wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 02:10 PM BST

PDB ID	:	5A22
EMDB ID:	:	EMD-6337
Title	:	Structure of the L protein of vesicular stomatitis virus from electron cryomicroscopy
Authors	:	Liang, B.; Li, Z.; Jenni, S.; Rameh, A.A.; Morin, B.M.; Grant, T.; Grigorieff, N.; Harrison, S.C.; Whelan, S.P.J.
Deposited on	:	2015-05-06
Resolution	:	3.80 Å(reported)

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could
stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/EMValidationReportHelp

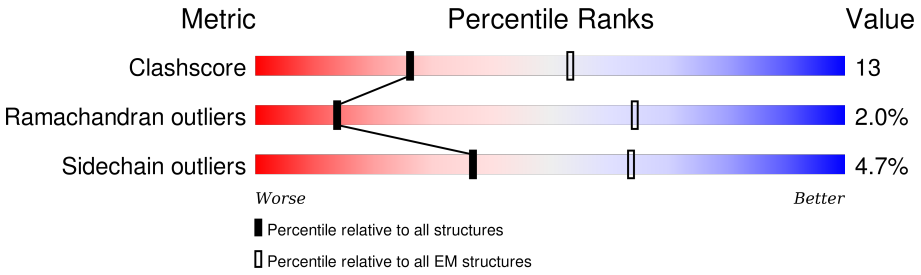
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 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)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	2109	64% 28% • 5%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 32187 atoms, of which 16110 are hydrogens and 0 are deuteriums.

In the tables below, 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 VESICULAR STOMATITIS VIRUS L POLYMERASE.

Mol	Chain	Residues	Atoms						AltConf	Trace
			Total	C	H	N	O	S		
1	A	2002	32185	10249	16110	2803	2934	89	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	228	ARG	PRO	CONFLICT	UNP P03523
A	467	ASP	HIS	CONFLICT	UNP P03523
A	548	LEU	PHE	CONFLICT	UNP P03523
A	549	ARG	PRO	CONFLICT	UNP P03523
A	670	ARG	PRO	CONFLICT	UNP P03523
A	910	PHE	SER	CONFLICT	UNP P03523
A	1026	ALA	PRO	CONFLICT	UNP P03523
A	1348	GLY	ALA	CONFLICT	UNP P03523
A	1589	ALA	PRO	CONFLICT	UNP P03523

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

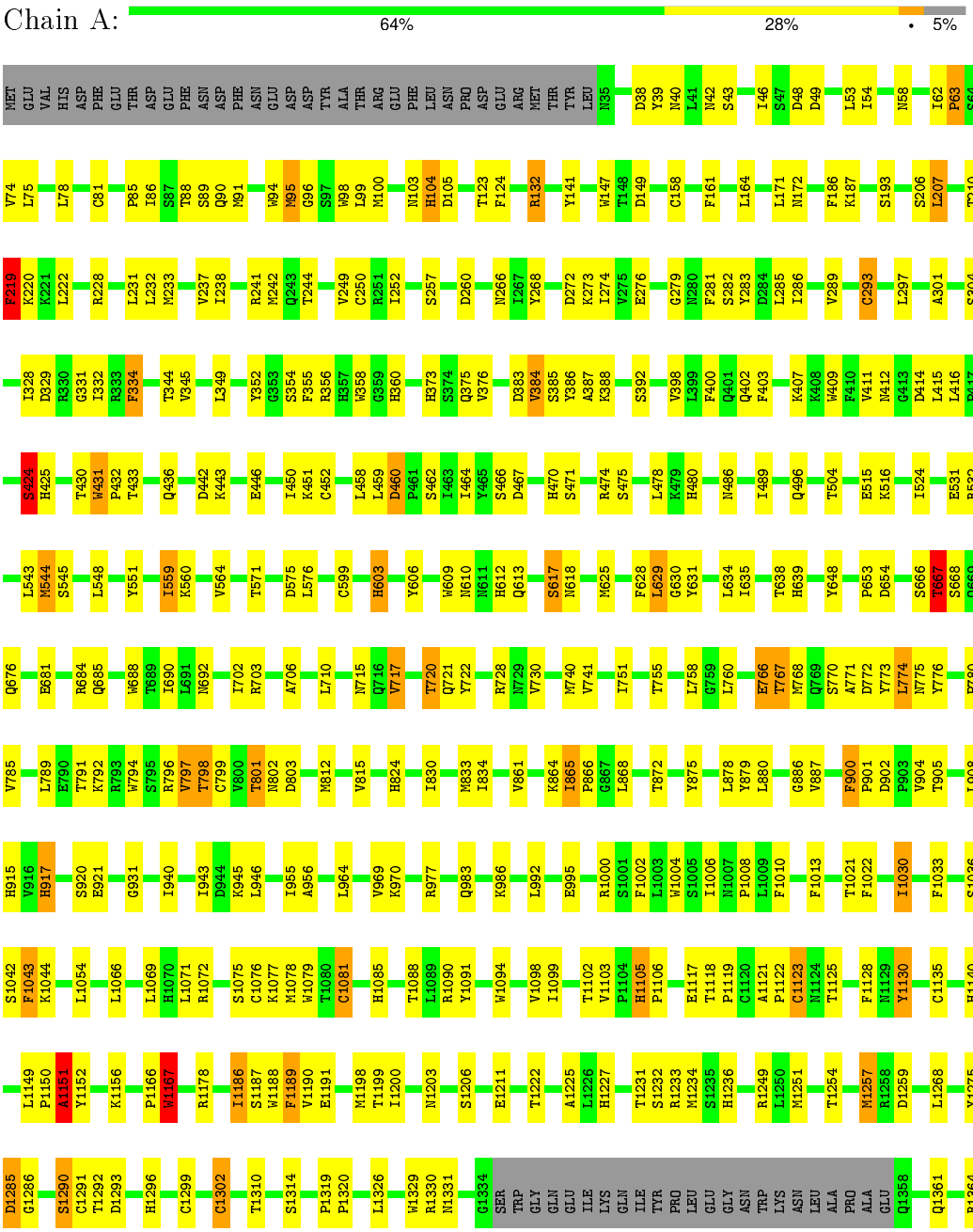
Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
2	A	2	2	2	0

