Full wwPDB X-ray Structure Validation Report (i)

Feb 28, 2023 – 12:20 pm GMT

PDB ID	:	8BCH
Title	:	Human Brr2 Helicase Region in complex with Sulfaguanidine
Authors	:	Vester, K.; Loll, B.; Wahl, M.C.
Deposited on	:	2022-10-15
Resolution	:	2.87 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

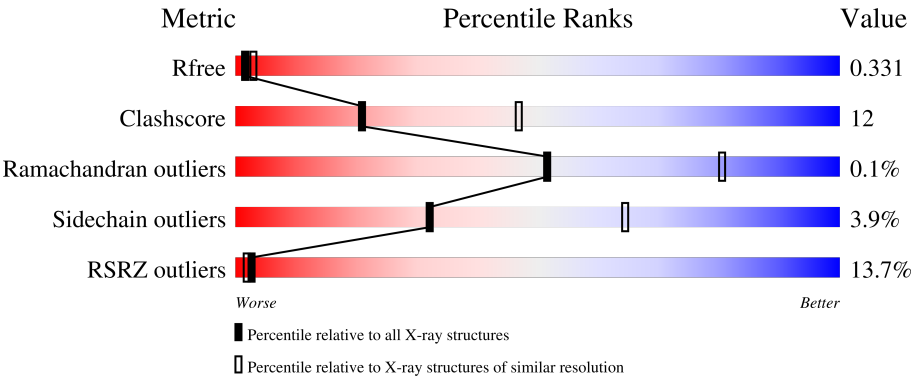
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.32.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.32.1

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 2.87 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	2691 (2.90-2.86)
Clashscore	141614	2947 (2.90-2.86)
Ramachandran outliers	138981	2868 (2.90-2.86)
Sidechain outliers	138945	2871 (2.90-2.86)
RSRZ outliers	127900	2629 (2.90-2.86)

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 of 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 <=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	B	1747	14% 69% 28% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 13884 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.

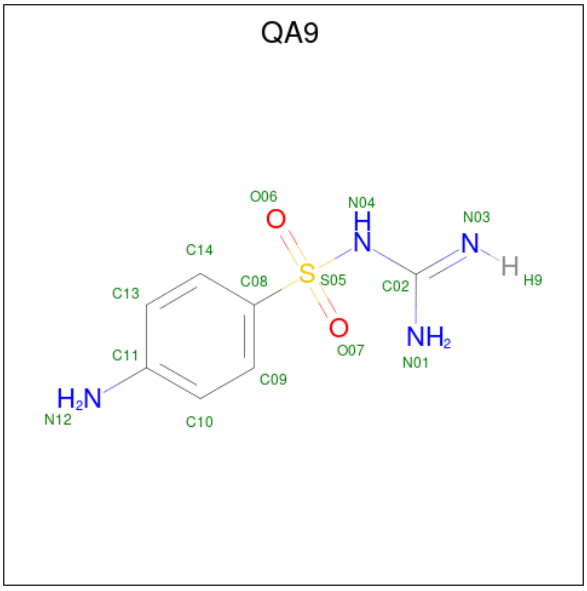
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	1724	13859	8857	2371	2559	72	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	390	GLY	-	expression tag	UNP O75643
B	391	ALA	-	expression tag	UNP O75643
B	392	GLU	-	expression tag	UNP O75643
B	393	PHE	-	expression tag	UNP O75643

- Molecule 2 is 1-(4-aminophenyl)sulfonylguanidine (three-letter code: QA9) (formula: $C_7H_{10}N_4O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	14	7	4	2	1	0	0

- Molecule 3 is water.

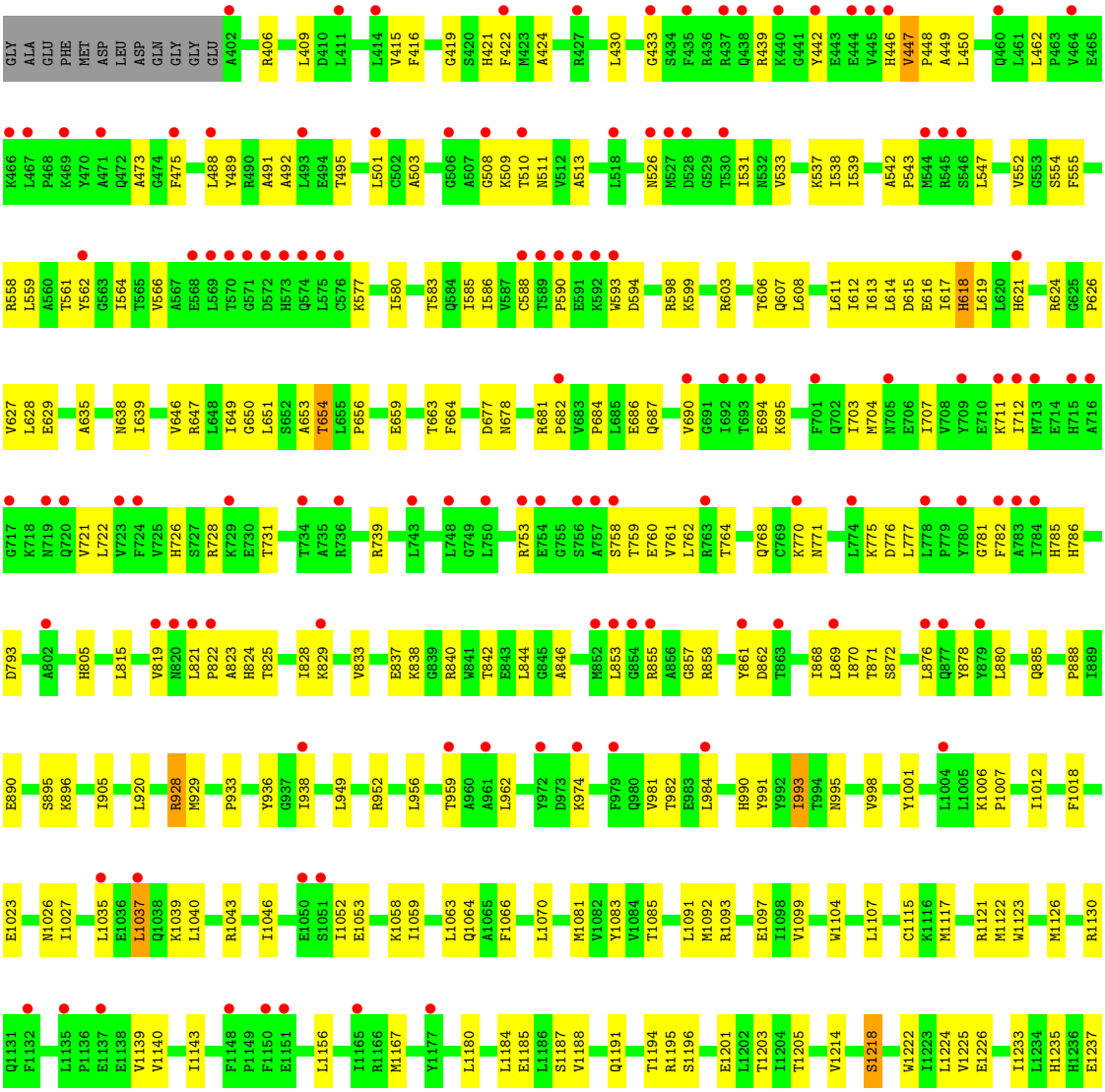
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	11	Total O 11 11	0	0

