



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:19 PM UTC

PDB ID : 1YCP / pdb_00001ycp
Title : THE CRYSTAL STRUCTURE OF FIBRINOGEN-AA PEPTIDE 1-23 (F8Y) BOUND TO BOVINE THROMBIN EXPLAINS WHY THE MUTATION OF PHE-8 TO TYROSINE STRONGLY INHIBITS NORMAL CLEAVAGE AT ARGININE-16
Authors : Malkowski, M.G.; Edwards, B.F.P.
Deposited on : 1997-05-01
Resolution : 2.50 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

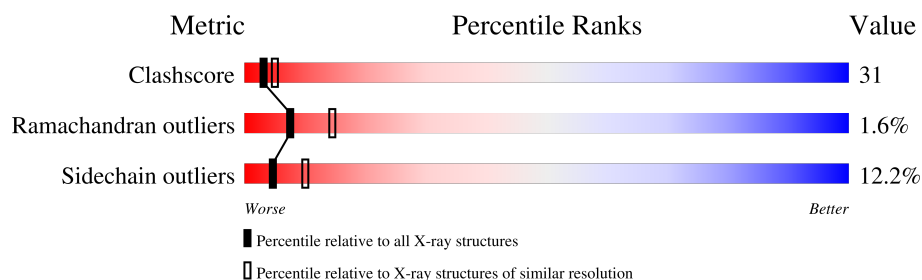
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)

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	J	49	27% 29% • 41%
1	L	49	35% 24% 41%
2	H	259	38% 44% 12% • 5%
3	F	23	17% 9% 74%
3	N	23	• 22% 74%
4	K	150	39% 48% 10% • •
5	M	109	42% 41% 9% 7%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4846 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 EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	29	Total	C	N	O	S	0	0	0
			238	150	38	49	1			
1	J	29	Total	C	N	O	S	0	0	0
			238	150	38	49	1			

- Molecule 2 is a protein called ALPHA THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	247	Total	C	N	O	S	0	0	0
			2002	1281	360	349	12			

- Molecule 3 is a protein called FIBRINOPEPTIDE A-ALPHA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	6	Total	C	N	O	0	0	0
			45	29	9	7			
3	N	6	Total	C	N	O	0	0	0
			45	29	9	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	308	TYR	PHE	engineered mutation	UNP P02671
N	308	TYR	PHE	engineered mutation	UNP P02671

- Molecule 4 is a protein called EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	146	Total	C	N	O	S	0	0	0
			1199	770	217	207	5			

- Molecule 5 is a protein called EPSILON THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	M	101	Total 803	C 511	N 143	O 142	S 7	0	0	0

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	L	27	Total 27	O 27	0	0
6	H	148	Total 148	O 148	0	0
6	F	6	Total 6	O 6	0	0
6	J	11	Total 11	O 11	0	0
6	K	61	Total 61	O 61	0	0
6	M	23	Total 23	O 23	0	0

3 Residue-property plots

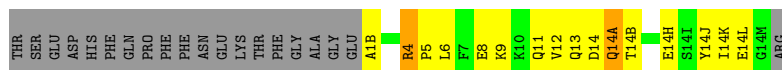
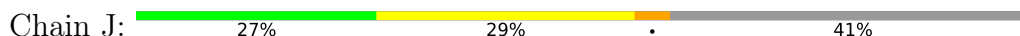
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

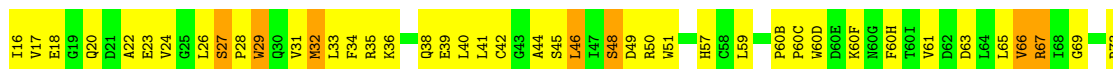
- Molecule 1: EPSILON THROMBIN



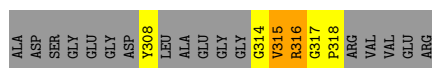
- Molecule 1: EPSILON THROMBIN



- Molecule 2: ALPHA THROMBIN



● Molecule 3: FIBRINOPEPTIDE A-ALPHA



• Molecule 3: FIBRINOPEPTIDE A-ALPHA

Chain N:  22% 74%

ALA	ASP	SER	GLY	GLY	ASP	Y308	LEU	ALA	GLY	GLY	G314	V315	R316	G317	P318	ARG	VAL	VAL	GLU	ARG
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• Molecule 4: EPSILON THROMBIN

