



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 28, 2020 – 10:09 AM BST

PDB ID : 2UV8  
Title : Crystal structure of yeast fatty acid synthase with stalled acyl carrier protein at 3.1 angstrom resolution  
Authors : Leibundgut, M.; Jenni, S.; Frick, C.; Ban, N.  
Deposited on : 2007-03-09  
Resolution : 3.10 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 : 2.13  
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) : 2.13

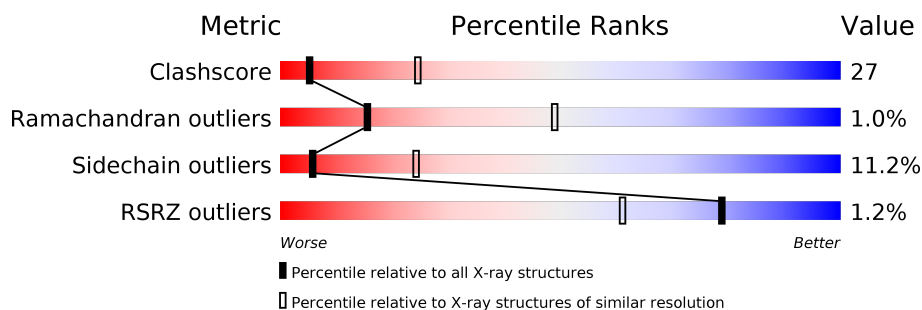
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

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	1887	 2% 50% 31% 5% 14%
1	B	1887	 % 51% 30% 5% 14%
1	C	1887	 2% 49% 31% 5% 14%
2	G	2051	 % 51% 41% 7% •
2	H	2051	 % 52% 40% 7% •
2	I	2051	 % 51% 41% 8% •

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 85962 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 SUBUNIT ALPHA (FAS2).

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			
1	B	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			
1	C	1614	Total	C	N	O	P	S	0	0	0
			12628	8003	2128	2448	1	48			

- Molecule 2 is a protein called FATTY ACID SYNTHASE SUBUNIT BETA (FAS1).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	G	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	H	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			
2	I	2033	Total	C	N	O	S	0	0	0
			15995	10253	2660	3026	56			

- Molecule 3 is FLAVIN MONONUCLEOTIDE (three-letter code: FMN) (formula: C<sub>17</sub>H<sub>21</sub>N<sub>4</sub>O<sub>9</sub>P).

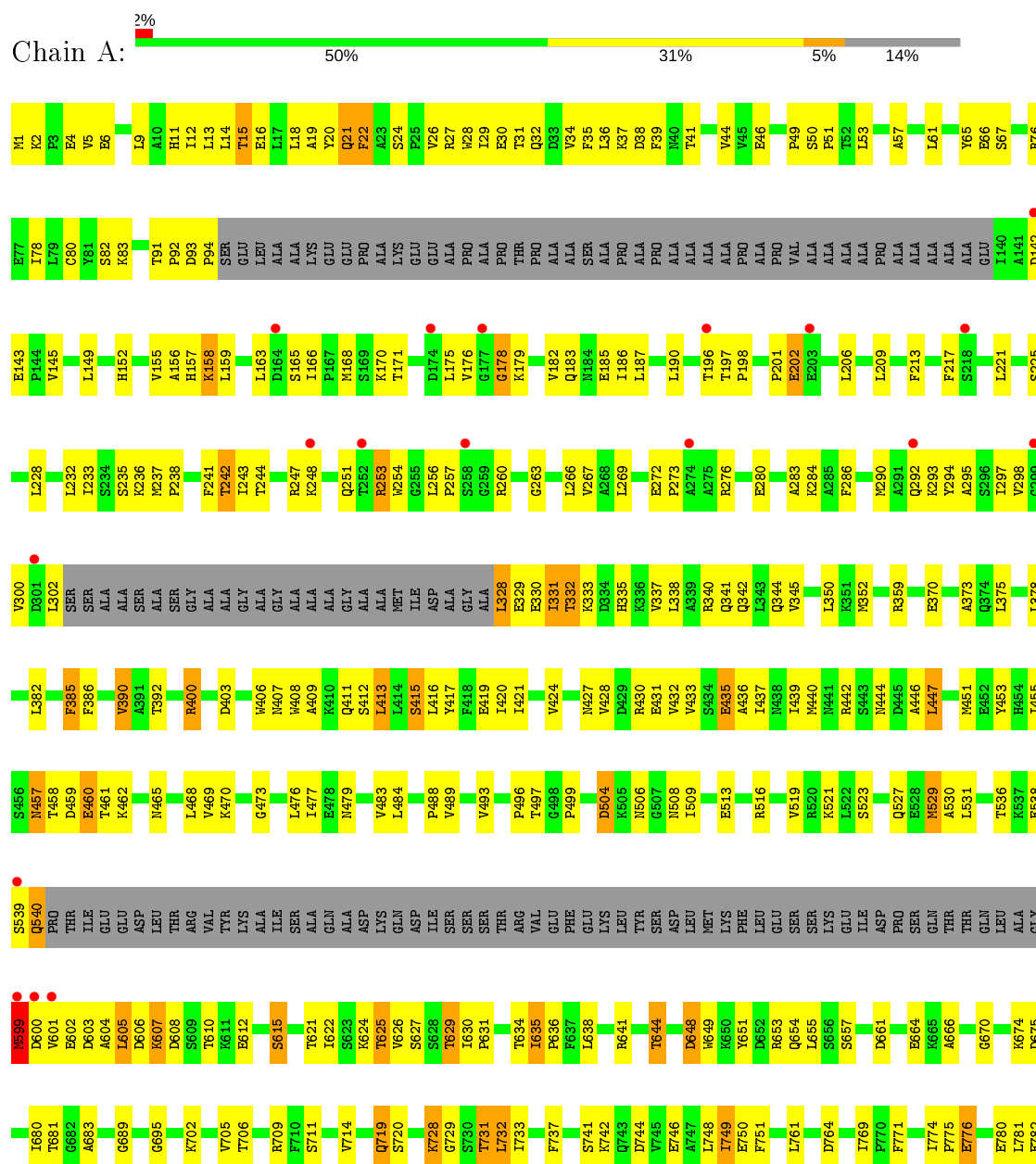


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	H	1	Total	C	N	O	P	0	0
			31	17	4	9	1		
3	I	1	Total	C	N	O	P	0	0
			31	17	4	9	1		

