



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:16 AM UTC

PDB ID : 3AU5 / pdb_00003au5
Title : Structure of the human myosin-X MyTH4-FERM cassette
Authors : Hirano, Y.; Takahashi, A.; Hakoshima, T.
Deposited on : 2011-01-28
Resolution : 2.55 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

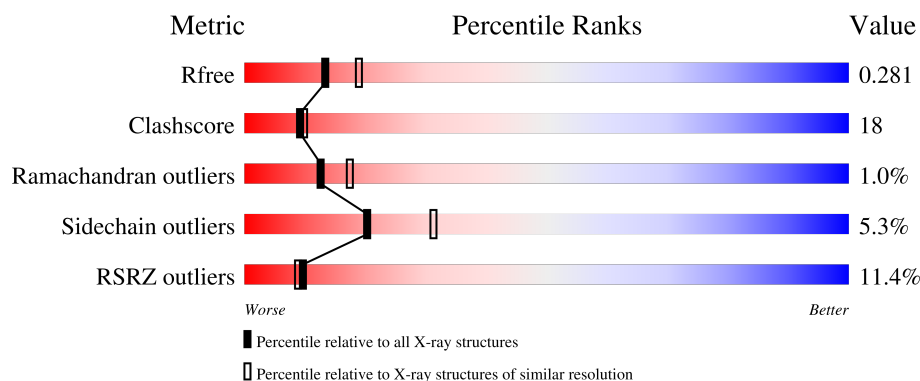
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	A	555	7% 65% 21% • 11%
1	B	555	13% 53% 30% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7782 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 Myosin-X.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			3856	2479	644	713	20			
1	B	484	Total	C	N	O	S	0	0	0
			3832	2465	642	706	19			

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1484	GLY	-	expression tag	UNP Q9HD67
A	1485	PRO	-	expression tag	UNP Q9HD67
A	1663	THR	SER	SEE REMARK 999	UNP Q9HD67
A	?	-	THR	deletion	UNP Q9HD67
A	?	-	PRO	deletion	UNP Q9HD67
A	?	-	CYS	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	LEU	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67
A	?	-	LYS	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	THR	deletion	UNP Q9HD67
A	?	-	SER	deletion	UNP Q9HD67
A	?	-	PHE	deletion	UNP Q9HD67
A	?	-	LEU	deletion	UNP Q9HD67
A	?	-	GLU	deletion	UNP Q9HD67
A	?	-	GLY	deletion	UNP Q9HD67
A	?	-	THR	deletion	UNP Q9HD67
A	?	-	LEU	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
A	?	-	ARG	deletion	UNP Q9HD67
B	1484	GLY	-	expression tag	UNP Q9HD67
B	1485	PRO	-	expression tag	UNP Q9HD67

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1663	THR	SER	SEE REMARK 999	UNP Q9HD67
B	?	-	THR	deletion	UNP Q9HD67
B	?	-	PRO	deletion	UNP Q9HD67
B	?	-	CYS	deletion	UNP Q9HD67
B	?	-	GLU	deletion	UNP Q9HD67
B	?	-	ARG	deletion	UNP Q9HD67
B	?	-	LEU	deletion	UNP Q9HD67
B	?	-	GLU	deletion	UNP Q9HD67
B	?	-	LYS	deletion	UNP Q9HD67
B	?	-	ARG	deletion	UNP Q9HD67
B	?	-	ARG	deletion	UNP Q9HD67
B	?	-	THR	deletion	UNP Q9HD67
B	?	-	SER	deletion	UNP Q9HD67
B	?	-	PHE	deletion	UNP Q9HD67
B	?	-	LEU	deletion	UNP Q9HD67
B	?	-	GLU	deletion	UNP Q9HD67
B	?	-	GLY	deletion	UNP Q9HD67
B	?	-	THR	deletion	UNP Q9HD67
B	?	-	LEU	deletion	UNP Q9HD67
B	?	-	ARG	deletion	UNP Q9HD67
B	?	-	ARG	deletion	UNP Q9HD67

