



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:14 AM UTC

PDB ID : 5MV7 / pdb_00005mv7
Title : Structure of human Myosin 7b C-terminal MyTH4-FERM MF2 domain
Authors : Planelles-Herrero, V.J.; Sourigues, Y.; Titus, M.A.; Houdusse, A.
Deposited on : 2017-01-15
Resolution : 2.44 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
Mogul	:	2022.3.0, CSD as543be (2022)
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

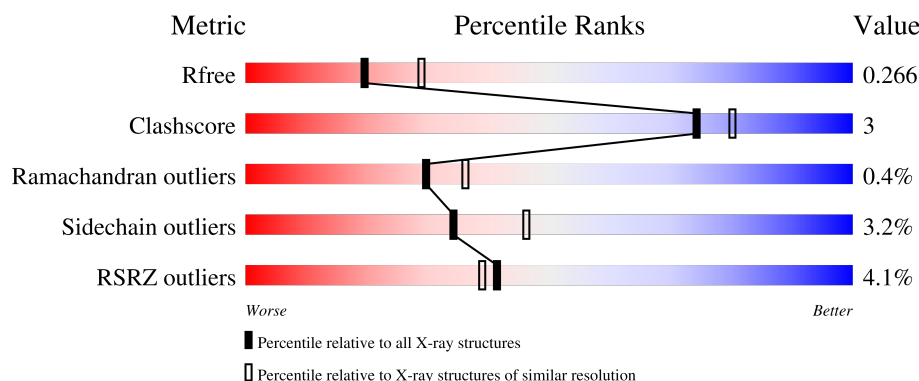
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	2340 (2.46-2.42)
Clashscore	190562	2400 (2.46-2.42)
Ramachandran outliers	187476	2379 (2.46-2.42)
Sidechain outliers	187428	2379 (2.46-2.42)
RSRZ outliers	180081	2340 (2.46-2.42)

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	522	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	TAM	A	2202	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4202 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.

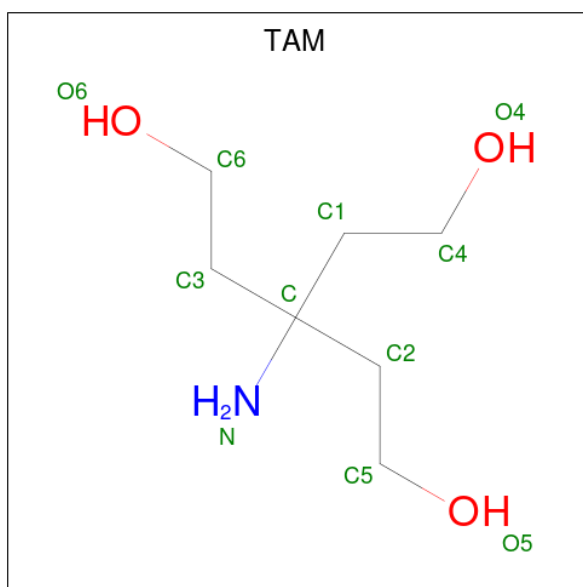
- Molecule 1 is a protein called Unconventional myosin-VIIb.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	493	4026	2590	708	710	18	0	0	0

There are 11 discrepancies between the modelled and reference sequences:

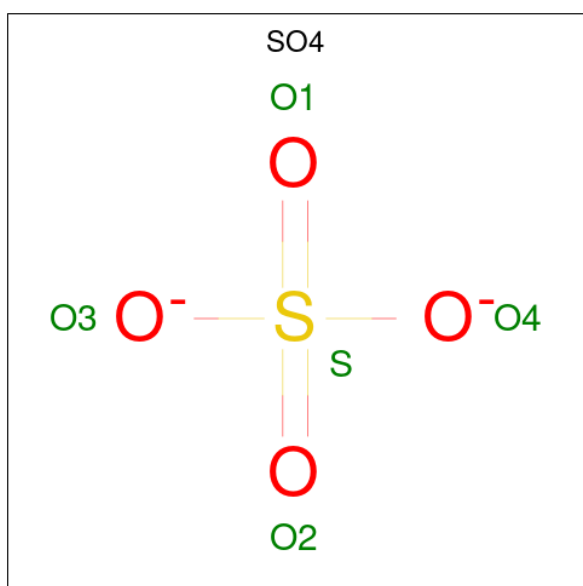
Chain	Residue	Modelled	Actual	Comment	Reference
A	1	HIS	-	expression tag	UNP Q6PIF6
A	2	HIS	-	expression tag	UNP Q6PIF6
A	3	HIS	-	expression tag	UNP Q6PIF6
A	4	HIS	-	expression tag	UNP Q6PIF6
A	5	HIS	-	expression tag	UNP Q6PIF6
A	6	HIS	-	expression tag	UNP Q6PIF6
A	7	SER	-	expression tag	UNP Q6PIF6
A	8	SER	-	expression tag	UNP Q6PIF6
A	9	GLY	-	expression tag	UNP Q6PIF6
A	10	HIS	-	expression tag	UNP Q6PIF6
A	1626	ALA	MET	conflict	UNP Q6PIF6

- Molecule 2 is TRIS(HYDROXYETHYL)AMINOMETHANE (CCD ID: TAM) (formula: $C_7H_{17}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	7	1	3		
2	A	1	Total	C	N	O	0	0
			11	7	1	3		

- Molecule 3 is SULFATE ION (CCD ID: SO₄) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

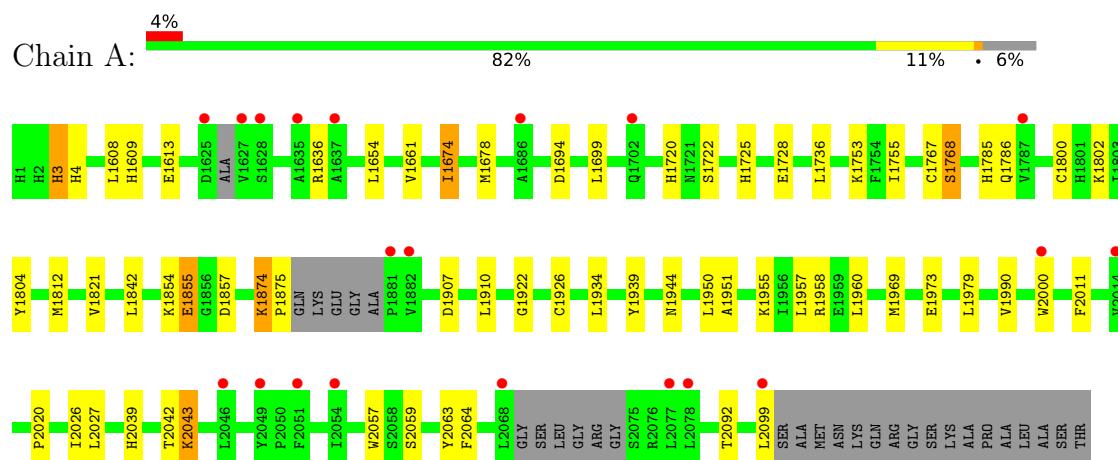
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	139	Total	O	0	0
			139	139		

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: Unconventional myosin-VIIIb



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	123.67Å 42.81Å 118.37Å 90.00° 97.69° 90.00°	Depositor
Resolution (Å)	35.17 – 2.44 35.17 – 2.44	Depositor EDS
% Data completeness (in resolution range)	96.9 (35.17-2.44) 97.5 (35.17-2.44)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.45Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.209 , 0.258 0.215 , 0.266	Depositor DCC
R_{free} test set	1132 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	52.0	Xtriage
Anisotropy	0.730	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 57.6	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	0.95	EDS
Total number of atoms	4202	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.59% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SO4, TAM

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	0.87	0/4135	1.41	29/5602 (0.5%)

