



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 12:12 AM UTC

PDB ID : 2PF1 / pdb_00002pf1
Title : STRUCTURE OF BOVINE PROTHROMBIN FRAGMENT 1 REFINED AT
2.25 ANGSTROMS RESOLUTION
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Deposited on : 1992-09-17
Resolution : 2.80 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)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

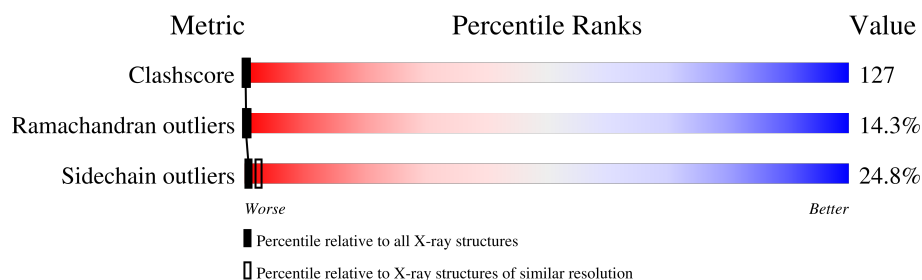
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)

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	156	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 1111 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 PROTHROMBIN FRAGMENT 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	121	Total	C	N	O	S	0	0	0
			947	576	177	185	9			

There are 10 discrepancies between the modelled and reference sequences:

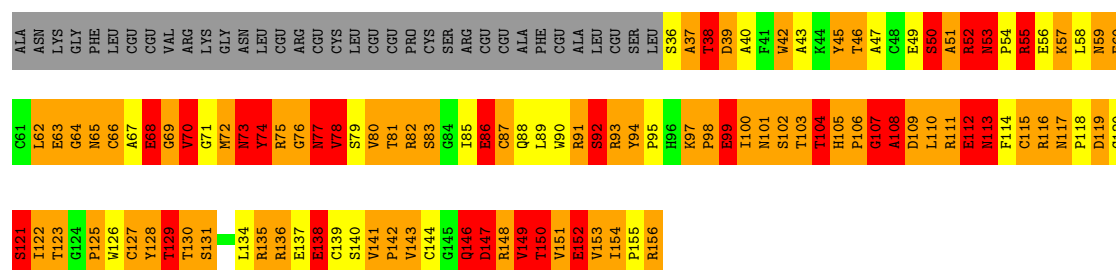
Chain	Residue	Modelled	Actual	Comment	Reference
A	7	CGU	GLU	conflict	UNP P00735
A	8	CGU	GLU	conflict	UNP P00735
A	15	CGU	GLU	conflict	UNP P00735
A	17	CGU	GLU	conflict	UNP P00735
A	20	CGU	GLU	conflict	UNP P00735
A	21	CGU	GLU	conflict	UNP P00735
A	26	CGU	GLU	conflict	UNP P00735
A	27	CGU	GLU	conflict	UNP P00735
A	30	CGU	GLU	conflict	UNP P00735
A	33	CGU	GLU	conflict	UNP P00735

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	164	Total	O	0	0
			164	164		

Note EDS was not executed.

Chain A: 6% 17% 37% 17% 22%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	77.62Å 77.62Å 85.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	5.00 – 2.80	Depositor
% Data completeness (in resolution range)	(Not available) (5.00-2.80)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.175 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	1111	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

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	1.66	9/969 (0.9%)	3.60	185/1316 (14.1%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	94	TYR	N-CA	7.23	1.56	1.46
1	A	71	GLY	N-CA	6.69	1.55	1.45
1	A	103	THR	CA-CB	6.68	1.62	1.53
1	A	63	GLU	N-CA	5.78	1.53	1.46
1	A	70	VAL	C-N	5.54	1.41	1.33
1	A	81	THR	CB-OG1	5.34	1.52	1.43
1	A	81	THR	N-CA	5.22	1.52	1.45
1	A	64	GLY	N-CA	5.06	1.52	1.45
1	A	121	SER	CA-C	-5.05	1.46	1.52

