



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 07:26 AM GMT

PDB ID : 3AU4
Title : Structure of the human myosin-X MyTH4-FERM cassette bound to its specific cargo, DCC
Authors : Hirano, Y.; Hatano, T.; Hakoshima, T.
Deposited on : 2011-01-28
Resolution : 1.90 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

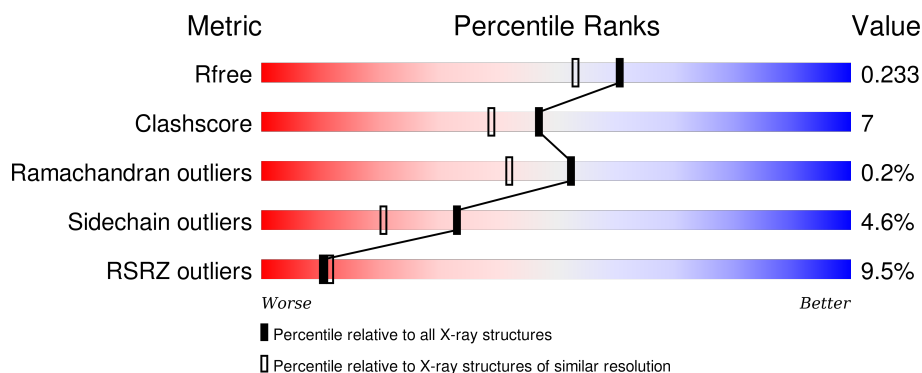
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	4755 (1.90-1.90)
Clashscore	102246	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

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>8%</div> <div>79%</div> <div>14%</div> <div>• 6%</div> </div>
2	B	63	<div> <div>10%</div> <div>32%</div> <div>16%</div> <div>• 49%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4677 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	524	Total	C	N	O	S	0	0	0
			4200	2696	703	779	22			

There are 23 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

- Molecule 2 is a protein called Netrin receptor DCC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	32	Total 234	C 141	N 38	O 53	S 2	0	0	0

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1385	GLY	-	EXPRESSION TAG	UNP P43146
B	1386	PRO	-	EXPRESSION TAG	UNP P43146
B	1387	GLY	-	EXPRESSION TAG	UNP P43146
B	1388	TYR	-	EXPRESSION TAG	UNP P43146
B	1389	GLN	-	EXPRESSION TAG	UNP P43146

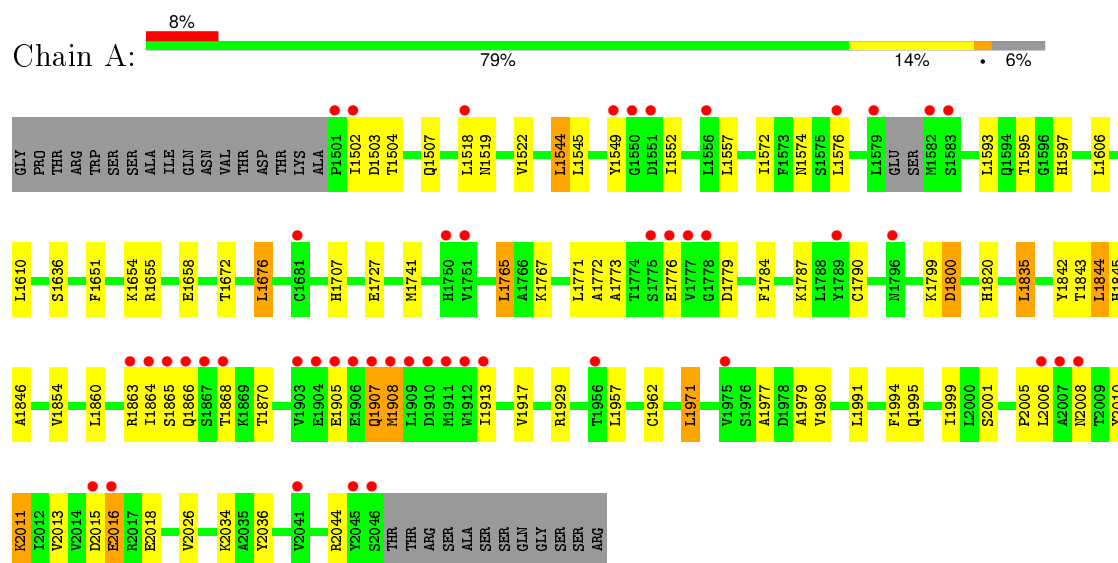
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	241	Total 241	O 241	0	0
3	B	2	Total 2	O 2	0	0

