



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:27 AM GMT

PDB ID : 3AU5
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
<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

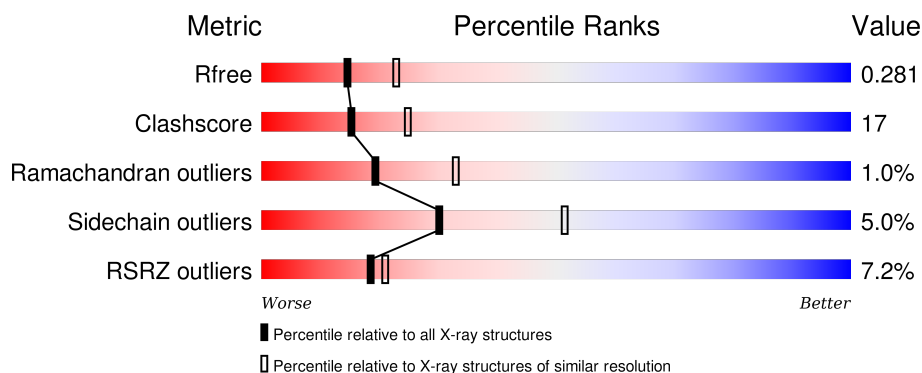
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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}	91344	4549 (2.58-2.50)
Clashscore	102246	5292 (2.58-2.50)
Ramachandran outliers	100387	5194 (2.58-2.50)
Sidechain outliers	100360	5196 (2.58-2.50)
RSRZ outliers	91569	4561 (2.58-2.50)

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 $\leq 5\%$. 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	<div> <div>5%</div> <div>65%</div> <div>21%</div> <div>•</div> <div>11%</div> </div>
1	B	555	<div> <div>8%</div> <div>54%</div> <div>30%</div> <div>•</div> <div>13%</div> </div>

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

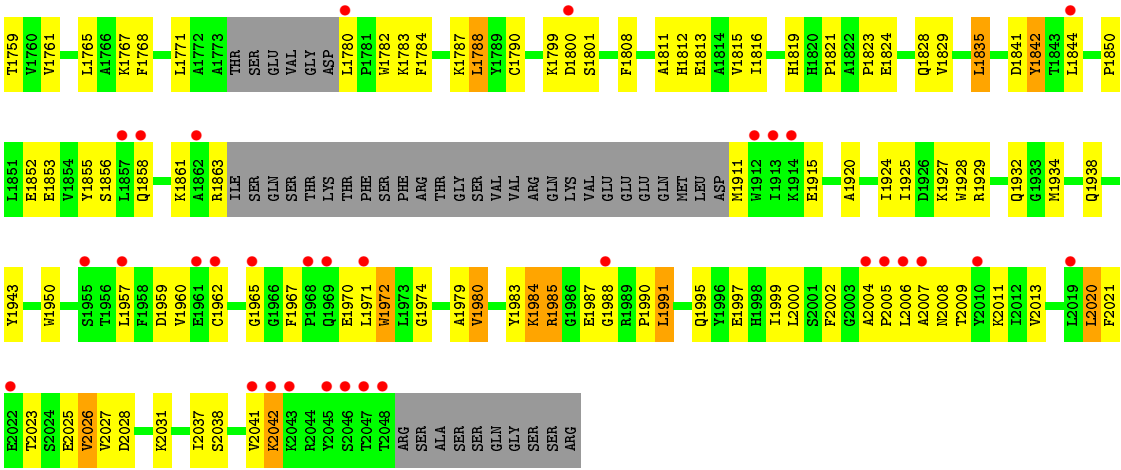
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Chain	Residue	Modelled	Actual	Comment	Reference
B	1663	THR	SER	SEE REMARK 999	UNP Q9HD67
B	?	-	THR	DELETION	UNP Q9HD67
B	?	-	PRO	DELETION	UNP Q9HD67
B	?	-	CYS	DELETION	UNP Q9HD67
B	?	-	GLU	DELETION	UNP Q9HD67
B	?	-	ARG	DELETION	UNP Q9HD67
B	?	-	LEU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



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) 92.0 (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 (5.02%)	DCC
Wilson B-factor (Å ²)	35.3	Xtriage
Anisotropy	0.378	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	2 of 42623 reflections (0.005%)	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, 0.375 respectively for untwinned datasets, and 0.333, 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	A	0.50	0/3945	0.62	0/5355
1	B	0.39	0/3921	0.55	0/5314
All	All	0.45	0/7866	0.59	0/10669

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3856	0	3751	101	0
1	B	3832	0	3740	167	0
2	A	62	0	0	2	0
2	B	32	0	0	2	0
All	All	7782	0	7491	264	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 17.