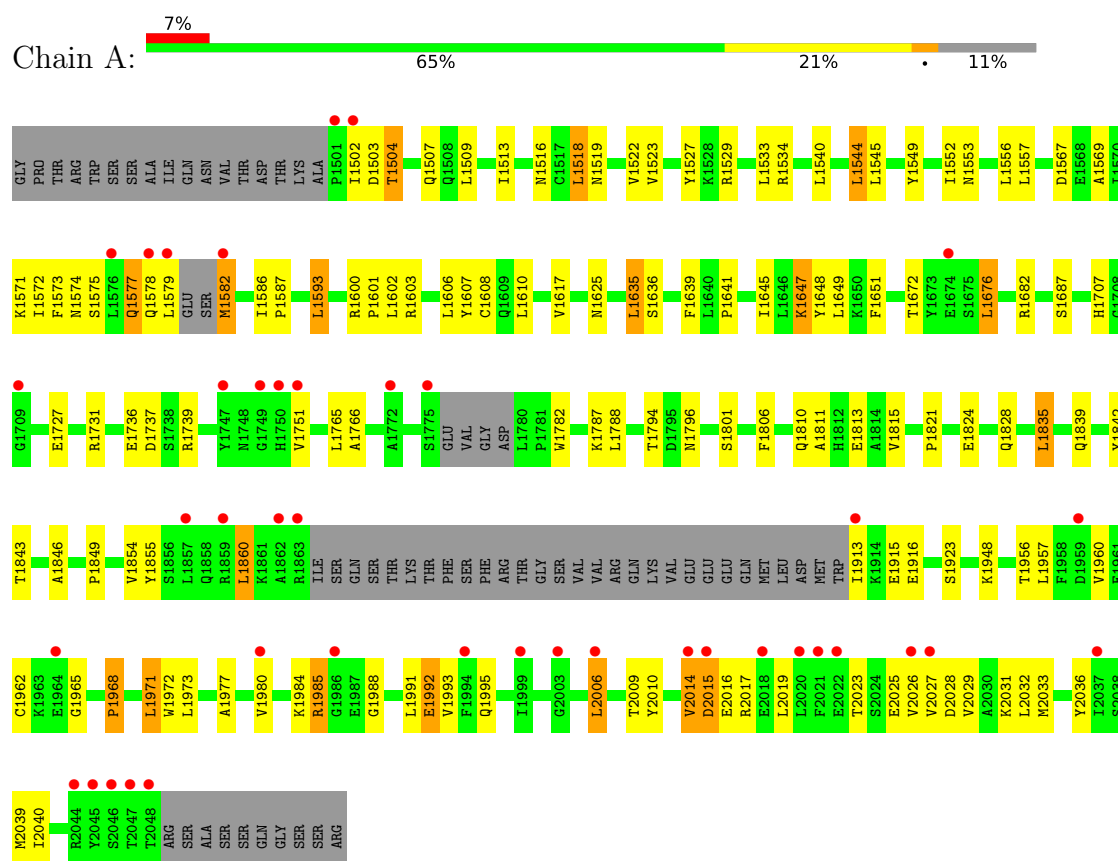
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	62	Total O 62 62	0	0
2	B	32	Total O 32 32	0	0

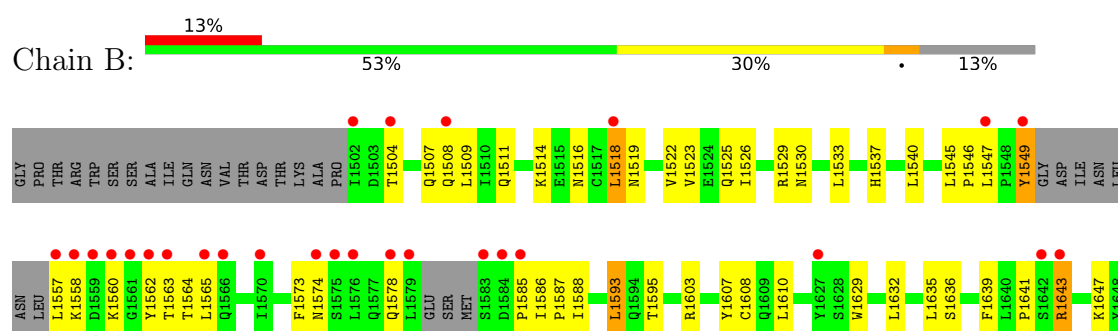
3 Residue-property plots

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: Myosin-X



• Molecule 1: Myosin-X





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.56Å 49.31Å 158.41Å 90.00° 93.58° 90.00°	Depositor
Resolution (Å)	32.68 – 2.55 32.68 – 2.55	Depositor EDS
% Data completeness (in resolution range)	91.9 (32.68-2.55) 91.9 (32.68-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.11 (at 2.54Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.236 , 0.281 0.236 , 0.281	Depositor DCC
R_{free} test set	2021 reflections (4.74%)	wwPDB-VP
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 52.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7782	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.67 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.0648e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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	A	0.60	0/3945	0.91	3/5355 (0.1%)
1	B	0.47	0/3921	0.88	9/5314 (0.2%)
All	All	0.54	0/7866	0.90	12/10669 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	2016	GLU	N-CA-C	-7.99	103.51	113.18
1	A	1577	GLN	N-CA-C	-7.17	104.15	114.12
1	A	2014	VAL	N-CA-C	-6.88	98.21	108.12
1	B	1530	ASN	CA-C-N	6.73	126.52	119.05
1	B	1530	ASN	C-N-CA	6.73	126.52	119.05
1	B	1733	LEU	N-CA-C	-6.10	105.13	113.30
1	B	1787	LYS	N-CA-C	6.03	117.41	108.60
1	A	1971	LEU	N-CA-C	5.79	119.12	110.14
1	B	1685	VAL	CA-C-N	5.67	126.93	119.84
1	B	1685	VAL	C-N-CA	5.67	126.93	119.84
1	B	1936	GLN	N-CA-C	5.24	117.00	111.28
1	B	1748	ASN	N-CA-C	-5.06	106.36	112.88

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	A	3856	0	3751	105	0
1	B	3832	0	3740	175	0
2	A	62	0	0	2	0
2	B	32	0	0	2	0
All	All	7782	0	7491	276	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 18.

