



wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 14, 2017 – 02:47 PM EST

PDB ID : 4U2P
Title : Full-length AMPA subtype ionotropic glutamate receptor GluA2 in the apo state
Authors : Duerr, K.L.; Gouaux, E.
Deposited on : unknown
Resolution : 3.24 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 ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030345
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : rb-20030345

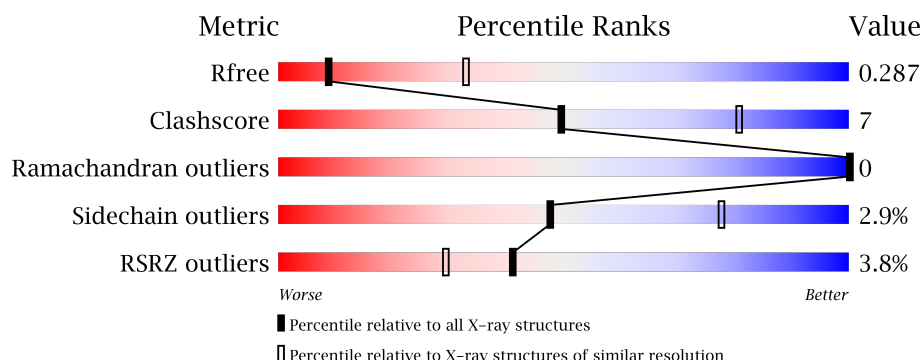
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.24 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}	100719	1247 (3.28-3.20)
Clashscore	112137	1383 (3.28-3.20)
Ramachandran outliers	110173	1358 (3.28-3.20)
Sidechain outliers	110143	1357 (3.28-3.20)
RSRZ outliers	101464	1252 (3.28-3.20)

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 $\leq 5\%$. 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	824	<div> <div>5%</div> <div> <div></div> <div>78%</div> <div>13%</div> <div>8%</div> </div> </div>
1	B	824	<div> <div>2%</div> <div> <div></div> <div>76%</div> <div>16%</div> <div>8%</div> </div> </div>
1	C	824	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>8%</div> </div> </div>
1	D	824	<div> <div>4%</div> <div> <div></div> <div>76%</div> <div>15%</div> <div>9%</div> </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	B	1001	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 22388 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 Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	755	Total	C	N	O	S	0	0	0
			5496	3519	909	1045	23			
1	B	761	Total	C	N	O	S	0	0	0
			5653	3626	933	1070	24			
1	D	751	Total	C	N	O	S	0	0	0
			5548	3548	912	1062	26			
1	C	755	Total	C	N	O	S	0	0	0
			5587	3578	934	1051	24			

There are 72 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	239	GLU	ASN	conflict	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	?	-	GLY	deletion	UNP P19491
A	385	ASP	ASN	conflict	UNP P19491
A	392	GLN	ASN	conflict	UNP P19491
A	528	ALA	CYS	conflict	UNP P19491
A	585	PHE	MET	conflict	UNP P19491
A	589	ALA	CYS	conflict	UNP P19491
A	598	ALA	GLY	conflict	UNP P19491
A	602	ALA	GLY	conflict	UNP P19491
A	815	ALA	CYS	conflict	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	239	GLU	ASN	conflict	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491