### 3 Residue-property plots

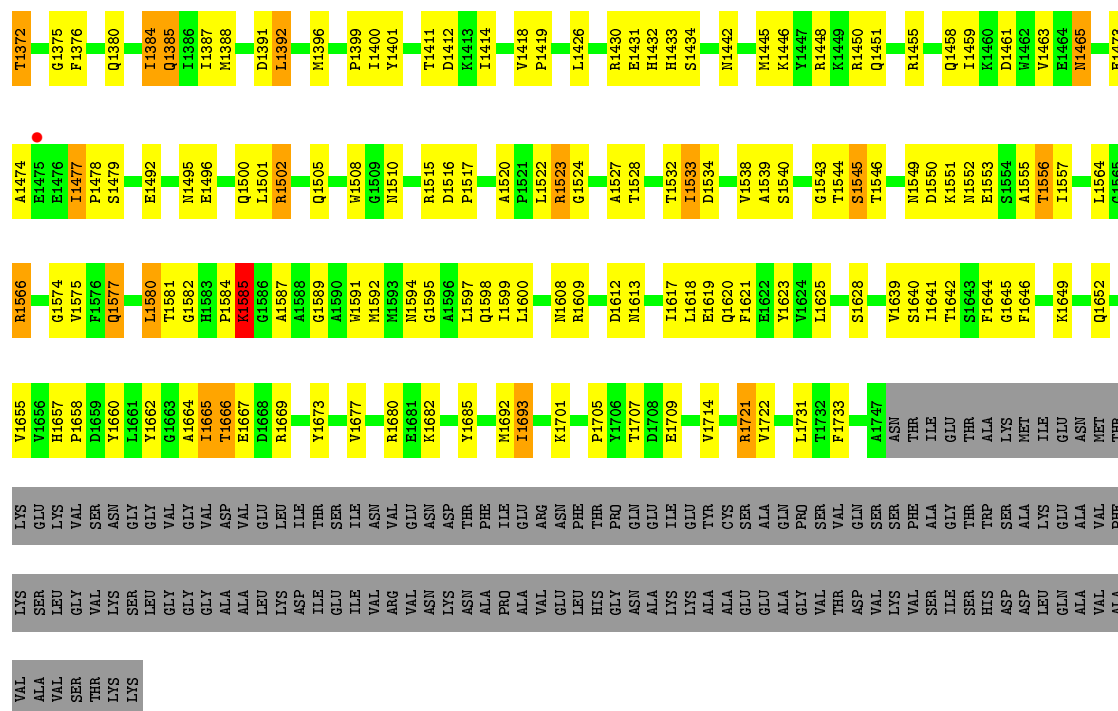
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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 SUBUNIT ALPHA (FAS2)

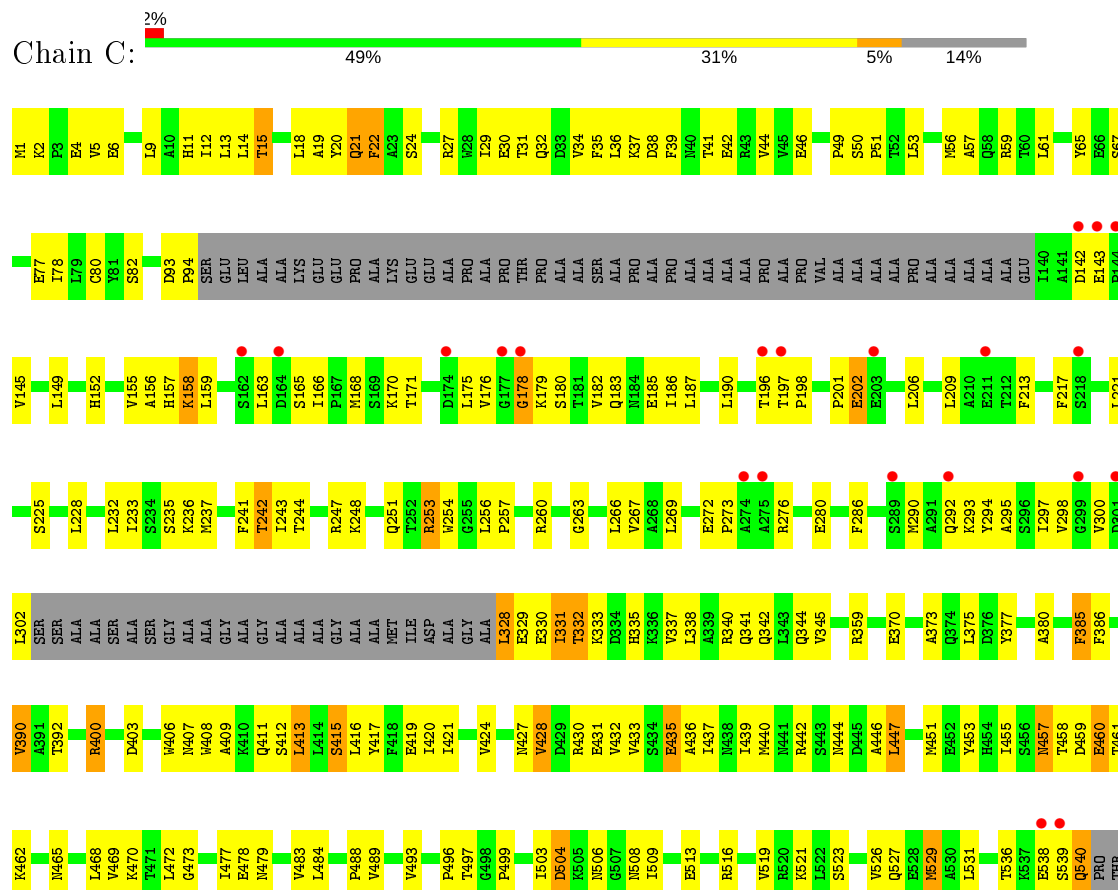




M1283	S1284	M1193	V1089	I988	E989	H792	K702	V601	E452	A373	A295	T216	I140	E66
A1285	M1194	R793	T1095	Q989	R890	R793	V705	E602	Y453	Q374	S296	F217	A141	E77
M1286	A1195	I794	S1096	L990	R891	I794	T706	A604	N457	L375	I297	L221	D142	I78
V1287	K1196	L796	I1097	F992	R893	L796	R709	L605	T458	L378	G299	S225	V144	L79
M1288	T1197	T797	K797	R894	R894	T797	F710	D606	D459	F385	V300	L228	V145	C80
M1289		M798	S711			M798	S711	K607	E460	F386	D301			Y81
		R801	V714			R801	V714	D608	T461		L302		L149	X83
		C805				C805		S609	K462		SER			S82
		V806	Q719			V806	Q719	T610	N465	V390	ALA	L232	H152	K83
		K807	S720			K807	S720	E612		T392	ALA	L233		Y90
		R818	G726			R818	G726	S615	L468		ALA	S234	V155	T91
		V822	K728			V822	K728	T621	V469	R400	ALA	S235	P156	P92
		I823	S730			I823	S730	G623	K470	F402	GLY	M237	H157	D93
		L824	T731			L824	T731	T625		D403	ALA	G239	K188	P94
		P825	I732			P825	I732	V626		W406	ALA	G240	L163	SER
		S827	I733			S827	I733	S627		W407	ALA	G241	D164	LEU
		P828	F737			P828	F737	G628		W408	ALA	T242	S165	GLU
		F833				F833		T629		W409	ALA	T243	I166	ALA
		G834	S741			G834	S741	L630		A409	ALA	T244	P167	GLU
		G835	K742			G835	K742	P631		Q411	ALA	R247	S169	PRO
		D836	Q743			D836	Q743	I638		S412	GLY		K170	ALA
		Y839	D744			Y839	D744	T644		L413	ALA	Q251	T171	LYS
		K843	E746			K843	E746	P636		L414	ALA	T252	L175	GLU
		E949	F637			E949	F637	L638		L416	ILE	R253	V176	GLU
		F953	L748			F953	L748	P499		Y417	ILE	Q254	G177	ALA
		A956	I749			A956	I749	G498		A494	ASP	Q255	G178	PRO
		E964	E750			E964	E750	P499		P636	ALA	L256	K179	ALA
		V968	F751			V968	F751	D648		E419	GLY	P257	S180	PRO
		N969	L761			N969	L761	K605		E419	GLY	R260	T181	THR
		G970	D764			G970	D764	N506		I421	ALA	G263	Q183	PRO
		V972	I769			V972	I769	N508		V424	ASP	L266	N184	ALA
		A973	F771			A973	F771	T510		D504	ASP	V267	E185	SER
		A976	E776			A976	E776	E513		N427	ASP	L268	I186	ALA
		Y977	I774			Y977	I774	V519		V428	ASP	A288	L187	PRO
		Y978	E776			Y978	E776	D675		D429	ASP	L269	G188	ALA
		Y979	E780			Y979	E780	F668		N430	ASP	L269	D189	PRO
		Y980	L781			Y980	L781	D661		E431	ASP	E272	L190	ALA
		Y981	E782			Y981	E782	P668		V432	ASP	P273	G191	ALA
		Y982	H783			Y982	H783	F668		V433	ASP	A274	K192	ALA
		Y983	SER			Y983	SER	D675		S434	ASP	A275	T196	PRO
		Y984	ALA			Y984	ALA	K674		A436	ASP	R276	T197	ALA
		Y985	ALA			Y985	ALA	D675		I437	ASP	E280	P198	PRO
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		Y987	ALA			Y987	ALA	F668		I439	ASP	E280	P198	ALA
		Y988	ALA			Y988	ALA	F668		N440	ASP	E280	P198	ALA
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		Y990	ALA			Y990	ALA	F668		N442	ASP	E280	P198	ALA
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		Y999	ALA			Y999	ALA	F668		N451	ASP	E280	P198	ALA
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		Y1003	ALA			Y1003	ALA	F668		N455	ASP	E280	P198	ALA
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		Y1048	ALA			Y1048	ALA	F668		N500	ASP	E280	P198	ALA
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• Molecule 1: FATTY ACID SYNTHASE SUBUNIT ALPHA (FAS2)

