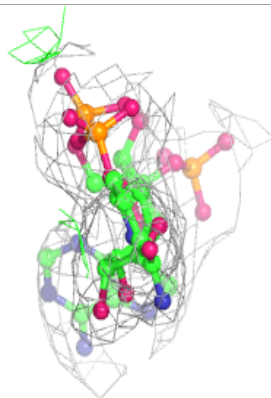
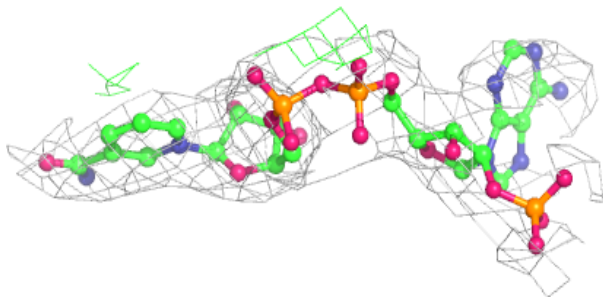
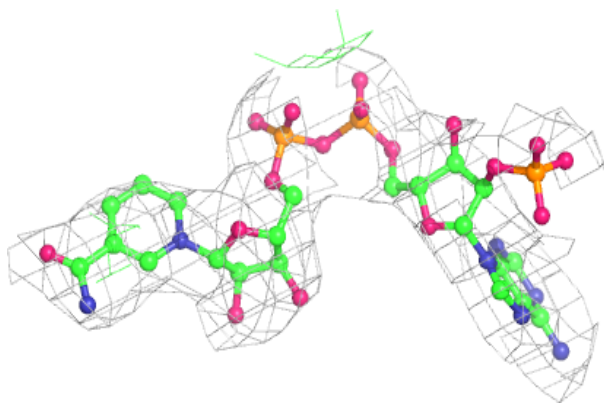
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAP	A	3001	48/48	0.90	0.32	100,122,179,189	0
2	NAP	B	3001	48/48	0.92	0.26	99,123,160,163	0
2	NAP	A	3002	48/48	0.95	0.20	96,135,161,194	0
2	NAP	B	3002	48/48	0.95	0.18	99,122,153,198	0

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.

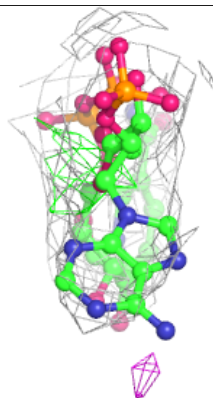
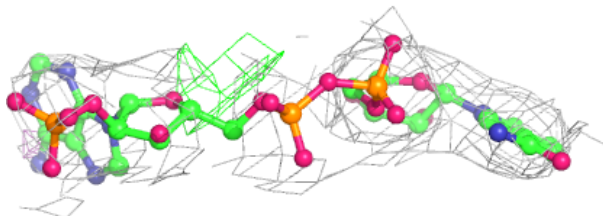
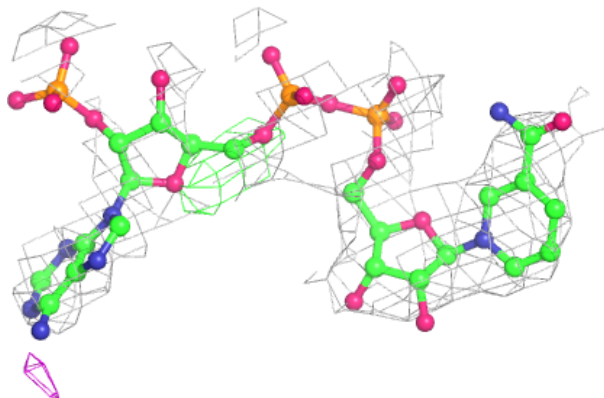


Electron density around NAP B 3001:

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

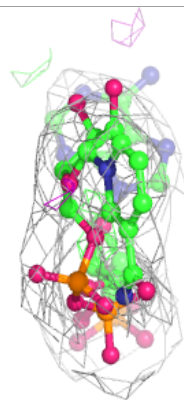
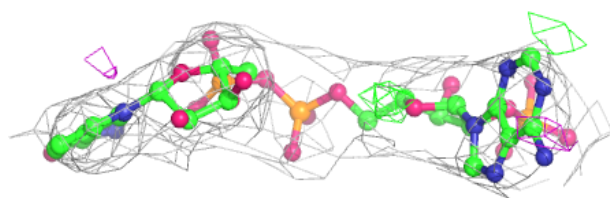
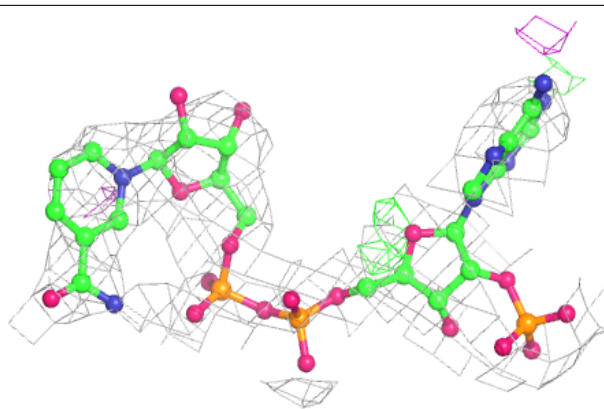
**Electron density around NAP A 3002:**

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



Electron density around NAP B 3002:

$2mF_o-DF_c$ (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.