



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:18 AM UTC

PDB ID : 2B9C / pdb_00002b9c
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 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
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

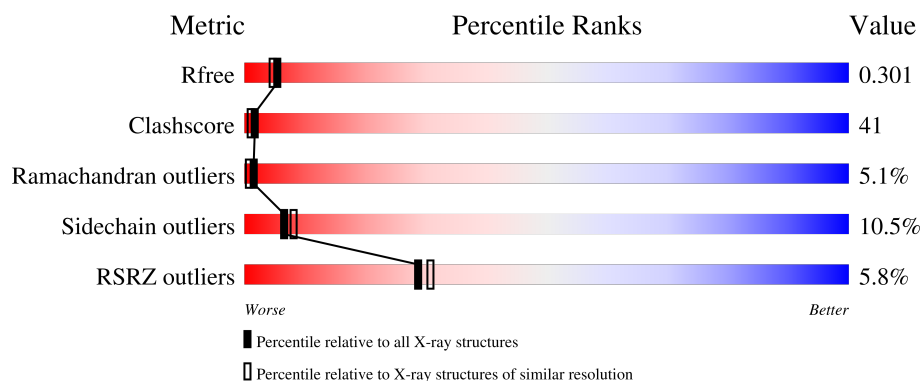
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	180053	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (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 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	147	
1	B	147	

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 methionine	UNP P04692
A	209	ASP	-	expression tag	UNP P04692
A	210	LYS	-	expression tag	UNP P04692
A	211	VAL	-	expression tag	UNP P04692
A	212	GLU	-	expression tag	UNP P04692
A	213	GLU	-	expression tag	UNP P04692
A	214	LEU	-	expression tag	UNP P04692
A	215	LEU	-	expression tag	UNP P04692
A	216	SER	-	expression tag	UNP P04692
A	217	LYS	-	expression tag	UNP P04692
A	218	ASN	-	expression tag	UNP P04692
A	219	TYR	-	expression tag	UNP P04692
A	220	HIS	-	expression tag	UNP P04692
A	221	LEU	-	expression tag	UNP P04692
A	222	GLU	-	expression tag	UNP P04692
A	223	ASN	-	expression tag	UNP P04692
A	224	GLU	-	expression tag	UNP P04692
A	225	VAL	-	expression tag	UNP P04692
A	226	ALA	-	expression tag	UNP P04692
A	227	ARG	-	expression tag	UNP P04692
A	228	LEU	-	expression tag	UNP P04692
A	229	LYS	-	expression tag	UNP P04692
A	230	LYS	-	expression tag	UNP P04692
A	231	LEU	-	expression tag	UNP P04692
A	232	VAL	-	expression tag	UNP P04692

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

- Molecule 2 is water.

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

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 20.00 – 2.30	Depositor EDS
% Data completeness (in resolution range)	96.8 (20.00-2.30) 96.7 (20.00-2.30)	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)	0.33 , 114.4	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	2.98	106/1156 (9.2%)	2.47	91/1543 (5.9%)
1	B	3.01	113/1153 (9.8%)	2.64	91/1539 (5.9%)
All	All	2.99	219/2309 (9.5%)	2.56	182/3082 (5.9%)

