Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:30 PM GMT

PDB ID	:	4F92
Title	:	Brr2 Helicase Region S1087L
Authors	:	Santos, K.F.; Jovin, S.M.; Weber, G.; Pena, V.; Luehrmann, R.; Wahl, M.C.
Deposited on	:	2012-05-18
Resolution	:	2.66 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

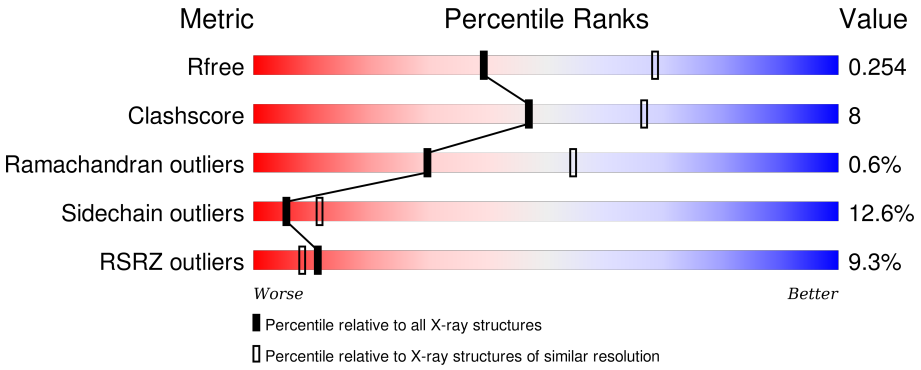
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.66 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}	91344	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1724	9% 74% 22%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAN	B	2201[A]	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAN	B	2201[B]	-	-	-	X

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 14019 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.

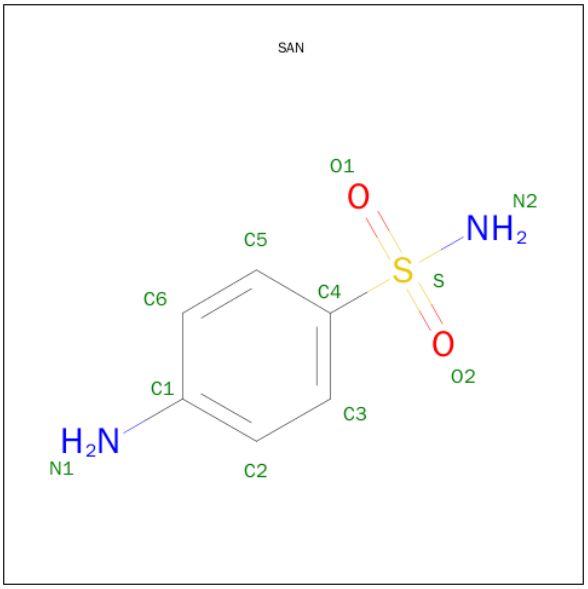
- Molecule 1 is a protein called U5 small nuclear ribonucleoprotein 200 kDa helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	1723	13866	8863	2373	2558	72	0	1	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1087	LEU	SER	ENGINEERED MUTATION	UNP O75643

- Molecule 2 is SULFANILAMIDE (three-letter code: SAN) (formula: $C_6H_8N_2O_2S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
2	B	1	22	12	4	4	2	0	1

- Molecule 3 is water.

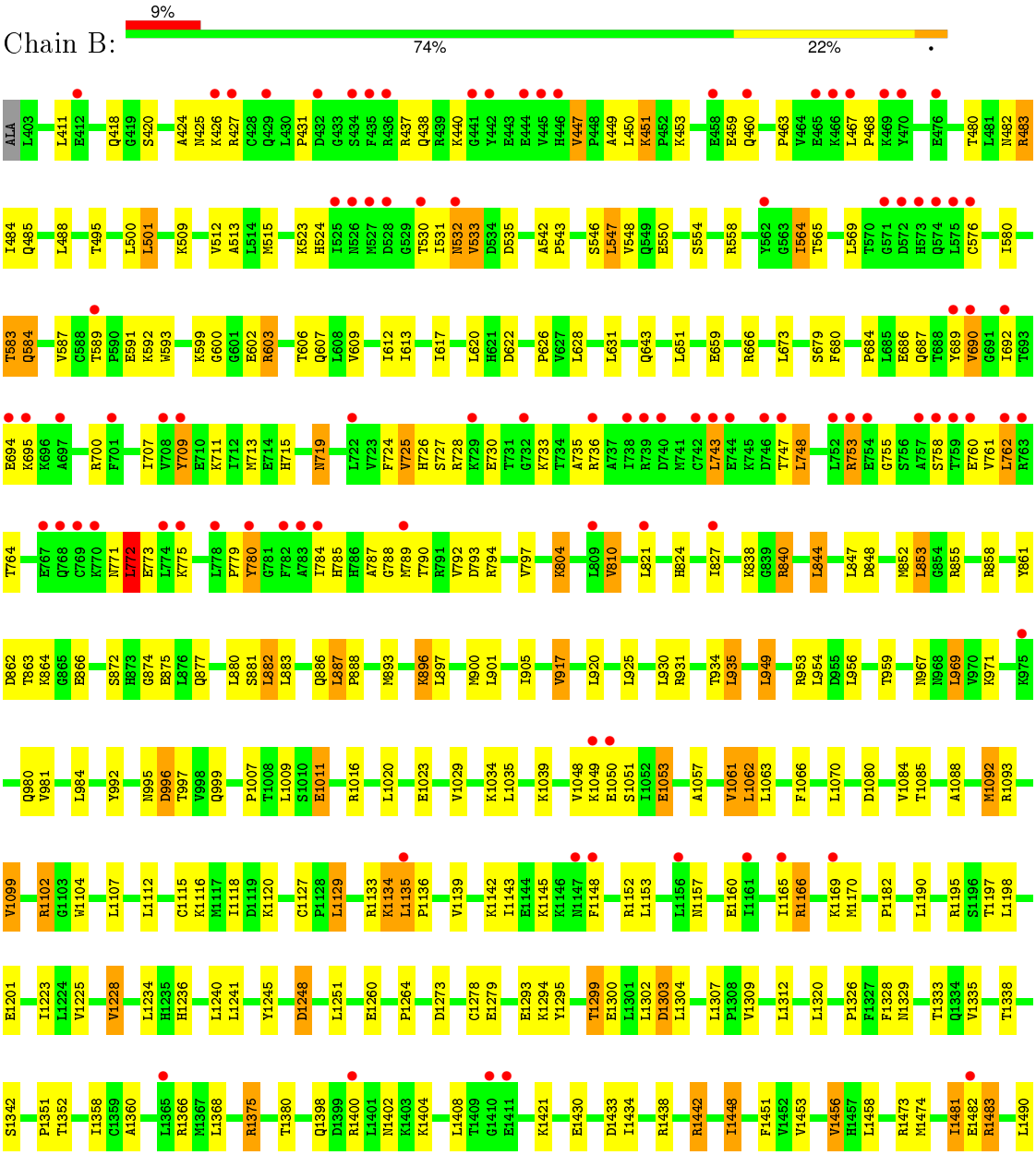
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	131	Total	O	0	0
			131	131		

