



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:24 AM UTC

PDB ID : 6S8O / pdb_00006s8o
Title : Human Brr2 Helicase Region M641C/A1582C
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Deposited on : 2019-07-10
Resolution : 3.17 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

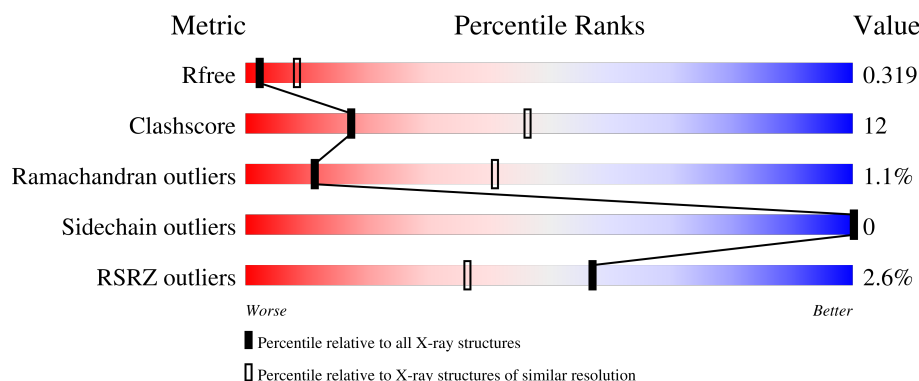
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

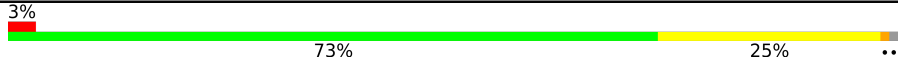
The reported resolution of this entry is 3.17 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2001 (3.20-3.16)
Clashscore	190562	2119 (3.20-3.16)
Ramachandran outliers	187476	2070 (3.20-3.16)
Sidechain outliers	187428	2069 (3.20-3.16)
RSRZ outliers	180081	2001 (3.20-3.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1747	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 13878 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	1724	Total	C	N	O	S	0	0	0
			13858	8855	2371	2559	73			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	390	GLY	-	expression tag	UNP O75643
B	391	ALA	-	expression tag	UNP O75643
B	392	GLU	-	expression tag	UNP O75643
B	393	PHE	-	expression tag	UNP O75643
B	641	CYS	MET	engineered mutation	UNP O75643
B	1582	CYS	ALA	engineered mutation	UNP O75643

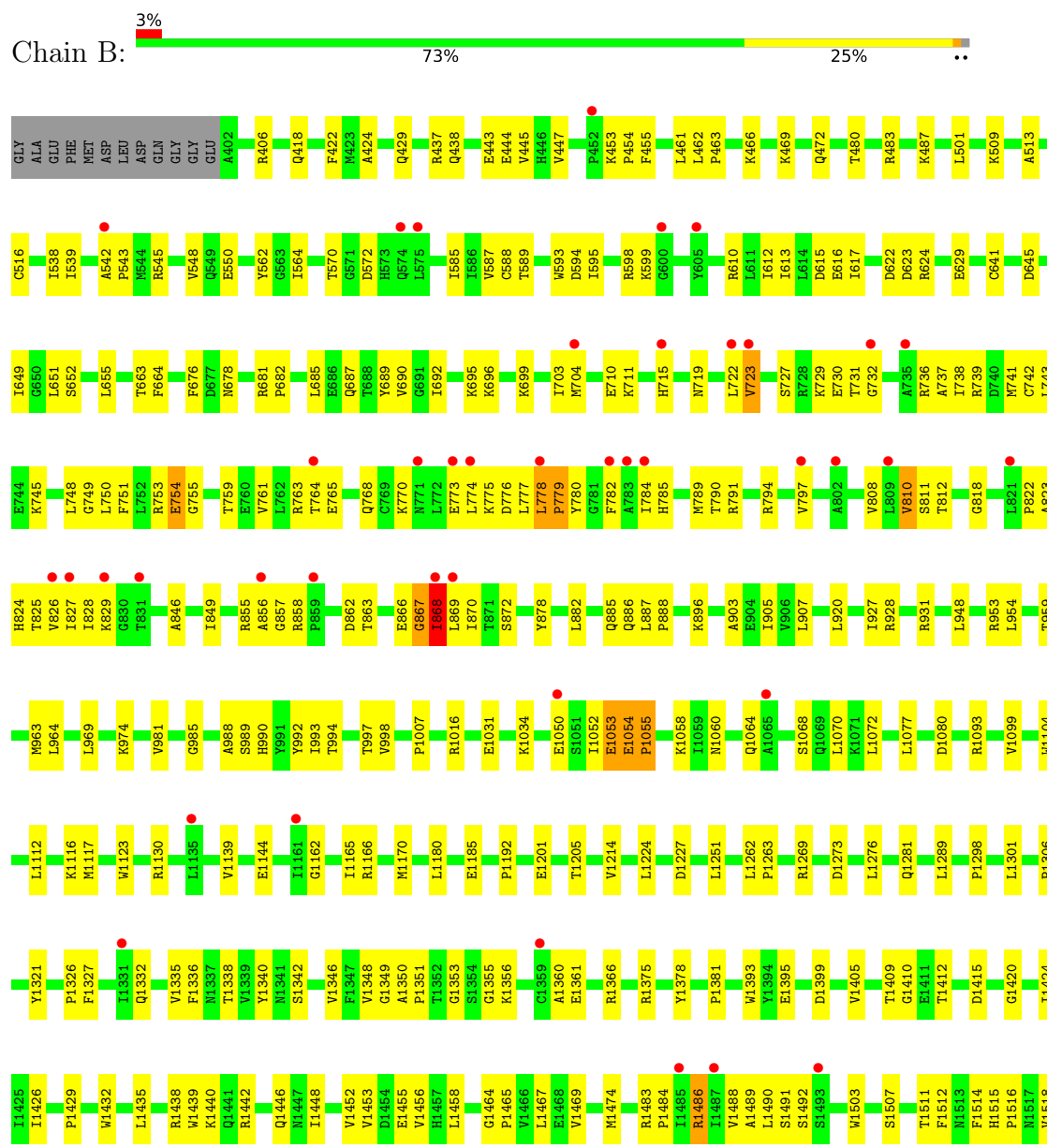
- Molecule 2 is water.