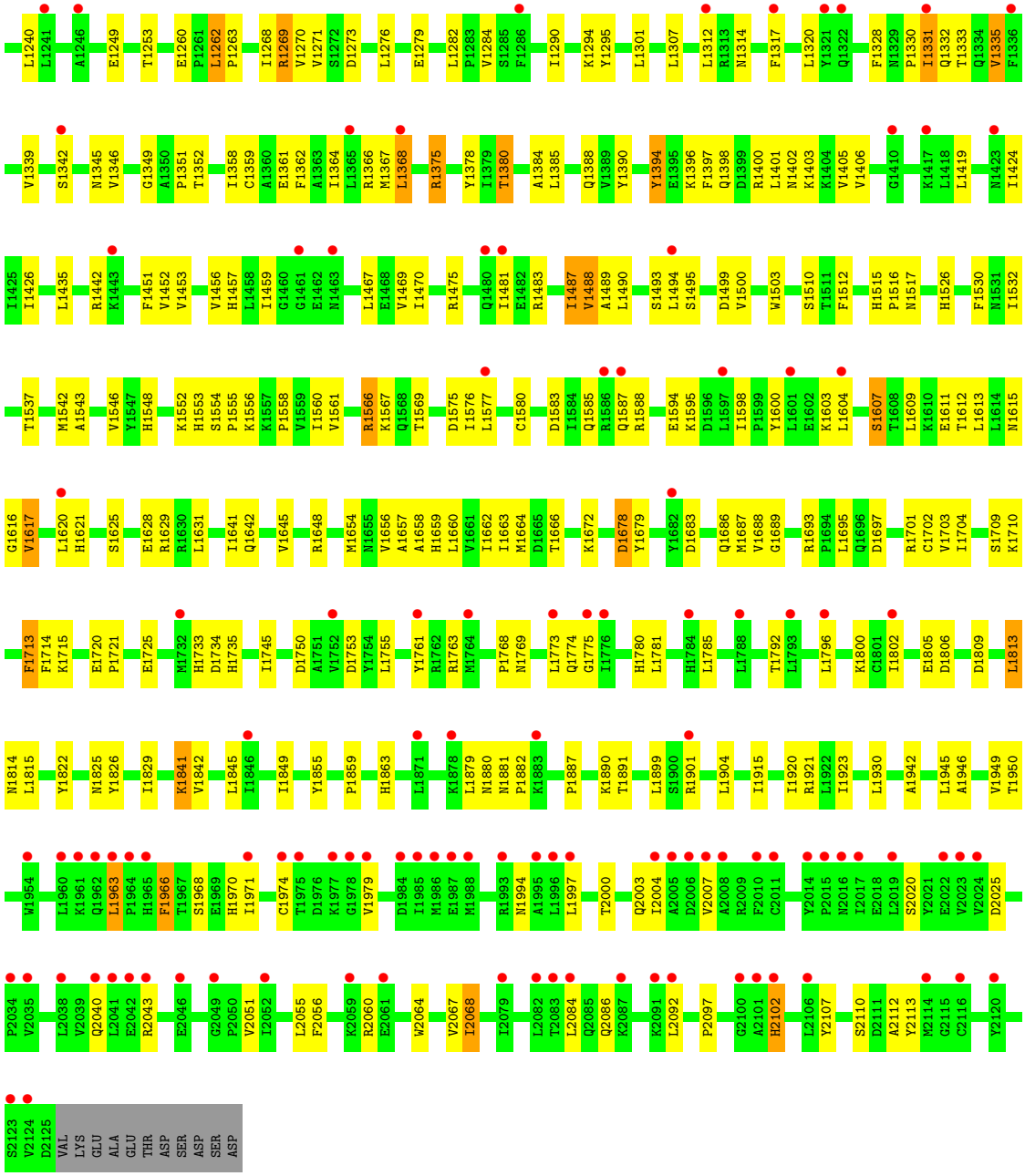
3 Residue-property plots (i)

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: U5 small nuclear ribonucleoprotein 200 kDa helicase

Chain B:




L1240 L1241 A1246 E1249 T1253 E1260 P1261 L1262 P1263 I1268 R1269 V1270 V1271 S1272 D1273 L1276 E1279 L1282 P1283 V1284 S1285 F1286 I1290 K1294 Y1295 L1301 L1307 L1312 R1313 N1314 F1317 L1320 Y1321 Q1322 F1328 N1329 P1330 I1331 Q1332 T1333 Q1334 V1335 F1336
V1339 S1342 N1345 V1346 G1349 A1350 P1351 T1352 I1358 C1359 A1360 E1361 F1362 A1363 I1364 L1365 R1366 M1367 L1368 R1375 Y1378 I1379 T1380 A1384 L1385 Q1388 V1389 Y1390 Y1394 E1395 K1396 F1397 Q1398 D1399 R1400 L1401 N1402 K1403 K1404 V1405 V1406 G1410 K1417 L1418 L1419 N1423 I1424
I1425 I1426 L1435 R1442 K1443 F1451 V1452 V1453 V1456 H1457 L1458 I1459 G1460 G1461 E1462 N1463 L1467 E1468 V1469 I1470 R1475 Q1480 I1481 E1482 R1483 I1487 V1488 A1489 L1490 S1493 L1494 S1495 D1499 V1500 W1503 S1510 Y1511 F1512 H1515 P1516 N1517 H1526 F1530 N1531 I1532
T1537 M1542 A1543 V1546 Y1547 H1548 K1552 H1553 S1554 P1555 K1556 K1557 P1558 V1559 I1560 V1561 R1566 K1567 Q1568 T1569 D1575 I1576 L1577 C1580 D1583 I1584 Q1585 R1586 Q1587 R1588 E1594 K1595 D1596 L1597 I1598 P1599 Y1600 L1601 E1602 K1603 L1604 S1607 T1608 L1609 K1610 E1611 T1612 L1613 L1614 N1615
G1616 V1617 L1620 H1621 S1625 E1628 R1629 R1630 L1631 I1641 Q1642 V1645 R1648 M1654 N1655 V1656 K1657 A1658 H1659 L1660 V1661 I1662 I1663 M1664 D1665 T1666 K1672 D1678 Y1679 Y1682 D1683 Q1686 M1687 V1688 G1689 R1693 P1694 L1695 Q1696 D1697 R1701 C1702 V1703 I1704 S1709 K1710
F1713 F1714 K1715 E1720 P1721 E1725 M1732 H1733 D1734 H1735 I1745 D1750 A1751 V1752 D1753 Y1754 L1755 Y1761 R1762 R1763 M1764 P1768 N1769 L1773 Q1774 G1775 I1776 H1780 L1781 H1784 L1785 L1788 T1792 L1793 L1796 K1800 C1801 I1802 E1805 D1806 D1809 L1813
N1814 L1815 Y1822 N1825 Y1826 I1829 K1841 V1842 L1845 I1846 I1849 Y1855 P1859 H1863 L1871 K1878 L1879 N1880 N1881 P1882 K1883 P1887 K1890 T1891 L1899 S1900 R1901 L1904 I1915 I1920 R1921 L1922 I1923 L1930 A1942 L1945 A1946 V1949 T1950
W1954 L1960 K1961 Q1962 L1963 P1964 H1965 F1966 T1967 S1968 E1969 H1970 I1971 C1974 T1975 D1976 K1977 G1978 V1979 D1984 I1985 M1986 E1987 M1988 R1993 N1994 A1995 L1996 L1997 T2000 Q2003 I2004 A2005 D2006 V2007 A2008 R2009 F2010 C2011 Y2014 P2015 N2016 I2017 E2018 L2019 S2020 Y2021 E2022 V2023 V2024 D2025
P2034 V2035 L2038 V2039 Q2040 L2041 E2042 R2043 E2046 G2049 P2050 V2051 I2052 L2055 F2056 K2059 R2060 E2061 W2064 V2067 I2068 I2079 L2082 T2083 L2084 Q2085 Q2086 K2087 K2091 L2092 P2097 G2100 A2101 H2102 L2106 Y2107 S2110 D2111 A2112 Y2113 M2114 G2115 C2116 Y2120
S2123 V2124 D2125 VAL LYS GLU ALA GLU THR ASP SER ASP SER ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.29Å 149.53Å 141.49Å 90.00° 120.32° 90.00°	Depositor
Resolution (Å)	47.20 – 2.87 47.20 – 2.87	Depositor EDS
% Data completeness (in resolution range)	93.2 (47.20-2.87) 93.3 (47.20-2.87)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 2.86Å)	Xtriage
Refinement program	PHENIX 1.20_4459	Depositor
R, R_{free}	0.281 , 0.337 0.278 , 0.331	Depositor DCC
R_{free} test set	2013 reflections (3.58%)	wwPDB-VP
Wilson B-factor (Å^2)	82.8	Xtriage
Anisotropy	0.412	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 64.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.001 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13884	wwPDB-VP
Average B, all atoms (Å^2)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% 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, 0.333 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: QA9

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	B	0.26	0/14153	0.50	0/19177

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

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	B	13859	0	14001	341	0
2	B	14	0	0	0	0
3	B	11	0	0	0	0
All	All	13884	0	14001	341	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 12.