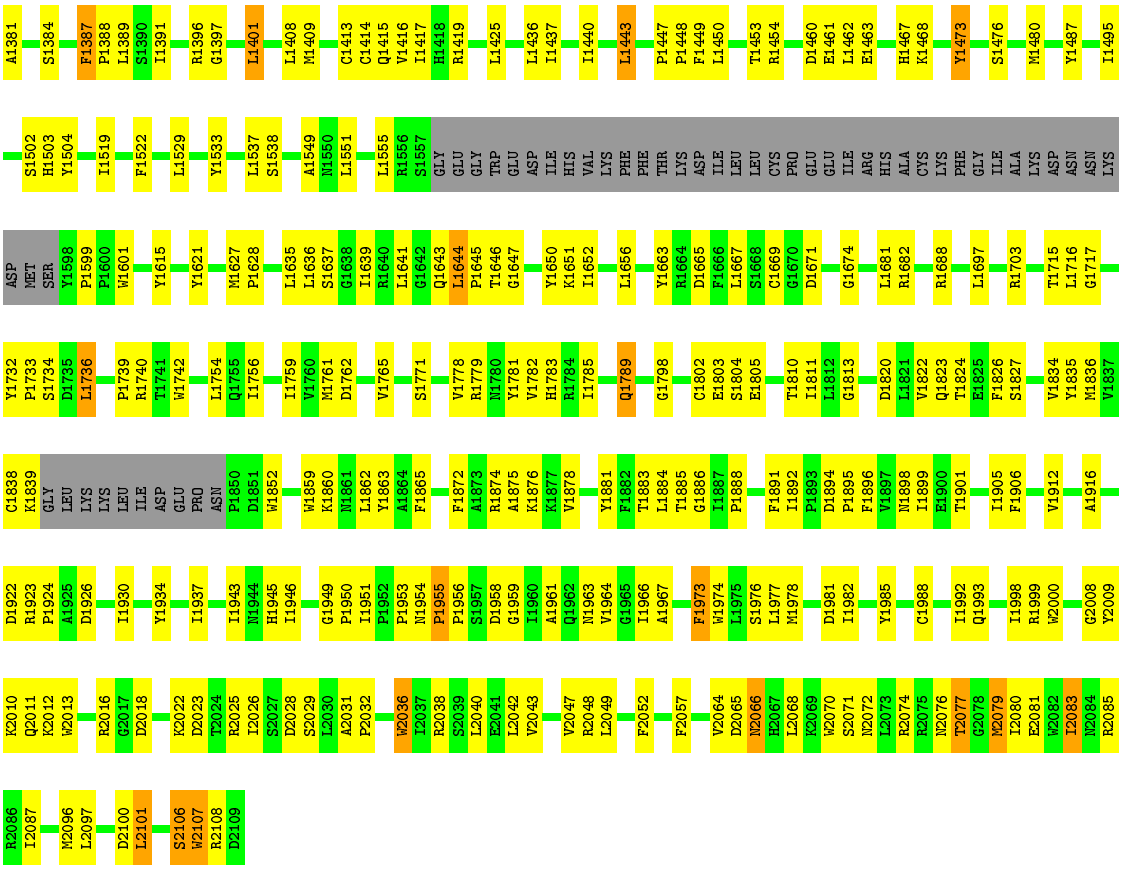
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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: VESICULAR STOMATITIS VIRUS L POLYMERASE

Chain A:




A1381 S1384 F1387 P1388 L1389 S1390 I1391 R1396 G1397 L1401 L1408 M1409 C1413 C1414 Q1415 V1416 I1417 H1418 R1419 L1425 L1436 I1437 I1440 L1443 P1447 P1448 F1449 L1450 T1453 R1454 D1460 E1461 L1462 E1463 H1467 K1468 Y1473 S1476 M1480 Y1487 I1495
S1502 H1503 Y1504 I1519 F1522 L1529 Y1533 L1537 S1538 A1549 N1550 L1551 L1555 R1556 S1557 GLY GLU GLY TRP GLU ASP ILE HIS VAL LYS PHE PHE THR LYS ASP ILE LEU LEU CYS PRO GLU GLU ILE ARG HIS ALA CYS LYS PHE GLY ILE ALA LYS ASP ASN LYS
ASP MET SER Y1598 P1599 P1600 W1601 Y1615 Y1621 M1627 P1628 L1635 L1636 S1637 G1638 I1639 R1640 L1641 G1642 Q1643 L1644 P1645 T1646 G1647 Y1650 K1651 I1652 L1656 Y1663 R1664 D1665 F1666 L1667 S1668 C1669 G1670 D1671 G1674 L1681 R1682 R1688 L1697 R1703 T1715 L1716 G1717
Y1732 P1733 S1734 D1735 L1736 P1739 R1740 T1741 W1742 L1754 Q1755 I1756 I1759 V1760 M1761 D1762 V1765 S1771 V1778 R1779 N1780 Y1781 V1782 H1783 R1784 I1785 Q1789 G1798 C1802 E1803 S1804 E1805 T1810 I1811 L1812 G1813 D1820 L1821 V1822 Q1823 T1824 E1825 F1826 S1827 V1834 Y1835 M1836 V1837
C1838 K1839 GLY LEU LYS LYS LEU ILE ASP GLU PRO ASN P1850 D1851 W1852 W1859 K1860 N1861 L1862 Y1863 A1864 F1865 F1872 A1873 R1874 A1875 K1876 K1877 V1878 Y1881 F1882 T1883 L1884 T1885 G1886 I1887 P1888 F1891 I1892 P1893 D1894 P1895 F1896 V1897 N1898 I1899 E1900 T1901 I1905 F1906 V1912 A1916
D1922 R1923 P1924 A1925 D1926 I1930 Y1934 I1937 I1943 N1944 H1945 I1946 G1949 P1950 I1951 P1952 P1953 N1954 P1955 P1956 S1957 D1958 G1959 I1960 A1961 Q1962 N1963 V1964 G1965 I1966 A1967 F1973 W1974 L1975 S1976 L1977 M1978 D1981 I1982 Y1985 C1988 I1992 Q1993 I1998 R1999 W2000 G2008 Y2009
K2010 Q2011 K2012 W2013 R2016 G2017 D2018 K2022 D2023 T2024 R2025 I2026 S2027 D2028 S2029 L2030 A2031 P2032 W2036 I2037 R2038 S2039 L2040 E2041 L2042 V2043 V2047 R2048 L2049 F2052 F2057 V2064 D2065 N2066 H2067 L2068 K2069 W2070 S2071 N2072 L2073 R2074 R2075 N2076 T2077 G2078 M2079 I2080 E2081 W2082 I2083 N2084 R2085
R2086 I2087 M2096 L2097 D2100 L2101 S2106 W2107 R2108 D2109

4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	Not provided	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	INDIVIDUAL PARTICLES	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	100	Depositor
Minimum defocus (nm)	900	Depositor
Maximum defocus (nm)	2300	Depositor
Magnification	29000	Depositor
Image detector	K2 DIRECT DETECTION CAMERA	Depositor

5 Model quality

5.1 Standard geometry

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

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	$\#\|Z\| > 2$	RMSZ	$\#\|Z\| > 2$
1	A	0.46	0/16456	0.67	0/22270

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	A	0	14

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1071	LEU	Peptide
1	A	1125	THR	Peptide
1	A	1151	ALA	Peptide
1	A	1167	TRP	Peptide
1	A	1285	ASP	Peptide
1	A	1380	HIS	Peptide
1	A	1621	TYR	Peptide
1	A	1789	GLN	Peptide
1	A	1955	PRO	Peptide
1	A	2066	ASN	Peptide
1	A	2106	SER	Peptide
1	A	431	TRP	Peptide
1	A	63	PRO	Peptide

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Mol	Chain	Res	Type	Group
1	A	766	GLU	Peptide

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	16075	16110	16109	427	0
2	A	2	0	0	0	0
All	All	16077	16110	16109	427	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 13.