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 (219) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ILE	CA-CB	-14.89	1.37	1.54
1	B	1170	VAL	C-O	-13.71	1.08	1.24
1	B	1179	ALA	N-CA	-13.31	1.29	1.46
1	A	169	LEU	CA-C	-12.84	1.36	1.52
1	A	143	ILE	CA-C	12.29	1.68	1.52
1	A	172	ILE	CA-C	-11.76	1.37	1.52
1	B	1132	SER	CA-C	11.49	1.68	1.52
1	A	166	ALA	N-CA	-11.47	1.31	1.46
1	A	172	ILE	CA-CB	-11.21	1.40	1.54
1	B	1176	LEU	C-O	10.74	1.36	1.24
1	B	1179	ALA	CA-CB	10.61	1.70	1.53
1	B	1151	ALA	N-CA	-10.43	1.33	1.46
1	A	178	ARG	CZ-NH1	10.36	1.47	1.32
1	B	1154	ILE	C-O	-10.36	1.11	1.24
1	A	181	GLU	N-CA	-10.28	1.33	1.46
1	B	1218	ASN	N-CA	-10.24	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1211	VAL	CA-CB	-9.97	1.40	1.54
1	A	158	ALA	N-CA	-9.88	1.34	1.46
1	B	1226	ALA	CA-CB	-9.65	1.37	1.53
1	B	1166	ALA	C-N	-9.62	1.20	1.33
1	A	128	LYS	CA-C	9.62	1.65	1.52
1	A	212	GLU	C-O	-9.62	1.11	1.24
1	B	1162	TYR	CZ-OH	9.54	1.58	1.38
1	B	1166	ALA	CA-C	9.49	1.65	1.52
1	A	182	ARG	CA-CB	-9.47	1.38	1.53
1	A	187	GLU	CA-C	-9.43	1.39	1.52
1	A	163	GLU	C-O	-9.38	1.12	1.24
1	A	181	GLU	C-O	-9.30	1.13	1.24
1	A	174	SER	N-CA	-9.13	1.35	1.46
1	A	164	GLU	N-CA	-9.00	1.35	1.46
1	A	179	ALA	CA-C	-8.85	1.40	1.52
1	A	162	TYR	CA-CB	-8.83	1.39	1.53
1	A	186	SER	N-CA	-8.72	1.34	1.46
1	A	175	ASP	CG-OD2	8.72	1.42	1.25
1	B	1095	VAL	CA-CB	8.63	1.66	1.54
1	B	1128	LYS	CA-C	8.55	1.64	1.52
1	B	1183	ALA	C-O	-8.55	1.14	1.24
1	A	195	GLU	N-CA	-8.43	1.36	1.46
1	A	171	ILE	N-CA	-8.22	1.36	1.46
1	A	174	SER	CA-CB	8.18	1.66	1.53
1	B	1176	LEU	CA-CB	8.14	1.66	1.53
1	B	1155	ALA	C-O	-8.04	1.13	1.24
1	A	181	GLU	CG-CD	7.98	1.72	1.52
1	A	231	LEU	CA-C	7.94	1.63	1.52
1	B	1179	ALA	C-O	-7.93	1.14	1.24
1	A	176	LEU	C-O	7.91	1.33	1.24
1	B	1167	ARG	CZ-NH2	7.91	1.43	1.33
1	A	172	ILE	C-N	-7.90	1.23	1.33
1	B	1156	GLU	C-O	-7.78	1.13	1.24
1	A	188	GLY	C-O	-7.75	1.14	1.23
1	A	134	ALA	CA-CB	-7.71	1.41	1.53
1	A	105	ARG	CA-C	7.70	1.63	1.52
1	B	1191	ALA	CA-CB	-7.69	1.39	1.53
1	B	1188	GLY	CA-C	7.66	1.62	1.51
1	B	1173	GLU	CA-C	-7.65	1.43	1.52
1	A	148	LEU	CA-CB	-7.59	1.41	1.53
1	B	1161	LYS	C-O	-7.56	1.15	1.24
1	B	1216	SER	C-O	-7.53	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	157	ASP	C-O	-7.51	1.15	1.24
1	B	1168	LYS	N-CA	7.51	1.56	1.46
1	A	177	GLU	C-O	-7.50	1.14	1.24
1	A	191	ALA	N-CA	-7.50	1.37	1.46
1	A	173	GLU	C-N	7.46	1.44	1.33
1	B	1232	VAL	CA-CB	7.46	1.64	1.54
1	A	170	VAL	C-O	-7.45	1.15	1.24
1	A	127	MET	CG-SD	7.44	1.99	1.80
1	A	189	LYS	C-O	-7.44	1.15	1.24
1	A	117	GLU	CA-CB	-7.38	1.41	1.53
1	B	1199	THR	CA-C	7.38	1.62	1.52
1	A	144	GLN	N-CA	-7.36	1.36	1.46
1	A	222	GLU	CA-C	7.34	1.62	1.52