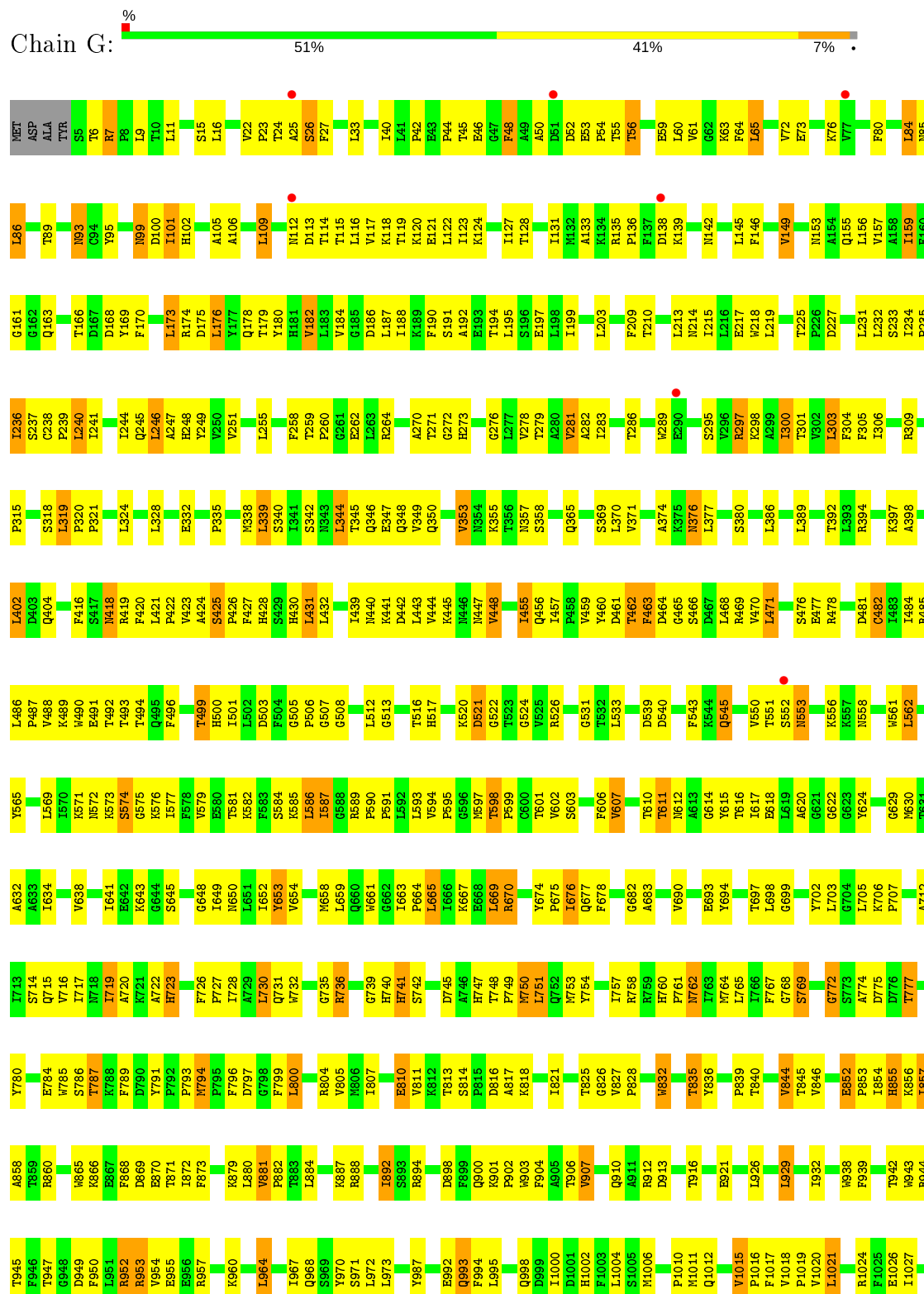


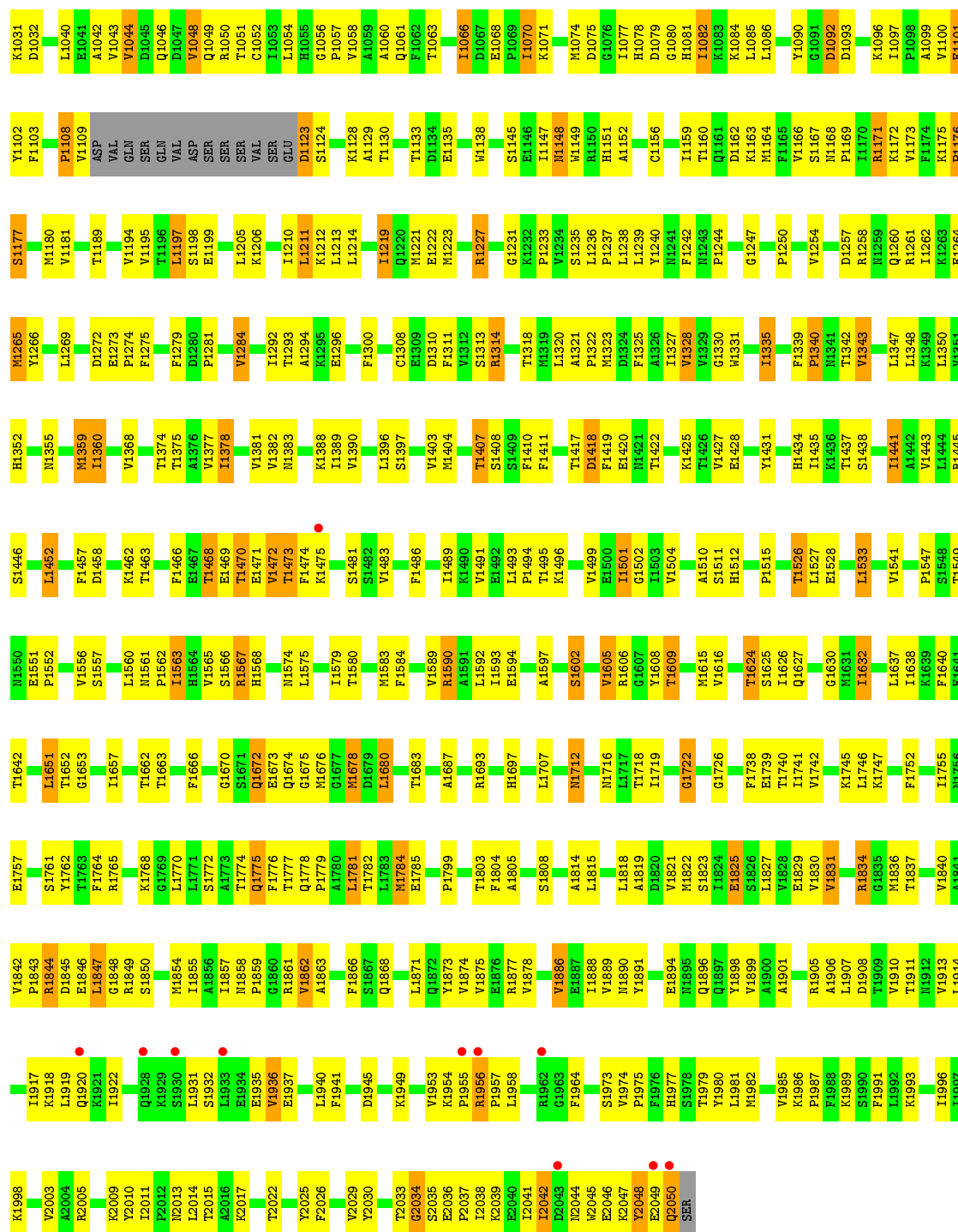


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ASP	T1707	F1621	S1540	Q1451	P1362	Q1276	P1190	V1099	V980	I883	A791	D606	GLU
THR	D1708	E1622	G1543	R1455	A1363	F1279	W1193	D1088	Q983	I888	R792	K607	ASP
PHE	E1709	E1623	T1544	R1455	E1364	I1280	M1194	D1089	Q984	E889	R793	D608	LEU
ILE	Y1714	Y1624	S1545	Q1458	S1366	W1281	A1195	V1099	R885	R890	R794	S609	THR
ARG	Y1714	L1625	T1546	Q1458	A1367	T1282	K1196	T1095	I988	R891	L796	T610	ARG
ASN	D1717	Y1627	T1546	I1459	R1367	M1283	T1197	S1096	Q989	R892	T797	K611	VAL
PHE	S1628	S1628	M1549	K1460	T1370	A1285	D1202	I1097	Q989	R894	N798	E612	LYS
THR	L1719	F1644	D1550	K1461	T1371	A1285	V1208	G1102	F952	R901	R709	E612	ALA
PRO	A1720	F1644	K1551	W1462	T1372	M1289	D1208	G1102	F952	R901	R709	S615	ILE
GLN	R1721	S1640	N1552	W1463	R1373	L1290	D1209	I1103	Y988	O805	S711	L616	SER
GLU	Y1722	I1641	E1553	E1464	E1574	L1291	D1209	I1103	Y988	O805	S711	P617	ALA
ILE	L1731	S1642	S1554	N1465	F1376	I1292	T1212	R1104	I1004	R806	V714	P617	GLN
GLU	L1732	S1643	A1555	N1465	F1376	I1292	T1212	R1104	I1004	R806	V714	P617	ALA
THR	F1733	F1644	T1556	E1473	Q1380	G1296	F1214	Y1114	L1009	R818	Q719	I622	ASP
CYS	F1733	F1646	I1557	E1475	G1381	P1297	V1215	N1115	E1010	R818	Q719	I622	LYS
SER	Y1738	F1646	L1564	E1475	A1382	P1297	V1215	P1116	E1010	R818	Q719	I622	GLN
ALA	Q1739	K1649	G1565	E1475	A1382	P1297	V1215	P1116	E1010	R818	Q719	I622	GLN
GLN	Y1744	G1650	R1566	E1475	A1382	P1297	V1215	P1116	E1010	R818	Q719	I622	ASP
PRO	Y1744	G1650	R1566	E1475	A1382	P1297	V1215	P1116	E1010	R818	Q719	I622	GLN
SER	Y1744	G1650	R1566	E1475	A1382	P1297	V1215	P1116	E1010	R818	Q719	I622	GLN
VAL	N1746	Q1652	I1573	E1480	I1386	A1304	I1224	E1124	I1019	N927	S730	T629	SER
SER	A1747	Q1652	I1573	E1480	I1386	A1304	I1224	E1124	I1019	N927	S730	T629	THR
SER	ASN	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
SER	THR	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
PHE	THR	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
GLY	GLU	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
GLY	GLU	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