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

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: U5 small nuclear ribonucleoprotein 200 kDa helicase



Q2086	E1992	E1864	V1661	R1519
K2089	A1995	L1867	I1662	H1534
V2090	L1996		T1663	T1535
K2091	L1997	K1883	D1665	Q1536
L2092		D1886	K1672	T1537
A2096	V2007			R1538
	K2008	T1891	Y1679	L1539
G2100	R2009	L1895	M1687	K1544
	F2010			P1545
N2103	R2013	H1898	N1692	V1559
L2106	L2019	R1901	I1704	I1560
S2110	S2020			R1566
	Z2021	L1904	V1724	T1569
C2116	V2024	S1905	E1725	T1572
Y2120	V2025	A1906	D1729	
	K2026	E1907		L1577
S2123	D2027	L1908	D1734	
V2124		Q1909	H1735	
D2125	S2031	S1910		C1582
VAL	V2037	D1911	E1739	
LYS	L2038	M1943		Q1587
GLU	V2039	E1944	T1744	
ALA	Q2040	L1945		E1594
GLU		A1946	W1757	K1595
THR	R2043	Q1947		I1598
ASP	E2044	M1948	L1760	
SER		V1949		L1601
ASP	G2049	T1950	R1763	
SER	P2050	Q1951	M1764	
ASP	V2051	A1952		K1610
	L2052	M1953	L1793	E1611
	A2053			T1612
	P2054	K1961	E1797	
	L2055	Q1962		V1617
	F2056	L1963	T1804	
	P2057	P1964		H1621
	Q2058	H1965	V1810	E1622
	K2059	F1966		S1625
	R2060	T1967	A1819	
	E2061			E1628
	E2062	H1970	N1825	
	G2063	R1973	I1829	V1632
	W2064	C1974		
	W2065		L1845	V1643
	V2066	G1978		V1644
	V2067		I1849	V1645
		S1981		R1648
	D2070		Y1855	S1649
	A2071	D1984	E1856	L1650
	K2072		M1857	
		M1988	I1858	V1656
	R2081	E1989		
		D1990	R1861	L1660
	L2084			
	Q2085	E1991		

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	145.56Å 152.53Å 142.51Å 90.00° 120.69° 90.00°	Depositor
Resolution (Å)	48.38 – 3.17 48.38 – 3.17	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.38-3.17) 97.2 (48.38-3.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.14 _3260	Depositor
R, R_{free}	0.264 , 0.318 0.266 , 0.319	Depositor DCC
R_{free} test set	2100 reflections (4.63%)	wwPDB-VP
Wilson B-factor (Å ²)	109.4	Xtriage
Anisotropy	0.450	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 78.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-1/2*h-1/2*k-l 0.000 for -k,-h,-1/2*h+1/2*k-l 0.000 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13878	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% of the height of the origin peak. No significant pseudotranslation is detected.*

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 [i](#)

5.1 Standard geometry [i](#)

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	0.11	0/14152	0.31	1/19176 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	868	ILE	N-CA-C	5.03	119.81	109.34