1	B	1225	VAL	CA-CB	7.33	1.64	1.54
1	B	1173	GLU	N-CA	-7.32	1.37	1.46
1	B	1166	ALA	C-O	7.27	1.33	1.24
1	B	1227	ARG	C-O	7.24	1.33	1.24
1	A	162	TYR	CA-C	7.16	1.62	1.52
1	A	209	ASP	N-CA	-7.11	1.37	1.46
1	B	1150	GLU	CA-C	7.10	1.61	1.52
1	A	215	LEU	CA-C	-7.04	1.43	1.52
1	A	162	TYR	CD1-CE1	7.03	1.59	1.38
1	A	164	GLU	CA-C	-7.03	1.44	1.52
1	A	182	ARG	CZ-NH1	-7.00	1.23	1.32
1	B	1105	ARG	N-CA	-6.95	1.37	1.46
1	B	1149	LYS	N-CA	-6.95	1.37	1.46
1	B	1153	HIS	N-CA	-6.90	1.38	1.46
1	A	172	ILE	CB-CG2	-6.89	1.29	1.52
1	B	1171	ILE	CB-CG2	6.89	1.75	1.52
1	B	1165	VAL	N-CA	6.85	1.55	1.46
1	A	171	ILE	CG1-CD1	6.84	1.78	1.51
1	A	187	GLU	N-CA	-6.81	1.37	1.46
1	A	162	TYR	CD2-CE2	6.79	1.59	1.38
1	B	1177	GLU	CD-OE1	6.77	1.38	1.25
1	B	1169	LEU	CG-CD2	6.75	1.74	1.52
1	B	1188	GLY	C-O	6.75	1.31	1.24
1	A	157	ASP	CA-C	6.68	1.61	1.52
1	A	162	TYR	N-CA	-6.68	1.38	1.46
1	B	1162	TYR	N-CA	-6.65	1.38	1.46
1	B	1147	GLN	N-CA	-6.65	1.37	1.46
1	A	185	LEU	C-O	-6.64	1.16	1.24
1	A	144	GLN	CA-C	6.63	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1177	GLU	CD-OE2	6.63	1.38	1.25
1	B	1203	ASN	N-CA	-6.59	1.37	1.46
1	A	162	TYR	CE2-CZ	-6.59	1.22	1.38
1	B	1203	ASN	CA-C	-6.55	1.43	1.52
1	A	162	TYR	C-O	-6.54	1.16	1.24
1	B	1190	CYS	C-O	-6.53	1.16	1.24
1	B	1216	SER	CA-C	-6.53	1.44	1.52
1	A	154	ILE	CA-CB	-6.51	1.45	1.54
1	A	216	SER	C-O	6.49	1.31	1.23
1	B	1167	ARG	NE-CZ	6.49	1.40	1.33
1	A	208	GLU	N-CA	6.45	1.54	1.46
1	B	1153	HIS	CA-CB	-6.44	1.43	1.53
1	A	107	ALA	CA-C	6.43	1.61	1.52
1	B	1193	LEU	C-O	-6.42	1.15	1.24
1	B	1106	LEU	N-CA	-6.38	1.38	1.46
1	A	130	ILE	C-O	-6.37	1.16	1.24
1	B	1161	LYS	C-N	-6.34	1.25	1.34
1	B	1174	SER	CA-CB	6.31	1.63	1.53
1	B	1153	HIS	CG-CD2	6.30	1.42	1.35
1	A	129	VAL	C-O	-6.26	1.16	1.24
1	B	1181	GLU	CA-C	-6.25	1.44	1.52
1	B	1157	ASP	C-O	-6.25	1.16	1.24
1	B	1186	SER	CA-C	-6.23	1.44	1.52
1	B	1155	ALA	N-CA	-6.15	1.37	1.46
1	A	147	GLN	CA-C	6.13	1.61	1.52
1	B	1106	LEU	C-O	6.13	1.31	1.24
1	A	173	GLU	CG-CD	6.11	1.67	1.52
1	B	1157	ASP	C-N	-6.10	1.24	1.33
1	B	1179	ALA	C-N	-6.08	1.26	1.33
1	A	169	LEU	CG-CD1	-6.07	1.32	1.52
1	B	1165	VAL	CA-C	-6.04	1.45	1.52
1	A	127	MET	CA-C	-6.03	1.45	1.53
1	B	1162	TYR	C-O	6.02	1.31	1.24
1	A	219	TYR	C-O	-6.00	1.17	1.24
1	B	1151	ALA	C-O	-5.98	1.16	1.24
1	B	1227	ARG	NE-CZ	5.98	1.39	1.33
1	B	1187	GLU	CB-CG	-5.97	1.34	1.52
1	A	156	GLU	C-O	-5.97	1.16	1.24
1	B	1175	ASP	N-CA	5.97	1.53	1.46
1	B	1170	VAL	N-CA	5.96	1.53	1.46
1	B	1180	GLU	CD-OE1	5.92	1.36	1.25
1	B	1095	VAL	CA-C	5.91	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	141	MET	SD-CE	5.91	1.94	1.79
1	A	116	ALA	CA-CB	5.86	1.64	1.53