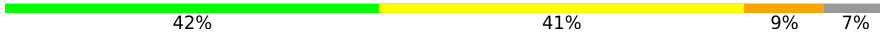
Chain K:  39% 48% 10%

I16	V17	E18	G19	Q20	E23	V24	G25	L26	S27	P28	W29	M32	L33	F34	R35	K36	Q38	E39	L40	L41	S45	L46	I47	S48	D49	R50	W51	A55	A56	H57	C58	L59	L60	Y60A	P60B	P60C	W60D	D60E	K60F	D62	D63	L64	L65	V66	R67	I68	G69	K70	H71	T74	R75	Y76
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E77	R77A	E80	K81	I82	S83	R84	L85	D86	K87	I88	Y89	I90	H91	P92	R93	K97	E97A	R101	D102	I103	A104	L105	L106	K107	L108	K109	R110	P111	I112	E113	L114	S115	D116	L123	F124	D125	K126	Q127	K129B	L129C	L130	H131	F134	K135	T139	N143	R144	R145	E146	THR	TRP
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THR	THR
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• Molecule 5: EPSILON THROMBIN

Chain M:  42% 41% 9% 7%

SER	VAL	ALA	GLU	V150	Q151	P152	S153	V154	V157	G226	V158	N159	L160	P161	E164	R165	P166	V167	C168	K169	A170	S171	D178	M179	M180	F181	C182	P186	G186A	E186B	G186C	K186D	R187	G188	D189	A190	C191	E192	G193	D194	S195	F199	V200	N201	K202	S203	P204	Y204A	N204B	N205	R206	W207	Y208	Q209
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V213	S214	W215	G216	D221	R221A	D222	Y225	G226	F227	Y228	R233	K236	W237	I238	Q239	K240	V241	I242	D243	ARG	LEU	GLY	SER
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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	88.27Å 88.27Å 195.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.50	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.50)	Depositor
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.183 , 0.245	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4846	wwPDB-VP
Average B, all atoms (Å ²)	20.0	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	J	0.51	0/241	1.02	1/321 (0.3%)
1	L	0.68	0/241	1.04	0/321
2	H	0.69	1/2053 (0.0%)	1.26	24/2774 (0.9%)
3	F	0.62	0/45	1.16	0/58
3	N	0.62	0/45	0.76	0/58
4	K	0.63	0/1229	1.25	14/1663 (0.8%)
5	M	0.73	0/824	1.24	6/1111 (0.5%)
All	All	0.67	1/4678 (0.0%)	1.23	45/6306 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	213	VAL	CA-CB	-5.11	1.48	1.54

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	75	ARG	N-CA-C	10.10	124.88	109.23
4	K	20	GLN	N-CA-C	8.47	120.83	110.41
5	M	199	PHE	N-CA-C	-8.29	93.27	108.02
4	K	60(B)	PRO	N-CA-C	8.18	120.67	110.70
2	H	194	ASP	N-CA-C	-7.75	103.80	113.18
4	K	51	TRP	N-CA-C	7.34	121.81	109.76
2	H	204(B)	ASN	N-CA-C	-6.97	98.99	109.94
4	K	86	ASP	N-CA-C	-6.97	103.66	112.93
2	H	27	SER	CA-C-N	6.93	126.74	119.05
2	H	27	SER	C-N-CA	6.93	126.74	119.05
2	H	36	LYS	N-CA-C	6.87	119.40	111.02
4	K	84	MET	N-CA-C	-6.84	99.54	110.14
5	M	221	ASP	N-CA-C	6.74	120.71	111.54
4	K	143	ASN	N-CA-C	6.73	119.99	110.23
2	H	206	ARG	N-CA-C	6.67	120.35	110.48
2	H	60(B)	PRO	N-CA-C	6.57	118.71	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	186(D)	LYS	N-CA-C	-6.57	97.52	108.75
2	H	203	SER	CA-C-N	6.53	125.97	118.85
2	H	203	SER	C-N-CA	6.53	125.97	118.85
4	K	97	LYS	N-CA-C	6.53	119.22	111.71
2	H	110	ARG	CA-C-N	6.47	127.92	119.84
2	H	110	ARG	C-N-CA	6.47	127.92	119.84
4	K	65	LEU	N-CA-C	-6.33	99.60	109.72
4	K	97(A)	GLU	N-CA-C	6.04	121.21	113.18
2	H	137	ARG	N-CA-C	6.03	119.03	109.50
2	H	190	ALA	N-CA-C	-5.97	101.63	110.46
5	M	194	ASP	N-CA-C	-5.89	106.14	113.38
2	H	133	GLY	N-CA-C	-5.67	106.87	114.25
2	H	199	PHE	N-CA-C	-5.67	98.10	108.02
2	H	44	ALA	N-CA-C	-5.62	99.96	107.88
2	H	136	GLY	N-CA-C	-5.57	103.51	111.42
2	H	98	ASN	N-CA-C	5.45	120.62	112.94
2	H	153	SER	N-CA-C	-5.34	106.61	113.23
2	H	86	ASP	N-CA-C	-5.32	105.86	112.93
2	H	143	ASN	N-CA-C	5.28	117.73	110.35
4	K	60	LEU	N-CA-C	5.24	116.86	107.80
4	K	123	LEU	N-CA-C	-5.20	103.51	110.07
4	K	80	GLU	N-CA-C	5.15	117.94	109.76
1	J	14(A)	GLN	N-CA-C	5.12	121.72	110.80
2	H	61	VAL	CB-CA-C	-5.11	104.25	112.16
5	M	179	ASN	N-CA-C	-5.05	106.97	112.72
2	H	65	LEU	N-CA-C	-5.04	101.45	108.96
5	M	151	GLN	CA-C-N	5.04	125.44	119.99
5	M	151	GLN	C-N-CA	5.04	125.44	119.99
4	K	116	ASP	N-CA-C	-5.03	106.41	112.54