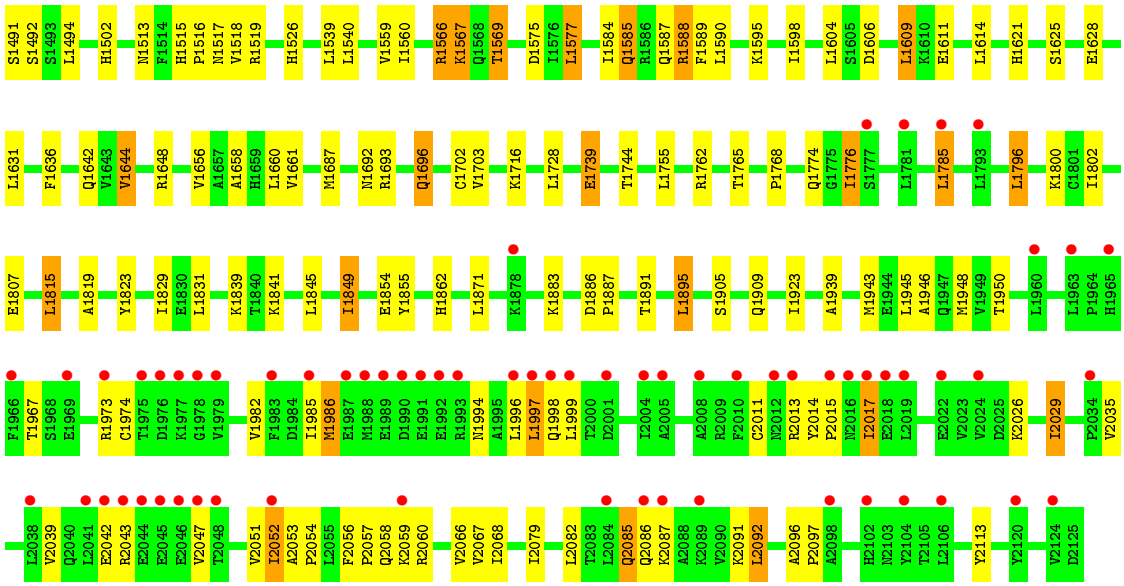
3 Residue-property plots (i)

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 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:




S1491 S1492 S1493 L1494 H1502 N1513 F1514 H1515 P1516 N1517 V1518 R1519 H1526 L1539 L1540 V1559 I1560 R1566 K1567 Q1568 T1569 D1575 I1576 L1577 I1584 Q1585 R1586 Q1587 R1588 F1589 L1590 K1595 I1598 L1604 S1605 D1606 L1609 K1610 E1611 L1614 H1621 S1625 E1628
L1631 F1636 Q1642 V1643 V1644 R1648 V1656 A1657 A1658 H1659 L1660 V1661 M1687 N1692 R1693 Q1696 C1702 V1703 K1716 L1728 E1739 T1744 L1755 R1762 T1765 P1768 Q1774 G1775 I1776 S1777 L1781 L1785 L1793 L1796 K1800 C1801 I1802
E1807 L1815 A1819 Y1823 I1829 E1830 L1831 K1839 T1840 K1841 L1845 I1849 E1854 Y1855 H1862 L1871 K1878 K1883 D1886 P1887 T1891 L1895 S1905 Q1909 I1923 A1939 M1943 E1944 L1945 A1946 Q1947 M1948 V1949 T1950 L1960 L1963 P1964 H1965
F1966 T1967 S1968 E1969 R1973 C1974 T1975 D1976 K1977 G1978 V1979 V1982 F1983 D1984 I1985 M1986 E1987 M1988 E1989 D1990 E1991 E1992 R1993 N1994 A1995 L1996 L1997 Q1998 L1999 T2000 D2001 I2004 A2005 A2008 R2009 F2010 C2011 N2012 R2013 Y2014 P2015 N2016 I2017 E2018 L2019 E2022 V2023 V2024 D2025 K2026 I2029 P2034 V2035
L2038 V2039 Q2040 L2041 E2042 R2043 E2044 E2045 E2046 V2047 T2048 V2051 I2052 A2053 P2054 L2055 F2056 P2057 Q2058 K2059 R2060 V2066 V2067 I2068 I2079 L2082 T2083 L2084 Q2085 Q2086 K2087 A2088 K2089 V2090 K2091 L2092 A2096 P2097 A2098 H2102 M2103 Y2104 T2105 L2106 Y2113 Y2120 V2124 D2125