1	A	183	ALA	CA-C	-5.86	1.44	1.52
1	B	1122	GLU	CG-CD	5.86	1.66	1.52
1	A	182	ARG	N-CA	-5.86	1.39	1.46
1	B	1224	GLU	CA-C	-5.84	1.46	1.53
1	B	1110	LEU	CA-C	-5.83	1.45	1.52
1	B	1144	GLN	C-O	-5.80	1.16	1.24
1	B	1189	LYS	CB-CG	5.80	1.69	1.52
1	B	1181	GLU	CB-CG	5.77	1.69	1.52
1	A	147	GLN	C-O	5.76	1.31	1.24
1	A	156	GLU	CA-C	-5.75	1.44	1.52
1	A	156	GLU	C-N	-5.74	1.26	1.33
1	A	210	LYS	C-O	-5.73	1.16	1.24
1	A	155	ALA	CA-CB	5.72	1.62	1.53
1	A	150	GLU	N-CA	-5.72	1.39	1.46
1	B	1157	ASP	N-CA	-5.71	1.39	1.46
1	B	1125	ARG	CA-CB	-5.71	1.44	1.53
1	B	1175	ASP	CA-CB	5.70	1.62	1.53
1	A	108	THR	CA-CB	5.65	1.62	1.53
1	A	190	CYS	N-CA	-5.65	1.38	1.46
1	B	1217	LYS	CA-CB	-5.65	1.44	1.53
1	B	1102	ALA	CA-C	-5.62	1.45	1.53
1	B	1177	GLU	N-CA	5.60	1.53	1.46
1	A	165	VAL	C-O	-5.60	1.17	1.24
1	B	1171	ILE	CG1-CD1	5.57	1.73	1.51
1	A	171	ILE	C-N	5.56	1.41	1.33
1	A	198	LYS	C-O	-5.54	1.17	1.24
1	B	1123	SER	CA-CB	-5.53	1.44	1.53
1	B	1102	ALA	CA-CB	-5.53	1.44	1.53
1	B	1134	ALA	C-O	5.51	1.30	1.24
1	B	1176	LEU	CB-CG	-5.50	1.42	1.53
1	B	1178	ARG	CG-CD	5.50	1.69	1.52
1	A	187	GLU	CG-CD	5.47	1.65	1.52
1	A	143	ILE	CA-CB	5.47	1.61	1.54
1	A	163	GLU	CD-OE2	5.46	1.35	1.25
1	B	1158	ALA	C-N	-5.46	1.25	1.33
1	A	176	LEU	CG-CD2	-5.45	1.34	1.52
1	B	1111	GLN	N-CA	-5.40	1.39	1.46
1	A	231	LEU	C-O	5.40	1.30	1.24
1	B	1181	GLU	CD-OE1	5.38	1.35	1.25
1	B	1103	GLN	CA-C	5.36	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	171	ILE	CB-CG2	5.36	1.70	1.52
1	A	194	GLU	C-N	-5.36	1.26	1.33
1	B	1176	LEU	CG-CD1	5.35	1.70	1.52
1	B	1182	ARG	CD-NE	5.35	1.53	1.46
1	A	167[A]	ARG	CG-CD	5.34	1.68	1.52
1	A	167[B]	ARG	CG-CD	5.34	1.68	1.52
1	B	1132	SER	C-O	5.34	1.30	1.24
1	B	1190	CYS	CA-CB	5.32	1.61	1.53
1	B	1169	LEU	CB-CG	-5.31	1.42	1.53
1	A	165	VAL	CA-CB	5.30	1.59	1.54
1	B	1156	GLU	CG-CD	5.30	1.65	1.52
1	B	1158	ALA	C-O	5.30	1.30	1.24
1	B	1189	LYS	N-CA	-5.29	1.40	1.46
1	B	1167	ARG	CD-NE	5.29	1.53	1.46
1	B	1177	GLU	CA-CB	5.28	1.61	1.53
1	A	175	ASP	CB-CG	5.28	1.65	1.52
1	A	137	ASP	N-CA	-5.27	1.39	1.46
1	B	1096	GLU	C-O	5.25	1.30	1.24
1	B	1180	GLU	N-CA	-5.23	1.40	1.46
1	A	159	ASP	CG-OD1	5.21	1.35	1.25
1	A	178	ARG	CB-CG	5.21	1.68	1.52
1	A	140	LYS	N-CA	-5.20	1.39	1.46
1	B	1212	GLU	C-O	-5.16	1.17	1.24
1	B	1187	GLU	CA-C	5.14	1.59	1.52
1	A	193	LEU	C-O	-5.13	1.17	1.24
1	B	1220	HIS	N-CA	-5.12	1.40	1.46
1	A	206	SER	CA-C	5.11	1.60	1.52
1	A	179	ALA	CA-CB	5.10	1.61	1.53
1	A	214	LEU	N-CA	-5.10	1.40	1.46
1	B	1214	LEU	N-CA	-5.10	1.39	1.46
1	B	1160	ARG	CZ-NH2	-5.09	1.26	1.33
1	B	1154	ILE	CA-CB	5.08	1.60	1.54
1	A	148	LEU	C-O	5.06	1.30	1.24
1	B	1184	GLU	N-CA	5.05	1.52	1.46
1	A	201	THR	CA-C	5.02	1.59	1.52

