



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 10:55 am GMT

PDB ID : 2B9C
Title : Structure of tropomyosin's mid-region: bending and binding sites for actin
Authors : Brown, J.H.; Zhou, Z.; Reshetnikova, L.; Robinson, H.; Yammani, R.D.; Tobacman, L.S.; Cohen, C.
Deposited on : 2005-10-11
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

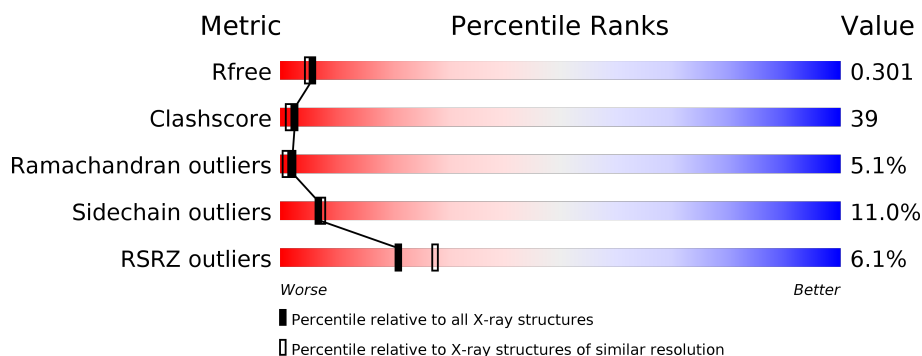
1 Overall quality at a glance

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	147	<div> <div>9%</div> <div>25% 41% 24% 7%</div> </div>
1	B	147	<div> <div>3%</div> <div>25% 44% 23%</div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2650 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 striated-muscle alpha tropomyosin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	136	Total	C	N	O	S	0	8	0
			1151	701	211	236	3			
1	B	142	Total	C	N	O	S	0	3	0
			1150	700	199	248	3			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	88	MET	-	INITIATING MET	UNP P04692
A	209	ASP	-	GCN4 TAG	UNP P04692
A	210	LYS	-	GCN4 TAG	UNP P04692
A	211	VAL	-	GCN4 TAG	UNP P04692
A	212	GLU	-	GCN4 TAG	UNP P04692
A	213	GLU	-	GCN4 TAG	UNP P04692
A	214	LEU	-	GCN4 TAG	UNP P04692
A	215	LEU	-	GCN4 TAG	UNP P04692
A	216	SER	-	GCN4 TAG	UNP P04692
A	217	LYS	-	GCN4 TAG	UNP P04692
A	218	ASN	-	GCN4 TAG	UNP P04692
A	219	TYR	-	GCN4 TAG	UNP P04692
A	220	HIS	-	GCN4 TAG	UNP P04692
A	221	LEU	-	GCN4 TAG	UNP P04692
A	222	GLU	-	GCN4 TAG	UNP P04692
A	223	ASN	-	GCN4 TAG	UNP P04692
A	224	GLU	-	GCN4 TAG	UNP P04692
A	225	VAL	-	GCN4 TAG	UNP P04692
A	226	ALA	-	GCN4 TAG	UNP P04692
A	227	ARG	-	GCN4 TAG	UNP P04692
A	228	LEU	-	GCN4 TAG	UNP P04692
A	229	LYS	-	GCN4 TAG	UNP P04692
A	230	LYS	-	GCN4 TAG	UNP P04692
A	231	LEU	-	GCN4 TAG	UNP P04692
A	232	VAL	-	GCN4 TAG	UNP P04692

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Chain	Residue	Modelled	Actual	Comment	Reference
A	233	GLY	-	GCN4 TAG	UNP P04692
A	234	GLU	-	GCN4 TAG	UNP P04692
B	1088	MET	-	INITIATING MET	UNP P04692
B	1209	ASP	-	GCN4 TAG	UNP P04692
B	1210	LYS	-	GCN4 TAG	UNP P04692
B	1211	VAL	-	GCN4 TAG	UNP P04692
B	1212	GLU	-	GCN4 TAG	UNP P04692
B	1213	GLU	-	GCN4 TAG	UNP P04692
B	1214	LEU	-	GCN4 TAG	UNP P04692
B	1215	LEU	-	GCN4 TAG	UNP P04692
B	1216	SER	-	GCN4 TAG	UNP P04692
B	1217	LYS	-	GCN4 TAG	UNP P04692
B	1218	ASN	-	GCN4 TAG	UNP P04692
B	1219	TYR	-	GCN4 TAG	UNP P04692
B	1220	HIS	-	GCN4 TAG	UNP P04692
B	1221	LEU	-	GCN4 TAG	UNP P04692
B	1222	GLU	-	GCN4 TAG	UNP P04692
B	1223	ASN	-	GCN4 TAG	UNP P04692
B	1224	GLU	-	GCN4 TAG	UNP P04692
B	1225	VAL	-	GCN4 TAG	UNP P04692
B	1226	ALA	-	GCN4 TAG	UNP P04692
B	1227	ARG	-	GCN4 TAG	UNP P04692
B	1228	LEU	-	GCN4 TAG	UNP P04692
B	1229	LYS	-	GCN4 TAG	UNP P04692
B	1230	LYS	-	GCN4 TAG	UNP P04692
B	1231	LEU	-	GCN4 TAG	UNP P04692
B	1232	VAL	-	GCN4 TAG	UNP P04692
B	1233	GLY	-	GCN4 TAG	UNP P04692
B	1234	GLU	-	GCN4 TAG	UNP P04692

