wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 06:07 AM GMT

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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

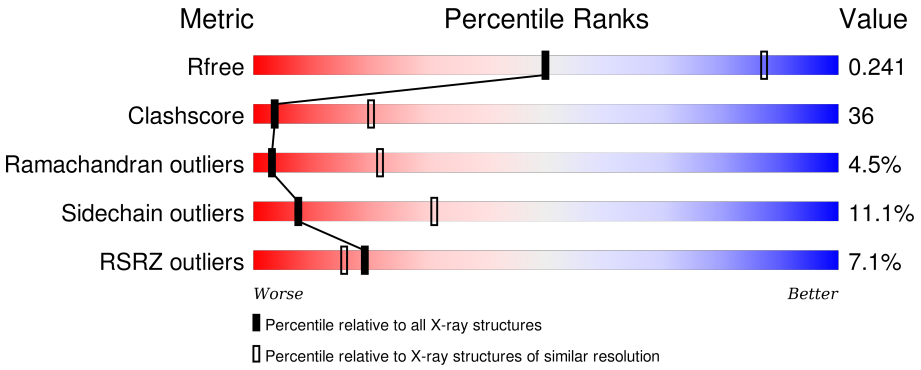
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 >=3, 2, 1 and 0 types of geometric quality criteria. 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 <=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	5% 38% 38% 7% 17%
1	B	2512	7% 36% 40% 7% 17%

2 Entry composition

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.

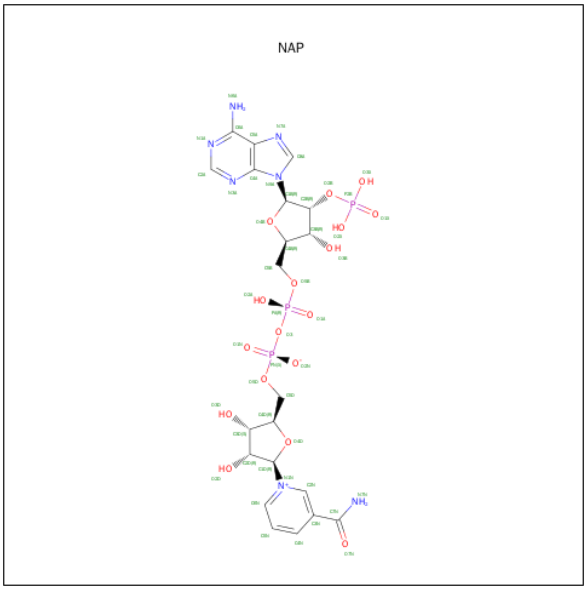
- Molecule 1 is a protein called FATTY ACID SYNTHASE.

