



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:28 PM UTC

PDB ID : 1MKX / pdb_00001mkx
Title : THE CO-CRYSTAL STRUCTURE OF UNLIGANDED BOVINE ALPHA-THROMBIN AND PRETHROMBIN-2: MOVEMENT OF THE YPPW SEGMENT AND ACTIVE SITE RESIDUES UPON LIGAND BINDING
Authors : Malkowski, M.G.; Edwards, B.F.P.
Deposited on : 1997-03-13
Resolution : 2.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

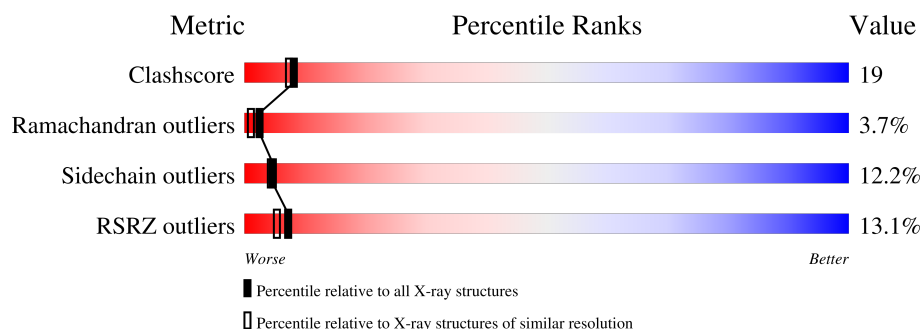
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	L	49	
2	H	259	
3	K	308	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5012 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 ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	29	Total	C	N	O	S	0	0	0
			243	153	38	51	1			

- Molecule 2 is a protein called ALPHA-THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	255	Total	C	N	O	S	0	0	0
			2064	1320	369	363	12			

- Molecule 3 is a protein called PRETHROMBIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	K	287	Total	C	N	O	S	0	0	0
			2326	1483	413	417	13			

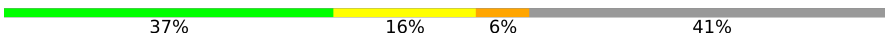
- Molecule 4 is water.

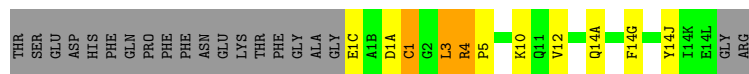
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	32	Total	O	0	0
			32	32		
4	H	205	Total	O	0	0
			205	205		
4	K	142	Total	O	0	0
			142	142		

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

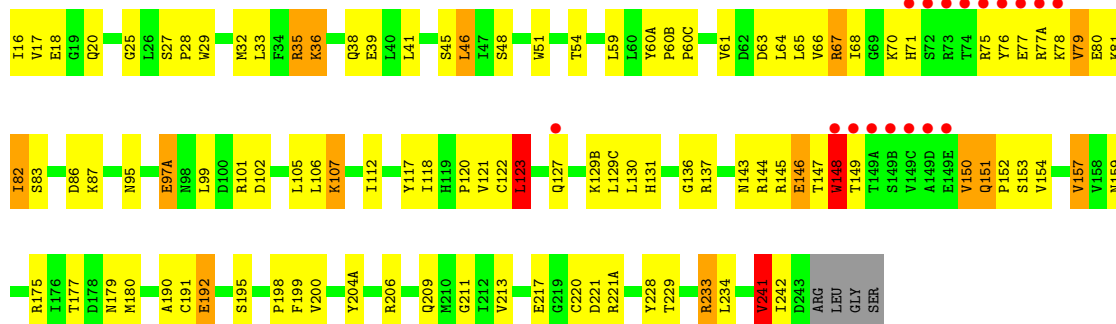
• Molecule 1: ALPHA-THROMBIN

Chain L: 