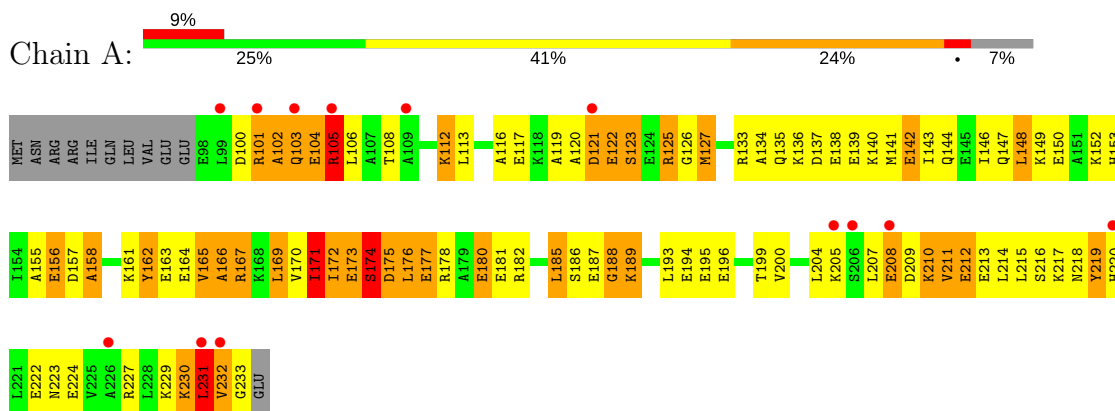
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	156	Total	O	0	0
			156	156		
2	B	193	Total	O	0	0
			193	193		

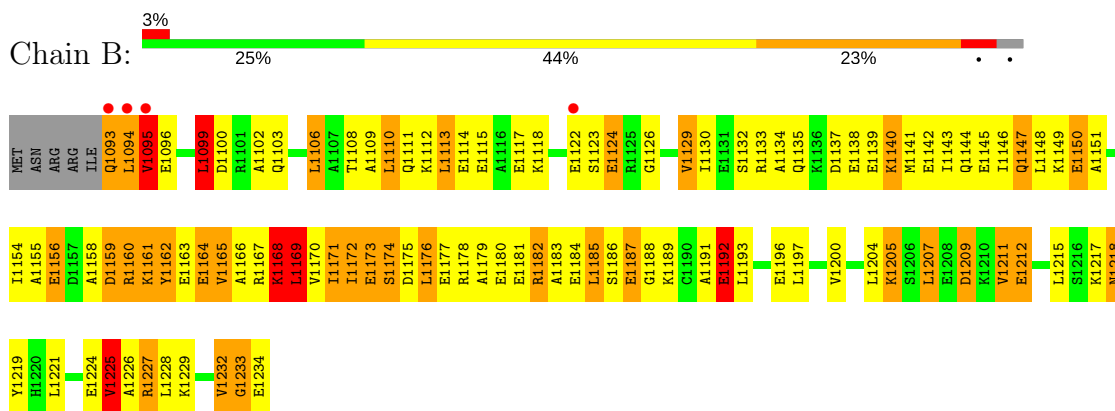
3 Residue-property plots

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: striated-muscle alpha tropomyosin



• Molecule 1: striated-muscle alpha tropomyosin



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	80.52Å 80.52Å 112.45Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.30 19.63 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-2.30) 96.8 (19.63-2.30)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.30Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.256 , 0.296 0.267 , 0.301	Depositor DCC
R_{free} test set	706 reflections (3.98%)	wwPDB-VP
Wilson B-factor (Å ²)	44.3	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 101.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.052 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	2650	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.86% 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

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	2.48	63/1156 (5.4%)	2.06	38/1543 (2.5%)
1	B	2.52	58/1153 (5.0%)	2.13	46/1539 (3.0%)
All	All	2.50	121/2309 (5.2%)	2.10	84/3082 (2.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	4
All	All	0	8