TRP	ALA	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
SER	LYS	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
ALA	MET	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
LYS	ILE	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
GLU	GLU	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
ALA	ASN	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
VAL	MET	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
PHE	THR	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
LYS	LYS	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
SER	GLU	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
LEU	LYS	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
GLY	VAL	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
SER	ASN	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
LYS	LYS	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
SER	GLY	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
LEU	GLY	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
GLY	VAL	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
GLY	VAL	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
ALA	ASP	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
ALA	VAL	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
LEU	GLU	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
LEU	LEU	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
LYS	LEU	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
ASP	ILE	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
THR	THR	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
GLU	SER	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
ILE	ILE	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
VAL	VAL	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG
ARG	ARG	Y1655	V1576	L1487	M1388	C1305	A1226	Y1126	V1020	G929	S731	I630	ARG

VAL	ASP	ASN	LYS	ASN	ALA	PRO	ALA	ALA	VAL	GLU	HIS	GLY	ASN	ALA	LYS	LYS	ALA	ALA	GLU	GLU	GLY	VAL	THR	ASP	VAL	LYS	VAL	SER	ILE	SER	HIS	ASP	ASP	LEU	GLN	ALA	VAL	ALA	VAL	ALA	VAL	SER	THR	LYS	LYS
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----

• Molecule 2: FATTY ACID SYNTHASE SUBUNIT BETA (FAS1)