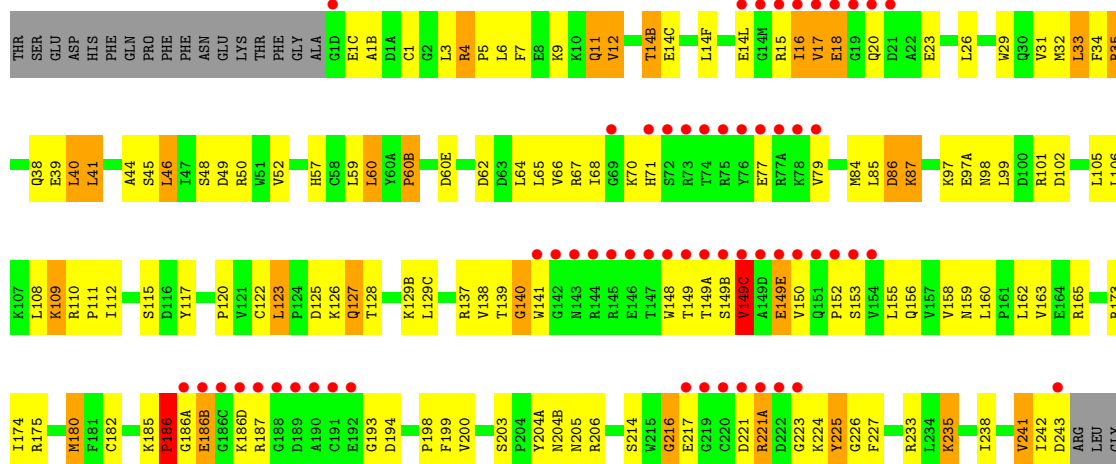
• Molecule 2: ALPHA-THROMBIN

Chain H: 



• Molecule 3: PRETHROMBIN-2

Chain K: 



SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	87.52Å 87.99Å 101.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.20 7.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.20) 86.0 (7.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.73 (at 1.93Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , 0.255 0.220 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	21.6	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.22 , 99.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.054 for k,h,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	5012	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	L	1.09	1/246 (0.4%)	1.32	3/328 (0.9%)
2	H	1.07	5/2118 (0.2%)	1.28	18/2867 (0.6%)
3	K	1.00	4/2384 (0.2%)	1.32	33/3222 (1.0%)
All	All	1.04	10/4748 (0.2%)	1.30	54/6417 (0.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	K	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	54	THR	CA-CB	7.74	1.64	1.53
3	K	174	ILE	CA-CB	7.27	1.62	1.54
3	K	200	VAL	CA-CB	6.17	1.62	1.54
2	H	241	VAL	CA-CB	6.01	1.61	1.54
2	H	118	ILE	CA-CB	5.96	1.62	1.54
3	K	241	VAL	CA-CB	5.77	1.61	1.54
2	H	83	SER	CA-C	-5.21	1.46	1.52
1	L	4	ARG	CA-C	-5.20	1.46	1.53
3	K	84	MET	SD-CE	5.13	1.92	1.79
2	H	86	ASP	CA-C	-5.00	1.47	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	17	VAL	N-CA-C	12.47	135.28	109.34
3	K	16	ILE	N-CA-C	9.66	129.44	109.34
2	H	147	THR	N-CA-C	8.65	129.23	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	157	VAL	CB-CA-C	-8.55	97.33	110.50
1	L	4	ARG	CA-C-N	8.49	129.00	119.32
1	L	4	ARG	C-N-CA	8.49	129.00	119.32
3	K	60(B)	PRO	N-CA-C	8.16	120.66	110.70
2	H	51	TRP	N-CA-C	7.59	121.29	109.07
2	H	129(C)	LEU	N-CA-C	7.29	121.42	112.23
3	K	199	PHE	N-CA-C	-6.94	97.20	108.52
2	H	123	LEU	N-CA-C	-6.82	101.22	110.36
3	K	123	LEU	N-CA-C	-6.69	101.64	110.07
3	K	200	VAL	N-CA-C	6.64	118.16	108.53
2	H	97(A)	GLU	N-CA-C	6.60	121.86	113.55
3	K	35	ARG	N-CA-C	-6.55	98.58	109.46
1	L	14(A)	GLN	N-CA-C	6.45	119.13	111.33
3	K	140	GLY	N-CA-C	6.36	122.75	110.66
2	H	36	LYS	N-CA-C	6.36	117.87	111.07
3	K	149(C)	VAL	N-CA-C	6.27	122.39	109.34
3	K	194	ASP	N-CA-C	6.16	119.16	110.23
3	K	186(B)	GLU	N-CA-C	-5.96	104.59	112.34
3	K	153	SER	N-CA-C	-5.93	102.48	111.56
3	K	86	ASP	N-CA-C	-5.88	106.14	113.55
3	K	64	LEU	N-CA-C	5.86	118.76	110.14
3	K	15	ARG	N-CA-C	5.84	115.72	108.19
3	K	125	ASP	N-CA-C	-5.80	101.61	110.14
2	H	82	ILE	N-CA-C	-5.78	99.79	108.12
3	K	18	GLU	N-CA-C	5.76	123.08	110.80
3	K	60	LEU	N-CA-C	5.66	117.93	108.02
3	K	110	ARG	CA-C-N	5.57	125.58	119.90
3	K	110	ARG	C-N-CA	5.57	125.58	119.90
2	H	147	THR	CA-C-N	5.54	132.12	121.54
2	H	147	THR	C-N-CA	5.54	132.12	121.54
3	K	120	PRO	N-CA-C	5.54	119.71	111.41
2	H	190	ALA	N-CA-C	-5.52	103.10	110.55
2	H	35	ARG	N-CA-C	-5.50	100.32	109.46
3	K	242	ILE	N-CA-C	5.46	116.19	110.62
3	K	97(A)	GLU	N-CA-C	5.41	120.37	113.18
3	K	16	ILE	CA-C-N	5.39	131.67	121.97
3	K	16	ILE	C-N-CA	5.39	131.67	121.97
2	H	130	LEU	N-CA-C	5.37	117.86	108.52
3	K	205	ASN	N-CA-C	5.28	119.56	113.38
2	H	60(B)	PRO	N-CA-C	5.27	117.13	110.70
3	K	214	SER	N-CA-C	5.25	119.00	111.02
2	H	18	GLU	N-CA-C	5.20	118.92	112.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	186(A)	GLY	N-CA-C	-5.12	101.04	113.18
3	K	14(B)	THR	N-CA-CB	-5.11	103.69	111.15
3	K	4	ARG	CA-C-N	5.10	124.27	118.97
3	K	4	ARG	C-N-CA	5.10	124.27	118.97
2	H	195	SER	N-CA-C	5.08	117.25	110.35
2	H	198	PRO	N-CA-C	5.05	121.30	112.01
3	K	14(B)	THR	CB-CA-C	5.03	115.65	109.16
3	K	162	LEU	N-CA-C	-5.03	102.25	110.20
2	H	64	LEU	N-CA-C	5.02	117.76	109.72