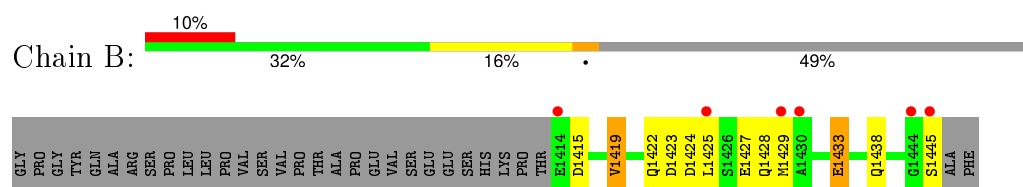
3 Residue-property plots [i](#)

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

• Molecule 1: Myosin-X



• Molecule 2: Netrin receptor DCC



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	85.22Å 49.56Å 93.98Å 90.00° 116.71° 90.00°	Depositor
Resolution (Å)	34.06 – 1.90 34.06 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.7 (34.06-1.90) 95.5 (34.06-1.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 1.89Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.215 , 0.233 0.215 , 0.233	Depositor DCC
R_{free} test set	2685 reflections (5.04%)	DCC
Wilson B-factor (Å ²)	30.9	Xtriage
Anisotropy	0.351	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 49.1	EDS
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55548 reflections	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4677	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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, 0.375 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	0.45	5/4297 (0.1%)	0.57	0/5816
2	B	0.31	0/234	0.44	0/314
All	All	0.44	5/4531 (0.1%)	0.56	0/6130

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1507	GLN	C-O	-9.37	1.05	1.23
1	A	1507	GLN	CB-CG	-6.72	1.34	1.52
1	A	1507	GLN	CD-NE2	-6.50	1.16	1.32
1	A	1507	GLN	CD-OE1	-6.43	1.09	1.24
1	A	1597	HIS	C-O	-5.54	1.12	1.23

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	4200	0	4168	61	0
2	B	234	0	217	10	0
3	A	241	0	0	5	0
3	B	2	0	0	0	0
All	All	4677	0	4385	66	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 7.