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	867	GLY	Peptide

5.2 Too-close contacts [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	B	13858	0	13995	347	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	20	0	0	7	0
All	All	13878	0	13995	347	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (347) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:723:VAL:HA	1:B:827:ILE:HG13	1.46	0.98
1:B:773:GLU:HG3	1:B:789:MET:CE	1.93	0.97
1:B:773:GLU:HG3	1:B:789:MET:HE1	1.56	0.87
1:B:773:GLU:HG3	1:B:789:MET:HE3	1.61	0.83
1:B:1456:VAL:HG11	1:B:1489:ALA:HB1	1.66	0.77
1:B:695:LYS:HA	1:B:696:LYS:HB2	1.67	0.76
1:B:687:GLN:HA	1:B:867:GLY:HA3	1.67	0.75
1:B:753:ARG:HD2	1:B:754:GLU:H	1.52	0.74
1:B:1904:LEU:HB3	1:B:1909:GLN:HB2	1.71	0.72
1:B:444:GLU:HA	1:B:690:VAL:HG12	1.74	0.70
1:B:463:PRO:O	1:B:466:LYS:NZ	2.24	0.70
1:B:826:VAL:HG23	1:B:868:ILE:HG12	1.73	0.69
1:B:1950:THR:OG1	1:B:2060:ARG:NH1	2.25	0.69
1:B:617:ILE:HG22	1:B:652:SER:HB2	1.74	0.69
1:B:823:ALA:HA	1:B:858:ARG:HE	1.58	0.69
1:B:2039:VAL:HG23	1:B:2090:VAL:HG11	1.76	0.68
1:B:689:TYR:HA	1:B:869:LEU:HD11	1.77	0.67
1:B:1951:GLN:HG2	1:B:1962:GLN:HG2	1.77	0.67
1:B:1559:VAL:HG22	1:B:1660:LEU:HB3	1.76	0.67
1:B:610:ARG:NH1	1:B:645:ASP:O	2.28	0.67
1:B:753:ARG:H	1:B:759:THR:HG22	1.59	0.66
1:B:969:LEU:HD22	1:B:985:GLY:HA2	1.78	0.66
1:B:1375:ARG:HH22	1:B:1420:GLY:HA2	1.60	0.65
1:B:2064:TRP:HH2	1:B:2116:CYS:HB2	1.61	0.65
1:B:1883:LYS:HE3	1:B:1886:ASP:HB2	1.79	0.65
1:B:483:ARG:NH1	1:B:681:ARG:O	2.29	0.65
1:B:692:ILE:HG13	1:B:872:SER:HA	1.77	0.65
1:B:445:VAL:N	1:B:689:TYR:O	2.29	0.65
1:B:406:ARG:NH1	1:B:974:LYS:O	2.26	0.64
1:B:538:ILE:HB	1:B:585:ILE:HG13	1.78	0.64
1:B:988:ALA:HB2	1:B:998:VAL:HG21	1.79	0.64
1:B:711:LYS:O	2:B:2201:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:LYS:HD2	1:B:775:LYS:HG2	1.78	0.64
1:B:687:GLN:OE1	1:B:689:TYR:OH	2.16	0.63
1:B:727:SER:HB2	1:B:730:GLU:HB2	1.79	0.63
1:B:846:ALA:HA	1:B:849:ILE:HD12	1.80	0.63
1:B:437:ARG:O	1:B:444:GLU:N	2.29	0.62
1:B:1895:LEU:HA	1:B:1898:HIS:HB3	1.81	0.62
1:B:699:LYS:HG2	1:B:703:ILE:HG13	1.81	0.62
1:B:1739:GLU:HG3	1:B:1744:THR:HB	1.81	0.62
1:B:615:ASP:HA	1:B:651:LEU:HB2	1.81	0.62
1:B:1099:VAL:HG13	1:B:1104:TRP:HB2	1.82	0.62
1:B:622:ASP:OD1	1:B:623:ASP:N	2.33	0.61
1:B:770:LYS:HB3	1:B:775:LYS:HD2	1.83	0.61
1:B:545:ARG:NH1	1:B:570:THR:OG1	2.33	0.61
1:B:811:SER:O	2:B:2202:HOH:O	2.16	0.61
1:B:1456:VAL:HG22	1:B:1491:SER:HB2	1.81	0.61
1:B:689:TYR:HA	1:B:869:LEU:CD1	2.30	0.61
1:B:406:ARG:HG2	1:B:954:LEU:HD22	1.83	0.60
1:B:1112:LEU:HG	1:B:1116:LYS:HE3	1.82	0.60
1:B:1415:ASP:HB3	1:B:1435:LEU:HD11	1.83	0.60
1:B:989:SER:OG	2:B:2203:HOH:O	2.17	0.60
1:B:732:GLY:O	1:B:736:ARG:N	2.34	0.60
1:B:1963:LEU:HD23	1:B:1965:HIS:H	1.66	0.60
1:B:784:ILE:HD12	1:B:794:ARG:HH12	1.67	0.60
1:B:827:ILE:HA	1:B:868:ILE:HD13	1.84	0.60
1:B:1375:ARG:HB2	1:B:1448:ILE:HA	1.84	0.60
1:B:1725:GLU:O	2:B:2204:HOH:O	2.17	0.59
1:B:595:ILE:HD11	1:B:992:TYR:HB2	1.86	0.58
1:B:1855:TYR:HB3	1:B:1891:THR:HG21	1.85	0.58
1:B:1906:ALA:O	1:B:1908:LEU:N	2.37	0.58
1:B:1943:MET:HE1	1:B:2067:VAL:HG21	1.85	0.58
1:B:778:LEU:C	1:B:780:TYR:H	2.12	0.57
1:B:1052:ILE:HD12	1:B:1053:GLU:N	2.20	0.57