All (341) 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:415:VAL:HG21	1:B:895:SER:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:406:ARG:NH2	1:B:974:LYS:O	2.19	0.74
1:B:1950:THR:HG22	1:B:2060:ARG:HH12	1.52	0.74
1:B:1526:HIS:HB2	1:B:1703:VAL:HG12	1.69	0.74
1:B:1710:LYS:O	1:B:1713:PHE:HB3	1.88	0.73
1:B:1378:TYR:HB3	1:B:1426:ILE:HG22	1.71	0.73
1:B:1328:PHE:HB3	1:B:1332:GLN:HG3	1.70	0.72
1:B:492:ALA:HA	1:B:647:ARG:HH22	1.53	0.72
1:B:1950:THR:HG21	1:B:2112:ALA:HA	1.72	0.72
1:B:626:PRO:HG2	1:B:896:LYS:HG3	1.72	0.71
1:B:1974:CYS:HB3	1:B:1979:VAL:HB	1.74	0.70
1:B:1320:LEU:HG	1:B:1396:LYS:HD3	1.72	0.70
1:B:1405:VAL:HG22	1:B:1424:ILE:HB	1.74	0.69
1:B:1734:ASP:OD2	1:B:1825:ASN:ND2	2.22	0.69
1:B:531:ILE:HD13	1:B:533:VAL:HG13	1.75	0.68
1:B:1577:LEU:HD11	1:B:1615:ASN:HB3	1.73	0.68
1:B:1800:LYS:HB2	1:B:1815:LEU:HD12	1.76	0.68
1:B:1345:ASN:HB3	1:B:1487:ILE:HG22	1.76	0.68
1:B:1966:PHE:HE1	1:B:1970:HIS:HB2	1.58	0.68
1:B:753:ARG:HD2	1:B:760:GLU:HB2	1.75	0.67
1:B:758:SER:OG	1:B:759:THR:N	2.27	0.67
1:B:1027:ILE:HG21	1:B:1059:ILE:HD11	1.77	0.67
1:B:566:VAL:HG12	1:B:585:ILE:HB	1.77	0.66
1:B:1301:LEU:HD21	1:B:1330:PRO:HB2	1.76	0.66
1:B:1359:CYS:O	1:B:1362:PHE:HB2	1.96	0.66
1:B:1301:LEU:HD22	1:B:1331:ILE:HG22	1.76	0.66
1:B:1660:LEU:HA	1:B:1701:ARG:O	1.97	0.65
1:B:2051:VAL:HG13	1:B:2113:TYR:HE1	1.60	0.65
1:B:1185:GLU:HB2	1:B:1205:THR:HB	1.78	0.65
1:B:1390:TYR:HB2	1:B:1426:ILE:HD11	1.77	0.65
1:B:993:ILE:HD11	1:B:998:VAL:HG23	1.78	0.65
1:B:1225:VAL:HG22	1:B:1268:ILE:HG22	1.78	0.65
1:B:768:GLN:HE21	1:B:775:LYS:HA	1.60	0.65
1:B:690:VAL:HG22	1:B:870:ILE:HA	1.79	0.64
1:B:678:ASN:OD1	1:B:885:GLN:NE2	2.31	0.64
1:B:758:SER:HB2	1:B:762:LEU:HB2	1.80	0.64
1:B:1226:GLU:OE2	1:B:1269:ARG:NH1	2.31	0.64
1:B:1222:TRP:NE1	1:B:1273:ASP:OD2	2.30	0.63
1:B:991:TYR:HE2	1:B:1097:GLU:HG3	1.63	0.63
1:B:1585:GLN:HB3	1:B:1588:ARG:HB2	1.81	0.63
1:B:777:LEU:HB3	1:B:782:PHE:HB2	1.81	0.62
1:B:539:ILE:HG22	1:B:586:ILE:HB	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:VAL:HG21	1:B:1489:ALA:HB1	1.81	0.62
1:B:659:GLU:O	1:B:663:THR:HG23	2.00	0.62
1:B:1339:VAL:HG22	1:B:1346:VAL:HG21	1.80	0.62
1:B:929:MET:HE2	1:B:949:LEU:HD13	1.82	0.62
1:B:1081:MET:O	1:B:1085:THR:HG23	2.00	0.61
1:B:858:ARG:HE	1:B:861:TYR:HB2	1.65	0.61
1:B:858:ARG:N	1:B:862:ASP:OD2	2.31	0.61
1:B:543:PRO:HD2	1:B:547:LEU:HD23	1.83	0.61
1:B:753:ARG:HH21	1:B:761:VAL:HG22	1.66	0.61
1:B:1195:ARG:NH1	1:B:1260:GLU:OE2	2.32	0.61
1:B:2043:ARG:HB3	1:B:2086:GLN:HA	1.83	0.60
1:B:419:GLY:O	1:B:421:HIS:N	2.32	0.60
1:B:1859:PRO:O	1:B:1890:LYS:NZ	2.31	0.60
1:B:1966:PHE:CE1	1:B:1970:HIS:HB2	2.37	0.59
1:B:537:LYS:NZ	1:B:583:THR:O	2.36	0.59
1:B:1451:PHE:HB3	1:B:1487:ILE:HD12	1.84	0.58
1:B:488:LEU:HD21	1:B:501:LEU:HD13	1.86	0.58
1:B:656:PRO:HG2	1:B:888:PRO:HA	1.84	0.58
1:B:768:GLN:NE2	1:B:775:LYS:HA	2.18	0.58
1:B:555:PHE:O	1:B:559:LEU:HG	2.03	0.58
1:B:2043:ARG:HH21	1:B:2084:LEU:HD23	1.68	0.58
1:B:508:GLY:O	1:B:510:THR:N	2.35	0.57
1:B:984:LEU:HD12	1:B:998:VAL:HG13	1.84	0.57
1:B:619:LEU:HD11	1:B:624:ARG:HB2	1.85	0.57
1:B:712:ILE:HG12	1:B:721:VAL:HB	1.87	0.57
1:B:982:THR:HG22	1:B:984:LEU:H	1.69	0.57
1:B:1066:PHE:O	1:B:1121:ARG:NH1	2.36	0.57
1:B:1368:LEU:HD21	1:B:1403:LYS:HE2	1.86	0.57
1:B:1842:VAL:HA	1:B:1845:LEU:HD22	1.87	0.57
1:B:552:VAL:HG23	1:B:566:VAL:HG23	1.87	0.57
1:B:1312:LEU:HD21	1:B:1317:PHE:HB3	1.87	0.56
1:B:1235:HIS:NE2	1:B:1237:GLU:HG3	2.21	0.56
1:B:1994:ASN:HA	1:B:1997:LEU:HD12	1.88	0.56
1:B:1364:ILE:O	1:B:1367:MET:HB3	2.05	0.56
1:B:1397:PHE:O	1:B:1402:ASN:N	2.39	0.56
1:B:1595:LYS:HD3	1:B:1598:ILE:HD12	1.87	0.56
1:B:694:GLU:HG2	1:B:695:LYS:H	1.71	0.55
1:B:1500:VAL:HG23	1:B:1503:TRP:HE3	1.69	0.55
1:B:1575:ASP:OD1	1:B:1576:ILE:N	2.40	0.55
1:B:1099:VAL:HG21	1:B:1107:LEU:HB3	1.88	0.55
1:B:1920:ILE:HA	1:B:1923:ILE:HG22	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.88	0.54
1:B:929:MET:HE3	1:B:938:ILE:HD11	1.89	0.54
1:B:1130:ARG:HG2	1:B:1140:VAL:HG11	1.88	0.54
1:B:1368:LEU:HD11	1:B:1403:LYS:HG2	1.88	0.54
1:B:824:HIS:ND1	1:B:862:ASP:OD1	2.40	0.54
1:B:424:ALA:HB3	1:B:888:PRO:HG2	1.88	0.54
1:B:1566:ARG:HB2	1:B:1621:HIS:HB2	1.90	0.54
1:B:1332:GLN:HA	1:B:1335:VAL:HG12	1.89	0.54
1:B:1384:ALA:O	1:B:1388:GLN:HG2	2.08	0.54
1:B:1092:MET:HB3	1:B:1115:CYS:SG	2.47	0.53
1:B:1018:PHE:CE2	1:B:1063:LEU:HD22	2.43	0.53
1:B:447:VAL:HG22	1:B:687:GLN:HG3	1.91	0.53
1:B:1688:VAL:HG22	1:B:1702:CYS:SG	2.49	0.53
1:B:539:ILE:HD11	1:B:612:ILE:HG23	1.91	0.53
1:B:677:ASP:HB2	1:B:885:GLN:HE22	1.73	0.53
1:B:1035:LEU:O	1:B:1039:LYS:HG2	2.09	0.53
1:B:728:ARG:HG2	1:B:786:HIS:CG	2.44	0.52
1:B:1543:ALA:O	1:B:1546:VAL:HG22	2.10	0.52
1:B:1733:HIS:CD2	1:B:1792:THR:HG22	2.44	0.52
1:B:1813:LEU:HD22	1:B:1814:ASN:H	1.74	0.52
1:B:1997:LEU:HD13	1:B:2004:ILE:HG22	1.92	0.52
1:B:491:ALA:O	1:B:495:THR:OG1	2.19	0.52
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.90	0.52
1:B:538:ILE:O	1:B:585:ILE:HA	2.10	0.52
1:B:1845:LEU:HB3	1:B:1945:LEU:HD22	1.90	0.52
1:B:933:PRO:HB2	1:B:938:ILE:HB	1.92	0.52
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.91	0.52
1:B:1612:THR:OG1	1:B:1617:VAL:HG13	2.09	0.52
1:B:635:ALA:O	1:B:639:ILE:HG23	2.10	0.52
1:B:1453:VAL:HG22	1:B:1456:VAL:HG22	1.92	0.52
