



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 22, 2024 – 09:46 PM EST

PDB ID : 4TNC
Title : REFINED STRUCTURE OF CHICKEN SKELETAL MUSCLE TROPONIN C IN THE TWO-CALCIUM STATE AT 2-ANGSTROMS RESOLUTION
Authors : Sundaralingam, M.
Deposited on : 1987-09-28
Resolution : 2.00 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 : 4.02b-467
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

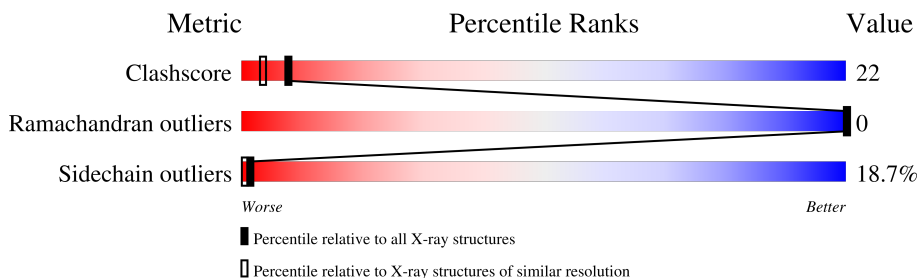
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)

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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	162	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 1327 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 TROPONIN C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	160	1257	774	199	272	12	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	ALA	MET	conflict	UNP P02588
A	4	MET	THR	conflict	UNP P02588
A	100	ASP	ASN	conflict	UNP P02588

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Ca	0	0
			2	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	68	Total	O	0	0
			68	68		

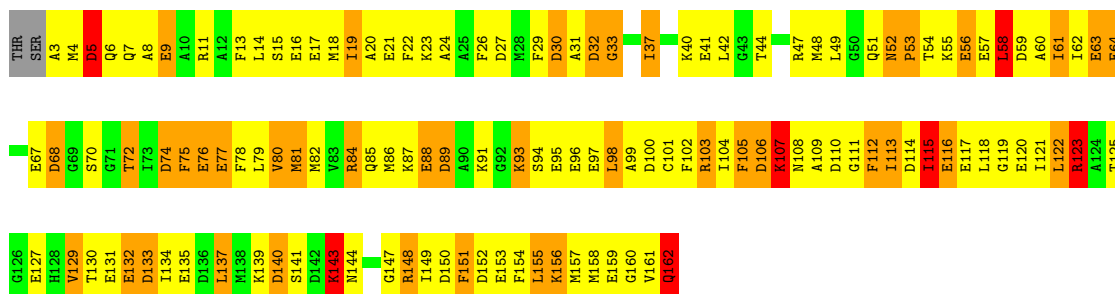
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: TROPONIN C

Chain A: 18% 51% 25%



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	66.70Å 66.70Å 60.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	8.00 – 2.00	Depositor
% Data completeness (in resolution range)	(Not available) (8.00-2.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.172 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1327	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	2.23	45/1269 (3.5%)	3.79	211/1694 (12.5%)