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	225	TYR	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	L	243	0	233	6	0
2	H	2064	0	2065	79	0
3	K	2326	0	2318	79	0
4	H	205	0	0	7	0
4	K	142	0	0	7	0
4	L	32	0	0	0	0
All	All	5012	0	4616	159	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (159) 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)
3:K:129(B):LYS:NZ	3:K:204(A):TYR:HB2	1.75	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:1(C):GLU:HG3	3:K:1:CYS:HB3	1.42	1.01
3:K:14(B):THR:HG22	3:K:137:ARG:NH2	1.78	0.99
2:H:145:ARG:NH1	2:H:150:VAL:HG13	1.81	0.95
2:H:32:MET:HE1	2:H:70:LYS:HE2	1.53	0.88
3:K:216:GLY:HA2	3:K:226:GLY:HA2	1.60	0.84
3:K:129(B):LYS:HZ2	3:K:204(A):TYR:HB2	1.44	0.82
3:K:129(B):LYS:HZ3	3:K:204(A):TYR:HB2	1.47	0.80
3:K:14(B):THR:HG22	3:K:137:ARG:HH21	1.45	0.80
3:K:141:TRP:CZ3	3:K:155:LEU:HD13	2.18	0.79
3:K:14(C):GLU:HA	3:K:14(F):LEU:HD13	1.66	0.75
2:H:145:ARG:HB3	2:H:150:VAL:CG1	2.18	0.73
2:H:32:MET:HE1	2:H:70:LYS:CE	2.19	0.72
3:K:14(F):LEU:HD23	4:K:296:HOH:O	1.90	0.71
2:H:36:LYS:HE3	2:H:65:LEU:HG	1.72	0.71
2:H:123:LEU:HB2	4:H:395:HOH:O	1.92	0.70
2:H:60(A):TYR:CE2	2:H:60(C):PRO:HB2	2.27	0.70
3:K:7:PHE:HA	3:K:12:VAL:HG13	1.73	0.70
2:H:144:ARG:NH2	2:H:152:PRO:HA	2.08	0.69
3:K:65:LEU:HD23	4:K:339:HOH:O	1.93	0.67
2:H:32:MET:CE	2:H:70:LYS:HE2	2.25	0.67
2:H:87:LYS:HD2	2:H:107:LYS:NZ	2.12	0.65
3:K:32:MET:HG2	4:K:284:HOH:O	1.95	0.65
2:H:70:LYS:HB3	4:H:316:HOH:O	1.98	0.64
3:K:141:TRP:CH2	3:K:155:LEU:HD13	2.33	0.63
1:L:10:LYS:O	1:L:12:VAL:HG23	1.98	0.63
2:H:95:ASN:ND2	2:H:97(A):GLU:HG2	2.14	0.63
3:K:50:ARG:HA	3:K:108:LEU:HD12	1.80	0.62
3:K:128:THR:HG22	3:K:129(C):LEU:HD12	1.81	0.62
2:H:144:ARG:NH1	2:H:151:GLN:H	1.97	0.62
3:K:46:LEU:HD22	3:K:48:SER:O	1.99	0.61
1:L:3:LEU:HD12	2:H:206:ARG:HG2	1.80	0.61
2:H:213:VAL:HG13	4:H:263:HOH:O	2.01	0.61
3:K:216:GLY:HA2	3:K:227:PHE:H	1.66	0.61
2:H:27:SER:O	2:H:71:HIS:HE1	1.84	0.61
2:H:175:ARG:NH1	4:H:321:HOH:O	2.34	0.61
3:K:204(B):ASN:ND2	3:K:206:ARG:H	1.98	0.60
3:K:14(B):THR:HG23	3:K:159:ASN:HD21	1.67	0.59
2:H:242:ILE:HG22	2:H:242:ILE:O	2.01	0.58
3:K:86:ASP:HB2	3:K:109:LYS:HA	1.85	0.58
2:H:35:ARG:HD2	2:H:39:GLU:HG2	1.85	0.58
2:H:46:LEU:HD13	2:H:120:PRO:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:38:GLN:HG3	4:K:277:HOH:O	2.03	0.58
2:H:145:ARG:HH11	2:H:150:VAL:HG13	1.68	0.58
3:K:34:PHE:CE2	3:K:67:ARG:HD2	2.39	0.57
3:K:139:THR:HG22	3:K:156:GLN:O	2.03	0.57