All (276) 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:1643:ARG:H	1:B:1643:ARG:HD2	1.21	1.01
1:A:1962:CYS:HB2	1:A:1971:LEU:HD22	1.47	0.97
1:B:2027:VAL:HG12	1:B:2031:LYS:HE3	1.52	0.91
1:B:2006:LEU:HD13	1:B:2008:ASN:H	1.37	0.89
1:B:1504:THR:HG22	1:B:1507:GLN:HB2	1.55	0.88
1:B:1518:LEU:H	1:B:1518:LEU:HD22	1.36	0.88
1:A:1540:LEU:H	1:A:1574:ASN:HD21	1.18	0.86
1:B:2000:LEU:HD12	1:B:2013:VAL:HG12	1.60	0.83
1:B:1747:TYR:HD1	1:B:1752:ASP:HB3	1.42	0.83
1:B:1960:VAL:HG23	1:B:1971:LEU:HB3	1.62	0.82
1:B:1516:ASN:HB3	1:B:1522:VAL:HG11	1.62	0.81
1:B:2009:THR:HG23	1:B:2020:LEU:HD11	1.63	0.80
1:A:1707:HIS:HE1	1:A:1787:LYS:HE3	1.47	0.80
1:B:1984:LYS:HG3	1:B:1987:GLU:CD	2.07	0.79
1:A:1835:LEU:HD13	1:A:1854:VAL:HG11	1.64	0.79
1:B:1549:TYR:HB3	1:B:1565:LEU:HD22	1.66	0.77
1:A:1567:ASP:OD2	1:A:1571:LYS:HE3	1.85	0.77
1:A:1860:LEU:HD13	1:A:1913:ILE:HD12	1.68	0.75
1:A:1636:SER:HB2	1:A:1676:LEU:HD13	1.67	0.75
1:B:1636:SER:HB2	1:B:1676:LEU:HD13	1.68	0.75
1:A:1739:ARG:HH21	1:A:1796:ASN:HB2	1.51	0.74
1:B:2006:LEU:HB3	1:B:2009:THR:HB	1.70	0.73
1:A:1843:THR:OG1	1:A:1846:ALA:HB2	1.89	0.73
1:A:1647:LYS:NZ	1:A:1647:LYS:HB3	2.04	0.72
1:B:2006:LEU:CD1	1:B:2008:ASN:H	2.02	0.72
1:B:1747:TYR:CD1	1:B:1752:ASP:HB3	2.25	0.71
1:B:1643:ARG:H	1:B:1643:ARG:CD	2.02	0.71
1:A:1504:THR:HG21	1:A:1544:LEU:O	1.90	0.71
1:B:1721:THR:HB	1:B:1757:SER:O	1.90	0.71
1:B:1984:LYS:H	1:B:1984:LYS:CD	2.04	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2029:VAL:HG12	1:A:2033:MET:HE3	1.72	0.71
1:A:1504:THR:HG22	1:A:1507:GLN:HG3	1.72	0.71
1:A:1739:ARG:HH21	1:A:1796:ASN:CB	2.06	0.69
1:A:2029:VAL:CG1	1:A:2033:MET:HE3	2.24	0.68
1:B:1607:TYR:CD2	1:B:1641:PRO:HB3	2.28	0.68
1:B:2020:LEU:HD13	1:B:2021:PHE:N	2.07	0.68
1:B:1509:LEU:HB3	1:B:1533:LEU:HD11	1.75	0.68
1:B:1782:TRP:O	1:B:1783:LYS:HG3	1.94	0.68
1:B:1522:VAL:HG13	1:B:1523:VAL:N	2.09	0.68
1:A:1835:LEU:CD1	1:A:1854:VAL:HG11	2.24	0.67
1:B:1657:ARG:HG2	1:B:1666:GLU:HG2	1.76	0.67
1:B:1746:GLU:HG2	1:B:1782:TRP:CE3	2.29	0.67
1:A:1593:LEU:HD12	1:A:1635:LEU:HD12	1.76	0.66
1:B:1700:MET:HE2	1:B:1765:LEU:HD23	1.77	0.66
1:B:1744:LEU:HB3	1:B:1755:ILE:HD12	1.79	0.65
1:A:1636:SER:HB3	1:A:1672:THR:HG23	1.78	0.65
1:A:1647:LYS:HD2	1:B:2000:LEU:HD21	1.78	0.65
1:B:1522:VAL:HG13	1:B:1523:VAL:H	1.60	0.65
1:B:1979:ALA:HB2	1:B:1995:GLN:HA	1.78	0.65
1:A:1519:ASN:HB3	1:A:1522:VAL:CG1	2.27	0.65
1:A:1579:LEU:HG	1:A:1582:MET:HE1	1.80	0.64
1:B:1507:GLN:HE22	1:B:1546:PRO:HG2	1.62	0.64
1:A:1962:CYS:HB2	1:A:1971:LEU:CD2	2.27	0.64
1:B:1962:CYS:SG	1:B:1967:PHE:HB2	2.38	0.63
1:B:1657:ARG:NH1	1:B:1670:LEU:HD13	2.14	0.63
1:B:1984:LYS:HD2	1:B:1991:LEU:HD13	1.80	0.63
1:B:1649:LEU:O	1:B:1653:LEU:HG	1.98	0.63
1:A:1519:ASN:HB3	1:A:1522:VAL:HG12	1.80	0.63
1:B:1696:HIS:O	1:B:1698:GLN:HG3	1.99	0.62
1:B:1850:PRO:O	1:B:1853:GLU:HB2	1.99	0.61
1:B:2009:THR:HG23	1:B:2020:LEU:CD1	2.30	0.61
1:B:2005:PRO:HD2	1:B:2009:THR:HG22	1.83	0.61
1:A:1502:ILE:HG13	1:A:1503:ASP:H	1.64	0.60
1:A:1647:LYS:HD2	1:B:2000:LEU:CD2	2.31	0.60
1:A:1977:ALA:HA	1:A:2036:TYR:CD1	2.37	0.60
1:B:1546:PRO:O	1:B:1547:LEU:HD23	2.02	0.60
1:A:1603:ARG:HG2	1:A:1639:PHE:CE2	2.37	0.60
1:A:1575:SER:O	1:A:1578:GLN:HG2	2.02	0.59
1:A:2010:TYR:HB2	1:A:2026:VAL:HG12	1.84	0.59