All (427) 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:A:100:MET:SD	1:A:241:ARG:NH1	2.51	0.84
1:A:88:THR:O	1:A:91:MET:N	2.21	0.73
1:A:767:THR:OG1	1:A:768:MET:N	2.22	0.72
1:A:977:ARG:O	1:A:986:LYS:NZ	2.22	0.72
1:A:419:ASP:HB2	1:A:421:PRO:HD2	1.71	0.71
1:A:1361:GLN:OE1	1:A:1364:ARG:NH2	2.23	0.70
1:A:147:TRP:NE1	1:A:250:CYS:SG	2.65	0.70
1:A:471:SER:N	1:A:544:MET:O	2.25	0.69
1:A:1637:SER:O	1:A:2038:ARG:NH1	2.27	0.68
1:A:354:SER:O	1:A:356:ARG:N	2.26	0.68
1:A:1128:PHE:O	1:A:1130:TYR:N	2.28	0.67
1:A:1117:GLU:OE1	1:A:1740:ARG:NH2	2.28	0.66
1:A:147:TRP:HE1	1:A:250:CYS:HG	1.45	0.65
1:A:384:VAL:O	1:A:387:ALA:N	2.31	0.64
1:A:474:ARG:NH2	1:A:674:GLN:OE1	2.32	0.62
1:A:375:GLN:OE1	1:A:612:HIS:NE2	2.33	0.62
1:A:424:SER:OG	1:A:425:HIS:N	2.28	0.62
1:A:1254:THR:O	1:A:1257:MET:N	2.31	0.61
1:A:132:ARG:NH2	1:A:917:HIS:O	2.33	0.61
1:A:301:ALA:O	1:A:304:SER:OG	2.13	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1838:CYS:SG	1:A:1839:LYS:N	2.75	0.60
1:A:1290:SER:OG	1:A:1291:CYS:N	2.30	0.60
1:A:629:LEU:O	1:A:631:TYR:N	2.31	0.59
1:A:354:SER:C	1:A:356:ARG:H	2.05	0.58
1:A:940:ILE:HA	1:A:943:ILE:HG22	1.84	0.58
1:A:1963:ASN:HA	1:A:1966:ILE:HG22	1.86	0.58
1:A:228:ARG:HG2	1:A:232:LEU:HD12	1.84	0.58
1:A:1945:HIS:HB2	1:A:2077:THR:HG23	1.84	0.58
1:A:467:ASP:OD1	1:A:1041:ASN:ND2	2.34	0.58
1:A:1798:GLY:HA2	1:A:1859:TRP:HH2	1.69	0.58
1:A:2074:ARG:HA	1:A:2080:ILE:HG13	1.86	0.58
1:A:902:ASP:OD2	1:A:1103:VAL:N	2.37	0.57
1:A:206:SER:OG	1:A:207:LEU:N	2.38	0.57
1:A:1822:VAL:HG11	1:A:1863:TYR:CE2	2.39	0.57
1:A:74:VAL:HG21	1:A:216:TRP:CD1	2.39	0.57
1:A:1973:PHE:CE1	1:A:1988:CYS:HB3	2.40	0.57
1:A:1551:LEU:O	1:A:1555:LEU:N	2.38	0.57
1:A:486:ASN:N	1:A:486:ASN:OD1	2.38	0.57
1:A:286:ILE:O	1:A:289:VAL:N	2.38	0.57
1:A:1906:PHE:CD1	1:A:1963:ASN:HB2	2.39	0.56
1:A:309:PRO:HG2	1:A:741:VAL:HG21	1.86	0.56
1:A:2016:ARG:HA	1:A:2087:ILE:CG1	2.35	0.56
1:A:880:LEU:HD11	1:A:886:GLY:HA3	1.87	0.56
1:A:1206:SER:OG	1:A:1211:GLU:OE2	2.23	0.56
1:A:613:GLN:HG3	1:A:688:TRP:CD2	2.41	0.56
1:A:946:LEU:HB2	1:A:1094:TRP:HH2	1.70	0.56
1:A:419:ASP:CB	1:A:421:PRO:HD2	2.34	0.55
1:A:1495:ILE:O	1:A:1533:TYR:OH	2.23	0.55
1:A:1949:GLY:O	1:A:2009:TYR:N	2.38	0.55
1:A:571:THR:OG1	1:A:776:TYR:OH	2.24	0.55
1:A:1537:LEU:HG	1:A:1538:SER:H	1.70	0.55
1:A:2080:ILE:O	1:A:2083:ILE:N	2.35	0.55
1:A:158:CYS:HA	1:A:242:MET:HE3	1.88	0.55
1:A:1186:ILE:HG22	1:A:1187:SER:N	2.21	0.55
1:A:432:PRO:HB3	1:A:436:GLN:HB2	1.89	0.55
1:A:409:TRP:CZ2	1:A:431:TRP:HE3	2.25	0.55
1:A:42:ASN:ND2	1:A:802:ASN:OD1	2.39	0.55
1:A:1006:ILE:HG22	1:A:1008:PRO:HD2	1.88	0.54
1:A:1130:TYR:HB2	1:A:1296:HIS:CE1	2.42	0.54
1:A:1079:TRP:CD1	1:A:1085:HIS:CG	2.95	0.54
1:A:1187:SER:HA	1:A:1191:GLU:HA	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:943:ILE:CD1	1:A:1004:TRP:CE3	2.90	0.54
1:A:443:LYS:O	1:A:446:GLU:N	2.35	0.54
1:A:1982:ILE:O	1:A:1985:TYR:N	2.40	0.54
1:A:880:LEU:CD1	1:A:886:GLY:HA3	2.37	0.53
1:A:403:PHE:CE2	1:A:431:TRP:HB2	2.43	0.53
1:A:88:THR:OG1	1:A:89:SER:N	2.41	0.53
1:A:1894:ASP:O	1:A:1896:PHE:N	2.40	0.53
1:A:286:ILE:O	1:A:289:VAL:HG12	2.08	0.53
1:A:1976:SER:OG	1:A:1981:ASP:O	2.26	0.53
1:A:1682:ARG:HE	1:A:1715:THR:HG21	1.72	0.53
1:A:1503:HIS:HB2	1:A:1504:TYR:HD2	1.74	0.53
1:A:1943:ILE:O	1:A:2011:GLN:NE2	2.37	0.53
1:A:416:LEU:O	1:A:418:HIS:N	2.39	0.53
1:A:1641:LEU:HB3	1:A:1883:THR:HB	1.91	0.52
1:A:755:THR:HG22	1:A:760:LEU:HB2	1.92	0.52
1:A:219:PHE:CD1	1:A:219:PHE:N	2.77	0.52
1:A:420:HIS:N	1:A:421:PRO:HD2	2.24	0.52
1:A:450:ILE:HG23	1:A:451:LYS:N	2.23	0.52
1:A:2031:ALA:HB3	1:A:2032:PRO:HD3	1.92	0.52
1:A:2000:TRP:CH2	1:A:2011:GLN:HB2	2.45	0.52
1:A:1923:ARG:HB2	1:A:1930:ILE:HD11	1.92	0.52
1:A:1934:TYR:HA	1:A:1937:ILE:HG22	1.91	0.52
1:A:706:ALA:HB3	1:A:721:GLN:HB2	1.92	0.52
1:A:1950:PRO:HA	1:A:2008:GLY:HA3	1.92	0.52
1:A:2012:LYS:NZ	1:A:2076:ASN:O	2.43	0.51
