



# Full wwPDB X-ray Structure Validation Report ⓘ

May 29, 2020 – 06:23 am BST

PDB ID : 4ZLK  
Title : Crystal structure of mouse myosin-5a in complex with calcium-bound calmodulin  
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Deposited on : 2015-05-01  
Resolution : 2.50 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](mailto: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.

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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	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

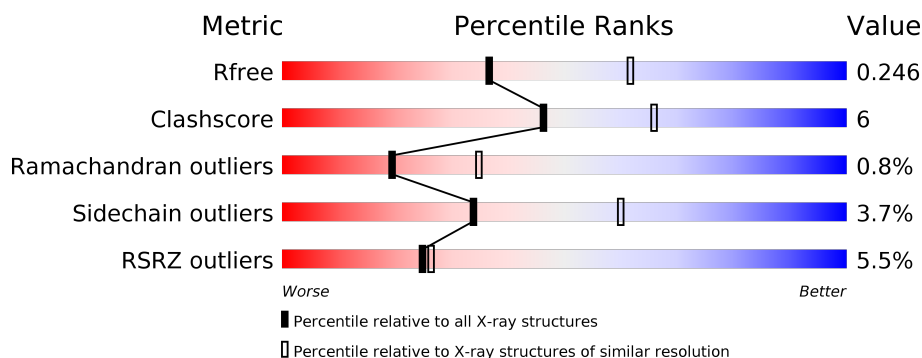
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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  $\geq 3$ , 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	839	<div> <div>2%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>13%</div> </div> </div>
2	B	149	<div> <div>21%</div> <div> <div></div> <div>60%</div> <div>23%</div> <div>5%</div> <div>11%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7289 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-Va.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	733	5997	3846	1029	1086	36	31	1	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-47	MET	-	expression tag	UNP Q99104
A	-46	SER	-	expression tag	UNP Q99104
A	-45	TYR	-	expression tag	UNP Q99104
A	-44	TYR	-	expression tag	UNP Q99104
A	-43	HIS	-	expression tag	UNP Q99104
A	-42	HIS	-	expression tag	UNP Q99104
A	-41	HIS	-	expression tag	UNP Q99104
A	-40	HIS	-	expression tag	UNP Q99104
A	-39	HIS	-	expression tag	UNP Q99104
A	-38	HIS	-	expression tag	UNP Q99104
A	-37	ASP	-	expression tag	UNP Q99104
A	-36	TYR	-	expression tag	UNP Q99104
A	-35	LYS	-	expression tag	UNP Q99104
A	-34	ASP	-	expression tag	UNP Q99104
A	-33	ASP	-	expression tag	UNP Q99104
A	-32	ASP	-	expression tag	UNP Q99104
A	-31	ASP	-	expression tag	UNP Q99104
A	-30	LYS	-	expression tag	UNP Q99104
A	-29	ASN	-	expression tag	UNP Q99104
A	-28	ILE	-	expression tag	UNP Q99104
A	-27	PRO	-	expression tag	UNP Q99104
A	-26	THR	-	expression tag	UNP Q99104
A	-25	THR	-	expression tag	UNP Q99104
A	-24	GLU	-	expression tag	UNP Q99104
A	-23	ASN	-	expression tag	UNP Q99104
A	-22	LEU	-	expression tag	UNP Q99104
A	-21	TYR	-	expression tag	UNP Q99104

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	PHE	-	expression tag	UNP Q99104
A	-19	GLN	-	expression tag	UNP Q99104
A	-18	GLY	-	expression tag	UNP Q99104
A	-17	ALA	-	expression tag	UNP Q99104
A	-16	MET	-	expression tag	UNP Q99104
A	-15	GLY	-	expression tag	UNP Q99104
A	-14	ILE	-	expression tag	UNP Q99104
A	-13	ARG	-	expression tag	UNP Q99104
A	-12	ASN	-	expression tag	UNP Q99104
A	-11	SER	-	expression tag	UNP Q99104
A	-10	LYS	-	expression tag	UNP Q99104
A	-9	ALA	-	expression tag	UNP Q99104
A	-8	TYR	-	expression tag	UNP Q99104
A	-7	VAL	-	expression tag	UNP Q99104
A	-6	ASP	-	expression tag	UNP Q99104
A	-5	GLU	-	expression tag	UNP Q99104
A	-4	LEU	-	expression tag	UNP Q99104
A	-3	THR	-	expression tag	UNP Q99104
A	-2	SER	-	expression tag	UNP Q99104
A	-1	PRO	-	expression tag	UNP Q99104
A	0	ALA	-	expression tag	UNP Q99104