All (121) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	TYR	CD1-CE1	13.60	1.59	1.39
1	A	181	GLU	CG-CD	13.37	1.72	1.51
1	A	162	TYR	CD2-CE2	13.11	1.59	1.39
1	A	162	TYR	CE2-CZ	-12.40	1.22	1.38
1	B	1162	TYR	CZ-OH	11.91	1.58	1.37
1	B	1177	GLU	CD-OE1	11.43	1.38	1.25
1	B	1177	GLU	CD-OE2	11.18	1.38	1.25
1	A	178	ARG	CZ-NH1	10.93	1.47	1.33
1	A	173	GLU	CG-CD	10.24	1.67	1.51
1	B	1180	GLU	CD-OE1	9.96	1.36	1.25
1	B	1122	GLU	CG-CD	9.84	1.66	1.51
1	B	1187	GLU	CB-CG	-9.28	1.34	1.52
1	B	1181	GLU	CB-CG	9.27	1.69	1.52
1	A	187	GLU	CG-CD	9.19	1.65	1.51
1	A	163	GLU	CD-OE2	9.15	1.35	1.25
1	B	1181	GLU	CD-OE1	9.02	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1156	GLU	CG-CD	8.89	1.65	1.51
1	A	174	SER	CA-CB	8.89	1.66	1.52
1	B	1179	ALA	CA-CB	8.43	1.70	1.52
1	B	1181	GLU	CG-CD	8.27	1.64	1.51
1	B	1167	ARG	CZ-NH2	8.21	1.43	1.33
1	B	1179	ALA	N-CA	-8.18	1.29	1.46
1	B	1170	VAL	C-O	-8.01	1.08	1.23
1	B	1192	GLU	CD-OE1	8.01	1.34	1.25
1	B	1164[A]	GLU	CB-CG	8.00	1.67	1.52
1	B	1164[B]	GLU	CB-CG	8.00	1.67	1.52
1	A	163	GLU	CD-OE1	7.93	1.34	1.25
1	B	1173	GLU	CD-OE1	7.81	1.34	1.25
1	A	182	ARG	CZ-NH1	-7.77	1.23	1.33
1	A	164	GLU	CD-OE1	7.66	1.34	1.25
1	A	139	GLU	CD-OE1	7.64	1.34	1.25
1	B	1129	VAL	CB-CG1	-7.57	1.36	1.52
1	A	211	VAL	CB-CG2	-7.56	1.36	1.52
1	A	166	ALA	N-CA	-7.48	1.31	1.46
1	A	208	GLU	CD-OE2	7.46	1.33	1.25
1	A	181	GLU	CD-OE1	7.45	1.33	1.25
1	A	172	ILE	CB-CG2	-7.43	1.29	1.52
1	A	171	ILE	CA-CB	-7.41	1.37	1.54
1	B	1171	ILE	CB-CG2	7.24	1.75	1.52
1	B	1226	ALA	CA-CB	-7.23	1.37	1.52
1	A	175	ASP	CG-OD2	7.20	1.42	1.25
1	A	180	GLU	CD-OE1	7.16	1.33	1.25
1	A	182	ARG	CA-CB	-7.15	1.38	1.53
1	B	1176	LEU	C-O	7.02	1.36	1.23
1	B	1211	VAL	CB-CG1	7.01	1.67	1.52
1	A	127	MET	CG-SD	7.00	1.99	1.81
1	B	1173	GLU	CD-OE2	6.98	1.33	1.25
1	B	1174	SER	CA-CB	6.91	1.63	1.52
1	A	177	GLU	CB-CG	6.84	1.65	1.52
1	B	1178	ARG	CG-CD	6.79	1.69	1.51
1	B	1211	VAL	CA-CB	-6.75	1.40	1.54
1	B	1151	ALA	N-CA	-6.65	1.33	1.46
1	A	167[A]	ARG	CG-CD	6.61	1.68	1.51
1	A	167[B]	ARG	CG-CD	6.61	1.68	1.51
1	B	1218	ASN	N-CA	-6.58	1.33	1.46
1	A	162	TYR	CA-CB	-6.56	1.39	1.53
1	B	1188	GLY	CA-C	6.55	1.62	1.51
1	A	156	GLU	CB-CG	6.49	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1124	GLU	CD-OE1	6.47	1.32	1.25
1	B	1196	GLU	CB-CG	-6.47	1.39	1.52
1	B	1156	GLU	CD-OE1	-6.44	1.18	1.25
1	A	175	ASP	CB-CG	6.43	1.65	1.51
1	B	1189	LYS	CB-CG	6.41	1.69	1.52
1	B	1173	GLU	CB-CG	6.36	1.64	1.52
1	A	169	LEU	CA-C	-6.32	1.36	1.52
1	A	172	ILE	CA-CB	-6.26	1.40	1.54
1	B	1169	LEU	CG-CD2	6.21	1.74	1.51
1	A	181	GLU	N-CA	-6.21	1.33	1.46
1	B	1139	GLU	CD-OE2	6.18	1.32	1.25
1	A	212	GLU	C-O	-6.15	1.11	1.23
1	B	1191	ALA	CA-CB	-6.07	1.39	1.52
1	B	1187	GLU	CG-CD	6.02	1.60	1.51
1	B	1154	ILE	C-O	-6.00	1.11	1.23
1	B	1166	ALA	C-N	-5.99	1.20	1.34
1	B	1132	SER	CA-C	5.97	1.68	1.52
1	A	143	ILE	CA-C	5.96	1.68	1.52
1	A	158	ALA	N-CA	-5.87	1.34	1.46
1	A	177	GLU	CD-OE2	5.86	1.32	1.25
1	A	173	GLU	CD-OE2	5.83	1.32	1.25
1	A	181	GLU	CB-CG	5.81	1.63	1.52
1	A	172	ILE	CA-C	-5.81	1.37	1.52
1	B	1150	GLU	CG-CD	5.80	1.60	1.51
1	B	1156	GLU	CB-CG	-5.80	1.41	1.52
1	A	163	GLU	C-O	-5.78	1.12	1.23
1	B	1184	GLU	CB-CG	-5.75	1.41	1.52
1	A	178	ARG	CB-CG	5.75	1.68	1.52
1	A	186	SER	N-CA	-5.71	1.34	1.46
1	A	116	ALA	CA-CB	5.68	1.64	1.52
1	A	188	GLY	C-O	-5.63	1.14	1.23
1	B	1224	GLU	CB-CG	5.63	1.62	1.52
1	A	162	TYR	CE1-CZ	5.62	1.45	1.38
1	B	1163	GLU	CD-OE1	5.62	1.31	1.25
1	A	174	SER	N-CA	-5.61	1.35	1.46
1	A	171	ILE	CB-CG2	5.61	1.70	1.52
1	A	212	GLU	CD-OE2	5.60	1.31	1.25
1	A	194	GLU	CB-CG	5.55	1.62	1.52
1	A	117	GLU	CA-CB	-5.53	1.41	1.53
1	A	212	GLU	CD-OE1	5.53	1.31	1.25
1	B	1123	SER	CA-CB	-5.52	1.44	1.52
1	B	1167	ARG	NE-CZ	5.49	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	148	LEU	CA-CB	-5.45	1.41	1.53
1	B	1095	VAL	CA-CB	5.45	1.66	1.54
1	B	1166	ALA	C-O	5.44	1.33	1.23
1	B	1173	GLU	CG-CD	5.40	1.60	1.51
1	A	164	GLU	N-CA	-5.39	1.35	1.46
1	B	1176	LEU	CA-CB	5.32	1.66	1.53
1	A	181	GLU	C-O	-5.32	1.13	1.23
1	A	142	GLU	CG-CD	5.31	1.59	1.51
1	A	176	LEU	C-O	5.28	1.33	1.23
1	B	1155	ALA	C-O	-5.23	1.13	1.23
1	A	169	LEU	CG-CD1	-5.22	1.32	1.51
1	A	187	GLU	CA-C	-5.21	1.39	1.52
1	A	134	ALA	CA-CB	-5.21	1.41	1.52
1	A	181	GLU	CD-OE2	5.14	1.31	1.25
1	B	1227	ARG	C-O	5.13	1.33	1.23
1	A	182	ARG	CB-CG	-5.12	1.38	1.52
1	B	1227	ARG	NE-CZ	5.06	1.39	1.33
1	A	195	GLU	N-CA	-5.05	1.36	1.46
1	B	1156	GLU	C-O	-5.03	1.13	1.23
1	A	189	LYS	CD-CE	5.03	1.63	1.51
1	B	1188	GLY	C-O	5.00	1.31	1.23