1:A:931:GLY:HA3	1:A:1079:TRP:CZ2	2.45	0.51
1:A:460:ASP:OD1	1:A:462:SER:N	2.43	0.51
1:A:1943:ILE:HG21	1:A:2013:TRP:CD1	2.46	0.51
1:A:2016:ARG:HA	1:A:2087:ILE:HG12	1.93	0.51
1:A:1417:ILE:CD1	1:A:1549:ALA:HB2	2.41	0.51
1:A:1974:TRP:CE2	1:A:2040:LEU:HB3	2.46	0.51
1:A:1038:THR:O	1:A:1042:SER:N	2.44	0.51
1:A:931:GLY:HA3	1:A:1079:TRP:HZ2	1.76	0.50
1:A:78:LEU:HG	1:A:219:PHE:CZ	2.45	0.50
1:A:124:PHE:HD2	1:A:141:TYR:HB2	1.76	0.50
1:A:470:HIS:HA	1:A:543:LEU:HB2	1.93	0.50
1:A:1822:VAL:C	1:A:1824:THR:H	2.13	0.50
1:A:1896:PHE:O	1:A:1899:ILE:N	2.45	0.50
1:A:1804:SER:OG	1:A:1805:GLU:N	2.44	0.50
1:A:1450:LEU:HG	1:A:1480:MET:HB3	1.94	0.50
1:A:1732:TYR:HB3	1:A:1733:PRO:HD2	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1644:LEU:CB	1:A:1645:PRO:CD	2.89	0.50
1:A:797:VAL:HG12	1:A:798:THR:N	2.26	0.50
1:A:1123:CYS:SG	1:A:1296:HIS:CD2	3.04	0.50
1:A:2040:LEU:HA	1:A:2043:VAL:HG22	1.94	0.50
1:A:1644:LEU:HB3	1:A:1645:PRO:CD	2.42	0.50
1:A:1076:CYS:SG	1:A:1077:LYS:N	2.81	0.50
1:A:782:PHE:CD1	1:A:783:ARG:HG3	2.47	0.50
1:A:244:THR:CG2	1:A:791:THR:HG23	2.41	0.50
1:A:1291:CYS:SG	1:A:1292:THR:N	2.85	0.49
1:A:1703:ARG:HA	1:A:2107:TRP:CZ2	2.47	0.49
1:A:54:ILE:HD12	1:A:85:PRO:HG3	1.94	0.49
1:A:2081:GLU:O	1:A:2085:ARG:N	2.43	0.49
1:A:78:LEU:HD23	1:A:219:PHE:HE2	1.77	0.49
1:A:911:TRP:HA	1:A:914:ILE:HG22	1.93	0.49
1:A:1234:MET:HB2	1:A:1236:HIS:ND1	2.28	0.49
1:A:104:HIS:CD2	1:A:206:SER:HA	2.47	0.49
1:A:1636:LEU:CD1	1:A:1875:ALA:HA	2.42	0.49
1:A:311:PHE:CD2	1:A:768:MET:HG3	2.47	0.49
1:A:420:HIS:N	1:A:421:PRO:CD	2.76	0.49
1:A:1742:TRP:HB3	1:A:1781:TYR:CD2	2.47	0.49
1:A:1105:HIS:ND1	1:A:1106:PRO:HD2	2.27	0.49
1:A:1152:TYR:HB3	1:A:1277:GLN:HE22	1.77	0.49
1:A:1636:LEU:HD22	1:A:1874:ARG:NH2	2.28	0.49
1:A:272:ASP:O	1:A:276:GLU:N	2.46	0.49
1:A:147:TRP:CD1	1:A:250:CYS:SG	3.06	0.49
1:A:617:SER:OG	1:A:618:ASN:N	2.45	0.49
1:A:1779:ARG:NH1	1:A:1810:THR:O	2.45	0.48
1:A:1998:ILE:HG22	1:A:2023:ASP:HA	1.94	0.48
1:A:430:THR:O	1:A:430:THR:HG22	2.13	0.48
1:A:904:VAL:HG12	1:A:908:LEU:HD12	1.94	0.48
1:A:53:LEU:HD13	1:A:71:TRP:CG	2.47	0.48
1:A:1203:ASN:HA	1:A:1206:SER:HB3	1.94	0.48
1:A:900:PHE:CZ	1:A:1105:HIS:HB2	2.48	0.48
1:A:376:VAL:HG11	1:A:676:GLN:CG	2.43	0.48
1:A:964:LEU:HB3	1:A:1054:LEU:HD11	1.96	0.48
1:A:1409:MET:CE	1:A:1495:ILE:HD13	2.42	0.48
1:A:1644:LEU:CB	1:A:1645:PRO:HD2	2.43	0.48
1:A:297:LEU:HB3	1:A:773:TYR:CE1	2.48	0.48
1:A:373:HIS:CG	1:A:670:ARG:HD3	2.48	0.48
1:A:1956:PRO:CG	1:A:2022:LYS:HG3	2.43	0.48
1:A:48:ASP:OD1	1:A:49:ASP:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:SER:OG	1:A:921:GLU:N	2.46	0.48
1:A:99:LEU:HD13	1:A:241:ARG:NH2	2.29	0.48
1:A:1823:GLN:HA	1:A:1878:VAL:HG22	1.94	0.48
1:A:1388:PRO:HD3	1:A:1396:ARG:CZ	2.44	0.48
1:A:432:PRO:CB	1:A:436:GLN:HB2	2.44	0.47
1:A:638:THR:OG1	1:A:639:HIS:N	2.47	0.47
1:A:1079:TRP:HD1	1:A:1085:HIS:CG	2.33	0.47
1:A:1916:ALA:HB1	1:A:1934:TYR:HE1	1.78	0.47
1:A:466:SER:HB3	1:A:1167:TRP:HB3	1.96	0.47
1:A:702:ILE:HD12	1:A:703:ARG:HB2	1.96	0.47
1:A:872:THR:HG23	1:A:1069:LEU:HD23	1.96	0.47
1:A:2070:TRP:O	1:A:2074:ARG:N	2.48	0.47
1:A:1387:PHE:HB3	1:A:1388:PRO:CD	2.45	0.47
1:A:164:LEU:HD12	1:A:238:ILE:HG21	1.97	0.47
1:A:524:ILE:HG22	1:A:648:TYR:HE1	1.78	0.47
1:A:1667:LEU:HB3	1:A:1759:ILE:HD13	1.96	0.47
1:A:43:SER:C	1:A:531:GLU:HB3	2.35	0.47
1:A:666:SER:OG	1:A:667:THR:N	2.48	0.47
1:A:409:TRP:CZ2	1:A:431:TRP:CE3	3.02	0.47
1:A:1895:PRO:HB3	1:A:2042:LEU:HG	1.97	0.47
1:A:576:LEU:HD21	1:A:824:HIS:CE1	2.49	0.47
1:A:1091:TYR:C	1:A:1091:TYR:CD1	2.87	0.47
1:A:1387:PHE:HB3	1:A:1388:PRO:HD2	1.97	0.46
1:A:123:THR:HG23	1:A:879:TYR:CE1	2.50	0.46
1:A:1075:SER:OG	1:A:1076:CYS:N	2.48	0.46
1:A:1090:ARG:HD2	1:A:1098:VAL:HG21	1.98	0.46
1:A:945:LYS:HB3	1:A:946:LEU:HD12	1.97	0.46
1:A:864:LYS:O	1:A:865:ILE:HG23	2.16	0.46
1:A:2040:LEU:HD12	1:A:2040:LEU:N	2.30	0.46