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	J	238	0	230	15	0
1	L	238	0	230	21	0
2	H	2002	0	2008	141	3
3	F	45	0	42	14	0
3	N	45	0	42	7	1
4	K	1199	0	1221	79	1
5	M	803	0	787	49	1
6	F	6	0	0	2	0
6	H	148	0	0	18	0
6	J	11	0	0	2	0
6	K	61	0	0	9	0
6	L	27	0	0	1	0
6	M	23	0	0	2	0
All	All	4846	0	4560	284	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 31.

All (284) 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)
2:H:192:GLU:HB3	3:F:318:PRO:HA	1.46	0.97
4:K:66:VAL:HG21	4:K:85:LEU:HD21	1.51	0.93
2:H:76:TYR:HB3	6:H:575:HOH:O	1.69	0.93
5:M:213:VAL:HG22	5:M:228:TYR:HE1	1.34	0.91
4:K:86:ASP:HB3	4:K:107:LYS:HG2	1.60	0.83
2:H:67:ARG:HH12	2:H:76:TYR:HB2	1.46	0.81
3:F:308:TYR:HH	3:F:314:GLY:N	1.79	0.80
4:K:65:LEU:HD23	4:K:84:MET:SD	2.23	0.79
2:H:235:LYS:O	2:H:239:GLN:HG2	1.83	0.78
2:H:213:VAL:HG22	2:H:228:TYR:CE2	2.20	0.76
2:H:137:ARG:HD3	2:H:157:VAL:HG12	1.67	0.76
2:H:173:ARG:HH11	2:H:173:ARG:HB2	1.51	0.76
2:H:187:ARG:HD3	2:H:221:ASP:OD2	1.85	0.75
2:H:32:MET:HE2	2:H:141:TRP:CZ3	2.22	0.75
2:H:213:VAL:HG22	2:H:228:TYR:HE2	1.51	0.75
4:K:35:ARG:O	4:K:38:GLN:HA	1.88	0.72
2:H:34:PHE:CE2	2:H:38:GLN:HB3	2.24	0.72
2:H:26:LEU:HD21	2:H:137:ARG:HH11	1.55	0.71
2:H:57:HIS:CD2	3:F:315:VAL:HG13	2.25	0.71
4:K:32:MET:HE2	4:K:40:LEU:CD1	2.20	0.71
1:L:3:LEU:HB2	1:L:9:LYS:HE3	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:135:LYS:O	5:M:201:MET:HE3	1.90	0.71
2:H:26:LEU:HD21	2:H:137:ARG:NH1	2.06	0.70
2:H:122:CYS:SG	2:H:206:ARG:HD3	2.32	0.69
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.00	0.69
1:L:1(B):ALA:HB1	2:H:206:ARG:NH2	2.07	0.68
5:M:213:VAL:HG22	5:M:228:TYR:CE1	2.22	0.68
2:H:35:ARG:HG2	2:H:39:GLU:HB3	1.74	0.68
5:M:204(B):ASN:O	5:M:206:ARG:N	2.26	0.67
4:K:89:TYR:HB2	4:K:105:LEU:HB2	1.74	0.67
2:H:67:ARG:NH1	2:H:76:TYR:HD2	1.91	0.67
1:J:14(K):ILE:HG13	1:J:14(L):GLU:N	2.08	0.67
2:H:213:VAL:HG21	6:H:549:HOH:O	1.96	0.66
4:K:75:ARG:HG2	4:K:76:TYR:N	2.09	0.66
4:K:70:LYS:NZ	4:K:70:LYS:HB3	2.10	0.66
5:M:190:ALA:O	5:M:191:CYS:HB2	1.96	0.66
4:K:113:GLU:HB3	6:K:607:HOH:O	1.95	0.65
5:M:165:ARG:HD3	6:M:611:HOH:O	1.96	0.65
2:H:73:ARG:HD3	2:H:141:TRP:HB3	1.78	0.65
4:K:125:ASP:OD1	4:K:127:GLN:HG3	1.97	0.65
1:J:6:LEU:HD12	4:K:25:GLY:HA3	1.79	0.64
1:L:14(K):ILE:HG13	1:L:14(K):ILE:O	1.96	0.64
2:H:197:GLY:HA3	6:H:401:HOH:O	1.98	0.64
5:M:195:SER:HB2	3:N:316:ARG:O	1.97	0.64
4:K:67:ARG:HD2	4:K:80:GLU:OE2	1.97	0.64
2:H:124:PRO:HB3	2:H:210:MET:HE1	1.79	0.64
2:H:137:ARG:HD3	2:H:157:VAL:CG1	2.27	0.63
3:N:308:TYR:CE1	3:N:314:GLY:HA2	2.33	0.63
2:H:105:LEU:HD13	2:H:241:VAL:CG2	2.28	0.63
2:H:86:ASP:HB3	2:H:107:LYS:HG2	1.81	0.63
4:K:17:VAL:O	5:M:188:GLY:HA2	1.98	0.62