All (84) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ARG	NE-CZ-NH2	-24.50	108.05	120.30
1	B	1182	ARG	NE-CZ-NH1	-20.30	110.15	120.30
1	A	178	ARG	NE-CZ-NH1	15.52	128.06	120.30
1	A	182	ARG	NE-CZ-NH1	15.08	127.84	120.30
1	B	1175	ASP	CB-CG-OD2	14.46	131.31	118.30
1	B	1159	ASP	CB-CG-OD1	-12.95	106.64	118.30
1	B	1182	ARG	NE-CZ-NH2	12.64	126.62	120.30
1	A	175	ASP	CB-CG-OD2	11.31	128.48	118.30
1	A	170	VAL	CG1-CB-CG2	-11.10	93.15	110.90
1	B	1160	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	B	1159	ASP	CB-CG-OD2	11.04	128.23	118.30
1	B	1176	LEU	CB-CG-CD1	-10.78	92.67	111.00
1	A	172	ILE	CG1-CB-CG2	-10.38	88.55	111.40
1	A	169	LEU	CA-CB-CG	9.99	138.27	115.30
1	A	176	LEU	CB-CG-CD1	-9.74	94.44	111.00
1	A	182	ARG	NH1-CZ-NH2	-9.08	109.41	119.40
1	B	1175	ASP	CB-CA-C	-8.82	92.76	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	ASP	CB-CA-C	-8.67	93.06	110.40
1	B	1168	LYS	O-C-N	-8.60	108.94	122.70
1	B	1166	ALA	N-CA-CB	-7.96	98.95	110.10
1	A	174	SER	O-C-N	-7.86	110.13	122.70
1	A	171	ILE	CG1-CB-CG2	-7.76	94.33	111.40
1	A	157	ASP	CB-CG-OD2	7.71	125.24	118.30
1	A	182	ARG	CG-CD-NE	7.67	127.91	111.80
1	A	121	ASP	CB-CG-OD1	7.53	125.08	118.30
1	B	1106	LEU	CB-CG-CD1	-7.50	98.26	111.00
1	A	176	LEU	O-C-N	-7.28	111.06	122.70
1	A	181	GLU	O-C-N	-7.26	111.08	122.70
1	A	157	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	B	1162	TYR	CZ-CE2-CD2	7.13	126.22	119.80
1	A	113	LEU	CB-CG-CD1	-7.11	98.92	111.00
1	A	176	LEU	CA-CB-CG	7.00	131.41	115.30
1	B	1160	ARG	NE-CZ-NH2	-6.95	116.82	120.30
1	B	1176	LEU	CD1-CG-CD2	-6.94	89.67	110.50
1	A	173	GLU	CB-CA-C	-6.94	96.52	110.40
1	B	1162	TYR	CB-CG-CD1	-6.94	116.84	121.00
1	B	1181	GLU	CB-CA-C	-6.90	96.61	110.40
1	B	1167	ARG	N-CA-C	-6.68	92.97	111.00
1	B	1165	VAL	C-N-CA	-6.62	105.14	121.70
1	A	113	LEU	CB-CG-CD2	6.60	122.22	111.00
1	B	1169	LEU	CB-CG-CD2	-6.55	99.87	111.00
1	A	188	GLY	O-C-N	-6.49	112.31	122.70
1	A	185	LEU	CB-CG-CD2	6.48	122.02	111.00
1	B	1189	LYS	CA-CB-CG	-6.46	99.19	113.40
1	A	182	ARG	CB-CA-C	-6.42	97.55	110.40
1	A	133	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	B	1162	TYR	C-N-CA	-6.34	105.86	121.70
1	B	1167	ARG	CB-CA-C	-6.28	97.85	110.40
1	A	166	ALA	CB-CA-C	-6.20	100.80	110.10
1	B	1133	ARG	CA-CB-CG	-6.18	99.80	113.40
1	B	1176	LEU	CB-CA-C	-6.15	98.51	110.20
1	B	1168	LYS	N-CA-CB	-6.12	99.59	110.60
1	B	1176	LEU	O-C-N	-5.96	113.16	122.70
1	B	1207	LEU	CB-CG-CD1	-5.95	100.89	111.00
1	B	1170	VAL	CA-CB-CG1	-5.92	102.01	110.90
1	B	1209	ASP	CB-CG-OD1	5.83	123.55	118.30
1	B	1174	SER	O-C-N	-5.80	113.43	122.70
1	A	165	VAL	CA-CB-CG2	-5.78	102.23	110.90
1	B	1183	ALA	O-C-N	-5.74	113.52	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1192	GLU	CG-CD-OE2	-5.67	106.97	118.30
1	B	1173	GLU	CB-CA-C	-5.62	99.16	110.40
1	B	1225	VAL	N-CA-C	-5.59	95.91	111.00
1	B	1161	LYS	CD-CE-NZ	-5.57	98.88	111.70
1	B	1175	ASP	C-N-CA	-5.53	107.88	121.70
1	B	1113	LEU	CB-CG-CD1	-5.47	101.71	111.00
1	A	155	ALA	N-CA-CB	5.42	117.69	110.10
1	B	1176	LEU	CA-CB-CG	5.38	127.68	115.30
1	B	1110	LEU	C-N-CA	-5.37	108.28	121.70
1	B	1137	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	1171	ILE	CG1-CB-CG2	-5.28	99.78	111.40
1	A	170	VAL	C-N-CA	5.27	134.88	121.70
1	B	1099	LEU	N-CA-C	-5.27	96.77	111.00
1	B	1140	LYS	CD-CE-NZ	5.26	123.80	111.70
1	B	1147	GLN	N-CA-C	-5.20	96.96	111.00
1	A	125[A]	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	125[B]	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	A	185	LEU	O-C-N	-5.19	114.40	122.70
1	B	1227	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	177	GLU	CB-CA-C	-5.13	100.13	110.40
1	A	104	GLU	N-CA-C	-5.09	97.25	111.00
1	B	1205	LYS	CD-CE-NZ	-5.09	99.98	111.70
1	A	162	TYR	N-CA-CB	-5.09	101.44	110.60
1	A	174	SER	C-N-CA	-5.02	109.16	121.70
1	A	162	TYR	CG-CD2-CE2	5.01	125.31	121.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	169	LEU	Mainchain
1	A	171	ILE	Mainchain
1	A	180	GLU	Mainchain
1	A	219	TYR	Sidechain
1	B	1162	TYR	Sidechain
1	B	1168	LYS	Mainchain
1	B	1173	GLU	Mainchain
1	B	1219	TYR	Sidechain