All (264) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD22	1:B:1518:LEU:H	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: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:B:1636:SER:HB2	1:B:1676:LEU:HD13	1.68	0.75
1:A:1636:SER:HB2	1:A:1676:LEU:HD13	1.67	0.75
1:B:1984:LYS:HG3	1:B:1987:GLU:CD	2.07	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:B:2006:LEU:CD1	1:B:2008:ASN:H	2.02	0.72
1:A:1647:LYS:NZ	1:A:1647:LYS:HB3	2.04	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:B:1984:LYS:H	1:B:1984:LYS:CD	2.04	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: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:B:2020:LEU:HD13	1:B:2021:PHE:N	2.07	0.68
1:B:1607:TYR:CD2	1:B:1641:PRO:HB3	2.28	0.68
1:B:1782:TRP:O	1:B:1783:LYS:HG3	1.94	0.68
1:B:1509:LEU:HB3	1:B:1533:LEU:HD11	1.75	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:1744:LEU:HB3	1:B:1755:ILE:HD12	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1647:LYS:HD2	1:B:2000:LEU:CD2	2.31	0.60
1:A:1502:ILE:HG13	1:A:1503:ASP:H	1.64	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:A:1707:HIS:CE1	1:A:1787:LYS:HE3	2.33	0.59
1:B:1863:ARG:O	1:B:1863:ARG:HD2	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:2006:LEU:HD13	1:B:2007:ALA:N	2.19	0.58
1:B:1707:HIS:ND1	1:B:1813:GLU:HG3	2.18	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:B:1984:LYS:HD3	1:B:1984:LYS:H	1.68	0.57
1:A:1727:GLU:O	1:A:1731:ARG:HG2	2.04	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1518:LEU:CD2	1:B:1518:LEU:H	2.13	0.56
1:A:2023:THR:HG23	1:A:2026:VAL:HG13	1.88	0.55
1:A:2029:VAL:HG12	1:A:2033:MET:HE3	1.87	0.55
1:B:1816:ILE:HA	1:B:1856:SER:HB2	1.89	0.55
1:A:1811:ALA:O	1:A:1815:VAL:HG23	2.05	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:A:1582:MET:HE1	1:A:1588:ILE:HD12	1.87	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:B:1643:ARG:N	1:B:1643:ARG:HD2	2.05	0.55
1:B:2037:ILE:O	1:B:2041:VAL:HG23	2.06	0.55
1:A:1824:GLU:O	1:A:1828:GLN:HG3	2.06	0.55
1:B:1782:TRP:C	1:B:1783:LYS:HG3	2.27	0.54
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:B:2004:ALA:HA	1:B:2009:THR:O	2.08	0.54
1:B:1650:LYS:HE2	1:B:1673:TYR:HE1	1.72	0.54
1:B:1984:LYS:HG3	1:B:1987:GLU:OE2	2.07	0.54
1:B:1852:GLU:HA	1:B:1855:TYR:O	2.08	0.54
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
1:B:2006:LEU:HD13	1:B:2008:ASN:N	2.17	0.53
1:B:1984:LYS:CD	1:B:1991:LEU:HD13	2.38	0.53
1:B:1979:ALA:CB	1:B:1995:GLN:HA	2.39	0.53
1:A:1824:GLU:OE2	1:A:1855:TYR:OH	2.27	0.53
1:A:1518:LEU:HD11	1:B:1997:GLU:HG2	1.91	0.53
1:B:1726:VAL:HG21	1:B:1743:ALA:HA	1.91	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:1959:ASP:CG	1:B:1985:ARG:HH12	2.13	0.52