1:A:1021:THR:HG22	1:A:1022:PHE:N	2.30	0.46
1:A:1823:GLN:HG2	1:A:1881:TYR:CE2	2.50	0.46
1:A:560:LYS:HA	1:A:564:VAL:CG2	2.45	0.46
1:A:81:CYS:SG	1:A:220:LYS:HD2	2.56	0.46
1:A:1135:CYS:SG	1:A:1291:CYS:HB3	2.56	0.46
1:A:95:MET:HG3	1:A:96:GLY:N	2.30	0.46
1:A:1955:PRO:HD2	1:A:2000:TRP:CZ2	2.50	0.46
1:A:1827:SER:HA	1:A:1874:ARG:HH22	1.81	0.46
1:A:1503:HIS:HB2	1:A:1504:TYR:CD2	2.51	0.46
1:A:1022:PHE:CE1	1:A:1326:LEU:HD22	2.51	0.46
1:A:458:LEU:HD23	1:A:464:ILE:HG12	1.96	0.46
1:A:241:ARG:HH21	1:A:358:TRP:HB3	1.81	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:PHE:HD2	1:A:431:TRP:HZ2	1.64	0.46
1:A:219:PHE:HD1	1:A:219:PHE:N	2.14	0.46
1:A:1473:TYR:C	1:A:1473:TYR:CD1	2.89	0.46
1:A:415:LEU:HD23	1:A:421:PRO:HB2	1.98	0.46
1:A:1151:ALA:CB	1:A:2106:SER:HB3	2.46	0.46
1:A:94:TRP:CE3	1:A:222:LEU:HD13	2.52	0.46
1:A:360:HIS:NE2	1:A:532:ARG:HD3	2.31	0.45
1:A:1010:PHE:CD2	1:A:1099:ILE:HG21	2.51	0.45
1:A:1231:THR:C	1:A:1233:ARG:H	2.19	0.45
1:A:915:HIS:NE2	1:A:1078:MET:HG3	2.31	0.45
1:A:1782:VAL:HG12	1:A:1783:HIS:N	2.31	0.45
1:A:1739:PRO:O	1:A:1740:ARG:HB3	2.16	0.45
1:A:1066:LEU:N	1:A:1066:LEU:HD23	2.31	0.45
1:A:1958:ASP:OD1	1:A:1959:GLY:N	2.50	0.45
1:A:1646:THR:HG22	1:A:1647:GLY:N	2.31	0.45
1:A:283:TYR:N	1:A:283:TYR:CD1	2.85	0.45
1:A:1142:VAL:HG23	1:A:1249:ARG:HE	1.82	0.45
1:A:2096:MET:C	1:A:2097:LEU:HG	2.37	0.45
1:A:1999:ARG:NH1	1:A:2018:ASP:OD1	2.48	0.45
1:A:720:THR:HG22	1:A:722:TYR:CE2	2.52	0.45
1:A:1891:PHE:CD1	1:A:1891:PHE:N	2.83	0.45
1:A:304:SER:HB2	1:A:783:ARG:CZ	2.47	0.45
1:A:1454:ARG:HG3	1:A:1480:MET:HG3	1.99	0.45
1:A:551:TYR:OH	1:A:684:ARG:NH2	2.50	0.45
1:A:610:ASN:HB3	1:A:681:GLU:H	1.82	0.45
1:A:1121:ALA:N	1:A:1122:PRO:HD2	2.32	0.45
1:A:609:TRP:HH2	1:A:692:ASN:HB2	1.82	0.45
1:A:983:GLN:HB2	1:A:1329:TRP:CZ3	2.52	0.45
1:A:1416:VAL:HA	1:A:1419:ARG:HB3	1.99	0.45
1:A:1156:LYS:HA	1:A:2108:ARG:HB3	1.99	0.45
1:A:75:LEU:HA	1:A:78:LEU:HD12	1.99	0.44
1:A:1189:PHE:HD1	1:A:1189:PHE:H	1.66	0.44
1:A:331:GLY:HA2	1:A:334:PHE:CD2	2.51	0.44
1:A:392:SER:OG	1:A:442:ASP:HB3	2.18	0.44
1:A:995:GLU:HG2	1:A:1320:PRO:HG2	1.98	0.44
1:A:1128:PHE:HB2	1:A:1259:ASP:CG	2.38	0.44
1:A:575:ASP:CG	1:A:576:LEU:H	2.20	0.44
1:A:710:LEU:HB3	1:A:776:TYR:CE2	2.52	0.44
1:A:1010:PHE:HD1	1:A:1013:PHE:H	1.65	0.44
1:A:334:PHE:N	1:A:334:PHE:CD1	2.85	0.44
1:A:1118:THR:HB	1:A:1119:PRO:HD2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:GLN:NE2	1:A:1043:PHE:CE1	2.85	0.44
1:A:430:THR:O	1:A:431:TRP:C	2.56	0.44
1:A:915:HIS:CG	1:A:1078:MET:SD	3.11	0.44
1:A:865:ILE:HD11	1:A:868:LEU:HD21	1.99	0.44
1:A:803:ASP:HB2	1:A:1036:SER:HB2	1.99	0.44
1:A:1081:CYS:SG	1:A:1299:CYS:HB2	2.57	0.44
1:A:1284:ARG:O	1:A:1286:GLY:N	2.43	0.44
1:A:1140:HIS:CG	1:A:1141:ASP:H	2.36	0.44
1:A:1231:THR:O	1:A:1233:ARG:N	2.51	0.44
1:A:1227:HIS:HB3	1:A:1268:LEU:HD21	1.99	0.44
1:A:424:SER:HA	1:A:430:THR:CB	2.48	0.44
1:A:1951:ILE:HA	1:A:2009:TYR:CZ	2.53	0.44
1:A:1081:CYS:HB3	1:A:1302:CYS:HB3	1.99	0.44
1:A:545:SER:O	1:A:548:LEU:N	2.51	0.44
1:A:1190:VAL:HB	1:A:1198:MET:SD	2.58	0.44
1:A:1834:VAL:CG1	1:A:1835:TYR:N	2.80	0.44
1:A:1644:LEU:O	1:A:1645:PRO:C	2.54	0.44
1:A:376:VAL:HG11	1:A:676:GLN:HG3	1.98	0.44
1:A:1443:LEU:HD21	1:A:1449:PHE:CE2	2.53	0.44
1:A:789:LEU:HB2	1:A:792:LYS:HB2	2.00	0.44
1:A:1822:VAL:C	1:A:1824:THR:N	2.71	0.44
1:A:812:MET:HA	1:A:815:VAL:HG12	1.99	0.44
1:A:1967:ALA:HA	1:A:2036:TRP:NE1	2.33	0.44
1:A:1943:ILE:HG21	1:A:2013:TRP:NE1	2.32	0.43
1:A:1992:ILE:HG13	1:A:1993:GLN:N	2.32	0.43
1:A:1389:LEU:HD23	1:A:1391:ILE:CD1	2.48	0.43
1:A:774:LEU:HD12	1:A:775:ASN:H	1.82	0.43
1:A:1002:PHE:CZ	1:A:1200:ILE:HD13	2.53	0.43
1:A:419:ASP:HB2	1:A:421:PRO:CD	2.42	0.43
1:A:946:LEU:HB2	1:A:1094:TRP:CH2	2.52	0.43
1:A:861:VAL:HG13	1:A:864:LYS:HB3	1.98	0.43
1:A:1895:PRO:O	1:A:2043:VAL:HG12	2.18	0.43
1:A:2100:ASP:OD1	1:A:2100:ASP:N	2.52	0.43