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	1151	0	1130	103	0
1	B	1150	0	1119	105	0
2	A	156	0	0	11	0
2	B	193	0	0	11	0
All	All	2650	0	2249	178	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 39.

All (178) 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:1171:ILE:CB	1:B:1171:ILE:CG2	1.75	1.60
1:B:1169:LEU:CD2	1:B:1169:LEU:CG	1.74	1.59
1:A:171:ILE:CG1	1:A:171:ILE:CD1	1.78	1.59
1:A:122[A]:GLU:OE1	1:A:122[A]:GLU:HA	1.51	1.11
1:B:1169:LEU:CD2	1:B:1169:LEU:CD1	2.36	1.02
1:B:1185:LEU:HD23	1:B:1186:SER:N	1.76	1.00
1:B:1169:LEU:CD2	1:B:1169:LEU:CB	2.43	0.96
1:A:149:LYS:HZ3	1:A:152:LYS:HE3	1.28	0.96
1:B:1114:GLU:HA	2:B:206:HOH:O	1.67	0.95
1:A:105:ARG:O	1:A:108:THR:HG22	1.71	0.91
1:B:1134:ALA:O	1:B:1138[A]:GLU:HG2	1.71	0.90
1:A:171:ILE:HG21	1:A:171:ILE:HD13	1.52	0.90
1:B:1171:ILE:CG1	1:B:1171:ILE:CG2	2.50	0.89
1:B:1229:LYS:O	1:B:1234:GLU:OXT	1.91	0.89
1:B:1192:GLU:HG2	1:B:1193:LEU:N	1.89	0.86
1:A:171:ILE:CB	1:A:171:ILE:CD1	2.54	0.85
1:A:149:LYS:HZ3	1:A:152:LYS:CE	1.93	0.79
1:B:1225:VAL:O	1:B:1229:LYS:HB2	1.82	0.79
1:B:1143:ILE:O	1:B:1146:ILE:N	2.16	0.78
1:B:1164[A]:GLU:OE2	1:B:1168:LYS:HE3	1.84	0.78
1:A:231:LEU:O	1:A:231:LEU:HG	1.86	0.76
1:B:1171:ILE:CG2	1:B:1171:ILE:CA	2.64	0.76
1:B:1185:LEU:HD23	1:B:1186:SER:CA	2.15	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:ASN:HB2	1:B:1218:ASN:OD1	1.88	0.74
1:A:171:ILE:CG2	1:A:171:ILE:CD1	2.66	0.73
1:B:1232:VAL:HG12	1:B:1233:GLY:H	1.52	0.73
1:B:1093:GLN:O	1:B:1093:GLN:HG3	1.90	0.72
1:A:141:MET:HE3	1:B:1140:LYS:HG2	1.71	0.72
1:A:141:MET:CE	1:B:1140:LYS:HG2	2.19	0.72
1:A:171:ILE:HG21	1:A:171:ILE:CD1	2.20	0.71
1:A:207:LEU:O	1:A:211:VAL:HG23	1.92	0.70
1:B:1185:LEU:HD23	1:B:1186:SER:HA	1.75	0.68
1:A:141:MET:HG2	1:B:1141:MET:HG2	1.75	0.67
1:A:209:ASP:O	1:A:211:VAL:N	2.28	0.66
1:B:1099:LEU:O	1:B:1103:GLN:HG3	1.96	0.66
1:A:171:ILE:CG2	1:A:171:ILE:HD13	2.23	0.66
1:B:1232:VAL:HG12	1:B:1233:GLY:N	2.11	0.66
2:A:313:HOH:O	1:B:1232:VAL:HG21	1.97	0.65
1:A:137:ASP:O	1:A:141:MET:HG3	1.97	0.65
1:A:176:LEU:HD13	1:B:1176:LEU:HA	1.78	0.65
1:A:149:LYS:NZ	1:A:152:LYS:CE	2.60	0.65
1:A:136:LYS:NZ	2:A:286:HOH:O	2.21	0.65
1:A:193:LEU:HB2	1:B:1193:LEU:HD23	1.79	0.64
1:B:1129:VAL:HG23	1:B:1130:ILE:HD13	1.78	0.64
1:B:1185:LEU:CD2	1:B:1186:SER:N	2.58	0.64
1:A:119:ALA:O	1:A:122[B]:GLU:HB3	1.98	0.64
1:B:1232:VAL:O	1:B:1233:GLY:O	2.16	0.64
1:B:1234:GLU:O	1:B:1234:GLU:HG2	1.96	0.63
1:B:1186:SER:O	1:B:1186:SER:OG	2.14	0.63
1:A:232:VAL:HG12	1:A:232:VAL:O	1.99	0.63
1:A:122[B]:GLU:O	1:A:125[B]:ARG:HB3	1.99	0.62
2:A:258:HOH:O	1:B:1217:LYS:HD3	1.97	0.62
1:B:1227:ARG:NH2	2:B:61:HOH:O	2.31	0.62
1:A:138[B]:GLU:O	1:A:142:GLU:HG2	1.99	0.62
1:A:200:VAL:CG1	1:B:1200:VAL:HG12	2.28	0.62
1:B:1169:LEU:CD2	1:B:1169:LEU:HB3	2.29	0.62