1:B:1660:PHE:O	1:B:1666:GLU:HB2	2.02	0.59
1:B:1782:TRP:C	1:B:1783:LYS:HG3	2.27	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1707:HIS:CE1	1:A:1787:LYS:HE3	2.33	0.59
1:B:1863:ARG:HD2	1:B:1863:ARG:O	2.03	0.59
1:A:1553:ASN:HB3	1:A:1556:LEU:HB2	1.85	0.58
1:A:1645:ILE:N	1:A:1645:ILE:HD12	2.18	0.58
1:B:1593:LEU:HD12	1:B:1635:LEU:HD12	1.85	0.58
1:B:1707:HIS:ND1	1:B:1813:GLU:HG3	2.18	0.58
1:B:2006:LEU:HD13	1:B:2007:ALA:N	2.19	0.58
1:B:1767:LYS:HG2	1:B:1771:LEU:HD12	1.84	0.58
1:A:1980:VAL:O	1:A:1980:VAL:HG23	2.02	0.58
1:A:2039:MET:HA	1:A:2039:MET:HE2	1.85	0.58
1:A:1727:GLU:O	1:A:1731:ARG:HG2	2.04	0.57
1:B:1984:LYS:H	1:B:1984:LYS:HD3	1.68	0.57
1:A:1549:TYR:HD1	1:A:1552:ILE:HG21	1.70	0.57
1:A:1962:CYS:HB3	1:A:1968:PRO:O	2.05	0.57
1:B:1959:ASP:CG	1:B:1985:ARG:HH12	2.13	0.57
1:B:1504:THR:HG21	1:B:1545:LEU:HA	1.87	0.56
1:B:1522:VAL:O	1:B:1526:ILE:HG13	2.05	0.56
1:B:1842:TYR:CD1	1:B:1842:TYR:C	2.84	0.56
1:B:1511:GLN:HE22	1:B:1514:LYS:HD3	1.69	0.56
1:B:1920:ALA:O	1:B:1924:ILE:HG13	2.05	0.56
1:B:1518:LEU:H	1:B:1518:LEU:CD2	2.13	0.56
1:A:2023:THR:HG23	1:A:2026:VAL:HG13	1.88	0.55
1:A:1811:ALA:O	1:A:1815:VAL:HG23	2.05	0.55
1:B:1816:ILE:HA	1:B:1856:SER:HB2	1.89	0.55
1:B:1562:TYR:CE1	1:B:1595:THR:HG23	2.42	0.55
1:B:1959:ASP:HB3	1:B:1985:ARG:HH22	1.72	0.55
1:A:1647:LYS:HB3	1:A:1647:LYS:HZ2	1.71	0.55
1:B:1516:ASN:HB3	1:B:1522:VAL:CG1	2.35	0.55
1:A:1553:ASN:CB	1:A:1556:LEU:HD12	2.37	0.55
1:A:1824:GLU:O	1:A:1828:GLN:HG3	2.06	0.55
1:B:1643:ARG:HD2	1:B:1643:ARG:N	2.05	0.55
1:B:2037:ILE:O	1:B:2041:VAL:HG23	2.06	0.55
1:A:2017:ARG:HG2	1:A:2019:LEU:HD21	1.88	0.54
1:B:2025:GLU:HB2	1:B:2028:ASP:OD2	2.07	0.54
1:A:1557:LEU:HD23	1:A:1557:LEU:C	2.33	0.54
1:B:1650:LYS:HE2	1:B:1673:TYR:HE1	1.72	0.54
1:B:2004:ALA:HA	1:B:2009:THR:O	2.08	0.54
1:B:1852:GLU:HA	1:B:1855:TYR:O	2.08	0.54
1:B:1799:LYS:O	1:B:1800:ASP:CG	2.50	0.53
1:A:1607:TYR:CD2	1:A:1641:PRO:HB3	2.44	0.53
1:B:1690:GLU:HG3	1:B:1700:MET:SD	2.48	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1979:ALA:CB	1:B:1995:GLN:HA	2.39	0.53
1:B:1984:LYS:CD	1:B:1991:LEU:HD13	2.38	0.53
1:B:2006:LEU:HD13	1:B:2008:ASN:N	2.17	0.53
1:A:1518:LEU:HD11	1:B:1997:GLU:HG2	1.91	0.53
1:A:1824:GLU:OE2	1:A:1855:TYR:OH	2.27	0.53
1:B:1726:VAL:HG21	1:B:1743:ALA:HA	1.91	0.53
1:B:1984:LYS:HG3	1:B:1987:GLU:OE2	2.07	0.53
1:B:1700:MET:HE2	1:B:1765:LEU:CD2	2.39	0.53
1:B:2023:THR:O	1:B:2026:VAL:HG13	2.09	0.53
1:B:2006:LEU:HB3	1:B:2009:THR:CB	2.37	0.53
1:B:1765:LEU:HD13	1:B:1784:PHE:CE2	2.44	0.52
1:B:1925:ILE:O	1:B:1929:ARG:HG3	2.09	0.52
1:B:1800:ASP:OD2	1:B:1800:ASP:C	2.53	0.52
1:A:1682:ARG:HD3	2:A:49:HOH:O	2.08	0.52
1:B:1740:ASN:HB3	1:B:1790:CYS:O	2.09	0.52
1:B:1746:GLU:HG3	1:B:1768:PHE:CE1	2.45	0.52
1:B:1821:PRO:HA	2:B:92:HOH:O	2.09	0.51
1:A:1645:ILE:HD12	1:A:1645:ILE:H	1.76	0.51
1:A:1572:ILE:HD13	1:A:1606:LEU:HD21	1.92	0.50
1:A:1518:LEU:CD1	1:B:1997:GLU:HG2	2.41	0.50
1:B:1700:MET:CE	1:B:1765:LEU:HD23	2.42	0.50
1:A:1649:LEU:HD23	1:A:1676:LEU:HD21	1.93	0.50
1:A:1617:VAL:HG11	1:A:1625:ASN:ND2	2.26	0.50
1:A:1593:LEU:CD1	1:A:1635:LEU:HD12	2.40	0.50
1:B:1545:LEU:HD11	1:B:1608:CYS:SG	2.52	0.50
1:B:1746:GLU:HG3	1:B:1768:PHE:HE1	1.76	0.50
