Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 09:36 PM EDT

PDB ID	:	2PF1
Title	:	STRUCTURE OF BOVINE PROTHROMBIN FRAGMENT 1 REFINED AT 2.25 ANGSTROMS RESOLUTION
Authors	:	Seshadri, T.P.; Tulinsky, A.; Skrzypczak-Jankun, E.; Park, C.H.
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 (i) 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 (i)) were used in the production of this report:

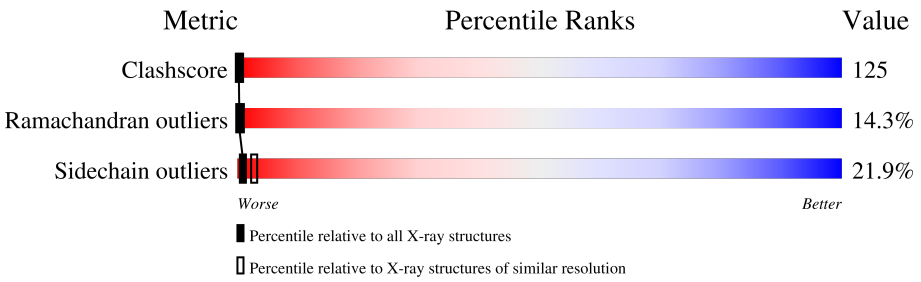
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	156	8% 28% 29% 12% 22%

2 Entry composition (i)

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
			Total	C	N	O	S			
1	A	121	947	576	177	185	9	0	0	0

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
			Total	O		
2	A	164	164	164	0	0

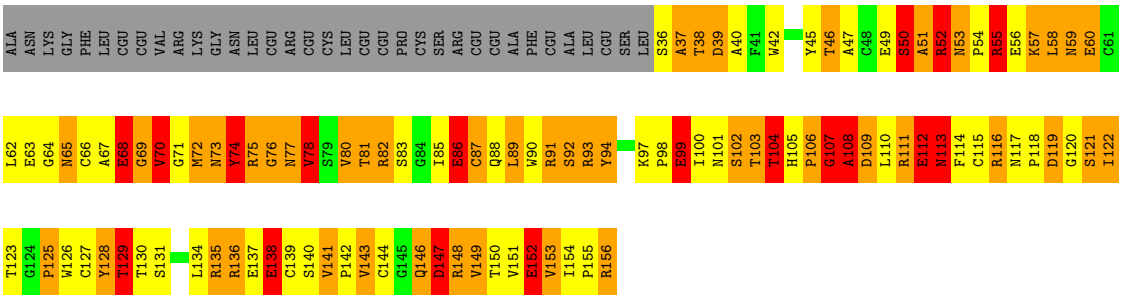
3 Residue-property plots (i)

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: PROTHROMBIN FRAGMENT 1

Chain A: 8% 28% 29% 12% 22%



4 Data and refinement statistics (i)

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 (i)

5.1 Standard geometry (i)

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	1.31	3/969 (0.3%)	2.91	101/1316 (7.7%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	71	GLY	N-CA	6.01	1.55	1.46
1	A	94	TYR	N-CA	5.18	1.56	1.46
1	A	99	GLU	CD-OE2	-5.00	1.20	1.25