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	146.15Å 149.54Å 141.32Å 90.00° 120.33° 90.00°	Depositor
Resolution (Å)	35.32 – 2.66 46.36 – 2.66	Depositor EDS
% Data completeness (in resolution range)	99.2 (35.32-2.66) 88.2 (46.36-2.66)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.66 (at 2.65Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.212 , 0.259 0.204 , 0.254	Depositor DCC
R_{free} test set	3747 reflections (5.97%)	DCC
Wilson B-factor (Å^2)	52.6	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.0	EDS
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
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.35$	Xtriage
Outliers	2 of 74395 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14019	wwPDB-VP
Average B, all atoms (Å^2)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.92% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: SAN

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	0.30	0/14161	0.51	1/19188 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	969	LEU	CA-CB-CG	5.48	127.91	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	13866	0	14008	210	0
2	B	22	0	16	0	0
3	B	131	0	0	8	0
All	All	14019	0	14024	210	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 8.

All (210) 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:1351:PRO:HG3	1:B:1516:PRO:HA	1.64	0.80
1:B:600:GLY:N	3:B:2315:HOH:O	2.17	0.72
1:B:1049:LYS:O	1:B:1051:SER:N	2.24	0.71
1:B:501:LEU:HD13	1:B:509:LYS:HG2	1.74	0.68
1:B:564:ILE:HG12	1:B:584:GLN:HG3	1.75	0.68
1:B:753:ARG:NH1	1:B:779:PRO:O	2.27	0.68
1:B:1051:SER:HB3	1:B:1057:ALA:HB2	1.76	0.67
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.76	0.67
1:B:997:THR:OG1	1:B:1023:GLU:OE1	2.12	0.65
1:B:771:ASN:HB3	1:B:772:LEU:HD13	1.79	0.64
1:B:447:VAL:HG13	1:B:687:GLN:HG3	1.81	0.62
1:B:1973:ARG:HB2	1:B:1997:LEU:HD11	1.82	0.62
1:B:626:PRO:HG2	1:B:896:LYS:HG3	1.80	0.61
1:B:1768:PRO:HG3	1:B:1776:ILE:HG22	1.82	0.61
1:B:882:LEU:HG	1:B:887:LEU:HD12	1.83	0.60
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	1.81	0.60
1:B:1604:LEU:HD21	1:B:1631:LEU:HD22	1.83	0.60
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.84	0.59
1:B:967:ASN:ND2	1:B:995:ASN:OD1	2.35	0.59
1:B:524:HIS:HB3	1:B:532:ASN:HB2	1.84	0.58
1:B:1456:VAL:HG23	1:B:1491:SER:HB2	1.85	0.58
1:B:758:SER:HB2	1:B:762:LEU:HB2	1.85	0.58
1:B:2068:ILE:HD11	1:B:2092:LEU:HD13	1.86	0.57
1:B:761:VAL:HA	1:B:764:THR:HG22	1.86	0.57
1:B:971:LYS:HB2	1:B:980:GLN:HB2	1.85	0.57
1:B:743:LEU:HA	1:B:747:THR:HA	1.87	0.57
1:B:715:HIS:HB3	1:B:719:ASN:HB3	1.86	0.57
1:B:949:LEU:O	1:B:953:ARG:HG3	2.05	0.56
1:B:690:VAL:HG21	1:B:707:ILE:HD13	1.87	0.56
1:B:1049:LYS:C	1:B:1051:SER:H	2.09	0.56
1:B:603:ARG:O	1:B:607:GLN:HB2	2.05	0.56
1:B:603:ARG:HB3	1:B:1540:LEU:HD13	1.88	0.56
1:B:1945:LEU:HA	1:B:1948:MET:HG2	1.87	0.56
1:B:736:ARG:HH21	1:B:773:GLU:HG2	1.71	0.55
1:B:1157:ASN:HB3	1:B:1160:GLU:OE1	2.07	0.55
1:B:512:VAL:HA	1:B:515:MET:HE2	1.89	0.54
1:B:787:ALA:O	1:B:789:MET:N	2.36	0.54
1:B:1228:VAL:HG11	1:B:1264:PRO:HD2	1.89	0.54
1:B:543:PRO:HD2	1:B:547:LEU:HD12	1.89	0.54
1:B:1329:ASN:O	1:B:1333:THR:HG23	2.07	0.54
1:B:858:ARG:HD2	1:B:861:TYR:HB2	1.90	0.53
1:B:617:ILE:HD12	1:B:628:LEU:HD13	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:692:ILE:HG13	1:B:872:SER:HA	1.90	0.53
1:B:1307:LEU:HB2	1:B:1333:THR:HB	1.90	0.53
1:B:1604:LEU:HD13	1:B:1609:LEU:HD13	1.91	0.53
1:B:606:THR:HA	1:B:609:VAL:HG23	1.91	0.53
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.91	0.53
1:B:1606:ASP:OD1	1:B:1609:LEU:N	2.41	0.53
1:B:725:VAL:HG11	1:B:730:GLU:HG2	1.91	0.53
1:B:1739:GLU:HG3	1:B:1744:THR:HB	1.90	0.53
1:B:1559:VAL:HG22	1:B:1660:LEU:HB3	1.90	0.53
