



wwPDB X-ray Structure Validation Summary Report ⓘ

May 14, 2020 – 04:15 am BST

PDB ID : 2VZ8
Title : Crystal Structure of Mammalian Fatty Acid Synthase
Authors : Maier, T.; Leibundgut, M.; Ban, N.
Deposited on : 2008-07-31
Resolution : 3.22 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
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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

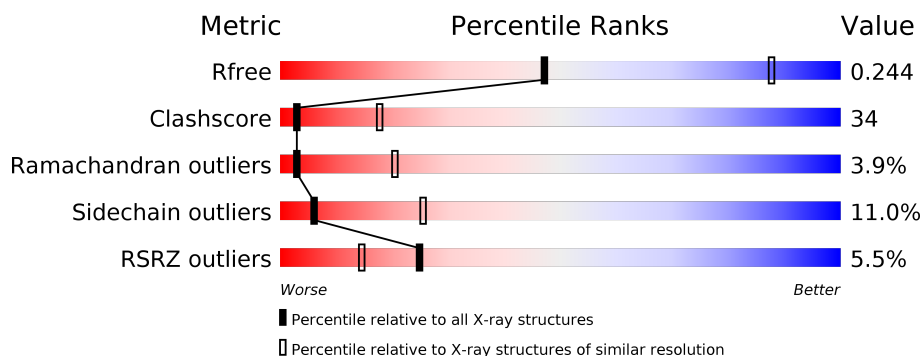
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)

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 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>4%</div> <div>35%</div> <div>36%</div> <div>6%</div> <div>22%</div> </div>
1	B	2512	<div> <div>5%</div> <div>36%</div> <div>37%</div> <div>6%</div> <div>20%</div> </div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 30281 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	1962	Total	C	N	O	S	0	0	0
			14977	9466	2630	2803	78			
1	B	2004	Total	C	N	O	S	0	0	0
			15304	9671	2684	2869	80			

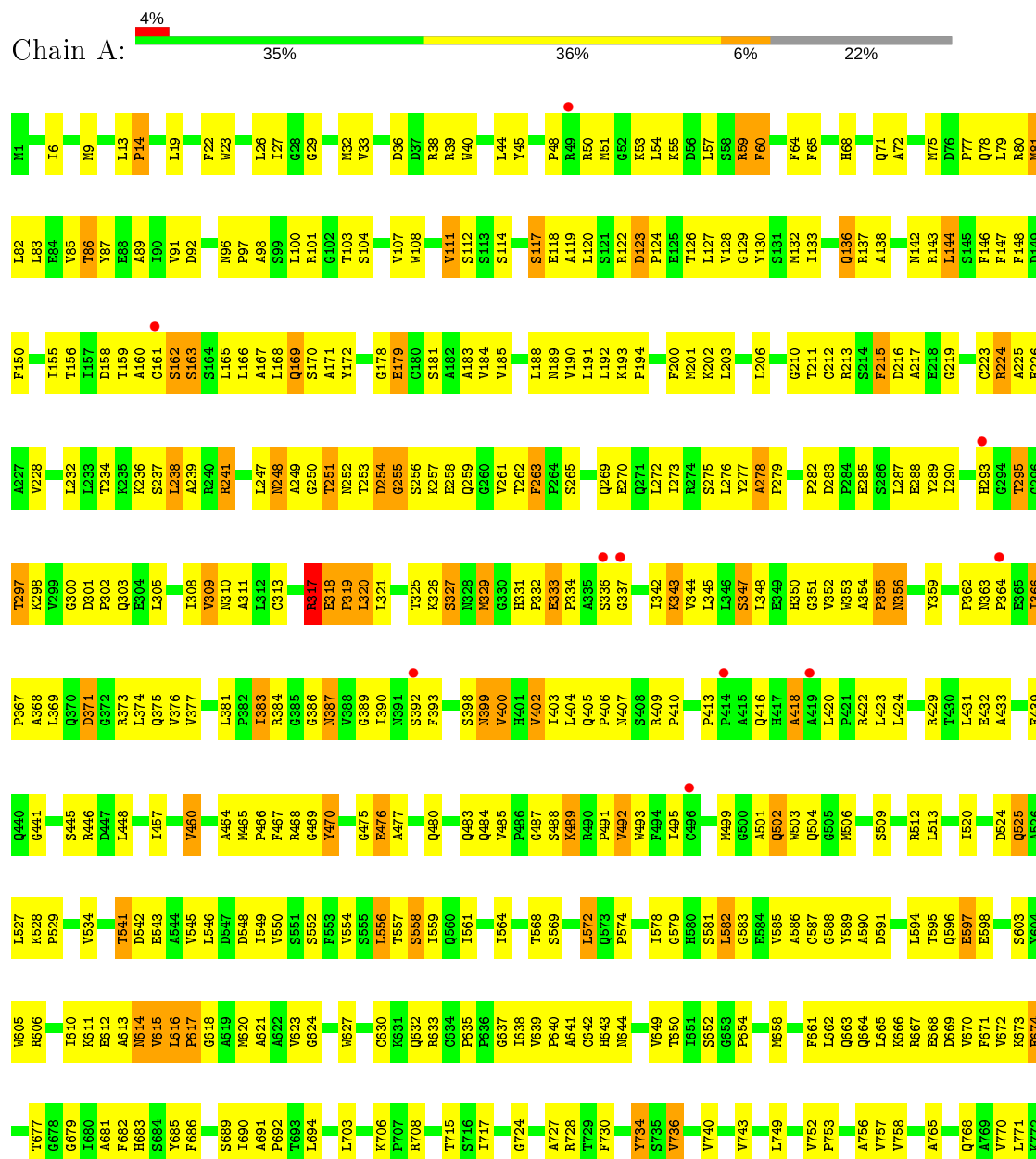
There are 2 discrepancies between the modelled and reference sequences:

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

3 Residue-property plots

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







LEU	THR	GLN	LEU	G2081	T2006	R1930	L1854	G1770	F1696	S1625	C1548	L1473	D1411	F1343
PHE	GLY	ALA	ASP	G2082	R2007	E1931	Q1855	D1773	T1697	V1626	C1549	V1474	S1412	L1344
LEU	ALA	THR	SER	I2088	C2010	V1932	R1856	L1774	T1698	V1627	P1550	N1476	P1413	L1345
ASP	PRO	ASN	MET	L2096	L2013	R1934	E1858	N1777	E1703	L1628	H1551	L1477	F1415	L1346
GLY	LEU	LEU	GLY	I2097	V2014	V1937	E1860	H1778	R1705	L1629	H1552	T1480	S1417	H1347
SER	ASP	SER	VAL	F2098	V2015	Q1936	Q1861	H1779	A1706	Q1630	A1553	L1349	LEU	L1348
HIS	SER	THR	GLU	L2099	V2016	V1939	L1862	L1780	A1707	H1631	A1554	S1481	ALA	L1347
THR	THR	VAL	VAL	F2016	V2017	Q1938	P1863	L1781	R1706	V1636	L1555	P1482	GLY	L1346
PHE	GLN	VAL	ARG	S2100	L2018	L1940	P1863	M1782	E1703	L1628	A1483	A1483	HIS	H1347
VAL	SER	VAL	GLN	Q2101	I2018	V1941	P1865	M1783	K1704	Q1630	P1482	T1421	GLY	H1347
LEU	LEU	ASN	ILE	P2102	T2019	V1941	P1865	F1712	E1859	A1557	E1485	P1422	PRO	H1347
ALA	ALA	PRO	LEU	S2020	S2020	V1944	P1865	A1784	R1704	Q1559	M1486	F1423	LEU	H1347
GLY	SER	GLY	GLU	S2021	S2021	V1944	P1865	F1785	P1713	T1641	H1487	A1424	GLY	H1347
THR	THR	GLY	ARG	V2022	S2022	G1951	L1868	L1786	F1720	L1642	P1488	M1425	GLU	H1347
GLN	THR	PRO	GLU	S2023	S2023	A1952	P1869	K1787	A1721	E1643	S1491	S1428	VAL	H1347
SER	THR	THR	THR	C2024	S2024	R1953	L1871	M1788	N1722	E1644	S1491	L1429	GLY	H1347
VAL	GLU	LEU	ASP	G2025	G2025	S1954	A1872	V1789	S1723	S1647	L1497	L1430	PHE	H1347
ARG	THR	THR	LEU	R2026	R2026	L1955	L1873	T1790	R1724	V1566	L1497	D1431	LEU	H1347
ALA	ILE	ARG	VAL	G2027	G2027	T1956	T1874	F1791	D1725	Y1567	L1497	D1431	LEU	H1347
LYS	ARG	ARG	LEU	N2028	N2028	T1957	G1875	H1792	P1648	Y1568	L1497	D1431	LEU	H1347
ALA	ALA	ALA	ALA	Q2031	Q2031	E1958	S1877	G1793	T1569	T1569	L1497	D1431	LEU	H1347
ALA	ALA	ALA	ALA	N2033	N2033	G1966	K1878	L1795	F1728	S1570	L1497	D1431	LEU	H1347
PRO	GLY	GLN	GLU	Y2034	Y2034	G1967	T1879	L1795	E1729	T1653	L1497	D1431	LEU	H1347
ARG	GLY	SER	VAL	G2035	G2035	L1971	P1882	F1800	V1732	Y1656	L1497	D1431	LEU	H1347
ALA	GLY	ALA	GLY	F2036	F2036	A1972	E1801	R1733	L1733	Y1656	L1497	D1431	LEU	H1347
GLY	GLY	GLY	GLY	G2039	G2039	M1973	K1885	G1803	R1734	Y1656	L1497	D1431	LEU	H1347