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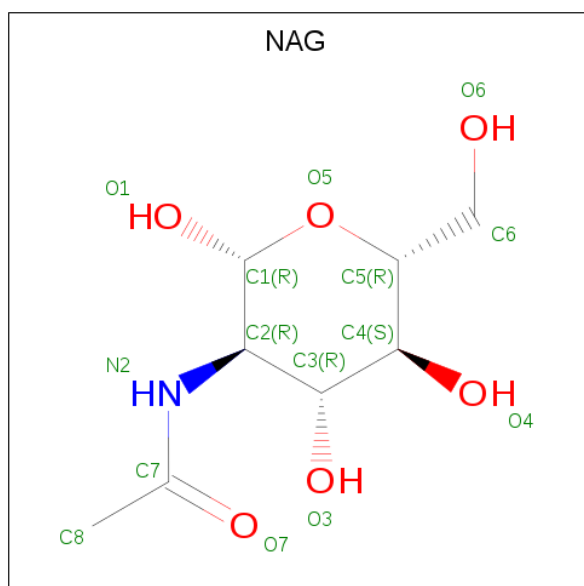
Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	SER	deletion	UNP P19491
B	?	-	GLY	deletion	UNP P19491
B	385	ASP	ASN	conflict	UNP P19491
B	392	GLN	ASN	conflict	UNP P19491
B	528	ALA	CYS	conflict	UNP P19491
B	585	PHE	MET	conflict	UNP P19491
B	589	ALA	CYS	conflict	UNP P19491
B	598	ALA	GLY	conflict	UNP P19491
B	602	ALA	GLY	conflict	UNP P19491
B	815	ALA	CYS	conflict	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
D	239	GLU	ASN	conflict	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	?	-	GLY	deletion	UNP P19491
D	385	ASP	ASN	conflict	UNP P19491
D	392	GLN	ASN	conflict	UNP P19491
D	528	ALA	CYS	conflict	UNP P19491
D	585	PHE	MET	conflict	UNP P19491
D	589	ALA	CYS	conflict	UNP P19491
D	598	ALA	GLY	conflict	UNP P19491
D	602	ALA	GLY	conflict	UNP P19491
D	815	ALA	CYS	conflict	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491
C	239	GLU	ASN	conflict	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	?	-	GLY	deletion	UNP P19491
C	385	ASP	ASN	conflict	UNP P19491
C	392	GLN	ASN	conflict	UNP P19491
C	528	ALA	CYS	conflict	UNP P19491
C	585	PHE	MET	conflict	UNP P19491

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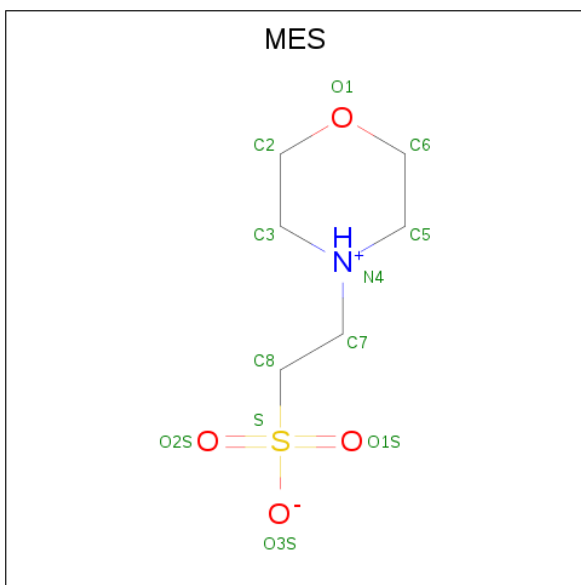
Chain	Residue	Modelled	Actual	Comment	Reference
C	589	ALA	CYS	conflict	UNP P19491
C	598	ALA	GLY	conflict	UNP P19491
C	602	ALA	GLY	conflict	UNP P19491
C	815	ALA	CYS	conflict	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



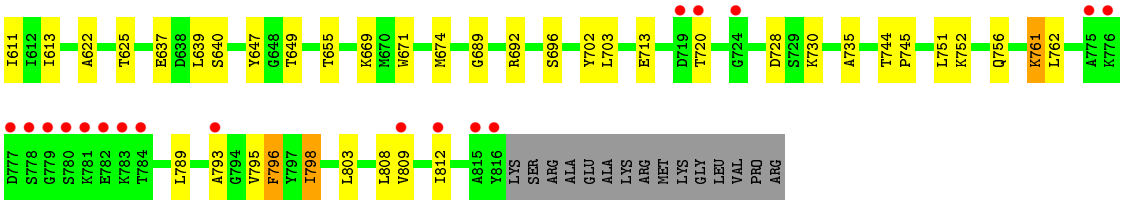
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	D	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
3	C	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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 ($\text{RSRZ} > 2$). 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.