1:A:186:PHE:O	1:A:187:LYS:HB3	2.17	0.43
1:A:710:LEU:HB2	1:A:717:VAL:HG22	2.00	0.43
1:A:911:TRP:CE3	1:A:914:ILE:HG21	2.53	0.43
1:A:1992:ILE:HA	1:A:2026:ILE:HD11	2.00	0.43
1:A:1872:PHE:CZ	1:A:1977:LEU:HA	2.53	0.43
1:A:1912:VAL:HG13	1:A:2064:VAL:HG11	2.01	0.43
1:A:915:HIS:ND1	1:A:1078:MET:SD	2.92	0.43
1:A:1188:TRP:CE3	1:A:1189:PHE:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1652:ILE:HA	1:A:1652:ILE:HD13	1.89	0.43
1:A:740:MET:HE2	1:A:2097:LEU:HD22	2.01	0.43
1:A:1440:ILE:HA	1:A:1440:ILE:HD13	1.92	0.43
1:A:403:PHE:O	1:A:407:LYS:HA	2.19	0.43
1:A:123:THR:CG2	1:A:879:TYR:CE1	3.02	0.43
1:A:40:ASN:O	1:A:232:LEU:HD13	2.19	0.43
1:A:1954:ASN:C	1:A:1956:PRO:HD2	2.39	0.43
1:A:1178:ARG:HA	1:A:1231:THR:HG21	2.00	0.43
1:A:515:GLU:HG3	1:A:516:LYS:N	2.33	0.43
1:A:603:HIS:CD2	1:A:767:THR:HG23	2.53	0.43
1:A:880:LEU:C	1:A:880:LEU:HD12	2.39	0.43
1:A:794:TRP:HA	1:A:797:VAL:HG23	2.00	0.43
1:A:983:GLN:HB2	1:A:1329:TRP:HZ3	1.83	0.43
1:A:969:VAL:HG21	1:A:1033:PHE:CD2	2.54	0.43
1:A:86:ILE:HG22	1:A:90:GLN:CB	2.48	0.43
1:A:65:MET:HB3	1:A:486:ASN:HB3	2.01	0.42
1:A:1453:THR:OG1	1:A:1462:LEU:HD12	2.19	0.42
1:A:770:SER:C	1:A:772:ASP:N	2.72	0.42
1:A:784:GLY:HA3	1:A:1146:ARG:HD2	2.01	0.42
1:A:983:GLN:HG3	1:A:1329:TRP:HZ3	1.84	0.42
1:A:1189:PHE:O	1:A:1310:THR:HA	2.19	0.42
1:A:2028:ASP:N	1:A:2028:ASP:OD1	2.52	0.42
1:A:241:ARG:HD2	1:A:268:TYR:CE2	2.54	0.42
1:A:1946:ILE:HG21	1:A:2068:LEU:HB3	2.00	0.42
1:A:398:VAL:CG2	1:A:628:PHE:CZ	3.02	0.42
1:A:1330:ARG:HG3	1:A:1331:ASN:N	2.34	0.42
1:A:354:SER:C	1:A:356:ARG:N	2.72	0.42
1:A:1951:ILE:HA	1:A:2009:TYR:CE1	2.55	0.42
1:A:1090:ARG:NH1	1:A:1102:THR:OG1	2.53	0.42
1:A:887:VAL:HG23	1:A:1066:LEU:HD21	2.02	0.42
1:A:1149:LEU:CD2	1:A:1251:MET:HB2	2.49	0.42
1:A:1251:MET:SD	1:A:1697:LEU:HD21	2.59	0.42
1:A:1898:ASN:HA	1:A:1901:THR:HG22	2.01	0.42
1:A:2065:ASP:HB3	1:A:2068:LEU:HD21	2.02	0.42
1:A:1601:TRP:CZ3	1:A:1682:ARG:HD3	2.55	0.42
1:A:515:GLU:CG	1:A:516:LYS:N	2.82	0.42
1:A:1627:MET:HE2	1:A:1802:CYS:C	2.40	0.42
1:A:666:SER:O	1:A:668:SER:N	2.53	0.42
1:A:293:CYS:SG	1:A:352:TYR:HB2	2.58	0.42
1:A:2057:PHE:CE2	1:A:2070:TRP:HE3	2.38	0.42
1:A:880:LEU:HD12	1:A:880:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:685:GLN:HA	1:A:685:GLN:NE2	2.35	0.42
1:A:599:CYS:O	1:A:771:ALA:HA	2.20	0.42
1:A:1487:TYR:CD1	1:A:1487:TYR:C	2.93	0.42
1:A:1943:ILE:HD13	1:A:2013:TRP:CG	2.54	0.42
1:A:2052:PHE:HE1	1:A:2057:PHE:HB2	1.84	0.42
1:A:74:VAL:HG21	1:A:216:TRP:CG	2.54	0.42
1:A:1199:THR:O	1:A:1203:ASN:ND2	2.48	0.42
1:A:1319:PRO:HA	1:A:1320:PRO:HD3	1.85	0.42
1:A:1397:GLY:C	1:A:1461:GLU:HG3	2.39	0.42
1:A:796:ARG:HB3	1:A:799:CYS:SG	2.60	0.42
1:A:1945:HIS:HE1	1:A:2068:LEU:HB2	1.84	0.42
1:A:1206:SER:HB2	1:A:1211:GLU:HG3	2.01	0.42
1:A:634:LEU:HG	1:A:635:ILE:N	2.35	0.42
1:A:834:ILE:HD12	1:A:834:ILE:N	2.34	0.42
1:A:1974:TRP:HE1	1:A:2040:LEU:CD2	2.33	0.42
1:A:865:ILE:HD11	1:A:868:LEU:HG	2.01	0.42
1:A:1140:HIS:CG	1:A:1141:ASP:N	2.88	0.42
1:A:1330:ARG:CG	1:A:1331:ASN:N	2.82	0.42
1:A:1671:ASP:HB3	1:A:1674:GLY:HA2	2.02	0.42
1:A:249:VAL:HG13	1:A:250:CYS:N	2.34	0.41
1:A:1651:LYS:CB	1:A:1824:THR:HG21	2.50	0.41
1:A:1425:LEU:HD23	1:A:1538:SER:CB	2.49	0.41
1:A:1425:LEU:HD23	1:A:1538:SER:HA	2.02	0.41
1:A:1078:MET:HA	1:A:1078:MET:HE3	2.02	0.41
1:A:1078:MET:HE3	1:A:1079:TRP:CE3	2.55	0.41
1:A:164:LEU:HD22	1:A:231:LEU:HD11	2.02	0.41
1:A:99:LEU:HD11	1:A:237:VAL:HG11	2.02	0.41
1:A:2010:LYS:HG2	1:A:2011:GLN:N	2.34	0.41
1:A:2009:TYR:N	1:A:2009:TYR:CD1	2.87	0.41
1:A:720:THR:CG2	1:A:722:TYR:CE2	3.03	0.41
1:A:1401:LEU:HD23	1:A:1487:TYR:CE1	2.55	0.41
1:A:1436:LEU:HD23	1:A:1437:ILE:HD13	2.02	0.41
1:A:386:TYR:CD2	1:A:758:LEU:HD21	2.55	0.41
1:A:794:TRP:O	1:A:797:VAL:HG23	2.21	0.41
1:A:609:TRP:CH2	1:A:692:ASN:HB2	2.55	0.41
1:A:1149:LEU:HD23	1:A:1251:MET:HB2	2.02	0.41
1:A:1669:CYS:HB2	1:A:1736:LEU:HD13	2.02	0.41