1:B:473:ALA:HB3	1:B:562:TYR:CZ	2.45	0.51
1:B:823:ALA:O	1:B:857:GLY:N	2.40	0.51
1:B:1946:ALA:O	1:B:1950:THR:HG23	2.11	0.51
1:B:1290:ILE:HD13	1:B:1768:PRO:HD2	1.92	0.51
1:B:1335:VAL:HG23	1:B:1512:PHE:CD2	2.45	0.51
1:B:1218:SER:HB2	1:B:1240:LEU:HD21	1.93	0.51
1:B:1796:LEU:HB3	1:B:1802:ILE:HG23	1.93	0.51
1:B:1188:VAL:HG11	1:B:1284:VAL:HG12	1.92	0.51
1:B:614:LEU:HD23	1:B:628:LEU:HD22	1.92	0.51
1:B:446:HIS:NE2	1:B:686:GLU:HG2	2.25	0.51
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:539:ILE:HD11	1:B:612:ILE:HG12	1.93	0.51
1:B:704:MET:HE3	1:B:829:LYS:HG2	1.93	0.51
1:B:442:TYR:HE1	1:B:707:ILE:HG12	1.76	0.51
1:B:611:LEU:HD11	1:B:649:ILE:HG12	1.93	0.50
1:B:1560:ILE:HD11	1:B:1656:VAL:HG12	1.92	0.50
1:B:711:LYS:HG3	1:B:868:ILE:HD13	1.93	0.50
1:B:681:ARG:HG3	1:B:682:PRO:HD2	1.93	0.50
1:B:1553:HIS:O	1:B:1701:ARG:NH1	2.44	0.50
1:B:629:GLU:HA	1:B:664:PHE:HZ	1.76	0.50
1:B:503:ALA:HB3	1:B:509:LYS:HD3	1.94	0.50
1:B:1349:GLY:N	1:B:1512:PHE:O	2.32	0.50
1:B:1001:TYR:OH	1:B:1091:LEU:HD12	2.12	0.49
1:B:603:ARG:NH2	1:B:607:GLN:HA	2.27	0.49
1:B:722:LEU:HD22	1:B:823:ALA:HB2	1.94	0.49
1:B:1678:ASP:OD1	1:B:1710:LYS:NZ	2.40	0.49
1:B:599:LYS:HA	1:B:990:HIS:CD2	2.48	0.49
1:B:1314:ASN:HB3	1:B:1317:PHE:HB2	1.95	0.49
1:B:1585:GLN:O	1:B:1587:GLN:N	2.42	0.49
1:B:2068:ILE:HD11	1:B:2092:LEU:HD13	1.95	0.49
1:B:1307:LEU:HG	1:B:1333:THR:HG23	1.95	0.49
1:B:768:GLN:HB3	1:B:775:LYS:NZ	2.28	0.49
1:B:2020:SER:OG	1:B:2040:GLN:HB2	2.13	0.49
1:B:1352:THR:HG22	1:B:1689:GLY:HA3	1.95	0.48
1:B:1566:ARG:HG3	1:B:1567:LYS:H	1.78	0.48
1:B:1364:ILE:HG21	1:B:1424:ILE:HD11	1.94	0.48
1:B:1515:HIS:ND1	1:B:1516:PRO:HD2	2.29	0.48
1:B:449:ALA:HB1	1:B:684:PRO:HB2	1.95	0.48
1:B:1271:VAL:HG13	1:B:1279:GLU:HB2	1.94	0.48
1:B:1046:ILE:HB	1:B:1064:GLN:NE2	2.28	0.48
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.53	0.48
1:B:1194:THR:HG23	1:B:1196:SER:H	1.78	0.48
1:B:1620:LEU:HD22	1:B:1629:ARG:HG2	1.95	0.48
1:B:1469:VAL:HG21	1:B:1735:HIS:NE2	2.28	0.48
1:B:1604:LEU:HD21	1:B:1631:LEU:HD23	1.95	0.48
1:B:1346:VAL:HA	1:B:1510:SER:HB3	1.96	0.48
1:B:1775:GLY:HA3	1:B:1780:HIS:CG	2.49	0.47
1:B:433:GLY:O	1:B:448:PRO:HD3	2.15	0.47
1:B:1664:MET:O	1:B:1666:THR:N	2.41	0.47
1:B:838:LYS:HB3	1:B:840:ARG:HG2	1.96	0.47
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	1.96	0.47
1:B:1725:GLU:OE2	1:B:1763:ARG:NH2	2.37	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1139:VAL:O	1:B:1143:ILE:HG13	2.14	0.47
1:B:1295:TYR:CG	1:B:1495:SER:HB2	2.48	0.47
1:B:871:THR:OG1	1:B:872:SER:N	2.48	0.47
1:B:2064:TRP:CZ3	1:B:2110:SER:HB3	2.50	0.47
1:B:450:LEU:HD12	1:B:678:ASN:HB2	1.96	0.47
1:B:928:ARG:HD2	1:B:928:ARG:HA	1.71	0.47
1:B:599:LYS:HA	1:B:990:HIS:HD2	1.80	0.47
1:B:837:GLU:HG3	1:B:1083:TYR:CE1	2.49	0.47
1:B:1224:LEU:HD23	1:B:1233:ILE:HD13	1.96	0.46
1:B:1452:VAL:HA	1:B:1488:VAL:O	2.15	0.46
1:B:776:ASP:OD1	1:B:777:LEU:N	2.48	0.46
1:B:1290:ILE:HG13	1:B:1769:ASN:OD1	2.14	0.46
1:B:678:ASN:ND2	1:B:681:ARG:HH21	2.13	0.46
1:B:538:ILE:HB	1:B:585:ILE:HG12	1.98	0.46
1:B:876:LEU:O	1:B:880:LEU:HG	2.15	0.46
1:B:1352:THR:HG21	1:B:1686:GLN:HA	1.97	0.46
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.98	0.46
1:B:639:ILE:HG21	1:B:646:VAL:HG22	1.97	0.46
1:B:1037:LEU:HD21	1:B:1058:LYS:HG3	1.98	0.46
1:B:562:TYR:HB2	1:B:564:ILE:HG12	1.98	0.46
1:B:890:GLU:HG3	1:B:936:TYR:OH	2.15	0.46
1:B:753:ARG:NH1	1:B:781:GLY:HA2	2.30	0.46
1:B:1720:GLU:HB2	1:B:1721:PRO:HD2	1.98	0.46
1:B:1657:ALA:HB1	1:B:1693:ARG:HB3	1.98	0.46
1:B:1774:GLN:N	1:B:1774:GLN:OE1	2.49	0.46
1:B:678:ASN:HD22	1:B:681:ARG:HH21	1.64	0.45
1:B:1467:LEU:O	1:B:1470:ILE:HG13	2.16	0.45
1:B:1733:HIS:CD2	1:B:1733:HIS:N	2.84	0.45
1:B:1481:ILE:HG22	1:B:1483:ARG:HG2	1.97	0.45
1:B:1493:SER:HB3	1:B:1516:PRO:HD3	1.98	0.45
1:B:1452:VAL:HB	1:B:1488:VAL:HG13	1.98	0.45
1:B:777:LEU:HD22	1:B:782:PHE:HD2	1.82	0.45
1:B:2097:PRO:HG2	1:B:2102:HIS:CD2	2.52	0.45
1:B:815:LEU:HD12	1:B:819:VAL:HB	1.99	0.45
1:B:1184:LEU:HD12	1:B:1270:VAL:HG11	1.99	0.45
1:B:1923:ILE:HD11	1:B:1942:ALA:HB1	1.98	0.45
1:B:421:HIS:CE1	1:B:846:ALA:HB2	2.52	0.45
1:B:704:MET:HG2	1:B:870:ILE:HG21	1.98	0.44
1:B:819:VAL:O	1:B:855:ARG:NH2	2.41	0.44
1:B:1345:ASN:HA	1:B:1487:ILE:O	2.17	0.44
1:B:577:LYS:NZ	1:B:1537:THR:HG21	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:920:LEU:HD23	1:B:920:LEU:HA	1.78	0.44
1:B:1180:LEU:HD23	1:B:1214:VAL:HG21	1.98	0.44
1:B:1554:SER:HB3	1:B:1659:HIS:ND1	2.32	0.44
1:B:442:TYR:CE1	1:B:707:ILE:HG12	2.52	0.44
1:B:409:LEU:H	1:B:959:THR:CG2	2.30	0.44
1:B:991:TYR:CE2	1:B:1097:GLU:HG3	2.48	0.44
1:B:1156:LEU:HD12	1:B:1156:LEU:HA	1.70	0.44
1:B:1733:HIS:HB2	1:B:1826:TYR:CE1	2.52	0.44
1:B:1829:ILE:HD13	1:B:1829:ILE:HA	1.75	0.44
1:B:475:PHE:CE2	1:B:511:ASN:HB3	2.53	0.44
1:B:554:SER:O	1:B:558:ARG:HG2	2.17	0.44
1:B:822:PRO:HB2	1:B:858:ARG:HA	1.99	0.44
1:B:2067:VAL:HB	1:B:2107:TYR:HB2	1.97	0.44
1:B:703:ILE:O	1:B:707:ILE:HG13	2.17	0.44
1:B:1122:MET:SD	1:B:1130:ARG:HB2	2.57	0.44
1:B:588:CYS:SG	1:B:593:TRP:HB2	2.58	0.44
1:B:1201:GLU:HG2	1:B:1253:THR:HG23	2.00	0.44
1:B:1294:LYS:HD3	1:B:1295:TYR:H	1.82	0.44
1:B:1052:ILE:HG13	1:B:1053:GLU:H	1.82	0.44
1:B:1262:LEU:HD23	1:B:1263:PRO:HD2	1.99	0.44
1:B:1577:LEU:HD13	1:B:1617:VAL:HG12	1.99	0.44
