Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 06:15 am BST

PDB ID	:	6S8O
Title	:	Human Brr2 Helicase Region M641C/A1582C
Authors	:	Vester, K.; Santos, K.F.; Wahl, M.C.
Deposited on	:	2019-07-10
Resolution	:	3.17 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 ⓘ symbol.

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

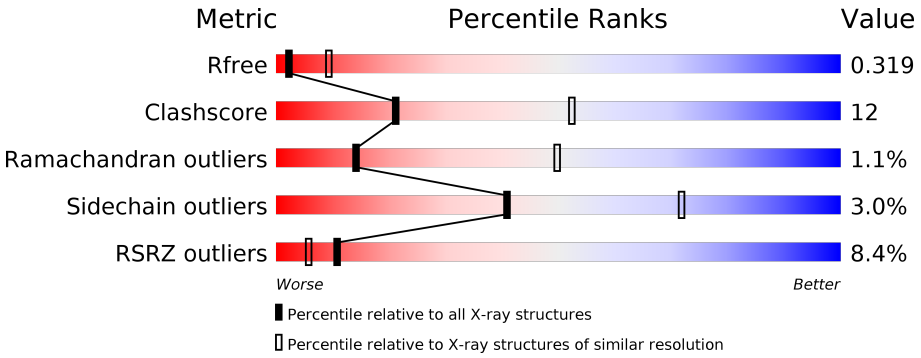
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 3.17 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	1467 (3.20-3.16)
Clashscore	141614	1599 (3.20-3.16)
Ramachandran outliers	138981	1574 (3.20-3.16)
Sidechain outliers	138945	1573 (3.20-3.16)
RSRZ outliers	127900	1423 (3.20-3.16)

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 <=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	8% 72% 25%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 13878 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
1	B	1724	Total	C	N	O	S	0	0	0
			13858	8855	2371	2559	73			

There are 6 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
B	641	CYS	MET	engineered mutation	UNP O75643
B	1582	CYS	ALA	engineered mutation	UNP O75643

- Molecule 2 is water.

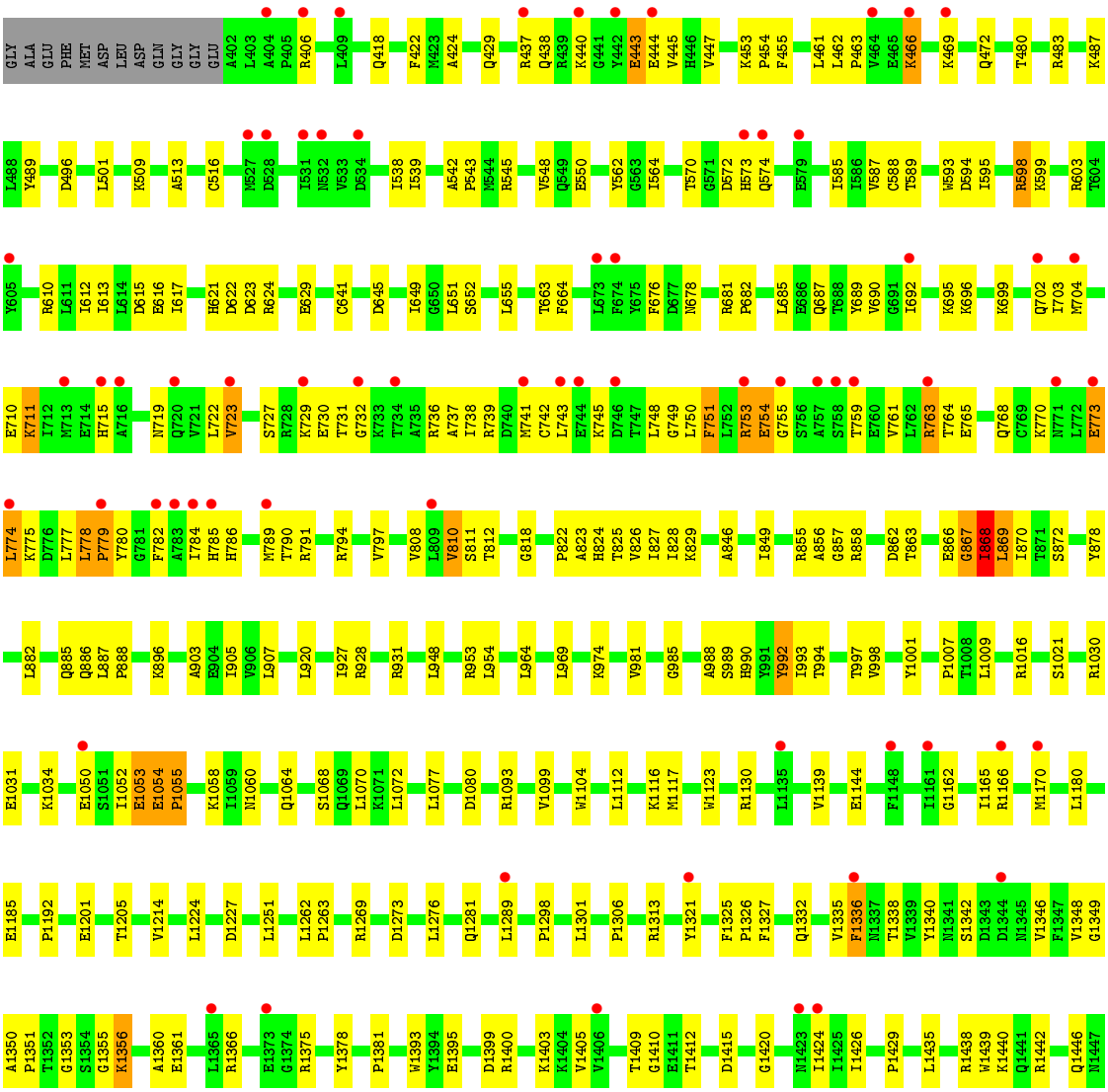
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	20	Total	O	0	0
			20	20		