All (182) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1167	ARG	N-CA-C	-15.11	92.97	111.40
1	B	1099	LEU	N-CA-C	-13.60	96.77	113.50
1	A	104	GLU	N-CA-C	-13.12	97.25	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	178	ARG	NE-CZ-NH2	-12.39	108.05	119.20
1	B	1178	ARG	N-CA-C	12.11	124.48	111.28
1	A	170	VAL	CA-C-N	11.35	134.88	120.70
1	A	170	VAL	C-N-CA	11.35	134.88	120.70
1	B	1182	ARG	NE-CZ-NH1	-11.35	110.15	121.50
1	B	1156	GLU	N-CA-C	-10.95	100.05	113.41
1	A	174	SER	O-C-N	-10.54	110.13	122.15
1	A	176	LEU	O-C-N	-10.43	111.06	122.12
1	A	181	GLU	O-C-N	-10.41	111.08	122.12
1	A	165	VAL	N-CA-C	10.31	120.96	110.23
1	A	188	GLY	O-C-N	-10.18	112.31	122.19
1	B	1168	LYS	O-C-N	-10.14	108.94	122.43
1	B	1174	SER	N-CA-C	-10.13	100.32	111.36
1	B	1165	VAL	N-CA-C	-9.97	98.30	113.16
1	A	212	GLU	N-CA-C	-9.86	99.80	112.23
1	B	1175	ASP	CB-CA-C	-9.66	92.76	110.63
1	B	1176	LEU	CD1-CG-CD2	-9.61	89.67	110.80
1	B	1112	LYS	N-CA-C	-9.58	98.25	112.04
1	A	174	SER	N-CA-C	-9.53	100.97	111.36
1	A	175	ASP	CB-CA-C	-9.50	93.06	110.63
1	A	169	LEU	N-CA-C	9.40	121.13	111.07
1	A	111	GLN	N-CA-C	-9.38	100.15	111.69
1	B	1165	VAL	CA-C-N	-9.39	105.14	121.66
1	B	1165	VAL	C-N-CA	-9.39	105.14	121.66
1	B	1175	ASP	CA-C-N	-9.25	107.88	120.28
1	B	1175	ASP	C-N-CA	-9.25	107.88	120.28
1	A	150	GLU	N-CA-C	-8.93	101.51	111.07
1	A	173	GLU	N-CA-C	8.80	120.87	111.28
1	A	106	LEU	N-CA-C	-8.77	100.70	111.40
1	B	1162	TYR	CA-C-N	-8.72	105.86	120.68
1	B	1162	TYR	C-N-CA	-8.72	105.86	120.68
1	B	1173	GLU	N-CA-C	8.67	120.81	111.36
1	B	1168	LYS	N-CA-C	8.66	123.26	112.87
1	B	1110	LEU	CA-C-N	-8.65	108.28	122.65
1	B	1110	LEU	C-N-CA	-8.65	108.28	122.65
1	B	1168	LYS	CA-C-O	8.61	129.94	119.10
1	A	173	GLU	CB-CA-C	-8.60	96.52	110.79
1	A	170	VAL	CA-C-O	-8.55	110.10	120.78
1	B	1176	LEU	O-C-N	-8.45	113.16	122.12
1	B	1171	ILE	N-CA-CB	-8.40	99.81	110.57
1	B	1176	LEU	CA-C-O	8.32	129.37	120.55
1	A	174	SER	CA-C-O	8.31	129.23	120.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1195	GLU	N-CA-C	-8.29	102.95	113.23
1	B	1182	ARG	NE-CZ-NH2	8.24	126.62	119.20
1	A	171	ILE	N-CA-CB	-8.21	101.67	110.62
1	B	1192	GLU	N-CA-C	-8.19	101.07	112.45
1	A	170	VAL	CG1-CB-CG2	-8.02	93.15	110.80
1	B	1177	GLU	CA-C-N	-7.98	109.59	120.28
1	B	1177	GLU	C-N-CA	-7.98	109.59	120.28
1	B	1183	ALA	O-C-N	-7.94	113.52	122.09
1	A	148	LEU	N-CA-C	-7.93	102.71	111.36
1	A	195	GLU	N-CA-C	-7.89	102.62	111.14
1	B	1226	ALA	N-CA-C	-7.87	102.69	111.82
1	A	182	ARG	CB-CA-C	-7.82	97.55	110.85
1	B	1187	GLU	CA-C-O	7.79	127.62	119.05
1	A	174	SER	CA-C-N	-7.72	109.16	120.28
1	A	174	SER	C-N-CA	-7.72	109.16	120.28
1	B	1158	ALA	CA-C-O	7.72	128.99	119.11
1	B	1167	ARG	CB-CA-C	-7.71	97.85	110.79
1	B	1181	GLU	CB-CA-C	-7.70	96.61	110.70
1	B	1174	SER	O-C-N	-7.65	113.43	122.15
1	A	182	ARG	NH1-CZ-NH2	-7.61	109.41	119.30
1	A	164	GLU	N-CA-C	-7.52	103.02	111.14
1	B	1189	LYS	CA-CB-CG	-7.46	99.19	114.10
1	B	1165	VAL	CA-C-O	7.42	127.73	119.42
1	B	1148	LEU	N-CA-C	-7.42	103.49	112.54
1	A	185	LEU	O-C-N	-7.40	114.40	122.09
1	B	1176	LEU	CB-CA-C	-7.40	98.51	110.79
1	A	172	ILE	CG1-CB-CG2	-7.38	88.55	110.70
1	B	1166	ALA	N-CA-CB	-7.36	98.95	110.44
1	A	119	ALA	N-CA-C	-7.36	102.95	110.97
1	B	1219	TYR	N-CA-C	-7.34	103.22	111.14
1	A	182	ARG	CG-CD-NE	7.23	127.91	112.00
1	B	1173	GLU	CB-CG-CD	7.20	124.83	112.60
1	B	1133	ARG	CA-CB-CG	-7.15	99.80	114.10
1	A	185	LEU	N-CA-C	-7.13	102.55	111.11
1	B	1183	ALA	N-CA-C	-7.10	103.47	111.14
1	A	203	ASN	N-CA-C	-6.99	103.10	111.69
1	A	99	LEU	N-CA-C	-6.94	102.23	113.19
1	B	1173	GLU	CB-CA-C	-6.88	99.16	110.85
1	B	1129	VAL	N-CA-C	-6.86	104.17	110.82
1	B	1166	ALA	CA-C-O	6.73	127.14	119.27
1	B	1158	ALA	CA-C-N	-6.67	109.24	121.52
1	B	1158	ALA	C-N-CA	-6.67	109.24	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1169	LEU	CD1-CG-CD2	-6.66	96.15	110.80
1	A	178	ARG	NE-CZ-NH1	6.56	128.06	121.50
1	A	169	LEU	O-C-N	-6.51	115.37	122.07
