



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:49 am BST

PDB ID : 4F91
Title : Brr2 Helicase Region
Authors : Santos, K.F.; Jovin, S.M.; Weber, G.; Pena, V.; Luehrmann, R.; Wahl, M.C.
Deposited on : 2012-05-18
Resolution : 2.70 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 ⓘ](#)) 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

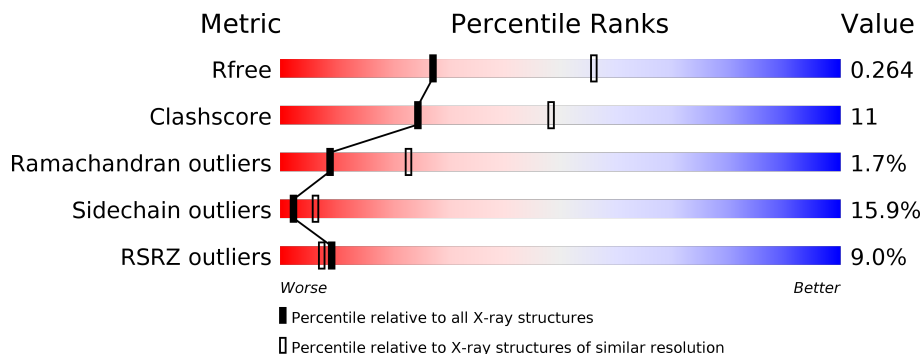
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	1724	 9% 65% 28% 7%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13865 atoms, of which 0 are hydrogens and 0 are deuteriums.

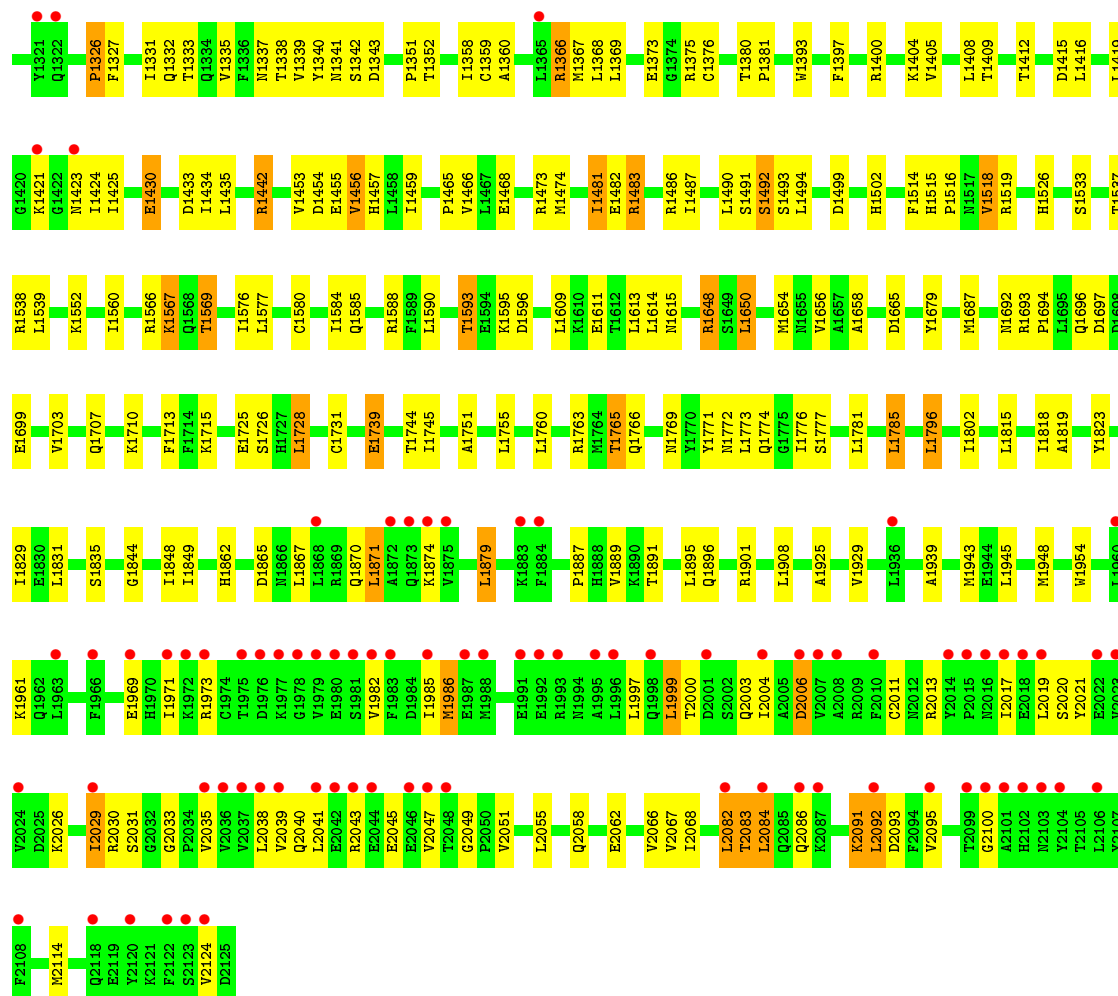
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

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

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

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	6	Total	O	0	0
			6	6		



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	146.26Å 150.50Å 141.96Å 90.00° 120.21° 90.00°	Depositor
Resolution (Å)	48.39 – 2.70 48.39 – 2.70	Depositor EDS
% Data completeness (in resolution range)	97.3 (48.39-2.70) 98.3 (48.39-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 2.69Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7.3_928)	Depositor
R, R_{free}	0.224 , 0.272 0.213 , 0.264	Depositor DCC
R_{free} test set	3656 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	65.0	Xtriage
Anisotropy	0.542	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	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 0.007 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	13865	wwPDB-VP
Average B, all atoms (Å ²)	100.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.60% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

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	0.44	0/14153	0.65	4/19177 (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 (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1773	LEU	CA-CB-CG	6.03	129.18	115.30
1	B	969	LEU	CA-CB-CG	5.40	127.71	115.30
1	B	441	GLY	N-CA-C	-5.24	100.01	113.10
1	B	1312	LEU	CA-CB-CG	5.17	127.19	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	440	LYS	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	13859	0	14001	303	0
2	B	6	0	0	0	0
All	All	13865	0	14001	303	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 11.