1:B:828:ILE:HD12	1:B:869:LEU:HD12	2.00	0.43
1:B:1268:ILE:HG13	1:B:1282:LEU:HB3	2.00	0.43
1:B:1963:LEU:HD13	1:B:2007:VAL:HG13	1.99	0.43
1:B:1380:THR:HG21	1:B:1385:LEU:HB2	1.99	0.43
1:B:1693:ARG:HB2	1:B:1695:LEU:HD12	1.99	0.43
1:B:409:LEU:HB2	1:B:959:THR:HG21	1.99	0.43
1:B:760:GLU:HG2	1:B:805:HIS:HA	2.00	0.43
1:B:1205:THR:HG23	1:B:1249:GLU:HG2	2.00	0.43
1:B:608:LEU:HD23	1:B:608:LEU:HA	1.85	0.43
1:B:819:VAL:HG12	1:B:821:LEU:HB2	1.99	0.43
1:B:1099:VAL:CG2	1:B:1104:TRP:HB2	2.48	0.43
1:B:1375:ARG:NH2	1:B:1419:LEU:O	2.52	0.43
1:B:1763:ARG:HA	1:B:1763:ARG:HD2	1.77	0.43
1:B:952:ARG:HD3	1:B:956:LEU:HD13	2.00	0.43
1:B:448:PRO:HA	1:B:686:GLU:HG3	1.99	0.43
1:B:559:LEU:HD13	1:B:564:ILE:HB	1.99	0.43
1:B:1006:LYS:HD3	1:B:1006:LYS:HA	1.83	0.43
1:B:1026:ASN:OD1	1:B:1026:ASN:N	2.52	0.43
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	2.00	0.43
1:B:1364:ILE:HA	1:B:1367:MET:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1007:PRO:HG3	1:B:1104:TRP:CE2	2.53	0.43
1:B:1290:ILE:HG13	1:B:1290:ILE:H	1.71	0.43
1:B:1367:MET:HE1	1:B:1375:ARG:N	2.33	0.43
1:B:1600:TYR:O	1:B:1603:LYS:HG2	2.18	0.43
1:B:1577:LEU:HD11	1:B:1615:ASN:CB	2.46	0.43
1:B:1683:ASP:O	1:B:1687:MET:HG3	2.19	0.43
1:B:513:ALA:HB2	1:B:651:LEU:HD11	2.01	0.43
1:B:1469:VAL:HG21	1:B:1735:HIS:CD2	2.54	0.43
1:B:1755:LEU:O	1:B:1761:TYR:HB2	2.19	0.43
1:B:726:HIS:HB3	1:B:833:VAL:HG23	2.01	0.42
1:B:1394:TYR:CD1	1:B:1398:GLN:HB3	2.53	0.42
1:B:1648:ARG:HD3	1:B:1679:TYR:CZ	2.54	0.42
1:B:1750:ASP:HA	1:B:1753:ASP:HB2	2.00	0.42
1:B:616:GLU:HA	1:B:618:HIS:CE1	2.54	0.42
1:B:1457:HIS:HB3	1:B:1494:LEU:HD11	2.01	0.42
1:B:1662:ILE:HG12	1:B:1703:VAL:HG22	2.01	0.42
1:B:1594:GLU:O	1:B:1598:ILE:HG13	2.19	0.42
1:B:1733:HIS:HD1	1:B:1826:TYR:HH	1.66	0.42
1:B:619:LEU:HD23	1:B:628:LEU:HG	2.02	0.42
1:B:1012:ILE:H	1:B:1012:ILE:HD12	1.83	0.42
1:B:1332:GLN:NE2	1:B:1358:ILE:HD11	2.33	0.42
1:B:1459:ILE:H	1:B:1459:ILE:HG12	1.63	0.42
1:B:624:ARG:O	1:B:627:VAL:HG22	2.20	0.42
1:B:731:THR:HG21	1:B:786:HIS:HD2	1.84	0.42
1:B:785:HIS:CE1	1:B:815:LEU:HD13	2.55	0.42
1:B:1556:LYS:HE2	1:B:1556:LYS:HB3	1.72	0.42
1:B:1187:SER:OG	1:B:1203:THR:HB	2.19	0.42
1:B:1558:PRO:HA	1:B:1642:GLN:O	2.20	0.42
1:B:1805:GLU:HG3	1:B:1806:ASP:OD1	2.20	0.42
1:B:1849:ILE:HD13	1:B:1849:ILE:HA	1.95	0.42
1:B:577:LYS:O	1:B:580:ILE:HG22	2.19	0.42
1:B:628:LEU:HD23	1:B:628:LEU:HA	1.84	0.42
1:B:722:LEU:HA	1:B:722:LEU:HD12	1.85	0.42
1:B:962:LEU:HD23	1:B:962:LEU:HA	1.93	0.42
1:B:1530:PHE:O	1:B:1532:ILE:N	2.51	0.42
1:B:618:HIS:CE1	1:B:653:ALA:H	2.38	0.42
1:B:1435:LEU:O	1:B:1442:ARG:NH1	2.53	0.42
1:B:1566:ARG:CB	1:B:1621:HIS:HB2	2.50	0.42
1:B:1899:LEU:HD23	1:B:1899:LEU:HA	1.93	0.42
1:B:1043:ARG:NH2	1:B:1070:LEU:HD22	2.35	0.42
1:B:1400:ARG:HA	1:B:1400:ARG:HD3	1.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:617:ILE:HD11	1:B:650:GLY:HA2	2.02	0.41
1:B:739:ARG:NH2	1:B:777:LEU:HD23	2.35	0.41
1:B:1117:MET:HG2	1:B:1276:LEU:HD11	2.02	0.41
1:B:1123:TRP:HD1	1:B:1126:MET:HE1	1.85	0.41
1:B:1493:SER:CB	1:B:1516:PRO:HD3	2.50	0.41
1:B:654:THR:HG21	1:B:677:ASP:HA	2.02	0.41
1:B:760:GLU:O	1:B:764:THR:HG23	2.19	0.41
1:B:1613:LEU:HD23	1:B:1613:LEU:HA	1.87	0.41
1:B:1666:THR:HA	1:B:1679:TYR:CE2	2.55	0.41
1:B:1881:ASN:N	1:B:1882:PRO:HD3	2.34	0.41
1:B:1609:LEU:HA	1:B:1612:THR:HG22	2.02	0.41
1:B:1855:TYR:CZ	1:B:1915:ILE:HG23	2.56	0.41
1:B:1023:GLU:OE1	1:B:1023:GLU:N	2.50	0.41
1:B:1035:LEU:HG	1:B:1039:LYS:HE2	2.01	0.41
1:B:1335:VAL:HG22	1:B:1339:VAL:HG23	2.02	0.41
1:B:1358:ILE:O	1:B:1361:GLU:HB2	2.21	0.41
1:B:1768:PRO:HB3	1:B:1773:LEU:HG	2.03	0.41
1:B:594:ASP:O	1:B:598:ARG:HG2	2.20	0.41
1:B:542:ALA:O	1:B:590:PRO:HD3	2.21	0.41
1:B:2000:THR:HG23	1:B:2003:GLN:H	1.86	0.41
1:B:1714:PHE:O	1:B:1715:LYS:C	2.59	0.41
1:B:1781:LEU:O	1:B:1785:LEU:HG	2.20	0.41
1:B:603:ARG:HE	1:B:607:GLN:HG3	1.86	0.41
1:B:1139:VAL:HG22	1:B:1167:MET:SD	2.61	0.41
1:B:1346:VAL:O	1:B:1488:VAL:HA	2.21	0.41
1:B:1397:PHE:HD1	1:B:1401:LEU:HD12	1.85	0.41
1:B:1566:ARG:HG3	1:B:1567:LYS:N	2.34	0.41
1:B:1822:TYR:O	1:B:1921:ARG:HD3	2.21	0.41
1:B:1879:LEU:HD23	1:B:1880:ASN:O	2.21	0.41
1:B:416:PHE:HB3	1:B:422:PHE:HB2	2.03	0.41
1:B:840:ARG:NH1	1:B:842:THR:HG22	2.36	0.41
1:B:1342:SER:C	1:B:1366:ARG:HH22	2.24	0.41
1:B:1945:LEU:O	1:B:1949:VAL:HG13	2.21	0.41
1:B:721:VAL:HA	1:B:825:THR:HB	2.02	0.40
1:B:1237:GLU:HG2	1:B:1709:SER:HB2	2.02	0.40
1:B:1542:MET:O	1:B:1546:VAL:HG13	2.21	0.40
1:B:1577:LEU:HA	1:B:1577:LEU:HD12	1.73	0.40
1:B:1800:LYS:O	1:B:1813:LEU:HD12	2.20	0.40
1:B:1887:PRO:O	1:B:1891:THR:HG23	2.21	0.40
1:B:853:LEU:HA	1:B:853:LEU:HD23	1.84	0.40
1:B:1901:ARG:HH21	1:B:2055:LEU:HD11	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1616:GLY:O	1:B:1641:ILE:HG23	2.21	0.40
1:B:1654:MET:HE2	1:B:1654:MET:HB3	1.87	0.40
1:B:1841:LYS:O	1:B:1845:LEU:HD13	2.21	0.40
1:B:603:ARG:O	1:B:607:GLN:HB2	2.22	0.40
1:B:615:ASP:HA	1:B:651:LEU:HB2	2.02	0.40
1:B:1548:HIS:HB3	1:B:1552:LYS:HZ2	1.87	0.40
1:B:1566:ARG:O	1:B:1569:THR:OG1	2.21	0.40
1:B:1607:SER:O	1:B:1611:GLU:HG2	2.21	0.40
1:B:1813:LEU:HD13	1:B:1814:ASN:N	2.36	0.40
1:B:1968:SER:HA	1:B:1971:ILE:HG12	2.04	0.40
1:B:1561:VAL:O	1:B:1645:VAL:HA	2.21	0.40
1:B:1672:LYS:HD2	1:B:1887:PRO:HG3	2.04	0.40