K2009	I1917	T1837	K1745	T1642	S1548
Y2010	K1918	M1838	L1746		T1549
T2011	L1919		K1747	V1650	I1550
P2012	Q1920	V1842		L1651	E1551
N2013	K1921	P1843	F1752	T1652	P1552
L2014	I1922	R1844	E1757	G1653	
L2015	K1929	D1845		I1657	V1556
T2016	S1930	E1846	S1761		S1557
A2016	L1931	L1847	F1764	T1662	L1560
K2017	S1932	R1848	R1765	T1663	N1561
		S1850			P1562
Q2020	E1936	M1854	L1770	F1666	I1563
V2021	V1936	I1855			H1564
T2022	E1937		T1774	G1670	V1565
Y2025	L1940	P1859	Q1775	S1671	S1566
F2026	F1941	G1860	F1776	Q1672	R1567
		R1861	T1777	E1673	H1568
V2029	D1945	V1862	Q1778	Q1674	
Y2030		A1863	P1779	Q1675	L1575
	K1949		A1780	M1676	
T2033	V1953	F1866	L1781	G1677	I1579
G2034	K1954	S1867	T1782	M1678	T1580
S2035	P1955	Q1868	L1783	D1679	
E2036	R1956		H1784	L1680	M1583
P2037	R1957	L1871	E1785	Y1881	F1584
I2038	L1958	Q1872	K1793	A1882	V1589
K2039	K1959	Y1873		T1683	R1590
E2040		V1874	I1798	S1684	A1591
L2041	F1964		P1799	A1687	L1592
T2042	I1967	R1877		Q1688	I1593
E2043	P1968	V1878	T1803		E1594
N2044		V1886	F1804	R1693	
W2045		E1887	A1805	H1697	A1597
E2046	S1973	I1888			
K2047	V1974	V1889	S1808	L1707	S1602
Y2048	P1975	M1890	A1814		V1605
E2049	F1976	Y1891	L1815	M1712	Y1608
Q2050	H1977	M1892		N1716	T1609
SER		V1893	L1818	N1716	
	Y1980		A1819	L1717	M1615
	L1981	Q1896	D1820	T1718	V1616
		Q1897	V1821	L1719	
	V1985	Y1898	M1822		T1624
	K1986	V1899	S1823	G1722	S1625
	P1987	A1900	H1824		I1626
	F1988	A1901	E1825	G1726	Q1627
	K1989		S1826		
		A1906	L1827	A1735	G1630
	K1993	L1907	V1828	M1736	
		D1908	E1829	I1737	M1631
	I1996	T1909	V1830	F1738	I1632
	I1997	V1910	V1831	E1739	
	K1998	T1911		T1740	L1637
		H1912	R1834	I1741	I1638
	V2003	V1913	G1835	V1742	F1640
	A2004	L1914		D1743	
	R2005			G1744	E1641

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	230.60 Å   230.60 Å   784.30 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	12.00 – 3.10 12.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	86.1 (12.00-3.10) 91.5 (12.00-3.10)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.94 (at 3.09 Å)	Xtriage
Refinement program	PHENIX, PHENIX	Depositor
R, $R_{free}$	0.200 ,   0.250 0.202 ,   (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	74.1	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	85962	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.36% 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

### 5.1 Standard geometry

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

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	0.41	0/12848	0.59	2/17358 (0.0%)
1	B	0.42	0/12848	0.59	2/17358 (0.0%)
1	C	0.41	0/12848	0.59	2/17358 (0.0%)
2	G	0.37	0/16360	0.56	0/22198
2	H	0.37	0/16360	0.57	0/22198
2	I	0.37	0/16360	0.56	0/22198
All	All	0.39	0/87624	0.58	6/118668 (0.0%)

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
2	G	0	1
2	H	0	1
2	I	0	1
All	All	0	3

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	599	MET	N-CA-C	-6.92	92.32	111.00
1	B	599	MET	N-CA-C	-6.91	92.36	111.00
1	C	599	MET	N-CA-C	-6.90	92.36	111.00
1	B	540	GLN	N-CA-C	-5.67	95.69	111.00
1	C	540	GLN	N-CA-C	-5.63	95.81	111.00

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	G	1108	PRO	Peptide
2	H	1108	PRO	Peptide
2	I	1108	PRO	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	12628	0	12603	572	0
1	B	12628	0	12603	587	0
1	C	12628	0	12603	584	0
2	G	15995	0	15978	984	0
2	H	15995	0	15978	995	0
2	I	15995	0	15978	996	0
3	G	31	0	19	7	0
3	H	31	0	19	6	0
3	I	31	0	19	6	0
All	All	85962	0	85800	4562	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 27.

The worst 5 of 4562 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)
2:I:1956:ARG:HB2	2:I:1957:PRO:HD3	1.23	1.21
2:G:499:THR:HB	2:G:500:HIS:HD2	1.07	1.16
2:G:1956:ARG:HB2	2:G:1957:PRO:HD3	1.23	1.14
2:H:490:TRP:HE1	2:H:516:THR:HG22	1.11	1.13
2:G:490:TRP:HE1	2:G:516:THR:HG22	1.12	1.13

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	1603/1887 (85%)	1498 (93%)	91 (6%)	14 (1%)	17	52
1	B	1603/1887 (85%)	1495 (93%)	95 (6%)	13 (1%)	19	54
1	C	1603/1887 (85%)	1498 (93%)	90 (6%)	15 (1%)	17	52
2	G	2029/2051 (99%)	1841 (91%)	163 (8%)	25 (1%)	13	44
2	H	2029/2051 (99%)	1841 (91%)	166 (8%)	22 (1%)	14	46
2	I	2029/2051 (99%)	1837 (90%)	168 (8%)	24 (1%)	13	44
All	All	10896/11814 (92%)	10010 (92%)	773 (7%)	113 (1%)	15	49

5 of 113 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	504	ASP
1	A	538	GLU
1	A	605	LEU
1	A	834	GLY
1	A	1252	GLY

### 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	1366/1565 (87%)	1220 (89%)	146 (11%)	6	26
1	B	1366/1565 (87%)	1222 (90%)	144 (10%)	7	26
1	C	1366/1565 (87%)	1224 (90%)	142 (10%)	7	27

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	G	1772/1789 (99%)	1564 (88%)	208 (12%)	5	22
2	H	1772/1789 (99%)	1564 (88%)	208 (12%)	5	22
2	I	1772/1789 (99%)	1562 (88%)	210 (12%)	5	20
All	All	9414/10062 (94%)	8356 (89%)	1058 (11%)	6	24

5 of 1058 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	402	LEU
2	G	1501	ILE
2	I	1171	ARG
2	G	539	ASP
2	G	929	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 276 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1000	GLN
2	G	440	ASN
2	I	910	GLN
1	C	1066	ASN
1	C	1563	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
1	GVL	C	180	1	15,18,19	0.77	0	20,26,28	0.98	1 (5%)
1	GVL	B	180	1	15,18,19	0.70	0	20,26,28	0.86	1 (5%)
1	GVL	A	180	1	15,18,19	0.73	0	20,26,28	0.81	0

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
1	GVL	C	180	1	-	6/21/25/27	-
1	GVL	B	180	1	-	6/21/25/27	-
1	GVL	A	180	1	-	6/21/25/27	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	180	GVL	C30-C29-C32	2.47	113.10	108.82
1	B	180	GVL	O35-C34-C32	2.20	121.15	119.04

There are no chirality outliers.