All (303) 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:1049:LYS:O	1:B:1051:SER:N	2.09	0.85
1:B:700:ARG:HA	1:B:703:ILE:HD12	1.57	0.85
1:B:753:ARG:NH1	1:B:779:PRO:O	2.12	0.81
1:B:2013:ARG:HE	1:B:2049:GLY:HA3	1.49	0.78
1:B:569:LEU:HD11	1:B:575:LEU:HD11	1.67	0.76
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.68	0.76
1:B:660:ASP:OD1	1:B:928:ARG:NH1	2.19	0.76
1:B:2043:ARG:HH11	1:B:2084:LEU:HD21	1.49	0.76
1:B:770:LYS:HD3	1:B:793:ASP:HB3	1.66	0.76
1:B:715:HIS:ND1	1:B:719:ASN:OD1	2.20	0.75
1:B:626:PRO:HG2	1:B:896:LYS:HG3	1.71	0.72
1:B:474:GLY:O	1:B:558:ARG:NH2	2.24	0.71
1:B:948:LEU:O	1:B:953:ARG:NH1	2.24	0.71
1:B:2068:ILE:HD11	1:B:2092:LEU:HD13	1.74	0.69
1:B:997:THR:OG1	1:B:1023:GLU:OE1	2.06	0.69
1:B:1901:ARG:HH12	1:B:1961:LYS:HE3	1.58	0.69
1:B:2066:VAL:HG23	1:B:2082:LEU:HD21	1.73	0.69
1:B:1765:THR:HG23	1:B:1781:LEU:HD13	1.73	0.69
1:B:701:PHE:O	1:B:705:ASN:ND2	2.25	0.69
1:B:1459:ILE:HD11	1:B:1468:GLU:HG3	1.75	0.69
1:B:735:ALA:HB2	1:B:810:VAL:HG11	1.74	0.69
1:B:1360:ALA:HB2	1:B:1490:LEU:HD11	1.75	0.68
1:B:720:GLN:NE2	1:B:801:PHE:O	2.27	0.68
1:B:1519:ARG:HH22	1:B:1692:ASN:HB2	1.60	0.67
1:B:438:GLN:HB3	1:B:440:LYS:HG2	1.77	0.67
1:B:566:VAL:HB	1:B:585:ILE:HB	1.76	0.67
1:B:759:THR:OG1	1:B:760:GLU:N	2.28	0.66
1:B:1201:GLU:HB3	1:B:1251:LEU:HD11	1.78	0.66
1:B:785:HIS:HB3	1:B:811:SER:HB2	1.76	0.66
1:B:727:SER:HB3	1:B:729:LYS:CG	2.26	0.65
1:B:777:LEU:HA	1:B:780:TYR:HE1	1.62	0.65
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:738:ILE:HD11	1:B:782:PHE:CZ	2.32	0.64
1:B:1815:LEU:HB3	1:B:1829:ILE:HD13	1.79	0.64
1:B:1456:VAL:HG23	1:B:1491:SER:HB2	1.78	0.64
1:B:703:ILE:O	1:B:707:ILE:HG12	1.98	0.64
1:B:1519:ARG:NH2	1:B:1692:ASN:HB2	2.13	0.63
1:B:2029:ILE:HD11	1:B:2035:VAL:HA	1.81	0.63
1:B:1249:GLU:CD	1:B:1249:GLU:H	2.02	0.62
1:B:969:LEU:HD13	1:B:985:GLY:HA2	1.81	0.62
1:B:763:ARG:HD2	1:B:805:HIS:CE1	2.34	0.62
1:B:882:LEU:HG	1:B:887:LEU:HD12	1.82	0.62
1:B:1093:ARG:NH1	1:B:1273:ASP:OD2	2.32	0.61
1:B:1228:VAL:HG11	1:B:1264:PRO:HD2	1.81	0.61
1:B:550:GLU:HB2	1:B:818:GLY:O	2.01	0.61
1:B:1262:LEU:HD22	1:B:1263:PRO:HD2	1.83	0.60
1:B:793:ASP:N	1:B:793:ASP:OD1	2.33	0.60
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.82	0.60
1:B:577:LYS:HB2	1:B:579:GLU:HG2	1.84	0.60
1:B:694:GLU:CD	1:B:695:LYS:H	2.05	0.60
1:B:781:GLY:O	1:B:807:GLN:N	2.33	0.60
1:B:708:VAL:O	1:B:712:ILE:HG12	2.01	0.60
1:B:1901:ARG:NH2	1:B:1961:LYS:O	2.36	0.59
1:B:761:VAL:O	1:B:765:GLU:N	2.31	0.59
1:B:735:ALA:HB1	1:B:782:PHE:HE1	1.68	0.58
1:B:1210:TRP:HZ3	1:B:1241:LEU:HD13	1.69	0.58
1:B:824:HIS:HD2	1:B:825:THR:HG22	1.68	0.58
1:B:1405:VAL:HG22	1:B:1424:ILE:HB	1.84	0.58
1:B:743:LEU:HA	1:B:747:THR:HA	1.85	0.58
1:B:768:GLN:HA	1:B:778:LEU:HD12	1.84	0.58
1:B:2043:ARG:NH1	1:B:2084:LEU:HD21	2.19	0.57
1:B:871:THR:OG1	1:B:872:SER:N	2.35	0.57
1:B:1538:ARG:NH1	1:B:1665:ASP:OD2	2.38	0.57
1:B:738:ILE:HD11	1:B:782:PHE:HZ	1.69	0.57
1:B:763:ARG:HD2	1:B:805:HIS:NE2	2.20	0.56
1:B:1301:LEU:HD22	1:B:1518:VAL:HG22	1.88	0.56