1:A:1682:ARG:HD3	2:A:49:HOH:O	2.08	0.52
1:B:1746:GLU:HG3	1:B:1768:PHE:CE1	2.45	0.52
1:B:1740:ASN:HB3	1:B:1790:CYS:O	2.09	0.52
1:B:1842:TYR:CD1	1:B:1842:TYR:C	2.84	0.52
1:B:1821:PRO:HA	2:B:92:HOH:O	2.09	0.51
1:A:1645:ILE:H	1:A:1645:ILE:HD12	1.76	0.51
1:B:1700:MET:HE1	1:B:1765:LEU:HD23	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1572:ILE:HD13	1:A:1606:LEU:HD21	1.92	0.50
1:B:1700:MET:CE	1:B:1765:LEU:HD23	2.42	0.50
1:A:1518:LEU:CD1	1:B:1997:GLU:HG2	2.41	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: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:1593:LEU:CD1	1:A:1635:LEU:HD12	2.40	0.50
1:A:2029:VAL:CG1	1:A:2033:MET:HE3	2.42	0.50
1:B:2020:LEU:HD13	1:B:2021:PHE:H	1.74	0.49
1:A:2036:TYR:O	1:A:2040:ILE:HG13	2.11	0.49
1:A:1557:LEU:C	1:A:1557:LEU:HD23	2.33	0.49
1:B:1812:HIS:HA	1:B:1943:TYR:OH	2.12	0.49
1:B:1799:LYS:O	1:B:1800:ASP:CG	2.50	0.49
1:B:1504:THR:HG22	1:B:1507:GLN:CB	2.33	0.49
1:A:2017:ARG:NH1	1:A:2019:LEU:HD21	2.27	0.49
1:B:1841:ASP:OD1	1:B:1932:GLN:HA	2.12	0.49
1:A:1736:GLU:HG2	1:A:1737:ASP:N	2.28	0.49
1:A:2028:ASP:HA	1:A:2031:LYS:HZ2	1.76	0.49
1:A:1860:LEU:HD11	1:A:1916:GLU:CB	2.43	0.48
1:B:1507:GLN:HE22	1:B:1546:PRO:CG	2.25	0.48
1:B:1861:LYS:HG2	1:B:1861:LYS:O	2.12	0.48
1:B:1984:LYS:N	1:B:1984:LYS:CD	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:1518:LEU:HD22	1:B:1518:LEU:N	2.17	0.48
1:A:1649:LEU:CD2	1:A:1676:LEU:HD21	2.44	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:1800:ASP:C	1:B:1800:ASP:OD2	2.53	0.47
1:A:1960:VAL:HG12	1:A:2023:THR:HB	1.97	0.47
1:B:1765:LEU:HD13	1:B:1784:PHE:HE2	1.79	0.47
1:A:1801:SER:HB2	2:A:52:HOH:O	2.14	0.47
1:B:1970:GLU:O	1:B:1984:LYS:O	2.32	0.47
1:B:1707:HIS:CG	1:B:1813:GLU:HG3	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1522:VAL:CG1	1:B:1523:VAL:N	2.77	0.46
1:A:2017:ARG:HG2	1:A:2019:LEU:CD2	2.44	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: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:B:1603:ARG:HG2	1:B:1639:PHE:CE2	2.50	0.46
1:A:1647:LYS:HZ3	1:A:1647:LYS:HB3	1.80	0.46
1:B:1974:GLY:O	1:B:1980:VAL:HA	2.14	0.46
1:A:1509:LEU:HB3	1:A:1533:LEU:HD11	1.98	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:2015:ASP:OD1	1:A:2017:ARG:HB2	2.17	0.45
1:A:1839:GLN:OE1	1:A:1849:PRO:HD3	2.16	0.45
1:A:1519:ASN:CB	1:A:1522:VAL:HG12	2.44	0.45
1:B:1578:GLN:NE2	2:B:67:HOH:O	2.50	0.45
1:A:1751:VAL:HG11	1:A:1782:TRP:HH2	1.82	0.45
1:B:2038:SER:O	1:B:2042:LYS:HD3	2.17	0.45
1:A:1545:LEU:HD11	1:A:1608:CYS:SG	2.57	0.45
1:B:1746:GLU:HG2	1:B:1782:TRP:CZ3	2.52	0.45
1:A:1586:ILE:HB	1:A:1587:PRO:HD3	1.98	0.45
1:A:1980:VAL:O	1:A:1980:VAL:CG2	2.65	0.45