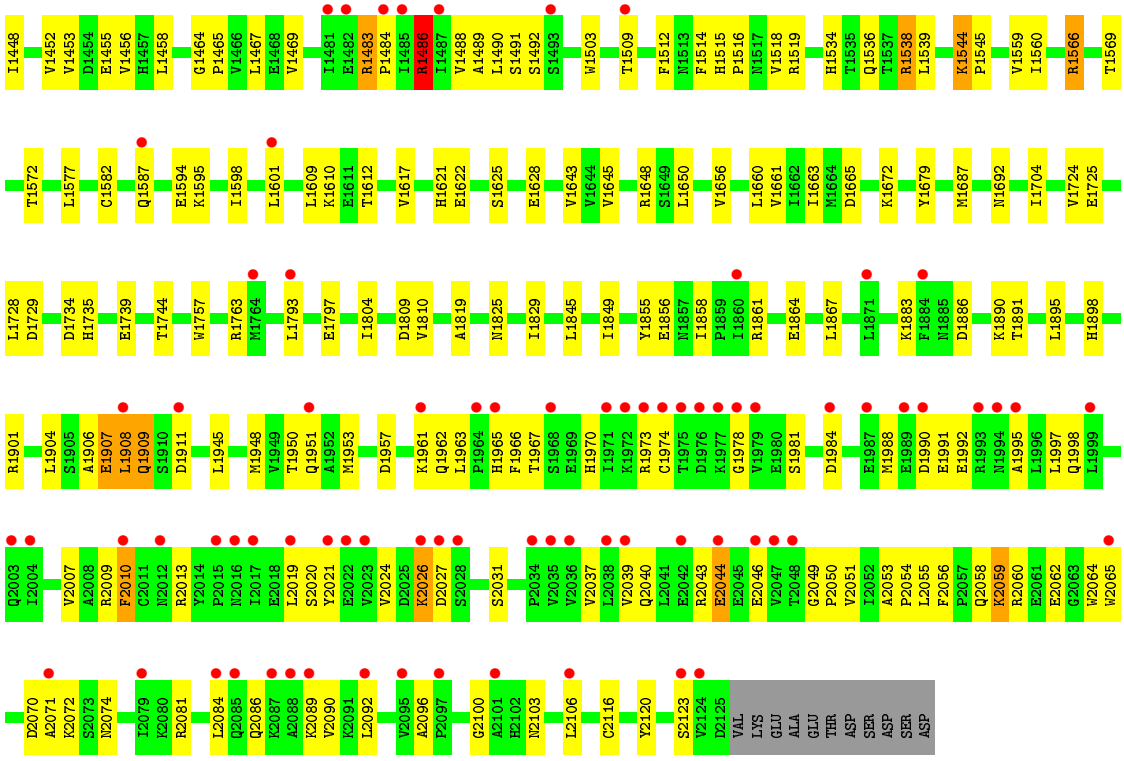
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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:




I1448 V1452 V1453 D1454 E1455 V1456 H1457 L1458 G1464 P1465 V1466 L1467 E1468 V1469 I1481 E1482 R1483 P1484 I1485 R1486 I1487 V1488 A1489 L1490 S1491 S1492 S1493 W1503 T1509 F1512 N1513 F1514 H1515 P1516 N1517 V1518 R1519 H1534 T1535 Q1536 T1537 R1538 L1539 K1544 P1545 V1559 I1560 R1566 T1569
T1572 L1577 C1582 Q1587 E1594 K1595 I1598 L1601 L1609 K1610 E1611 T1612 V1617 H1621 E1622 S1625 E1628 V1643 V1644 V1645 R1648 S1649 L1650 V1656 L1660 V1661 I1662 I1663 M1664 D1665 K1672 Y1679 M1687 N1692 I1704 V1724 E1725
L1728 D1729 D1734 H1735 E1739 T1744 W1757 R1763 M1764 L1793 E1797 I1804 D1809 V1810 A1819 N1825 I1829 L1845 I1849 Y1855 E1856 N1857 I1858 P1859 I1860 R1861 E1864 L1867 L1871 K1883 F1884 N1885 D1886 K1890 T1891 L1895 H1898
R1901 L1904 S1905 A1906 E1907 L1908 Q1909 S1910 D1911 L1945 M1948 V1949 T1950 Q1951 A1952 M1953 D1957 K1961 Q1962 L1963 P1964 H1965 F1966 T1967 S1968 E1969 H1970 I1971 K1972 R1973 C1974 T1975 D1976 K1977 G1978 V1979 E1980 S1981 D1984 E1987 M1988 E1989 D1990 E1991 E1992 R1993 N1994 A1995 L1996 L1997 Q1998 L1999
Q2003 I2004 V2007 A2008 R2009 F2010 C2011 N2012 R2013 Y2014 P2015 N2016 I2017 E2018 L2019 S2020 Y2021 E2022 V2023 V2024 D2025 K2026 D2027 S2028 S2031 P2034 V2035 V2036 W2037 I2038 V2039 Q2040 I2041 E2042 R2043 E2044 E2045 E2046 V2047 T2048 G2049 P2050 V2051 I2052 A2053 P2054 L2055 F2056 P2057 Q2058 K2059 R2060 E2061 E2062 G2063 W2064 W2065
D2070 A2071 K2072 S2073 N2074 I2079 K2080 R2081 L2084 Q2085 Q2086 K2087 A2088 K2089 V2090 K2091 L2092 V2095 A2096 P2097 G2100 A2101 H2102 N2103 L2106 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	145.56Å 152.53Å 142.51Å 90.00° 120.69° 90.00°	Depositor
Resolution (Å)	48.38 – 3.17 48.38 – 3.17	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.38-3.17) 97.3 (48.38-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.06 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.264 , 0.318 0.264 , 0.319	Depositor DCC
R_{free} test set	2100 reflections (4.76%)	wwPDB-VP
Wilson B-factor (Å^2)	109.4	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 66.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	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 0.000 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	13878	wwPDB-VP
Average B, all atoms (Å^2)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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