1:B:1887:PRO:O	1:B:1891:THR:HG23	2.05	0.56
1:B:1188:VAL:HG12	1:B:1282:LEU:HD21	1.87	0.56
1:B:2051:VAL:HG22	1:B:2062:GLU:HG3	1.88	0.56
1:B:752:LEU:HD22	1:B:807:GLN:HB3	1.88	0.56
1:B:993:ILE:HD11	1:B:998:VAL:HG22	1.88	0.56
1:B:688:THR:HB	1:B:868:ILE:HG23	1.88	0.56
1:B:2091:LYS:HD2	1:B:2091:LYS:H	1.71	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:543:PRO:O	1:B:624:ARG:NH2	2.21	0.55
1:B:785:HIS:CE1	1:B:794:ARG:HG3	2.42	0.55
1:B:1193:ILE:HB	1:B:1197:THR:HG23	1.88	0.55
1:B:577:LYS:HG3	1:B:580:ILE:HD13	1.88	0.54
1:B:707:ILE:HA	1:B:710:GLU:OE1	2.08	0.54
1:B:736:ARG:HA	1:B:739:ARG:HB3	1.89	0.54
1:B:1269:ARG:HD2	1:B:1279:GLU:OE2	2.08	0.54
1:B:864:LYS:HG3	1:B:865:GLY:H	1.72	0.54
1:B:1430:GLU:H	1:B:1430:GLU:CD	2.10	0.54
1:B:548:VAL:HG13	1:B:587:VAL:HG12	1.88	0.54
1:B:482:ASN:HB3	1:B:485:GLN:CD	2.28	0.53
1:B:1896:GLN:HB3	1:B:1954:TRP:HZ2	1.72	0.53
1:B:569:LEU:O	1:B:573:HIS:NE2	2.41	0.53
1:B:509:LYS:HE2	1:B:652:SER:O	2.07	0.53
1:B:781:GLY:HA3	1:B:807:GLN:HB2	1.89	0.53
1:B:1739:GLU:HG3	1:B:1744:THR:HB	1.91	0.53
1:B:1533:SER:HA	1:B:1707:GLN:NE2	2.23	0.53
1:B:402:ALA:O	1:B:406:ARG:NH2	2.41	0.53
1:B:2020:SER:HB3	1:B:2040:GLN:HB2	1.92	0.53
1:B:493:LEU:O	1:B:519:ARG:NH2	2.37	0.53
1:B:1456:VAL:CG2	1:B:1491:SER:HB2	2.39	0.52
1:B:727:SER:HB3	1:B:729:LYS:HG3	1.89	0.52
1:B:734:THR:OG1	1:B:829:LYS:NZ	2.36	0.52
1:B:2000:THR:HG23	1:B:2003:GLN:H	1.73	0.52
1:B:1526:HIS:HB2	1:B:1703:VAL:HG22	1.90	0.52
1:B:777:LEU:HA	1:B:780:TYR:CE1	2.44	0.52
1:B:1312:LEU:HD12	1:B:1340:TYR:CZ	2.45	0.52
1:B:1560:ILE:HG13	1:B:1658:ALA:HB2	1.92	0.52
1:B:840:ARG:NH2	1:B:842:THR:HG22	2.23	0.52
1:B:1157:ASN:HB3	1:B:1160:GLU:OE1	2.10	0.52
1:B:1728:LEU:HB3	1:B:1760:LEU:HD22	1.92	0.52
1:B:1925:ALA:O	1:B:1929:VAL:HG23	2.10	0.52
1:B:1796:LEU:HB3	1:B:1802:ILE:HG12	1.91	0.51
1:B:439:ARG:HB2	1:B:442:TYR:CZ	2.45	0.51
1:B:467:LEU:HB2	1:B:468:PRO:HD2	1.93	0.51
1:B:1057:ALA:O	1:B:1061:VAL:HG13	2.11	0.51
1:B:1650:LEU:O	1:B:1654:MET:HG3	2.10	0.51
1:B:1648:ARG:HD3	1:B:1679:TYR:CE1	2.46	0.51
1:B:796:LEU:HA	1:B:799:ASP:OD1	2.11	0.50
1:B:1945:LEU:HA	1:B:1948:MET:HG2	1.93	0.50
1:B:1066:PHE:CG	1:B:1085:THR:HG21	2.46	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:594:ASP:O	1:B:598:ARG:HG3	2.12	0.50
1:B:712:ILE:CD1	1:B:721:VAL:HG11	2.41	0.50
1:B:853:LEU:HD22	1:B:883:LEU:HD22	1.94	0.50
1:B:453:LYS:HB3	1:B:483:ARG:HH12	1.77	0.50
1:B:725:VAL:HG11	1:B:730:GLU:HG2	1.94	0.50
1:B:542:ALA:HB1	1:B:547:LEU:HD13	1.94	0.49
1:B:578:GLU:O	1:B:581:SER:HB3	2.12	0.49
1:B:1982:VAL:O	1:B:1986:MET:HG2	2.12	0.49
1:B:552:VAL:HG13	1:B:566:VAL:HG22	1.94	0.49
1:B:1035:LEU:O	1:B:1039:LYS:HG2	2.11	0.49
1:B:1338:THR:O	1:B:1342:SER:HB2	2.12	0.49
1:B:516:CYS:SG	1:B:649:ILE:HG12	2.52	0.49
1:B:768:GLN:O	1:B:770:LYS:N	2.43	0.49
1:B:1939:ALA:O	1:B:1943:MET:HG3	2.13	0.49
1:B:538:ILE:HB	1:B:585:ILE:HG13	1.95	0.49
1:B:690:VAL:HG13	1:B:870:ILE:HA	1.94	0.49
1:B:729:LYS:HB3	1:B:1075:PHE:CE1	2.47	0.49
1:B:853:LEU:HD12	1:B:853:LEU:N	2.28	0.48
1:B:1271:VAL:HG13	1:B:1279:GLU:HB2	1.96	0.48