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	141	VAL	CB-CA-C	16.55	125.55	109.33
1	A	109	ASP	CA-CB-CG	14.95	127.55	112.60
1	A	59	ASN	CA-CB-CG	13.74	126.34	112.60
1	A	78	VAL	CB-CA-C	13.18	125.43	110.41
1	A	113	ASN	CA-CB-CG	12.51	125.11	112.60
1	A	129	THR	CA-CB-OG1	-12.35	91.07	109.60
1	A	147	ASP	CA-CB-CG	-12.34	100.26	112.60
1	A	136	ARG	CD-NE-CZ	12.19	141.46	124.40
1	A	91	ARG	CD-NE-CZ	11.81	140.94	124.40
1	A	60	GLU	CA-C-N	11.75	135.71	120.44
1	A	60	GLU	C-N-CA	11.75	135.71	120.44
1	A	141	VAL	N-CA-CB	-11.49	99.34	111.64
1	A	147	ASP	CA-C-O	11.19	133.68	120.92
1	A	103	THR	N-CA-CB	-10.95	95.22	111.43
1	A	72	MET	CB-CA-C	10.81	129.23	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	ARG	CD-NE-CZ	10.79	139.51	124.40
1	A	94	TYR	O-C-N	-10.69	113.50	121.84
1	A	91	ARG	N-CA-CB	10.38	125.90	110.33
1	A	105	HIS	O-C-N	10.10	130.56	121.17
1	A	46	THR	CA-C-N	9.82	134.71	120.38
1	A	46	THR	C-N-CA	9.82	134.71	120.38
1	A	70	VAL	CA-C-O	-9.79	108.55	120.78
1	A	56	GLU	CB-CG-CD	9.59	128.91	112.60
1	A	38	THR	N-CA-C	-9.59	101.71	113.50
1	A	87	CYS	CA-C-O	-9.57	110.67	121.19
1	A	152	GLU	CA-C-O	-9.55	110.46	121.16
1	A	39	ASP	N-CA-C	-9.32	101.01	111.82
1	A	100	ILE	N-CA-CB	9.15	120.70	110.72
1	A	122	ILE	CB-CA-C	9.06	124.73	112.22
1	A	137	GLU	CA-CB-CG	9.06	132.22	114.10
1	A	107	GLY	CA-C-N	9.01	138.75	121.54
1	A	107	GLY	C-N-CA	9.01	138.75	121.54
1	A	111	ARG	CD-NE-CZ	-8.90	111.94	124.40
1	A	152	GLU	O-C-N	8.84	133.68	122.89
1	A	99	GLU	N-CA-C	-8.83	101.58	111.82
1	A	135	ARG	CD-NE-CZ	-8.75	112.14	124.40
1	A	119	ASP	CA-C-O	-8.73	108.03	120.51
1	A	148	ARG	NE-CZ-NH2	8.69	127.02	119.20
1	A	156	ARG	CD-NE-CZ	8.68	136.56	124.40
1	A	86	GLU	CA-C-O	8.67	130.15	120.43
1	A	148	ARG	NE-CZ-NH1	-8.53	112.97	121.50
1	A	129	THR	CA-C-O	-8.51	112.29	121.99
1	A	53	ASN	CA-CB-CG	-8.39	104.21	112.60
1	A	135	ARG	O-C-N	8.36	130.68	122.07
1	A	62	LEU	N-CA-C	-8.24	102.38	111.36
1	A	99	GLU	N-CA-CB	8.10	122.83	110.28
1	A	81	THR	CA-CB-OG1	-8.07	97.50	109.60
1	A	131	SER	N-CA-C	-8.04	99.67	109.72
1	A	66	CYS	CA-C-N	7.99	132.93	121.50
1	A	66	CYS	C-N-CA	7.99	132.93	121.50
1	A	141	VAL	O-C-N	7.93	126.69	121.69
1	A	53	ASN	OD1-CG-ND2	7.90	130.50	122.60
1	A	137	GLU	N-CA-CB	7.88	125.18	111.39
1	A	50	SER	O-C-N	-7.83	112.18	122.59
1	A	39	ASP	CA-CB-CG	7.82	120.42	112.60
1	A	149	VAL	CB-CA-C	7.82	122.55	110.50
1	A	127	CYS	CA-C-O	-7.79	112.53	121.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	153	VAL	N-CA-CB	7.76	121.28	110.56
1	A	129	THR	O-C-N	7.73	132.08	122.65
1	A	137	GLU	CG-CD-OE2	7.60	135.88	118.40
1	A	67	ALA	O-C-N	7.56	131.89	123.04
1	A	138	GLU	CA-C-N	7.53	134.24	122.94
1	A	138	GLU	C-N-CA	7.53	134.24	122.94
1	A	86	GLU	CG-CD-OE2	7.46	135.56	118.40
1	A	93	ARG	N-CA-C	7.45	119.69	109.11
1	A	52	ARG	CD-NE-CZ	-7.44	113.99	124.40
1	A	146	GLN	OE1-CD-NE2	7.41	130.01	122.60
1	A	111	ARG	NE-CZ-NH1	-7.38	114.12	121.50
1	A	62	LEU	O-C-N	7.23	130.40	122.15
1	A	149	VAL	O-C-N	7.22	130.83	123.10
1	A	82	ARG	NH1-CZ-NH2	7.22	128.69	119.30
1	A	87	CYS	O-C-N	7.18	131.71	122.87
1	A	106	PRO	N-CA-C	-7.16	97.72	112.47
1	A	125	PRO	N-CA-C	-7.14	99.62	111.26
1	A	108	ALA	CA-C-O	-7.14	110.30	120.51
1	A	39	ASP	N-CA-CB	7.11	121.30	110.28
1	A	45	TYR	O-C-N	7.08	130.22	122.15
1	A	147	ASP	CB-CA-C	7.03	120.87	109.90
1	A	104	THR	CB-CA-C	-6.99	96.51	110.42
1	A	55	ARG	O-C-N	6.95	130.35	122.22
1	A	50	SER	CA-CB-OG	6.94	124.98	111.10
1	A	129	THR	OG1-CB-CG2	6.93	123.17	109.30
1	A	113	ASN	N-CA-C	6.91	125.52	110.80
1	A	122	ILE	N-CA-CB	-6.90	100.23	110.58
1	A	67	ALA	CB-CA-C	-6.88	98.62	109.84
1	A	105	HIS	CA-CB-CG	-6.88	106.92	113.80
1	A	153	VAL	O-C-N	6.80	130.72	122.83
1	A	75	ARG	CA-C-O	6.74	128.21	121.20
1	A	77	ASN	CA-C-O	-6.72	110.89	120.51
1	A	75	ARG	N-CA-CB	-6.69	102.28	111.65
1	A	53	ASN	O-C-N	6.68	129.00	121.32
1	A	82	ARG	NE-CZ-NH1	-6.67	114.83	121.50