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	0.24	0/14152	0.42	2/19176 (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
1	B	0	1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	774	LEU	CA-CB-CG	5.74	128.50	115.30
1	B	868	ILE	CG1-CB-CG2	5.41	123.30	111.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	867	GLY	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	B	13858	0	13995	337	0
2	B	20	0	0	6	0
All	All	13878	0	13995	337	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 (337) 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:723:VAL:HA	1:B:827:ILE:HG13	1.46	0.98
1:B:773:GLU:HG3	1:B:789:MET:CE	1.93	0.97
1:B:773:GLU:HG3	1:B:789:MET:HE3	1.54	0.89
1:B:773:GLU:HG3	1:B:789:MET:HE1	1.63	0.81
1:B:1456:VAL:HG11	1:B:1489:ALA:HB1	1.66	0.77
1:B:695:LYS:HA	1:B:696:LYS:HB2	1.67	0.76
1:B:687:GLN:HA	1:B:867:GLY:HA3	1.67	0.75
1:B:753:ARG:HD2	1:B:754:GLU:H	1.52	0.74
1:B:1904:LEU:HB3	1:B:1909:GLN:HB2	1.71	0.72
1:B:444:GLU:HA	1:B:690:VAL:HG12	1.74	0.70
1:B:463:PRO:O	1:B:466:LYS:NZ	2.24	0.70
1:B:1950:THR:OG1	1:B:2060:ARG:NH1	2.25	0.69
1:B:826:VAL:HG23	1:B:868:ILE:HG12	1.73	0.69
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.74	0.69
1:B:823:ALA:HA	1:B:858:ARG:HE	1.58	0.69
1:B:2039:VAL:HG23	1:B:2090:VAL:HG11	1.76	0.68
1:B:689:TYR:HA	1:B:869:LEU:HD11	1.77	0.67
1:B:1951:GLN:HG2	1:B:1962:GLN:HG2	1.77	0.67
1:B:1559:VAL:HG22	1:B:1660:LEU:HB3	1.76	0.67
1:B:610:ARG:NH1	1:B:645:ASP:O	2.28	0.67
1:B:753:ARG:H	1:B:759:THR:HG22	1.59	0.66
1:B:969:LEU:HD22	1:B:985:GLY:HA2	1.78	0.66
1:B:1375:ARG:HH22	1:B:1420:GLY:HA2	1.60	0.65
1:B:2064:TRP:HH2	1:B:2116:CYS:HB2	1.61	0.65
1:B:1883:LYS:HE3	1:B:1886:ASP:HB2	1.79	0.65
1:B:483:ARG:NH1	1:B:681:ARG:O	2.29	0.65
1:B:692:ILE:HG13	1:B:872:SER:HA	1.77	0.65
1:B:445:VAL:N	1:B:689:TYR:O	2.29	0.65
1:B:406:ARG:NH1	1:B:974:LYS:O	2.26	0.64
1:B:538:ILE:HB	1:B:585:ILE:HG13	1.78	0.64
1:B:988:ALA:HB2	1:B:998:VAL:HG21	1.79	0.64
1:B:711:LYS:O	2:B:2201:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:LYS:HD2	1:B:775:LYS:HG2	1.78	0.64
1:B:687:GLN:OE1	1:B:689:TYR:OH	2.16	0.63
1:B:727:SER:HB2	1:B:730:GLU:HB2	1.79	0.63
1:B:846:ALA:HA	1:B:849:ILE:HD12	1.80	0.63
1:B:1895:LEU:HA	1:B:1898:HIS:HB3	1.81	0.62
1:B:437:ARG:O	1:B:444:GLU:N	2.29	0.62
1:B:699:LYS:HG2	1:B:703:ILE:HG13	1.81	0.62
1:B:1739:GLU:HG3	1:B:1744:THR:HB	1.81	0.62
1:B:1099:VAL:HG13	1:B:1104:TRP:HB2	1.82	0.62
1:B:615:ASP:HA	1:B:651:LEU:HB2	1.81	0.62
1:B:622:ASP:OD1	1:B:623:ASP:N	2.33	0.61
1:B:770:LYS:HB3	1:B:775:LYS:HD2	1.83	0.61
1:B:1456:VAL:HG22	1:B:1491:SER:HB2	1.81	0.61
1:B:545:ARG:NH1	1:B:570:THR:OG1	2.33	0.61
1:B:811:SER:O	2:B:2202:HOH:O	2.16	0.61
1:B:689:TYR:HA	1:B:869:LEU:CD1	2.30	0.61
1:B:406:ARG:HG2	1:B:954:LEU:HD22	1.83	0.60
1:B:1112:LEU:HG	1:B:1116:LYS:HE3	1.82	0.60
1:B:1415:ASP:HB3	1:B:1435:LEU:HD11	1.83	0.60
1:B:732:GLY:O	1:B:736:ARG:N	2.34	0.60
1:B:1963:LEU:HD23	1:B:1965:HIS:H	1.66	0.60
1:B:1375:ARG:HB2	1:B:1448:ILE:HA	1.84	0.60
1:B:784:ILE:HD12	1:B:794:ARG:HH12	1.67	0.60
1:B:827:ILE:HA	1:B:868:ILE:HD13	1.84	0.60
1:B:1725:GLU:O	2:B:2204:HOH:O	2.17	0.59
1:B:595:ILE:HD11	1:B:992:TYR:HB2	1.86	0.58
1:B:1409:THR:OG1	1:B:1410:GLY:N	2.35	0.58
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.85	0.58
1:B:1906:ALA:O	1:B:1908:LEU:N	2.37	0.58
1:B:1052:ILE:HD12	1:B:1053:GLU:N	2.20	0.57
1:B:2054:PRO:HG2	1:B:2055:LEU:HD12	1.86	0.57
1:B:948:LEU:O	1:B:953:ARG:NH1	2.38	0.57
1:B:1797:GLU:HB2	1:B:1804:ILE:HD13	1.86	0.57
1:B:599:LYS:NZ	1:B:990:HIS:O	2.38	0.57
1:B:731:THR:OG1	1:B:810:VAL:O	2.22	0.57
1:B:1130:ARG:NH2	1:B:1144:GLU:OE2	2.35	0.57
1:B:1595:LYS:HD3	1:B:1598:ILE:HD12	1.88	0.56
1:B:539:ILE:HB	1:B:612:ILE:HG22	1.87	0.56
1:B:743:LEU:HB2	1:B:748:LEU:HD22	1.87	0.56
1:B:749:GLY:O	1:B:751:PHE:N	2.38	0.56
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:826:VAL:HG22	1:B:856:ALA:HB2	1.87	0.56
1:B:2031:SER:HA	1:B:2096:ALA:HB3	1.86	0.56
1:B:690:VAL:CG2	1:B:870:ILE:HG12	2.36	0.56