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	21	GLU	CD-OE1	-8.81	1.16	1.25
1	A	132	GLU	CD-OE1	-8.05	1.16	1.25
1	A	41	GLU	CD-OE1	-7.86	1.17	1.25
1	A	94	SER	CA-CB	7.78	1.64	1.52
1	A	114	ASP	C-O	7.39	1.37	1.23
1	A	130	THR	C-O	7.26	1.37	1.23
1	A	111	GLY	N-CA	7.13	1.56	1.46
1	A	13	PHE	CE2-CZ	6.91	1.50	1.37
1	A	61	ILE	CA-CB	6.80	1.70	1.54
1	A	17	GLU	CB-CG	6.72	1.65	1.52
1	A	62	ILE	C-N	-6.38	1.19	1.34
1	A	97	GLU	CG-CD	-6.36	1.42	1.51
1	A	47	ARG	NE-CZ	6.26	1.41	1.33
1	A	76	GLU	CG-CD	-6.18	1.42	1.51
1	A	76	GLU	CD-OE2	6.16	1.32	1.25
1	A	26	PHE	CE2-CZ	6.12	1.49	1.37
1	A	147	GLY	C-O	6.08	1.33	1.23
1	A	53	PRO	C-O	5.93	1.35	1.23
1	A	100	ASP	C-N	-5.87	1.20	1.34
1	A	130	THR	CB-OG1	5.83	1.54	1.43
1	A	13	PHE	CD1-CE1	5.80	1.50	1.39
1	A	157	MET	CG-SD	5.80	1.96	1.81
1	A	9	GLU	CB-CG	5.75	1.63	1.52
1	A	20	ALA	C-O	5.63	1.34	1.23
1	A	131	GLU	CD-OE2	5.62	1.31	1.25
1	A	16	GLU	CD-OE1	-5.56	1.19	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	16	GLU	N-CA	-5.48	1.35	1.46
1	A	76	GLU	N-CA	5.47	1.57	1.46
1	A	84	ARG	CD-NE	-5.46	1.37	1.46
1	A	147	GLY	N-CA	5.45	1.54	1.46
1	A	88	GLU	CD-OE2	-5.36	1.19	1.25
1	A	17	GLU	N-CA	5.31	1.56	1.46
1	A	76	GLU	CB-CG	5.24	1.62	1.52
1	A	27	ASP	CA-CB	5.23	1.65	1.53
1	A	154	PHE	CE1-CZ	5.22	1.47	1.37
1	A	20	ALA	N-CA	5.19	1.56	1.46
1	A	137	LEU	C-O	5.17	1.33	1.23
1	A	22	PHE	CD2-CE2	5.15	1.49	1.39
1	A	70	SER	CB-OG	5.13	1.49	1.42
1	A	76	GLU	C-O	5.12	1.33	1.23
1	A	151	PHE	CG-CD2	5.10	1.46	1.38
1	A	152	ASP	CB-CG	5.10	1.62	1.51
1	A	53	PRO	N-CD	-5.09	1.40	1.47
1	A	17	GLU	CD-OE2	-5.06	1.20	1.25
1	A	29	PHE	N-CA	5.02	1.56	1.46