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.91	0.52
1:B:1201:GLU:HB3	1:B:1251:LEU:HD11	1.92	0.52
1:B:1307:LEU:H	1:B:1333:THR:HG21	1.74	0.52
1:B:2059:LYS:HD2	1:B:2059:LYS:H	1.74	0.52
1:B:617:ILE:HG22	1:B:651:LEU:O	2.10	0.52
1:B:853:LEU:HD22	1:B:883:LEU:HD22	1.92	0.52
1:B:1909:GLN:HG3	3:B:2396:HOH:O	2.10	0.51
1:B:425:ASN:HB2	1:B:888:PRO:HD3	1.92	0.51
1:B:1093:ARG:NH1	1:B:1273:ASP:OD2	2.43	0.51
1:B:565:THR:HB	1:B:583:THR:HA	1.94	0.50
1:B:709:TYR:O	1:B:713:MET:HG2	2.10	0.50
1:B:692:ILE:HD11	1:B:700:ARG:NH1	2.27	0.50
1:B:1716:LYS:NZ	3:B:2382:HOH:O	2.30	0.50
1:B:896:LYS:O	1:B:900:MET:HG2	2.12	0.50
1:B:753:ARG:HD3	1:B:780:TYR:HA	1.94	0.49
1:B:735:ALA:HB2	1:B:810:VAL:HG11	1.94	0.49
1:B:684:PRO:HB2	1:B:864:LYS:HD2	1.94	0.49
1:B:1845:LEU:O	1:B:1849:ILE:HG22	2.13	0.49
1:B:1438:ARG:O	1:B:1442:ARG:HG2	2.13	0.49
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.95	0.49
1:B:1481:ILE:HD13	1:B:1483:ARG:HD2	1.94	0.49
1:B:1502[B]:HIS:CE1	1:B:1762:ARG:HE	2.31	0.49
1:B:1099:VAL:HG21	1:B:1107:LEU:HD23	1.95	0.49
1:B:758:SER:HA	1:B:761:VAL:HB	1.95	0.48
1:B:1566:ARG:O	1:B:1569:THR:HG22	2.13	0.48
1:B:709:TYR:HE1	1:B:748:LEU:HD22	1.78	0.48
1:B:692:ILE:HD13	1:B:700:ARG:HG3	1.95	0.48
1:B:1986:MET:SD	1:B:2011:CYS:HB3	2.53	0.48
1:B:1994:ASN:HB2	1:B:1999:LEU:HD13	1.95	0.48
1:B:1526:HIS:HB2	1:B:1703:VAL:HG22	1.95	0.48
1:B:1099:VAL:HG22	1:B:1104:TRP:HB2	1.94	0.48
1:B:1169:LYS:HD2	1:B:1169:LYS:H	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1519:ARG:NH2	1:B:1692:ASN:HB2	2.29	0.48
1:B:484:ILE:HD11	1:B:680:PHE:HB3	1.96	0.48
1:B:736:ARG:HH21	1:B:773:GLU:CG	2.27	0.47
1:B:709:TYR:CE1	1:B:748:LEU:HD22	2.49	0.47
1:B:1796:LEU:HB3	1:B:1802:ILE:HG12	1.94	0.47
1:B:930:LEU:HD23	1:B:949:LEU:HD22	1.95	0.47
1:B:793:ASP:O	1:B:797:VAL:HG23	2.14	0.47
1:B:542:ALA:O	1:B:589:THR:HA	2.14	0.47
1:B:509:LYS:NZ	3:B:2307:HOH:O	2.37	0.47
1:B:1007:PRO:HG3	1:B:1104:TRP:CE2	2.49	0.47
1:B:1430:GLU:CD	1:B:1430:GLU:H	2.18	0.47
1:B:1080:ASP:O	1:B:1084:VAL:HG13	2.15	0.47
1:B:1636:PHE:CE1	1:B:1644:VAL:HG22	2.49	0.47
1:B:1148:PHE:CZ	1:B:1152:ARG:HD2	2.50	0.47
1:B:1939:ALA:O	1:B:1943:MET:HG3	2.15	0.47
1:B:1112:LEU:HG	1:B:1116:LYS:HE2	1.96	0.47
1:B:877:GLN:HB2	1:B:880:LEU:HD12	1.97	0.47
1:B:2029:ILE:HG12	1:B:2035:VAL:HG22	1.96	0.47
1:B:694:GLU:HB3	3:B:2428:HOH:O	2.14	0.47
1:B:1245:TYR:O	1:B:1248:ASP:HB2	2.14	0.47
1:B:1011:GLU:OE2	3:B:2398:HOH:O	2.19	0.46
1:B:482:ASN:OD1	1:B:483:ARG:N	2.48	0.46
1:B:420:SER:HB2	1:B:622:ASP:HA	1.97	0.46
1:B:593:TRP:HD1	1:B:631:LEU:HD22	1.79	0.46
1:B:569:LEU:O	1:B:592:LYS:HG2	2.15	0.46
1:B:1839:LYS:O	1:B:1841:LYS:HE3	2.16	0.46
1:B:2039:VAL:HG21	1:B:2066:VAL:HG11	1.98	0.46
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.96	0.46
1:B:753:ARG:C	1:B:755:GLY:H	2.19	0.46
1:B:1328:PHE:HB2	1:B:1333:THR:HG22	1.97	0.46
1:B:1338:THR:O	1:B:1342:SER:HB2	2.15	0.46
1:B:1182:PRO:HB2	1:B:1278:CYS:SG	2.56	0.45
1:B:1102:ARG:NH1	3:B:2392:HOH:O	2.43	0.45
1:B:1585:GLN:O	1:B:1588:ARG:HB3	2.16	0.45
1:B:411:LEU:HD13	1:B:959:THR:HG21	1.98	0.45
1:B:424:ALA:HB1	1:B:935:LEU:HD11	1.97	0.45
1:B:1165:ILE:O	1:B:1166:ARG:HG3	2.17	0.45
1:B:1135:LEU:HD13	1:B:1136:PRO:HD2	1.98	0.45
1:B:449:ALA:H	1:B:686:GLU:HG2	1.81	0.45
1:B:450:LEU:H	1:B:450:LEU:HD22	1.82	0.45
1:B:687:GLN:HG3	1:B:689:TYR:HE1	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1062:LEU:HA	1:B:1062:LEU:HD12	1.73	0.44
1:B:1595:LYS:HA	1:B:1598:ILE:HD12	1.98	0.44
1:B:1190:LEU:HD11	1:B:1198:LEU:HD13	1.99	0.44
1:B:1302:LEU:O	1:B:1304:LEU:N	2.51	0.44
1:B:1887:PRO:O	1:B:1891:THR:HG23	2.18	0.44
1:B:996:ASP:N	1:B:996:ASP:OD1	2.50	0.44
1:B:463:PRO:HA	1:B:480:THR:HA	1.99	0.44
1:B:1375:ARG:HH11	1:B:1375:ARG:HB2	1.82	0.44