1:A:2036:TYR:O	1:A:2040:ILE:HG13	2.11	0.49
1:B:2020:LEU:HD13	1:B:2021:PHE:H	1.74	0.49
1:B:1812:HIS:HA	1:B:1943:TYR:OH	2.12	0.49
1:A:1736:GLU:HG2	1:A:1737:ASP:N	2.28	0.49
1:A:2017:ARG:NH1	1:A:2019:LEU:HD21	2.27	0.49
1:B:1504:THR:HG22	1:B:1507:GLN:CB	2.33	0.49
1:B:1841:ASP:OD1	1:B:1932:GLN:HA	2.12	0.49
1:A:1860:LEU:HD11	1:A:1916:GLU:CB	2.43	0.48
1:A:2028:ASP:HA	1:A:2031:LYS:HZ2	1.76	0.48
1:B:1507:GLN:HE22	1:B:1546:PRO:CG	2.25	0.48
1:B:1861:LYS:O	1:B:1861:LYS:HG2	2.12	0.48
1:B:1984:LYS:CD	1:B:1984:LYS:N	2.72	0.48
1:B:1995:GLN:O	1:B:1999:ILE:HG13	2.12	0.48
1:A:1553:ASN:HB3	1:A:1556:LEU:HD12	1.96	0.48
1:B:1558:LYS:C	1:B:1560:LYS:H	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1649:LEU:CD2	1:A:1676:LEU:HD21	2.44	0.48
1:B:1518:LEU:HD22	1:B:1518:LEU:N	2.17	0.48
1:B:1504:THR:HG23	1:B:1507:GLN:H	1.79	0.48
1:A:1962:CYS:CB	1:A:1971:LEU:HD22	2.32	0.48
1:B:1716:ILE:HD13	1:B:1761:VAL:CG1	2.43	0.48
1:B:1934:MET:HA	1:B:1938:GLN:NE2	2.28	0.47
1:B:1657:ARG:HH11	1:B:1670:LEU:HD13	1.79	0.47
1:B:1824:GLU:HG3	1:B:1828:GLN:NE2	2.29	0.47
1:B:2006:LEU:HD13	1:B:2006:LEU:C	2.39	0.47
1:A:1960:VAL:HG12	1:A:2023:THR:HB	1.97	0.47
1:A:1801:SER:HB2	2:A:52:HOH:O	2.14	0.47
1:B:1765:LEU:HD13	1:B:1784:PHE:HE2	1.79	0.47
1:B:1707:HIS:CG	1:B:1813:GLU:HG3	2.50	0.47
1:B:1730:ILE:C	1:B:1732:GLY:H	2.23	0.47
1:B:1823:PRO:O	1:B:1824:GLU:C	2.57	0.47
1:B:1970:GLU:O	1:B:1984:LYS:O	2.32	0.47
1:A:1575:SER:C	1:A:1577:GLN:H	2.22	0.47
1:A:1860:LEU:HD11	1:A:1916:GLU:HB2	1.97	0.47
1:B:1574:ASN:O	1:B:1578:GLN:HG2	2.16	0.47
1:A:2017:ARG:HG2	1:A:2019:LEU:CD2	2.44	0.46
1:B:1522:VAL:CG1	1:B:1523:VAL:N	2.77	0.46
1:B:1950:TRP:HE1	1:B:1988:GLY:HA2	1.79	0.46
1:A:1821:PRO:CG	1:A:1988:GLY:HA2	2.45	0.46
1:A:2015:ASP:C	1:A:2017:ARG:H	2.24	0.46
1:B:1603:ARG:HG2	1:B:1639:PHE:CE2	2.50	0.46
1:B:1756:GLU:OE2	1:B:2031:LYS:HE2	2.15	0.46
1:B:2002:PHE:HA	1:B:2011:LYS:O	2.15	0.46
1:A:1509:LEU:HB3	1:A:1533:LEU:HD11	1.98	0.46
1:A:1647:LYS:HB3	1:A:1647:LYS:HZ3	1.80	0.46
1:B:1974:GLY:O	1:B:1980:VAL:HA	2.14	0.46
1:B:1808:PHE:HE1	1:B:1943:TYR:CG	2.33	0.46
1:A:1806:PHE:O	1:A:1810:GLN:HB2	2.16	0.46
1:B:1523:VAL:HA	1:B:1526:ILE:HD12	1.98	0.45
1:B:1799:LYS:O	1:B:1800:ASP:OD2	2.34	0.45
1:A:1569:ALA:HB2	1:A:1602:LEU:HD21	1.99	0.45
1:B:1767:LYS:HG2	1:B:1771:LEU:CD1	2.46	0.45
1:A:1839:GLN:OE1	1:A:1849:PRO:HD3	2.16	0.45
1:A:2015:ASP:OD1	1:A:2017:ARG:HB2	2.17	0.45
1:A:1519:ASN:CB	1:A:1522:VAL:HG12	2.44	0.45
1:A:1751:VAL:HG11	1:A:1782:TRP:HH2	1.82	0.45
1:B:1578:GLN:NE2	2:B:67:HOH:O	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1545:LEU:HD11	1:A:1608:CYS:SG	2.57	0.45
1:B:2038:SER:O	1:B:2042:LYS:HD3	2.17	0.45
1:A:1586:ILE:HB	1:A:1587:PRO:HD3	1.98	0.45
1:B:1746:GLU:HG2	1:B:1782:TRP:CZ3	2.52	0.45
1:A:1828:GLN:NE2	1:A:1923:SER:OG	2.47	0.45
1:A:1980:VAL:O	1:A:1980:VAL:CG2	2.65	0.45
1:A:1984:LYS:O	1:A:1985:ARG:C	2.60	0.44
1:A:1687:SER:HB3	1:A:1766:ALA:HA	1.99	0.44
1:B:1733:LEU:HD13	1:B:1735:MET:HE2	1.99	0.44
1:B:1525:GLN:O	1:B:1529:ARG:HB2	2.17	0.44
1:A:1502:ILE:HG13	1:A:1503:ASP:N	2.32	0.44
1:B:2006:LEU:HD22	1:B:2007:ALA:H	1.83	0.44
1:B:2027:VAL:O	1:B:2031:LYS:HG3	2.18	0.44
1:A:2025:GLU:O	1:A:2029:VAL:HG23	2.17	0.44
1:B:1522:VAL:HG13	1:B:1523:VAL:HG23	1.99	0.44