5 of 18 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	180	GVL	CB-O25-P24-O23
1	C	180	GVL	CB-O25-P24-O27
1	C	180	GVL	C28-O27-P24-O26
1	B	180	GVL	CB-O25-P24-O23
1	B	180	GVL	CB-O25-P24-O27

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

3 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
3	FMN	H	3051	-	31,33,33	6.72	18 (58%)	40,50,50	1.90	8 (20%)
3	FMN	I	3051	-	31,33,33	6.75	20 (64%)	40,50,50	1.82	7 (17%)
3	FMN	G	3051	-	31,33,33	6.89	18 (58%)	40,50,50	1.95	7 (17%)

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
3	FMN	H	3051	-	-	5/18/18/18	0/3/3/3
3	FMN	I	3051	-	-	5/18/18/18	0/3/3/3
3	FMN	G	3051	-	-	5/18/18/18	0/3/3/3

The worst 5 of 56 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	3051	FMN	C4A-C10	16.15	1.55	1.38
3	H	3051	FMN	C4A-C10	15.08	1.53	1.38
3	I	3051	FMN	C4A-C10	14.93	1.53	1.38
3	G	3051	FMN	C4A-N5	12.72	1.51	1.33
3	I	3051	FMN	C4A-N5	12.29	1.50	1.33

The worst 5 of 22 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	3051	FMN	C4-N3-C2	7.49	121.47	115.14
3	G	3051	FMN	C4-N3-C2	7.30	121.30	115.14
3	I	3051	FMN	C4-N3-C2	6.98	121.03	115.14
3	G	3051	FMN	C1'-N10-C9A	4.66	121.96	118.29

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Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
3	H	3051	FMN	C1'-N10-C9A	4.18	121.58	118.29

There are no chirality outliers.

5 of 15 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	3051	FMN	C2'-C3'-C4'-C5'
3	H	3051	FMN	O3'-C3'-C4'-C5'
3	I	3051	FMN	C2'-C3'-C4'-C5'
3	I	3051	FMN	O3'-C3'-C4'-C5'
3	G	3051	FMN	C2'-C3'-C4'-C5'

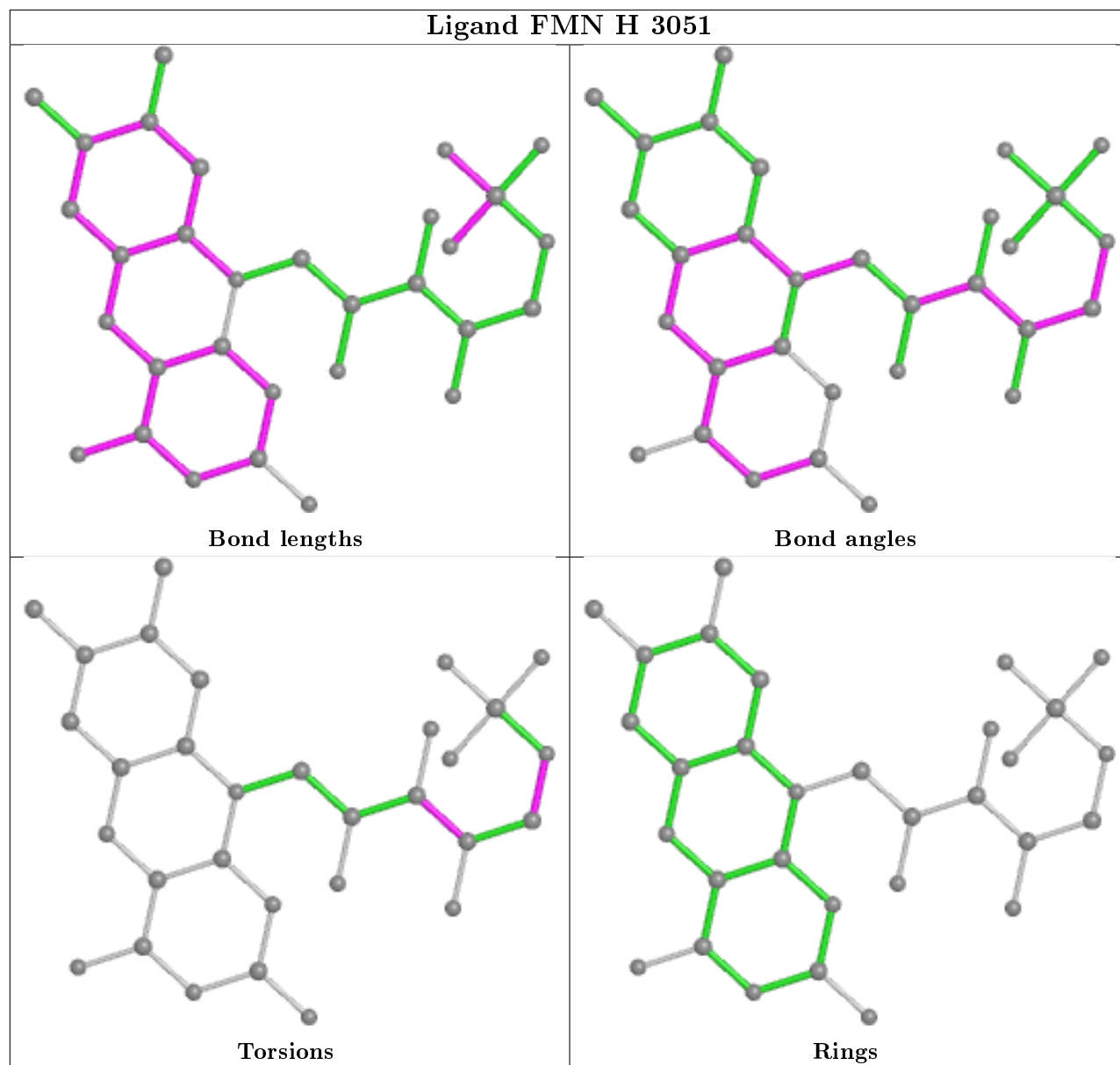
There are no ring outliers.

3 monomers are involved in 19 short contacts:

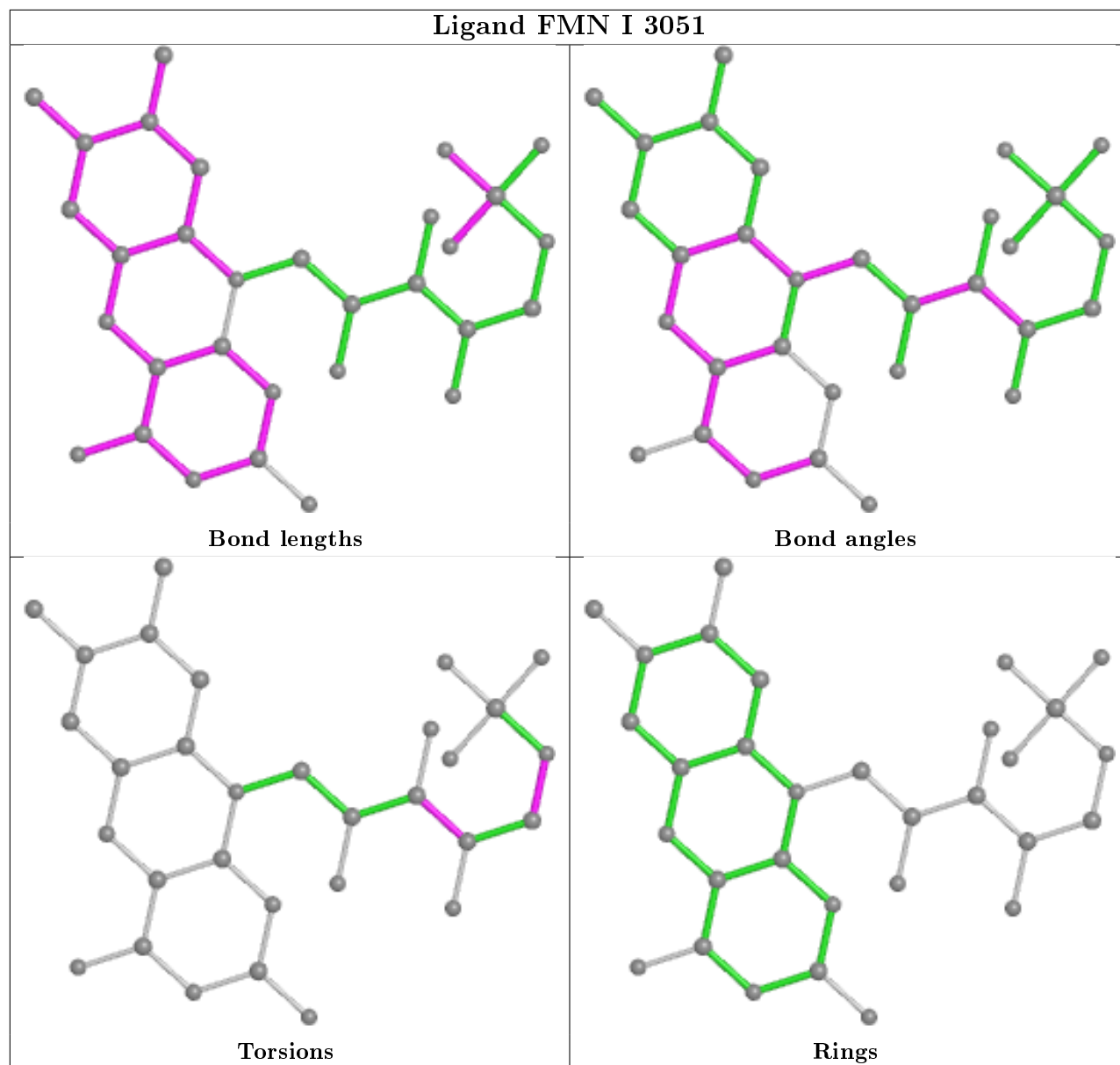
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	3051	FMN	6	0
3	I	3051	FMN	6	0
3	G	3051	FMN	7	0

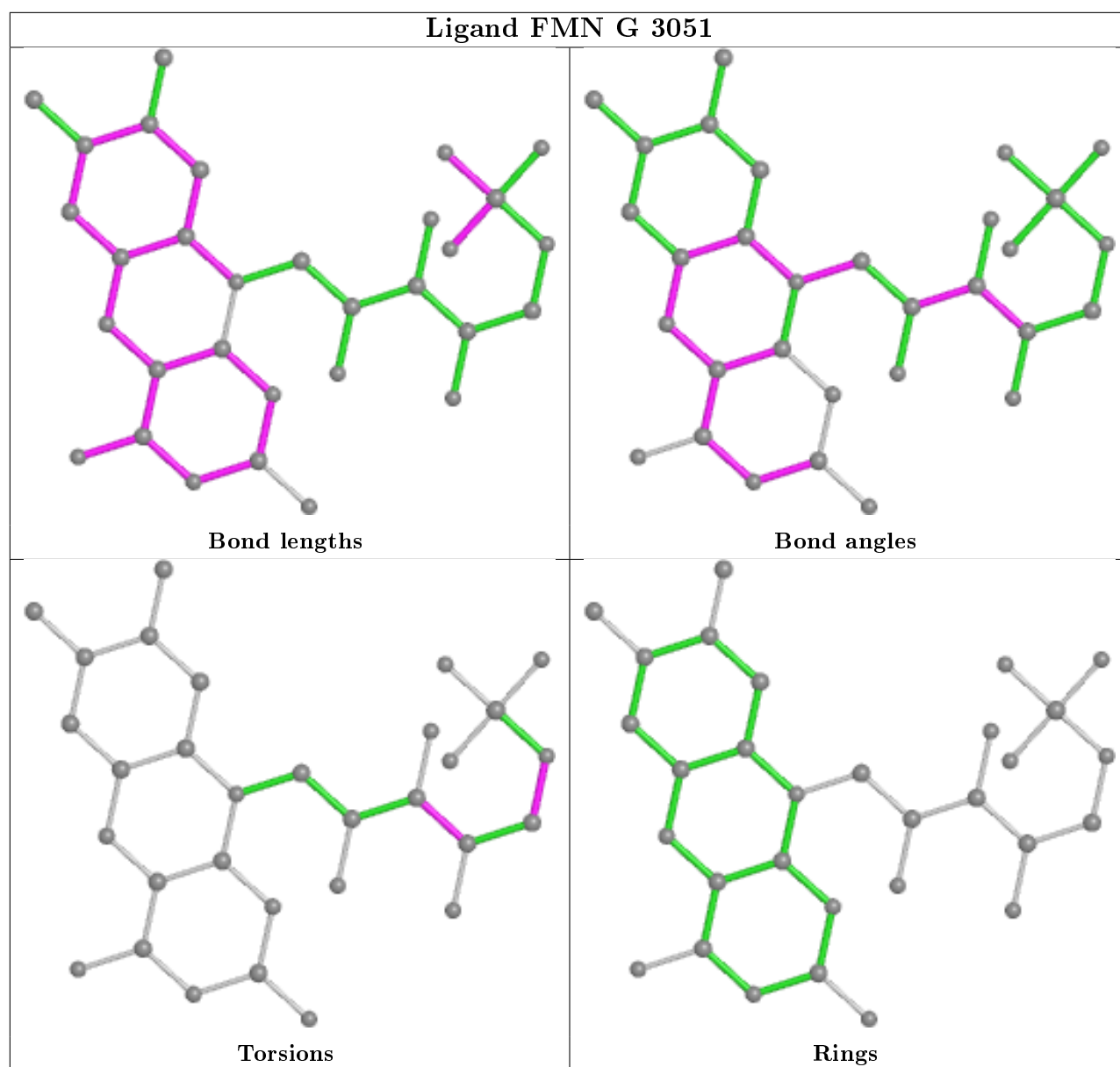
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand FMN H 3051









## 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, 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	1613/1887 (85%)	-0.60	29 (1%) 68 47	28, 59, 126, 166	0
1	B	1613/1887 (85%)	-0.59	26 (1%) 72 51	30, 59, 127, 170	0
1	C	1613/1887 (85%)	-0.59	31 (1%) 66 46	29, 61, 126, 170	0
2	G	2033/2051 (99%)	-0.52	18 (0%) 84 69	39, 73, 114, 151	0
2	H	2033/2051 (99%)	-0.54	17 (0%) 86 72	41, 73, 113, 152	0
2	I	2033/2051 (99%)	-0.53	14 (0%) 87 75	42, 74, 113, 150	0
All	All	10938/11814 (92%)	-0.56	135 (1%) 79 61	28, 69, 119, 170	0

The worst 5 of 135 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	977	TYR	5.6
1	C	976	ALA	5.2
2	H	35	GLU	5.2
1	C	975	ALA	5.2
1	C	1475	GLU	4.7