1:B:2054:PRO:HG2	1:B:2055:LEU:HD12	1.86	0.57
1:B:948:LEU:O	1:B:953:ARG:NH1	2.38	0.57
1:B:1797:GLU:HB2	1:B:1804:ILE:HD13	1.86	0.57
1:B:599:LYS:NZ	1:B:990:HIS:O	2.38	0.57
1:B:731:THR:OG1	1:B:810:VAL:O	2.22	0.57
1:B:1130:ARG:NH2	1:B:1144:GLU:OE2	2.35	0.57
1:B:539:ILE:HB	1:B:612:ILE:HG22	1.87	0.56
1:B:743:LEU:HB2	1:B:748:LEU:HD22	1.87	0.56
1:B:749:GLY:O	1:B:751:PHE:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:905:ILE:HG22	1:B:981:VAL:HG22	1.87	0.56
1:B:1595:LYS:HD3	1:B:1598:ILE:HD12	1.88	0.56
1:B:826:VAL:HG22	1:B:856:ALA:HB2	1.87	0.56
1:B:1432:TRP:HE1	1:B:1474:MET:HE3	1.70	0.56
1:B:2031:SER:HA	1:B:2096:ALA:HB3	1.86	0.56
1:B:690:VAL:CG2	1:B:870:ILE:HG12	2.36	0.56
1:B:775:LYS:HA	1:B:778:LEU:HD12	1.87	0.56
1:B:1338:THR:O	1:B:1342:SER:OG	2.21	0.55
1:B:753:ARG:O	1:B:755:GLY:N	2.37	0.55
1:B:827:ILE:HA	1:B:868:ILE:HB	1.88	0.55
1:B:469:LYS:HA	1:B:472:GLN:HG3	1.88	0.55
1:B:2019:LEU:HD12	1:B:2040:GLN:HB2	1.88	0.55
1:B:1262:LEU:HD21	1:B:1289:LEU:HD23	1.88	0.55
1:B:1378:TYR:HD2	1:B:1426:ILE:HG23	1.72	0.55
1:B:719:ASN:ND2	2:B:2201:HOH:O	2.39	0.55
1:B:1185:GLU:HB2	1:B:1205:THR:HB	1.89	0.55
1:B:1601:LEU:HB3	1:B:1610:LYS:HG3	1.89	0.54
1:B:1625:SER:HB2	1:B:1628:GLU:HG3	1.88	0.54
1:B:2059:LYS:H	1:B:2059:LYS:HD3	1.71	0.54
1:B:1346:VAL:HG12	1:B:1488:VAL:HG12	1.89	0.54
1:B:453:LYS:HD2	1:B:454:PRO:HD2	1.90	0.54
1:B:723:VAL:HA	1:B:827:ILE:CG1	2.30	0.54
1:B:1409:THR:OG1	1:B:1410:GLY:N	2.35	0.54
1:B:2024:VAL:HG11	1:B:2026:LYS:HE3	1.88	0.54
1:B:1336:PHE:HE1	1:B:1340:TYR:HD2	1.53	0.54
1:B:1162:GLY:HA2	1:B:1165:ILE:HG22	1.90	0.54
1:B:1617:VAL:HG22	1:B:1643:VAL:HB	1.90	0.54
1:B:2007:VAL:HG23	1:B:2010:PHE:HE1	1.73	0.54
1:B:777:LEU:HB2	1:B:782:PHE:HB3	1.90	0.53
1:B:447:VAL:HG22	1:B:687:GLN:HB2	1.90	0.53
1:B:463:PRO:HA	1:B:480:THR:HA	1.89	0.53
1:B:1587:GLN:NE2	1:B:1594:GLU:OE2	2.41	0.53
1:B:2019:LEU:HB3	1:B:2120:TYR:HE2	1.73	0.53
1:B:1901:ARG:NH2	1:B:1951:GLN:O	2.42	0.52
1:B:1566:ARG:HB2	1:B:1621:HIS:HB2	1.90	0.52
1:B:2070:ASP:OD1	1:B:2071:ALA:N	2.42	0.52
1:B:1262:LEU:HD12	1:B:1263:PRO:HD2	1.91	0.52
1:B:2019:LEU:HB3	1:B:2120:TYR:CE2	2.45	0.52
1:B:827:ILE:HG22	1:B:868:ILE:CG2	2.40	0.52
1:B:742:CYS:HB3	1:B:748:LEU:HD13	1.91	0.52
1:B:1093:ARG:NH1	1:B:1273:ASP:OD1	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2037:VAL:HB	1:B:2092:LEU:HD11	1.92	0.51
1:B:1729:ASP:OD1	1:B:1729:ASP:N	2.37	0.51
1:B:1908:LEU:HD23	1:B:1908:LEU:H	1.75	0.51
1:B:1405:VAL:HG22	1:B:1424:ILE:HB	1.93	0.51
1:B:1984:ASP:OD1	1:B:1984:ASP:N	2.36	0.51
1:B:1342:SER:O	1:B:1486:ARG:NH1	2.43	0.51
1:B:2051:VAL:HG22	1:B:2062:GLU:HG3	1.91	0.51
1:B:775:LYS:O	1:B:778:LEU:HB2	2.10	0.51
1:B:826:VAL:HG23	1:B:868:ILE:CG1	2.39	0.51
1:B:1566:ARG:O	1:B:1569:THR:OG1	2.21	0.51
1:B:1068:SER:OG	1:B:1123:TRP:NE1	2.37	0.51
1:B:1901:ARG:NH2	1:B:1961:LYS:O	2.44	0.51
1:B:1904:LEU:HB3	1:B:1909:GLN:CB	2.40	0.51
1:B:1180:LEU:HD13	1:B:1214:VAL:HG21	1.93	0.50
1:B:2043:ARG:O	1:B:2086:GLN:NE2	2.44	0.50
1:B:761:VAL:HA	1:B:764:THR:HB	1.94	0.50
1:B:466:LYS:H	1:B:466:LYS:HD3	1.76	0.50
1:B:704:MET:O	1:B:829:LYS:NZ	2.43	0.50
1:B:741:MET:O	1:B:745:LYS:HG2	2.12	0.50
1:B:429:GLN:N	1:B:886:GLN:OE1	2.41	0.50
1:B:743:LEU:HA	1:B:748:LEU:HB2	1.94	0.50