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 SEE REMARK 9	UNP A5YV76
B	834	ILE	UNK	CONFLICT SEE REMARK 9	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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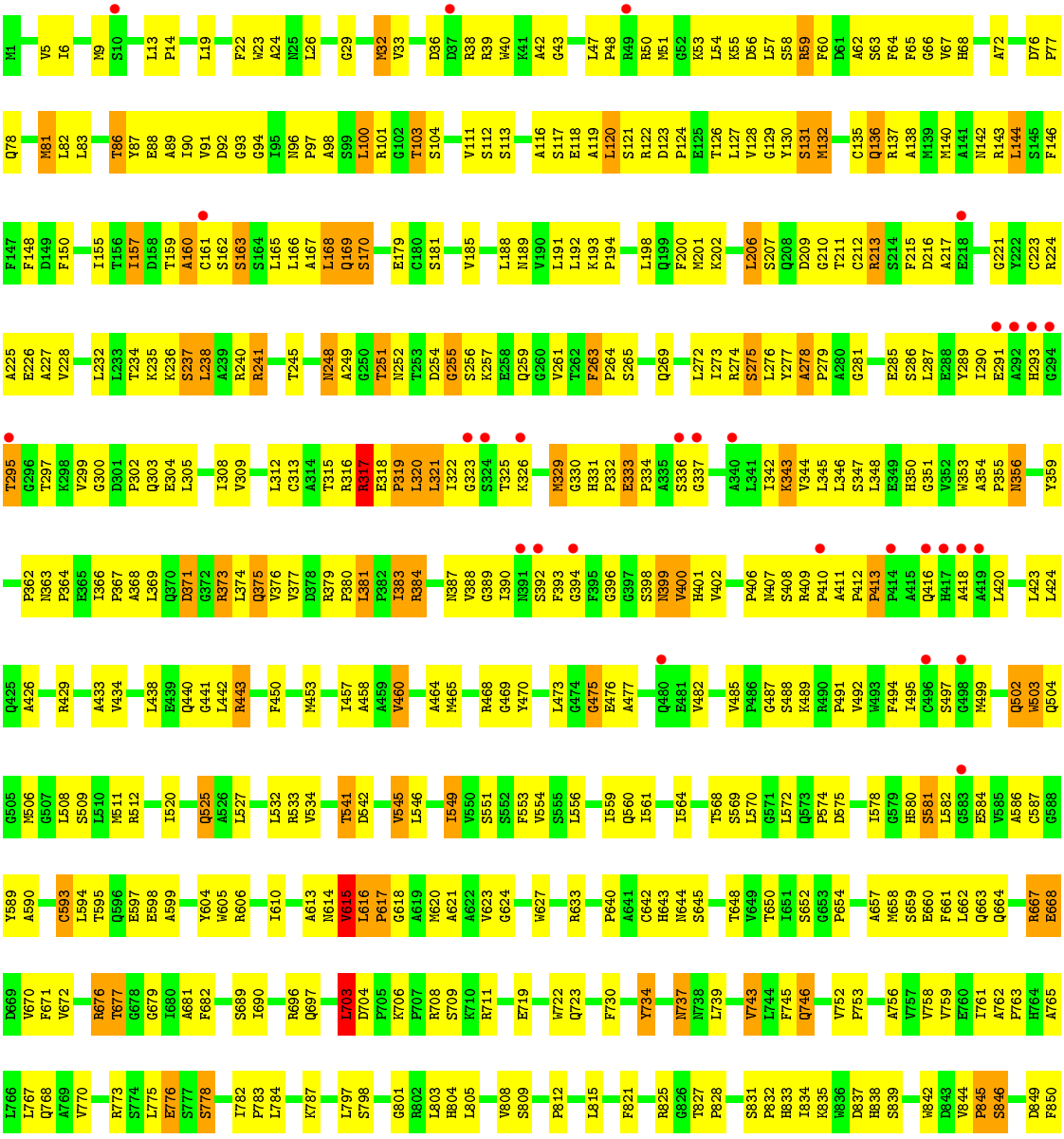
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		
2	B	1	Total	C	N	O	P	0	0
			48	21	7	17	3		

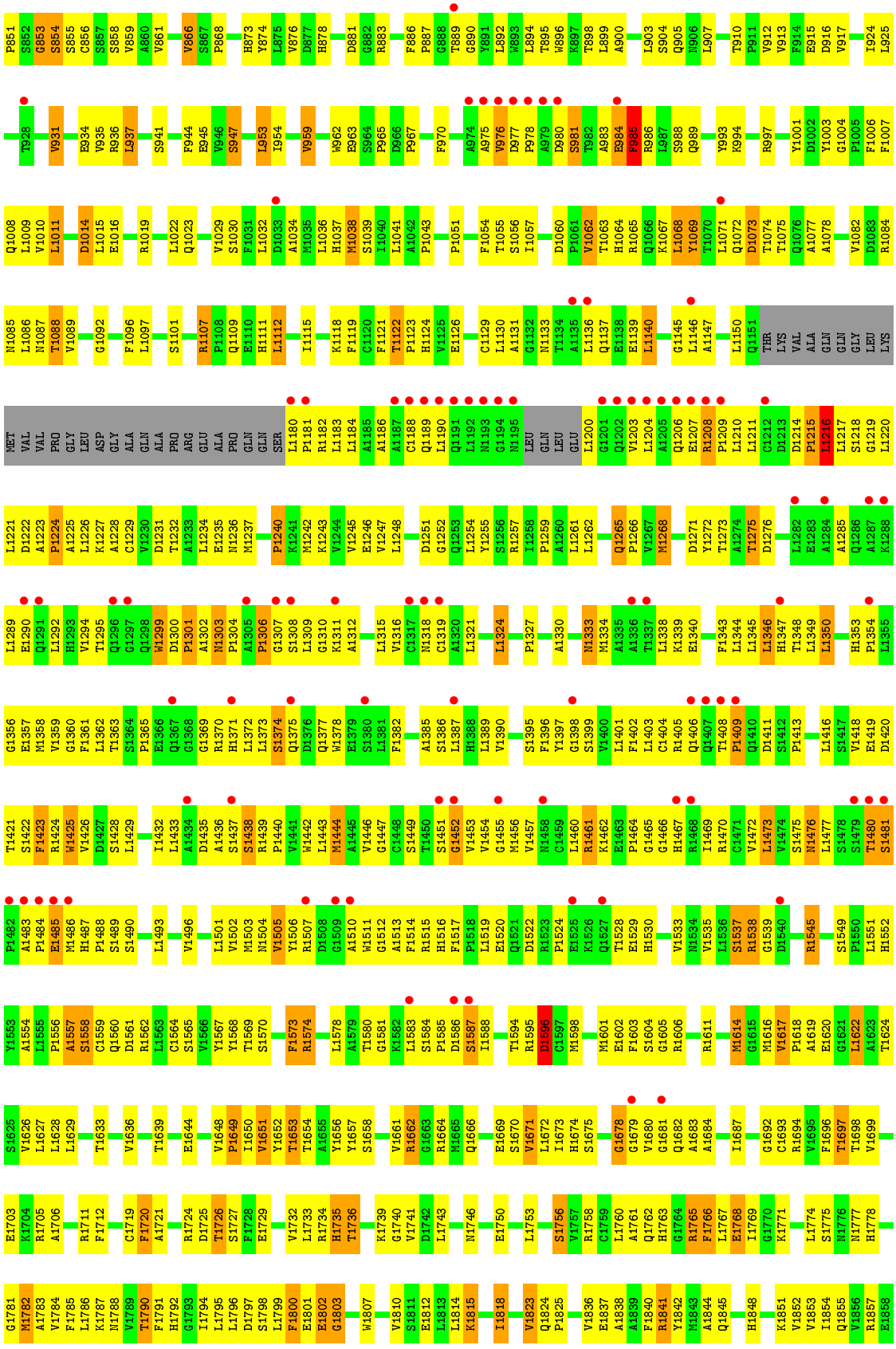
3 Residue-property plots (i)