4:K:36:LYS:HB2	6:K:532:HOH:O	1.98	0.62
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.34	0.62
2:H:105:LEU:HD13	2:H:241:VAL:HG21	1.82	0.62
2:H:192:GLU:HG2	6:F:481:HOH:O	1.98	0.62
4:K:50:ARG:CZ	4:K:111:PRO:HB3	2.30	0.62
2:H:173:ARG:HD3	6:H:433:HOH:O	2.00	0.62
2:H:23:GLU:O	2:H:26:LEU:HB2	2.00	0.61
2:H:139:THR:HG22	2:H:157:VAL:HG13	1.81	0.61
2:H:165:ARG:O	2:H:169:LYS:HG3	2.00	0.61
1:L:14(D):LYS:HG2	6:L:641:HOH:O	2.01	0.61
2:H:60(F):LYS:HE2	2:H:60(H):PHE:HE2	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:110:ARG:HG2	6:K:454:HOH:O	2.01	0.60
2:H:145:ARG:HG2	2:H:146:GLU:N	2.15	0.60
4:K:68:ILE:HD13	4:K:112:ILE:HD12	1.82	0.60
5:M:216:GLY:O	3:N:314:GLY:N	2.34	0.60
2:H:172:THR:HG21	2:H:176:ILE:HD11	1.84	0.59
2:H:46:LEU:HD13	2:H:48:SER:O	2.01	0.59
6:K:442:HOH:O	3:N:315:VAL:HG11	2.02	0.59
5:M:204(B):ASN:O	5:M:204(B):ASN:ND2	2.35	0.59
2:H:145:ARG:NE	6:H:414:HOH:O	2.36	0.58
2:H:137:ARG:HB2	2:H:159:ASN:OD1	2.04	0.58
2:H:119:HIS:HB3	6:H:616:HOH:O	2.04	0.58
1:J:1(B):ALA:HA	6:J:590:HOH:O	2.03	0.58
1:J:11:GLN:HB2	6:J:573:HOH:O	2.04	0.57
4:K:35:ARG:HD2	4:K:41:LEU:HD21	1.87	0.57
2:H:131:HIS:O	2:H:134:PHE:HB2	2.04	0.57
4:K:66:VAL:CG2	4:K:85:LEU:HD21	2.30	0.57
4:K:47:ILE:HD11	5:M:242:ILE:HD11	1.87	0.57
4:K:70:LYS:HB3	4:K:70:LYS:HZ2	1.69	0.56
2:H:34:PHE:CZ	2:H:38:GLN:HB3	2.39	0.56
4:K:84:MET:HB2	4:K:109:LYS:HD3	1.87	0.56
4:K:70:LYS:HG2	4:K:80:GLU:HG3	1.88	0.56
1:L:3:LEU:HD13	1:L:8:GLU:HG2	1.88	0.56
2:H:69:GLY:HA2	6:H:406:HOH:O	2.06	0.55
2:H:97(A):GLU:O	3:F:308:TYR:HA	2.05	0.55
2:H:99:LEU:HD11	3:F:315:VAL:HG22	1.88	0.55
4:K:60(D):TRP:O	4:K:60(E):ASP:HB2	2.06	0.55
4:K:55:ALA:O	4:K:58:CYS:HB2	2.07	0.55
2:H:41:LEU:O	3:F:318:PRO:HD3	2.07	0.55
2:H:28:PRO:HG2	6:H:616:HOH:O	2.07	0.54
2:H:78:LYS:HB3	6:H:569:HOH:O	2.08	0.54
2:H:163:VAL:HG13	2:H:185:LYS:HE2	1.90	0.54
4:K:51:TRP:HH2	4:K:89:TYR:CE1	2.25	0.54
4:K:103:ILE:HD11	5:M:238:ILE:HD11	1.89	0.54
4:K:18:GLU:HG3	5:M:187:ARG:HB2	1.89	0.53
2:H:177:THR:H	2:H:180:MET:HE3	1.72	0.53
4:K:32:MET:SD	4:K:34:PHE:HD1	2.32	0.53
2:H:16:ILE:HD11	2:H:138:VAL:HG12	1.91	0.53
1:J:14(B):THR:HB	5:M:159:ASN:HD21	1.73	0.53
4:K:85:LEU:HD22	4:K:106:LEU:HB3	1.91	0.53
1:L:3:LEU:CD2	2:H:206:ARG:HH11	2.21	0.53
2:H:17:VAL:O	2:H:188:GLY:HA2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(B):ALA:HB1	2:H:206:ARG:HH22	1.73	0.52
2:H:22:ALA:HB1	2:H:26:LEU:HD13	1.92	0.52
2:H:135:LYS:HA	2:H:161:PRO:HA	1.92	0.52
2:H:51:TRP:NE1	2:H:242:ILE:HG23	2.24	0.52
2:H:145:ARG:CB	2:H:145:ARG:HH11	2.23	0.51
4:K:105:LEU:HD12	5:M:241:VAL:HG23	1.92	0.51
1:J:14(J):TYR:CE2	5:M:204:PRO:HG3	2.45	0.51
2:H:130:LEU:HD21	2:H:210:MET:HG3	1.92	0.51
5:M:236:LYS:H	5:M:236:LYS:HD2	1.74	0.51