1:A:230:LYS:O	1:A:231:LEU:HB3	1.99	0.62
1:B:1106:LEU:HG	1:B:1110:LEU:CD1	2.30	0.62
1:B:1115:GLU:O	1:B:1118:LYS:HB3	2.00	0.61
1:A:138[A]:GLU:O	1:A:142:GLU:HG2	1.99	0.61
1:A:210:LYS:O	1:A:210:LYS:HG2	2.00	0.61
1:B:1146:ILE:O	1:B:1146:ILE:HG22	2.01	0.60
1:B:1169:LEU:CD2	1:B:1169:LEU:HD13	2.30	0.60
1:A:173:GLU:HA	1:B:1172:ILE:HD11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1227:ARG:HG2	1:B:1228:LEU:N	2.17	0.60
1:B:1099:LEU:HD12	1:B:1099:LEU:O	2.02	0.59
1:A:209:ASP:C	1:A:211:VAL:H	2.06	0.59
1:A:125[B]:ARG:HE	1:A:126:GLY:N	2.01	0.59
1:A:119:ALA:O	1:A:120:ALA:C	2.40	0.58
1:A:104:GLU:C	1:A:106:LEU:H	2.05	0.57
1:A:222:GLU:HG3	2:A:301:HOH:O	2.03	0.57
1:B:1143:ILE:O	1:B:1145:GLU:N	2.37	0.56
1:A:204:LEU:CD1	1:B:1204:LEU:HA	2.34	0.56
1:B:1217:LYS:O	1:B:1221:LEU:HG	2.06	0.56
1:B:1117:GLU:O	1:B:1118:LYS:C	2.45	0.55
1:B:1126:GLY:O	1:B:1129:VAL:HG22	2.05	0.55
1:A:222:GLU:C	1:A:224:GLU:H	2.08	0.55
1:A:219:TYR:CD2	1:A:220[A]:HIS:CD2	2.95	0.55
1:A:146:ILE:HD13	1:A:146:ILE:N	2.22	0.55
1:A:149:LYS:HZ2	1:A:152:LYS:HD2	1.71	0.55
1:A:200:VAL:HG12	1:B:1200:VAL:CG1	2.37	0.55
1:B:1160:ARG:NH1	2:B:136:HOH:O	2.39	0.55
1:A:173:GLU:O	1:A:177:GLU:HG3	2.07	0.54
2:A:313:HOH:O	1:B:1232:VAL:HG11	2.06	0.53
1:B:1108:THR:HB	2:B:280:HOH:O	2.08	0.53
1:A:217:LYS:NZ	2:A:281:HOH:O	2.42	0.53
1:B:1106:LEU:HG	1:B:1110:LEU:HD11	1.89	0.53
1:B:1204:LEU:O	1:B:1204:LEU:HG	2.09	0.53
1:A:212:GLU:HA	1:A:215:LEU:HD12	1.90	0.52
1:A:176:LEU:CD1	1:B:1176:LEU:HA	2.40	0.52
1:A:148:LEU:N	1:B:1148:LEU:HD13	2.23	0.52
1:B:1209:ASP:O	1:B:1212:GLU:N	2.43	0.52
1:A:140:LYS:HE3	1:A:144:GLN:HG3	1.92	0.52
1:A:141:MET:HE1	1:B:1140:LYS:HG2	1.92	0.52
1:A:174:SER:O	1:A:175:ASP:C	2.45	0.52
1:B:1156:GLU:HB3	1:B:1160:ARG:NH2	2.25	0.52
1:A:209:ASP:C	1:A:211:VAL:N	2.64	0.51
1:A:173:GLU:CA	1:B:1172:ILE:HD11	2.40	0.51
1:A:193:LEU:CB	1:B:1193:LEU:HD23	2.39	0.51
1:A:222:GLU:C	1:A:224:GLU:N	2.61	0.51
1:B:1168:LYS:HD3	2:B:53:HOH:O	2.10	0.51
1:A:149:LYS:NZ	1:A:152:LYS:HD2	2.25	0.51
1:B:1111:GLN:OE1	1:B:1114:GLU:OE2	2.29	0.51
1:B:1164[A]:GLU:OE2	1:B:1168:LYS:CE	2.57	0.50
1:B:1197:LEU:O	1:B:1197:LEU:HG	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLU:HA	2:A:295:HOH:O	2.11	0.50
1:A:188:GLY:O	1:A:189:LYS:C	2.45	0.50
1:A:153[A]:HIS:O	1:A:156:GLU:N	2.45	0.50
1:A:141:MET:HG2	1:B:1141:MET:CG	2.41	0.50
1:A:165:VAL:HG12	1:B:1165:VAL:HG22	1.93	0.50
1:B:1108:THR:CB	2:B:280:HOH:O	2.58	0.50
1:A:204:LEU:O	1:A:208:GLU:HG2	2.11	0.49
1:B:1096:GLU:HA	1:B:1099:LEU:HB3	1.93	0.49
1:A:103:GLN:CB	1:B:1102:ALA:HB1	2.43	0.49
1:A:161:LYS:HD2	2:A:241:HOH:O	2.12	0.49
1:A:196:GLU:OE2	1:B:1197:LEU:HD21	2.13	0.48
1:A:227:ARG:HG2	1:A:227:ARG:O	2.12	0.48
1:B:1093:GLN:HA	2:B:115:HOH:O	2.14	0.48
1:A:102:ALA:O	1:A:104:GLU:N	2.47	0.48