1	B	1147	GLN	N-CA-C	-6.50	96.96	110.80
1	B	1201	THR	N-CA-C	-6.47	104.86	112.89
1	B	1225	VAL	N-CA-C	-6.46	95.91	109.34
1	B	1169	LEU	N-CA-C	-6.45	105.56	113.50
1	A	183	ALA	N-CA-C	-6.43	104.36	111.82
1	A	171	ILE	CA-C-O	-6.43	114.41	121.29
1	B	1094	LEU	N-CA-C	6.43	124.49	110.80
1	A	189	LYS	N-CA-C	-6.38	104.02	110.97
1	B	1136	LYS	N-CA-C	-6.38	105.15	113.12
1	B	1116	ALA	CA-C-O	-6.37	114.08	120.90
1	A	100	ASP	N-CA-C	-6.35	102.64	111.52
1	A	182	ARG	NE-CZ-NH1	6.34	127.84	121.50
1	B	1217	LYS	N-CA-C	6.33	117.84	111.07
1	A	169	LEU	CA-CB-CG	6.28	138.27	116.30
1	A	108	THR	N-CA-C	-6.25	104.46	111.28
1	B	1106	LEU	N-CA-C	-6.19	104.61	111.36
1	A	223	ASN	N-CA-C	-6.17	104.86	113.37
1	B	1105	ARG	N-CA-C	-6.16	104.47	112.23
1	A	223	ASN	CA-C-N	-6.15	112.67	122.08
1	A	223	ASN	C-N-CA	-6.15	112.67	122.08
1	A	229	LYS	N-CA-C	-6.08	105.35	112.89
1	A	110	LEU	N-CA-C	-6.07	106.52	114.04
1	B	1223	ASN	CA-C-N	-6.04	113.01	122.08
1	B	1223	ASN	C-N-CA	-6.04	113.01	122.08
1	A	173	GLU	CB-CG-CD	6.02	122.84	112.60
1	B	1176	LEU	CB-CG-CD1	-6.01	92.67	110.70
1	A	172	ILE	CB-CA-C	-5.96	104.10	112.14
1	A	168	LYS	O-C-N	-5.95	115.81	122.12
1	A	176	LEU	CD1-CG-CD2	-5.92	97.78	110.80
1	A	162	TYR	N-CA-CB	-5.90	101.44	110.12
1	B	1168	LYS	N-CA-CB	-5.90	99.59	110.32
1	B	1205	LYS	N-CA-C	-5.84	104.50	111.69
1	B	1171	ILE	N-CA-C	5.82	116.00	110.53
1	A	199	THR	CA-C-N	5.81	129.85	120.55
1	A	199	THR	C-N-CA	5.81	129.85	120.55
1	A	122[A]	GLU	N-CA-C	-5.80	104.33	111.40
1	A	122[B]	GLU	N-CA-C	-5.80	104.33	111.40
1	A	221	LEU	N-CA-C	-5.79	105.01	111.32
1	A	188	GLY	CA-C-O	5.78	126.79	120.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1179	ALA	N-CA-C	-5.77	105.08	111.36
1	A	179	ALA	O-C-N	-5.75	115.49	122.22
1	A	197	LEU	N-CA-C	-5.74	106.11	113.23
1	B	1169	LEU	O-C-N	-5.72	114.83	122.49
1	B	1145	GLU	N-CA-C	-5.71	106.35	113.38
1	A	186	SER	CA-C-N	-5.71	111.02	121.52
1	A	186	SER	C-N-CA	-5.71	111.02	121.52
1	B	1177	GLU	O-C-N	-5.69	115.56	122.22
1	B	1107	ALA	CA-C-N	5.68	128.68	120.79
1	B	1107	ALA	C-N-CA	5.68	128.68	120.79
1	B	1171	ILE	O-C-N	-5.68	116.00	121.90
1	A	177	GLU	CB-CA-C	-5.67	100.13	110.63
1	A	211	VAL	CB-CA-C	-5.67	106.07	111.06
1	B	1187	GLU	O-C-N	-5.63	115.43	122.35
1	B	1175	ASP	CB-CG-OD2	5.61	131.31	118.40
1	B	1169	LEU	CA-C-O	5.61	125.31	119.14
1	B	1165	VAL	O-C-N	-5.53	115.65	122.18
1	B	1180	GLU	CB-CG-CD	-5.50	103.25	112.60
1	B	1224	GLU	CA-CB-CG	-5.46	103.18	114.10
1	A	171	ILE	CG1-CB-CG2	-5.46	94.33	110.70
1	A	217	LYS	CA-C-N	5.45	128.60	120.31
1	A	217	LYS	C-N-CA	5.45	128.60	120.31
1	A	176	LEU	CB-CG-CD1	-5.42	94.44	110.70
1	A	207	LEU	N-CA-C	-5.41	106.52	113.23
1	A	146	ILE	CA-C-N	5.41	129.87	120.68
1	A	146	ILE	C-N-CA	5.41	129.87	120.68
1	A	184	GLU	CA-C-N	5.37	127.79	120.54
1	A	184	GLU	C-N-CA	5.37	127.79	120.54
1	B	1188	GLY	N-CA-C	-5.37	108.01	114.66
1	A	134	ALA	N-CA-C	-5.35	106.43	113.12
1	A	172	ILE	CA-C-N	-5.33	113.14	120.28
1	A	172	ILE	C-N-CA	-5.33	113.14	120.28
1	A	172	ILE	O-C-N	-5.30	116.73	121.87
1	B	1215	LEU	N-CA-C	-5.29	105.57	112.23
1	A	176	LEU	N-CA-C	-5.26	105.55	111.28
1	A	219	TYR	CB-CA-C	-5.22	101.97	110.85
1	A	148	LEU	CA-C-N	-5.21	112.89	120.29
1	A	148	LEU	C-N-CA	-5.21	112.89	120.29
1	A	138[A]	GLU	N-CA-C	-5.17	105.71	112.23
1	A	138[B]	GLU	N-CA-C	-5.17	105.71	112.23
1	B	1217	LYS	CB-CA-C	-5.13	102.82	110.88
1	B	1159	ASP	CB-CG-OD1	-5.11	106.64	118.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1172	ILE	CB-CG1-CD1	-5.11	103.07	113.80
1	A	166	ALA	N-CA-C	5.10	121.67	110.80
1	A	171	ILE	CB-CG1-CD1	-5.10	103.08	113.80
1	A	158	ALA	CA-C-O	-5.09	115.47	120.82
1	B	1151	ALA	CA-C-O	-5.09	114.50	120.20
1	B	1218	ASN	N-CA-C	5.07	117.70	111.82
1	B	1160	ARG	N-CA-C	-5.06	105.85	111.36
1	B	1177	GLU	N-CA-C	-5.05	105.91	111.71
1	A	217	LYS	N-CA-C	-5.04	105.06	111.11
1	B	1111	GLN	CB-CA-C	5.03	119.50	110.81
1	A	215	LEU	O-C-N	5.01	129.75	122.43