- Chain A:
-
- 78% 13% 8%
- ASN I10 G14 D21 Y24 T36 I45 F60 G61 S62 Q63 F64 Y69 F72 Y75 F86 T86 P97 S98 F99 P100 T101 Q110 M111 R112 A118 Y126 Q127 W128 A132 Y133 L134 Y135 D136 L148 A151 W156 G164 Y171

- Chain B:
-
- 76% 16% 8%
- 2%
- 1369 1398 1400 1401 1402 1403 1404 1405 1406 1407 1408 1409 1410 1411 1412 1413 1414 1415 1416 1417 1418 1419 1420 1421 1422 1423 1424 1425 1426 1427 1428 1429 1430 1431 1432 1433 1434 1435 1436 1437 1438 1439 1440 1441 1442 1443 1444 1445 1446 1447 1448 1449 1450 1451 1452 1453 1454 1455 1456 1457 1458 1459 1460 1461 1462 1463 1464 1465 1466 1467 1468 1469 1470 1471 1472 1473 1474 1475 1476 1477 1478 1479 1480 1481 1482 1483 1484 1485 1486 1487 1488 1489 1490 1491 1492 1493 1494 1495 1496 1497 1498 1499 1500 1501 1502 1503 1504 1505 1506 1507 1508 1509 1510 1511 1512 1513 1514 1515 1516 1517 1518 1519 1520 1521 1522 1523 1524 1525 1526 1527 1528 1529 1530 1531 1532 1533 1534 1535 1536 1537 1538 1539 1540 1541 1542 1543 1544 1545 1546 1547 1548 1549 1550 1551 1552 1553 1554 1555 1556 1557 1558 1559 1560 1561 1562 1563 1564 1565 1566 1567 1568 1569 1570 1571 1572 1573 1574 1575 1576 1577 1578 1579 1580 1581 1582 1583 1584 1585 1586 1587 1588 1589 1590 1591 1592 1593 1594 1595 1596 1597 1598 1599 1600 1601 1602 1603 1604 1605 1606 1607 1608 1609 1610 1611 1612 1613 1614 1615 1616 1617 1618 1619 1620 1621 1622 1623 1624 1625 1626 1627 1628 1629 1630 1631 1632 1633 1634 1635 1636 1637 1638 1639 1640 1641 1642 1643 1644 1645 1646 1647 1648 1649 1650 1651 1652 1653 1654 1655 1656 1657 1658 1659 1660 1661 1662 1663 1664 1665 1666 1667 1668 1669 1670 1671 1672 1673 1674 1675 1676 1677 1678 1679 1680 1681 1682 1683 1684 1685 1686 1687 1688 1689 1690 1691 1692 1693 1694 1695 1696 1697 1698 1699 1700 1701 1702 1703 1704 1705 1706 1707 1708 1709 1710 1711 1712 1713 1714 1715 1716 1717 1718 1719 1720 1721 1722 1723 1724 1725 1726 1727 1728 1729 1730 1731 1732 1733 1734 1735 1736 1737 1738 1739 1740 1741 1742 1743 1744 1745 1746 1747 1748 1749 1750 1751 1752 1753 1754 1755 1756 1757 1758 1759 1760 1761 1762 1763 1764 1765 1766 1767 1768 1769 1770 1771 1772 1773 1774 1775 1776 1777 1778 1779 1780 1781 1782 1783 1784 1785 1786 1787 1788 1789 1790 1791 1792 1793 1794 1795 1796 1797 1798 1799 1800 1801 1802 1803 1804 1805 1806 1807 1808 1809 1810 1811 1812 1813 1814 1815 1816 1817 1818 1819 1820 1821 1822 1823 1824 1825 1826 1827 1828 1829 1830 1831 1832 1833 1834 1835 1836 1837 1838 1839 1840 1841 1842 1843 1844 1845 1846 1847 1848 1849 1850 1851 1852 1853 1854 1855 1856 1857 1858 1859 1860 1861 1862 1863 1864 1865 1866 1867 1868 1869 1870 1871 1872 1873 1874 1875 1876 1877 1878 1879 1880 1881 1882 1883 1884 1885 1886 1887 1888 1889 1890 1891 1892 1893 1894 1895 1896 1897 1898 1899 1900 1901 1902 1903 1904 1905 1906 1907 1908 1909 1910 1911 1912 1913 1914 1915 1916 1917 1918 1919 1920 1921 1922 1923 1924 1925 1926 1927 1928 1929 1930 1931 1932 1933 1934 1935 1936 1937 1938 1939 1940 1941 1942 1943 1944 1945 1946 1947 1948 1949 1950 1951 1952 1953 1954 1955 1956 1957 1958 1959 1960 1961 1962 1963 1964 1965 1966 1967 1968 1969 1970 1971 1972 1973 1974 1975 1976 1977 1978 1979 1980 1981 1982 1983 1984 1985 1986 1987 1988 1989 1990 1991 1992 1993 1994 1995 1996 1997 1998 1999 2000 2001 2002 2003 2004 2005 2006 2007 2008 2009 2010 2011 2012 2013 2014 2015 2016 2017 2018 2019 2020 2021 2022 2023 2024 2025 2026 2027 2028 2029 2030 2031 2032 2033 2034 2035 2036 2037 2038 2039 2040 2041 2042 2043 2044 2045 2046 2047 2048 2049 2050 2051 2052 2053 2054 2055 2056 2057 2058 2059 2060 2061 2062 2063 2064 2065 2066 2067 2068 2069 2070 2071 2072 2073 2074 2075 2076 2077 2078 2079 2080 2081 2082 2083 2084 2085 2086 2087 2088 2089 2090 2091 2092 2093 2094 2095 2096 2097 2098 2099 2100 2101 2102 2103 2104 2105 2106 2107 2108 2109 2110 2111 2112 2113 2114 2115 2116 2117 2118 2119 2120 2121 2122 2123 2124 2125 2126 2127 2128 2129 2130 2131 2132 2133 2134 2135 2136 2137 2138 2139 2140 2141 2142 2143 2144 2145 2146 2147 2148 2149 2150 2151 2152 2153 2154 2155 2156 2157 2158 2159 2160 2161 2162 2163 2164 2165 2166 2167 2168 2169 2170 2171 2172 2173 2174 2175 2176 2177 2178 2179 2180 2181 2182 2183 2184 2185 2186 2187 2188 2189 2190 2191 2192 2193 2194 2195 2196 2197 2198 2199 220