1:B:531:ILE:HD12	1:B:533:VAL:HG23	1.99	0.44
1:B:2067:VAL:HG22	1:B:2079:ILE:HG13	1.99	0.44
1:B:467:LEU:HB2	1:B:468:PRO:HD2	2.00	0.44
1:B:2017:ILE:HG23	1:B:2043:ARG:HB3	1.98	0.44
1:B:542:ALA:HB1	1:B:547:LEU:HD13	2.00	0.43
1:B:848:ASP:O	1:B:852:MET:HG2	2.18	0.43
1:B:719:ASN:HA	1:B:719:ASN:HD22	1.51	0.43
1:B:1048:VAL:HG12	1:B:1051:SER:HB2	2.00	0.43
1:B:1165:ILE:HD13	1:B:1165:ILE:HA	1.84	0.43
1:B:2042:GLU:HG3	1:B:2087:LYS:HB3	2.01	0.43
1:B:1195:ARG:NH1	1:B:1260:GLU:OE1	2.51	0.43
1:B:1299:THR:CG2	1:B:1513:ASN:H	2.31	0.43
1:B:532:ASN:HB3	1:B:535:ASP:OD2	2.19	0.43
1:B:753:ARG:HD2	1:B:761:VAL:HG22	2.00	0.43
1:B:1127:CYS:SG	1:B:1129:LEU:HB2	2.58	0.43
1:B:1442:ARG:H	1:B:1442:ARG:HG2	1.72	0.43
1:B:874:GLY:HA2	3:B:2323:HOH:O	2.18	0.43
1:B:785:HIS:CD2	1:B:794:ARG:HB2	2.54	0.43
1:B:1223:ILE:O	1:B:1236:HIS:HA	2.18	0.43
1:B:917:VAL:HG23	1:B:953:ARG:NH2	2.34	0.43
1:B:603:ARG:NH2	1:B:1575:ASP:OD1	2.52	0.43
1:B:425:ASN:HD21	1:B:886:GLN:HB3	1.83	0.43
1:B:2043:ARG:HD3	1:B:2085:GLN:O	2.19	0.43
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	2.01	0.43
1:B:2013:ARG:HD3	1:B:2052:ILE:HD13	2.01	0.43
1:B:727:SER:HB2	1:B:730:GLU:HB2	2.01	0.43
1:B:2096:ALA:HA	1:B:2097:PRO:HD3	1.85	0.43
1:B:1448:ILE:HD11	1:B:1451:PHE:HB2	2.00	0.43
1:B:580:ILE:HA	1:B:583:THR:HG23	2.01	0.43
1:B:548:VAL:HG13	1:B:587:VAL:HG12	2.00	0.42
1:B:426:LYS:HG2	1:B:427:ARG:HG3	2.00	0.42
1:B:1661:VAL:O	1:B:1702:CYS:HA	2.19	0.42
1:B:707:ILE:O	1:B:711:LYS:HD3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1589:PHE:HD2	1:B:1642:GLN:OE1	2.02	0.42
1:B:666:ARG:HD2	1:B:666:ARG:HA	1.89	0.42
1:B:1883:LYS:HD3	1:B:1883:LYS:HA	1.78	0.42
1:B:1515:HIS:ND1	1:B:1517:ASN:OD1	2.52	0.42
1:B:1997:LEU:HB3	1:B:1998:GLN:H	1.71	0.42
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.60	0.42
1:B:482:ASN:HB3	1:B:485:GLN:CD	2.40	0.42
1:B:724:PHE:CE2	1:B:852:MET:HB2	2.54	0.42
1:B:1398:GLN:O	1:B:1402:ASN:HA	2.20	0.42
1:B:1577:LEU:HA	1:B:1577:LEU:HD12	1.84	0.42
1:B:1950:THR:OG1	1:B:2060:ARG:NH2	2.38	0.42
1:B:1800:LYS:HB3	1:B:1815:LEU:HD23	2.00	0.42
1:B:1648:ARG:HB2	1:B:1687:MET:HE2	2.01	0.42
1:B:554:SER:O	1:B:558:ARG:HG2	2.20	0.42
1:B:1309:VAL:HG23	1:B:1326:PRO:O	2.20	0.42
1:B:1433:ASP:OD2	1:B:1473:ARG:NH2	2.53	0.41
1:B:1567:LYS:HE3	1:B:1567:LYS:HB3	1.81	0.41
1:B:726:HIS:CD2	1:B:844:LEU:HD13	2.56	0.41
1:B:1088:ALA:HB1	1:B:1118:ILE:HD13	2.02	0.41
1:B:1886:ASP:HA	1:B:1887:PRO:HD2	1.90	0.41
1:B:2014:TYR:HA	1:B:2015:PRO:HD3	1.85	0.41
1:B:821:LEU:HD12	1:B:821:LEU:O	2.19	0.41
1:B:1502[B]:HIS:CE1	1:B:1762:ARG:HH11	2.39	0.41
1:B:1923:ILE:HG21	1:B:1946:ALA:HB2	2.02	0.41
1:B:1092:MET:HB3	1:B:1115:CYS:SG	2.60	0.41
1:B:631:LEU:HA	1:B:631:LEU:HD23	1.76	0.41
1:B:838:LYS:O	1:B:840:ARG:HG2	2.20	0.41
1:B:824:HIS:ND1	1:B:862:ASP:OD2	2.50	0.41
1:B:1982:VAL:O	1:B:1985:ILE:HG13	2.20	0.41
1:B:1693:ARG:CZ	1:B:1696:GLN:HG3	2.51	0.41
1:B:1134:LYS:HD3	1:B:1134:LYS:HA	1.84	0.41
1:B:1895:LEU:HD12	1:B:1895:LEU:HA	1.89	0.41
1:B:531:ILE:O	1:B:533:VAL:N	2.52	0.40
1:B:2047:VAL:HG21	1:B:2085:GLN:HA	2.04	0.40
1:B:2051:VAL:HG13	1:B:2113:TYR:CZ	2.56	0.40
1:B:451:LYS:HG3	1:B:451:LYS:H	1.40	0.40
1:B:2056:PHE:HA	1:B:2057:PRO:HD3	1.84	0.40
1:B:1057:ALA:O	1:B:1061:VAL:HG13	2.22	0.40
1:B:1569:THR:HG21	1:B:1621:HIS:HB3	2.02	0.40
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.57	0.40
1:B:1755:LEU:HD13	1:B:1785:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1456:VAL:CG2	1:B:1491:SER:HB2	2.49	0.40
1:B:1307:LEU:H	1:B:1333:THR:CG2	2.35	0.40
1:B:1136:PRO:HB2	1:B:1139:VAL:HG23	2.03	0.40
1:B:2053:ALA:HA	1:B:2054:PRO:HD2	1.90	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	1722/1724 (100%)	1632 (95%)	79 (5%)	11 (1%)	30 54