All (211) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	103	ARG	NE-CZ-NH1	46.80	143.70	120.30
1	A	103	ARG	CD-NE-CZ	31.16	167.22	123.60
1	A	123	ARG	NE-CZ-NH1	-29.22	105.69	120.30
1	A	140	ASP	CB-CG-OD2	-23.77	96.91	118.30
1	A	103	ARG	NE-CZ-NH2	-21.44	109.58	120.30
1	A	59	ASP	CB-CG-OD1	20.85	137.07	118.30
1	A	76	GLU	OE1-CD-OE2	-16.77	103.17	123.30
1	A	47	ARG	NE-CZ-NH1	16.43	128.51	120.30
1	A	148	ARG	NE-CZ-NH1	-15.73	112.44	120.30
1	A	117	GLU	OE1-CD-OE2	-14.80	105.53	123.30
1	A	47	ARG	NE-CZ-NH2	-14.44	113.08	120.30
1	A	143	LYS	CB-CG-CD	14.38	149.00	111.60
1	A	74	ASP	CB-CG-OD2	13.51	130.46	118.30
1	A	140	ASP	OD1-CG-OD2	13.49	148.93	123.30
1	A	11	ARG	CD-NE-CZ	13.28	142.19	123.60
1	A	76	GLU	CG-CD-OE1	12.95	144.20	118.30
1	A	148	ARG	NE-CZ-NH2	12.20	126.40	120.30
1	A	5	ASP	CA-C-O	12.13	145.57	120.10
1	A	103	ARG	NH1-CZ-NH2	-11.54	106.70	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	133	ASP	CB-CG-OD2	-11.15	108.27	118.30
1	A	84	ARG	CD-NE-CZ	10.95	138.92	123.60
1	A	93	LYS	O-C-N	10.58	139.63	122.70
1	A	159	GLU	CA-C-N	10.44	137.07	116.20
1	A	160	GLY	N-CA-C	10.43	139.17	113.10
1	A	115	ILE	O-C-N	10.31	139.19	122.70
1	A	117	GLU	CG-CD-OE1	10.12	138.55	118.30
1	A	153	GLU	OE1-CD-OE2	-10.11	111.17	123.30
1	A	75	PHE	O-C-N	10.02	138.73	122.70
1	A	110	ASP	CB-CG-OD1	-9.95	109.34	118.30
1	A	75	PHE	CB-CG-CD2	-9.86	113.90	120.80
1	A	106	ASP	CB-CG-OD2	-9.84	109.44	118.30
1	A	101	CYS	CA-CB-SG	9.82	131.68	114.00
1	A	79	LEU	CA-CB-CG	9.76	137.74	115.30
1	A	5	ASP	CB-CG-OD2	-9.55	109.70	118.30
1	A	123	ARG	NE-CZ-NH2	9.52	125.06	120.30
1	A	129	VAL	O-C-N	9.23	137.47	122.70
1	A	72	THR	CA-CB-CG2	9.20	125.29	112.40
1	A	63	GLU	CB-CG-CD	9.11	138.79	114.20
1	A	111	GLY	O-C-N	-9.11	108.13	122.70
1	A	123	ARG	NH1-CZ-NH2	8.94	129.24	119.40
1	A	160	GLY	C-N-CA	8.78	143.66	121.70
1	A	159	GLU	CB-CA-C	8.74	127.88	110.40
1	A	107	LYS	CB-CA-C	-8.66	93.08	110.40
1	A	89	ASP	CB-CG-OD1	8.65	126.08	118.30
1	A	27	ASP	CB-CG-OD1	8.62	126.06	118.30
1	A	133	ASP	CB-CG-OD1	8.57	126.01	118.30
1	A	16	GLU	OE1-CD-OE2	-8.51	113.08	123.30
1	A	116	GLU	O-C-N	-8.49	109.11	122.70
1	A	139	LYS	CA-C-O	8.40	137.73	120.10
1	A	13	PHE	CB-CG-CD2	-8.39	114.93	120.80
1	A	113	ILE	CA-C-N	8.20	135.24	117.20
1	A	64	GLU	O-C-N	-8.13	109.68	122.70
1	A	127	GLU	OE1-CD-OE2	-8.13	113.55	123.30
1	A	150	ASP	CB-CG-OD2	8.11	125.59	118.30
1	A	108	ASN	O-C-N	8.09	135.64	122.70
1	A	16	GLU	CG-CD-OE1	8.08	134.46	118.30
1	A	150	ASP	CB-CG-OD1	-7.98	111.12	118.30
1	A	162	GLN	CA-C-O	-7.95	103.41	120.10
1	A	58	LEU	CB-CG-CD2	-7.88	97.61	111.00
1	A	75	PHE	CB-CG-CD1	7.75	126.23	120.80
1	A	81	MET	CG-SD-CE	7.72	112.55	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	ASP	CB-CG-OD1	7.57	125.11	118.30
1	A	84	ARG	NE-CZ-NH1	-7.55	116.52	120.30
1	A	157	MET	O-C-N	-7.48	110.73	122.70
1	A	26	PHE	CB-CG-CD1	-7.46	115.58	120.80
1	A	135	GLU	N-CA-CB	7.44	124.00	110.60
1	A	96	GLU	OE1-CD-OE2	7.43	132.22	123.30
1	A	32	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	132	GLU	OE1-CD-OE2	7.36	132.13	123.30