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	107.81Å 149.13Å 352.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.00 – 3.24 49.00 – 3.24	Depositor EDS
% Data completeness (in resolution range)	72.2 (49.00-3.24) 72.2 (49.00-3.24)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.68 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.250 , 0.288 0.246 , 0.287	Depositor DCC
R_{free} test set	3374 reflections (5.12%)	DCC
Wilson B-factor (Å ²)	107.7	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.20 , 79.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.37$, $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	22388	wwPDB-VP
Average B, all atoms (Å ²)	181.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.80% 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: NAG, MES

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	0.25	0/5614	0.46	0/7661
1	B	0.25	0/5773	0.45	0/7854
1	C	0.26	0/5703	0.46	0/7759
1	D	0.26	0/5664	0.48	0/7721
All	All	0.26	0/22754	0.46	0/30995

There are no bond length outliers.

There are no bond angle outliers.

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	5496	0	5031	67	0
1	B	5653	0	5313	91	0
1	C	5587	0	5248	83	0
1	D	5548	0	5169	78	0
2	A	14	0	13	1	0
2	B	14	0	12	0	0
2	C	14	0	13	0	0
2	D	14	0	13	1	0
3	A	12	0	13	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	12	0	13	0	0
3	C	12	0	13	0	0
3	D	12	0	13	1	0
All	All	22388	0	20864	291	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 7.

The worst 5 of 291 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:D:626:VAL:HG13	1:D:628:ARG:H	1.39	0.88
1:C:175:TYR:HD2	1:C:205:GLN:HG3	1.44	0.81
1:C:475:ALA:HB3	1:C:735:ALA:HB3	1.63	0.79
1:B:664:ILE:HG12	1:C:761:LYS:HE2	1.64	0.78
1:B:475:ALA:HB3	1:B:735:ALA:HB3	1.65	0.78

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	751/824 (91%)	728 (97%)	23 (3%)	0	100	100
1	B	757/824 (92%)	741 (98%)	16 (2%)	0	100	100
1	C	749/824 (91%)	728 (97%)	21 (3%)	0	100	100
1	D	747/824 (91%)	727 (97%)	20 (3%)	0	100	100
All	All	3004/3296 (91%)	2924 (97%)	80 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	521/701 (74%)	504 (97%)	17 (3%)	43	75
1	B	556/701 (79%)	543 (98%)	13 (2%)	56	82
1	C	545/701 (78%)	531 (97%)	14 (3%)	51	80
1	D	546/701 (78%)	528 (97%)	18 (3%)	43	75
All	All	2168/2804 (77%)	2106 (97%)	62 (3%)	48	78