All (66) 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:A:1864:ILE:HD12	1:A:1913:ILE:HG22	1.52	0.91
1:A:1868:THR:HG23	1:A:1870:THR:H	1.41	0.85
2:B:1415:ASP:O	2:B:1419:VAL:HG12	1.88	0.72
1:A:1504:THR:HG21	1:A:1544:LEU:O	1.91	0.70
1:A:2013:VAL:HG22	1:A:2018:GLU:HG2	1.78	0.66
1:A:2001:SER:HB2	2:B:1438:GLN:HE22	1.61	0.64
1:A:1606:LEU:O	1:A:1610:LEU:HD23	1.98	0.63
1:A:1636:SER:HB2	1:A:1676:LEU:HD13	1.80	0.62
1:A:1905:GLU:HG2	1:A:1907:GLN:HG3	1.80	0.62
1:A:2008:ASN:HB2	3:A:168:HOH:O	2.00	0.61
1:A:1905:GLU:HB3	1:A:1908:MET:HB2	1.83	0.61
1:A:1572:ILE:HD13	1:A:1606:LEU:HD21	1.82	0.60
1:A:2010:TYR:HD1	1:A:2026:VAL:HG13	1.67	0.59
2:B:1425:LEU:O	2:B:1429:MET:HG2	2.03	0.59
1:A:2044:ARG:HH12	2:B:1428:GLN:CD	2.05	0.58
1:A:1776:GLU:HB2	1:A:1779:ASP:OD2	2.02	0.58
1:A:1741:MET:HB3	1:A:1790:CYS:HB2	1.86	0.57
1:A:1502:ILE:HG12	3:A:231:HOH:O	2.05	0.56
1:A:1502:ILE:HG13	1:A:1503:ASP:N	2.20	0.56
1:A:1863:ARG:O	1:A:1866:GLN:HG2	2.05	0.56
1:A:1574:ASN:ND2	3:A:110:HOH:O	2.38	0.56
1:A:1502:ILE:HG13	1:A:1503:ASP:H	1.71	0.55
1:A:1977:ALA:HA	1:A:2036:TYR:CD1	2.42	0.54
1:A:1843:THR:OG1	1:A:1846:ALA:HB2	2.07	0.54
1:A:1844:LEU:HD22	1:A:1845:HIS:CE1	2.42	0.54
1:A:2011:LYS:HD3	1:A:2013:VAL:HG23	1.88	0.54
1:A:1504:THR:HG21	1:A:1545:LEU:HA	1.90	0.53
1:A:1654:LYS:O	1:A:1658:GLU:HG3	2.09	0.53
1:A:2005:PRO:O	1:A:2006:LEU:HD22	2.08	0.53
1:A:1651:PHE:CZ	1:A:1655:ARG:HD2	2.44	0.52
1:A:1519:ASN:HB3	1:A:1522:VAL:HG12	1.91	0.52
1:A:1707:HIS:CG	1:A:1787:LYS:HG2	2.45	0.52
2:B:1424:ASP:HB2	2:B:1427:GLU:OE1	2.09	0.52
1:A:1519:ASN:HB3	1:A:1522:VAL:CG1	2.40	0.52
1:A:1835:LEU:HD13	1:A:1854:VAL:HG11	1.91	0.51
1:A:1636:SER:HB3	1:A:1672:THR:HG23	1.92	0.51
1:A:1707:HIS:HB2	1:A:1787:LYS:HG2	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2044:ARG:HG3	2:B:1425:LEU:HD13	1.93	0.51
1:A:2044:ARG:HB3	2:B:1429:MET:HE2	1.94	0.50
1:A:1549:TYR:HD1	1:A:1552:ILE:HG21	1.76	0.50
2:B:1429:MET:O	2:B:1433:GLU:HB2	2.12	0.49
1:A:1771:LEU:C	1:A:1773:ALA:H	2.17	0.48
1:A:1799:LYS:O	1:A:1800:ASP:OD2	2.32	0.48
1:A:1860:LEU:HD12	1:A:1863:ARG:NH2	2.29	0.48
1:A:2005:PRO:C	1:A:2006:LEU:HD22	2.35	0.46
1:A:1707:HIS:CE1	1:A:1787:LYS:HE3	2.51	0.46
1:A:1980:VAL:CG1	1:A:1999:ILE:HD11	2.45	0.46
1:A:1765:LEU:HD13	1:A:1784:PHE:CE2	2.50	0.46
1:A:2011:LYS:HD3	1:A:2013:VAL:CG2	2.46	0.46
1:A:1962:CYS:HB2	1:A:1971:LEU:HD22	1.99	0.45
1:A:1549:TYR:HD1	1:A:1552:ILE:CG2	2.29	0.45
1:A:1979:ALA:HB1	1:A:1994:PHE:O	2.16	0.44
1:A:1865:SER:O	1:A:1868:THR:HG22	2.17	0.44
1:A:1727:GLU:HG2	3:A:229:HOH:O	2.16	0.44
1:A:1913:ILE:O	1:A:1917:VAL:HG23	2.17	0.44
1:A:1905:GLU:OE1	1:A:1907:GLN:NE2	2.51	0.43
1:A:1549:TYR:CD1	1:A:1552:ILE:HG21	2.54	0.43
1:A:1979:ALA:HB2	1:A:1995:GLN:HA	2.01	0.42
1:A:1557:LEU:C	1:A:1557:LEU:HD23	2.40	0.42
1:A:1799:LYS:O	1:A:1800:ASP:CB	2.67	0.41
1:A:1820:HIS:HE1	3:A:3:HOH:O	2.01	0.41
1:A:2016:GLU:HG3	1:A:2016:GLU:H	1.63	0.41
1:A:1767:LYS:O	1:A:1771:LEU:HG	2.21	0.41
1:A:2034:LYS:NZ	2:B:1445:SER:OG	2.53	0.41
2:B:1419:VAL:HA	2:B:1422:GLN:OE1	2.21	0.41
1:A:1572:ILE:HD11	1:A:1595:THR:HG21	2.03	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	520/555 (94%)	505 (97%)	14 (3%)	1 (0%)	52	42
2	B	30/63 (48%)	30 (100%)	0	0	100	100
All	All	550/618 (89%)	535 (97%)	14 (2%)	1 (0%)	52	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1772	ALA