1	A	139	LYS	O-C-N	-7.31	111.01	122.70
1	A	80	VAL	CA-CB-CG1	7.27	121.81	110.90
1	A	85	GLN	O-C-N	-7.27	111.07	122.70
1	A	161	VAL	N-CA-C	-7.25	91.41	111.00
1	A	55	LYS	CD-CE-NZ	7.24	128.36	111.70
1	A	76	GLU	CB-CG-CD	7.23	133.71	114.20
1	A	9	GLU	CG-CD-OE2	-7.20	103.91	118.30
1	A	59	ASP	CB-CG-OD2	-7.16	111.86	118.30
1	A	144	ASN	O-C-N	-7.13	111.29	122.70
1	A	151	PHE	N-CA-CB	-7.09	97.84	110.60
1	A	27	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	A	18	MET	CA-CB-CG	-7.06	101.30	113.30
1	A	104	ILE	C-N-CA	7.05	139.32	121.70
1	A	155	LEU	CB-CG-CD1	-7.03	99.05	111.00
1	A	94	SER	CA-CB-OG	-6.96	92.42	111.20
1	A	30	ASP	CB-CG-OD1	6.95	124.55	118.30
1	A	94	SER	N-CA-CB	6.94	120.91	110.50
1	A	120	GLU	O-C-N	-6.91	111.64	122.70
1	A	115	ILE	CG1-CB-CG2	6.86	126.48	111.40
1	A	102	PHE	CB-CG-CD1	6.82	125.57	120.80
1	A	24	ALA	O-C-N	-6.78	111.85	122.70
1	A	5	ASP	O-C-N	-6.78	111.86	122.70
1	A	54	THR	O-C-N	-6.75	111.89	122.70
1	A	22	PHE	CB-CG-CD2	-6.71	116.10	120.80
1	A	101	CYS	O-C-N	6.71	133.43	122.70
1	A	57	GLU	N-CA-CB	6.70	122.66	110.60
1	A	112	PHE	CA-CB-CG	6.67	129.92	113.90
1	A	5	ASP	CA-C-N	-6.66	102.55	117.20
1	A	148	ARG	CG-CD-NE	-6.66	97.81	111.80
1	A	152	ASP	CA-CB-CG	-6.60	98.88	113.40
1	A	151	PHE	CB-CA-C	6.58	123.56	110.40
1	A	149	ILE	O-C-N	6.56	133.19	122.70
1	A	113	ILE	CA-C-O	-6.55	106.33	120.10
1	A	22	PHE	CZ-CE2-CD2	-6.55	112.24	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	31	ALA	C-N-CA	6.55	138.07	121.70
1	A	19	ILE	O-C-N	6.51	133.12	122.70
1	A	72	THR	CA-CB-OG1	-6.51	95.33	109.00
1	A	110	ASP	CB-CG-OD2	6.51	124.16	118.30
1	A	131	GLU	CG-CD-OE1	6.49	131.28	118.30
1	A	158	MET	CA-C-O	6.47	133.70	120.10
1	A	58	LEU	CB-CG-CD1	6.47	121.99	111.00
1	A	8	ALA	N-CA-CB	6.44	119.11	110.10
1	A	59	ASP	OD1-CG-OD2	-6.43	111.08	123.30
1	A	159	GLU	CA-C-O	-6.43	106.61	120.10
1	A	55	LYS	CG-CD-CE	6.41	131.13	111.90
1	A	11	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	A	22	PHE	CE1-CZ-CE2	6.37	131.47	120.00
1	A	84	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	A	115	ILE	CA-C-O	-6.33	106.80	120.10
1	A	116	GLU	CG-CD-OE1	6.33	130.97	118.30
1	A	84	ARG	NH1-CZ-NH2	6.31	126.34	119.40
1	A	150	ASP	N-CA-CB	6.31	121.96	110.60
1	A	130	THR	CA-CB-OG1	-6.30	95.77	109.00
1	A	112	PHE	CB-CG-CD2	-6.30	116.39	120.80
1	A	96	GLU	CG-CD-OE2	-6.26	105.78	118.30
1	A	143	LYS	CG-CD-CE	6.24	130.61	111.90
1	A	9	GLU	CA-CB-CG	-6.23	99.69	113.40
1	A	122	LEU	CA-C-O	6.23	133.19	120.10
1	A	101	CYS	CA-C-O	-6.20	107.08	120.10
1	A	9	GLU	CG-CD-OE1	6.19	130.69	118.30
1	A	17	GLU	OE1-CD-OE2	-6.19	115.87	123.30
1	A	154	PHE	CD1-CE1-CZ	-6.15	112.72	120.10
1	A	97	GLU	CA-CB-CG	-6.15	99.87	113.40
1	A	9	GLU	N-CA-CB	6.09	121.57	110.60
1	A	48	MET	C-N-CA	6.09	136.92	121.70
1	A	67	GLU	CA-C-N	6.05	130.52	117.20
1	A	56	GLU	CG-CD-OE2	-6.04	106.21	118.30
1	A	115	ILE	CB-CA-C	-6.04	99.53	111.60
1	A	99	ALA	CA-C-O	6.03	132.76	120.10
1	A	129	VAL	CA-C-O	-6.03	107.44	120.10
1	A	130	THR	CA-CB-CG2	6.03	120.84	112.40