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1050	GLU
1	B	1584	ILE
1	B	788	GLY
1	B	431	PRO
1	B	772	LEU
1	B	804	LYS
1	B	875	GLU
1	B	530	THR
1	B	532	ASN
1	B	1053	GLU
1	B	1303	ASP

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	1543/1542 (100%)	1349 (87%)	194 (13%)	5 11

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	GLN
1	B	437	ARG
1	B	438	GLN
1	B	440	LYS
1	B	447	VAL
1	B	451	LYS
1	B	453	LYS
1	B	459	GLU
1	B	460	GLN
1	B	483	ARG
1	B	488	LEU
1	B	495	THR
1	B	500	LEU
1	B	501	LEU
1	B	523	LYS
1	B	533	VAL
1	B	546	SER
1	B	547	LEU
1	B	550	GLU
1	B	564	ILE
1	B	576	CYS
1	B	583	THR
1	B	584	GLN
1	B	591	GLU
1	B	599	LYS
1	B	602	GLU
1	B	603	ARG
1	B	612	ILE
1	B	620	LEU
1	B	643	GLN
1	B	659	GLU
1	B	673	LEU
1	B	679	SER
1	B	690	VAL

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Mol	Chain	Res	Type
1	B	695	LYS
1	B	709	TYR
1	B	719	ASN
1	B	725	VAL
1	B	728	ARG
1	B	733	LYS
1	B	743	LEU
1	B	748	LEU
1	B	753	ARG
1	B	760	GLU
1	B	762	LEU
1	B	772	LEU
1	B	775	LYS
1	B	780	TYR
1	B	784	ILE
1	B	790	THR
1	B	792	VAL
1	B	804	LYS
1	B	810	VAL
1	B	827	ILE
1	B	840	ARG
1	B	844	LEU
1	B	847	LEU
1	B	853	LEU
1	B	855	ARG
1	B	863	THR
1	B	866	GLU
1	B	881	SER
1	B	882	LEU
1	B	887	LEU
1	B	893	MET
1	B	896	LYS
1	B	897	LEU
1	B	901	LEU
1	B	917	VAL
1	B	920	LEU
1	B	925	LEU
1	B	931	ARG
1	B	934	THR
1	B	935	LEU
1	B	949	LEU
1	B	954	LEU