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	458/492 (93%)	439 (96%)	19 (4%)	37	25
2	B	25/53 (47%)	22 (88%)	3 (12%)	6	2
All	All	483/545 (89%)	461 (95%)	22 (5%)	33	21

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1518	LEU
1	A	1544	LEU
1	A	1576	LEU
1	A	1593	LEU
1	A	1676	LEU
1	A	1765	LEU
1	A	1800	ASP
1	A	1835	LEU
1	A	1842	TYR
1	A	1844	LEU
1	A	1907	GLN
1	A	1908	MET
1	A	1929	ARG
1	A	1957	LEU
1	A	1971	LEU

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Mol	Chain	Res	Type
1	A	1991	LEU
1	A	2011	LYS
1	A	2015	ASP
1	A	2016	GLU
2	B	1419	VAL
2	B	1423	ASP
2	B	1433	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1574	ASN
1	A	1659	GLN
1	A	1796	ASN
1	A	1817	HIS
1	A	1820	HIS
1	A	1845	HIS
1	A	1907	GLN
1	A	1938	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	524/555 (94%)	0.41	47 (8%) 12 13	21, 35, 67, 86	3 (0%)
2	B	32/63 (50%)	1.28	6 (18%) 2 2	41, 58, 70, 73	0
All	All	556/618 (89%)	0.46	53 (9%) 10 12	21, 36, 69, 86	3 (0%)

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1777	VAL	7.1
1	A	1778	GLY	5.7
1	A	1864	ILE	5.3
1	A	1501	PRO	5.3
1	A	1502	ILE	5.1
1	A	2045	TYR	4.8
1	A	2046	SER	4.8
1	A	1582	MET	4.7
2	B	1445	SER	4.7
1	A	1868	THR	4.3
1	A	1867	SER	4.3
1	A	1912	TRP	4.1
2	B	1425	LEU	4.1
1	A	1903	VAL	3.9
1	A	1750	HIS	3.9
1	A	1866	GLN	3.8
1	A	1905	GLU	3.6
1	A	2016	GLU	3.4
1	A	1775	SER	3.4
1	A	1865	SER	3.4
1	A	1909	LEU	3.4
1	A	1751	VAL	3.4
1	A	1776	GLU	3.3
2	B	1414	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	2007	ALA	3.2
1	A	1907	GLN	3.2
1	A	1908	MET	3.1
1	A	1910	ASP	3.1
1	A	1549	TYR	3.0
1	A	1551	ASP	3.0
1	A	1796	ASN	3.0
2	B	1429	MET	2.9
1	A	2008	ASN	2.9
1	A	1583	SER	2.9
2	B	1444	GLY	2.7
1	A	2015	ASP	2.7
1	A	1579	LEU	2.6
1	A	1518	LEU	2.5
1	A	1550	GLY	2.5
1	A	1911	MET	2.4
1	A	1556	LEU	2.4
1	A	1904	GLU	2.4
2	B	1430	ALA	2.4
1	A	1681	CYS	2.3
1	A	1956	THR	2.3
1	A	1913	ILE	2.3
1	A	1906	GLU	2.3
1	A	1975	VAL	2.2
1	A	1789	TYR	2.2
1	A	2041	VAL	2.1
1	A	1863	ARG	2.1
1	A	1576	LEU	2.1
1	A	2006	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.