1	A	113	ILE	CB-CG1-CD1	-6.02	97.04	113.90
1	A	11	ARG	CG-CD-NE	-6.02	99.16	111.80
1	A	26	PHE	O-C-N	-6.02	113.07	122.70
1	A	13	PHE	CG-CD2-CE2	5.99	127.39	120.80
1	A	4	MET	N-CA-CB	-5.97	99.85	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	131	GLU	N-CA-CB	5.95	121.31	110.60
1	A	78	PHE	CG-CD1-CE1	5.94	127.33	120.80
1	A	57	GLU	CB-CA-C	-5.91	98.58	110.40
1	A	144	ASN	C-N-CA	5.86	136.35	121.70
1	A	77	GLU	OE1-CD-OE2	5.86	130.33	123.30
1	A	80	VAL	O-C-N	-5.86	113.33	122.70
1	A	132	GLU	N-CA-CB	-5.86	100.06	110.60
1	A	111	GLY	CA-C-O	5.84	131.11	120.60
1	A	13	PHE	CG-CD1-CE1	-5.80	114.42	120.80
1	A	95	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	A	95	GLU	N-CA-CB	5.80	121.04	110.60
1	A	75	PHE	CA-C-O	-5.80	107.93	120.10
1	A	40	LYS	O-C-N	-5.78	113.44	122.70
1	A	122	LEU	O-C-N	-5.76	113.48	122.70
1	A	84	ARG	N-CA-CB	5.76	120.97	110.60
1	A	116	GLU	CG-CD-OE2	-5.73	106.84	118.30
1	A	57	GLU	OE1-CD-OE2	-5.65	116.52	123.30
1	A	114	ASP	CB-CA-C	5.64	121.69	110.40
1	A	125	THR	OG1-CB-CG2	5.64	122.98	110.00
1	A	68	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	A	151	PHE	CG-CD2-CE2	-5.63	114.61	120.80
1	A	79	LEU	O-C-N	-5.62	113.71	122.70
1	A	27	ASP	CA-CB-CG	-5.57	101.14	113.40
1	A	135	GLU	CG-CD-OE1	5.57	129.43	118.30
1	A	44	THR	O-C-N	-5.55	113.81	122.70
1	A	100	ASP	CA-C-O	-5.55	108.45	120.10
1	A	118	LEU	O-C-N	-5.54	113.77	123.20
1	A	127	GLU	CG-CD-OE2	5.54	129.38	118.30
1	A	42	LEU	CB-CG-CD1	-5.53	101.60	111.00
1	A	131	GLU	CG-CD-OE2	-5.53	107.24	118.30
1	A	37	ILE	CA-C-O	5.52	131.69	120.10
1	A	74	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	A	116	GLU	C-N-CA	5.50	135.45	121.70
1	A	106	ASP	CA-C-O	5.50	131.65	120.10
1	A	114	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	A	117	GLU	N-CA-CB	5.49	120.48	110.60
1	A	13	PHE	CZ-CE2-CD2	-5.47	113.53	120.10
1	A	18	MET	CG-SD-CE	-5.46	91.46	100.20
1	A	87	LYS	O-C-N	5.45	131.42	122.70
1	A	161	VAL	CA-C-N	-5.44	105.22	117.20
1	A	21	GLU	OE1-CD-OE2	5.44	129.83	123.30
1	A	56	GLU	OE1-CD-OE2	5.42	129.81	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	PHE	O-C-N	5.41	131.35	122.70
1	A	161	VAL	CA-CB-CG1	5.41	119.01	110.90
1	A	100	ASP	CA-C-N	5.39	129.06	117.20
1	A	160	GLY	CA-C-O	5.37	130.27	120.60
1	A	47	ARG	CD-NE-CZ	-5.28	116.21	123.60
1	A	86	MET	O-C-N	-5.26	114.28	122.70
1	A	29	PHE	CD1-CE1-CZ	-5.25	113.80	120.10
1	A	77	GLU	CG-CD-OE2	-5.24	107.82	118.30
1	A	98	LEU	O-C-N	5.24	131.08	122.70
1	A	115	ILE	N-CA-CB	5.24	122.84	110.80
1	A	107	LYS	CA-C-N	-5.23	105.69	117.20
1	A	33	GLY	O-C-N	5.23	132.09	123.20
1	A	135	GLU	CB-CA-C	-5.19	100.02	110.40
1	A	143	LYS	CD-CE-NZ	5.18	123.61	111.70
1	A	123	ARG	CA-CB-CG	-5.15	102.07	113.40
1	A	131	GLU	CA-CB-CG	5.14	124.72	113.40
1	A	140	ASP	CB-CA-C	-5.14	100.12	110.40
1	A	24	ALA	CB-CA-C	5.14	117.81	110.10
1	A	48	MET	CB-CG-SD	-5.12	97.04	112.40
1	A	54	THR	CA-C-N	5.07	128.34	117.20
1	A	120	GLU	CA-C-O	5.06	130.73	120.10
1	A	63	GLU	CG-CD-OE1	5.06	128.42	118.30
1	A	20	ALA	CB-CA-C	5.05	117.67	110.10
1	A	14	LEU	N-CA-CB	-5.03	100.34	110.40

