



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2018 – 11:52 pm GMT

PDB ID : 4L79
Title : Crystal Structure of nucleotide-free Myosin 1b residues 1-728 with bound Calmodulin
Authors : Shuman, H.; Zwolak, A.; Dominguez, R.; Ostap, E.M.
Deposited on : 2013-06-13
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : trunk30967
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30967

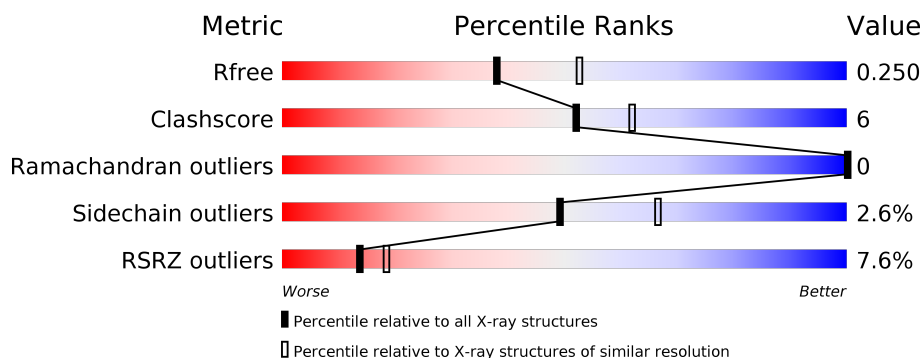
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	111664	4477 (2.30-2.30)
Clashscore	122126	5072 (2.30-2.30)
Ramachandran outliers	120053	5022 (2.30-2.30)
Sidechain outliers	120020	5021 (2.30-2.30)
RSRZ outliers	108989	4374 (2.30-2.30)

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	744	<div> <div>5%</div> <div>84%</div> <div>14%</div> <div>••</div> </div>
2	B	149	<div> <div>19%</div> <div>77%</div> <div>21%</div> <div>•</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7631 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-Ib.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	734	6010	3820	1035	1130	25	0	7	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	729	GLY	-	EXPRESSION TAG	UNP Q05096
A	730	LEU	-	EXPRESSION TAG	UNP Q05096
A	731	ASN	-	EXPRESSION TAG	UNP Q05096
A	732	ASP	-	EXPRESSION TAG	UNP Q05096
A	733	ILE	-	EXPRESSION TAG	UNP Q05096
A	734	PHE	-	EXPRESSION TAG	UNP Q05096
A	735	GLU	-	EXPRESSION TAG	UNP Q05096
A	736	ALA	-	EXPRESSION TAG	UNP Q05096
A	737	GLN	-	EXPRESSION TAG	UNP Q05096
A	738	LYS	-	EXPRESSION TAG	UNP Q05096
A	739	ILE	-	EXPRESSION TAG	UNP Q05096
A	740	GLU	-	EXPRESSION TAG	UNP Q05096
A	741	TRP	-	EXPRESSION TAG	UNP Q05096
A	742	HIS	-	EXPRESSION TAG	UNP Q05096
A	743	GLU	-	EXPRESSION TAG	UNP Q05096
A	744	ASP	-	EXPRESSION TAG	UNP Q05096

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	147	1161	711	187	254	9	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total 1	Mg 1	0	0

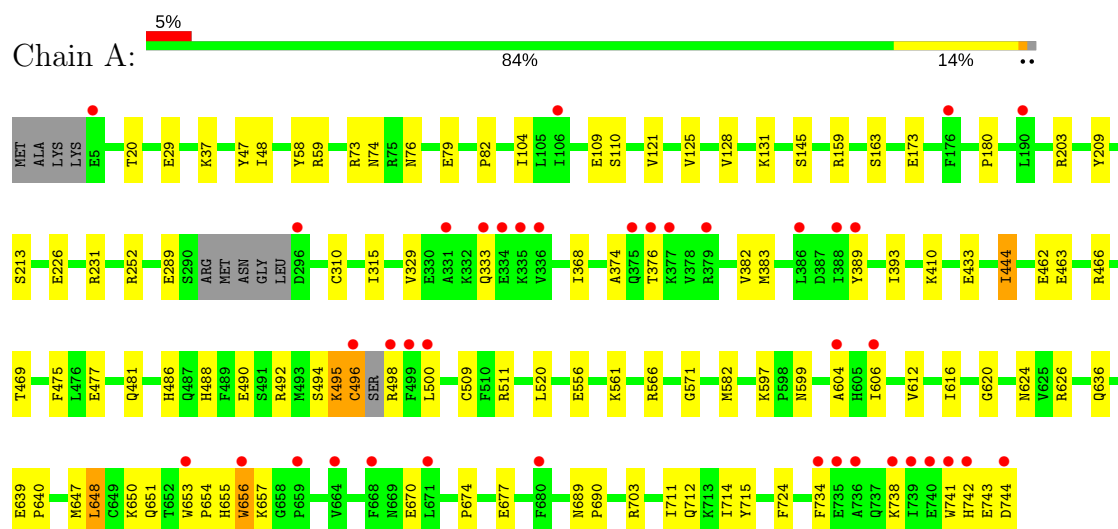
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	440	Total 440	O 440	0	0
4	B	19	Total 19	O 19	0	0