1:B:1911:MET:O	1:B:1915:GLU:CB	2.66	0.44
1:B:1959:ASP:CG	1:B:1985:ARG:NH1	2.76	0.44
1:A:1648:TYR:O	1:A:1651:PHE:HB3	2.17	0.44
1:B:1636:SER:HB3	1:B:1672:THR:HG23	1.98	0.44
1:B:1519:ASN:HB3	1:B:1522:VAL:CG1	2.48	0.43
1:B:1819:HIS:HD2	1:B:1957:LEU:HB2	1.83	0.43
1:B:1745:PHE:CE2	1:B:1787:LYS:HG3	2.54	0.43
1:B:1972:TRP:HB2	1:B:1983:TYR:HB2	2.00	0.43
1:A:1582:MET:N	1:A:1582:MET:HE2	2.34	0.43
1:B:1655:ARG:HH11	1:B:1655:ARG:HG2	1.83	0.43
1:B:1740:ASN:HB3	1:B:1788:LEU:HD11	2.01	0.43
1:B:1983:TYR:CE2	1:B:1990:PRO:HB3	2.54	0.43
1:A:2006:LEU:HB3	1:A:2009:THR:OG1	2.19	0.43
1:B:1753:LYS:HB2	1:B:1753:LYS:HE3	1.81	0.43
1:B:1522:VAL:CG1	1:B:1523:VAL:H	2.27	0.43
1:B:1721:THR:HA	1:B:1759:THR:O	2.19	0.43
1:A:2010:TYR:HE2	1:A:2033:MET:HE1	1.83	0.42
1:B:1686:PRO:HA	1:B:1690:GLU:OE1	2.19	0.42
1:B:1984:LYS:HG2	1:B:1987:GLU:HB2	2.00	0.42
1:B:2009:THR:CG2	1:B:2020:LEU:HD11	2.42	0.42
1:A:1569:ALA:HB2	1:A:1602:LEU:CD2	2.49	0.42
1:A:2014:VAL:O	1:A:2015:ASP:CG	2.62	0.42
1:B:1842:TYR:HB2	1:B:1928:TRP:CD2	2.54	0.42
1:B:1557:LEU:HG	1:B:1558:LYS:N	2.34	0.42
1:A:1573:PHE:O	1:A:1577:GLN:HB2	2.19	0.42
1:B:1911:MET:O	1:B:1915:GLU:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1707:HIS:CD2	1:A:1813:GLU:HG3	2.55	0.42
1:B:1636:SER:CB	1:B:1672:THR:HG23	2.49	0.42
1:A:1960:VAL:HG21	1:A:1973:LEU:HD13	2.01	0.42
1:B:1643:ARG:O	1:B:1647:LYS:HG3	2.19	0.42
1:B:1735:MET:C	1:B:1737:ASP:N	2.77	0.42
1:A:1956:THR:HB	1:A:2032:LEU:HD21	2.02	0.41
1:A:1991:LEU:O	1:A:1992:GLU:HB2	2.20	0.41
1:B:1562:TYR:OH	1:B:1595:THR:HA	2.19	0.41
1:B:1585:PRO:O	1:B:1586:ILE:C	2.63	0.41
1:B:1586:ILE:HB	1:B:1587:PRO:HD3	2.02	0.41
1:B:1629:TRP:CZ3	1:B:1632:LEU:HD23	2.54	0.41
1:B:1657:ARG:CG	1:B:1666:GLU:HG2	2.47	0.41
1:A:1794:THR:O	1:A:1948:LYS:NZ	2.33	0.41
1:B:1649:LEU:HD23	1:B:1676:LEU:HD21	2.02	0.41
1:B:1563:THR:OG1	1:B:1564:THR:N	2.53	0.41
1:B:1971:LEU:HA	1:B:1984:LYS:O	2.20	0.41
1:A:1516:ASN:HB3	1:A:1522:VAL:HG11	2.03	0.41
1:B:1835:LEU:HD12	1:B:1835:LEU:HA	1.94	0.41
1:A:1960:VAL:HG12	1:A:2023:THR:CB	2.51	0.41
1:B:1540:LEU:HB2	1:B:1573:PHE:CD2	2.56	0.41
1:B:1950:TRP:NE1	1:B:1988:GLY:HA2	2.35	0.41
1:B:1585:PRO:O	1:B:1588:ILE:N	2.53	0.41
1:B:1562:TYR:HE1	1:B:1595:THR:HG23	1.83	0.41
1:B:1851:LEU:C	1:B:1853:GLU:H	2.29	0.41
1:B:1984:LYS:CE	1:B:1991:LEU:HD13	2.50	0.41
1:A:1600:ARG:HB2	1:A:1601:PRO:HD3	2.03	0.41
1:A:1915:GLU:OE2	1:A:1915:GLU:HA	2.19	0.41
1:B:1800:ASP:OD2	1:B:1801:SER:N	2.53	0.41
1:B:1991:LEU:HD12	1:B:1991:LEU:HA	1.91	0.41
1:A:1503:ASP:HA	1:A:1507:GLN:OE1	2.21	0.41
1:B:1657:ARG:NE	1:B:1666:GLU:OE2	2.54	0.41
1:A:1527:TYR:O	1:A:1534:ARG:NE	2.49	0.40
1:B:1735:MET:C	1:B:1737:ASP:H	2.29	0.40
1:B:1858:GLN:C	1:B:1860:LEU:N	2.78	0.40
1:B:1811:ALA:O	1:B:1815:VAL:HG23	2.21	0.40
1:A:1513:ILE:HG23	1:A:1523:VAL:HG22	2.03	0.40
1:A:1516:ASN:HB3	1:A:1522:VAL:CG1	2.51	0.40
1:B:1829:VAL:HG22	1:B:1927:LYS:HD3	2.03	0.40
1:B:1522:VAL:HG22	1:B:1526:ILE:HD11	2.03	0.40
1:B:1748:ASN:ND2	1:B:1780:LEU:HD13	2.36	0.40
1:B:2006:LEU:O	1:B:2007:ALA:C	2.64	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	A	485/555 (87%)	450 (93%)	29 (6%)	6 (1%)	10	13
1	B	474/555 (85%)	424 (90%)	46 (10%)	4 (1%)	16	22
All	All	959/1110 (86%)	874 (91%)	75 (8%)	10 (1%)	12	17