1:A:279:GLY:O	1:A:281:PHE:N	2.53	0.41
1:A:274:ILE:HG22	1:A:282:SER:HB3	2.02	0.41
1:A:402:GLN:HE21	1:A:452:CYS:HB3	1.86	0.41
1:A:1827:SER:CA	1:A:1874:ARG:HH22	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:915:HIS:CG	1:A:1078:MET:CE	3.04	0.41
1:A:1732:TYR:O	1:A:1734:SER:N	2.54	0.41
1:A:865:ILE:HG13	1:A:866:PRO:N	2.35	0.41
1:A:1118:THR:HB	1:A:1119:PRO:CD	2.51	0.41
1:A:257:SER:O	1:A:260:ASP:N	2.53	0.41
1:A:728:ARG:HB2	1:A:2025:ARG:HH12	1.85	0.41
1:A:2047:VAL:HG12	1:A:2048:ARG:N	2.35	0.41
1:A:1778:VAL:CG2	1:A:1811:ILE:HD11	2.50	0.41
1:A:1765:VAL:HG11	1:A:1771:SER:HB2	2.02	0.41
1:A:1789:GLN:N	1:A:1789:GLN:OE1	2.53	0.41
1:A:606:TYR:HD2	1:A:609:TRP:HB2	1.86	0.41
1:A:770:SER:C	1:A:772:ASP:H	2.23	0.41
1:A:1665:ASP:OD1	1:A:1688:ARG:N	2.43	0.41
1:A:1862:LEU:HG	1:A:1863:TYR:N	2.36	0.41
1:A:946:LEU:HD22	1:A:1094:TRP:CH2	2.55	0.41
1:A:1106:PRO:HB2	1:A:1275:TYR:CD1	2.56	0.41
1:A:559:ILE:CD1	1:A:625:MET:CE	2.98	0.41
1:A:1961:ALA:HA	1:A:1964:VAL:HG12	2.03	0.41
1:A:1885:THR:HG22	1:A:1886:GLY:N	2.35	0.41
1:A:2013:TRP:HZ2	1:A:2079:MET:HE2	1.85	0.41
1:A:1822:VAL:CB	1:A:1874:ARG:HD2	2.51	0.41
1:A:1656:LEU:HD23	1:A:1663:TYR:HE1	1.86	0.41
1:A:411:VAL:HG12	1:A:412:ASN:N	2.35	0.41
1:A:2010:LYS:CG	1:A:2011:GLN:N	2.84	0.41
1:A:1945:HIS:CB	1:A:2077:THR:HG23	2.49	0.41
1:A:104:HIS:ND1	1:A:105:ASP:O	2.54	0.41
1:A:865:ILE:HD11	1:A:868:LEU:CG	2.50	0.41
1:A:344:THR:HG22	1:A:345:VAL:N	2.36	0.41
1:A:1447:PRO:HG2	1:A:1448:PRO:HD3	2.01	0.41
1:A:1813:GLY:HA3	1:A:1836:MET:SD	2.61	0.41
1:A:328:ILE:HG22	1:A:329:ASP:N	2.36	0.41
1:A:1636:LEU:HA	1:A:1639:ILE:HG12	2.03	0.41
1:A:801:THR:HG22	1:A:802:ASN:H	1.86	0.41
1:A:878:LEU:C	1:A:879:TYR:CD1	2.94	0.41
1:A:1888:PRO:HG2	1:A:1891:PHE:CE2	2.56	0.41
1:A:496:GLN:HE22	1:A:1044:LYS:HB3	1.85	0.41
1:A:1901:THR:O	1:A:1905:ILE:N	2.53	0.41
1:A:955:ILE:HG22	1:A:956:ALA:N	2.35	0.41
1:A:285:LEU:HB3	1:A:332:ILE:HD12	2.02	0.41
1:A:252:ILE:HD12	1:A:830:ILE:CG2	2.51	0.41
1:A:1884:LEU:HD11	1:A:1892:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:654:ASP:N	1:A:654:ASP:OD1	2.54	0.41
1:A:970:LYS:HB2	1:A:1030:ILE:CD1	2.51	0.41
1:A:1387:PHE:CB	1:A:1388:PRO:HD2	2.51	0.40
1:A:1627:MET:HG3	1:A:1628:PRO:HD2	2.03	0.40
1:A:1922:ASP:C	1:A:1924:PRO:HD3	2.40	0.40
1:A:459:LEU:HD23	1:A:459:LEU:HA	1.99	0.40
1:A:1599:PRO:HD3	1:A:1716:LEU:C	2.42	0.40
1:A:1636:LEU:HB3	1:A:1826:PHE:HA	2.03	0.40
1:A:1409:MET:HG3	1:A:1529:LEU:HD21	2.04	0.40
1:A:1106:PRO:HB2	1:A:1275:TYR:CG	2.56	0.40
1:A:875:TYR:O	1:A:879:TYR:HB2	2.21	0.40
1:A:1599:PRO:HD3	1:A:1717:GLY:HA3	2.02	0.40
1:A:1860:LYS:HA	1:A:1865:PHE:CD2	2.56	0.40
1:A:1460:ASP:O	1:A:1463:GLU:N	2.50	0.40
1:A:385:SER:HA	1:A:388:LYS:HB2	2.03	0.40
1:A:1643:GLN:O	1:A:1643:GLN:HG3	2.21	0.40
1:A:1963:ASN:HA	1:A:1966:ILE:CG2	2.51	0.40
1:A:78:LEU:HD23	1:A:219:PHE:CE2	2.56	0.40
1:A:1414:CYS:O	1:A:1417:ILE:HG22	2.20	0.40
1:A:1781:TYR:HB3	1:A:1785:ILE:HD12	2.04	0.40
1:A:2100:ASP:CG	1:A:2101:LEU:H	2.25	0.40
1:A:252:ILE:HD12	1:A:830:ILE:HG22	2.03	0.40
1:A:830:ILE:O	1:A:833:MET:N	2.53	0.40
1:A:39:TYR:CE1	1:A:172:ASN:HB3	2.56	0.40
1:A:781:ILE:HG23	1:A:785:VAL:O	2.21	0.40
1:A:403:PHE:HE2	1:A:431:TRP:CB	2.35	0.40
1:A:2013:TRP:O	1:A:2077:THR:OG1	2.31	0.40
1:A:1450:LEU:HA	1:A:1453:THR:HG22	2.03	0.40
1:A:1188:TRP:CH2	1:A:1225:ALA:HA	2.57	0.40
1:A:1284:ARG:NH2	1:A:1293:ASP:OD1	2.54	0.40
1:A:480:HIS:ND1	1:A:480:HIS:O	2.52	0.40
1:A:1375:TYR:CD1	1:A:1415:GLN:HG2	2.56	0.40
1:A:1951:ILE:O	1:A:1953:PRO:HD3	2.22	0.40
1:A:94:TRP:HZ3	1:A:98:TRP:CG	2.39	0.40
1:A:1872:PHE:CD2	1:A:1876:LYS:HE3	2.56	0.40
1:A:489:ILE:HD11	1:A:653:PRO:HB3	2.04	0.40
1:A:349:LEU:HD11	1:A:780:PRO:HG3	2.04	0.40
1:A:1978:MET:HB3	1:A:2049:LEU:HD13	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 PDB entries followed by that with respect to all EM entries.