1	A	111	ARG	O-C-N	6.67	130.93	122.93
1	A	92	SER	CA-C-O	-6.66	110.98	120.51
1	A	68	GLU	CA-C-O	-6.61	113.05	120.32
1	A	99	GLU	CG-CD-OE1	-6.60	103.23	118.40
1	A	128	TYR	N-CA-CB	6.58	121.22	110.17
1	A	125	PRO	CA-C-N	6.58	135.85	123.09
1	A	125	PRO	C-N-CA	6.58	135.85	123.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	107	GLY	CA-C-O	6.54	131.95	120.57
1	A	143	VAL	CA-C-O	-6.53	114.89	122.13
1	A	78	VAL	CA-C-N	6.47	134.09	122.38
1	A	78	VAL	C-N-CA	6.47	134.09	122.38
1	A	116	ARG	CA-C-N	6.47	137.59	121.80
1	A	116	ARG	C-N-CA	6.47	137.59	121.80
1	A	122	ILE	CA-CB-CG2	6.38	121.34	110.50
1	A	55	ARG	CA-C-O	-6.37	112.91	120.10
1	A	123	THR	CA-C-O	-6.35	113.69	120.42
1	A	104	THR	CA-C-O	6.35	129.59	120.51
1	A	135	ARG	NE-CZ-NH2	6.32	124.88	119.20
1	A	154	ILE	O-C-N	6.31	128.29	121.10
1	A	103	THR	CB-CA-C	6.29	122.21	111.46
1	A	130	THR	O-C-N	6.29	129.84	122.24
1	A	83	SER	CA-C-O	-6.22	112.28	119.56
1	A	92	SER	CA-C-N	-6.13	114.57	122.79
1	A	92	SER	C-N-CA	-6.13	114.57	122.79
1	A	62	LEU	CA-C-N	-6.11	112.13	121.66
1	A	62	LEU	C-N-CA	-6.11	112.13	121.66
1	A	104	THR	CA-CB-OG1	-6.09	100.47	109.60
1	A	55	ARG	CD-NE-CZ	-6.09	115.88	124.40
1	A	62	LEU	N-CA-CB	6.08	119.16	110.16
1	A	116	ARG	NE-CZ-NH2	6.04	124.63	119.20
1	A	99	GLU	CB-CA-C	-6.01	99.12	110.67
1	A	75	ARG	CA-C-N	6.00	133.17	121.41
1	A	75	ARG	C-N-CA	6.00	133.17	121.41
1	A	112	GLU	CA-C-N	5.96	132.93	121.54
1	A	112	GLU	C-N-CA	5.96	132.93	121.54
1	A	151	VAL	O-C-N	5.96	129.55	123.00
1	A	148	ARG	N-CA-CB	5.92	118.92	110.51
1	A	101	ASN	OD1-CG-ND2	5.91	128.51	122.60
1	A	43	ALA	O-C-N	5.87	128.37	122.08
1	A	38	THR	CB-CA-C	5.87	119.98	109.29
1	A	46	THR	O-C-N	5.85	128.11	122.03
1	A	109	ASP	CA-C-N	5.79	130.78	122.21
1	A	109	ASP	C-N-CA	5.79	130.78	122.21
1	A	79	SER	CA-C-O	-5.79	112.27	119.28
1	A	80	VAL	CB-CA-C	-5.78	101.44	110.69
1	A	79	SER	N-CA-C	5.75	120.28	113.16
1	A	111	ARG	CG-CD-NE	-5.72	99.41	112.00
1	A	74	TYR	CA-CB-CG	-5.70	103.65	113.90
1	A	115	CYS	O-C-N	5.67	129.67	123.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	143	VAL	CA-CB-CG1	5.66	120.01	110.40
1	A	78	VAL	CA-C-O	5.65	125.25	120.22
1	A	94	TYR	CA-CB-CG	-5.64	103.75	113.90
1	A	130	THR	N-CA-CB	5.62	119.10	110.61
1	A	138	GLU	CB-CG-CD	5.54	122.03	112.60
1	A	92	SER	O-C-N	5.51	129.92	122.59
1	A	125	PRO	N-CA-CB	5.51	108.15	103.19
1	A	142	PRO	CB-CA-C	-5.50	104.72	111.64
1	A	111	ARG	CA-C-O	-5.49	114.70	120.58
1	A	141	VAL	CA-CB-CG1	5.49	119.73	110.40
1	A	75	ARG	NE-CZ-NH1	-5.41	116.09	121.50
1	A	154	ILE	N-CA-CB	5.39	118.76	111.21
1	A	98	PRO	CB-CA-C	-5.39	104.81	111.11
1	A	99	GLU	CA-C-N	-5.38	115.44	122.37
1	A	99	GLU	C-N-CA	-5.38	115.44	122.37
1	A	117	ASN	O-C-N	5.36	127.49	121.32
1	A	123	THR	CA-CB-OG1	-5.33	101.61	109.60
1	A	63	GLU	CB-CA-C	5.29	118.71	110.67
1	A	59	ASN	CB-CG-ND2	-5.29	108.47	116.40
1	A	73	ASN	CA-CB-CG	-5.29	107.31	112.60
1	A	63	GLU	N-CA-C	-5.28	101.55	109.15
1	A	150	THR	O-C-N	-5.26	116.62	122.09
1	A	108	ALA	N-CA-CB	-5.25	101.62	110.49
1	A	39	ASP	CA-C-N	5.24	127.30	120.28
1	A	39	ASP	C-N-CA	5.24	127.30	120.28
1	A	148	ARG	O-C-N	5.22	128.89	122.88
1	A	97	LYS	CB-CA-C	-5.22	104.08	110.08
1	A	101	ASN	CA-C-N	5.21	131.50	121.54
1	A	101	ASN	C-N-CA	5.21	131.50	121.54
1	A	52	ARG	NE-CZ-NH2	5.20	123.88	119.20
1	A	81	THR	CB-CA-C	5.19	120.33	110.51
1	A	95	PRO	N-CD-CG	5.18	110.02	103.80
1	A	125	PRO	CA-C-O	-5.18	115.68	121.32
1	A	45	TYR	CA-C-N	-5.17	113.82	120.65
1	A	45	TYR	C-N-CA	-5.17	113.82	120.65
1	A	148	ARG	N-CA-C	-5.17	101.10	108.23
1	A	68	GLU	CG-CD-OE2	-5.16	106.54	118.40
1	A	86	GLU	OE1-CD-OE2	-5.16	110.52	122.90
1	A	68	GLU	CA-CB-CG	5.15	124.40	114.10
1	A	152	GLU	CB-CG-CD	5.13	121.32	112.60
1	A	104	THR	OG1-CB-CG2	5.13	119.55	109.30
1	A	100	ILE	O-C-N	5.12	128.79	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	56	GLU	N-CA-CB	5.01	117.24	109.98
1	A	42	TRP	O-C-N	5.00	127.85	122.15