1:B:775:LYS:HA	1:B:778:LEU:HD12	1.87	0.56
1:B:1338:THR:O	1:B:1342:SER:OG	2.21	0.55
1:B:753:ARG:O	1:B:755:GLY:N	2.37	0.55
1:B:827:ILE:HA	1:B:868:ILE:HB	1.88	0.55
1:B:469:LYS:HA	1:B:472:GLN:HG3	1.88	0.55
1:B:2019:LEU:HD12	1:B:2040:GLN:HB2	1.88	0.55
1:B:1262:LEU:HD21	1:B:1289:LEU:HD23	1.88	0.55
1:B:1378:TYR:HD2	1:B:1426:ILE:HG23	1.72	0.55
1:B:719:ASN:ND2	2:B:2201:HOH:O	2.39	0.55
1:B:1185:GLU:HB2	1:B:1205:THR:HB	1.89	0.55
1:B:1601:LEU:HB3	1:B:1610:LYS:HG3	1.89	0.54
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	1.88	0.54
1:B:2059:LYS:HD3	1:B:2059:LYS:H	1.71	0.54
1:B:1346:VAL:HG12	1:B:1488:VAL:HG12	1.89	0.54
1:B:2024:VAL:HG11	1:B:2026:LYS:HE3	1.88	0.54
1:B:453:LYS:HD2	1:B:454:PRO:HD2	1.90	0.54
1:B:723:VAL:HA	1:B:827:ILE:CG1	2.30	0.54
1:B:1336:PHE:HE1	1:B:1340:TYR:HD2	1.53	0.54
1:B:1162:GLY:HA2	1:B:1165:ILE:HG22	1.90	0.54
1:B:1617:VAL:HG22	1:B:1643:VAL:HB	1.90	0.54
1:B:2007:VAL:HG23	1:B:2010:PHE:HE1	1.73	0.54
1:B:777:LEU:HB2	1:B:782:PHE:HB3	1.90	0.53
1:B:447:VAL:HG22	1:B:687:GLN:HB2	1.90	0.53
1:B:778:LEU:C	1:B:780:TYR:H	2.12	0.53
1:B:463:PRO:HA	1:B:480:THR:HA	1.89	0.53
1:B:1587:GLN:NE2	1:B:1594:GLU:OE2	2.41	0.53
1:B:2019:LEU:HB3	1:B:2120:TYR:HE2	1.73	0.53
1:B:1901:ARG:NH2	1:B:1951:GLN:O	2.42	0.52
1:B:1566:ARG:HB2	1:B:1621:HIS:HB2	1.90	0.52
1:B:2070:ASP:OD1	1:B:2071:ALA:N	2.42	0.52
1:B:1262:LEU:HD12	1:B:1263:PRO:HD2	1.91	0.52
1:B:2019:LEU:HB3	1:B:2120:TYR:CE2	2.45	0.52
1:B:827:ILE:HG22	1:B:868:ILE:CG2	2.40	0.52
1:B:1093:ARG:NH1	1:B:1273:ASP:OD1	2.41	0.52
1:B:742:CYS:HB3	1:B:748:LEU:HD13	1.91	0.52
1:B:2037:VAL:HB	1:B:2092:LEU:HD11	1.92	0.51
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.37	0.51
1:B:1908:LEU:H	1:B:1908:LEU:HD23	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1405:VAL:HG22	1:B:1424:ILE:HB	1.93	0.51
1:B:1984:ASP:OD1	1:B:1984:ASP:N	2.36	0.51
1:B:1342:SER:O	1:B:1486:ARG:NH1	2.43	0.51
1:B:2051:VAL:HG22	1:B:2062:GLU:HG3	1.91	0.51
1:B:1566:ARG:O	1:B:1569:THR:OG1	2.21	0.51
1:B:775:LYS:O	1:B:778:LEU:HB2	2.10	0.51
1:B:826:VAL:HG23	1:B:868:ILE:CG1	2.39	0.51
1:B:1068:SER:OG	1:B:1123:TRP:NE1	2.37	0.51
1:B:1901:ARG:NH2	1:B:1961:LYS:O	2.44	0.51
1:B:1904:LEU:HB3	1:B:1909:GLN:CB	2.40	0.51
1:B:1180:LEU:HD13	1:B:1214:VAL:HG21	1.93	0.50
1:B:2043:ARG:O	1:B:2086:GLN:NE2	2.44	0.50
1:B:761:VAL:HA	1:B:764:THR:HB	1.94	0.50
1:B:466:LYS:H	1:B:466:LYS:HD3	1.76	0.50
1:B:741:MET:O	1:B:745:LYS:HG2	2.12	0.50
1:B:429:GLN:N	1:B:886:GLN:OE1	2.41	0.50
1:B:743:LEU:HA	1:B:748:LEU:HB2	1.94	0.50
1:B:1016:ARG:HB2	1:B:1050:GLU:HG2	1.94	0.50
1:B:1861:ARG:HH21	1:B:1890:LYS:HZ3	1.60	0.50
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.92	0.50
1:B:1455:GLU:N	1:B:1490:LEU:O	2.45	0.49
1:B:1349:GLY:N	1:B:1512:PHE:O	2.36	0.49
1:B:1901:ARG:HH21	1:B:1961:LYS:HB3	1.77	0.49
1:B:1361:GLU:OE2	1:B:1393:TRP:NE1	2.42	0.49
1:B:1560:ILE:HD11	1:B:1656:VAL:HG12	1.93	0.49
1:B:681:ARG:NH2	1:B:856:ALA:O	2.44	0.49
1:B:1201:GLU:HB3	1:B:1251:LEU:HD11	1.94	0.49
1:B:1963:LEU:CD2	1:B:1965:HIS:H	2.25	0.49
1:B:418:GLN:HB2	1:B:422:PHE:HB2	1.93	0.49
1:B:2021:TYR:HB3	1:B:2106:LEU:HD22	1.94	0.49
1:B:882:LEU:HB2	1:B:887:LEU:HD13	1.93	0.49
1:B:1429:PRO:HG3	1:B:1467:LEU:HD13	1.94	0.49
1:B:1001:TYR:HH	1:B:1021:SER:HG	1.60	0.49
1:B:1192:PRO:HG3	1:B:1289:LEU:HD11	1.95	0.49
1:B:1060:ASN:OD1	1:B:1064:GLN:NE2	2.39	0.48
1:B:681:ARG:HD2	1:B:682:PRO:HD2	1.96	0.48
1:B:753:ARG:HD3	1:B:754:GLU:HG2	1.95	0.48
1:B:1395:GLU:HA	1:B:1399:ASP:HB2	1.96	0.48
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	1.95	0.48
1:B:1804:ILE:HG13	1:B:1810:VAL:HG12	1.95	0.48
1:B:2056:PHE:HE1	1:B:2058:GLN:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:710:GLU:OE1	1:B:710:GLU:N	2.46	0.48
1:B:988:ALA:HA	1:B:993:ILE:HG12	1.95	0.48
1:B:2059:LYS:HD3	1:B:2059:LYS:N	2.28	0.48
1:B:1353:GLY:H	1:B:1356:LYS:NZ	2.12	0.48
1:B:1464:GLY:H	1:B:1465:PRO:HD2	1.79	0.48
1:B:1332:GLN:NE2	1:B:1355:GLY:O	2.39	0.48