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	148	ARG	NE-CZ-NH1	-14.65	112.97	120.30
1	A	148	ARG	NE-CZ-NH2	13.44	127.02	120.30
1	A	136	ARG	CD-NE-CZ	12.76	141.46	123.60
1	A	91	ARG	CD-NE-CZ	12.39	140.94	123.60
1	A	111	ARG	NE-CZ-NH1	-12.36	114.12	120.30
1	A	93	ARG	NE-CZ-NH1	12.27	126.43	120.30
1	A	75	ARG	CD-NE-CZ	11.37	139.51	123.60
1	A	82	ARG	NE-CZ-NH1	-10.94	114.83	120.30
1	A	86	GLU	OE1-CD-OE2	-10.65	110.52	123.30
1	A	72	MET	CB-CA-C	9.41	129.23	110.40
1	A	128	TYR	CB-CG-CD1	9.36	126.61	121.00
1	A	93	ARG	NE-CZ-NH2	-9.33	115.64	120.30
1	A	156	ARG	CD-NE-CZ	9.26	136.56	123.60
1	A	135	ARG	NE-CZ-NH2	9.17	124.88	120.30
1	A	137	GLU	CG-CD-OE2	8.79	135.88	118.30
1	A	116	ARG	NE-CZ-NH2	8.67	124.63	120.30
1	A	86	GLU	CG-CD-OE2	8.63	135.56	118.30
1	A	137	GLU	CA-CB-CG	8.56	132.22	113.40
1	A	82	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	A	129	THR	CA-CB-OG1	-8.54	91.07	109.00
1	A	91	ARG	N-CA-CB	8.50	125.90	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	74	TYR	CB-CG-CD1	-8.49	115.90	121.00
1	A	82	ARG	NH1-CZ-NH2	8.44	128.69	119.40
1	A	75	ARG	NE-CZ-NH1	-8.43	116.09	120.30
1	A	111	ARG	CD-NE-CZ	-8.33	111.94	123.60
1	A	147	ASP	CB-CG-OD1	-8.28	110.84	118.30
1	A	135	ARG	CD-NE-CZ	-8.18	112.14	123.60
1	A	137	GLU	OE1-CD-OE2	-8.17	113.50	123.30
1	A	137	GLU	N-CA-CB	8.10	125.18	110.60
1	A	147	ASP	CB-CG-OD2	7.94	125.44	118.30
1	A	103	THR	N-CA-CB	-7.94	95.22	110.30
1	A	67	ALA	CB-CA-C	-7.65	98.62	110.10
1	A	99	GLU	OE1-CD-OE2	7.55	132.36	123.30
1	A	99	GLU	CG-CD-OE1	-7.54	103.23	118.30
1	A	141	VAL	CB-CA-C	7.45	125.55	111.40
1	A	78	VAL	CB-CA-C	7.38	125.43	111.40
1	A	52	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	52	ARG	CD-NE-CZ	-6.87	113.99	123.60
1	A	152	GLU	O-C-N	6.86	133.68	122.70
1	A	107	GLY	C-N-CA	6.82	138.75	121.70
1	A	99	GLU	N-CA-CB	6.80	122.83	110.60
1	A	50	SER	O-C-N	-6.58	112.18	122.70
1	A	122	ILE	CB-CA-C	6.56	124.73	111.60
1	A	91	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	A	55	ARG	NE-CZ-NH1	-6.49	117.05	120.30
1	A	147	ASP	CA-C-O	6.47	133.68	120.10
1	A	109	ASP	CA-CB-CG	6.43	127.55	113.40
1	A	116	ARG	C-N-CA	6.36	137.59	121.70
1	A	50	SER	CA-C-N	6.32	131.10	117.20
1	A	107	GLY	CA-C-O	6.31	131.95	120.60
1	A	58	LEU	CA-CB-CG	6.15	129.44	115.30
1	A	143	VAL	CA-CB-CG1	6.08	120.01	110.90
1	A	108	ALA	N-CA-CB	-6.06	101.62	110.10
1	A	94	TYR	CB-CG-CD2	6.06	124.64	121.00
1	A	56	GLU	OE1-CD-OE2	-6.02	116.08	123.30
1	A	147	ASP	CA-CB-CG	-5.97	100.26	113.40
1	A	39	ASP	N-CA-CB	5.95	121.30	110.60
1	A	111	ARG	CG-CD-NE	-5.90	99.41	111.80
1	A	128	TYR	N-CA-CB	5.90	121.22	110.60
1	A	141	VAL	CA-CB-CG1	5.89	119.73	110.90
1	A	59	ASN	CA-CB-CG	5.88	126.34	113.40
1	A	68	GLU	CG-CD-OE2	-5.88	106.54	118.30
1	A	149	VAL	CB-CA-C	5.87	122.55	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	129	THR	O-C-N	5.86	132.08	122.70
1	A	119	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	119	ASP	CA-C-N	5.75	127.70	116.20
1	A	119	ASP	CA-C-O	-5.75	108.03	120.10
1	A	67	ALA	O-C-N	5.74	131.89	122.70
1	A	129	THR	OG1-CB-CG2	5.72	123.17	110.00
1	A	125	PRO	C-N-CA	5.66	135.85	121.70
1	A	99	GLU	CB-CA-C	-5.64	99.12	110.40
1	A	87	CYS	O-C-N	5.63	131.71	122.70
1	A	60	GLU	C-N-CA	5.60	135.71	121.70
1	A	104	THR	CB-CA-C	-5.59	96.51	111.60
1	A	89	LEU	CA-CB-CG	5.58	128.12	115.30
1	A	106	PRO	N-CA-C	-5.53	97.72	112.10
1	A	141	VAL	N-CA-CB	-5.53	99.34	111.50
1	A	55	ARG	CD-NE-CZ	-5.51	115.88	123.60
1	A	136	ARG	NE-CZ-NH2	-5.51	117.54	120.30
1	A	70	VAL	CA-C-O	-5.50	108.55	120.10
1	A	81	THR	CA-CB-OG1	-5.48	97.50	109.00
1	A	56	GLU	CB-CG-CD	5.45	128.91	114.20
1	A	113	ASN	N-CA-C	5.38	125.52	111.00
1	A	56	GLU	CG-CD-OE2	5.36	129.02	118.30
1	A	113	ASN	CA-CB-CG	5.32	125.11	113.40
1	A	80	VAL	CB-CA-C	-5.24	101.44	111.40
1	A	147	ASP	CB-CA-C	5.23	120.87	110.40
1	A	122	ILE	CA-CB-CG2	5.22	121.34	110.90
1	A	46	THR	C-N-CA	5.21	134.71	121.70
1	A	156	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	A	75	ARG	C-N-CA	5.18	133.17	122.30
1	A	111	ARG	O-C-N	5.14	130.93	122.70
1	A	74	TYR	CA-CB-CG	-5.13	103.65	113.40
1	A	50	SER	CA-CB-OG	5.10	124.98	111.20
1	A	149	VAL	O-C-N	5.08	130.83	122.70
1	A	94	TYR	CA-CB-CG	-5.08	103.75	113.40
1	A	75	ARG	NH1-CZ-NH2	5.05	124.95	119.40
1	A	138	GLU	C-N-CA	5.01	134.24	121.70
1	A	147	ASP	CA-C-N	-5.01	106.18	117.20
1	A	153	VAL	O-C-N	5.01	130.72	122.70
1	A	68	GLU	CA-CB-CG	5.00	124.40	113.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	230	1
2	A	164	0	0	62	0
All	All	1111	0	890	230	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 125.