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	947	0	890	234	1
2	A	164	0	0	63	0
All	All	1111	0	890	234	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 127.

All (234) 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:122:ILE:HB	2:A:317:HOH:O	1.15	1.30
1:A:149:VAL:HG13	2:A:198:HOH:O	1.33	1.28
1:A:101:ASN:OD1	1:A:103:THR:HB	1.28	1.25
1:A:111:ARG:O	1:A:112:GLU:O	1.57	1.22
1:A:53:ASN:HB3	1:A:54:PRO:HD3	1.21	1.16
1:A:126:TRP:CZ3	1:A:136:ARG:HD2	1.80	1.16
1:A:39:ASP:HA	2:A:307:HOH:O	1.54	1.07
1:A:89:LEU:CB	1:A:92:SER:HB2	1.85	1.07
1:A:64:GLY:N	2:A:243:HOH:O	1.60	1.06
1:A:101:ASN:OD1	1:A:103:THR:CB	2.04	1.05
1:A:89:LEU:HB2	1:A:92:SER:CB	1.87	1.04
1:A:98:PRO:HB3	1:A:128:TYR:CE2	1.92	1.04
1:A:156:ARG:HD3	2:A:296:HOH:O	1.55	1.04
1:A:139:CYS:SG	2:A:177:HOH:O	2.16	1.02
1:A:138:GLU:C	2:A:177:HOH:O	2.03	1.01
1:A:37:ALA:H	1:A:40:ALA:HB2	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:TRP:CZ3	1:A:136:ARG:CD	2.48	0.96
1:A:136:ARG:NH1	2:A:252:HOH:O	1.64	0.95
1:A:93:ARG:HG2	2:A:258:HOH:O	1.66	0.93
1:A:154:ILE:HG23	1:A:155:PRO:HD2	1.50	0.93
1:A:53:ASN:HB3	1:A:54:PRO:CD	1.94	0.93
1:A:98:PRO:HG3	2:A:213:HOH:O	1.70	0.91
1:A:154:ILE:CG2	1:A:155:PRO:HD2	1.99	0.91
1:A:98:PRO:HB3	1:A:128:TYR:CZ	2.06	0.90
1:A:109:ASP:HA	2:A:286:HOH:O	1.71	0.90
1:A:122:ILE:HG12	2:A:202:HOH:O	1.71	0.89
1:A:156:ARG:HG3	2:A:277:HOH:O	1.73	0.88
1:A:101:ASN:C	1:A:103:THR:H	1.76	0.88
1:A:74:TYR:O	1:A:75:ARG:HD3	1.75	0.86
1:A:140:SER:C	1:A:141:VAL:HG23	1.99	0.86
1:A:150:THR:N	2:A:198:HOH:O	2.08	0.86
1:A:64:GLY:HA3	1:A:75:ARG:HB2	1.56	0.86
1:A:97:LYS:CD	2:A:161:HOH:O	2.24	0.86
1:A:129:THR:HG23	1:A:131:SER:H	1.37	0.86
1:A:73:ASN:CG	1:A:73:ASN:O	2.20	0.84
1:A:126:TRP:CH2	1:A:136:ARG:HD2	2.11	0.84
1:A:100:ILE:HG23	1:A:105:HIS:CD2	2.13	0.84
1:A:140:SER:C	1:A:141:VAL:CG2	2.51	0.84
1:A:58:LEU:O	1:A:62:LEU:HD12	1.77	0.83
1:A:126:TRP:CE3	1:A:136:ARG:HG2	2.15	0.82
1:A:37:ALA:H	1:A:40:ALA:CB	1.94	0.81
1:A:37:ALA:O	1:A:40:ALA:HB3	1.80	0.81
1:A:129:THR:CG2	1:A:131:SER:H	1.95	0.80
1:A:53:ASN:C	2:A:195:HOH:O	2.24	0.80
1:A:89:LEU:HD12	1:A:92:SER:OG	1.82	0.80
1:A:51:ALA:HB2	1:A:57:LYS:HE3	1.64	0.79
1:A:37:ALA:N	1:A:40:ALA:HB2	1.97	0.79
1:A:123:THR:HB	1:A:138:GLU:OE1	1.82	0.79
1:A:155:PRO:O	1:A:156:ARG:C	2.26	0.79
1:A:91:ARG:HA	2:A:188:HOH:O	1.83	0.79
1:A:122:ILE:CB	2:A:317:HOH:O	1.90	0.79
1:A:101:ASN:HB2	2:A:257:HOH:O	1.83	0.78
1:A:74:TYR:CZ	1:A:76:GLY:HA3	2.18	0.78
1:A:63:GLU:CD	2:A:281:HOH:O	2.27	0.77
1:A:39:ASP:CB	2:A:299:HOH:O	2.32	0.77