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Mol	Chain	Res	Type
1	B	956	LEU
1	B	969	LEU
1	B	984	LEU
1	B	992	TYR
1	B	996	ASP
1	B	999	GLN
1	B	1009	LEU
1	B	1011	GLU
1	B	1016	ARG
1	B	1020	LEU
1	B	1029	VAL
1	B	1034	LYS
1	B	1035	LEU
1	B	1039	LYS
1	B	1053	GLU
1	B	1061	VAL
1	B	1062	LEU
1	B	1063	LEU
1	B	1070	LEU
1	B	1092	MET
1	B	1099	VAL
1	B	1102	ARG
1	B	1120	LYS
1	B	1129	LEU
1	B	1133	ARG
1	B	1134	LYS
1	B	1135	LEU
1	B	1142	LYS
1	B	1143	ILE
1	B	1145	LYS
1	B	1153	LEU
1	B	1166	ARG
1	B	1170	MET
1	B	1197	THR
1	B	1225	VAL
1	B	1228	VAL
1	B	1234	LEU
1	B	1240	LEU
1	B	1241	LEU
1	B	1248	ASP
1	B	1279	GLU
1	B	1293	GLU

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Mol	Chain	Res	Type
1	B	1294	LYS
1	B	1295	TYR
1	B	1299	THR
1	B	1300	GLU
1	B	1303	ASP
1	B	1312	LEU
1	B	1320	LEU
1	B	1335	VAL
1	B	1352	THR
1	B	1358	ILE
1	B	1366	ARG
1	B	1368	LEU
1	B	1375	ARG
1	B	1380	THR
1	B	1400	ARG
1	B	1404	LYS
1	B	1408	LEU
1	B	1421	LYS
1	B	1442	ARG
1	B	1448	ILE
1	B	1453	VAL
1	B	1456	VAL
1	B	1458	LEU
1	B	1474	MET
1	B	1481	ILE
1	B	1482	GLU
1	B	1483	ARG
1	B	1492	SER
1	B	1494	LEU
1	B	1518	VAL
1	B	1539	LEU
1	B	1566	ARG
1	B	1567	LYS
1	B	1569	THR
1	B	1577	LEU
1	B	1585	GLN
1	B	1587	GLN
1	B	1588	ARG
1	B	1590	LEU
1	B	1609	LEU
1	B	1611	GLU
1	B	1614	LEU

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Mol	Chain	Res	Type
1	B	1644	VAL
1	B	1656	VAL
1	B	1696	GLN
1	B	1728	LEU
1	B	1739	GLU
1	B	1765	THR
1	B	1774	GLN
1	B	1776	ILE
1	B	1785	LEU
1	B	1796	LEU
1	B	1807	GLU
1	B	1815	LEU
1	B	1831	LEU
1	B	1849	ILE
1	B	1854	GLU
1	B	1862	HIS
1	B	1871	LEU
1	B	1895	LEU
1	B	1905	SER
1	B	1967	THR
1	B	1974	CYS
1	B	1986	MET
1	B	1996	LEU
1	B	1997	LEU
1	B	2017	ILE
1	B	2026	LYS
1	B	2029	ILE
1	B	2052	ILE
1	B	2058	GLN
1	B	2082	LEU
1	B	2085	GLN
1	B	2086	GLN
1	B	2091	LYS
1	B	2092	LEU

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

Mol	Chain	Res	Type
1	B	425	ASN
1	B	719	ASN
1	B	990	HIS

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

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	SAN	B	2201[A]	-	11,11,11	3.14	1 (9%)	16,16,16	2.29	3 (18%)
2	SAN	B	2201[B]	-	11,11,11	3.39	1 (9%)	16,16,16	2.20	3 (18%)

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	SAN	B	2201[A]	-	-	0/6/6/6	0/1/1/1
2	SAN	B	2201[B]	-	-	0/6/6/6	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2201[B]	SAN	C4-S	-11.19	1.60	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2201[A]	SAN	C4-S	-10.34	1.61	1.77

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	2201[A]	SAN	O2-S-O1	-7.57	108.16	118.80
2	B	2201[B]	SAN	O2-S-O1	-7.33	108.50	118.80
2	B	2201[A]	SAN	O2-S-C4	2.49	110.46	107.39
2	B	2201[B]	SAN	O1-S-N2	2.74	110.82	107.28
2	B	2201[A]	SAN	O1-S-C4	2.74	110.77	107.39
2	B	2201[B]	SAN	O2-S-C4	2.87	110.94	107.39

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.