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	B	1722/1747 (99%)	1625 (94%)	96 (6%)	1 (0%)	51 80

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1713	PHE

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	B	1542/1560 (99%)	1482 (96%)	60 (4%)	32 64

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	430	LEU
1	B	439	ARG
1	B	447	VAL
1	B	462	LEU
1	B	489	TYR
1	B	526	ASN
1	B	561	THR
1	B	606	THR
1	B	618	HIS
1	B	621	HIS
1	B	638	ASN
1	B	654	THR
1	B	770	LYS
1	B	771	ASN
1	B	793	ASP
1	B	844	LEU
1	B	878	TYR
1	B	928	ARG
1	B	993	ILE
1	B	995	ASN
1	B	1037	LEU
1	B	1040	LEU
1	B	1191	GLN
1	B	1218	SER
1	B	1262	LEU
1	B	1269	ARG
1	B	1331	ILE
1	B	1335	VAL
1	B	1368	LEU
1	B	1375	ARG
1	B	1380	THR
1	B	1394	TYR
1	B	1406	VAL
1	B	1475	ARG
1	B	1487	ILE
1	B	1488	VAL

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Mol	Chain	Res	Type
1	B	1490	LEU
1	B	1499	ASP
1	B	1517	ASN
1	B	1555	PRO
1	B	1566	ARG
1	B	1580	CYS
1	B	1583	ASP
1	B	1607	SER
1	B	1617	VAL
1	B	1678	ASP
1	B	1697	ASP
1	B	1745	ILE
1	B	1809	ASP
1	B	1813	LEU
1	B	1841	LYS
1	B	1863	HIS
1	B	1904	LEU
1	B	1930	LEU
1	B	1963	LEU
1	B	1966	PHE
1	B	2025	ASP
1	B	2056	PHE
1	B	2068	ILE
1	B	2102	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is 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	QA9	B	2201	-	13,14,14	1.78	4 (30%)	17,20,20	4.43	4 (23%)

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	QA9	B	2201	-	-	4/9/11/11	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2201	QA9	S05-N04	3.24	1.71	1.64
2	B	2201	QA9	C02-N01	2.79	1.46	1.34
2	B	2201	QA9	O07-S05	2.58	1.46	1.43
2	B	2201	QA9	C08-S05	2.51	1.80	1.76

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2201	QA9	O07-S05-O06	-16.67	99.06	119.55
2	B	2201	QA9	C08-S05-N04	4.82	113.28	105.97
2	B	2201	QA9	O07-S05-N04	3.53	116.67	106.74
2	B	2201	QA9	O06-S05-C08	2.96	111.62	107.97

There are no chirality outliers.