1:A:98:PRO:HB2	1:A:100:ILE:O	1.85	0.77
1:A:122:ILE:O	2:A:330:HOH:O	2.01	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:O	1:A:112:GLU:C	2.28	0.76
1:A:89:LEU:HB2	1:A:92:SER:HB2	0.90	0.76
1:A:97:LYS:HD3	2:A:161:HOH:O	1.84	0.76
1:A:53:ASN:CB	1:A:54:PRO:HD3	2.12	0.76
1:A:143:VAL:HG11	1:A:146:GLN:OE1	1.86	0.75
1:A:152:GLU:HG3	2:A:303:HOH:O	1.86	0.75
1:A:36:SER:HB2	1:A:40:ALA:HB2	1.68	0.75
1:A:52:ARG:HA	1:A:58:LEU:HB2	1.68	0.74
1:A:104:THR:HB	1:A:105:HIS:HD2	1.54	0.72
1:A:126:TRP:CE3	1:A:136:ARG:CG	2.73	0.72
1:A:57:LYS:O	2:A:172:HOH:O	2.08	0.72
1:A:122:ILE:CG2	2:A:317:HOH:O	2.27	0.71
1:A:86:GLU:O	1:A:130:THR:HG23	1.91	0.71
1:A:75:ARG:HH11	1:A:109:ASP:HB3	1.56	0.71
1:A:116:ARG:O	1:A:125:PRO:HA	1.91	0.71
1:A:151:VAL:N	2:A:198:HOH:O	2.14	0.70
1:A:50:SER:O	1:A:52:ARG:N	2.25	0.70
1:A:109:ASP:CA	2:A:286:HOH:O	2.35	0.70
1:A:108:ALA:O	2:A:286:HOH:O	2.10	0.69
1:A:143:VAL:O	1:A:147:ASP:OD2	2.09	0.69
1:A:147:ASP:OD1	1:A:148:ARG:N	2.25	0.69
1:A:73:ASN:O	1:A:74:TYR:HB2	1.93	0.69
1:A:63:GLU:OE1	2:A:281:HOH:O	2.11	0.68
1:A:152:GLU:CG	2:A:303:HOH:O	2.41	0.68
1:A:140:SER:O	1:A:141:VAL:HG22	1.94	0.68
1:A:94:TYR:HE2	2:A:282:HOH:O	1.75	0.68
1:A:69:GLY:O	1:A:70:VAL:C	2.37	0.67
1:A:59:ASN:O	1:A:63:GLU:N	2.22	0.67
1:A:101:ASN:O	1:A:103:THR:N	2.27	0.66
1:A:101:ASN:C	1:A:103:THR:N	2.52	0.66
1:A:81:THR:HG22	2:A:204:HOH:O	1.94	0.66
1:A:150:THR:HG21	2:A:199:HOH:O	1.96	0.66
1:A:111:ARG:C	1:A:112:GLU:O	2.39	0.65
1:A:53:ASN:CB	1:A:54:PRO:CD	2.67	0.65
1:A:51:ALA:CB	1:A:57:LYS:HE3	2.25	0.65
1:A:110:LEU:N	2:A:286:HOH:O	2.16	0.65
1:A:75:ARG:NH1	1:A:109:ASP:H	1.94	0.65
1:A:91:ARG:O	1:A:93:ARG:N	2.30	0.64
1:A:75:ARG:NH1	1:A:109:ASP:N	2.46	0.64
1:A:103:THR:C	1:A:104:THR:OG1	2.41	0.64
1:A:139:CYS:N	2:A:177:HOH:O	2.25	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:TRP:HD1	2:A:307:HOH:O	1.81	0.63
1:A:149:VAL:C	2:A:198:HOH:O	2.40	0.63
1:A:126:TRP:CZ3	1:A:136:ARG:CG	2.81	0.63
1:A:91:ARG:O	1:A:92:SER:C	2.39	0.63
1:A:140:SER:O	1:A:141:VAL:CG2	2.46	0.62
1:A:101:ASN:OD1	1:A:103:THR:CA	2.48	0.62
1:A:74:TYR:O	1:A:75:ARG:CD	2.46	0.61
1:A:52:ARG:HA	1:A:58:LEU:HD23	1.81	0.61
1:A:143:VAL:HG11	1:A:146:GLN:CD	2.25	0.61
1:A:39:ASP:HB2	2:A:299:HOH:O	1.97	0.60
1:A:36:SER:O	1:A:37:ALA:HB2	2.01	0.60
1:A:52:ARG:O	1:A:58:LEU:HG	2.01	0.60
1:A:75:ARG:HH12	1:A:109:ASP:N	2.00	0.59
1:A:52:ARG:HA	1:A:58:LEU:CB	2.33	0.59
1:A:97:LYS:HD2	2:A:161:HOH:O	1.94	0.59
1:A:42:TRP:CD1	2:A:307:HOH:O	2.55	0.59
1:A:150:THR:CG2	2:A:199:HOH:O	2.51	0.59
1:A:36:SER:CB	1:A:40:ALA:HB2	2.33	0.59