1:B:723:VAL:HG22	1:B:827:ILE:HG23	1.95	0.48
1:B:1184:LEU:HD12	1:B:1270:VAL:HG11	1.96	0.48
1:B:1335:VAL:HG11	1:B:1359:CYS:SG	2.53	0.48
1:B:531:ILE:HG12	1:B:562:TYR:O	2.13	0.48
1:B:603:ARG:O	1:B:607:GLN:HB2	2.13	0.48
1:B:484:ILE:HD11	1:B:680:PHE:HB3	1.94	0.48
1:B:876:LEU:HD22	1:B:879:TYR:CE1	2.48	0.48
1:B:760:GLU:O	1:B:764:THR:HB	2.13	0.48
1:B:1165:ILE:HG23	1:B:1167:MET:H	1.79	0.48
1:B:2006:ASP:OD1	1:B:2006:ASP:N	2.45	0.48
1:B:635:ALA:O	1:B:639:ILE:HD12	2.14	0.48
1:B:824:HIS:CD2	1:B:825:THR:HG22	2.48	0.48
1:B:941:ASP:N	1:B:941:ASP:OD1	2.32	0.48
1:B:1982:VAL:O	1:B:1985:ILE:HG13	2.13	0.48
1:B:1029:VAL:HG11	1:B:1053:GLU:O	2.14	0.48
1:B:1879:LEU:HD23	1:B:1889:VAL:HG13	1.97	0.47
1:B:626:PRO:HD3	1:B:892:GLN:HB2	1.96	0.47
1:B:794:ARG:HA	1:B:794:ARG:NE	2.29	0.47
1:B:1772:ASN:O	1:B:1774:GLN:NE2	2.46	0.47
1:B:1999:LEU:HB2	1:B:2004:ILE:HD11	1.96	0.47
1:B:967:ASN:HA	1:B:999:GLN:HG2	1.97	0.47
1:B:853:LEU:H	1:B:853:LEU:HD12	1.78	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:524:HIS:HB3	1:B:532:ASN:HB2	1.95	0.47
1:B:591:GLU:HG2	1:B:591:GLU:H	1.44	0.47
1:B:930:LEU:HD23	1:B:949:LEU:HD22	1.96	0.47
1:B:712:ILE:HD12	1:B:721:VAL:HG11	1.97	0.47
1:B:917:VAL:HG13	1:B:953:ARG:HB2	1.95	0.47
1:B:579:GLU:O	1:B:583:THR:HG23	2.14	0.47
1:B:1340:TYR:O	1:B:1366:ARG:HG3	2.15	0.47
1:B:1481:ILE:O	1:B:1483:ARG:HD2	2.15	0.47
1:B:1577:LEU:HD11	1:B:1615:ASN:HB3	1.96	0.47
1:B:726:HIS:HB3	1:B:833:VAL:HG23	1.96	0.47
1:B:654:THR:HG21	1:B:676:PHE:O	2.14	0.46
1:B:1099:VAL:HG21	1:B:1107:LEU:HG	1.97	0.46
1:B:758:SER:O	1:B:762:LEU:HB2	2.16	0.46
1:B:1140:VAL:HA	1:B:1143:ILE:HG23	1.98	0.46
1:B:1986:MET:SD	1:B:2011:CYS:HB3	2.56	0.46
1:B:727:SER:HB3	1:B:729:LYS:HG2	1.97	0.46
1:B:1961:LYS:HG2	1:B:1971:ILE:HD11	1.98	0.46
1:B:1973:ARG:HB2	1:B:1997:LEU:HD11	1.97	0.46
1:B:707:ILE:O	1:B:711:LYS:HD3	2.15	0.46
1:B:1165:ILE:HG23	1:B:1167:MET:N	2.31	0.46
1:B:1416:LEU:HD21	1:B:1442:ARG:HD2	1.96	0.46
1:B:1710:LYS:O	1:B:1713:PHE:HB3	2.16	0.46
1:B:1870:GLN:O	1:B:1874:LYS:HD3	2.16	0.46
1:B:542:ALA:O	1:B:589:THR:HA	2.16	0.46
1:B:858:ARG:H	1:B:862:ASP:HB2	1.81	0.46
1:B:1337:ASN:O	1:B:1341:ASN:HB2	2.16	0.46
1:B:1419:LEU:HD22	1:B:1435:LEU:HD13	1.97	0.46
1:B:1648:ARG:HH21	1:B:1648:ARG:HG2	1.80	0.46
1:B:1308:PRO:HA	1:B:1327:PHE:HD1	1.80	0.45
1:B:599:LYS:HA	1:B:599:LYS:HD2	1.64	0.45
1:B:601:GLY:HA3	1:B:1537:THR:HG23	1.97	0.45
1:B:481:LEU:HD22	1:B:485:GLN:HB3	1.98	0.45
1:B:869:LEU:HG	1:B:871:THR:HG22	1.98	0.45
1:B:1116:LYS:O	1:B:1120:LYS:HB2	2.16	0.45
1:B:1343:ASP:OD2	1:B:1366:ARG:NE	2.50	0.45
1:B:753:ARG:C	1:B:755:GLY:H	2.20	0.45
1:B:726:HIS:CE1	1:B:831:THR:HA	2.52	0.45
1:B:1225:VAL:HG13	1:B:1235:HIS:HB3	1.98	0.45
1:B:1307:LEU:H	1:B:1333:THR:HG21	1.82	0.45
1:B:1552:LYS:HE3	1:B:1552:LYS:HB2	1.66	0.45
1:B:1576:ILE:O	1:B:1580:CYS:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:743:LEU:HD21	1:B:750:LEU:HD13	1.99	0.45
1:B:848:ASP:O	1:B:852:MET:HG3	2.16	0.45
1:B:777:LEU:HB3	1:B:782:PHE:HB3	2.00	0.44
1:B:1457:HIS:ND1	1:B:1492:SER:HB2	2.32	0.44