1:B:1381:PRO:HG2	1:B:1458:LEU:HD12	1.97	0.47
1:B:2056:PHE:CE1	1:B:2058:GLN:HB2	2.49	0.47
1:B:964:LEU:HD22	1:B:969:LEU:HD12	1.95	0.47
1:B:2053:ALA:HB1	1:B:2056:PHE:HB3	1.96	0.47
1:B:778:LEU:O	1:B:780:TYR:N	2.48	0.47
1:B:774:LEU:O	1:B:778:LEU:HG	2.14	0.47
1:B:1990:ASP:O	1:B:1992:GLU:N	2.47	0.47
1:B:2027:ASP:N	1:B:2027:ASP:OD1	2.47	0.47
1:B:545:ARG:HH21	1:B:548:VAL:HG21	1.79	0.47
1:B:1335:VAL:HG21	1:B:1348:VAL:HG22	1.95	0.47
1:B:828:ILE:HD11	1:B:870:ILE:H	1.80	0.47
1:B:2064:TRP:CD1	1:B:2084:LEU:HD22	2.49	0.47
1:B:462:LEU:HB3	1:B:466:LYS:NZ	2.29	0.47
1:B:770:LYS:HD2	1:B:775:LYS:CG	2.45	0.47
1:B:785:HIS:HA	1:B:794:ARG:NH1	2.29	0.47
1:B:1117:MET:HG2	1:B:1276:LEU:HD11	1.97	0.46
1:B:1412:THR:HA	1:B:1415:ASP:HB2	1.96	0.46
1:B:1572:THR:HB	1:B:1645:VAL:HG11	1.96	0.46
1:B:825:THR:HB	1:B:866:GLU:HB3	1.97	0.46
1:B:1068:SER:HB2	1:B:1070:LEU:HD13	1.95	0.46
1:B:2020:SER:OG	1:B:2040:GLN:NE2	2.48	0.46
1:B:594:ASP:O	1:B:598:ARG:HB2	2.16	0.46
1:B:704:MET:O	1:B:829:LYS:NZ	2.43	0.46
1:B:928:ARG:HH12	1:B:931:ARG:HB2	1.79	0.46
1:B:1539:LEU:HD21	1:B:1665:ASP:HB2	1.98	0.46
1:B:1577:LEU:HD21	1:B:1612:THR:HA	1.98	0.46
1:B:1734:ASP:OD2	1:B:1825:ASN:ND2	2.46	0.46
1:B:920:LEU:HB3	1:B:953:ARG:HD2	1.97	0.46
1:B:1974:CYS:HB3	1:B:1978:GLY:HA3	1.96	0.46
1:B:731:THR:HA	1:B:810:VAL:HG22	1.97	0.46
1:B:867:GLY:HA2	1:B:868:ILE:HG13	1.96	0.46
1:B:1469:VAL:HG21	1:B:1735:HIS:CG	2.51	0.46
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.97	0.46
1:B:692:ILE:HD13	1:B:695:LYS:HE2	1.96	0.46
1:B:2039:VAL:HG12	1:B:2040:GLN:H	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2009:ARG:O	1:B:2013:ARG:HG2	2.15	0.46
1:B:445:VAL:O	1:B:689:TYR:N	2.49	0.46
1:B:903:ALA:O	1:B:907:LEU:HD12	2.16	0.46
1:B:785:HIS:O	1:B:811:SER:HA	2.16	0.45
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.97	0.45
1:B:1861:ARG:NH2	1:B:1911:ASP:OD2	2.50	0.45
1:B:2064:TRP:CH2	1:B:2116:CYS:HB2	2.48	0.45
1:B:424:ALA:HB3	1:B:888:PRO:HG2	1.98	0.45
1:B:543:PRO:O	1:B:624:ARG:NH2	2.31	0.45
1:B:572:ASP:N	1:B:572:ASP:OD1	2.49	0.45
1:B:768:GLN:HG3	1:B:770:LYS:HE2	1.98	0.45
1:B:1992:GLU:HG3	1:B:1995:ALA:HB3	1.99	0.45
1:B:678:ASN:H	1:B:885:GLN:NE2	2.14	0.45
1:B:1306:PRO:HB2	1:B:1327:PHE:HB3	1.99	0.45
1:B:1967:THR:OG1	1:B:1970:HIS:ND1	2.48	0.45
1:B:784:ILE:O	1:B:797:VAL:HG11	2.17	0.45
1:B:828:ILE:O	1:B:829:LYS:HD2	2.16	0.45
1:B:1356:LYS:H	1:B:1356:LYS:HD3	1.82	0.45
1:B:1544:LYS:HB3	1:B:1545:PRO:HD3	1.99	0.45
1:B:1519:ARG:NH2	1:B:1692:ASN:HB2	2.31	0.45
1:B:739:ARG:HE	1:B:748:LEU:HD21	1.82	0.45
1:B:588:CYS:SG	1:B:593:TRP:HB2	2.57	0.44
1:B:696:LYS:HD3	1:B:699:LYS:HD3	1.98	0.44
1:B:1966:PHE:CZ	1:B:1970:HIS:HB3	2.53	0.44
1:B:846:ALA:HB2	1:B:878:TYR:OH	2.17	0.44
1:B:655:LEU:HD22	1:B:887:LEU:HB3	1.98	0.44
1:B:1298:PRO:HG3	1:B:1515:HIS:HB2	2.00	0.44
1:B:1375:ARG:NH1	1:B:1420:GLY:O	2.33	0.44
1:B:1446:GLN:OE1	1:B:1446:GLN:N	2.50	0.44
1:B:2021:TYR:CE1	1:B:2120:TYR:HB3	2.53	0.44
1:B:689:TYR:CD2	1:B:869:LEU:HD21	2.52	0.44
1:B:1483:ARG:HG3	1:B:1484:PRO:HD2	1.98	0.44
1:B:2103:ASN:OD1	1:B:2123:SER:OG	2.36	0.44
1:B:681:ARG:HE	1:B:685:LEU:HD22	1.81	0.44
1:B:777:LEU:HA	1:B:780:TYR:CZ	2.52	0.44
1:B:824:HIS:ND1	1:B:862:ASP:OD2	2.35	0.44
1:B:1054:GLU:HB3	1:B:1055:PRO:HD2	1.99	0.44
1:B:763:ARG:NH1	1:B:764:THR:OG1	2.51	0.44
1:B:826:VAL:O	1:B:868:ILE:HG21	2.18	0.44
1:B:1321:TYR:OH	1:B:1361:GLU:OE1	2.26	0.44
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2072:LYS:HD2	1:B:2072:LYS:HA	1.80	0.44
1:B:438:GLN:HA	1:B:443:GLU:HA	2.00	0.44
1:B:487:LYS:HD3	1:B:676:PHE:CZ	2.53	0.44
1:B:1058:LYS:NZ	1:B:1080:ASP:OD2	2.39	0.43
1:B:1165:ILE:HD12	1:B:1165:ILE:HA	1.85	0.43
1:B:1438:ARG:HB2	1:B:1442:ARG:HD2	1.99	0.43
1:B:1227:ASP:OD1	1:B:1227:ASP:N	2.48	0.43
1:B:550:GLU:HB2	1:B:818:GLY:O	2.18	0.43
1:B:822:PRO:HA	1:B:855:ARG:HB3	1.99	0.43
1:B:862:ASP:OD1	1:B:863:THR:N	2.46	0.43
1:B:1515:HIS:O	1:B:1518:VAL:HG22	2.18	0.43
1:B:1269:ARG:HG2	1:B:1281:GLN:HG3	2.00	0.43
1:B:826:VAL:O	1:B:868:ILE:HG12	2.18	0.43