1:L:3:LEU:CD2	2:H:206:ARG:NH1	2.74	0.51
5:M:237:TRP:O	5:M:241:VAL:HG22	2.11	0.51
4:K:127:GLN:HB2	4:K:129(B):LYS:NZ	2.25	0.51
2:H:75:ARG:O	2:H:75:ARG:HG2	2.09	0.51
2:H:78:LYS:O	2:H:78:LYS:HG3	2.11	0.51
2:H:195:SER:HB2	3:F:316:ARG:O	2.11	0.51
3:F:316:ARG:HA	6:F:482:HOH:O	2.10	0.51
4:K:88:ILE:HG22	4:K:90:ILE:HD12	1.92	0.51
5:M:237:TRP:O	5:M:240:LYS:HG2	2.11	0.51
2:H:76:TYR:CE1	2:H:77(A):ARG:HA	2.46	0.51
5:M:180:MET:HG2	5:M:227:PHE:HD2	1.76	0.51
5:M:204(B):ASN:ND2	5:M:206:ARG:HB2	2.26	0.51
4:K:26:LEU:HD23	4:K:27:SER:HB2	1.93	0.50
4:K:84:MET:H	4:K:109:LYS:HE2	1.75	0.50
4:K:48:SER:OG	4:K:49:ASP:N	2.45	0.50
4:K:57:HIS:O	4:K:60(F):LYS:HE2	2.11	0.50
2:H:50:ARG:HG2	2:H:111:PRO:HG3	1.93	0.50
2:H:176:ILE:HG21	6:H:531:HOH:O	2.10	0.50
4:K:29:TRP:O	4:K:45:SER:HA	2.12	0.50
5:M:215:TRP:HB2	3:N:314:GLY:N	2.27	0.50
4:K:50:ARG:O	4:K:108:LEU:HG	2.11	0.50
2:H:39:GLU:HG3	6:H:558:HOH:O	2.12	0.50
4:K:129(C):LEU:O	4:K:134:PHE:HD2	1.95	0.50
2:H:119:HIS:CB	6:H:616:HOH:O	2.59	0.49
2:H:173:ARG:HH11	2:H:173:ARG:CB	2.24	0.49
2:H:232:PHE:O	2:H:235:LYS:HB3	2.12	0.49
2:H:17:VAL:HG11	2:H:221:ASP:CB	2.42	0.49
4:K:57:HIS:CD2	3:N:315:VAL:HG13	2.46	0.49
1:L:3:LEU:HD22	1:L:3:LEU:N	2.28	0.49
1:L:4:ARG:HD3	1:L:8:GLU:OE1	2.13	0.49
1:J:14:ASP:HB2	4:K:23:GLU:OE2	2.11	0.49
4:K:129(B):LYS:O	4:K:131:HIS:CD2	2.65	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:32:MET:HE2	2:H:141:TRP:CH2	2.47	0.49
4:K:84:MET:O	4:K:109:LYS:HG2	2.13	0.49
4:K:105:LEU:CD1	5:M:241:VAL:HG23	2.42	0.49
1:L:3:LEU:CD1	1:L:8:GLU:HG2	2.42	0.49
2:H:35:ARG:CG	2:H:39:GLU:HB3	2.43	0.49
2:H:165:ARG:NH2	2:H:177:THR:O	2.44	0.49
2:H:94:TYR:CZ	2:H:96:TRP:HB3	2.47	0.49
2:H:101:ARG:HG2	2:H:234:LEU:HD21	1.95	0.49
4:K:46:LEU:HD22	4:K:48:SER:O	2.12	0.49
5:M:164:GLU:H	5:M:164:GLU:CD	2.21	0.49
2:H:41:LEU:O	2:H:42:CYS:SG	2.71	0.48
2:H:97(A):GLU:HG2	6:H:509:HOH:O	2.12	0.48
1:J:4:ARG:HD3	1:J:8:GLU:OE1	2.13	0.48
1:L:10:LYS:O	1:L:11:GLN:HB3	2.13	0.48
2:H:29:TRP:O	2:H:45:SER:HA	2.13	0.48
4:K:60(A):TYR:CE2	4:K:60(C):PRO:HB2	2.49	0.48
5:M:187:ARG:NH1	5:M:221:ASP:O	2.47	0.48
2:H:50:ARG:CG	2:H:111:PRO:HG3	2.44	0.48
2:H:211:GLY:HA2	2:H:229:THR:O	2.13	0.48
2:H:46:LEU:O	2:H:120:PRO:HA	2.14	0.48
2:H:98:ASN:OD1	2:H:100:ASP:HB2	2.14	0.48
2:H:240:LYS:HE2	6:H:547:HOH:O	2.14	0.48
4:K:90:ILE:HG22	4:K:91:HIS:N	2.29	0.48
2:H:49:ASP:HB2	2:H:112:ILE:HG22	1.96	0.47
4:K:135:LYS:HE2	5:M:161:PRO:HG3	1.97	0.47
4:K:38:GLN:HG3	6:K:440:HOH:O	2.14	0.47
5:M:182:CYS:HA	5:M:226:GLY:O	2.14	0.47
2:H:73:ARG:HB2	2:H:141:TRP:CD1	2.50	0.47
2:H:138:VAL:HG13	6:H:549:HOH:O	2.14	0.47
2:H:150:VAL:N	6:H:438:HOH:O	2.48	0.47
4:K:41:LEU:HD11	4:K:64:LEU:CD2	2.45	0.47