1:B:1351:PRO:CG	1:B:1516:PRO:HA	2.46	0.44
1:B:1577:LEU:HD11	1:B:1615:ASN:CB	2.47	0.44
1:B:2031:SER:C	1:B:2033:GLY:H	2.21	0.44
1:B:745:LYS:O	1:B:748:LEU:HD13	2.17	0.44
1:B:728:ARG:HB2	1:B:786:HIS:HB2	1.98	0.44
1:B:1373:GLU:HG2	1:B:1423:ASN:HD21	1.83	0.44
1:B:1120:LYS:HG3	1:B:1131:GLN:HG2	1.99	0.44
1:B:1593:THR:O	1:B:1596:ASP:HB2	2.18	0.44
1:B:1499:ASP:OD1	1:B:1766:GLN:HG3	2.17	0.44
1:B:628:LEU:HD23	1:B:628:LEU:HA	1.74	0.44
1:B:949:LEU:HD12	1:B:949:LEU:HA	1.89	0.44
1:B:1381:PRO:HG2	1:B:1455:GLU:HB2	1.99	0.44
1:B:1648:ARG:HB2	1:B:1687:MET:CE	2.48	0.44
1:B:769:CYS:HA	1:B:775:LYS:HE2	1.99	0.44
1:B:656:PRO:HB2	1:B:888:PRO:HA	1.99	0.44
1:B:1493:SER:OG	1:B:1514:PHE:O	2.21	0.44
1:B:1367:MET:SD	1:B:1376:CYS:HB2	2.58	0.43
1:B:1080:ASP:O	1:B:1084:VAL:HG13	2.18	0.43
1:B:949:LEU:O	1:B:953:ARG:HG3	2.18	0.43
1:B:1062:LEU:HA	1:B:1062:LEU:HD12	1.71	0.43
1:B:1715:LYS:HE3	1:B:1715:LYS:HB3	1.77	0.43
1:B:877:GLN:O	1:B:877:GLN:HG2	2.18	0.43
1:B:1049:LYS:HB2	1:B:1049:LYS:HE3	1.75	0.43
1:B:1228:VAL:HG13	1:B:1265:GLN:O	2.19	0.43
1:B:1986:MET:HA	1:B:1986:MET:HE2	2.01	0.43
1:B:1763:ARG:HD2	1:B:1763:ARG:HA	1.86	0.43
1:B:1844:GLY:O	1:B:1848:ILE:HG13	2.19	0.43
1:B:1117:MET:HG2	1:B:1122:MET:O	2.18	0.43
1:B:543:PRO:HG3	1:B:616:GLU:HB2	2.01	0.43
1:B:548:VAL:O	1:B:552:VAL:HG23	2.18	0.43
1:B:1430:GLU:O	1:B:1434:ILE:HG22	2.18	0.43
1:B:1515:HIS:CG	1:B:1516:PRO:HD2	2.54	0.43
1:B:2041:LEU:HD13	1:B:2041:LEU:HA	1.86	0.43
1:B:845:GLY:O	1:B:849:ILE:HD12	2.18	0.43
1:B:1095:ILE:HG22	1:B:1111:THR:HG21	2.00	0.42
1:B:1433:ASP:OD2	1:B:1473:ARG:NH2	2.52	0.42
1:B:2000:THR:HG22	1:B:2003:GLN:CD	2.40	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:GLN:HG3	1:B:422:PHE:HA	2.01	0.42
1:B:1871:LEU:HA	1:B:1871:LEU:HD23	1.86	0.42
1:B:533:VAL:O	1:B:584:GLN:NE2	2.52	0.42
1:B:801:PHE:HA	1:B:806:ILE:HB	2.00	0.42
1:B:1331:ILE:O	1:B:1335:VAL:HB	2.19	0.42
1:B:1409:THR:H	1:B:1415:ASP:CG	2.21	0.42
1:B:1697:ASP:HB3	1:B:1699:GLU:O	2.18	0.42
1:B:490:ARG:HE	1:B:490:ARG:HB2	1.71	0.42
1:B:617:ILE:HG22	1:B:651:LEU:O	2.20	0.42
1:B:1332:GLN:CD	1:B:1358:ILE:HD11	2.39	0.42
1:B:1339:VAL:HA	1:B:1486:ARG:HH22	1.84	0.42
1:B:1755:LEU:HD13	1:B:1785:LEU:HD12	2.01	0.42
1:B:801:PHE:HD1	1:B:806:ILE:CG2	2.31	0.42
1:B:1339:VAL:HA	1:B:1486:ARG:NH2	2.35	0.42
1:B:745:LYS:HB2	1:B:748:LEU:HD22	2.00	0.42
1:B:1077:LEU:HA	1:B:1077:LEU:HD12	1.84	0.42
1:B:1693:ARG:HA	1:B:1694:PRO:HD2	1.78	0.42
1:B:1244:LYS:HG3	1:B:1244:LYS:H	1.36	0.42
1:B:500:LEU:HB2	1:B:667:VAL:HG21	2.01	0.42
1:B:1120:LYS:HD2	1:B:1120:LYS:HA	1.89	0.42
1:B:719:ASN:HA	1:B:719:ASN:HD22	1.47	0.42
1:B:1393:TRP:O	1:B:1397:PHE:N	2.51	0.42
1:B:2062:GLU:O	1:B:2083:THR:HG22	2.20	0.42
1:B:455:PHE:CE1	1:B:460:GLN:HA	2.54	0.42
1:B:547:LEU:HD22	1:B:551:MET:HG2	2.01	0.42
1:B:554:SER:O	1:B:558:ARG:HG2	2.20	0.42
1:B:1567:LYS:H	1:B:1567:LYS:CE	2.33	0.41
1:B:748:LEU:O	1:B:750:LEU:N	2.53	0.41
1:B:1099:VAL:HG22	1:B:1104:TRP:HE3	1.85	0.41
1:B:1093:ARG:HD2	1:B:1115:CYS:SG	2.61	0.41
1:B:1142:LYS:HD2	1:B:1142:LYS:HA	1.96	0.41
1:B:440:LYS:HA	1:B:440:LYS:HD2	1.76	0.41