1:B:1648:ARG:HD3	1:B:1679:TYR:CE1	2.53	0.43
1:B:443:GLU:O	1:B:690:VAL:HA	2.19	0.43
1:B:542:ALA:O	1:B:589:THR:HA	2.19	0.43
1:B:1052:ILE:HD12	1:B:1053:GLU:H	1.81	0.43
1:B:1353:GLY:O	1:B:1692:ASN:ND2	2.52	0.43
1:B:509:LYS:HD2	1:B:651:LEU:HB3	2.01	0.43
1:B:739:ARG:NE	1:B:748:LEU:HD21	2.34	0.43
1:B:827:ILE:HG21	1:B:827:ILE:HD13	1.77	0.43
1:B:1053:GLU:HB3	1:B:1054:GLU:H	1.59	0.43
1:B:1503:TRP:NE1	1:B:1757:TRP:O	2.48	0.43
1:B:1861:ARG:NH1	1:B:1907:GLU:OE1	2.52	0.43
1:B:811:SER:N	2:B:2202:HOH:O	2.52	0.43
1:B:1340:TYR:O	1:B:1366:ARG:HD3	2.18	0.42
1:B:715:HIS:ND1	1:B:719:ASN:OD1	2.46	0.42
1:B:739:ARG:NH2	1:B:780:TYR:OH	2.48	0.42
1:B:722:LEU:HD11	1:B:823:ALA:CB	2.49	0.42
1:B:737:ALA:O	1:B:741:MET:HB3	2.19	0.42
1:B:768:GLN:NE2	1:B:768:GLN:HA	2.34	0.42
1:B:828:ILE:HG13	1:B:869:LEU:HA	2.01	0.42
1:B:765:GLU:HA	1:B:768:GLN:OE1	2.19	0.42
1:B:768:GLN:NE2	1:B:770:LYS:HD3	2.33	0.42
1:B:1855:TYR:HA	1:B:1858:ILE:HD13	2.00	0.42
1:B:2007:VAL:HG23	1:B:2010:PHE:CE1	2.52	0.42
1:B:1981:SER:OG	1:B:1984:ASP:OD1	2.33	0.42
1:B:598:ARG:HD3	1:B:989:SER:O	2.19	0.42
1:B:1793:LEU:HD13	1:B:1810:VAL:HG11	2.02	0.42
1:B:641:CYS:HA	1:B:1582:CYS:HB2	2.01	0.42
1:B:768:GLN:HE21	1:B:770:LYS:HD3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:PHE:CE2	1:B:461:LEU:HG	2.54	0.42
1:B:827:ILE:CA	1:B:868:ILE:HD13	2.50	0.42
1:B:1301:LEU:HD22	1:B:1518:VAL:HB	2.02	0.42
1:B:1672:LYS:NZ	1:B:1856:GLU:O	2.48	0.42
1:B:1945:LEU:HD12	1:B:1945:LEU:HA	1.91	0.42
1:B:406:ARG:HH11	1:B:974:LYS:HD2	1.84	0.42
1:B:562:TYR:HB2	1:B:564:ILE:HD13	2.01	0.42
1:B:1360:ALA:HB1	1:B:1452:VAL:HG11	2.02	0.42
1:B:1350:ALA:O	1:B:1492:SER:HA	2.20	0.42
1:B:1538:ARG:NH1	1:B:1665:ASP:OD1	2.53	0.42
1:B:782:PHE:HA	1:B:808:VAL:O	2.19	0.42
1:B:753:ARG:CD	1:B:754:GLU:H	2.28	0.41
1:B:1007:PRO:HG3	1:B:1104:TRP:CE2	2.55	0.41
1:B:1950:THR:HG1	1:B:2060:ARG:NH1	2.16	0.41
1:B:548:VAL:HG13	1:B:587:VAL:HG12	2.02	0.41
1:B:722:LEU:O	1:B:810:VAL:HA	2.20	0.41
1:B:994:THR:HG23	1:B:997:THR:H	1.84	0.41
1:B:1072:LEU:HD23	1:B:1077:LEU:HB3	2.01	0.41
1:B:1901:ARG:HE	1:B:1961:LYS:HD3	1.84	0.41
1:B:738:ILE:HG13	1:B:739:ARG:N	2.35	0.41
1:B:777:LEU:HB2	1:B:782:PHE:CB	2.50	0.41
1:B:1439:TRP:O	1:B:1446:GLN:NE2	2.53	0.41
1:B:1973:ARG:HD2	1:B:1997:LEU:HD23	2.02	0.41
1:B:629:GLU:HA	1:B:664:PHE:HZ	1.85	0.41
1:B:722:LEU:HD11	1:B:823:ALA:HB3	2.02	0.41
1:B:1661:VAL:HG11	1:B:1687:MET:O	2.20	0.41
1:B:1763:ARG:HD2	1:B:1763:ARG:HA	1.91	0.41
1:B:784:ILE:HG22	1:B:810:VAL:HG13	2.01	0.41
1:B:663:THR:HB	1:B:927:ILE:HD13	2.02	0.41
1:B:1031:GLU:HA	1:B:1034:LYS:HD3	2.03	0.41
1:B:1724:VAL:HB	2:B:2204:HOH:O	2.19	0.41
1:B:1948:MET:HB2	1:B:1953:MET:O	2.21	0.41
1:B:681:ARG:HH21	1:B:685:LEU:HB3	1.86	0.41
1:B:729:LYS:HA	1:B:729:LYS:HD2	1.89	0.41
1:B:753:ARG:HG3	1:B:753:ARG:H	1.71	0.41
1:B:1139:VAL:HG21	1:B:1170:MET:SD	2.61	0.41
1:B:867:GLY:O	1:B:868:ILE:HG23	2.21	0.41
1:B:1440:LYS:HD2	1:B:1440:LYS:HA	1.95	0.41
1:B:1622:GLU:HG2	1:B:1650:LEU:HD21	2.02	0.41
1:B:1864:GLU:HA	1:B:1867:LEU:HB3	2.02	0.41
1:B:1453:VAL:HG12	1:B:1456:VAL:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:811:SER:OG	1:B:812:THR:N	2.54	0.41
1:B:2049:GLY:HA2	1:B:2050:PRO:HD3	1.93	0.41
1:B:2065:TRP:NE1	1:B:2081:ARG:HB2	2.36	0.41
1:B:501:LEU:HD13	1:B:509:LYS:HG3	2.02	0.41
1:B:823:ALA:HA	1:B:858:ARG:NE	2.32	0.41
1:B:1224:LEU:O	1:B:1269:ARG:N	2.53	0.40
1:B:1845:LEU:O	1:B:1849:ILE:HD12	2.21	0.40
1:B:2089:LYS:HA	1:B:2089:LYS:HD3	1.89	0.40
1:B:516:CYS:SG	1:B:649:ILE:HG12	2.60	0.40
1:B:461:LEU:HA	1:B:461:LEU:HD23	1.84	0.40
1:B:509:LYS:HB2	1:B:509:LYS:HE3	1.78	0.40
1:B:543:PRO:HG3	1:B:616:GLU:HB2	2.03	0.40
1:B:778:LEU:H	1:B:779:PRO:HD2	1.86	0.40
1:B:1165:ILE:O	1:B:1166:ARG:HG2	2.21	0.40
1:B:1534:HIS:CE1	1:B:1536:GLN:HB2	2.56	0.40
1:B:791:ARG:H	1:B:791:ARG:HG2	1.69	0.40
1:B:896:LYS:HE2	1:B:896:LYS:HB3	1.88	0.40
1:B:2024:VAL:HG12	1:B:2026:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	1559 (90%)	144 (8%)	19 (1%)	14 50