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	1257	0	1171	53	1
2	A	2	0	0	0	0
3	A	68	0	0	5	3
All	All	1327	0	1171	53	3

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 22.

All (53) 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:119:GLY:HA2	1:A:134:ILE:HD13	1.24	1.13
1:A:141:SER:O	1:A:143:LYS:HD3	1.61	0.98
1:A:6:GLN:NE2	3:A:199:HOH:O	1.94	0.94
1:A:105:PHE:CE2	1:A:121:ILE:HG21	2.05	0.92
1:A:60:ALA:O	1:A:63:GLU:HG2	1.73	0.88
1:A:151:PHE:O	1:A:155:LEU:HD13	1.74	0.87
1:A:119:GLY:HA2	1:A:134:ILE:CD1	2.05	0.84
1:A:143:LYS:HE2	1:A:156:LYS:CE	2.16	0.76
1:A:77:GLU:HG2	3:A:188:HOH:O	1.87	0.75
1:A:156:LYS:HG2	1:A:162:GLN:O	1.87	0.75
1:A:143:LYS:HE2	1:A:156:LYS:HE2	1.73	0.70
1:A:60:ALA:O	1:A:63:GLU:CG	2.39	0.70
1:A:105:PHE:CE2	1:A:121:ILE:CG2	2.75	0.69
1:A:51:GLN:NE2	1:A:89:ASP:OD2	2.28	0.67
1:A:107:LYS:NZ	1:A:121:ILE:HG12	2.10	0.65
1:A:5:ASP:O	1:A:9:GLU:HG3	1.97	0.65
1:A:105:PHE:CZ	1:A:121:ILE:HG21	2.34	0.62
1:A:107:LYS:HZ1	1:A:121:ILE:HG12	1.63	0.61
1:A:119:GLY:CA	1:A:134:ILE:HD13	2.16	0.61
1:A:77:GLU:CG	3:A:188:HOH:O	2.46	0.60
1:A:151:PHE:CZ	1:A:155:LEU:HD11	2.36	0.60
1:A:63:GLU:HG3	1:A:64:GLU:N	2.16	0.60
1:A:155:LEU:HD12	1:A:155:LEU:N	2.17	0.59
1:A:156:LYS:HA	1:A:162:GLN:HB3	1.83	0.59
1:A:23:LYS:HD3	1:A:75:PHE:CD2	2.39	0.58
1:A:119:GLY:O	1:A:123:ARG:HD2	2.04	0.57
1:A:143:LYS:HE2	1:A:156:LYS:HE3	1.87	0.56
1:A:63:GLU:HB3	3:A:215:HOH:O	2.05	0.55
1:A:156:LYS:HG2	1:A:162:GLN:C	2.27	0.54
1:A:53:PRO:HG2	1:A:58:LEU:HD21	1.90	0.54
1:A:37:ILE:O	1:A:72:THR:HA	2.08	0.53
1:A:23:LYS:HD3	1:A:75:PHE:CE2	2.45	0.51
1:A:122:LEU:HD11	1:A:137:LEU:HD23	1.92	0.51
1:A:106:ASP:OD1	1:A:109:ALA:HA	2.11	0.50
1:A:30:ASP:OD1	1:A:33:GLY:N	2.46	0.49
1:A:3:ALA:O	1:A:7:GLN:HG3	2.13	0.49
1:A:112:PHE:CD2	1:A:148:ARG:HG3	2.48	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ALA:C	1:A:63:GLU:HG2	2.33	0.47
1:A:115:ILE:H	1:A:115:ILE:HG13	1.46	0.47
1:A:56:GLU:CD	1:A:56:GLU:C	2.74	0.46
1:A:80:VAL:O	1:A:84:ARG:HG3	2.15	0.46
1:A:155:LEU:N	1:A:155:LEU:CD1	2.79	0.46
1:A:53:PRO:HG2	1:A:58:LEU:CD2	2.47	0.44
1:A:123:ARG:HH11	1:A:123:ARG:HD3	1.33	0.44
1:A:151:PHE:O	1:A:155:LEU:CD1	2.57	0.43
1:A:121:ILE:HD13	1:A:121:ILE:HA	1.84	0.43
1:A:61:ILE:CG2	1:A:81:MET:HG3	2.50	0.42
1:A:156:LYS:HE2	1:A:156:LYS:HB2	1.67	0.42
1:A:141:SER:C	1:A:143:LYS:HD3	2.37	0.41
1:A:15:SER:O	1:A:19:ILE:HG13	2.20	0.41
1:A:115:ILE:HG13	3:A:170:HOH:O	2.22	0.40
1:A:52:ASN:HD22	1:A:52:ASN:HA	1.43	0.40
1:A:113:ILE:HD13	1:A:113:ILE:HG21	1.65	0.40