1:B:1016:ARG:HB2	1:B:1050:GLU:HG2	1.94	0.50
1:B:1351:PRO:HG3	1:B:1516:PRO:HA	1.92	0.50
1:B:1349:GLY:N	1:B:1512:PHE:O	2.36	0.49
1:B:1455:GLU:N	1:B:1490:LEU:O	2.45	0.49
1:B:1901:ARG:HH21	1:B:1961:LYS:HB3	1.77	0.49
1:B:1361:GLU:OE2	1:B:1393:TRP:NE1	2.42	0.49
1:B:681:ARG:NH2	1:B:856:ALA:O	2.44	0.49
1:B:1560:ILE:HD11	1:B:1656:VAL:HG12	1.93	0.49
1:B:418:GLN:HB2	1:B:422:PHE:HB2	1.93	0.49
1:B:1201:GLU:HB3	1:B:1251:LEU:HD11	1.94	0.49
1:B:1963:LEU:CD2	1:B:1965:HIS:H	2.25	0.49
1:B:1988:MET:HE3	1:B:1990:ASP:HB3	1.94	0.49
1:B:2021:TYR:HB3	1:B:2106:LEU:HD22	1.94	0.49
1:B:882:LEU:HB2	1:B:887:LEU:HD13	1.93	0.49
1:B:1429:PRO:HG3	1:B:1467:LEU:HD13	1.94	0.49
1:B:1192:PRO:HG3	1:B:1289:LEU:HD11	1.95	0.49
1:B:1060:ASN:OD1	1:B:1064:GLN:NE2	2.39	0.48
1:B:681:ARG:HD2	1:B:682:PRO:HD2	1.96	0.48
1:B:753:ARG:HD3	1:B:754:GLU:HG2	1.95	0.48
1:B:1395:GLU:HA	1:B:1399:ASP:HB2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1663:ILE:HD12	1:B:1704:ILE:HG12	1.95	0.48
1:B:773:GLU:CG	1:B:789:MET:HE1	2.38	0.48
1:B:1804:ILE:HG13	1:B:1810:VAL:HG12	1.95	0.48
1:B:2056:PHE:HE1	1:B:2058:GLN:HB2	1.79	0.48
1:B:710:GLU:OE1	1:B:710:GLU:N	2.46	0.48
1:B:959:THR:HG22	1:B:963:MET:HE3	1.94	0.48
1:B:988:ALA:HA	1:B:993:ILE:HG12	1.95	0.48
1:B:2059:LYS:HD3	1:B:2059:LYS:N	2.28	0.48
1:B:1353:GLY:H	1:B:1356:LYS:NZ	2.12	0.48
1:B:1464:GLY:H	1:B:1465:PRO:HD2	1.79	0.48
1:B:1332:GLN:NE2	1:B:1355:GLY:O	2.39	0.48
1:B:1381:PRO:HG2	1:B:1458:LEU:HD12	1.97	0.47
1:B:964:LEU:HD22	1:B:969:LEU:HD12	1.95	0.47
1:B:2056:PHE:CE1	1:B:2058:GLN:HB2	2.49	0.47
1:B:2053:ALA:HB1	1:B:2056:PHE:HB3	1.96	0.47
1:B:778:LEU:O	1:B:780:TYR:N	2.48	0.47
1:B:545:ARG:HH21	1:B:548:VAL:HG21	1.79	0.47
1:B:774:LEU:O	1:B:778:LEU:HG	2.14	0.47
1:B:1990:ASP:O	1:B:1992:GLU:N	2.47	0.47
1:B:828:ILE:HD11	1:B:870:ILE:H	1.80	0.47
1:B:1335:VAL:HG21	1:B:1348:VAL:HG22	1.95	0.47
1:B:462:LEU:HB3	1:B:466:LYS:NZ	2.29	0.47
1:B:770:LYS:HD2	1:B:775:LYS:CG	2.45	0.47
1:B:1953:MET:HE2	1:B:1961:LYS:HB2	1.95	0.47
1:B:2064:TRP:CD1	1:B:2084:LEU:HD22	2.49	0.47
1:B:785:HIS:HA	1:B:794:ARG:NH1	2.29	0.47
1:B:825:THR:HB	1:B:866:GLU:HB3	1.97	0.46
1:B:1117:MET:HG2	1:B:1276:LEU:HD11	1.97	0.46
1:B:1412:THR:HA	1:B:1415:ASP:HB2	1.96	0.46
1:B:1572:THR:HB	1:B:1645:VAL:HG11	1.96	0.46
1:B:594:ASP:O	1:B:598:ARG:HB2	2.16	0.46
1:B:928:ARG:HH12	1:B:931:ARG:HB2	1.79	0.46
1:B:1068:SER:HB2	1:B:1070:LEU:HD13	1.95	0.46
1:B:2020:SER:OG	1:B:2040:GLN:NE2	2.48	0.46
1:B:2027:ASP:OD1	1:B:2027:ASP:N	2.47	0.46
1:B:1539:LEU:HD21	1:B:1665:ASP:HB2	1.98	0.46
1:B:920:LEU:HB3	1:B:953:ARG:HD2	1.97	0.46
1:B:1577:LEU:HD21	1:B:1612:THR:HA	1.98	0.46
1:B:1734:ASP:OD2	1:B:1825:ASN:ND2	2.46	0.46
1:B:731:THR:HA	1:B:810:VAL:HG22	1.97	0.46
1:B:867:GLY:HA2	1:B:868:ILE:HG13	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1974:CYS:HB3	1:B:1978:GLY:HA3	1.96	0.46
1:B:513:ALA:HB1	1:B:613:ILE:HD13	1.97	0.46
1:B:692:ILE:HD13	1:B:695:LYS:HE2	1.96	0.46
1:B:1469:VAL:HG21	1:B:1735:HIS:CG	2.51	0.46
1:B:2039:VAL:HG12	1:B:2040:GLN:H	1.81	0.46
1:B:2009:ARG:O	1:B:2013:ARG:HG2	2.15	0.46
1:B:445:VAL:O	1:B:689:TYR:N	2.49	0.46
1:B:903:ALA:O	1:B:907:LEU:HD12	2.16	0.46
1:B:785:HIS:O	1:B:811:SER:HA	2.16	0.45