1:A:152:GLU:OE1	1:A:152:GLU:HA	2.03	0.58
1:A:37:ALA:HB2	2:A:314:HOH:O	2.02	0.58
1:A:54:PRO:N	2:A:195:HOH:O	2.34	0.58
1:A:73:ASN:O	1:A:73:ASN:OD1	2.21	0.58
1:A:129:THR:CG2	1:A:131:SER:HB3	2.34	0.58
1:A:115:CYS:O	1:A:116:ARG:HD3	2.04	0.58
1:A:122:ILE:CG1	2:A:202:HOH:O	2.41	0.57
1:A:112:GLU:OE1	1:A:114:PHE:CZ	2.57	0.57
1:A:149:VAL:CG1	2:A:198:HOH:O	2.14	0.57
1:A:147:ASP:OD1	1:A:148:ARG:O	2.22	0.57
1:A:66:CYS:HB2	1:A:143:VAL:C	2.30	0.57
1:A:37:ALA:C	1:A:40:ALA:HB3	2.29	0.56
1:A:42:TRP:O	1:A:46:THR:N	2.31	0.56
1:A:68:GLU:C	1:A:69:GLY:O	2.48	0.56
1:A:68:GLU:O	1:A:69:GLY:O	2.23	0.56
1:A:126:TRP:HA	2:A:177:HOH:O	2.05	0.56
1:A:111:ARG:C	1:A:112:GLU:HG3	2.31	0.56
1:A:75:ARG:HH11	1:A:109:ASP:CB	2.19	0.56
1:A:97:LYS:O	1:A:135:ARG:NH2	2.36	0.56
1:A:106:PRO:O	1:A:107:GLY:C	2.48	0.56
1:A:93:ARG:NH2	1:A:97:LYS:CG	2.69	0.56
1:A:52:ARG:CA	1:A:58:LEU:HD23	2.37	0.55
1:A:126:TRP:CE3	1:A:136:ARG:CD	2.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:122:ILE:HG22	2:A:317:HOH:O	2.01	0.55
1:A:60:GLU:O	1:A:63:GLU:O	2.24	0.54
1:A:77:ASN:O	1:A:78:VAL:HG12	2.08	0.54
1:A:88:GLN:HG2	1:A:89:LEU:N	2.23	0.54
1:A:99:GLU:OE1	1:A:99:GLU:N	2.35	0.54
1:A:66:CYS:HA	1:A:142:PRO:O	2.08	0.54
1:A:129:THR:HG21	1:A:131:SER:HB3	1.89	0.54
1:A:150:THR:O	1:A:151:VAL:CG1	2.57	0.53
1:A:154:ILE:HG22	1:A:155:PRO:HD2	1.85	0.53
1:A:60:GLU:HA	2:A:281:HOH:O	2.07	0.53
1:A:82:ARG:HA	1:A:153:VAL:HG12	1.89	0.53
1:A:154:ILE:CG2	1:A:155:PRO:CD	2.82	0.53
1:A:36:SER:O	1:A:37:ALA:CB	2.56	0.53
1:A:64:GLY:HA3	1:A:75:ARG:CB	2.33	0.53
1:A:123:THR:CB	1:A:138:GLU:OE1	2.56	0.53
1:A:70:VAL:HB	1:A:121:SER:O	2.10	0.52
1:A:126:TRP:CZ2	1:A:136:ARG:CZ	2.92	0.52
1:A:80:VAL:C	2:A:204:HOH:O	2.52	0.52
1:A:129:THR:HG21	1:A:134:LEU:HB3	1.92	0.52
1:A:138:GLU:HG3	1:A:151:VAL:HG21	1.91	0.52
1:A:104:THR:C	1:A:106:PRO:HD3	2.35	0.52
1:A:93:ARG:HH21	1:A:97:LYS:HB3	1.75	0.51
1:A:141:VAL:CG1	1:A:142:PRO:HD2	2.41	0.51
1:A:68:GLU:N	1:A:73:ASN:OD1	2.43	0.51
1:A:52:ARG:HA	1:A:58:LEU:CG	2.41	0.51
1:A:112:GLU:O	1:A:114:PHE:N	2.44	0.51
1:A:46:THR:O	1:A:49:GLU:OE1	2.29	0.51
1:A:74:TYR:C	1:A:75:ARG:HG2	2.36	0.51
1:A:102:SER:HB2	1:A:110:LEU:HB2	1.93	0.50
1:A:88:GLN:HG2	1:A:89:LEU:O	2.11	0.50
1:A:146:GLN:OE1	1:A:146:GLN:O	2.29	0.50
1:A:73:ASN:HB3	2:A:159:HOH:O	2.10	0.49
1:A:91:ARG:HB3	2:A:165:HOH:O	2.12	0.49
1:A:52:ARG:HB2	1:A:58:LEU:HD23	1.94	0.49
1:A:153:VAL:HG11	2:A:253:HOH:O	2.12	0.49
1:A:47:ALA:HB2	2:A:326:HOH:O	2.13	0.48
1:A:52:ARG:HB2	1:A:58:LEU:CD2	2.43	0.48