1:B:517:MET:HG2	1:B:538:ILE:HG21	2.03	0.41
1:B:592:LYS:HE3	1:B:596:ILE:HD11	2.03	0.41
1:B:630:ALA:O	1:B:634:ARG:HB2	2.19	0.41
1:B:656:PRO:O	1:B:657:ASN:HB2	2.20	0.41
1:B:1726:SER:OG	1:B:1728:LEU:HB2	2.21	0.41
1:B:1745:ILE:HD13	1:B:1751:ALA:HA	2.02	0.41
1:B:1725:GLU:HB3	1:B:1771:TYR:OH	2.20	0.41
1:B:2000:THR:H	1:B:2003:GLN:HB2	1.86	0.41
1:B:954:LEU:HA	1:B:954:LEU:HD23	1.93	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1040:LEU:HD11	1:B:1072:LEU:HD11	2.02	0.41
1:B:532:ASN:O	1:B:534:ASP:N	2.53	0.41
1:B:733:LYS:O	1:B:736:ARG:HB3	2.20	0.41
1:B:738:ILE:C	1:B:738:ILE:HD12	2.41	0.41
1:B:1381:PRO:HD3	1:B:1454:ASP:O	2.20	0.41
1:B:437:ARG:HD3	1:B:439:ARG:HH11	1.85	0.41
1:B:696:LYS:O	1:B:700:ARG:N	2.34	0.41
1:B:1309:VAL:HG23	1:B:1326:PRO:O	2.20	0.40
1:B:1566:ARG:O	1:B:1569:THR:HG22	2.21	0.40
1:B:1908:LEU:HA	1:B:1908:LEU:HD23	1.87	0.40
1:B:686:GLU:O	1:B:866:GLU:HA	2.21	0.40
1:B:731:THR:HG21	1:B:786:HIS:CD2	2.55	0.40
1:B:827:ILE:HD11	1:B:870:ILE:HD11	2.02	0.40
1:B:1613:LEU:HD23	1:B:1613:LEU:HA	1.94	0.40
1:B:602:GLU:HA	1:B:605:TYR:CE2	2.56	0.40
1:B:1434:ILE:HD13	1:B:1823:TYR:HB2	2.02	0.40
1:B:2013:ARG:NE	1:B:2049:GLY:HA3	2.27	0.40
1:B:489:TYR:O	1:B:493:LEU:HB2	2.20	0.40
1:B:579:GLU:C	1:B:582:ALA:H	2.25	0.40
1:B:699:LYS:HA	1:B:702:GLN:HG2	2.04	0.40
1:B:827:ILE:HD11	1:B:870:ILE:CD1	2.51	0.40
1:B:1567:LYS:H	1:B:1567:LYS:HE3	1.85	0.40
1:B:617:ILE:O	1:B:617:ILE:HG13	2.21	0.40
1:B:718:LYS:HD3	1:B:719:ASN:N	2.37	0.40
1:B:831:THR:HG21	1:B:869:LEU:HD11	2.03	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%)	1566 (91%)	126 (7%)	30 (2%)	9 23

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	431	PRO
1	B	457	SER
1	B	577	LYS
1	B	747	THR
1	B	1050	GLU
1	B	533	VAL
1	B	602	GLU
1	B	695	LYS
1	B	697	ALA
1	B	719	ASN
1	B	746	ASP
1	B	769	CYS
1	B	789	MET
1	B	1584	ILE
1	B	2100	GLY
1	B	428	CYS
1	B	749	GLY
1	B	754	GLU
1	B	791	ARG
1	B	804	LYS
1	B	875	GLU
1	B	1074	GLY
1	B	1303	ASP
1	B	561	THR
1	B	1075	PHE
1	B	1051	SER
1	B	1326	PRO
1	B	1465	PRO
1	B	1045	PRO
1	B	717	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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
-----	-------	----------	-----------	----------	-------------

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	1542/1542 (100%)	1297 (84%)	245 (16%)	2 6

All (245) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	418	GLN
1	B	427	ARG
1	B	429	GLN
1	B	439	ARG
1	B	443	GLU
1	B	447	VAL
1	B	465	GLU
1	B	476	GLU
1	B	484	ILE
1	B	488	LEU
1	B	489	TYR
1	B	495	THR
1	B	500	LEU
1	B	501	LEU
1	B	525	ILE
1	B	530	THR
1	B	533	VAL
1	B	546	SER
1	B	547	LEU
1	B	550	GLU
1	B	557	LYS
1	B	558	ARG
1	B	564	ILE
1	B	566	VAL
1	B	572	ASP
1	B	577	LYS
1	B	580	ILE
1	B	584	GLN
1	B	591	GLU
1	B	595	ILE
1	B	599	LYS
1	B	602	GLU
1	B	603	ARG
1	B	610	ARG
1	B	612	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	617	ILE
1	B	620	LEU
1	B	639	ILE
1	B	643	GLN
1	B	654	THR
1	B	673	LEU
1	B	677	ASP
1	B	679	SER
1	B	688	THR
1	B	690	VAL
1	B	694	GLU
1	B	719	ASN