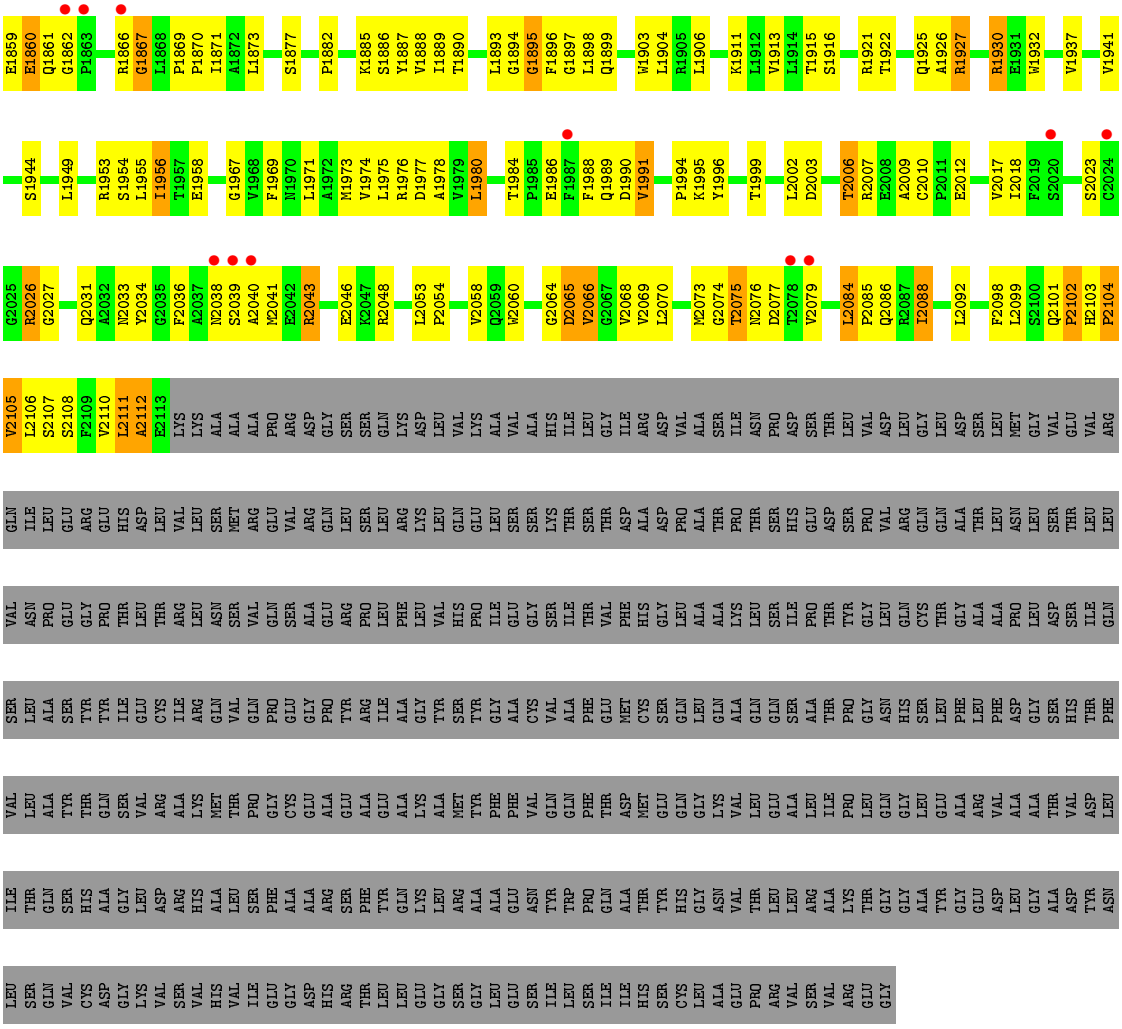
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