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1736	LEU	CA-C-N	7.41	130.54	120.54
1	A	1736	LEU	C-N-CA	7.41	130.54	120.54
1	A	1854	LYS	CA-C-N	6.67	129.51	120.38
1	A	1854	LYS	C-N-CA	6.67	129.51	120.38
1	A	1768	SER	CA-C-N	6.51	129.00	120.28
1	A	1768	SER	C-N-CA	6.51	129.00	120.28
1	A	1725	HIS	CA-C-N	6.21	128.61	120.28
1	A	1725	HIS	C-N-CA	6.21	128.61	120.28
1	A	1786	GLN	CA-C-N	5.67	127.70	120.56
1	A	1786	GLN	C-N-CA	5.67	127.70	120.56
1	A	2063	TYR	N-CA-C	5.61	116.48	108.74
1	A	1767	CYS	CA-C-N	5.57	128.01	120.44
1	A	1767	CYS	C-N-CA	5.57	128.01	120.44
1	A	1674	ILE	CA-C-N	5.48	127.57	120.44
1	A	1674	ILE	C-N-CA	5.48	127.57	120.44
1	A	1694	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	1951	ALA	CA-C-N	5.30	127.65	120.65
1	A	1951	ALA	C-N-CA	5.30	127.65	120.65
1	A	1907	ASP	CA-CB-CG	5.25	117.85	112.60
1	A	1728	GLU	CA-C-N	5.24	127.72	120.29
1	A	1728	GLU	C-N-CA	5.24	127.72	120.29
1	A	1654	LEU	CA-C-N	5.18	127.22	120.28
1	A	1654	LEU	C-N-CA	5.18	127.22	120.28
1	A	1910	LEU	CA-C-N	5.17	127.52	120.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1910	LEU	C-N-CA	5.17	127.52	120.54
1	A	2020	PRO	CA-C-N	5.14	127.16	120.28
1	A	2020	PRO	C-N-CA	5.14	127.16	120.28
1	A	1785	HIS	CA-C-N	5.11	128.48	120.82
1	A	1785	HIS	C-N-CA	5.11	128.48	120.82

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	4026	0	4020	24	0
2	A	22	0	34	6	0
3	A	15	0	0	0	0
4	A	139	0	0	0	0
All	All	4202	0	4054	25	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 3.

All (25) 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:1674:ILE:HG23	1:A:1678:MET:HE3	1.50	0.94
1:A:1720:HIS:H	2:A:2202:TAM:HN2	1.20	0.88
1:A:1608:LEU:HD23	2:A:2202:TAM:H22	1.77	0.65
1:A:1922:GLY:O	1:A:2043:LYS:HE2	1.97	0.64
1:A:1934:LEU:HD21	1:A:2000:TRP:CD1	2.41	0.56
1:A:1720:HIS:HA	2:A:2202:TAM:H32	1.87	0.56
1:A:1720:HIS:CE1	2:A:2202:TAM:H41	2.46	0.50
1:A:1874:LYS:HG3	1:A:1875:PRO:HD3	1.94	0.50
1:A:1950:LEU:HD23	1:A:1979:LEU:HG	1.95	0.48
1:A:2057:TRP:HE1	1:A:2092:THR:HG23	1.78	0.47
1:A:1800:CYS:HB3	1:A:1812:MET:HE3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2202:TAM:H12	2:A:2202:TAM:H61	1.70	0.45
1:A:2039:HIS:HB3	1:A:2042:THR:O	2.17	0.45
1:A:3:HIS:HD2	1:A:4:HIS:CD2	2.36	0.44
1:A:1955:LYS:HB3	1:A:1958:ARG:HD2	2.00	0.44
1:A:1969:MET:HE2	1:A:1973:GLU:HB3	2.00	0.43
1:A:1821:VAL:HG13	1:A:1842:LEU:HD12	2.00	0.43
1:A:2011:PHE:HB3	1:A:2027:LEU:HD11	1.99	0.43
1:A:1855:GLU:CD	1:A:1855:GLU:H	2.26	0.42
1:A:1802:LYS:HD3	1:A:1804:TYR:CZ	2.54	0.42
1:A:1720:HIS:ND1	2:A:2202:TAM:H32	2.36	0.41
1:A:1609:HIS:CD2	1:A:1753:LYS:HB3	2.56	0.41
1:A:1755:ILE:HG21	1:A:1768:SER:HB2	2.03	0.41
1:A:1939:TYR:HD2	1:A:1960:LEU:HD11	1.86	0.40
1:A:2059:SER:HB3	1:A:2064:PHE:HD1	1.86	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	485/522 (93%)	468 (96%)	15 (3%)	2 (0%)	30	36