### 6.2 Non-standard residues in protein, DNA, RNA chains [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, 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
1	GVL	C	180	19/20	0.76	0.38	49,130,161,187	0
1	GVL	B	180	19/20	0.82	0.30	48,119,172,190	0
1	GVL	A	180	19/20	0.86	0.26	44,125,164,189	0

## 6.3 Carbohydrates [i](#)

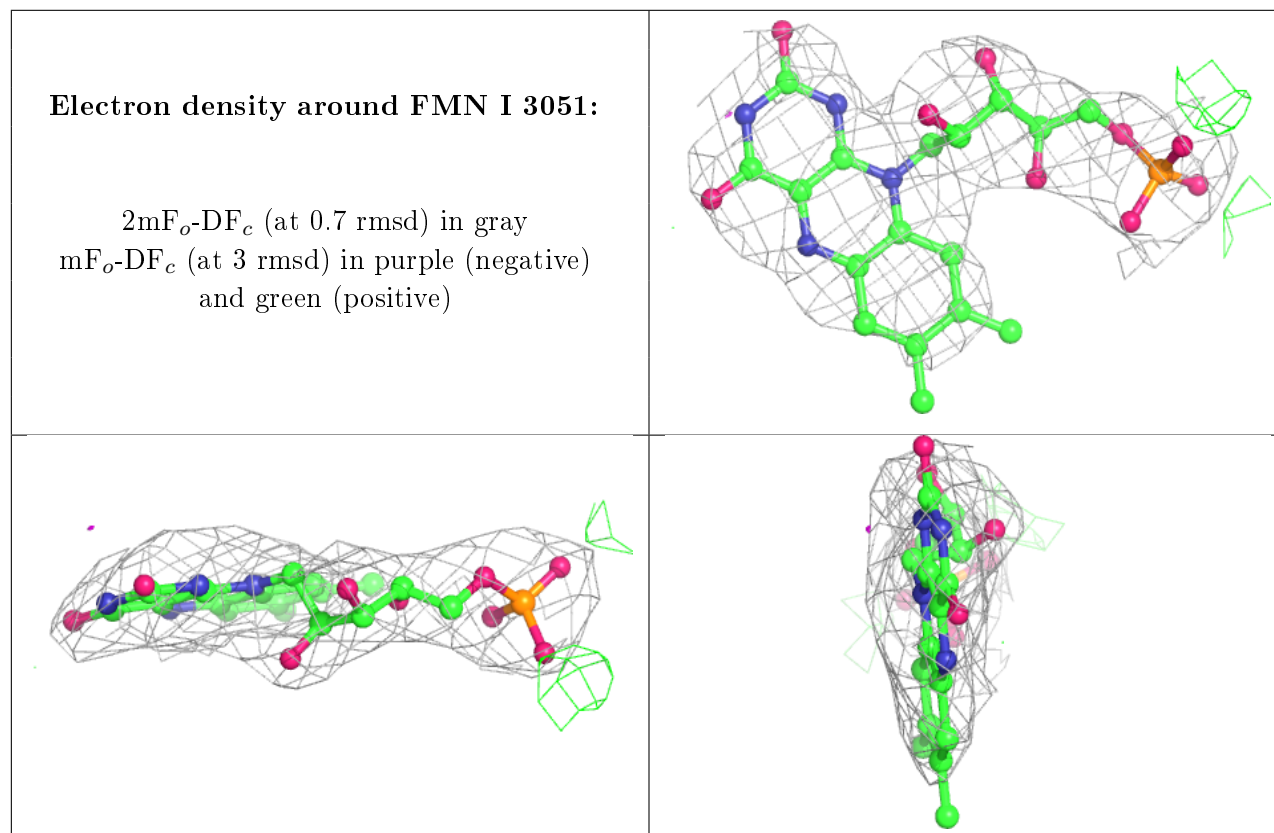
There are no monosaccharides in this entry.

## 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, 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.

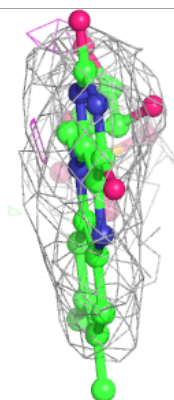
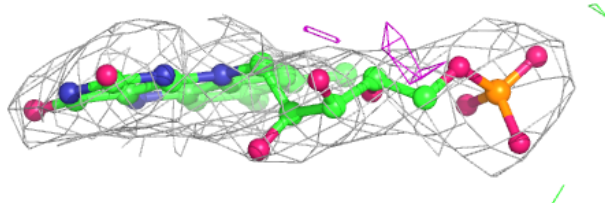
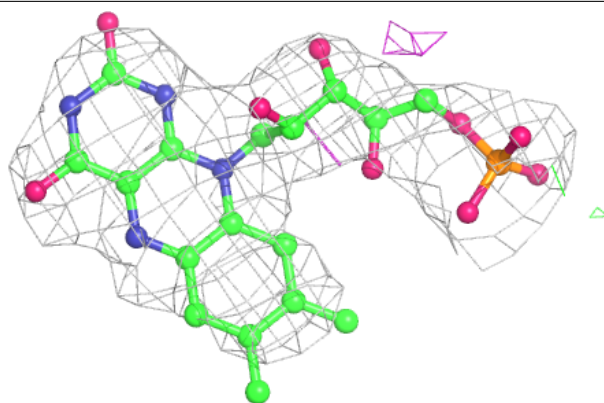
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	FMN	I	3051	31/31	0.96	0.13	26,57,75,97	0
3	FMN	G	3051	31/31	0.96	0.14	31,55,81,100	0
3	FMN	H	3051	31/31	0.97	0.14	27,54,78,82	0

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.

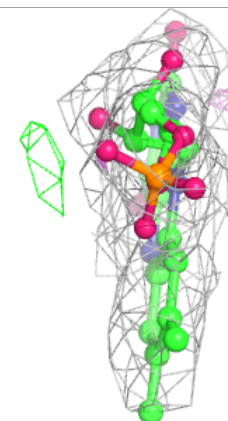
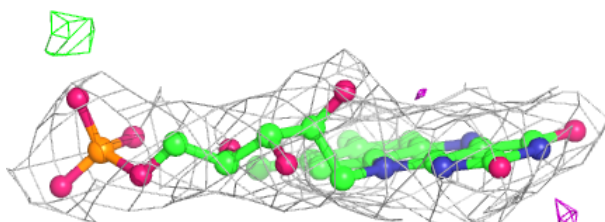
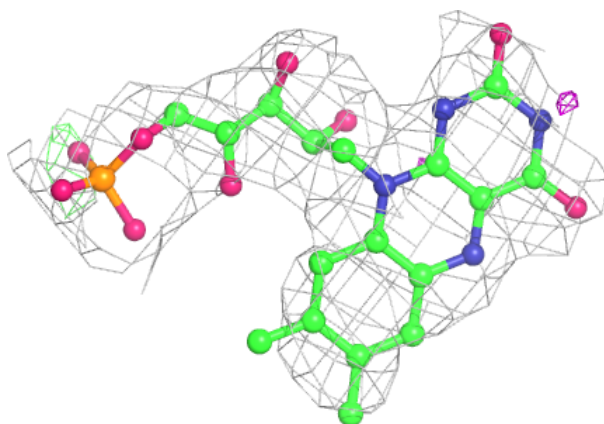


**Electron density around FMN G 3051:**

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

**Electron density around FMN H 3051:**

$2mF_o-DF_c$  (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.