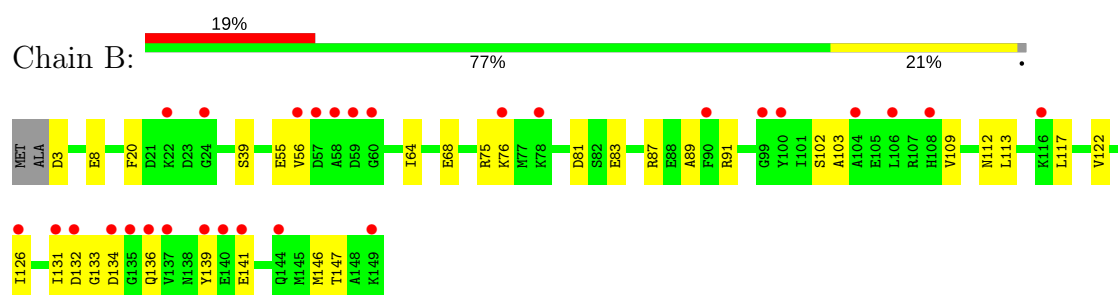
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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-Ib



• Molecule 2: Calmodulin



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	114.18Å 45.09Å 115.55Å 90.00° 117.18° 90.00°	Depositor
Resolution (Å)	39.21 – 2.30 39.21 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (39.21-2.30) 99.7 (39.21-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.98 (at 2.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1314)	Depositor
R, R_{free}	0.189 , 0.249 0.190 , 0.250	Depositor DCC
R_{free} test set	2381 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	31.5	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 53.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.015 for l,-k,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7631	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.62% 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: MG

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	0.44	0/6145	0.55	0/8287
2	B	0.30	0/1173	0.48	0/1573
All	All	0.42	0/7318	0.54	0/9860

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

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	6010	0	5982	67	1
2	B	1161	0	1088	23	0
3	A	1	0	0	0	0
4	A	440	0	0	14	1
4	B	19	0	0	6	0
All	All	7631	0	7070	86	2

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 6.