- Molecule 2 is a protein called Calmodulin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	133	Total	C	N	O	S	0	0	0
			1032	635	164	225	8			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	4	Total	Ca	0	0
			4	4		

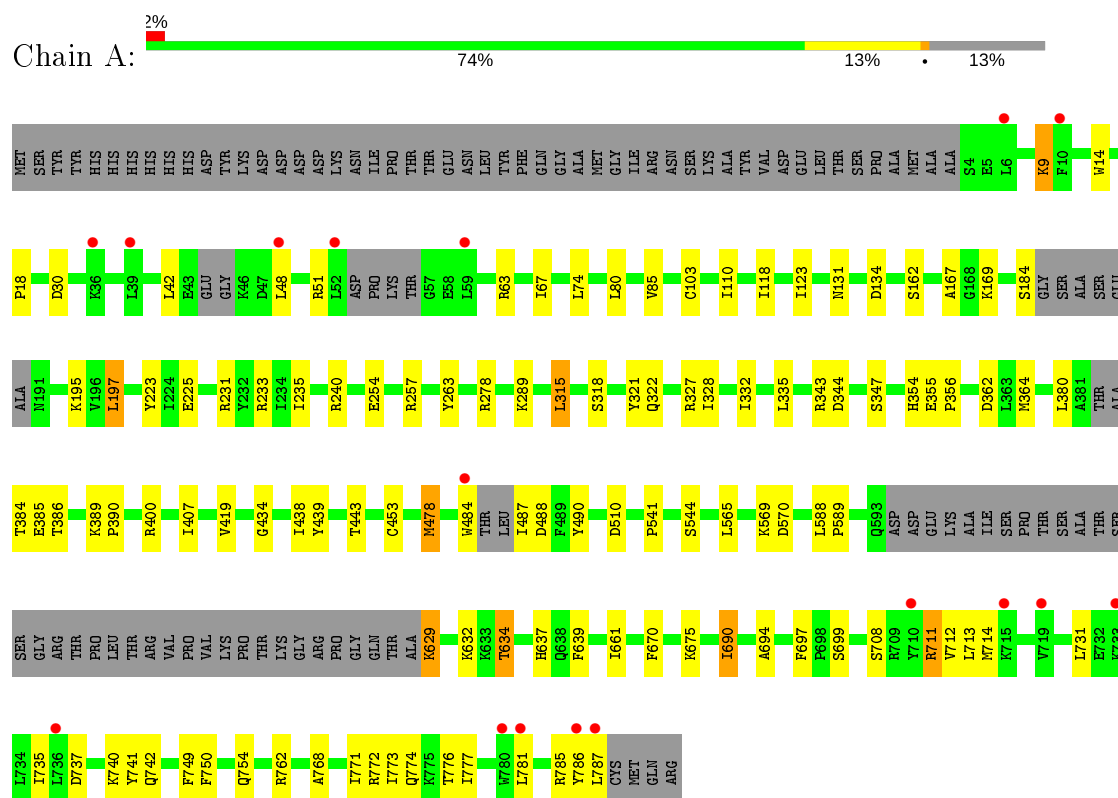
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	256	Total	O	0	0
			256	256		

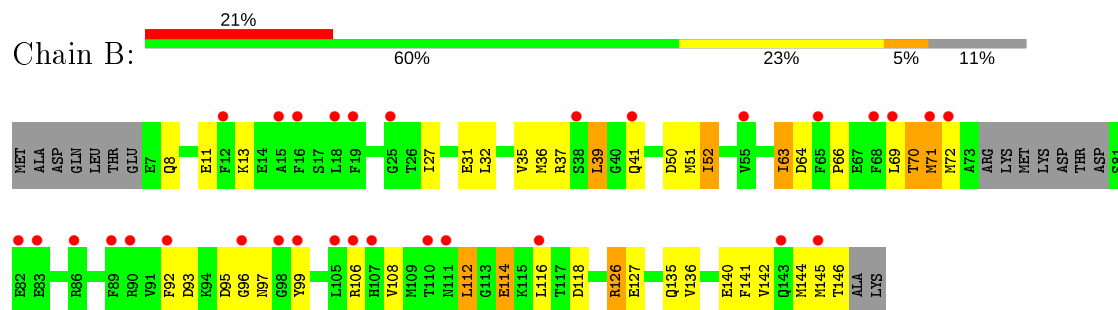
### 3 Residue-property plots [i](#)