5:M:236:LYS:HZ2	5:M:236:LYS:HB3	1.79	0.47
2:H:216:GLY:HA3	3:F:316:ARG:NH2	2.30	0.47
5:M:238:ILE:O	5:M:242:ILE:HB	2.15	0.47
4:K:51:TRP:CH2	4:K:89:TYR:CE1	3.03	0.47
4:K:81:LYS:HG2	6:K:562:HOH:O	2.15	0.47
1:J:12:VAL:HG12	1:J:13:GLN:N	2.31	0.46
4:K:38:GLN:O	4:K:39:GLU:HB2	2.14	0.46
4:K:32:MET:HE2	4:K:40:LEU:HD12	1.97	0.46
1:L:14(L):GLU:HA	1:L:14(L):GLU:OE1	2.14	0.46
2:H:105:LEU:HD11	2:H:238:ILE:HG23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:139:THR:HA	2:H:156:GLN:O	2.16	0.46
4:K:68:ILE:HG22	4:K:69:GLY:N	2.31	0.46
2:H:94:TYR:HE1	2:H:99:LEU:HD22	1.80	0.45
4:K:71:HIS:O	5:M:154:VAL:HB	2.15	0.45
5:M:157:VAL:HG12	5:M:158:VAL:N	2.31	0.45
2:H:76:TYR:CE2	2:H:82:ILE:HD11	2.51	0.45
2:H:188:GLY:O	2:H:189:ASP:HB2	2.16	0.45
2:H:31:VAL:HG12	2:H:32:MET:N	2.32	0.45
4:K:32:MET:HE2	4:K:40:LEU:HD11	1.99	0.45
4:K:81:LYS:HE2	4:K:82:ILE:H	1.82	0.45
1:L:3:LEU:HD23	2:H:206:ARG:NH1	2.32	0.45
1:J:9:LYS:C	1:J:11:GLN:H	2.25	0.45
4:K:146:GLU:OE2	5:M:221(A):ARG:NH1	2.50	0.45
5:M:192:GLU:HG3	3:N:317:GLY:O	2.16	0.45
1:L:3:LEU:CD2	2:H:206:ARG:HG2	2.47	0.45
4:K:90:ILE:CG2	4:K:91:HIS:N	2.80	0.45
4:K:76:TYR:HA	4:K:80:GLU:OE1	2.17	0.45
1:J:4:ARG:HA	1:J:5:PRO:HD2	1.85	0.44
2:H:32:MET:HE2	2:H:32:MET:HB2	1.78	0.44
4:K:115:SER:OG	4:K:116:ASP:N	2.50	0.44
4:K:93:ARG:O	4:K:101:ARG:HD2	2.18	0.44
5:M:187:ARG:HD3	5:M:221:ASP:OD2	2.17	0.44
2:H:110:ARG:HH11	2:H:110:ARG:HB3	1.83	0.44
2:H:136:GLY:HA3	2:H:199:PHE:CE1	2.52	0.44
4:K:101:ARG:NE	6:K:474:HOH:O	2.50	0.44
2:H:60(C):PRO:O	2:H:60(D):TRP:HD1	2.00	0.44
4:K:18:GLU:HG3	5:M:187:ARG:CB	2.48	0.44
1:J:6:LEU:HG	6:K:518:HOH:O	2.17	0.44
5:M:203:SER:HB2	5:M:208:TYR:CE2	2.52	0.44
2:H:16:ILE:CD1	2:H:138:VAL:HG12	2.46	0.44
2:H:204(B):ASN:ND2	2:H:206:ARG:H	2.15	0.44
2:H:49:ASP:HA	2:H:112:ILE:HG22	1.99	0.44
2:H:112:ILE:HG23	2:H:114:LEU:HD12	2.00	0.44
1:J:14(K):ILE:HG13	1:J:14(L):GLU:H	1.81	0.44
3:F:308:TYR:OH	3:F:314:GLY:N	2.45	0.44
2:H:42:CYS:HB3	2:H:195:SER:O	2.18	0.43
1:L:6:LEU:HD12	6:H:462:HOH:O	2.18	0.43
2:H:60(F):LYS:HE3	6:H:473:HOH:O	2.18	0.43
2:H:84:MET:CE	2:H:109:LYS:HE3	2.47	0.43
3:F:315:VAL:C	3:F:317:GLY:H	2.27	0.43
5:M:187:ARG:HB3	5:M:221:ASP:OD2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:ARG:CD	2:H:39:GLU:HB3	2.48	0.43
4:K:32:MET:SD	4:K:34:PHE:CD1	3.10	0.43
1:L:4:ARG:N	1:L:8:GLU:HB2	2.33	0.43
2:H:202:LYS:HG2	2:H:203:SER:N	2.33	0.43
4:K:71:HIS:CD2	5:M:154:VAL:HB	2.54	0.43
1:L:3:LEU:CB	1:L:9:LYS:HE3	2.42	0.43
2:H:31:VAL:CG1	2:H:32:MET:N	2.82	0.43
2:H:67:ARG:NH1	2:H:76:TYR:CD2	2.79	0.43
2:H:91:HIS:ND1	2:H:92:PRO:HD2	2.33	0.43
2:H:134:PHE:O	2:H:162:LEU:HD12	2.18	0.43
5:M:165:ARG:HG2	5:M:169:LYS:NZ	2.34	0.43