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	108	0
1	B	1150	0	1120	111	0
2	A	156	0	0	11	0
2	B	193	0	0	11	0
All	All	2650	0	2250	189	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 41.

All (189) 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:CD1	1:A:171:ILE:CG1	1.78	1.59
1:A:122[A]:GLU:HA	1:A:122[A]:GLU:OE1	1.51	1.11
1:A:141:MET:HE1	1:B:1140:LYS:HG2	1.37	1.05
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:HD13	1:A:171:ILE:HG21	1.52	0.90
1:B:1171:ILE:CG2	1:B:1171:ILE:CG1	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:CD1	1:A:171:ILE:CB	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
1:A:218:ASN:HB2	1:B:1218:ASN:OD1	1.88	0.74
1:A:136:LYS:NZ	2:A:286:HOH:O	2.21	0.74
1:A:171:ILE:CD1	1:A:171:ILE:CG2	2.66	0.73
1:B:1232:VAL:HG12	1:B:1233:GLY:H	1.52	0.73
1:B:1093:GLN:HG3	1:B:1093:GLN:O	1.90	0.72
1:A:171:ILE:CD1	1:A:171:ILE:HG21	2.20	0.71
1:A:207:LEU:O	1:A:211:VAL:HG23	1.92	0.70
1:A:141:MET:HE1	1:B:1140:LYS:CG	2.20	0.69
1:A:141:MET:CE	1:B:1140:LYS:HG2	2.19	0.68
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:HD13	1:A:171:ILE:CG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:A:209:ASP:C	1:A:211:VAL:H	2.06	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:104:GLU:C	1:A:106:LEU:H	2.05	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:119:ALA:O	1:A:120:ALA:C	2.40	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:HG2	1:A:210:LYS:O	2.00	0.61
1:A:222:GLU:C	1:A:224:GLU:H	2.08	0.61
1:B:1146:ILE:HG22	1:B:1146:ILE:O	2.01	0.60
1:B:1117:GLU:O	1:B:1118:LYS:C	2.45	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
1:B:1227:ARG:HG2	1:B:1228:LEU:N	2.17	0.60
1:B:1099:LEU:O	1:B:1099:LEU:HD12	2.02	0.59
1:A:125[B]:ARG:HE	1:A:126:GLY:N	2.01	0.59
1:A:222:GLU:HG3	2:A:301:HOH:O	2.03	0.57
1:A:174:SER:O	1:A:175:ASP:C	2.45	0.56
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:A:209:ASP:C	1:A:211:VAL:N	2.64	0.56
1:A:222:GLU:C	1:A:224:GLU:N	2.61	0.56
1:B:1126:GLY:O	1:B:1129:VAL:HG22	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:188:GLY:O	1:A:189:LYS:C	2.45	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:125[A]:ARG:C	1:A:127:MET:H	2.16	0.53
1:A:176:LEU:CD1	1:B:1176:LEU:HA	2.40	0.52
1:A:212:GLU:HA	1:A:215:LEU:HD12	1.90	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:B:1094:LEU:C	1:B:1096:GLU:H	2.17	0.52
1:B:1156:GLU:HB3	1:B:1160:ARG:NH2	2.25	0.52
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: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
1:A:104:GLU:HA	2:A:295:HOH:O	2.11	0.50
1:A:141:MET:HG2	1:B:1141:MET:CG	2.41	0.50
1:A:153[A]:HIS:O	1:A:156:GLU:N	2.45	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:147:GLN:C	1:B:1148:LEU:CD1	2.85	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:O	1:A:227:ARG:HG2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:125[A]:ARG:C	1:A:127:MET:N	2.72	0.47
1:A:205:LYS:O	1:A:208:GLU:N	2.43	0.47
1:A:208:GLU:HA	1:A:208:GLU:OE1	2.14	0.47
1:B:1227:ARG:NH1	2:B:137:HOH:O	2.28	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
1:A:213:GLU:O	1:A:214:LEU:C	2.57	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:HA	1:B:1135[A]:GLN:OE1	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:A:135[A]:GLN:O	1:A:136:LYS:C	2.55	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:162:TYR:CD2	1:A:162:TYR:C	2.94	0.45
1:B:1114:GLU:O	1:B:1115:GLU:C	2.59	0.45
1:A:100:ASP:O	1:A:101:ARG:C	2.60	0.45
1:A:125[B]:ARG:C	1:A:127:MET:H	2.22	0.45
1:A:162:TYR:CE1	1:B:1161:LYS:HE2	2.51	0.45
1:A:232:VAL:O	1:A:233:GLY:O	2.33	0.45
1:B:1156:GLU:HB3	1:B:1160:ARG:HH21	1.82	0.45
1:B:1182:ARG:O	1:B:1182:ARG:HG2	2.16	0.45
1:A:224:GLU:HG3	1:A:227:ARG:HD3	1.99	0.44
1:A:232:VAL:O	1:A:232:VAL:CG1	2.65	0.44
1:B:1109:ALA:O	1:B:1112:LYS:HB2	2.17	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
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:111:GLN:C	1:A:113:LEU:H	2.25	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:B:1185:LEU:HD23	1:B:1185:LEU:C	2.39	0.44
1:A:229:LYS:O	1:A:231:LEU:N	2.51	0.44
1:B:1171:ILE:CG2	1:B:1171:ILE:C	2.89	0.44
1:B:1143:ILE:C	1:B:1145:GLU:N	2.76	0.43
1:B:1207:LEU:O	1:B:1207:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:125[A]:ARG:O	1:A:127:MET:N	2.52	0.43
1:A:144:GLN:HE21	1:B:1145:GLU:CD	2.26	0.43
1:A:214:LEU:HA	1:A:214:LEU:HD23	1.76	0.43
1:A:104:GLU:C	1:A:106:LEU:N	2.74	0.43
1:A:149:LYS:HZ2	1:A:152:LYS:CD	2.32	0.43
1:B:1095:VAL:HG12	1:B:1095:VAL:O	2.19	0.42
1:B:1129:VAL:CG2	1:B:1130:ILE:N	2.82	0.42
1:B:1232:VAL:O	1:B:1233:GLY:C	2.63	0.42
1:B:1130:ILE:HD13	1:B:1130:ILE:N	2.35	0.42
1:A:189:LYS:O	1:A:190:CYS:C	2.59	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:1162:TYR:O	1:B:1163:GLU:C	2.61	0.41
1:B:1205:LYS:HD3	1:B:1205:LYS:HA	1.79	0.41
1:A:125[B]:ARG:C	1:A:127:MET:N	2.78	0.41
1:A:194:GLU:O	1:A:195:GLU:C	2.58	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:146:ILE:HG22	1:A:150:GLU:OE2	2.20	0.41
1:A:161:LYS:O	1:A:162:TYR:C	2.61	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:219:TYR:CE1	1:A:223:ASN:ND2	2.89	0.40
1:B:1227:ARG:C	1:B:1229:LYS:H	2.28	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	142/147 (97%)	119 (84%)	15 (11%)	8 (6%)	1 0