1:A:1828:GLN:NE2	1:A:1923:SER:OG	2.47	0.45
1:A:1687:SER:HB3	1:A:1766:ALA:HA	1.99	0.44
1:B:1525:GLN:O	1:B:1529:ARG:HB2	2.17	0.44
1:B:2006:LEU:HD22	1:B:2007:ALA:H	1.83	0.44
1:A:1502:ILE:HG13	1:A:1503:ASP:N	2.32	0.44
1:B:2027:VAL:O	1:B:2031:LYS:HG3	2.18	0.44
1:B:1522:VAL:HG13	1:B:1523:VAL:HG23	1.99	0.44
1:A:2025:GLU:O	1:A:2029:VAL:HG23	2.17	0.44
1:B:1911:MET:O	1:B:1915:GLU:CB	2.66	0.44
1:B:1636:SER:HB3	1:B:1672:THR:HG23	1.98	0.44
1:A:1648:TYR:O	1:A:1651:PHE:HB3	2.17	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1558:LYS:C	1:B:1560:LYS:H	2.21	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:B:1655:ARG:HH11	1:B:1655:ARG:HG2	1.83	0.43
1:A:2010:TYR:CE2	1:A:2033:MET:HE3	2.54	0.43
1:A:2006:LEU:HB3	1:A:2009:THR:OG1	2.19	0.43
1:A:1575:SER:C	1:A:1577:GLN:H	2.22	0.43
1:B:1823:PRO:O	1:B:1824:GLU:C	2.57	0.43
1:B:1753:LYS:HE3	1:B:1753:LYS:HB2	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:B:2006:LEU:HD13	1:B:2006:LEU:C	2.39	0.43
1:B:2009:THR:CG2	1:B:2020:LEU:HD11	2.42	0.42
1:B:1984:LYS:HG2	1:B:1987:GLU:HB2	2.00	0.42
1:B:1686:PRO:HA	1:B:1690:GLU:OE1	2.19	0.42
1:B:1842:TYR:HB2	1:B:1928:TRP:CD2	2.54	0.42
1:A:1569:ALA:HB2	1:A:1602:LEU:CD2	2.49	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
1:B:1730:ILE:C	1:B:1732:GLY:H	2.23	0.42
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:B:1643:ARG:O	1:B:1647:LYS:HG3	2.19	0.42
1:A:1960:VAL:HG21	1:A:1973:LEU:HD13	2.01	0.42
1:B:1657:ARG:CG	1:B:1666:GLU:HG2	2.47	0.41
1:B:1562:TYR:OH	1:B:1595:THR:HA	2.19	0.41
1:A:2015:ASP:C	1:A:2017:ARG:H	2.24	0.41
1:B:1586:ILE:HB	1:B:1587:PRO:HD3	2.02	0.41
1:A:1991:LEU:O	1:A:1992:GLU:HB2	2.20	0.41
1:B:1629:TRP:CZ3	1:B:1632:LEU:HD23	2.54	0.41
1:A:1956:THR:HB	1:A:2032:LEU:HD21	2.02	0.41
1:B:1649:LEU:HD23	1:B:1676:LEU:HD21	2.02	0.41
1:A:1794:THR:O	1:A:1948:LYS:NZ	2.33	0.41
1:B:1971:LEU:HA	1:B:1984:LYS:O	2.20	0.41
1:B:1563:THR:OG1	1:B:1564:THR:N	2.53	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:1950:TRP:NE1	1:B:1988:GLY:HA2	2.35	0.41
1:B:1540:LEU:HB2	1:B:1573:PHE:CD2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1585:PRO:O	1:B:1588:ILE:N	2.53	0.41
1:B:1984:LYS:CE	1:B:1991:LEU:HD13	2.50	0.41
1:B:1562:TYR:HE1	1:B:1595:THR:HG23	1.83	0.41
1:B:1991:LEU:HA	1:B:1991:LEU:HD12	1.91	0.41
1:B:1800:ASP:OD2	1:B:1801:SER:N	2.53	0.41
1:A:1600:ARG:HB2	1:A:1601:PRO:HD3	2.03	0.41
1:A:1915:GLU:HA	1:A:1915:GLU:OE2	2.19	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:1733:LEU:HD13	1:B:1735:MET:HE2	2.03	0.40
1:B:1811:ALA:O	1:B:1815:VAL:HG23	2.21	0.40
1:A:1516:ASN:HB3	1:A:1522:VAL:CG1	2.51	0.40
1:A:1513:ILE:HG23	1:A:1523:VAL:HG22	2.03	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