1:A:125[A]:ARG:C	1:A:127:MET:H	2.16	0.48
1:A:153[B]:HIS:O	1:A:156:GLU:N	2.47	0.48
1:A:172:ILE:HB	1:B:1172:ILE:HD13	1.95	0.48
1:B:1114:GLU:CA	2:B:206:HOH:O	2.42	0.47
1:A:205:LYS:O	1:A:208:GLU:N	2.43	0.47
1:B:1094:LEU:C	1:B:1096:GLU:H	2.17	0.47
1:B:1227:ARG:NH1	2:B:137:HOH:O	2.28	0.47
1:A:208:GLU:OE1	1:A:208:GLU:HA	2.14	0.47
1:B:1225:VAL:O	1:B:1229:LYS:CB	2.59	0.47
1:A:212:GLU:HB3	2:A:306:HOH:O	2.15	0.47
2:A:335:HOH:O	1:B:1217:LYS:HE2	2.15	0.47
1:A:167[A]:ARG:NH1	2:A:365:HOH:O	2.49	0.46
1:B:1135[A]:GLN:OE1	1:B:1135[A]:GLN:HA	2.16	0.46
1:A:123:SER:O	1:A:127:MET:HB2	2.14	0.46
1:B:1138[A]:GLU:O	1:B:1142:GLU:HG2	2.16	0.46
1:B:1146:ILE:HD13	1:B:1149:LYS:HD2	1.97	0.46
1:A:158:ALA:HB1	1:B:1158:ALA:O	2.16	0.46
1:A:232:VAL:O	1:A:233:GLY:O	2.33	0.45
1:A:162:TYR:CE1	1:B:1161:LYS:HE2	2.51	0.45
1:B:1156:GLU:HB3	1:B:1160:ARG:HH21	1.82	0.45
1:B:1182:ARG:HG2	1:B:1182:ARG:O	2.16	0.45
1:A:224:GLU:HG3	1:A:227:ARG:HD3	1.99	0.44
1:A:232:VAL:CG1	1:A:232:VAL:O	2.65	0.44
1:B:1109:ALA:O	1:B:1112:LYS:HB2	2.17	0.44
1:A:147:GLN:C	1:B:1148:LEU:CD1	2.85	0.44
1:B:1205:LYS:NZ	2:B:98:HOH:O	2.50	0.44
1:A:112:LYS:HD2	1:B:1113:LEU:HD21	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:VAL:CG1	1:B:1200:VAL:CG1	2.95	0.44
1:B:1135[B]:GLN:NE2	2:B:63:HOH:O	2.49	0.44
1:A:218:ASN:ND2	1:B:1218:ASN:OD1	2.48	0.44
1:A:149:LYS:NZ	1:A:152:LYS:CD	2.81	0.44
1:A:229:LYS:O	1:A:231:LEU:N	2.51	0.44
1:A:141:MET:HE1	1:B:1140:LYS:HE3	1.99	0.43
1:B:1207:LEU:HG	1:B:1207:LEU:O	2.18	0.43
1:A:125[A]:ARG:C	1:A:127:MET:N	2.72	0.43
1:A:125[A]:ARG:O	1:A:127:MET:N	2.52	0.43
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.76	0.43
1:A:149:LYS:HZ2	1:A:152:LYS:CD	2.32	0.43
1:B:1095:VAL:O	1:B:1095:VAL:HG12	2.19	0.42
1:B:1129:VAL:CG2	1:B:1130:ILE:N	2.82	0.42
1:A:213:GLU:O	1:A:214:LEU:C	2.57	0.42
1:B:1130:ILE:HD13	1:B:1130:ILE:N	2.35	0.42
1:B:1211:VAL:O	1:B:1215:LEU:HB2	2.20	0.42
1:A:106:LEU:HD23	1:B:1106:LEU:HD13	2.01	0.42
1:A:148:LEU:O	1:A:152:LYS:HG3	2.20	0.42
1:B:1205:LYS:HA	1:B:1205:LYS:HD3	1.79	0.41
1:A:200:VAL:HG12	1:B:1200:VAL:HG11	2.02	0.41
1:B:1106:LEU:CG	1:B:1110:LEU:HD11	2.51	0.41
1:A:135[A]:GLN:O	1:A:136:LYS:C	2.55	0.41
1:A:146:ILE:HG22	1:A:150:GLU:OE2	2.20	0.41
1:A:162:TYR:C	1:A:162:TYR:CD2	2.94	0.41
1:B:1114:GLU:O	1:B:1115:GLU:C	2.59	0.41
1:B:1215:LEU:HD12	1:B:1215:LEU:HA	1.94	0.41
1:A:106:LEU:HD23	1:B:1106:LEU:CD1	2.51	0.41
1:A:125[B]:ARG:C	1:A:127:MET:H	2.22	0.40
1:A:219:TYR:CE1	1:A:223:ASN:ND2	2.89	0.40
1:A:104:GLU:C	1:A:106:LEU:N	2.74	0.40
1:A:100:ASP:O	1:A:101:ARG:C	2.60	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	142/147 (97%)	119 (84%)	15 (11%)	8 (6%)	2	1
1	B	143/147 (97%)	122 (85%)	15 (10%)	6 (4%)	3	1
All	All	285/294 (97%)	241 (85%)	30 (10%)	14 (5%)	2	1