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-Va



#### • Molecule 2: Calmodulin



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	56.08 Å 99.45 Å 248.16 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.85 – 2.50 49.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.2 (48.85-2.50) 93.7 (49.73-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.43 (at 2.51 Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, $R_{free}$	0.196 , 0.246 0.197 , 0.246	Depositor DCC
$R_{free}$ test set	2410 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	39.6	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	7289	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: CA

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	0.46	0/6132	0.56	0/8253
2	B	0.42	0/1043	0.70	0/1402
All	All	0.46	0/7175	0.59	0/9655

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	5997	0	5984	68	1
2	B	1032	0	948	25	1
3	B	4	0	0	0	0
4	A	256	0	0	3	0
All	All	7289	0	6932	88	1

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 (88) 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:484:TRP:HB2	1:A:487:ILE:HB	1.62	0.79
1:A:772:ARG:HH11	2:B:114:GLU:HG3	1.52	0.74
1:A:634:THR:HG22	1:A:637:HIS:H	1.54	0.73
2:B:141:PHE:CZ	2:B:145:MET:HE2	2.23	0.73
1:A:510:ASP:OD1	1:A:634:THR:HG21	1.90	0.71
2:B:66:PRO:O	2:B:70:THR:OG1	2.10	0.68
2:B:92:PHE:HA	2:B:108:VAL:HG21	1.76	0.67
2:B:71:MET:HG3	2:B:72:MET:N	2.13	0.64
1:A:389:LYS:HG2	1:A:390:PRO:O	1.98	0.63
1:A:195:LYS:NZ	4:A:801:HOH:O	2.32	0.62
1:A:364:MET:HE2	1:A:364:MET:HA	1.81	0.62
2:B:141:PHE:CE2	2:B:145:MET:HE2	2.36	0.61
2:B:99:TYR:HD2	2:B:135:GLN:HG3	1.66	0.60
1:A:777:ILE:HG21	2:B:145:MET:HE1	1.85	0.58
1:A:18:PRO:O	1:A:675:LYS:NZ	2.35	0.56
2:B:37:ARG:HA	2:B:41:GLN:O	2.06	0.56
1:A:74:LEU:HD12	1:A:103:CYS:HB2	1.88	0.56
1:A:774:GLN:NE2	2:B:144:MET:O	2.39	0.56
1:A:711:ARG:HA	1:A:714:MET:SD	2.46	0.56
1:A:711:ARG:HB2	1:A:711:ARG:CZ	2.36	0.55
1:A:629:LYS:HA	1:A:632:LYS:H	1.71	0.55
1:A:787:LEU:HD12	2:B:39:LEU:HD12	1.87	0.55
1:A:9:LYS:N	1:A:30:ASP:OD1	2.41	0.54
1:A:777:ILE:HG21	2:B:145:MET:CE	2.38	0.53
1:A:731:LEU:HD11	1:A:735:ILE:HD12	1.89	0.53
1:A:588:LEU:HB3	1:A:589:PRO:HD3	1.90	0.53
2:B:95:ASP:O	2:B:97:ASN:N	2.42	0.52
2:B:32:LEU:HD21	2:B:51:MET:HE1	1.92	0.52
2:B:36:MET:O	2:B:41:GLN:HB2	2.10	0.52
1:A:131:ASN:HB2	1:A:134:ASP:OD2	2.10	0.51
1:A:169:LYS:HG3	4:A:819:HOH:O	2.11	0.51
1:A:785:ARG:HD2	1:A:786:TYR:HE1	1.77	0.50