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1985	ARG
1	A	1985	ARG
1	B	1844	LEU
1	A	2015	ASP
1	A	2016	GLU
1	B	1686	PRO
1	B	1965	GLY
1	A	1965	GLY
1	A	1992	GLU
1	A	1968	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 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	A	407/492 (83%)	386 (95%)	21 (5%)	21	32

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	406/492 (82%)	384 (95%)	22 (5%)	20	30
All	All	813/984 (83%)	770 (95%)	43 (5%)	20	31

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1504	THR
1	A	1518	LEU
1	A	1529	ARG
1	A	1544	LEU
1	A	1582	MET
1	A	1593	LEU
1	A	1610	LEU
1	A	1635	LEU
1	A	1647	LYS
1	A	1676	LEU
1	A	1765	LEU
1	A	1788	LEU
1	A	1835	LEU
1	A	1842	TYR
1	A	1860	LEU
1	A	1957	LEU
1	A	1972	TRP
1	A	1993	VAL
1	A	1995	GLN
1	A	2006	LEU
1	A	2027	VAL
1	B	1508	GLN
1	B	1518	LEU
1	B	1537	HIS
1	B	1549	TYR
1	B	1593	LEU
1	B	1610	LEU
1	B	1643	ARG
1	B	1676	LEU
1	B	1724	GLU
1	B	1737	ASP
1	B	1788	LEU
1	B	1835	LEU
1	B	1842	TYR
1	B	1858	GLN
1	B	1972	TRP