1:L:4:ARG:HH11	2:H:207:TRP:HE1	1.66	0.42
2:H:203:SER:HA	2:H:204:PRO:HD3	1.80	0.42
4:K:49:ASP:HA	6:K:441:HOH:O	2.19	0.42
2:H:41:LEU:O	3:F:318:PRO:CD	2.67	0.42
2:H:76:TYR:HE2	2:H:82:ILE:HD11	1.84	0.42
2:H:101:ARG:HG2	2:H:234:LEU:CD2	2.49	0.42
2:H:59:LEU:HD11	2:H:106:LEU:HD11	2.01	0.42
2:H:139:THR:CG2	2:H:157:VAL:HG13	2.47	0.42
1:J:14(H):GLU:O	1:J:14(L):GLU:HG3	2.19	0.42
5:M:164:GLU:O	5:M:167:VAL:HB	2.20	0.42
2:H:22:ALA:HB2	2:H:157:VAL:HG22	2.01	0.42
2:H:94:TYR:HB2	2:H:101:ARG:O	2.19	0.42
1:J:5:PRO:HA	1:J:9:LYS:HD2	2.01	0.42
5:M:178:ASP:O	5:M:233:ARG:NH1	2.52	0.42
2:H:152:PRO:HB2	2:H:154:VAL:O	2.20	0.42
4:K:109:LYS:HE3	4:K:110:ARG:HE	1.84	0.42
2:H:172:THR:CG2	2:H:176:ILE:HD11	2.50	0.42
4:K:75:ARG:HG2	4:K:76:TYR:O	2.20	0.42
5:M:203:SER:HA	5:M:204:PRO:HD3	1.84	0.42
2:H:29:TRP:CG	2:H:121:VAL:HB	2.55	0.41
2:H:48:SER:OG	2:H:49:ASP:N	2.54	0.41
2:H:215:TRP:HA	3:F:314:GLY:O	2.20	0.41
4:K:105:LEU:O	4:K:106:LEU:HD12	2.20	0.41
5:M:187:ARG:NH2	5:M:222:ASP:OD1	2.53	0.41
4:K:16:ILE:N	5:M:194:ASP:OD2	2.54	0.41
2:H:17:VAL:O	2:H:18:GLU:HB2	2.21	0.41
2:H:66:VAL:O	2:H:82:ILE:HA	2.20	0.41
2:H:160:LEU:HD23	2:H:184(A):TYR:CE2	2.55	0.41
2:H:174:ILE:HD12	3:F:308:TYR:HE1	1.84	0.41
4:K:82:ILE:HG22	4:K:83:SER:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:VAL:HG21	2:H:220:CYS:HB3	2.03	0.41
2:H:20:GLN:O	2:H:156:GLN:HA	2.21	0.41
2:H:34:PHE:HE2	2:H:38:GLN:HB3	1.81	0.41
2:H:35:ARG:HD3	2:H:39:GLU:OE1	2.21	0.41
4:K:49:ASP:OD2	4:K:111:PRO:HB2	2.21	0.41
1:L:1:CYS:C	2:H:122:CYS:SG	3.04	0.41
2:H:16:ILE:O	2:H:144:ARG:HA	2.20	0.41
1:L:1(B):ALA:O	2:H:206:ARG:NH1	2.53	0.40
4:K:33:LEU:HD23	4:K:33:LEU:HA	1.96	0.40
5:M:200:VAL:HG12	5:M:209:GLN:HA	2.03	0.40
5:M:171:SER:HB2	5:M:225:TYR:HE2	1.85	0.40
2:H:35:ARG:O	2:H:38:GLN:HA	2.22	0.40
5:M:203:SER:HB2	5:M:208:TYR:HE2	1.86	0.40
2:H:17:VAL:HG11	2:H:221:ASP:HB2	2.03	0.40
4:K:57:HIS:CE1	5:M:195:SER:OG	2.74	0.40
4:K:86:ASP:HB3	4:K:107:LYS:CG	2.41	0.40
5:M:236:LYS:HE2	6:M:586:HOH:O	2.21	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)
2:H:186(C):GLY:O	4:K:145:ARG:NH1[1_545]	1.97	0.23
2:H:145:ARG:NE	5:M:186(C):GLY:O[1_545]	2.05	0.15
2:H:60(D):TRP:NE1	3:N:308:TYR:N[8_655]	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	J	27/49 (55%)	22 (82%)	4 (15%)	1 (4%)	2 3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	L	27/49 (55%)	20 (74%)	7 (26%)	0	100	100
2	H	243/259 (94%)	213 (88%)	26 (11%)	4 (2%)	7	14
3	F	3/23 (13%)	1 (33%)	1 (33%)	1 (33%)	0	0
3	N	3/23 (13%)	1 (33%)	2 (67%)	0	100	100
4	K	144/150 (96%)	126 (88%)	16 (11%)	2 (1%)	9	17
5	M	99/109 (91%)	86 (87%)	12 (12%)	1 (1%)	12	24
All	All	546/662 (82%)	469 (86%)	68 (12%)	9 (2%)	7	14