5 of 62 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	813	GLU
1	D	168	ASN
1	C	498	LEU
1	D	139	ARG
1	D	183	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	168	ASN
1	C	162	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](#)

8 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	NAG	A	1001	1	14,14,15	1.42	3 (21%)	15,19,21	2.32	6 (40%)
3	MES	A	1002	-	12,12,12	1.74	3 (25%)	14,16,16	1.52	3 (21%)
2	NAG	B	1001	1	14,14,15	2.36	5 (35%)	15,19,21	4.61	8 (53%)
3	MES	B	1002	-	12,12,12	1.92	4 (33%)	14,16,16	10.26	5 (35%)
2	NAG	C	1001	1	14,14,15	0.29	0	15,19,21	1.04	1 (6%)
3	MES	C	1002	-	12,12,12	1.83	3 (25%)	14,16,16	1.48	3 (21%)
2	NAG	D	1001	1	14,14,15	2.05	4 (28%)	15,19,21	4.16	10 (66%)
3	MES	D	1002	-	12,12,12	1.79	3 (25%)	14,16,16	1.52	2 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
3	MES	A	1002	-	-	0/6/14/14	0/1/1/1
2	NAG	B	1001	1	-	0/6/23/26	0/1/1/1
3	MES	B	1002	-	-	0/6/14/14	0/1/1/1
2	NAG	C	1001	1	-	0/6/23/26	0/1/1/1
3	MES	C	1002	-	-	0/6/14/14	0/1/1/1
2	NAG	D	1001	1	-	0/6/23/26	0/1/1/1
3	MES	D	1002	-	-	0/6/14/14	0/1/1/1

The worst 5 of 25 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1001	NAG	O5-C5	2.00	1.47	1.43
2	A	1001	NAG	O5-C5	2.11	1.47	1.43
2	A	1001	NAG	O7-C7	2.15	1.28	1.23
3	B	1002	MES	O3S-S	2.17	1.54	1.47
2	D	1001	NAG	C4-C3	2.19	1.57	1.52

The worst 5 of 38 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1002	MES	O2S-S-C8	-24.52	85.73	106.79
3	B	1002	MES	O1S-S-C8	-24.30	85.92	106.79
3	B	1002	MES	O3S-S-C8	-15.86	86.55	106.06
2	D	1001	NAG	C2-N2-C7	-10.94	106.98	122.94
2	B	1001	NAG	C1-O5-C5	-10.24	98.06	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	NAG	1	0
2	D	1001	NAG	1	0
3	D	1002	MES	1	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 [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	755/824 (91%)	0.10	38 (5%)	30	19	110, 176, 267, 324	0
1	B	761/824 (92%)	-0.00	18 (2%)	59	47	103, 176, 267, 348	0
1	C	755/824 (91%)	0.04	31 (4%)	38	27	106, 175, 269, 334	0
1	D	751/824 (91%)	0.03	29 (3%)	40	29	105, 175, 261, 305	0
All	All	3022/3296 (91%)	0.04	116 (3%)	41	29	103, 176, 266, 348	0

The worst 5 of 116 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	777	ASP	7.1
1	A	540	LEU	6.7
1	A	811	LEU	6.3
1	A	390	LEU	5.5
1	B	792	VAL	5.3

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. 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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	NAG	B	1001	14/15	0.76	0.30	2.16	175,275,394,397	0
3	MES	A	1002	12/12	0.95	0.29	0.73	93,148,187,245	0
2	NAG	A	1001	14/15	0.94	0.24	0.13	104,192,258,311	0
2	NAG	C	1001	14/15	0.95	0.19	-0.19	117,155,252,264	0
2	NAG	D	1001	14/15	0.86	0.19	-0.47	166,292,335,356	0
3	MES	B	1002	12/12	0.97	0.23	-0.58	108,144,223,237	0
3	MES	C	1002	12/12	0.94	0.21	-0.81	116,147,179,195	0
3	MES	D	1002	12/12	0.96	0.17	-1.33	90,126,163,182	0

6.5 Other polymers [i](#)

There are no such residues in this entry.