Chain A:

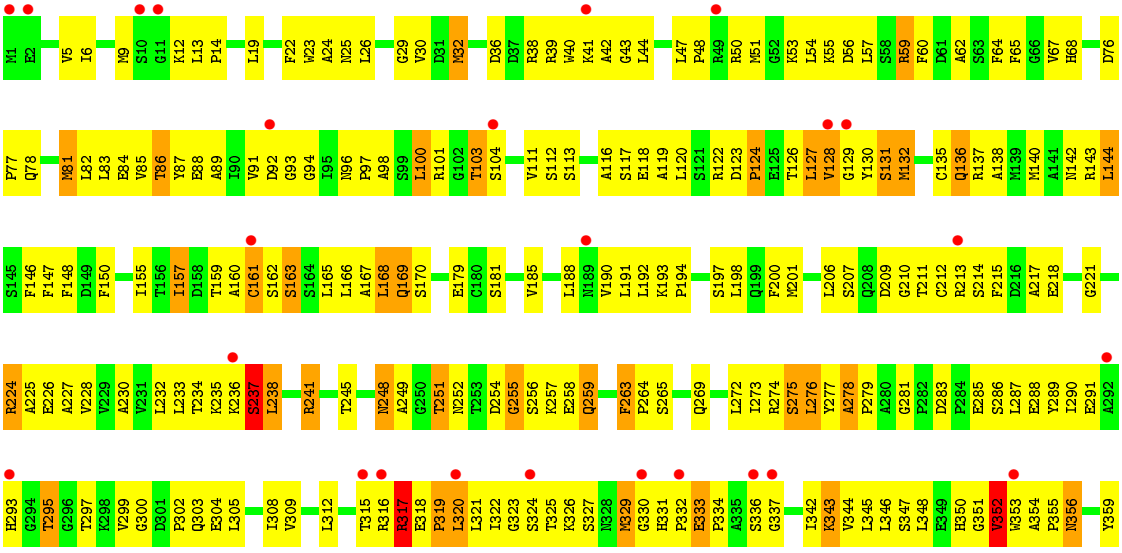


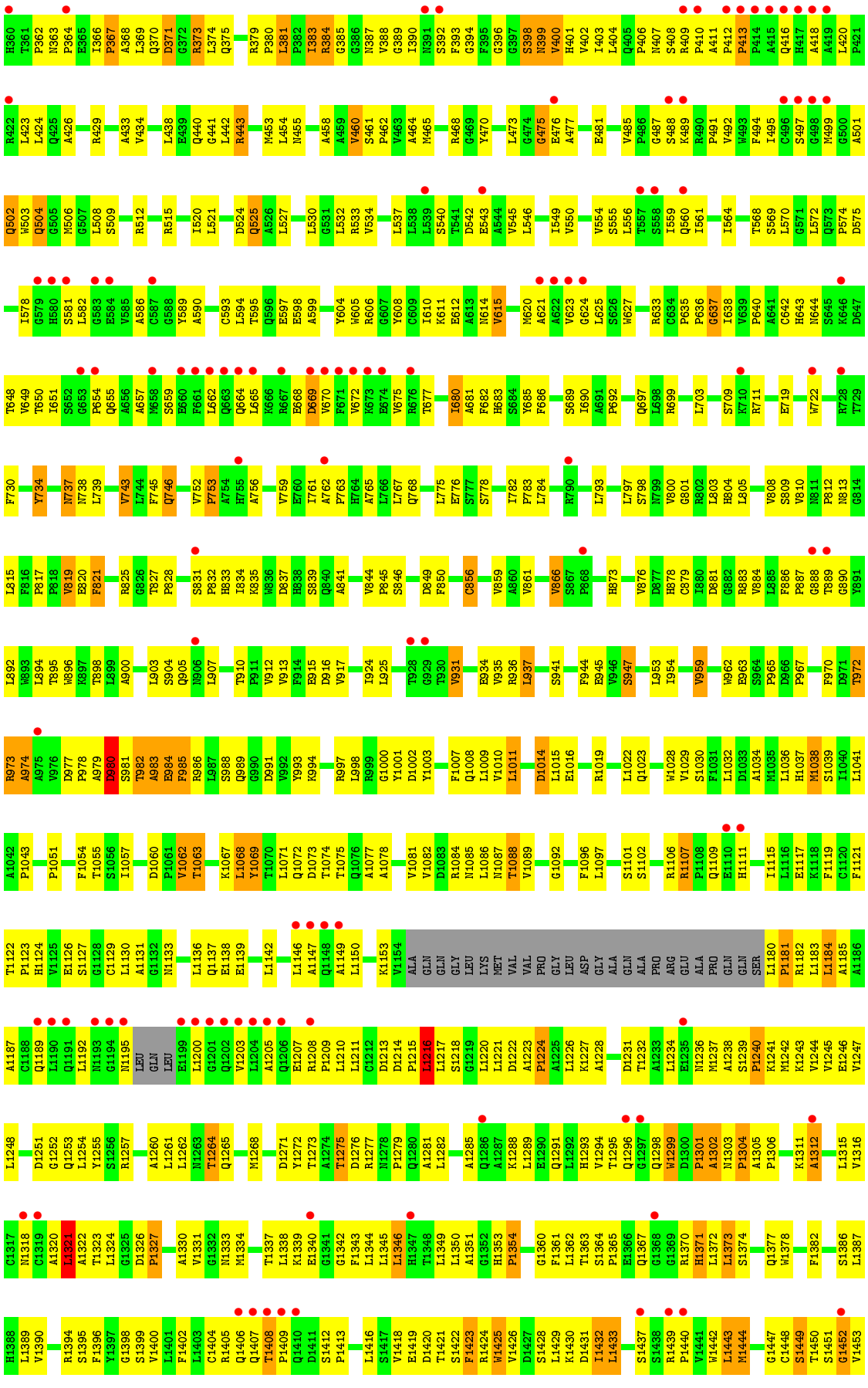

P851 S852 G853 S854 S855 C856 S857 S858 V859 A860 V861 V866 S867 P868 H873 Y874 L875 V876 D877 H878 D881 G882 R883 F886 P887 G888 T889 G890 Y891 L892 W893 L894 T895 W896 K897 T898 L899 A900 L903 S904 Q905 N906 L907 T910 P911 V912 V913 F914 E915 D916 V917 I924 L925
T928 V931 E934 V935 R936 L937 S941 F944 E945 V946 S947 L953 I954 V959 W962 E963 S964 P965 D966 P967 F970 A974 A975 V976 D977 P978 A979 D980 S981 T982 A983 E984 P985 R986 L987 S988 Q989 Y993 K994 R997 Y1001 D1002 Y1003 G1004 P1005 F1006 F1007
Q1008 L1009 V1010 L1011 D1014 L1015 E1016 R1019 L1022 Q1023 V1029 S1030 F1031 L1032 D1033 A1034 M1035 L1036 H1037 M1038 S1039 I1040 L1041 A1042 P1043 P1051 F1054 T1055 S1056 I1057 D1060 P1061 V1062 T1063 H1064 R1065 Q1066 K1067 L1068 Y1069 T1070 L1071 Q1072 D1073 T1074 T1075 Q1076 A1077 A1078 V1082 D1083 R1084
N1085 L1086 N1087 T1088 V1089 G1092 F1096 L1097 S1101 R1107 P1108 Q1109 E1110 H1111 L1112 I1115 K1118 F1119 C1120 F1121 T1122 P1123 H1124 V1125 E1126 C1129 L1130 A1131 G1132 N1133 T1134 A1135 L1136 Q1137 E1138 E1139 L1140 G1145 L1146 A1147 L1150 Q1151 THR LYS VAL ALA GLN GLN GLY LEU LYS
MET VAL VAL PRO GLY LEU ASP GLY ALA GLN ALA PRO ARG GLU ALA PRO GLN GLN SER L1180 P1181 R1182 L1183 L1184 A1185 A1186 A1187 C1188 Q1189 L1190 Q1191 L1192 N1193 G1194 N1195 LEU GLN LEU GLU L1200 G1201 Q1202 V1203 L1204 A1205 Q1206 E1207 R1208 P1209 L1210 L1211 C1212 D1213 D1214 P1215 L1216 L1217 S1218 G1219 G1220