All (4) torsion outliers are listed below:

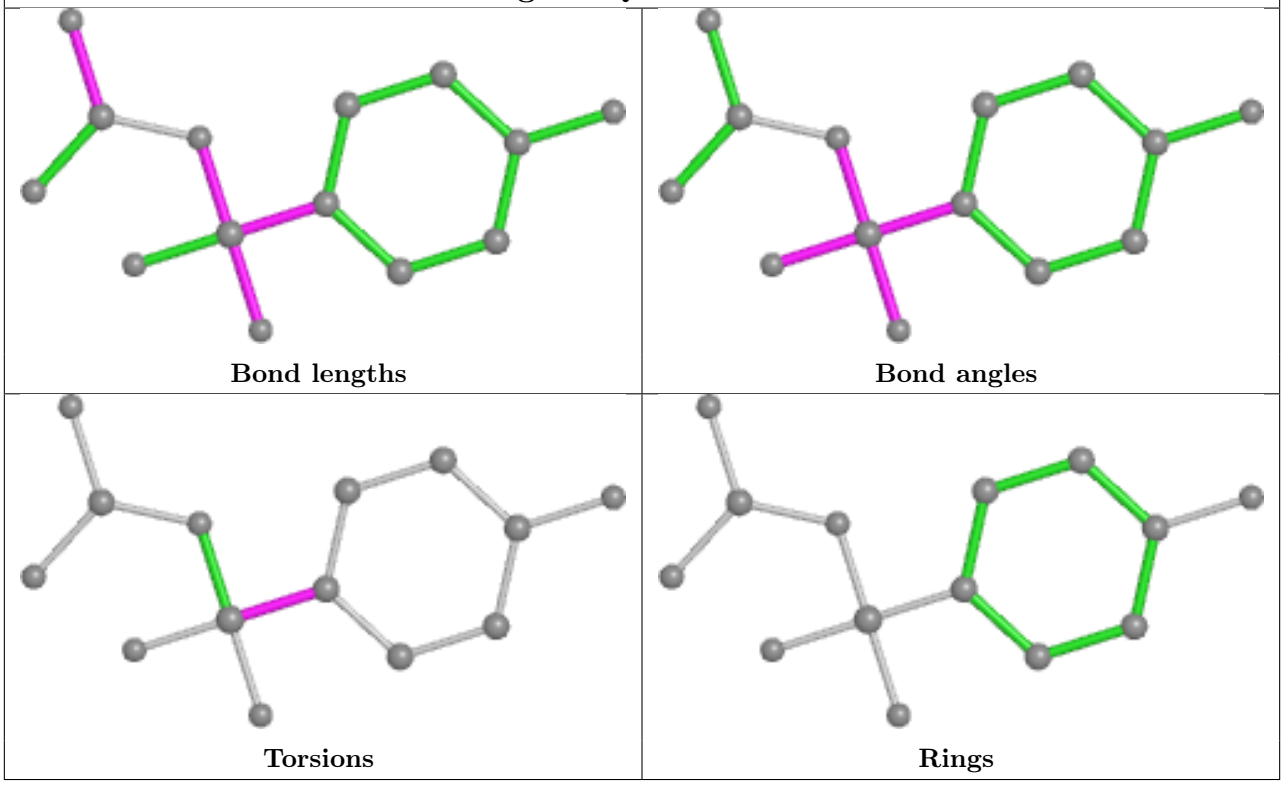
Mol	Chain	Res	Type	Atoms
2	B	2201	QA9	C14-C08-S05-O06
2	B	2201	QA9	C09-C08-S05-O06
2	B	2201	QA9	C14-C08-S05-N04
2	B	2201	QA9	C09-C08-S05-N04

There are no ring outliers.

No monomer is involved in short contacts.

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 then 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 QA9 B 2201



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	B	1724/1747 (98%)	0.75	236 (13%)	3	2	52, 112, 198, 330	0

All (236) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1985	ILE	10.4
1	B	572	ASP	9.2
1	B	1988	MET	8.5
1	B	571	GLY	8.1
1	B	783	ALA	7.9
1	B	757	ALA	7.7
1	B	573	HIS	7.4
1	B	2010	PHE	7.3
1	B	1587	GLN	7.1
1	B	2124	VAL	7.0
1	B	2015	PRO	6.6
1	B	1979	VAL	6.2
1	B	774	LEU	6.2
1	B	442	TYR	6.0
1	B	763	ARG	5.9
1	B	694	GLU	5.7
1	B	1997	LEU	5.7
1	B	692	ILE	5.6
1	B	1963	LEU	5.5
1	B	1481	ILE	5.4
1	B	829	LYS	5.3
1	B	756	SER	5.3
1	B	780	TYR	5.2
1	B	2014	TYR	5.2
1	B	1993	ARG	5.2
1	B	530	THR	5.2
1	B	784	ILE	5.2