PRO	ARG	ARG	SER	A2040	A2040	V1974	S1886	G1803	H1735	S1658	L1497	D1431	LEU	H1347
LEU	LEU	LEU	LEU	L2041	L2041	L1975	A1887	G1804	T1736	G1581	L1497	D1431	LEU	H1347
ARG	ARG	PHE	ARG	R2042	R2042	R1976	V1888	V1810	K1739	Y1660	L1497	D1431	LEU	H1347
LEU	LEU	VAL	LEU	E2042	E2042	D1977	I1889	V1810	G1740	Y1661	L1497	D1431	LEU	H1347
LEU	LEU	VAL	LEU	R2043	R2043	A1978	T1890	L1813	D1742	R1662	L1497	D1431	LEU	H1347
VAL	VAL	HIS	GLN	T2044	T2044	V1979	T1890	L1814	L1743	Q1666	L1497	D1431	LEU	H1347
LYS	LYS	PRO	GLY	R2048	R2048	L1930	L1893	K1815	V1744	S1587	L1497	D1431	LEU	H1347
ALA	ALA	ILE	LEU	R2049	R2049	E1981	G1894	V1744	L1745	L1583	L1497	D1431	LEU	H1347
VAL	VAL	GLY	SER	L2056	L2056	Q1982	G1895	Q1819	N1746	T1594	L1497	D1431	LEU	H1347
ALA	ALA	HIS	SER	V2060	V2060	T1984	L1898	V1823	S1747	R1595	L1497	D1431	LEU	H1347
ILE	ILE	ILE	THR	G2064	G2064	P1985	Q1899	V1823	H1674	D1596	L1497	D1431	LEU	H1347
ASP	ASP	THR	THR	D2065	D2065	E1986	L1903	Q1824	A1749	C1597	L1497	D1431	LEU	H1347
ALA	ALA	PHE	ASP	V2066	V2066	F1987	L1904	P1825	L1753	M1598	L1497	D1431	LEU	H1347
GLY	GLY	HIS	ALA	G2067	G2067	Q1988	L1904	K1835	Q1754	E1602	L1497	D1431	LEU	H1347
ASP	ASP	THR	THR	V2068	V2068	D1990	K1911	V1836	A1755	F1603	L1497	D1431	LEU	H1347
ALA	ALA	GLY	GLY	V2069	V2069	V1991	L1912	E1837	S1756	R1606	L1497	D1431	LEU	H1347
ALA	ALA	ALA	ALA	L2070	L2070	S1992	V1913	A1838	V1757	A1531	L1497	D1431	LEU	H1347
ILE	ILE	LYS	THR	E2071	E2071	K1993	L1914	A1839	R1758	D1607	L1497	D1431	LEU	H1347
ASN	ASN	LEU	THR	THR	THR	P1994	T1915	F1840	C1759	Q1682	L1497	D1431	LEU	H1347
PRO	PRO	LEU	THR	THR	THR	K1995	S1916	A1841	L1760	R1611	L1497	D1431	LEU	H1347
GLN	GLN	SER	SER	THR	THR	Y1996	R1917	Y1842	A1761	R1612	L1497	D1431	LEU	H1347
ASP	ASP	ILE	ASP	THR	THR	S1997	G1917	M1843	Q1762	V1613	L1497	D1431	LEU	H1347
GLY	GLY	PRO	GLY	THR	THR	G1998	R1921	A1944	H1763	M1614	L1497	D1431	LEU	H1347
LEU	LEU	THR	THR	THR	THR	THR	T1922	H1848	G1764	G1615	L1497	D1431	LEU	H1347
VAL	VAL	THR	THR	THR	THR	THR	Q1925	H1848	G1765	M1616	L1497	D1431	LEU	H1347
ASP	ASP	GLY	GLY	THR	THR	THR	A1926	K1851	F1766	V1617	L1497	D1431	LEU	H1347
LEU	LEU	GLN	GLN	THR	THR	THR	R1927	V1852	L1767	P1618	L1497	D1431	LEU	H1347
GLY	GLY	GLN	GLN	THR	THR	THR	R1927	V1853	I1769	L1622	L1497	D1431	LEU	H1347
LEU	LEU	CYS	GLN	THR	THR	THR	R1927	V1853	I1769	L1622	L1497	D1431	LEU	H1347