L1221 D1222 A1223 P1224 A1225 L1226 K1227 A1228 C1229 V1230 D1231 T1232 A1233 L1234 E1235 N1236 M1237 P1240 K1241 M1242 K1243 V1244 V1245 E1246 V1247 L1248 D1251 G1252 Q1253 L1254 Y1255 S1256 R1257 I1258 P1259 A1260 L1261 L1262 Q1265 P1266 V1267 M1268 D1271 Y1272 T1273 A1274 T1275 D1276 L1282 E1283 A1284 A1285 Q1286 A1287 K1288
L1289 E1290 Q1291 L1292 H1293 V1294 T1295 Q1296 G1297 Q1298 W1299 D1300 P1301 A1302 N1303 P1304 A1305 P1306 G1307 S1308 L1309 G1310 K1311 A1312 L1315 V1316 C1317 N1318 C1319 A1320 L1321 L1324 P1327 A1330 N1333 M1334 A1335 A1336 T1337 L1338 K1339 E1340 F1343 L1344 L1345 L1346 H1347 T1348 L1349 L1350 H1353 P1354 L1355
G1356 E1357 M1358 V1359 G1360 F1361 L1362 T1363 S1364 P1365 E1366 Q1367 G1368 G1369 R1370 H1371 L1372 L1373 S1374 Q1375 D1376 Q1377 W1378 E1379 S1380 L1381 F1382 A1385 S1386 L1387 H1388 L1389 V1390 S1395 F1396 Y1397 G1398 S1399 V1400 L1401 F1402 L1403 C1404 R1405 Q1406 Q1407 T1408 P1409 Q1410 D1411 S1412 P1413 L1416 S1417 V1418 E1419 D1420
T1421 S1422 F1423 R1424 W1425 V1426 D1427 S1428 L1429 I1432 L1433 A1434 D1435 A1436 S1437 S1438 R1439 P1440 V1441 W1442 L1443 M1444 A1445 V1446 G1447 C1448 S1449 T1450 S1451 G1452 V1453 V1454 G1455 M1456 V1457 N1458 C1459 L1460 R1461 K1462 E1463 P1464 G1465 G1466 H1467 R1468 I1469 R1470 C1471 V1472 L1473 V1474 S1475 N1476 L1477 S1478 S1479 T1480 S1481