2:H:35:ARG:HB3	2:H:39:GLU:HG2	1.86	0.57
3:K:67:ARG:NH1	4:K:344:HOH:O	2.38	0.56
2:H:36:LYS:HE2	4:H:319:HOH:O	2.04	0.56
2:H:25:GLY:H	2:H:71:HIS:CD2	2.22	0.56
2:H:129(B):LYS:O	2:H:131:HIS:CD2	2.59	0.56
3:K:216:GLY:CA	3:K:226:GLY:HA2	2.33	0.56
3:K:7:PHE:HZ	3:K:23:GLU:HG3	1.70	0.56
3:K:97:LYS:HB2	4:K:258:HOH:O	2.05	0.56
2:H:35:ARG:HH11	2:H:39:GLU:CD	2.14	0.56
2:H:221(A):ARG:HG2	3:K:173:ARG:CZ	2.36	0.55
3:K:105:LEU:HD11	3:K:238:ILE:HG23	1.89	0.54
3:K:141:TRP:CE3	3:K:155:LEU:HD13	2.42	0.54
3:K:14(B):THR:CG2	3:K:137:ARG:HH21	2.17	0.54
2:H:29:TRP:O	2:H:45:SER:HA	2.07	0.54
3:K:233:ARG:HD3	4:K:273:HOH:O	2.08	0.54
3:K:9:LYS:C	3:K:11:GLN:H	2.15	0.53
3:K:216:GLY:HA2	3:K:226:GLY:CA	2.34	0.53
2:H:87:LYS:HD2	2:H:107:LYS:HZ3	1.72	0.53
3:K:163:VAL:HG21	3:K:225:TYR:CD2	2.44	0.53
3:K:7:PHE:CZ	3:K:23:GLU:HG3	2.44	0.53
3:K:49:ASP:O	3:K:112:ILE:HG12	2.09	0.52
3:K:204(B):ASN:HD22	3:K:204(B):ASN:C	2.17	0.52
2:H:148:TRP:CZ3	3:K:175:ARG:HG3	2.45	0.52
3:K:123:LEU:HD13	3:K:235:LYS:HD3	1.92	0.52
2:H:46:LEU:CD1	2:H:120:PRO:HB3	2.39	0.52
1:L:4:ARG:HG2	2:H:28:PRO:HG3	1.91	0.51
2:H:17:VAL:HG23	2:H:191:CYS:HB2	1.93	0.51
1:L:14(G):PHE:HA	1:L:14(J):TYR:CD2	2.46	0.51
2:H:145:ARG:HB3	2:H:150:VAL:HG12	1.92	0.51
2:H:95:ASN:HD21	2:H:97(A):GLU:HG2	1.76	0.51
3:K:35:ARG:O	3:K:38:GLN:HA	2.11	0.51
2:H:35:ARG:O	2:H:38:GLN:HA	2.10	0.51
2:H:16:ILE:O	2:H:144:ARG:HA	2.11	0.50
2:H:71:HIS:CE1	4:H:314:HOH:O	2.64	0.50
3:K:14(B):THR:CG2	3:K:159:ASN:HD21	2.25	0.50
3:K:23:GLU:HG2	3:K:26:LEU:HD13	1.92	0.50
3:K:31:VAL:HG13	3:K:68:ILE:HG12	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:79:VAL:HB	2:H:117:TYR:CD2	2.47	0.49
2:H:129(B):LYS:HD3	2:H:204(A):TYR:CZ	2.48	0.49
2:H:95:ASN:O	2:H:99:LEU:HA	2.13	0.49
2:H:217:GLU:O	2:H:221(A):ARG:HD2	2.13	0.48
2:H:17:VAL:HG11	2:H:221:ASP:HB2	1.95	0.48
2:H:99:LEU:O	2:H:102:ASP:HB2	2.13	0.48
2:H:213:VAL:HG22	2:H:228:TYR:HE2	1.79	0.48
3:K:45:SER:OG	3:K:198:PRO:HB3	2.13	0.48
2:H:17:VAL:HG21	2:H:220:CYS:HB3	1.95	0.48
2:H:105:LEU:CD1	2:H:241:VAL:HG22	2.43	0.48
2:H:29:TRP:CG	2:H:121:VAL:HB	2.49	0.47
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.50	0.47
3:K:60(B):PRO:O	3:K:60(E):ASP:N	2.40	0.47
3:K:32:MET:HE2	3:K:40:LEU:HD22	1.96	0.47
3:K:59:LEU:HD11	3:K:106:LEU:HD21	1.98	0.46
2:H:97(A):GLU:CD	2:H:175:ARG:HH21	2.24	0.46
3:K:32:MET:O	3:K:66:VAL:HA	2.15	0.46
3:K:139:THR:HA	3:K:156:GLN:O	2.16	0.46