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ALA
1	A	103	GLN
1	A	210	LYS
1	A	231	LEU
1	B	1094	LEU
1	B	1095	VAL
1	B	1144	GLN
1	B	1233	GLY
1	A	101	ARG
1	A	230	LYS
1	B	1232	VAL
1	A	166	ALA
1	A	105	ARG
1	B	1225	VAL

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	119/129 (92%)	107 (90%)	12 (10%)	8	10
1	B	120/129 (93%)	106 (88%)	14 (12%)	6	6
All	All	239/258 (93%)	213 (89%)	26 (11%)	7	8

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	105	ARG
1	A	112	LYS
1	A	121	ASP
1	A	122[A]	GLU
1	A	122[B]	GLU
1	A	123	SER
1	A	174	SER
1	A	185	LEU
1	A	199	THR
1	A	216	SER
1	A	231	LEU
1	A	232	VAL
1	B	1093	GLN
1	B	1099	LEU
1	B	1100	ASP
1	B	1124	GLU
1	B	1147	GLN
1	B	1150	GLU
1	B	1159	ASP
1	B	1169	LEU
1	B	1172	ILE
1	B	1174	SER
1	B	1185	LEU
1	B	1187	GLU
1	B	1192	GLU
1	B	1212	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	144	GLN
1	B	1093	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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1166:ALA	C	1167:ARG	N	1.20

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	136/147 (92%)	0.51	13 (9%) 8 11	15, 71, 93, 101	0
1	B	142/147 (96%)	0.31	4 (2%) 53 60	15, 66, 87, 98	0
All	All	278/294 (94%)	0.41	17 (6%) 21 27	15, 68, 91, 101	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	232	VAL	4.9
1	B	1094	LEU	4.4
1	B	1093	GLN	4.0
1	A	231	LEU	3.9
1	A	109	ALA	3.8
1	B	1095	VAL	3.8
1	A	105	ARG	3.0
1	A	121	ASP	3.0
1	A	208	GLU	2.8
1	B	1122	GLU	2.6
1	A	101	ARG	2.3
1	A	99	LEU	2.3
1	A	205	LYS	2.3
1	A	226	ALA	2.3
1	A	206	SER	2.2
1	A	220[A]	HIS	2.1
1	A	103	GLN	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.