P1482 A1483 P1484 E1485 M1486 H1487 P1488 S1489 S1490 L1493 V1496 L1501 V1502 M1503 N1504 V1505 Y1506 R1507 D1508 G1509 A1510 W1511 G1512 A1513 F1514 R1515 H1516 F1517 P1518 L1519 E1520 Q1521 D1522 R1523 P1524 E1525 K1526 Q1527 T1528 E1529 H1530 V1533 N1534 V1535 L1536 S1537 R1538 G1539 D1540 R1545 S1549 P1550 L1551 H1552
Y1553 A1554 L1555 P1556 A1557 S1558 C1559 Q1560 D1561 R1562 L1563 C1564 S1565 V1566 Y1567 Y1568 T1569 S1570 F1573 R1574 L1578 A1579 T1580 G1581 K1582 L1583 S1584 P1585 D1586 S1587 I1588 T1594 R1595 D1596 C1597 M1598 M1601 E1602 F1603 S1604 G1605 R1606 R1611 M1614 G1615 M1616 V1617 P1618 A1619 E1620 G1621 L1622 A1623 T1624
S1625 V1626 L1627 L1628 L1629 T1633 V1636 T1639 E1644 V1648 P1649 I1650 V1651 Y1652 T1653 T1654 A1655 Y1656 Y1657 S1658 V1661 R1662 G1663 R1664 M1665 Q1666 E1669 S1670 V1671 L1672 I1673 H1674 S1675 G1678 G1679 V1680 G1681 Q1682 A1683 A1684 I1687 G1692 C1693 R1694 V1695 F1696 T1697 T1698 V1699
E1703 K1704 R1705 A1706 R1711 F1712 C1719 F1720 A1721 R1724 D1725 T1726 S1727 F1728 E1729 V1732 L1733 R1734 H1735 T1736 K1739 G1740 V1741 D1742 L1743 N1746 E1750 L1753 S1756 V1757 R1758 C1759 L1760 A1761 Q1762 H1763 G1764 R1765 F1766 L1767 E1768 I1769 G1770 K1771 L1774 S1775 N1776 N1777 H1778
G1781 M1782 A1783 V1784 F1785 L1786 K1787 N1788 V1789 T1790 F1791 H1792 G1793 I1794 L1795 L1796 D1797 S1798 L1799 F1800 E1801 E1802 G1803 W1807 V1810 S1811 E1812 L1813 L1814 K1815 I1818 V1823 Q1824 P1825 V1836 E1837 A1838 A1839 F1840 R1841 Y1842 M1843 A1844 Q1845 H1848 K1851 V1852 V1853 I1854 Q1855 V1856 R1857 E1858