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Mol	Chain	Res	Type	RSRZ
1	B	435	PHE	5.2
1	B	782	PHE	5.2
1	B	2007	VAL	5.0
1	B	754	GLU	5.0
1	B	2120	TYR	5.0
1	B	1964	PRO	5.0
1	B	1761	TYR	5.0
1	B	527	MET	4.7
1	B	575	LEU	4.7
1	B	2019	LEU	4.7
1	B	778	LEU	4.6
1	B	753	ARG	4.6
1	B	1321	TYR	4.6
1	B	467	LEU	4.5
1	B	2016	ASN	4.5
1	B	2052	ILE	4.4
1	B	1975	THR	4.3
1	B	2123	SER	4.3
1	B	1960	LEU	4.2
1	B	2041	LEU	4.2
1	B	2006	ASP	4.1
1	B	876	LEU	4.1
1	B	2101	ALA	4.0
1	B	1148	PHE	4.0
1	B	1165	ILE	3.9
1	B	2005	ALA	3.9
1	B	1775	GLY	3.8
1	B	1037	LEU	3.8
1	B	877	GLN	3.8
1	B	690	VAL	3.7
1	B	2106	LEU	3.7
1	B	1050	GLU	3.7
1	B	2092	LEU	3.6
1	B	422	PHE	3.6
1	B	1317	PHE	3.6
1	B	1773	LEU	3.6
1	B	2084	LEU	3.6
1	B	2042	GLU	3.5
1	B	743	LEU	3.5
1	B	736	ARG	3.5
1	B	2008	ALA	3.5
1	B	2004	ILE	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	712	ILE	3.4
1	B	588	CYS	3.3
1	B	2102	HIS	3.3
1	B	445	VAL	3.3
1	B	1336	PHE	3.3
1	B	1965	HIS	3.3
1	B	713	MET	3.3
1	B	879	TYR	3.2
1	B	1802	ILE	3.2
1	B	1135	LEU	3.2
1	B	1241	LEU	3.2
1	B	1776	ILE	3.2
1	B	1996	LEU	3.2
1	B	974	LYS	3.1
1	B	2059	LYS	3.1
1	B	545	ARG	3.1
1	B	1480	GLN	3.1
1	B	2017	ILE	3.1
1	B	589	THR	3.1
1	B	1423	ASN	3.1
1	B	1682	TYR	3.1
1	B	1986	MET	3.0
1	B	1732	MET	3.0
1	B	440	LYS	3.0
1	B	1977	LYS	3.0
1	B	1974	CYS	3.0
1	B	444	GLU	3.0
1	B	576	CYS	3.0
1	B	1443	LYS	2.9
1	B	1752	VAL	2.9
1	B	1132	PHE	2.9
1	B	1871	LEU	2.9
1	B	2061	GLU	2.9
1	B	1365	LEU	2.9
1	B	1601	LEU	2.9
1	B	464	VAL	2.8
1	B	506	GLY	2.8
1	B	437	ARG	2.8
1	B	2082	LEU	2.8
1	B	466	LYS	2.8
1	B	723	VAL	2.8
1	B	570	THR	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	709	TYR	2.8
1	B	1051	SER	2.8
1	B	861	TYR	2.8
1	B	1961	LYS	2.7
1	B	1342	SER	2.7
1	B	724	PHE	2.7
1	B	1987	GLU	2.7
1	B	574	GLN	2.7
1	B	1577	LEU	2.7
1	B	1796	LEU	2.7
1	B	562	TYR	2.7
1	B	591	GLU	2.7
1	B	402	ALA	2.7
1	B	508	GLY	2.7
1	B	822	PRO	2.7
1	B	720	GLN	2.7
1	B	1846	ILE	2.7
1	B	1604	LEU	2.7
1	B	1962	GLN	2.6
1	B	2035	VAL	2.6
1	B	715	HIS	2.6
1	B	1463	ASN	2.6
1	B	2091	LYS	2.6
1	B	475	PHE	2.6
1	B	2038	LEU	2.6
1	B	446	HIS	2.6
1	B	853	LEU	2.6
1	B	693	THR	2.6
1	B	682	PRO	2.6
1	B	528	ASP	2.5
1	B	869	LEU	2.5
1	B	546	SER	2.5
1	B	1312	LEU	2.5
1	B	471	ALA	2.5
1	B	569	LEU	2.5
1	B	961	ALA	2.5
1	B	493	LEU	2.5
1	B	2043	ARG	2.5
1	B	1368	LEU	2.5
1	B	820	ASN	2.5
1	B	2087	LYS	2.5
1	B	1984	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1788	LEU	2.5
1	B	1586	ARG	2.4
1	B	979	PHE	2.4
1	B	1417	LYS	2.4
1	B	1177	TYR	2.4
1	B	433	GLY	2.4
1	B	460	GLN	2.4
1	B	2040	GLN	2.4
1	B	526	ASN	2.4
1	B	1620	LEU	2.4
1	B	1784	HIS	2.4
1	B	1150	PHE	2.4
1	B	590	PRO	2.4
1	B	863	THR	2.4
1	B	1461	GLY	2.4
1	B	544	MET	2.4
1	B	719	ASN	2.4
1	B	1597	LEU	2.4
1	B	2034	PRO	2.3
1	B	1764	MET	2.3
1	B	770	LYS	2.3
1	B	518	LEU	2.3
1	B	1331	ILE	2.3
1	B	729	LYS	2.3
1	B	2049	GLY	2.3
1	B	972	TYR	2.3
1	B	1793	LEU	2.3
1	B	748	LEU	2.3
1	B	1995	ALA	2.3
1	B	701	PHE	2.3
1	B	758	SER	2.3
1	B	427	ARG	2.3
1	B	1971	ILE	2.3
1	B	1878	LYS	2.3
1	B	411	LEU	2.2
1	B	1494	LEU	2.2
1	B	938	ILE	2.2
1	B	2046	GLU	2.2
1	B	819	VAL	2.2
1	B	734	THR	2.2
1	B	469	LYS	2.2
1	B	592	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	1286	PHE	2.2
1	B	855	ARG	2.2
1	B	2116	CYS	2.2
1	B	711	LYS	2.2
1	B	716	ALA	2.2
1	B	2114	MET	2.2
1	B	488	LEU	2.2
1	B	750	LEU	2.2
1	B	802	ALA	2.2
1	B	1246	ALA	2.2
1	B	2079	ILE	2.2
1	B	1410	GLY	2.1
1	B	501	LEU	2.1
1	B	984	LEU	2.1
1	B	1901	ARG	2.1
1	B	717	GLY	2.1
1	B	2024	VAL	2.1
1	B	1035	LEU	2.1
1	B	1137	GLU	2.1
1	B	1954	TRP	2.1
1	B	510	THR	2.1
1	B	959	THR	2.1
1	B	414	LEU	2.1
1	B	821	LEU	2.1
1	B	2023	VAL	2.1
1	B	1883	LYS	2.1
1	B	2083	THR	2.1
1	B	2011	CYS	2.1
1	B	438	GLN	2.0
1	B	1004	LEU	2.0
1	B	1322	GLN	2.0
1	B	593	TRP	2.0
1	B	1978	GLY	2.0
1	B	2022	GLU	2.0
1	B	852	MET	2.0
1	B	705	ASN	2.0
1	B	621	HIS	2.0
1	B	568	GLU	2.0
1	B	854	GLY	2.0
1	B	1151	GLU	2.0
1	B	2100	GLY	2.0

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 monosaccharides in this entry.

6.4 Ligands (i)

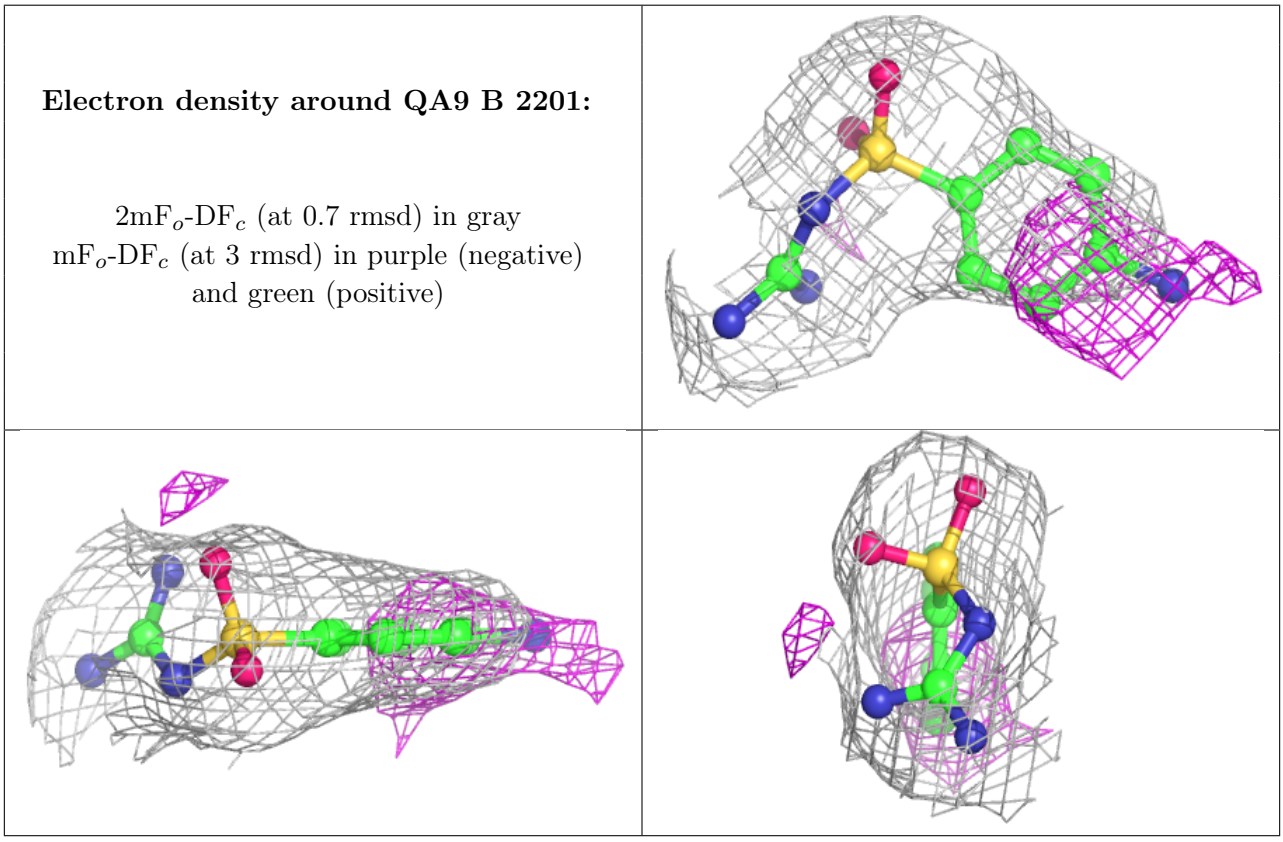
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	QA9	B	2201	14/14	0.91	0.25	50,57,66,94	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 QA9 B 2201:

$2mF_o$-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.