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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%)	16	27
1	B	474/555 (85%)	424 (90%)	46 (10%)	4 (1%)	24	40
All	All	959/1110 (86%)	874 (91%)	75 (8%)	10 (1%)	19	33

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1985	ARG

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Mol	Chain	Res	Type
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 ⓘ

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%)	387 (95%)	20 (5%)	31	52
1	B	406/492 (82%)	385 (95%)	21 (5%)	29	49
All	All	813/984 (83%)	772 (95%)	41 (5%)	30	51

All (41) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1503	ASP
1	A	1518	LEU
1	A	1520	SER
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	1747	TYR
1	A	1765	LEU
1	A	1788	LEU

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Mol	Chain	Res	Type
1	A	1835	LEU
1	A	1842	TYR
1	A	1860	LEU
1	A	1957	LEU
1	A	1972	TRP
1	A	1995	GLN
1	B	1508	GLN
1	B	1518	LEU
1	B	1537	HIS
1	B	1549	TYR
1	B	1559	ASP
1	B	1593	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
1	B	1980	VAL
1	B	1984	LYS
1	B	1991	LEU
1	B	2020	LEU
1	B	2026	VAL
1	B	2042	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1508	GLN
1	A	1538	HIS
1	A	1574	ASN
1	A	1707	HIS
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

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Mol	Chain	Res	Type
1	B	1597	HIS
1	B	1659	GLN
1	B	1748	ASN
1	B	1796	ASN
1	B	1817	HIS
1	B	1819	HIS
1	B	1826	ASN
1	B	1858	GLN
1	B	1969	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	A	493/555 (88%)	0.18	25 (5%)	32 37	12, 36, 77, 109	2 (0%)
1	B	484/555 (87%)	0.56	45 (9%)	11 12	30, 55, 86, 106	3 (0%)
All	All	977/1110 (88%)	0.37	70 (7%)	18 21	12, 47, 83, 109	5 (0%)

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	2045	TYR	8.4
1	A	1501	PRO	7.2
1	A	2047	THR	5.9
1	B	2048	THR	5.9
1	A	2007	ALA	5.9
1	B	1912	TRP	5.8
1	B	1913	ILE	5.8
1	A	1780	LEU	5.7
1	B	1549	TYR	5.6
1	B	2046	SER	5.4
1	B	1562	TYR	5.2
1	A	2045	TYR	4.9
1	A	2046	SER	4.9
1	A	2005	PRO	4.5
1	A	2048	THR	4.5
1	B	2047	THR	4.1
1	B	2041	VAL	4.0
1	B	1844	LEU	4.0
1	B	1518	LEU	4.0
1	B	1758	ARG	3.9
1	B	1968	PRO	3.9
1	B	1862	ALA	3.8
1	B	1750	HIS	3.6
1	B	2005	PRO	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	1914	LYS	3.5
1	B	1583	SER	3.3
1	B	1857	LEU	3.3
1	B	2042	LYS	3.3
1	B	2043	LYS	3.2
1	B	1780	LEU	3.2
1	A	1775	SER	3.1
1	A	2006	LEU	3.1
1	B	1737	ASP	3.1
1	B	2022	GLU	3.1
1	A	2004	ALA	3.1
1	B	1600	ARG	3.0
1	B	1502	ILE	3.0
1	B	1559	ASP	3.0
1	B	2004	ALA	3.0
1	B	1965	GLY	2.8
1	A	1980	VAL	2.8
1	A	1994	PHE	2.8
1	B	1969	GLN	2.8
1	A	1582	MET	2.8
1	A	1549	TYR	2.7
1	A	1991	LEU	2.6
1	A	1750	HIS	2.4
1	B	1800	ASP	2.4
1	B	2019	LEU	2.3
1	A	2008	ASN	2.3
1	A	1772	ALA	2.3
1	B	1659	GLN	2.3
1	B	1961	GLU	2.3
1	B	1955	SER	2.3
1	B	1971	LEU	2.3
1	B	1561	GLY	2.3
1	B	1988	GLY	2.3
1	A	1781	PRO	2.3
1	B	2007	ALA	2.2
1	A	2043	LYS	2.2
1	B	1957	LEU	2.2
1	A	1749	GLY	2.2
1	A	2018	GLU	2.2
1	B	1858	GLN	2.2
1	B	2010	TYR	2.1
1	B	2006	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	1962	CYS	2.1
1	B	1517	CYS	2.1
1	A	2044	ARG	2.0
1	A	1913	ILE	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.