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	1723/1724 (99%)	0.44	160 (9%)	11	8	38, 83, 156, 206	0

All (160) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	1993	ARG	6.5
1	B	2047	VAL	6.2
1	B	746	ASP	6.1
1	B	571	GLY	5.9
1	B	1977	LYS	5.8
1	B	2124	VAL	5.8
1	B	527	MET	5.5
1	B	575	LEU	5.5
1	B	572	ASP	5.3
1	B	1985	ILE	5.2
1	B	763	ARG	5.1
1	B	742	CYS	5.1
1	B	743	LEU	5.1
1	B	2043	ARG	5.0
1	B	2016	ASN	4.9
1	B	573	HIS	4.9
1	B	1999	LEU	4.8
1	B	2004	ILE	4.7
1	B	1973	ARG	4.7
1	B	1979	VAL	4.7
1	B	528	ASP	4.5
1	B	709	TYR	4.5
1	B	770	LYS	4.5
1	B	530	THR	4.4
1	B	774	LEU	4.4
1	B	2038	LEU	4.4
1	B	1966	PHE	4.4

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Mol	Chain	Res	Type	RSRZ
1	B	1991	GLU	4.3
1	B	695	LYS	4.3
1	B	435	PHE	4.2
1	B	1996	LEU	4.2
1	B	784	ILE	4.1
1	B	747	THR	4.1
1	B	574	GLN	4.0
1	B	738	ILE	3.9
1	B	470	TYR	3.9
1	B	768	GLN	3.9
1	B	758	SER	3.8
1	B	1988	MET	3.8
1	B	2086	GLN	3.7
1	B	1989	GLU	3.7
1	B	2001	ASP	3.7
1	B	1987	GLU	3.7
1	B	1050	GLU	3.7
1	B	2084	LEU	3.6
1	B	526	ASN	3.6
1	B	427	ARG	3.6
1	B	436	ARG	3.6
1	B	1963	LEU	3.6
1	B	759	THR	3.6
1	B	434	SER	3.5
1	B	469	LYS	3.5
1	B	783	ALA	3.4
1	B	2046	GLU	3.4
1	B	2010	PHE	3.3
1	B	426	LYS	3.3
1	B	2044	GLU	3.3
1	B	1976	ASP	3.3
1	B	767	GLU	3.3
1	B	446	HIS	3.2
1	B	441	GLY	3.2
1	B	2048	THR	3.2
1	B	2019	LEU	3.2
1	B	2120	TYR	3.2
1	B	1997	LEU	3.2
1	B	690	VAL	3.1
1	B	1960	LEU	3.1
1	B	789	MET	3.1
1	B	1990	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	780	TYR	3.1
1	B	692	ILE	3.1
1	B	1793	LEU	3.1
1	B	2042	GLU	3.1
1	B	1400	ARG	3.0
1	B	1135	LEU	3.0
1	B	1998	GLN	3.0
1	B	2022	GLU	3.0
1	B	1992	GLU	3.0
1	B	740	ASP	3.0
1	B	2041	LEU	2.9
1	B	1147	ASN	2.9
1	B	2087	LYS	2.9
1	B	2089	LYS	2.9
1	B	429	GLN	2.9
1	B	762	LEU	2.9
1	B	778	LEU	2.9
1	B	2024	VAL	2.9
1	B	694	GLU	2.9
1	B	445	VAL	2.8
1	B	432	ASP	2.8
1	B	467	LEU	2.8
1	B	525	ILE	2.8
1	B	757	ALA	2.8
1	B	532	ASN	2.8
1	B	2018	GLU	2.8
1	B	2013	ARG	2.8
1	B	576	CYS	2.8
1	B	744	GLU	2.7
1	B	821	LEU	2.7
1	B	2106	LEU	2.7
1	B	1165	ILE	2.7
1	B	1777	SER	2.7
1	B	1969	GLU	2.6
1	B	722	LEU	2.6
1	B	1983	PHE	2.6
1	B	1410	GLY	2.6
1	B	1978	GLY	2.6
1	B	775	LYS	2.6
1	B	739	ARG	2.6
1	B	782	PHE	2.6
1	B	2005	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	2015	PRO	2.6
1	B	458	GLU	2.5
1	B	2012	ASN	2.5
1	B	2098	ALA	2.5
1	B	1169	LYS	2.5
1	B	476	GLU	2.5
1	B	760	GLU	2.5
1	B	466	LYS	2.5
1	B	753	ARG	2.5
1	B	589	THR	2.5
1	B	1482	GLU	2.4
1	B	2045	GLU	2.4
1	B	689	TYR	2.4
1	B	2017	ILE	2.4
1	B	2052	ILE	2.4
1	B	975	LYS	2.4
1	B	1965	HIS	2.4
1	B	1975	THR	2.4
1	B	708	VAL	2.3
1	B	701	PHE	2.3
1	B	754	GLU	2.3
1	B	1156	LEU	2.3
1	B	729	LYS	2.3
1	B	1411	GLU	2.3
1	B	1148	PHE	2.3
1	B	809	LEU	2.2
1	B	2102	HIS	2.2
1	B	827	ILE	2.2
1	B	1878	LYS	2.2
1	B	697	ALA	2.2
1	B	732	GLY	2.2
1	B	442	TYR	2.1
1	B	2104	TYR	2.1
1	B	2034	PRO	2.1
1	B	2059	LYS	2.1
1	B	752	LEU	2.1
1	B	460	GLN	2.1
1	B	736	ARG	2.1
1	B	562	TYR	2.1
1	B	1049	LYS	2.1
1	B	444	GLU	2.0
1	B	769	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1365	LEU	2.0
1	B	412	GLU	2.0
1	B	465	GLU	2.0
1	B	1161	ILE	2.0
1	B	2008	ALA	2.0
1	B	1781	LEU	2.0
1	B	1785	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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	LLDF	B-factors(Å^2)	Q<0.9
2	SAN	B	2201[A]	11/11	0.98	0.22	2.53	28,37,50,52	11
2	SAN	B	2201[B]	11/11	0.98	0.22	2.31	18,25,49,54	11

6.5 Other polymers

There are no such residues in this entry.