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2043	LYS
1	A	1944	ASN

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	443/465 (95%)	429 (97%)	14 (3%)	34 46

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	1613	GLU
1	A	1636	ARG
1	A	1661	VAL
1	A	1699	LEU
1	A	1722	SER
1	A	1855	GLU
1	A	1857	ASP
1	A	1874	LYS
1	A	1926	CYS
1	A	1957	LEU
1	A	1990	VAL
1	A	2026	ILE
1	A	2099	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	3	HIS
1	A	1660	ASN
1	A	1752	GLN
1	A	1785	HIS
1	A	1786	GLN
1	A	1887	GLN
1	A	1897	ASN
1	A	1945	ASN
1	A	1949	GLN
1	A	2097	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](#)

5 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	2204	-	4,4,4	0.25	0	6,6,6	0.06	0
3	SO4	A	2203	-	4,4,4	0.26	0	6,6,6	0.09	0
3	SO4	A	2205	-	4,4,4	0.24	0	6,6,6	0.11	0
2	TAM	A	2202	-	10,10,10	0.78	0	12,12,12	1.33	2 (16%)
2	TAM	A	2201	-	10,10,10	0.82	0	12,12,12	1.64	2 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	TAM	A	2202	-	-	10/12/12/12	-
2	TAM	A	2201	-	-	4/12/12/12	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2201	TAM	C2-C-C1	-3.37	104.56	110.50
2	A	2202	TAM	C6-C3-C	3.21	119.76	115.97
2	A	2201	TAM	C4-C1-C	3.10	119.63	115.97
2	A	2202	TAM	C3-C-C2	-2.13	106.75	110.50

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2201	TAM	C2-C-C1-C4
2	A	2201	TAM	C3-C-C1-C4
2	A	2201	TAM	N-C-C1-C4
2	A	2202	TAM	C2-C-C1-C4
2	A	2202	TAM	C3-C-C1-C4
2	A	2202	TAM	N-C-C1-C4
2	A	2202	TAM	C1-C-C2-C5
2	A	2202	TAM	C3-C-C2-C5
2	A	2202	TAM	N-C-C2-C5
2	A	2202	TAM	C1-C-C3-C6
2	A	2202	TAM	C2-C-C3-C6
2	A	2202	TAM	N-C-C3-C6
2	A	2202	TAM	C-C3-C6-O6
2	A	2201	TAM	C-C2-C5-O5

There are no ring outliers.

1 monomer is involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2202	TAM	6	0

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	493/522 (94%)	0.37	20 (4%) 41 39	35, 64, 101, 131	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1637	ALA	4.5
1	A	1625	ASP	4.3
1	A	2099	LEU	4.2
1	A	1882	VAL	3.2
1	A	1635	ALA	3.1
1	A	1881	PRO	2.8
1	A	1628	SER	2.8
1	A	2049	TYR	2.7
1	A	2068	LEU	2.6
1	A	1627	VAL	2.6
1	A	2054	ILE	2.6
1	A	2046	LEU	2.5
1	A	2078	LEU	2.4
1	A	1702	GLN	2.4
1	A	2051	PHE	2.3
1	A	1686	ALA	2.3
1	A	1787	VAL	2.3
1	A	2077	LEU	2.1
1	A	2014	VAL	2.0
1	A	2000	TRP	2.0

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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	2205	5/5	0.74	0.08	149,150,150,150	0
2	TAM	A	2202	11/11	0.79	0.24	99,103,104,105	0
2	TAM	A	2201	11/11	0.86	0.13	70,81,85,85	0
3	SO4	A	2204	5/5	0.90	0.07	116,117,117,117	0
3	SO4	A	2203	5/5	0.92	0.09	108,109,109,110	0

6.5 Other polymers [i](#)

There are no such residues in this entry.