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	1994/2109 (94%)	1678 (84%)	277 (14%)	39 (2%)	9 54

All (39) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	355	PHE
1	A	730	VAL
1	A	1381	ALA
1	A	2066	ASN
1	A	384	VAL
1	A	1166	PRO
1	A	1232	SER
1	A	1803	GLU
1	A	58	ASN
1	A	218	TYR
1	A	667	THR
1	A	797	VAL
1	A	1186	ILE
1	A	219	PHE
1	A	539	ARG
1	A	901	PRO
1	A	1314	SER
1	A	1644	LEU
1	A	424	SER
1	A	774	LEU
1	A	1081	CYS
1	A	1151	ALA
1	A	1387	PHE
1	A	1468	LYS
1	A	1635	LEU
1	A	2083	ILE
1	A	2107	TRP

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Mol	Chain	Res	Type
1	A	62	ILE
1	A	104	HIS
1	A	630	GLY
1	A	1285	ASP
1	A	2101	LEU
1	A	46	ILE
1	A	559	ILE
1	A	900	PHE
1	A	1756	ILE
1	A	1519	ILE
1	A	1150	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

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	1794/1890 (95%)	1709 (95%)	85 (5%)	32 72

All (85) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ASP
1	A	95	MET
1	A	103	ASN
1	A	132	ARG
1	A	149	ASP
1	A	161	PHE
1	A	171	LEU
1	A	193	SER
1	A	207	LEU
1	A	210	THR
1	A	219	PHE
1	A	233	MET
1	A	266	ASN
1	A	273	LYS
1	A	293	CYS

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Mol	Chain	Res	Type
1	A	334	PHE
1	A	383	ASP
1	A	414	ASP
1	A	424	SER
1	A	433	THR
1	A	460	ASP
1	A	475	SER
1	A	478	LEU
1	A	504	THR
1	A	534	LEU
1	A	544	MET
1	A	603	HIS
1	A	617	SER
1	A	629	LEU
1	A	667	THR
1	A	690	ILE
1	A	715	ASN
1	A	717	VAL
1	A	720	THR
1	A	751	ILE
1	A	766	GLU
1	A	767	THR
1	A	798	THR
1	A	801	THR
1	A	865	ILE
1	A	905	THR
1	A	917	HIS
1	A	992	LEU
1	A	1000	ARG
1	A	1030	ILE
1	A	1043	PHE
1	A	1072	ARG
1	A	1088	THR
1	A	1105	HIS
1	A	1123	CYS
1	A	1130	TYR
1	A	1142	VAL
1	A	1167	TRP
1	A	1189	PHE
1	A	1222	THR
1	A	1257	MET
1	A	1290	SER

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Mol	Chain	Res	Type
1	A	1302	CYS
1	A	1384	SER
1	A	1401	LEU
1	A	1408	LEU
1	A	1413	CYS
1	A	1443	LEU
1	A	1467	HIS
1	A	1473	TYR
1	A	1476	SER
1	A	1502	SER
1	A	1522	PHE
1	A	1615	TYR
1	A	1650	TYR
1	A	1681	LEU
1	A	1736	LEU
1	A	1754	LEU
1	A	1761	MET
1	A	1762	ASP
1	A	1820	ASP
1	A	1852	TRP
1	A	1926	ASP
1	A	1973	PHE
1	A	2029	SER
1	A	2036	TRP
1	A	2071	SER
1	A	2072	ASN
1	A	2077	THR
1	A	2079	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	425	HIS
1	A	496	GLN
1	A	1277	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

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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.