All (86) 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:495:LYS:HE2	1:A:496:CYS:SG	2.02	0.98
1:A:462:GLU:OE2	4:A:1119:HOH:O	1.87	0.91
1:A:742:HIS:HB3	1:A:743:GLU:HB2	1.68	0.76
1:A:496:CYS:SG	1:A:498:ARG:HG3	2.26	0.74
1:A:109:GLU:OE2	4:A:1289:HOH:O	2.08	0.71
1:A:561:LYS:NZ	4:A:1165:HOH:O	2.16	0.69
2:B:102:SER:HA	2:B:136:GLN:HG2	1.75	0.69
1:A:252:ARG:NH1	4:A:1175:HOH:O	2.22	0.68
1:A:715:TYR:HA	2:B:146:MET:HE2	1.76	0.67
2:B:3:ASP:OD1	4:B:213:HOH:O	2.13	0.64
1:A:433:GLU:O	4:A:1222:HOH:O	2.15	0.64
2:B:20:PHE:O	4:B:214:HOH:O	2.15	0.64
2:B:55:GLU:OE1	2:B:75:ARG:NH2	2.31	0.63
1:A:712:GLN:HG2	2:B:117:LEU:HD13	1.79	0.63
2:B:103:ALA:H	2:B:136:GLN:HG2	1.64	0.62
1:A:656:TRP:CG	1:A:657:LYS:HA	2.34	0.62
1:A:496:CYS:HG	1:A:498:ARG:N	1.98	0.61
1:A:131:LYS:HG3	1:A:180:PRO:HD3	1.84	0.60
2:B:109:VAL:HG13	2:B:113:LEU:HD12	1.82	0.60
1:A:599:ASN:ND2	1:A:606:ILE:O	2.34	0.59
1:A:59:ARG:HD3	1:A:604:ALA:HB1	1.84	0.59
2:B:103:ALA:H	2:B:136:GLN:CG	2.15	0.58
1:A:492:ARG:O	4:A:1314:HOH:O	2.16	0.58
1:A:656:TRP:CE3	1:A:656:TRP:HA	2.38	0.57
1:A:20:THR:OG1	1:A:48:ILE:HG12	2.05	0.57
2:B:81:ASP:OD2	4:B:215:HOH:O	2.16	0.57
1:A:639:GLU:HB2	1:A:640:PRO:HD3	1.87	0.56
1:A:145:SER:HB2	1:A:368:ILE:HD13	1.87	0.56
1:A:556:GLU:HA	1:A:561:LYS:HD3	1.87	0.56
1:A:159:ARG:NH1	1:A:393:ILE:O	2.37	0.56
1:A:110:SER:OG	1:A:163:SER:HA	2.06	0.55
1:A:741:TRP:O	1:A:742:HIS:ND1	2.39	0.55
1:A:742:HIS:CB	1:A:743:GLU:HB2	2.36	0.54
1:A:636:GLN:OE1	4:A:1009:HOH:O	2.18	0.54
1:A:109:GLU:HG2	1:A:597:LYS:HE3	1.90	0.54
1:A:656:TRP:CB	1:A:657:LYS:HA	2.39	0.53
2:B:64:ILE:HG23	2:B:68:GLU:HG3	1.92	0.52
2:B:83:GLU:HG3	2:B:147:THR:HG21	1.89	0.52
1:A:612:VAL:O	1:A:616:ILE:HG12	2.09	0.52
1:A:734:PHE:O	4:A:1255:HOH:O	2.20	0.51
1:A:47:TYR:CZ	1:A:82:PRO:HA	2.46	0.50
1:A:73:ARG:HD3	1:A:128:VAL:HG23	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:VAL:O	2:B:126:ILE:HG12	2.10	0.50
1:A:571:GLY:HA3	4:A:1114:HOH:O	2.11	0.50
1:A:76:ASN:HB2	1:A:79:GLU:HG3	1.92	0.49
2:B:76:LYS:HB2	4:B:219:HOH:O	2.12	0.49
1:A:466:ARG:NH2	1:A:469:THR:O	2.43	0.49
1:A:444:ILE:HD11	1:A:488:HIS:ND1	2.29	0.48
1:A:333:GLN:HA	1:A:333:GLN:HE21	1.80	0.47
1:A:711:ILE:HD11	2:B:89:ALA:HB3	1.97	0.47
1:A:213:SER:O	4:A:1049:HOH:O	2.20	0.47
1:A:231:ARG:NH2	4:A:1024:HOH:O	2.47	0.47
1:A:463:GLU:HG3	1:A:475:PHE:HA	1.98	0.46
2:B:76:LYS:CB	4:B:219:HOH:O	2.62	0.46
1:A:73:ARG:HG2	1:A:74:ASN:ND2	2.31	0.46
1:A:410:LYS:HB3	1:A:582:MET:HE1	1.98	0.46
1:A:674:PRO:HG2	1:A:677:GLU:HG3	1.98	0.45
2:B:132:ASP:N	2:B:132:ASP:OD1	2.43	0.45
1:A:58:TYR:HB2	1:A:604:ALA:HA	1.99	0.45
2:B:8:GLU:OE1	2:B:8:GLU:N	2.48	0.45
2:B:87:ARG:HG2	2:B:91:ARG:CZ	2.47	0.44
2:B:133:GLY:HA2	2:B:134:ASP:HA	1.46	0.44
1:A:310:CYS:HB3	1:A:315:ILE:O	2.18	0.44
1:A:490:GLU:HB2	1:A:511:ARG:HB3	2.00	0.44
1:A:738:LYS:HG3	4:A:1255:HOH:O	2.18	0.44
2:B:112:ASN:ND2	4:B:216:HOH:O	2.36	0.43
1:A:651:GLN:HE22	1:A:670:GLU:HG3	1.84	0.43
1:A:203:ARG:HB3	1:A:209:TYR:CE2	2.54	0.43
1:A:477:GLU:O	1:A:481[A]:GLN:HG2	2.19	0.42
1:A:653:TRP:HA	1:A:654:PRO:HA	1.55	0.42
1:A:566:ARG:HE	1:A:566:ARG:HB3	1.64	0.42
1:A:689:ASN:HA	1:A:690:PRO:HD3	1.96	0.42
1:A:724:PHE:CG	2:B:39:SER:HB3	2.54	0.41
1:A:226:GLU:HB2	1:A:231:ARG:HD2	2.02	0.41
1:A:173:GLU:HG2	1:A:382:VAL:HG12	2.03	0.41
1:A:509:CYS:SG	1:A:520:LEU:HD11	2.60	0.41
1:A:104:ILE:HD12	1:A:121:VAL:HG11	2.02	0.41
1:A:620:GLY:HA2	4:A:952:HOH:O	2.20	0.41
1:A:648:LEU:HD12	1:A:648:LEU:HA	1.83	0.41
1:A:626:ARG:NH2	4:A:1095:HOH:O	2.53	0.41
1:A:125:VAL:HG21	1:A:383:MET:HG2	2.02	0.41
1:A:650:LYS:HA	1:A:650:LYS:HD3	1.74	0.40
1:A:125:VAL:HA	1:A:128:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:HB3	1:A:37:LYS:HE2	1.76	0.40
2:B:91:ARG:HG2	2:B:139:TYR:OH	2.22	0.40
1:A:374:ALA:O	1:A:376:THR:HG22	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:GLU:OE1	1:A:495:LYS:NZ[2_746]	2.03	0.17
4:A:914:HOH:O	4:A:1018:HOH:O[2_656]	2.14	0.06