All (3) 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)
3:A:236:HOH:O	3:A:239:HOH:O[3_564]	1.54	0.66
3:A:233:HOH:O	3:A:234:HOH:O[6_554]	2.00	0.20
1:A:133:ASP:OD1	3:A:218:HOH:O[2_664]	2.06	0.14

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	158/162 (98%)	156 (99%)	2 (1%)	0	100 100

There are no Ramachandran outliers to report.

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	134/136 (98%)	109 (81%)	25 (19%)	1 0

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

Mol	Chain	Res	Type
1	A	5	ASP
1	A	32	ASP
1	A	49	LEU
1	A	52	ASN
1	A	58	LEU
1	A	68	ASP
1	A	74	ASP
1	A	76	GLU
1	A	82	MET
1	A	88	GLU
1	A	91	LYS
1	A	93	LYS
1	A	98	LEU
1	A	103	ARG
1	A	105	PHE
1	A	107	LYS
1	A	115	ILE
1	A	116	GLU
1	A	123	ARG
1	A	129	VAL
1	A	132	GLU
1	A	140	ASP
1	A	143	LYS
1	A	156	LYS
1	A	162	GLN

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

Mol	Chain	Res	Type
1	A	52	ASN
1	A	162	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 2 ligands modelled in this entry, 2 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](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	62:ILE	C	63:GLU	N	1.19

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.