All (230) 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	0.97
1:A:37:ALA:H	1:A:40:ALA:HB2	1.29	0.96
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:74:TYR:O	1:A:75:ARG:HD3	1.75	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: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:58:LEU:O	1:A:62:LEU:HD12	1.77	0.83
1:A:101:ASN:C	1:A:103:THR:H	1.76	0.83
1:A:140:SER:C	1:A:141:VAL:HG23	1.99	0.82
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:73:ASN:CG	1:A:73:ASN:O	2.20	0.80
1:A:89:LEU:HD12	1:A:92:SER:OG	1.82	0.80
1:A:140:SER:C	1:A:141:VAL:CG2	2.51	0.79
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: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: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
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:C	2:A:195:HOH:O	2.24	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:155:PRO:O	1:A:156:ARG:C	2.26	0.74
1:A:52:ARG:HA	1:A:58:LEU:HB2	1.68	0.74
1:A:63:GLU:CD	2:A:281:HOH:O	2.27	0.73
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LYS:O	2:A:172:HOH:O	2.08	0.72
1:A:111:ARG:O	1:A:112:GLU:C	2.28	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:139:CYS:N	2:A:177:HOH:O	2.25	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: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: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:42:TRP:HD1	2:A:307:HOH:O	1.81	0.63
1:A:126:TRP:CZ3	1:A:136:ARG:CG	2.81	0.63
1:A:69:GLY:O	1:A:70:VAL:C	2.37	0.62
1:A:101:ASN:C	1:A:103:THR:N	2.52	0.62
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:36:SER:O	1:A:37:ALA:HB2	2.01	0.61
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:111:ARG:C	1:A:112:GLU:O	2.39	0.61
1:A:39:ASP:HB2	2:A:299:HOH:O	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:91:ARG:O	1:A:92:SER:C	2.39	0.58
1:A:129:THR:CG2	1:A:131:SER:HB3	2.34	0.58
1:A:103:THR:C	1:A:104:THR:OG1	2.41	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:42:TRP:O	1:A:46:THR:N	2.31	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:143:VAL:HG11	1:A:146:GLN:CD	2.25	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: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
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:149:VAL:C	2:A:198:HOH:O	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:VAL:HB	1:A:121:SER:O	2.10	0.52
1:A:66:CYS:HB2	1:A:143:VAL:C	2.30	0.52
1:A:126:TRP:CZ2	1:A:136:ARG:CZ	2.92	0.52
1:A:37:ALA:C	1:A:40:ALA:HB3	2.29	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:68:GLU:C	1:A:69:GLY:O	2.48	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:111:ARG:C	1:A:112:GLU:HG3	2.31	0.51
1:A:68:GLU:N	1:A:73:ASN:OD1	2.43	0.51
1:A:106:PRO:O	1:A:107:GLY:C	2.48	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: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:42:TRP:CD1	2:A:307:HOH:O	2.55	0.49
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: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
1:A:126:TRP:HA	1:A:138:GLU:HA	1.95	0.47
1:A:80:VAL:C	2:A:204:HOH:O	2.52	0.47
1:A:104:THR:C	1:A:106:PRO:HD3	2.35	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: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:49:GLU:N	2:A:283:HOH:O	2.49	0.46
1:A:74:TYR:C	1:A:75:ARG:HG2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:129:THR:HB	1:A:134:LEU:O	2.16	0.46
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:78:VAL:O	1:A:115:CYS:SG	2.75	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:139:CYS:C	1:A:141:VAL:HG23	2.39	0.42
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:46:THR:HA	1:A:49:GLU:CD	2.39	0.42
1:A:57:LYS:HZ1	1:A:144:CYS:HB3	1.85	0.42
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:150:THR:C	1:A:151:VAL:HG13	2.41	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:94:TYR:CD2	1:A:94:TYR:C	2.93	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: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 (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	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
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 (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	105/125 (84%)	82 (78%)	23 (22%)	1 3

All (23) 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
1	A	104	THR
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	152	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	65	ASN

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Mol	Chain	Res	Type
1	A	105	HIS

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)

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 (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains (i)

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.