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	735/744 (99%)	712 (97%)	23 (3%)	0	100	100
2	B	145/149 (97%)	144 (99%)	1 (1%)	0	100	100
All	All	880/893 (98%)	856 (97%)	24 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	663/664 (100%)	646 (97%)	17 (3%)	49	66
2	B	126/127 (99%)	123 (98%)	3 (2%)	52	69
All	All	789/791 (100%)	769 (98%)	20 (2%)	49	68

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	289	GLU
1	A	329	VAL
1	A	389	TYR
1	A	444	ILE
1	A	486	HIS
1	A	494	SER
1	A	495	LYS
1	A	496	CYS
1	A	500	LEU
1	A	624	ASN
1	A	647	MET
1	A	648	LEU
1	A	655	HIS
1	A	656	TRP
1	A	703	ARG
1	A	714	ILE
1	A	744	ASP
2	B	56	VAL
2	B	131	ILE
2	B	141	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	333	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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	734/744 (98%)	0.07	39 (5%) 26 33	14, 38, 72, 106	0
2	B	147/149 (98%)	0.87	28 (19%) 1 1	40, 73, 98, 109	0
All	All	881/893 (98%)	0.21	67 (7%) 14 18	14, 43, 84, 109	0

All (67) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	131	ILE	8.2
2	B	58	ALA	6.6
1	A	496	CYS	6.6
1	A	604	ALA	5.6
1	A	742	HIS	5.3
1	A	499	PHE	5.2
1	A	744	ASP	5.0
1	A	498	ARG	5.0
2	B	60	GLY	4.8
1	A	334	GLU	4.6
1	A	739	ILE	4.3
1	A	335	LYS	4.3
1	A	741	TRP	4.3
2	B	78	LYS	4.2
1	A	740	GLU	4.0
1	A	375	GLN	3.6
1	A	671	LEU	3.5
2	B	106	LEU	3.4
1	A	331	ALA	3.4
2	B	126	ILE	3.3
2	B	56	VAL	3.3
1	A	333	GLN	3.3
1	A	680	PHE	3.2
1	A	656	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	137	VAL	3.0
2	B	76	LYS	3.0
1	A	296	ASP	2.9
1	A	377	LYS	2.8
2	B	132	ASP	2.8
2	B	59	ASP	2.8
2	B	134	ASP	2.8
2	B	136	GLN	2.8
1	A	668	PHE	2.7
1	A	176	PHE	2.7
2	B	104	ALA	2.6
2	B	108	HIS	2.6
1	A	738	LYS	2.5
1	A	376	THR	2.5
1	A	388	ILE	2.5
1	A	734	PHE	2.4
1	A	735	GLU	2.4
2	B	100	TYR	2.4
2	B	141	GLU	2.4
2	B	116	LYS	2.4
2	B	24	GLY	2.4
1	A	379	ARG	2.4
2	B	57	ASP	2.3
2	B	149	LYS	2.3
1	A	659	PRO	2.3
1	A	653	TRP	2.2
1	A	106	ILE	2.2
1	A	386	LEU	2.2
1	A	336	VAL	2.2
1	A	736	ALA	2.2
1	A	606	ILE	2.2
1	A	190	LEU	2.2
2	B	144	GLN	2.2
1	A	5	GLU	2.1
1	A	500	LEU	2.1
2	B	22	LYS	2.1
2	B	99	GLY	2.1
1	A	389	TYR	2.1
1	A	664	VAL	2.0
2	B	90	PHE	2.0
2	B	140	GLU	2.0
2	B	135	GLY	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	139	TYR	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](#)

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(Å ²)	Q<0.9
3	MG	A	801	1/1	0.99	0.03	32,32,32,32	0

6.5 Other polymers [i](#)

There are no such residues in this entry.