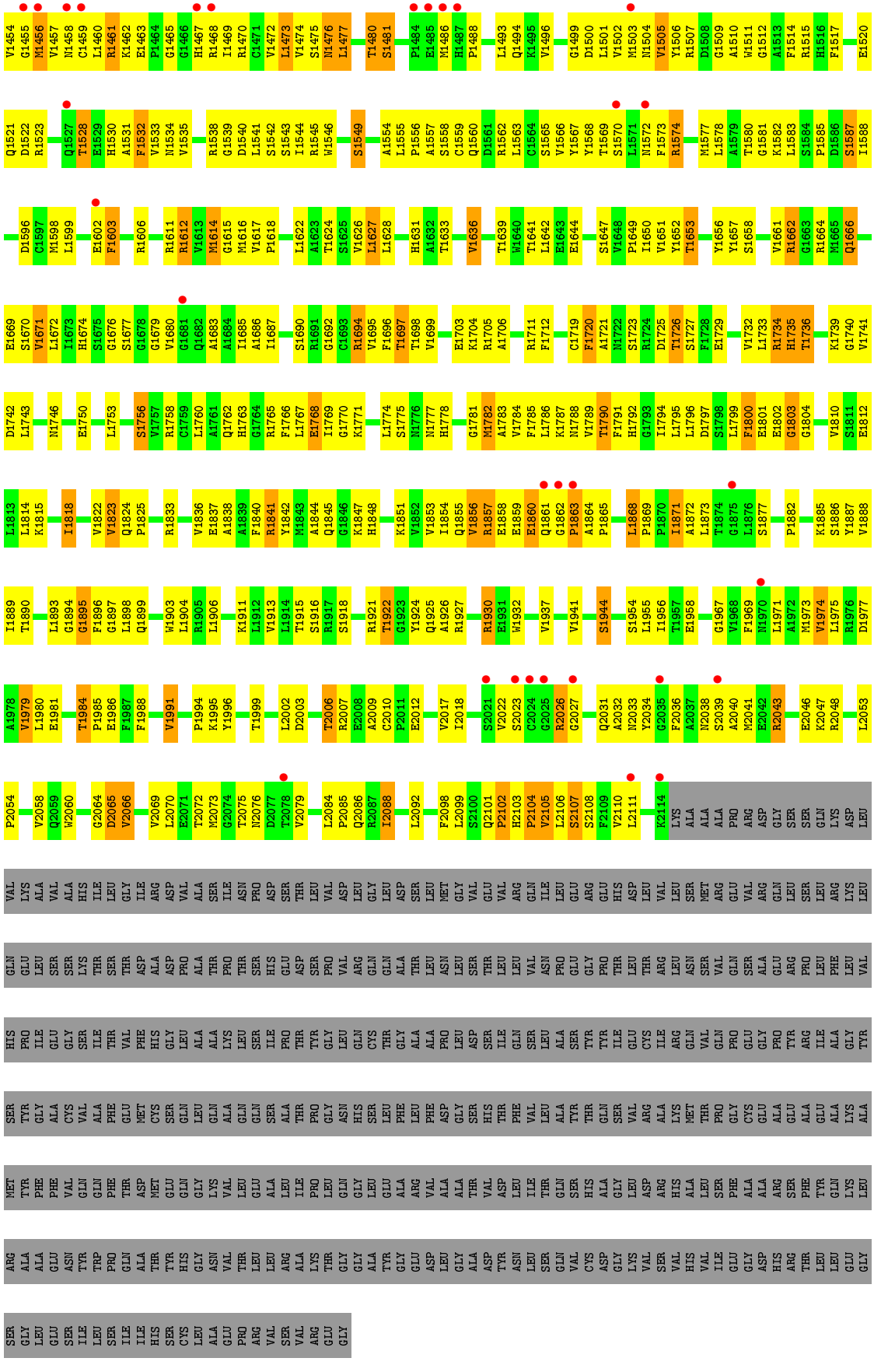


• Molecule 1: FATTY ACID SYNTHASE

Chain B:







4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.13 (at 3.31Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.193 , 0.244 0.198 , 0.241	Depositor DCC
R_{free} test set	4016 reflections (5.28%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.26$	Xtriage
Outliers	0 of 80013 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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(^{o})	Ideal(^{o})
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

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%)	3	21
1	B	2080/2512 (83%)	1713 (82%)	276 (13%)	91 (4%)	3	22
All	All	4155/5024 (83%)	3396 (82%)	572 (14%)	187 (4%)	3	21

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 (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1717/2072 (83%)	1522 (89%)	195 (11%)	7	29
1	B	1722/2072 (83%)	1534 (89%)	188 (11%)	8	32
All	All	3439/4144 (83%)	3056 (89%)	383 (11%)	8	31

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 (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no 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	A	3001	-	42,52,52	1.16	2 (4%)	54,80,80	1.97	4 (7%)
2	NAP	A	3002	-	42,52,52	0.99	2 (4%)	54,80,80	1.77	3 (5%)
2	NAP	B	3001	-	42,52,52	1.05	2 (4%)	54,80,80	1.97	6 (11%)
2	NAP	B	3002	-	42,52,52	1.09	3 (7%)	54,80,80	1.91	6 (11%)

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	A	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	A	3002	-	-	0/27/67/67	0/5/5/5
2	NAP	B	3001	-	-	0/27/67/67	0/5/5/5
2	NAP	B	3002	-	-	0/27/67/67	0/5/5/5

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	3002	NAP	C2A-N1A	2.08	1.37	1.33
2	B	3002	NAP	C6N-N1N	2.12	1.41	1.35
2	A	3002	NAP	C2A-N1A	2.13	1.38	1.33
2	B	3001	NAP	C2A-N1A	3.10	1.39	1.33
2	A	3001	NAP	C2A-N1A	3.13	1.39	1.33

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	3001	NAP	N3A-C2A-N1A	-12.43	119.37	128.89
2	A	3002	NAP	N3A-C2A-N1A	-11.35	120.20	128.89
2	B	3001	NAP	N3A-C2A-N1A	-11.11	120.39	128.89
2	B	3002	NAP	N3A-C2A-N1A	-10.52	120.84	128.89
2	B	3002	NAP	C4B-O4B-C1B	-5.34	103.85	109.72

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 15 short contacts:

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

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

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^{th} 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%)	0.06	132 (6%)	23	19	73, 131, 230, 299	0
1	B	2086/2512 (83%)	0.25	165 (7%)	15	12	72, 166, 228, 299	0
All	All	4167/5024 (82%)	0.15	297 (7%)	19	15	72, 145, 229, 299	0

The worst 5 of 297 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	416	GLN	9.8
1	A	977	ASP	9.6
1	A	976	VAL	9.4
1	A	1188	CYS	7.0
1	A	1297	GLY	7.0

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
2	NAP	A	3001	48/48	0.90	0.32	0.86	100,122,179,189	0
2	NAP	B	3001	48/48	0.92	0.26	0.12	99,123,160,163	0
2	NAP	A	3002	48/48	0.95	0.20	-0.36	96,135,161,194	0
2	NAP	B	3002	48/48	0.95	0.18	-0.51	99,122,153,198	0

6.5 Other polymers (i)

There are no such residues in this entry.