2:H:105:LEU:HD13	2:H:241:VAL:HG22	1.98	0.46
2:H:137:ARG:HB2	2:H:159:ASN:OD1	2.15	0.46
3:K:203:SER:HB3	3:K:204(B):ASN:ND2	2.31	0.46
1:L:4:ARG:HA	1:L:5:PRO:HD3	1.78	0.45
3:K:138:VAL:HG23	3:K:158:VAL:HG13	1.98	0.45
3:K:182:CYS:HA	3:K:226:GLY:O	2.16	0.45
3:K:185:LYS:O	3:K:186:PRO:C	2.59	0.45
2:H:143:ASN:OD1	2:H:192:GLU:CG	2.65	0.45
2:H:87:LYS:HB2	2:H:107:LYS:HZ3	1.82	0.45
2:H:211:GLY:HA2	2:H:229:THR:O	2.17	0.45
2:H:29:TRP:CD2	2:H:121:VAL:HB	2.52	0.45
2:H:17:VAL:HG11	2:H:221:ASP:CB	2.46	0.45
2:H:70:LYS:HD3	2:H:80:GLU:OE1	2.17	0.44
2:H:81:LYS:HD3	2:H:112:ILE:CG2	2.48	0.44
3:K:140:GLY:HA3	3:K:193:GLY:HA2	1.99	0.44
3:K:57:HIS:ND1	3:K:102:ASP:OD2	2.51	0.44
2:H:27:SER:O	2:H:71:HIS:CE1	2.68	0.44
3:K:33:LEU:O	3:K:40:LEU:HD12	2.17	0.44
1:L:1:CYS:O	2:H:122:CYS:SG	2.75	0.44
2:H:152:PRO:HB2	2:H:154:VAL:O	2.18	0.44
2:H:179:ASN:OD1	2:H:233:ARG:HD2	2.18	0.44
3:K:46:LEU:HD23	3:K:46:LEU:HA	1.88	0.44
2:H:32:MET:HE3	2:H:67:ARG:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:23:GLU:O	3:K:26:LEU:HB2	2.17	0.44
3:K:87:LYS:HA	3:K:87:LYS:HD2	1.77	0.43
2:H:61:VAL:HG22	4:H:295:HOH:O	2.17	0.43
3:K:203:SER:HB3	3:K:204(B):ASN:HD21	1.83	0.43
2:H:146:GLU:HB2	2:H:220:CYS:HB2	1.99	0.43
3:K:45:SER:O	3:K:52:VAL:HA	2.18	0.43
2:H:25:GLY:H	2:H:71:HIS:HD2	1.65	0.43
2:H:145:ARG:HB3	2:H:150:VAL:HG11	1.98	0.43
2:H:242:ILE:O	2:H:242:ILE:CG2	2.66	0.43
2:H:67:ARG:C	2:H:68:ILE:HG13	2.43	0.43
2:H:67:ARG:HD2	2:H:82:ILE:HG12	2.01	0.43
3:K:101:ARG:HH11	3:K:101:ARG:HD3	1.68	0.42
2:H:35:ARG:NH1	2:H:39:GLU:CD	2.77	0.42
2:H:175:ARG:NH1	2:H:177:THR:HG22	2.35	0.42
2:H:35:ARG:NH1	2:H:41:LEU:HD21	2.35	0.42
3:K:115:SER:C	3:K:117:TYR:N	2.77	0.42
2:H:87:LYS:HD2	2:H:107:LYS:HZ1	1.81	0.42
3:K:31:VAL:HB	3:K:44:ALA:HB3	2.01	0.42
3:K:60:LEU:HG	3:K:60(B):PRO:HD3	2.02	0.42
3:K:5:PRO:HA	3:K:9:LYS:HB2	2.00	0.42
3:K:35:ARG:HD2	3:K:39:GLU:OE2	2.19	0.42
3:K:41:LEU:HD12	3:K:41:LEU:HA	1.89	0.42
3:K:216:GLY:HA2	3:K:227:PHE:N	2.32	0.41
3:K:1:CYS:C	3:K:122:CYS:SG	3.03	0.41
3:K:4:ARG:HA	3:K:5:PRO:HD2	1.79	0.41
3:K:98:ASN:O	3:K:99:LEU:HB2	2.20	0.41
3:K:3:LEU:O	3:K:9:LYS:NZ	2.46	0.41
2:H:59:LEU:HD11	2:H:106:LEU:HD11	2.02	0.41
3:K:29:TRP:O	3:K:45:SER:HA	2.20	0.40
3:K:165:ARG:NH2	3:K:180:MET:O	2.54	0.40
3:K:9:LYS:C	3:K:11:GLN:N	2.79	0.40
2:H:101:ARG:HG2	2:H:234:LEU:HD11	2.03	0.40
2:H:129(B):LYS:O	2:H:131:HIS:NE2	2.55	0.40
2:H:200:VAL:HG12	2:H:209:GLN:HA	2.03	0.40
3:K:126:LYS:HG2	3:K:127:GLN:H	1.87	0.40