1:B:1819:ALA:HB2	1:B:1829:ILE:HG12	1.97	0.45
1:B:1861:ARG:NH2	1:B:1911:ASP:OD2	2.50	0.45
1:B:2064:TRP:CH2	1:B:2116:CYS:HB2	2.48	0.45
1:B:1507:SER:O	1:B:1511:THR:OG1	2.30	0.45
1:B:1760:LEU:HD11	1:B:1764:MET:HE3	1.98	0.45
1:B:424:ALA:HB3	1:B:888:PRO:HG2	1.98	0.45
1:B:543:PRO:O	1:B:624:ARG:NH2	2.31	0.45
1:B:572:ASP:OD1	1:B:572:ASP:N	2.49	0.45
1:B:768:GLN:HG3	1:B:770:LYS:HE2	1.98	0.45
1:B:678:ASN:H	1:B:885:GLN:NE2	2.14	0.45
1:B:1992:GLU:HG3	1:B:1995:ALA:HB3	1.99	0.45
1:B:784:ILE:O	1:B:797:VAL:HG11	2.17	0.45
1:B:828:ILE:O	1:B:829:LYS:HD2	2.16	0.45
1:B:1306:PRO:HB2	1:B:1327:PHE:HB3	1.99	0.45
1:B:1967:THR:OG1	1:B:1970:HIS:ND1	2.48	0.45
1:B:739:ARG:HE	1:B:748:LEU:HD21	1.82	0.45
1:B:1356:LYS:HD3	1:B:1356:LYS:H	1.82	0.45
1:B:1519:ARG:NH2	1:B:1692:ASN:HB2	2.31	0.45
1:B:1544:LYS:HB3	1:B:1545:PRO:HD3	1.99	0.45
1:B:588:CYS:SG	1:B:593:TRP:HB2	2.57	0.44
1:B:696:LYS:HD3	1:B:699:LYS:HD3	1.98	0.44
1:B:655:LEU:HD22	1:B:887:LEU:HB3	1.98	0.44
1:B:846:ALA:HB2	1:B:878:TYR:OH	2.17	0.44
1:B:1966:PHE:CZ	1:B:1970:HIS:HB3	2.53	0.44
1:B:1298:PRO:HG3	1:B:1515:HIS:HB2	2.00	0.44
1:B:1375:ARG:NH1	1:B:1420:GLY:O	2.33	0.44
1:B:1446:GLN:OE1	1:B:1446:GLN:N	2.50	0.44
1:B:2021:TYR:CE1	1:B:2120:TYR:HB3	2.53	0.44
1:B:689:TYR:CD2	1:B:869:LEU:HD21	2.52	0.44
1:B:681:ARG:HE	1:B:685:LEU:HD22	1.81	0.44
1:B:777:LEU:HA	1:B:780:TYR:CZ	2.52	0.44
1:B:1483:ARG:HG3	1:B:1484:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2103:ASN:OD1	1:B:2123:SER:OG	2.36	0.44
1:B:824:HIS:ND1	1:B:862:ASP:OD2	2.35	0.44
1:B:763:ARG:NH1	1:B:764:THR:OG1	2.51	0.44
1:B:826:VAL:O	1:B:868:ILE:HG21	2.18	0.44
1:B:1054:GLU:HB3	1:B:1055:PRO:HD2	1.99	0.44
1:B:438:GLN:HA	1:B:443:GLU:HA	2.00	0.44
1:B:487:LYS:HD3	1:B:676:PHE:CZ	2.53	0.44
1:B:1321:TYR:OH	1:B:1361:GLU:OE1	2.26	0.44
1:B:1514:PHE:HB3	1:B:1518:VAL:HG21	2.00	0.44
1:B:2072:LYS:HD2	1:B:2072:LYS:HA	1.80	0.44
1:B:1058:LYS:NZ	1:B:1080:ASP:OD2	2.39	0.43
1:B:1165:ILE:HD12	1:B:1165:ILE:HA	1.85	0.43
1:B:1438:ARG:HB2	1:B:1442:ARG:HD2	1.99	0.43
1:B:550:GLU:HB2	1:B:818:GLY:O	2.18	0.43
1:B:822:PRO:HA	1:B:855:ARG:HB3	1.99	0.43
1:B:1227:ASP:OD1	1:B:1227:ASP:N	2.48	0.43
1:B:862:ASP:OD1	1:B:863:THR:N	2.46	0.43
1:B:1515:HIS:O	1:B:1518:VAL:HG22	2.18	0.43
1:B:826:VAL:O	1:B:868:ILE:HG12	2.18	0.43
1:B:1269:ARG:HG2	1:B:1281:GLN:HG3	2.00	0.43
1:B:443:GLU:O	1:B:690:VAL:HA	2.19	0.43
1:B:1648:ARG:HD3	1:B:1679:TYR:CE1	2.53	0.43
1:B:542:ALA:O	1:B:589:THR:HA	2.19	0.43
1:B:1947:GLN:HE21	1:B:2110:SER:C	2.27	0.43
1:B:509:LYS:HD2	1:B:651:LEU:HB3	2.01	0.43
1:B:739:ARG:NE	1:B:748:LEU:HD21	2.34	0.43
1:B:827:ILE:HD13	1:B:827:ILE:HG21	1.77	0.43
1:B:1052:ILE:HD12	1:B:1053:GLU:H	1.81	0.43
1:B:1353:GLY:O	1:B:1692:ASN:ND2	2.52	0.43
1:B:811:SER:N	2:B:2202:HOH:O	2.52	0.43
1:B:1053:GLU:HB3	1:B:1054:GLU:H	1.59	0.43
1:B:1503:TRP:NE1	1:B:1757:TRP:O	2.48	0.43
1:B:1861:ARG:NH1	1:B:1907:GLU:OE1	2.52	0.43
1:B:715:HIS:ND1	1:B:719:ASN:OD1	2.46	0.42
1:B:722:LEU:HD11	1:B:823:ALA:CB	2.49	0.42
1:B:739:ARG:NH2	1:B:780:TYR:OH	2.48	0.42
1:B:1340:TYR:O	1:B:1366:ARG:HD3	2.18	0.42
1:B:737:ALA:O	1:B:741:MET:HB3	2.19	0.42
1:B:768:GLN:NE2	1:B:768:GLN:HA	2.34	0.42
1:B:828:ILE:HG13	1:B:869:LEU:HA	2.01	0.42