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

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	96.32Å 244.70Å 135.25Å 90.00° 101.65° 90.00°	Depositor
Resolution (Å)	29.50 – 3.22 29.50 – 3.22	Depositor EDS
% Data completeness (in resolution range)	94.8 (29.50-3.22) 97.6 (29.50-3.22)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.24Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.217 , 0.259 0.204 , 0.244	Depositor DCC
R_{free} test set	4839 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	95.2	Xtriage
Anisotropy	0.218	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 73.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	30281	wwPDB-VP
Average B, all atoms (Å ²)	143.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% 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

5.1 Standard geometry

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	0.45	1/15302 (0.0%)	0.63	0/20792
1	B	0.41	0/15634	0.60	1/21243 (0.0%)
All	All	0.43	1/30936 (0.0%)	0.61	1/42035 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1759	CYS	CB-SG	-5.79	1.72	1.81

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1694	ARG	NE-CZ-NH1	6.90	123.75	120.30

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	14977	0	14938	1049	0
1	B	15304	0	15266	1083	0
All	All	30281	0	30204	2085	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 34.

The worst 5 of 2085 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:1694:ARG:HH11	1:B:1694:ARG:HG3	1.17	1.10
1:B:1303:ASN:H	1:B:1304:PRO:HD3	1.25	1.02
1:A:1473:LEU:HD21	1:A:1503:MET:HG2	1.36	1.02
1:A:165:LEU:HD23	1:A:400:VAL:HG22	1.37	1.02
1:B:1456:MET:HG2	1:B:2036:PHE:HB2	1.41	1.01

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	1948/2512 (78%)	1586 (81%)	282 (14%)	80 (4%)	3	19
1	B	1992/2512 (79%)	1622 (81%)	296 (15%)	74 (4%)	3	21
All	All	3940/5024 (78%)	3208 (81%)	578 (15%)	154 (4%)	3	20

5 of 154 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	179	GLU
1	A	255	GLY
1	A	278	ALA
1	A	333	GLU
1	A	413	PRO

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	1624/2072 (78%)	1450 (89%)	174 (11%)	6	26
1	B	1660/2072 (80%)	1473 (89%)	187 (11%)	6	24
All	All	3284/4144 (79%)	2923 (89%)	361 (11%)	6	25

5 of 361 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1996	TYR
1	B	318	GLU
1	B	1823	VAL
1	A	2028	ASN
1	B	127	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2086	GLN
1	B	350	HIS
1	B	1777	ASN
1	A	2103	HIS
1	B	136	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	1962/2512 (78%)	-0.12	88 (4%)	33	21	63, 118, 226, 276	0
1	B	2004/2512 (79%)	0.09	131 (6%)	18	11	54, 158, 230, 276	0
All	All	3966/5024 (78%)	-0.01	219 (5%)	25	14	54, 136, 229, 276	0

The worst 5 of 219 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	581	SER	7.9
1	A	1297	GLY	7.7
1	B	496	CYS	7.4
1	B	579	GLY	7.3
1	B	672	VAL	7.1

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.