1:A:565:LEU:O	1:A:569:LYS:HG3	2.12	0.50
1:A:634:THR:CG2	1:A:637:HIS:H	2.23	0.50
1:A:741:TYR:O	1:A:742:GLN:NE2	2.45	0.50
2:B:142:VAL:O	2:B:146:THR:HG23	2.12	0.49
1:A:384:THR:HG23	1:A:385:GLU:HG2	1.95	0.49
1:A:711:ARG:HB2	1:A:711:ARG:NH1	2.27	0.49
1:A:14:TRP:NE1	1:A:63:ARG:HG2	2.27	0.49
1:A:167:ALA:HB3	4:A:819:HOH:O	2.13	0.48
1:A:737:ASP:HB3	1:A:740:LYS:HG2	1.95	0.48
1:A:772:ARG:O	1:A:776:THR:HG23	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:8:GLN:O	2:B:11:GLU:HB3	2.13	0.47
2:B:136:VAL:HA	2:B:140:GLU:OE2	2.15	0.47
1:A:332:ILE:HD11	1:A:407:ILE:HG22	1.96	0.47
1:A:231:ARG:HD3	1:A:233:ARG:HH21	1.79	0.46
1:A:708:SER:O	1:A:711:ARG:NH1	2.48	0.46
1:A:453:CYS:HB3	1:A:639:PHE:CZ	2.51	0.46
1:A:343:ARG:O	1:A:347:SER:HB3	2.15	0.45
1:A:42:LEU:HD11	1:A:48:LEU:HD11	1.98	0.45
2:B:31:GLU:O	2:B:35:VAL:HG23	2.15	0.45
1:A:478:MET:SD	1:A:484:TRP:HH2	2.40	0.45
2:B:106:ARG:NE	2:B:118:ASP:OD2	2.50	0.45
1:A:80:LEU:HB3	1:A:694:ALA:HB2	1.98	0.45
1:A:773:ILE:O	1:A:777:ILE:HG13	2.17	0.45
1:A:354:HIS:CD2	1:A:356:PRO:HD2	2.52	0.45
2:B:52:ILE:HG13	2:B:63:ILE:HG22	1.99	0.45
1:A:484:TRP:HB2	1:A:487:ILE:CB	2.42	0.45
1:A:768:ALA:HA	1:A:771:ILE:HG12	1.99	0.45
1:A:713:LEU:HD21	1:A:762:ARG:HA	1.98	0.44
1:A:355:GLU:HB3	1:A:356:PRO:HD3	1.98	0.44
1:A:118:ILE:HA	1:A:123:ILE:HD13	1.99	0.44
1:A:697:PHE:HB3	1:A:749:PHE:HB3	1.99	0.44
1:A:278:ARG:NH2	1:A:362:ASP:OD2	2.50	0.43
1:A:380:LEU:O	1:A:386:THR:HA	2.17	0.43
2:B:141:PHE:CZ	2:B:145:MET:CE	2.99	0.43
2:B:27:ILE:HB	2:B:63:ILE:HG23	2.00	0.43
1:A:318:SER:O	1:A:322:GLN:HG3	2.19	0.43
1:A:225:GLU:OE2	1:A:240:ARG:NE	2.51	0.43
1:A:110:ILE:HG12	1:A:661:ILE:HD11	2.00	0.43
1:A:488:ASP:HB3	1:A:490:TYR:CE1	2.54	0.43
1:A:634:THR:HG22	1:A:637:HIS:CB	2.49	0.43
2:B:32:LEU:HD21	2:B:51:MET:CE	2.49	0.42
1:A:328:ILE:HA	1:A:364:MET:HE1	2.01	0.42
1:A:781:LEU:HD23	1:A:781:LEU:HA	1.90	0.42
1:A:223:TYR:CZ	1:A:434:GLY:HA3	2.54	0.42
1:A:257:ARG:HB3	1:A:263:TYR:CE2	2.54	0.42
2:B:126:ARG:HG3	2:B:127:GLU:N	2.35	0.42
1:A:335:LEU:O	1:A:400:ARG:HD2	2.19	0.42
1:A:197:LEU:HA	1:A:197:LEU:HD13	1.88	0.41
1:A:162:SER:HA	1:A:438:ILE:O	2.21	0.41
1:A:315:LEU:HD22	1:A:419:VAL:HG13	2.03	0.41
1:A:85:VAL:HG21	1:A:690:ILE:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:750:PHE:HB3	1:A:754:GLN:HB2	2.03	0.41
1:A:541:PRO:HG2	1:A:544:SER:HB3	2.03	0.41
1:A:699:SER:HB2	1:A:750:PHE:HB2	2.03	0.41
1:A:632:LYS:O	1:A:632:LYS:HG2	2.21	0.40
1:A:235:ILE:HG12	1:A:235:ILE:H	1.75	0.40