1:B:765:GLU:HA	1:B:768:GLN:OE1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:768:GLN:NE2	1:B:770:LYS:HD3	2.33	0.42
1:B:1855:TYR:HA	1:B:1858:ILE:HD13	2.00	0.42
1:B:2007:VAL:HG23	1:B:2010:PHE:CE1	2.52	0.42
1:B:598:ARG:HD3	1:B:989:SER:O	2.19	0.42
1:B:1907:GLU:C	1:B:1909:GLN:H	2.28	0.42
1:B:1981:SER:OG	1:B:1984:ASP:OD1	2.33	0.42
1:B:641:CYS:HA	1:B:1582:CYS:HB2	2.01	0.42
1:B:768:GLN:HE21	1:B:770:LYS:HD3	1.84	0.42
1:B:1793:LEU:HD13	1:B:1810:VAL:HG11	2.02	0.42
1:B:455:PHE:CE2	1:B:461:LEU:HG	2.54	0.42
1:B:778:LEU:C	1:B:780:TYR:N	2.76	0.42
1:B:827:ILE:CA	1:B:868:ILE:HD13	2.50	0.42
1:B:1301:LEU:HD22	1:B:1518:VAL:HB	2.02	0.42
1:B:1672:LYS:NZ	1:B:1856:GLU:O	2.48	0.42
1:B:1945:LEU:HD12	1:B:1945:LEU:HA	1.91	0.42
1:B:406:ARG:HH11	1:B:974:LYS:HD2	1.84	0.42
1:B:562:TYR:HB2	1:B:564:ILE:HD13	2.01	0.42
1:B:782:PHE:HA	1:B:808:VAL:O	2.19	0.42
1:B:1350:ALA:O	1:B:1492:SER:HA	2.20	0.42
1:B:1360:ALA:HB1	1:B:1452:VAL:HG11	2.02	0.42
1:B:1538:ARG:NH1	1:B:1665:ASP:OD1	2.53	0.42
1:B:753:ARG:CD	1:B:754:GLU:H	2.28	0.41
1:B:548:VAL:HG13	1:B:587:VAL:HG12	2.02	0.41
1:B:722:LEU:O	1:B:810:VAL:HA	2.20	0.41
1:B:994:THR:HG23	1:B:997:THR:H	1.84	0.41
1:B:1007:PRO:HG3	1:B:1104:TRP:CE2	2.55	0.41
1:B:738:ILE:HG13	1:B:739:ARG:N	2.35	0.41
1:B:777:LEU:HB2	1:B:782:PHE:CB	2.50	0.41
1:B:1072:LEU:HD23	1:B:1077:LEU:HB3	2.01	0.41
1:B:1901:ARG:HE	1:B:1961:LYS:HD3	1.84	0.41
1:B:629:GLU:HA	1:B:664:PHE:HZ	1.85	0.41
1:B:722:LEU:HD11	1:B:823:ALA:HB3	2.02	0.41
1:B:1439:TRP:O	1:B:1446:GLN:NE2	2.53	0.41
1:B:1973:ARG:HD2	1:B:1997:LEU:HD23	2.02	0.41
1:B:663:THR:HB	1:B:927:ILE:HD13	2.02	0.41
1:B:784:ILE:HG22	1:B:810:VAL:HG13	2.01	0.41
1:B:1661:VAL:HG11	1:B:1687:MET:O	2.20	0.41
1:B:1763:ARG:HD2	1:B:1763:ARG:HA	1.91	0.41
1:B:681:ARG:HH21	1:B:685:LEU:HB3	1.86	0.41
1:B:729:LYS:HD2	1:B:729:LYS:HA	1.89	0.41
1:B:753:ARG:H	1:B:753:ARG:HG3	1.71	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1031:GLU:HA	1:B:1034:LYS:HD3	2.03	0.41
1:B:1724:VAL:HB	2:B:2204:HOH:O	2.19	0.41
1:B:1948:MET:HB2	1:B:1953:MET:O	2.21	0.41
1:B:776:ASP:O	1:B:780:TYR:OH	2.38	0.41
1:B:867:GLY:O	1:B:868:ILE:HG23	2.21	0.41
1:B:1139:VAL:HG21	1:B:1170:MET:SD	2.61	0.41
1:B:1440:LYS:HD2	1:B:1440:LYS:HA	1.95	0.41
1:B:1622:GLU:HG2	1:B:1650:LEU:HD21	2.02	0.41
1:B:1864:GLU:HA	1:B:1867:LEU:HB3	2.02	0.41
1:B:811:SER:OG	1:B:812:THR:N	2.54	0.41
1:B:1453:VAL:HG12	1:B:1456:VAL:HG12	2.03	0.41
1:B:501:LEU:HD13	1:B:509:LYS:HG3	2.02	0.41
1:B:823:ALA:HA	1:B:858:ARG:NE	2.32	0.41
1:B:2049:GLY:HA2	1:B:2050:PRO:HD3	1.93	0.41
1:B:2065:TRP:NE1	1:B:2081:ARG:HB2	2.36	0.41
1:B:516:CYS:SG	1:B:649:ILE:HG12	2.60	0.40
1:B:1224:LEU:O	1:B:1269:ARG:N	2.53	0.40
1:B:1845:LEU:O	1:B:1849:ILE:HD12	2.21	0.40
1:B:2089:LYS:HA	1:B:2089:LYS:HD3	1.89	0.40
1:B:461:LEU:HD23	1:B:461:LEU:HA	1.84	0.40
1:B:509:LYS:HE3	1:B:509:LYS:HB2	1.78	0.40
1:B:543:PRO:HG3	1:B:616:GLU:HB2	2.03	0.40
1:B:778:LEU:H	1:B:779:PRO:HD2	1.86	0.40
1:B:791:ARG:H	1:B:791:ARG:HG2	1.69	0.40
1:B:896:LYS:HE2	1:B:896:LYS:HB3	1.88	0.40
1:B:1165:ILE:O	1:B:1166:ARG:HG2	2.21	0.40
1:B:1534:HIS:CE1	1:B:1536:GLN:HB2	2.56	0.40
1:B:2024:VAL:HG12	1:B:2026:LYS:HG3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	1722/1747 (99%)	1559 (90%)	144 (8%)	19 (1%)	11	41