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Mol	Chain	Res	Type
1	B	1980	VAL
1	B	1984	LYS
1	B	1991	LEU
1	B	2011	LYS
1	B	2020	LEU
1	B	2026	VAL
1	B	2042	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1508	GLN
1	A	1538	HIS
1	A	1541	HIS
1	A	1566	GLN
1	A	1574	ASN
1	A	1707	HIS
1	A	1796	ASN
1	A	1817	HIS
1	A	1828	GLN
1	A	1938	GLN
1	B	1507	GLN
1	B	1508	GLN
1	B	1511	GLN
1	B	1574	ASN
1	B	1597	HIS
1	B	1659	GLN
1	B	1796	ASN
1	B	1819	HIS
1	B	1826	ASN
1	B	1858	GLN
1	B	1969	GLN
1	B	2008	ASN

5.3.3 RNA ⓘ

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 [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	A	493/555 (88%)	0.36	41 (8%) 17 17	12, 36, 77, 109	2 (0%)
1	B	484/555 (87%)	1.01	70 (14%) 6 5	30, 55, 86, 106	3 (0%)
All	All	977/1110 (88%)	0.68	111 (11%) 10 9	12, 47, 83, 109	5 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1501	PRO	6.5
1	B	1911	MET	5.1
1	B	1557	LEU	4.9
1	B	1562	TYR	4.7
1	B	1583	SER	4.5
1	A	2048	THR	4.4
1	B	1968	PRO	4.4
1	A	2045	TYR	4.4
1	B	2045	TYR	4.4
1	B	1969	GLN	4.3
1	B	1857	LEU	4.2
1	B	1912	TRP	4.1
1	B	1508	GLN	4.0
1	B	1561	GLY	4.0
1	B	1579	LEU	3.9
1	B	1549	TYR	3.9
1	A	1980	VAL	3.9
1	A	2027	VAL	3.8
1	B	1971	LEU	3.8
1	A	1579	LEU	3.7
1	B	1502	ILE	3.7
1	A	1747	TYR	3.7
1	B	1518	LEU	3.6
1	B	1844	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	1502	ILE	3.5
1	B	1913	ILE	3.4
1	B	1862	ALA	3.4
1	A	2046	SER	3.4
1	B	1780	LEU	3.3
1	A	2047	THR	3.3
1	B	1750	HIS	3.3
1	A	2014	VAL	3.2
1	A	1582	MET	3.1
1	A	1751	VAL	3.1
1	B	1989	ARG	3.0
1	A	1576	LEU	2.9
1	B	1967	PHE	2.9
1	A	2018	GLU	2.9
1	A	1863	ARG	2.9
1	B	2010	TYR	2.9
1	B	2048	THR	2.9
1	B	1560	LYS	2.9
1	B	2025	GLU	2.9
1	B	1570	ILE	2.9
1	B	1563	THR	2.8
1	A	1994	PHE	2.8
1	A	2026	VAL	2.7
1	A	1859	ARG	2.7
1	B	1736	GLU	2.7
1	B	1566	GLN	2.7
1	A	2003	GLY	2.7
1	A	2044	ARG	2.7
1	B	1961	GLU	2.7
1	A	2020	LEU	2.6
1	B	2006	LEU	2.6
1	B	1558	LYS	2.6
1	A	1964	GLU	2.6
1	B	1963	LYS	2.6
1	B	1627	TYR	2.6
1	B	2012	ILE	2.5
1	B	1773	ALA	2.5
1	B	1965	GLY	2.5
1	A	1999	ILE	2.5
1	A	2037	ILE	2.5
1	B	2047	THR	2.5
1	B	1986	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	2016	GLU	2.4
1	B	1576	LEU	2.4
1	A	1578	GLN	2.4
1	A	1772	ALA	2.4
1	A	1959	ASP	2.4
1	A	2021	PHE	2.4
1	B	2021	PHE	2.3
1	B	1575	SER	2.3
1	B	1643	ARG	2.3
1	B	1988	GLY	2.2
1	A	2006	LEU	2.2
1	A	1913	ILE	2.2
1	A	2022	GLU	2.2
1	B	2041	VAL	2.2
1	B	1504	THR	2.2
1	B	1578	GLN	2.2
1	B	1858	GLN	2.2
1	B	1860	LEU	2.2
1	B	1585	PRO	2.2
1	B	1993	VAL	2.2
1	B	1659	GLN	2.2
1	A	1749	GLY	2.2
1	A	1674	GLU	2.2
1	B	1987	GLU	2.2
1	B	2022	GLU	2.2
1	B	1859	ARG	2.2
1	A	1862	ALA	2.1
1	B	1584	ASP	2.1
1	B	1917	VAL	2.1
1	B	1574	ASN	2.1
1	B	1957	LEU	2.1
1	B	2000	LEU	2.1
1	A	1750	HIS	2.1
1	B	1565	LEU	2.1
1	A	1709	GLY	2.1
1	B	1937	GLU	2.1
1	A	1775	SER	2.1
1	B	1642	SER	2.1
1	B	1758	ARG	2.0
1	A	2015	ASP	2.0
1	B	1559	ASP	2.0
1	A	1857	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	1547	LEU	2.0
1	A	1986	GLY	2.0
1	B	1826	ASN	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.