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	723	VAL
1	B	750	LEU
1	B	868	ILE

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Mol	Chain	Res	Type
1	B	1907	GLU
1	B	754	GLU
1	B	1053	GLU
1	B	1054	GLU
1	B	1486	ARG
1	B	790	THR
1	B	1988	MET
1	B	2044	GLU
1	B	2100	GLY
1	B	1991	GLU
1	B	778	LEU
1	B	810	VAL
1	B	1055	PRO
1	B	779	PRO
1	B	1326	PRO
1	B	857	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	B	1543/1561 (99%)	1497 (97%)	46 (3%)	41 72

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	440	LYS
1	B	443	GLU
1	B	466	LYS
1	B	489	TYR
1	B	496	ASP
1	B	573	HIS
1	B	574	GLN
1	B	598	ARG
1	B	603	ARG
1	B	621	HIS

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Mol	Chain	Res	Type
1	B	702	GLN
1	B	711	LYS
1	B	751	PHE
1	B	753	ARG
1	B	763	ARG
1	B	773	GLU
1	B	786	HIS
1	B	869	LEU
1	B	992	TYR
1	B	1009	LEU
1	B	1030	ARG
1	B	1313	ARG
1	B	1325	PHE
1	B	1336	PHE
1	B	1356	LYS
1	B	1400	ARG
1	B	1403	LYS
1	B	1483	ARG
1	B	1486	ARG
1	B	1509	THR
1	B	1538	ARG
1	B	1544	LYS
1	B	1566	ARG
1	B	1609	LEU
1	B	1728	LEU
1	B	1809	ASP
1	B	1908	LEU
1	B	1909	GLN
1	B	1957	ASP
1	B	1998	GLN
1	B	2010	PHE
1	B	2026	LYS
1	B	2044	GLU
1	B	2046	GLU
1	B	2059	LYS
1	B	2074	ASN