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	723	VAL
1	B	750	LEU
1	B	868	ILE
1	B	1907	GLU
1	B	754	GLU
1	B	1053	GLU
1	B	1054	GLU
1	B	1486	ARG
1	B	790	THR
1	B	1988	MET
1	B	2044	GLU
1	B	2100	GLY
1	B	1991	GLU
1	B	778	LEU
1	B	810	VAL
1	B	1055	PRO
1	B	779	PRO
1	B	1326	PRO
1	B	857	GLY

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1543/1561 (99%)	1543 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	768	GLN
1	B	918	ASN
1	B	940	HIS
1	B	967	ASN
1	B	978	ASN
1	B	995	ASN
1	B	1175	HIS
1	B	1189	HIS
1	B	1329	ASN
1	B	1402	ASN
1	B	1536	GLN
1	B	1772	ASN
1	B	1784	HIS
1	B	1791	GLN
1	B	1814	ASN
1	B	1933	ASN
1	B	1951	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 oligosaccharides 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 ⓘ

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	1724/1747 (98%)	0.29	45 (2%) 57 36	64, 112, 181, 223	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	723	VAL	4.2
1	B	782	PHE	3.9
1	B	1487	ILE	3.7
1	B	797	VAL	3.3
1	B	605	TYR	3.2
1	B	722	LEU	3.1
1	B	856	ALA	3.1
1	B	783	ALA	3.0
1	B	575	LEU	2.9
1	B	859	PRO	2.9
1	B	869	LEU	2.9
1	B	784	ILE	2.8
1	B	1601	LEU	2.8
1	B	773	GLU	2.7
1	B	809	LEU	2.7
1	B	771	ASN	2.7
1	B	600	GLY	2.6
1	B	1493	SER	2.5
1	B	778	LEU	2.5
1	B	1485	ILE	2.5
1	B	715	HIS	2.5
1	B	827	ILE	2.4
1	B	826	VAL	2.4
1	B	1050	GLU	2.4
1	B	1577	LEU	2.4
1	B	704	MET	2.3
1	B	821	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	735	ALA	2.3
1	B	1632	VAL	2.3
1	B	1135	LEU	2.2
1	B	829	LYS	2.2
1	B	868	ILE	2.2
1	B	732	GLY	2.2
1	B	574	GLN	2.2
1	B	452	PRO	2.2
1	B	1065	ALA	2.1
1	B	1911	ASP	2.1
1	B	1161	ILE	2.1
1	B	831	THR	2.1
1	B	1331	ILE	2.1
1	B	764	THR	2.1
1	B	1359	CYS	2.1
1	B	542	ALA	2.0
1	B	802	ALA	2.0
1	B	774	LEU	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 oligosaccharides 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.