All (1) 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:327:ARG:NH2	2:B:50:ASP:OD2[2_555]	2.18	0.02

## 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	720/839 (86%)	692 (96%)	25 (4%)	3 (0%)	34	54
2	B	129/149 (87%)	118 (92%)	7 (5%)	4 (3%)	4	5
All	All	849/988 (86%)	810 (95%)	32 (4%)	7 (1%)	19	35

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	96	GLY
1	A	344	ASP
1	A	670	PHE
2	B	93	ASP
2	B	112	LEU
1	A	570	ASP
2	B	39	LEU

### 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	649/736 (88%)	632 (97%)	17 (3%)	46	72
2	B	110/127 (87%)	99 (90%)	11 (10%)	7	15
All	All	759/863 (88%)	731 (96%)	28 (4%)	34	60

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LYS
1	A	51	ARG
1	A	67	ILE
1	A	184	SER
1	A	197	LEU
1	A	254	GLU
1	A	289	LYS
1	A	315	LEU
1	A	321	TYR
1	A	439	TYR
1	A	443	THR
1	A	478	MET
1	A	629	LYS
1	A	634	THR
1	A	690	ILE
1	A	711	ARG
1	A	712	VAL
2	B	13	LYS
2	B	52	ILE
2	B	63	ILE
2	B	64	ASP
2	B	69	LEU
2	B	70	THR
2	B	71	MET
2	B	112	LEU
2	B	114	GLU
2	B	116	LEU

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Mol	Chain	Res	Type
2	B	126	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

Of 4 ligands modelled in this entry, 4 are 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	733/839 (87%)	0.02	17 (2%) 60 63	9, 26, 70, 91	6 (0%)
2	B	133/149 (89%)	1.16	31 (23%) 0 0	38, 77, 99, 105	0
All	All	866/988 (87%)	0.20	48 (5%) 25 26	9, 30, 84, 105	6 (0%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	65	PHE	6.4
2	B	12	PHE	5.6
2	B	96	GLY	5.1
1	A	787	LEU	5.0
2	B	116	LEU	4.9
2	B	68	PHE	4.7
2	B	18	LEU	4.4
2	B	98	GLY	4.2
2	B	69	LEU	3.8
2	B	92	PHE	3.8
1	A	786	TYR	3.6
2	B	19	PHE	3.5
1	A	48	LEU	3.5
2	B	107	HIS	3.5
2	B	16	PHE	3.3
1	A	36	LYS	3.3
2	B	110	THR	3.3
1	A	780	TRP	3.3
2	B	83	GLU	3.2
2	B	99	TYR	3.2
1	A	736	LEU	3.1
1	A	733	LYS	2.9
2	B	55	VAL	2.8
2	B	89	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	B	105	LEU	2.8
2	B	72	MET	2.8
1	A	781	LEU	2.8
2	B	25	GLY	2.8
2	B	111	ASN	2.8
1	A	39	LEU	2.8
2	B	38	SER	2.7
1	A	484	TRP	2.7
2	B	71	MET	2.7
2	B	106	ARG	2.7
1	A	719	VAL	2.7
1	A	10	PHE	2.7
2	B	15	ALA	2.6
2	B	145	MET	2.6
1	A	52	LEU	2.6
2	B	143	GLN	2.6
1	A	6	LEU	2.4
2	B	86	ARG	2.4
2	B	90	ARG	2.4
2	B	41	GLN	2.3
2	B	82	GLU	2.3
1	A	59	LEU	2.2
1	A	715	LYS	2.0
1	A	710	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, 95<sup>th</sup> 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	CA	B	203	1/1	0.32	0.09	87,87,87,87	0
3	CA	B	202	1/1	0.66	0.06	79,79,79,79	0
3	CA	B	201	1/1	0.92	0.03	83,83,83,83	0
3	CA	B	204	1/1	0.92	0.05	66,66,66,66	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.