1:A:51:ALA:HB1	1:A:57:LYS:O	2.14	0.48
1:A:39:ASP:CG	2:A:299:HOH:O	2.55	0.47
1:A:58:LEU:O	1:A:62:LEU:CD1	2.56	0.47
1:A:126:TRP:CH2	1:A:136:ARG:CD	2.88	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:CYS:C	1:A:141:VAL:HG23	2.39	0.47
1:A:126:TRP:HA	1:A:138:GLU:HA	1.95	0.47
1:A:52:ARG:CB	1:A:58:LEU:HD23	2.45	0.47
1:A:65:ASN:O	1:A:142:PRO:HG2	2.15	0.47
1:A:46:THR:HA	1:A:49:GLU:CD	2.39	0.47
1:A:90:TRP:O	2:A:188:HOH:O	2.21	0.46
1:A:52:ARG:HA	1:A:58:LEU:CD2	2.45	0.46
1:A:70:VAL:O	1:A:70:VAL:CG2	2.64	0.46
1:A:89:LEU:HD12	1:A:92:SER:CB	2.45	0.46
1:A:101:ASN:OD1	1:A:103:THR:N	2.47	0.46
1:A:57:LYS:HA	1:A:57:LYS:HD2	1.51	0.46
1:A:150:THR:C	1:A:151:VAL:HG13	2.41	0.46
1:A:49:GLU:N	2:A:283:HOH:O	2.49	0.46
1:A:129:THR:HB	1:A:134:LEU:O	2.16	0.46
1:A:94:TYR:CD2	1:A:94:TYR:C	2.93	0.45
1:A:104:THR:HB	1:A:105:HIS:CD2	2.42	0.45
1:A:112:GLU:HB3	2:A:300:HOH:O	2.17	0.45
1:A:117:ASN:HB2	1:A:125:PRO:HA	1.98	0.45
1:A:129:THR:HG23	1:A:130:THR:N	2.31	0.45
1:A:74:TYR:CE1	1:A:141:VAL:CG1	2.99	0.45
1:A:74:TYR:C	1:A:75:ARG:HD3	2.39	0.45
1:A:78:VAL:O	1:A:115:CYS:SG	2.75	0.44
1:A:74:TYR:C	1:A:75:ARG:CG	2.89	0.44
1:A:117:ASN:N	1:A:118:PRO:HD3	2.32	0.44
1:A:122:ILE:CD1	2:A:202:HOH:O	2.65	0.44
1:A:70:VAL:O	1:A:70:VAL:HG22	2.18	0.44
1:A:74:TYR:OH	1:A:78:VAL:HG13	2.18	0.44
1:A:85:ILE:HG21	1:A:129:THR:HG23	1.98	0.44
1:A:36:SER:HB3	1:A:40:ALA:N	2.33	0.44
1:A:143:VAL:CG1	1:A:146:GLN:OE1	2.63	0.43
1:A:65:ASN:HD22	1:A:65:ASN:HA	1.61	0.43
1:A:138:GLU:CA	2:A:177:HOH:O	2.59	0.43
1:A:55:ARG:HH11	1:A:55:ARG:HD3	1.50	0.43
1:A:100:ILE:N	1:A:100:ILE:HD12	2.33	0.43
1:A:74:TYR:OH	1:A:76:GLY:HA3	2.19	0.43
1:A:90:TRP:CZ3	1:A:128:TYR:CE2	3.06	0.42
1:A:122:ILE:CA	2:A:202:HOH:O	2.66	0.42
1:A:69:GLY:C	1:A:70:VAL:O	2.54	0.42
1:A:51:ALA:O	1:A:58:LEU:HA	2.19	0.42
1:A:111:ARG:HE	1:A:111:ARG:HB2	1.64	0.42
1:A:57:LYS:HZ1	1:A:144:CYS:HB3	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:TYR:O	1:A:49:GLU:HG3	2.20	0.42
1:A:82:ARG:HG2	1:A:83:SER:N	2.35	0.42
1:A:129:THR:CG2	1:A:130:THR:N	2.82	0.41
1:A:74:TYR:CZ	1:A:141:VAL:CG1	3.04	0.41
1:A:38:THR:O	1:A:42:TRP:CD1	2.73	0.41
1:A:112:GLU:HA	2:A:162:HOH:O	2.20	0.41
1:A:49:GLU:O	1:A:52:ARG:NE	2.47	0.41
1:A:129:THR:CB	2:A:214:HOH:O	2.69	0.41
1:A:87:CYS:O	1:A:113:ASN:ND2	2.53	0.40
1:A:57:LYS:NZ	1:A:144:CYS:HB3	2.37	0.40
1:A:74:TYR:C	1:A:75:ARG:CD	2.95	0.40
1:A:88:GLN:OE1	1:A:92:SER:O	2.40	0.40
1:A:103:THR:O	1:A:104:THR:OG1	2.35	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:138:GLU:OE1	1:A:156:ARG:NH2[3_554]	2.01	0.19