1	B	725	VAL
1	B	728	ARG
1	B	729	LYS
1	B	730	GLU
1	B	731	THR
1	B	733	LYS
1	B	738	ILE
1	B	748	LEU
1	B	752	LEU
1	B	753	ARG
1	B	758	SER
1	B	762	LEU
1	B	764	THR
1	B	765	GLU
1	B	769	CYS
1	B	773	GLU
1	B	780	TYR
1	B	782	PHE
1	B	784	ILE
1	B	790	THR
1	B	793	ASP
1	B	794	ARG
1	B	795	THR
1	B	799	ASP
1	B	807	GLN
1	B	810	VAL
1	B	811	SER
1	B	819	VAL
1	B	825	THR
1	B	827	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	835	SER
1	B	840	ARG
1	B	844	LEU
1	B	855	ARG
1	B	862	ASP
1	B	863	THR
1	B	866	GLU
1	B	868	ILE
1	B	871	THR
1	B	872	SER
1	B	877	GLN
1	B	882	LEU
1	B	887	LEU
1	B	893	MET
1	B	897	LEU
1	B	900	MET
1	B	901	LEU
1	B	911	GLN
1	B	920	LEU
1	B	925	LEU
1	B	931	ARG
1	B	934	THR
1	B	941	ASP
1	B	949	LEU
1	B	954	LEU
1	B	956	LEU
1	B	969	LEU
1	B	970	VAL
1	B	971	LYS
1	B	984	LEU
1	B	992	TYR
1	B	993	ILE
1	B	999	GLN
1	B	1009	LEU
1	B	1011	GLU
1	B	1020	LEU
1	B	1023	GLU
1	B	1028	THR
1	B	1029	VAL
1	B	1030	ARG
1	B	1035	LEU
1	B	1039	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1053	GLU
1	B	1061	VAL
1	B	1062	LEU
1	B	1063	LEU
1	B	1070	LEU
1	B	1072	LEU
1	B	1086	GLN
1	B	1092	MET
1	B	1099	VAL
1	B	1102	ARG
1	B	1120	LYS
1	B	1124	GLN
1	B	1129	LEU
1	B	1134	LYS
1	B	1135	LEU
1	B	1138	GLU
1	B	1143	ILE
1	B	1169	LYS
1	B	1170	MET
1	B	1172	LYS
1	B	1187	SER
1	B	1225	VAL
1	B	1228	VAL
1	B	1230	SER
1	B	1234	LEU
1	B	1240	LEU
1	B	1241	LEU
1	B	1244	LYS
1	B	1249	GLU
1	B	1262	LEU
1	B	1271	VAL
1	B	1274	ARG
1	B	1279	GLU
1	B	1287	ARG
1	B	1293	GLU
1	B	1294	LYS
1	B	1302	LEU
1	B	1307	LEU
1	B	1313	ARG
1	B	1352	THR
1	B	1366	ARG
1	B	1368	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1369	LEU
1	B	1375	ARG
1	B	1380	THR
1	B	1400	ARG
1	B	1404	LYS
1	B	1408	LEU
1	B	1412	THR
1	B	1421	LYS
1	B	1425	ILE
1	B	1430	GLU
1	B	1442	ARG
1	B	1453	VAL
1	B	1456	VAL
1	B	1466	VAL
1	B	1474	MET
1	B	1481	ILE
1	B	1482	GLU
1	B	1483	ARG
1	B	1487	ILE
1	B	1492	SER
1	B	1494	LEU
1	B	1502	HIS
1	B	1518	VAL
1	B	1539	LEU
1	B	1567	LYS
1	B	1569	THR
1	B	1585	GLN
1	B	1588	ARG
1	B	1590	LEU
1	B	1593	THR
1	B	1595	LYS
1	B	1609	LEU
1	B	1611	GLU
1	B	1614	LEU
1	B	1648	ARG
1	B	1650	LEU
1	B	1656	VAL
1	B	1696	GLN
1	B	1728	LEU
1	B	1731	CYS
1	B	1739	GLU
1	B	1765	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1769	ASN
1	B	1776	ILE
1	B	1777	SER
1	B	1785	LEU
1	B	1796	LEU
1	B	1818	ILE
1	B	1831	LEU
1	B	1835	SER
1	B	1849	ILE
1	B	1862	HIS
1	B	1865	ASP
1	B	1867	LEU
1	B	1871	LEU
1	B	1879	LEU
1	B	1895	LEU
1	B	1969	GLU
1	B	1986	MET
1	B	1999	LEU
1	B	2006	ASP
1	B	2017	ILE
1	B	2019	LEU
1	B	2021	TYR
1	B	2026	LYS
1	B	2029	ILE
1	B	2030	ARG
1	B	2038	LEU
1	B	2039	VAL
1	B	2045	GLU
1	B	2047	VAL
1	B	2055	LEU
1	B	2058	GLN
1	B	2067	VAL
1	B	2082	LEU
1	B	2083	THR
1	B	2084	LEU
1	B	2086	GLN
1	B	2091	LYS
1	B	2092	LEU
1	B	2093	ASP
1	B	2095	VAL
1	B	2114	MET
1	B	2124	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	425	ASN
1	B	584	GLN
1	B	771	ASN
1	B	785	HIS
1	B	786	HIS
1	B	1528	GLN
1	B	1690	HIS
1	B	1877	HIS
1	B	1924	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	B	1724/1724 (100%)	0.53	155 (8%) 9 7	45, 95, 166, 219	0