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

Mol	Chain	Res	Type
1	B	720	GLN
1	B	768	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

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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%)	0.52	144 (8%)	11	6	64, 112, 181, 223	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	758	SER	8.3
1	B	1968	SER	6.7
1	B	532	ASN	6.4
1	B	2035	VAL	6.4
1	B	771	ASN	6.2
1	B	1979	VAL	5.8
1	B	2084	LEU	5.4
1	B	784	ILE	5.3
1	B	763	ARG	5.2
1	B	1977	LYS	5.1
1	B	2028	SER	5.0
1	B	2015	PRO	4.8
1	B	2088	ALA	4.8
1	B	715	HIS	4.8
1	B	1482	GLU	4.7
1	B	757	ALA	4.6
1	B	783	ALA	4.4
1	B	741	MET	4.3
1	B	1989	GLU	4.3
1	B	692	ILE	4.3
1	B	782	PHE	4.1
1	B	1975	THR	4.1
1	B	528	ASP	4.1
1	B	2085	GLN	4.0
1	B	2022	GLU	3.9
1	B	779	PRO	3.8
1	B	527	MET	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	2048	THR	3.7
1	B	1990	ASP	3.7
1	B	1587	GLN	3.7
1	B	1974	CYS	3.6
1	B	2092	LEU	3.6
1	B	2089	LYS	3.6
1	B	1148	PHE	3.5
1	B	2021	TYR	3.5
1	B	2016	ASN	3.5
1	B	2087	LYS	3.5
1	B	2023	VAL	3.5
1	B	1321	TYR	3.4
1	B	2095	VAL	3.4
1	B	1050	GLU	3.4
1	B	2010	PHE	3.3
1	B	1995	ALA	3.3
1	B	732	GLY	3.2
1	B	1961	LYS	3.2
1	B	574	GLN	3.2
1	B	437	ARG	3.2
1	B	1908	LEU	3.2
1	B	1999	LEU	3.2
1	B	789	MET	3.2
1	B	2027	ASP	3.1
1	B	466	LYS	3.1
1	B	579	GLU	3.1
1	B	1406	VAL	3.1
1	B	2124	VAL	3.1
1	B	1971	ILE	3.1
1	B	704	MET	3.1
1	B	409	LEU	3.1
1	B	2038	LEU	3.1
1	B	2004	ILE	3.1
1	B	1964	PRO	3.0
1	B	605	TYR	3.0
1	B	2036	VAL	3.0
1	B	1973	ARG	3.0
1	B	1978	GLY	3.0
1	B	2065	TRP	2.9
1	B	1987	GLU	2.9
1	B	2071	ALA	2.8
1	B	1161	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	2106	LEU	2.8
1	B	673	LEU	2.8
1	B	1487	ILE	2.7
1	B	1484	PRO	2.7
1	B	2039	VAL	2.7
1	B	2017	ILE	2.7
1	B	716	ALA	2.7
1	B	774	LEU	2.6
1	B	753	ARG	2.6
1	B	2042	GLU	2.6
1	B	2019	LEU	2.6
1	B	1170	MET	2.5
1	B	1976	ASP	2.5
1	B	2012	ASN	2.5
1	B	1135	LEU	2.5
1	B	1289	LEU	2.5
1	B	713	MET	2.5
1	B	755	GLY	2.5
1	B	440	LYS	2.4
1	B	729	LYS	2.4
1	B	464	VAL	2.4
1	B	1860	ILE	2.4
1	B	1481	ILE	2.4
1	B	442	TYR	2.4
1	B	1493	SER	2.4
1	B	2034	PRO	2.4
1	B	1965	HIS	2.4
1	B	1373	GLU	2.3
1	B	1423	ASN	2.3
1	B	1972	LYS	2.3
1	B	573	HIS	2.3
1	B	1601	LEU	2.3
1	B	1764	MET	2.3
1	B	1993	ARG	2.3
1	B	1344	ASP	2.3
1	B	1994	ASN	2.3
1	B	2079	ILE	2.3
1	B	809	LEU	2.3
1	B	534	ASP	2.3
1	B	1911	ASP	2.3
1	B	2046	GLU	2.3
1	B	2097	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	759	THR	2.3
1	B	404	ALA	2.3
1	B	1365	LEU	2.2
1	B	743	LEU	2.2
1	B	746	ASP	2.2
1	B	2101	ALA	2.2
1	B	2123	SER	2.2
1	B	1336	PHE	2.2
1	B	2026	LYS	2.2
1	B	720	GLN	2.2
1	B	702	GLN	2.2
1	B	406	ARG	2.2
1	B	1871	LEU	2.2
1	B	744	GLU	2.2
1	B	674	PHE	2.1
1	B	785	HIS	2.1
1	B	444	GLU	2.1
1	B	723	VAL	2.1
1	B	1485	ILE	2.1
1	B	1509	THR	2.1
1	B	2047	VAL	2.1
1	B	1166	ARG	2.1
1	B	1984	ASP	2.1
1	B	1424	ILE	2.1
1	B	531	ILE	2.1
1	B	1884	PHE	2.0
1	B	1951	GLN	2.0
1	B	1793	LEU	2.0
1	B	734	THR	2.0
1	B	2044	GLU	2.0
1	B	2003	GLN	2.0
1	B	469	LYS	2.0
1	B	773	GLU	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 carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.