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	143/147 (97%)	122 (85%)	15 (10%)	6 (4%)	2	1
All	All	285/294 (97%)	241 (85%)	30 (10%)	14 (5%)	1	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 ⓘ

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%)	7	9
1	B	120/129 (93%)	107 (89%)	13 (11%)	6	7
All	All	239/258 (93%)	214 (90%)	25 (10%)	6	8

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LYS
1	A	121	ASP

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Mol	Chain	Res	Type
1	A	122[A]	GLU
1	A	122[B]	GLU
1	A	123	SER
1	A	174	SER
1	A	185	LEU
1	A	187	GLU
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	1124	GLU
1	B	1147	GLN
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	1194	GLU
1	B	1212	GLU

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

Mol	Chain	Res	Type
1	A	144	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 oligosaccharides 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%)	0.56	10 (7%)	20 22	15, 68, 93, 101	8 (5%)
1	B	142/147 (96%)	0.34	6 (4%)	40 42	14, 66, 87, 98	3 (2%)
All	All	278/294 (94%)	0.44	16 (5%)	29 31	14, 67, 91, 101	11 (3%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	208	GLU	4.8
1	A	232	VAL	3.5
1	A	109	ALA	3.4
1	A	107	ALA	2.9
1	B	1095	VAL	2.9
1	B	1110	LEU	2.6
1	B	1207	LEU	2.6
1	B	1228	LEU	2.6
1	A	204	LEU	2.6
1	A	105	ARG	2.4
1	B	1094	LEU	2.2
1	B	1102	ALA	2.1
1	A	121	ASP	2.1
1	A	108	THR	2.1
1	A	110	LEU	2.1
1	A	141	MET	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 oligosaccharides 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.