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	111	PRO
5	M	205	ASN
2	H	79	VAL
3	F	316	ARG
4	K	77(A)	ARG
1	J	14(A)	GLN
4	K	130	LEU
2	H	29	TRP
2	H	242	ILE

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	J	26/43 (60%)	25 (96%)	1 (4%)	29	56
1	L	26/43 (60%)	26 (100%)	0	100	100
2	H	216/226 (96%)	184 (85%)	32 (15%)	3	6
3	F	4/15 (27%)	3 (75%)	1 (25%)	0	1
3	N	4/15 (27%)	4 (100%)	0	100	100
4	K	130/134 (97%)	117 (90%)	13 (10%)	7	15

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	M	86/92 (94%)	73 (85%)	13 (15%)	3	5
All	All	492/568 (87%)	432 (88%)	60 (12%)	5	10

All (60) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	24	VAL
2	H	27	SER
2	H	32	MET
2	H	33	LEU
2	H	40	LEU
2	H	46	LEU
2	H	48	SER
2	H	63	ASP
2	H	66	VAL
2	H	67	ARG
2	H	75	ARG
2	H	76	TYR
2	H	99	LEU
2	H	105	LEU
2	H	110	ARG
2	H	111	PRO
2	H	113	GLU
2	H	126	LYS
2	H	127	GLN
2	H	137	ARG
2	H	145	ARG
2	H	150	VAL
2	H	153	SER
2	H	154	VAL
2	H	157	VAL
2	H	173	ARG
2	H	195	SER
2	H	210	MET
2	H	224	LYS
2	H	236	LYS
2	H	239	GLN
2	H	240	LYS
3	F	315	VAL
1	J	4	ARG
4	K	26	LEU
4	K	45	SER

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Mol	Chain	Res	Type
4	K	48	SER
4	K	50	ARG
4	K	62	ASP
4	K	70	LYS
4	K	74	THR
4	K	81	LYS
4	K	84	MET
4	K	107	LYS
4	K	130	LEU
4	K	139	THR
4	K	145	ARG
5	M	153	SER
5	M	154	VAL
5	M	164	GLU
5	M	169	LYS
5	M	171	SER
5	M	186	PRO
5	M	186(B)	GLU
5	M	186(D)	LYS
5	M	187	ARG
5	M	233	ARG
5	M	236	LYS
5	M	239	GLN
5	M	242	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	71	HIS
2	H	98	ASN
2	H	127	GLN
2	H	131	HIS
2	H	143	ASN
2	H	204(B)	ASN
1	J	11	GLN
1	J	13	GLN
4	K	20	GLN
4	K	30	GLN
4	K	71	HIS
4	K	131	HIS
5	M	159	ASN
5	M	204(B)	ASN

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Mol	Chain	Res	Type
5	M	239	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.