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2124	VAL	9.2
1	B	1963	LEU	7.8
1	B	1977	LYS	7.4
1	B	2038	LEU	7.4
1	B	758	SER	7.1
1	B	1979	VAL	7.1
1	B	2019	LEU	7.1
1	B	783	ALA	6.7
1	B	572	ASP	6.6
1	B	1978	GLY	6.4
1	B	1976	ASP	6.3
1	B	1988	MET	6.2
1	B	1985	ILE	5.9
1	B	469	LYS	5.9
1	B	2036	VAL	5.8
1	B	2102	HIS	5.8
1	B	2047	VAL	5.4
1	B	748	LEU	5.4
1	B	763	ARG	5.3
1	B	2104	TYR	5.1
1	B	2035	VAL	5.1
1	B	2001	ASP	4.9
1	B	774	LEU	4.8
1	B	2043	ARG	4.8
1	B	2016	ASN	4.6
1	B	743	LEU	4.6
1	B	2106	LEU	4.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1883	LYS	4.5
1	B	1998	GLN	4.5
1	B	1991	GLU	4.5
1	B	747	THR	4.5
1	B	757	ALA	4.5
1	B	2008	ALA	4.4
1	B	571	GLY	4.4
1	B	442	TYR	4.4
1	B	1975	THR	4.3
1	B	1983	PHE	4.3
1	B	2022	GLU	4.3
1	B	809	LEU	4.3
1	B	1365	LEU	4.2
1	B	530	THR	4.1
1	B	2015	PRO	4.1
1	B	435	PHE	4.1
1	B	528	ASP	4.0
1	B	1050	GLU	3.9
1	B	746	ASP	3.9
1	B	2122	PHE	3.9
1	B	1993	ARG	3.9
1	B	2123	SER	3.8
1	B	2010	PHE	3.8
1	B	2023	VAL	3.8
1	B	574	GLN	3.8
1	B	734	THR	3.8
1	B	527	MET	3.7
1	B	2092	LEU	3.7
1	B	1969	GLU	3.6
1	B	437	ARG	3.6
1	B	1960	LEU	3.6
1	B	521	ILE	3.5
1	B	2004	ILE	3.5
1	B	575	LEU	3.5
1	B	2101	ALA	3.5
1	B	2042	GLU	3.5
1	B	782	PHE	3.5
1	B	2044	GLU	3.5
1	B	2108	PHE	3.4
1	B	2041	LEU	3.4
1	B	402	ALA	3.4
1	B	2120	TYR	3.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1972	LYS	3.3
1	B	784	ILE	3.3
1	B	722	LEU	3.3
1	B	2017	ILE	3.2
1	B	467	LEU	3.2
1	B	2048	THR	3.2
1	B	732	GLY	3.2
1	B	2018	GLU	3.1
1	B	770	LYS	3.1
1	B	576	CYS	3.1
1	B	1966	PHE	3.0
1	B	1971	ILE	3.0
1	B	2087	LYS	3.0
1	B	719	ASN	3.0
1	B	464	VAL	2.9
1	B	2014	TYR	2.9
1	B	573	HIS	2.9
1	B	525	ILE	2.9
1	B	1874	LYS	2.8
1	B	690	VAL	2.8
1	B	1973	ARG	2.8
1	B	701	PHE	2.8
1	B	2037	VAL	2.7
1	B	1423	ASN	2.7
1	B	778	LEU	2.7
1	B	1147	ASN	2.7
1	B	1872	ALA	2.7
1	B	2039	VAL	2.7
1	B	1996	LEU	2.6
1	B	441	GLY	2.6
1	B	754	GLU	2.6
1	B	870	ILE	2.6
1	B	1987	GLU	2.6
1	B	752	LEU	2.6
1	B	1259	PHE	2.6
1	B	1884	PHE	2.6
1	B	705	ASN	2.5
1	B	2095	VAL	2.5
1	B	781	GLY	2.5
1	B	518	LEU	2.5
1	B	1980	GLU	2.5
1	B	974	LYS	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	741	MET	2.5
1	B	821	LEU	2.4
1	B	470	TYR	2.4
1	B	1321	TYR	2.4
1	B	1936	LEU	2.4
1	B	2029	ILE	2.4
1	B	2086	GLN	2.4
1	B	2100	GLY	2.4
1	B	2084	LEU	2.4
1	B	1992	GLU	2.4
1	B	762	LEU	2.4
1	B	2046	GLU	2.4
1	B	2006	ASP	2.4
1	B	436	ARG	2.4
1	B	875	GLU	2.4
1	B	1982	VAL	2.4
1	B	2007	VAL	2.4
1	B	466	LYS	2.4
1	B	458	GLU	2.4
1	B	2082	LEU	2.3
1	B	738	ILE	2.3
1	B	2118	GLN	2.3
1	B	1165	ILE	2.3
1	B	702	GLN	2.3
1	B	1873	GLN	2.3
1	B	2024	VAL	2.3
1	B	694	GLU	2.2
1	B	1421	LYS	2.2
1	B	736	ARG	2.2
1	B	2099	THR	2.1
1	B	753	ARG	2.1
1	B	1868	LEU	2.1
1	B	859	PRO	2.1
1	B	460	GLN	2.1
1	B	742	CYS	2.1
1	B	696	LYS	2.1
1	B	2103	ASN	2.1
1	B	708	VAL	2.0
1	B	1317	PHE	2.0
1	B	444	GLU	2.0
1	B	1875	VAL	2.0
1	B	1995	ALA	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	1322	GLN	2.0
1	B	1981	SER	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 [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.