There are no symmetry-related clashes.

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	L	27/49 (55%)	23 (85%)	4 (15%)	0	100	100
2	H	253/259 (98%)	233 (92%)	14 (6%)	6 (2%)	4	3
3	K	285/308 (92%)	237 (83%)	33 (12%)	15 (5%)	1	0
All	All	565/616 (92%)	493 (87%)	51 (9%)	21 (4%)	2	1

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	77(A)	ARG
2	H	149	THR
3	K	14(L)	GLU
3	K	17	VAL
3	K	149(C)	VAL
3	K	150	VAL
3	K	216	GLY
3	K	221(A)	ARG
2	H	148	TRP
2	H	150	VAL
3	K	1(B)	ALA
3	K	16	ILE
3	K	149(E)	GLU
3	K	77	GLU
3	K	152	PRO
3	K	217	GLU
3	K	223	GLY
2	H	146	GLU
3	K	18	GLU
2	H	77	GLU
3	K	186	PRO

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	L	27/43 (63%)	23 (85%)	4 (15%)	3	2
2	H	223/226 (99%)	201 (90%)	22 (10%)	7	8
3	K	251/269 (93%)	216 (86%)	35 (14%)	3	3
All	All	501/538 (93%)	440 (88%)	61 (12%)	5	4

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	1(A)	ASP
1	L	1	CYS
1	L	3	LEU
2	H	20	GLN
2	H	33	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	78	LYS
2	H	79	VAL
2	H	107	LYS
2	H	123	LEU
2	H	127	GLN
2	H	148	TRP
2	H	151	GLN
2	H	153	SER
2	H	157	VAL
2	H	180	MET
2	H	192	GLU
2	H	233	ARG
2	H	241	VAL