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	119/156 (76%)	92 (77%)	10 (8%)	17 (14%)	0 0

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	37	ALA
1	A	51	ALA
1	A	76	GLY

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Mol	Chain	Res	Type
1	A	102	SER
1	A	104	THR
1	A	112	GLU
1	A	113	ASN
1	A	50	SER
1	A	69	GLY
1	A	107	GLY
1	A	74	TYR
1	A	77	ASN
1	A	120	GLY
1	A	70	VAL
1	A	108	ALA
1	A	53	ASN
1	A	65	ASN

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	105/125 (84%)	79 (75%)	26 (25%)	1 2

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

Mol	Chain	Res	Type
1	A	38	THR
1	A	52	ARG
1	A	55	ARG
1	A	57	LYS
1	A	68	GLU
1	A	70	VAL
1	A	72	MET
1	A	73	ASN
1	A	78	VAL
1	A	86	GLU
1	A	92	SER
1	A	99	GLU

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Mol	Chain	Res	Type
1	A	104	THR
1	A	110	LEU
1	A	112	GLU
1	A	113	ASN
1	A	119	ASP
1	A	121	SER
1	A	127	CYS
1	A	129	THR
1	A	138	GLU
1	A	146	GLN
1	A	147	ASP
1	A	149	VAL
1	A	150	THR
1	A	152	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	65	ASN
1	A	105	HIS
1	A	146	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 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](#)

There are no chain breaks in this entry.

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.