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Mol	Chain	Res	Type
3	K	6	LEU
3	K	11	GLN
3	K	12	VAL
3	K	20	GLN
3	K	33	LEU
3	K	40	LEU
3	K	41	LEU
3	K	46	LEU
3	K	62	ASP
3	K	70	LYS
3	K	71	HIS
3	K	79	VAL
3	K	85	LEU
3	K	87	LYS
3	K	109	LYS
3	K	111	PRO
3	K	127	GLN
3	K	148	TRP
3	K	149	THR
3	K	149(A)	THR
3	K	149(B)	SER
3	K	149(C)	VAL
3	K	149(E)	GLU
3	K	160	LEU
3	K	180	MET
3	K	186	PRO
3	K	186(B)	GLU
3	K	186(D)	LYS
3	K	187	ARG
3	K	221	ASP
3	K	221(A)	ARG
3	K	224	LYS
3	K	235	LYS
3	K	241	VAL
3	K	243	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	95	ASN
3	K	11	GLN
3	K	127	GLN

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Mol	Chain	Res	Type
3	K	204(B)	ASN
3	K	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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	L	29/49 (59%)	-0.26	0 100 100	15, 28, 50, 56	0
2	H	255/259 (98%)	-0.21	17 (6%) 24 21	1, 18, 46, 88	14 (5%)
3	K	287/308 (93%)	0.87	58 (20%) 3 2	0, 21, 50, 71	53 (18%)
All	All	571/616 (92%)	0.33	75 (13%) 7 5	0, 20, 49, 88	67 (11%)

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	K	223	GLY	17.9
3	K	72	SER	12.5
3	K	222	ASP	9.6
3	K	219	GLY	9.3
3	K	190	ALA	9.1
3	K	191	CYS	9.0
3	K	14(M)	GLY	8.6
2	H	72	SER	8.3
3	K	149	THR	7.9
3	K	77	GLU	7.8
3	K	188	GLY	7.7
3	K	144	ARG	7.5
3	K	186(A)	GLY	7.2
2	H	149(A)	THR	7.2
2	H	149(D)	ALA	6.9
3	K	20	GLN	6.8
3	K	221(A)	ARG	6.7
3	K	142	GLY	6.6
3	K	148	TRP	6.5
2	H	76	TYR	6.5
2	H	149(E)	GLU	6.5
3	K	14(L)	GLU	6.4
3	K	76	TYR	6.1

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Mol	Chain	Res	Type	RSRZ
2	H	74	THR	6.1
3	K	147	THR	6.1
3	K	143	ASN	6.0
3	K	149(A)	THR	5.9
2	H	149(C)	VAL	5.9
3	K	79	VAL	5.6
3	K	75	ARG	5.5
3	K	189	ASP	5.4
3	K	71	HIS	5.4
3	K	186(D)	LYS	5.3
3	K	154	VAL	5.2
3	K	16	ILE	5.2
3	K	149(D)	ALA	5.2
3	K	149(B)	SER	5.2
3	K	15	ARG	5.1
3	K	187	ARG	5.1
2	H	149	THR	5.1
3	K	217	GLU	5.1
3	K	151	GLN	5.1
2	H	148	TRP	5.0
2	H	75	ARG	4.9
3	K	17	VAL	4.9
3	K	221	ASP	4.9
3	K	18	GLU	4.8
3	K	186(C)	GLY	4.7
3	K	145	ARG	4.7
3	K	19	GLY	4.6
3	K	220	CYS	4.6
3	K	73	ARG	4.6
3	K	192	GLU	4.5
3	K	78	LYS	4.4
2	H	77	GLU	4.4
3	K	186(B)	GLU	4.3
3	K	149(E)	GLU	4.2
3	K	153	SER	4.2
3	K	146	GLU	4.1
2	H	78	LYS	4.0
3	K	150	VAL	3.9
3	K	74	THR	3.9
3	K	149(C)	VAL	3.8
2	H	77(A)	ARG	3.6
3	K	77(A)	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
2	H	149(B)	SER	3.3
2	H	73	ARG	3.3
3	K	152	PRO	3.0
3	K	141	TRP	2.9
3	K	1(D)	GLY	2.7
3	K	21	ASP	2.3
2	H	71	HIS	2.2
2	H	127	GLN	2.0
3	K	69	GLY	2.0
3	K	243	ASP	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.