Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 08:53 PM GMT

PDB ID	:	1MKW
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	:	2.30 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

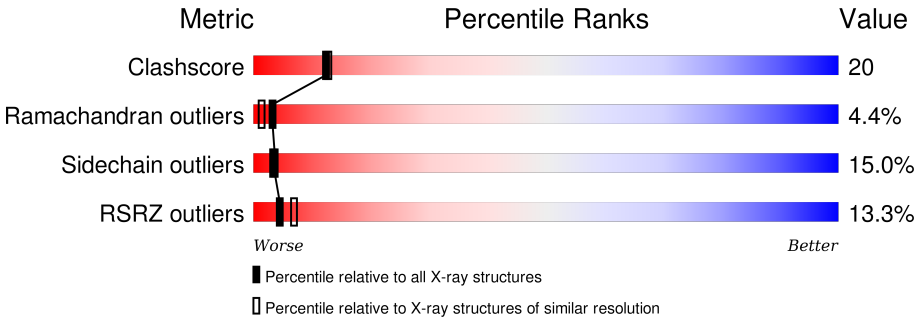
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 2.30 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	102246	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% 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	33% 22% • 41%
2	H	259	7% 63% 31% 5% •
3	K	308	19% 53% 31% 8% • 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4838 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.

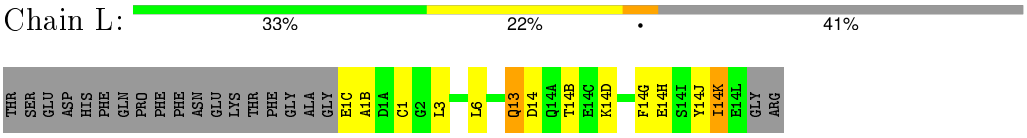
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	102	Total	O	0	0
			102	102		
4	K	87	Total	O	0	0
			87	87		
4	L	16	Total	O	0	0
			16	16		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

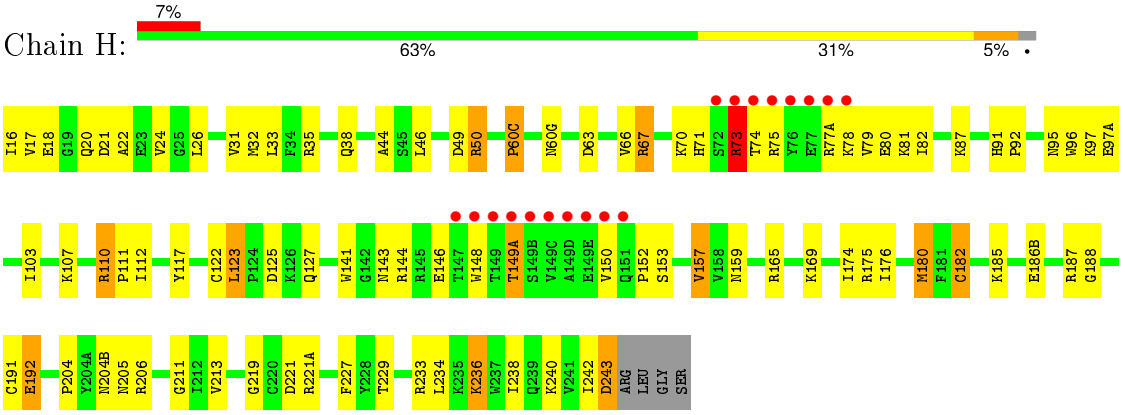
- Molecule 1: ALPHA-THROMBIN

Chain L:



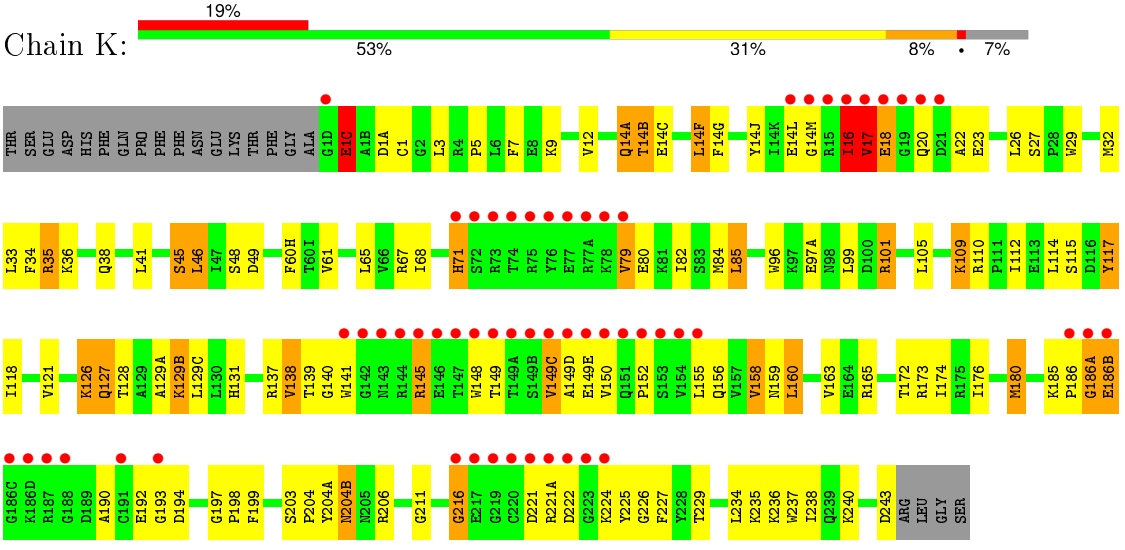
- Molecule 2: ALPHA-THROMBIN

Chain H:



- Molecule 3: PRETHROMBIN-2

Chain K:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	87.58Å 88.55Å 101.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	7.00 – 2.30 39.51 – 2.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (7.00-2.30) 83.1 (39.51-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	0.83 (at 2.00Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.190 , 0.282 0.219 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	20.1	Xtriage
Anisotropy	0.255	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.18 , 42.2	EDS
Estimated twinning fraction	0.053 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.46$, $< L^2 > = 0.29$	Xtriage
Outliers	0 of 44688 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	4838	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.67% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.90	0/246	1.01	0/328
2	H	0.86	0/2118	1.00	5/2867 (0.2%)
3	K	0.82	0/2384	1.03	5/3222 (0.2%)
All	All	0.84	0/4748	1.01	10/6417 (0.2%)

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	2

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	17	VAL	N-CA-C	9.71	137.22	111.00
3	K	16	ILE	N-CA-C	8.65	134.36	111.00
2	H	157	VAL	CB-CA-C	-6.97	98.15	111.40
3	K	186(A)	GLY	N-CA-C	-5.36	99.70	113.10
2	H	221	ASP	CB-CG-OD1	5.21	122.99	118.30
2	H	243	ASP	CB-CG-OD1	5.17	122.95	118.30
2	H	73	ARG	N-CA-C	5.11	124.80	111.00
3	K	14(F)	LEU	CA-CB-CG	5.10	127.04	115.30
2	H	35	ARG	N-CA-C	-5.09	97.27	111.00
3	K	18	GLU	N-CA-C	5.08	124.72	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	K	117	TYR	Sidechain
3	K	225	TYR	Sidechain

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	L	243	0	233	11	0
2	H	2064	0	2065	66	0
3	K	2326	0	2318	88	0
4	H	102	0	0	5	0
4	K	87	0	0	10	0
4	L	16	0	0	2	0
All	All	4838	0	4616	160	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 20.

All (160) 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:61:VAL:HG23	3:K:85:LEU:HB2	1.48	0.96
3:K:14(B):THR:HG22	3:K:137:ARG:NH2	1.81	0.94
2:H:81:LYS:HD3	2:H:112:ILE:HG23	1.48	0.94
2:H:50:ARG:HD2	4:H:322:HOH:O	1.72	0.88
3:K:216:GLY:HA2	3:K:226:GLY:HA2	1.59	0.84
2:H:87:LYS:HD2	2:H:107:LYS:HZ1	1.43	0.83
3:K:14(B):THR:HG22	3:K:137:ARG:HH21	1.40	0.81
3:K:14(C):GLU:HA	3:K:14(F):LEU:HD13	1.62	0.80
3:K:7:PHE:HA	3:K:12:VAL:HG13	1.65	0.76
2:H:67:ARG:HD2	2:H:82:ILE:HG12	1.66	0.76
2:H:107:LYS:HZ3	2:H:107:LYS:HB3	1.52	0.75
3:K:14(J):TYR:CZ	4:K:258:HOH:O	2.41	0.74
3:K:5:PRO:HA	3:K:9:LYS:HB2	1.70	0.74
3:K:14(B):THR:HG23	3:K:159:ASN:HD21	1.52	0.72
2:H:71:HIS:HD2	2:H:80:GLU:OE1	1.73	0.72
3:K:7:PHE:HZ	3:K:23:GLU:HG3	1.56	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:129(B):LYS:NZ	3:K:204(A):TYR:HB2	2.06	0.71
3:K:1(C):GLU:HG3	3:K:1:CYS:HB3	1.71	0.70
3:K:216:GLY:CA	3:K:226:GLY:HA2	2.22	0.69
3:K:165:ARG:NH2	3:K:180:MET:O	2.25	0.69
3:K:49:ASP:O	3:K:112:ILE:HG13	1.92	0.69
2:H:18:GLU:HG3	2:H:187:ARG:HB2	1.74	0.69
2:H:71:HIS:HB2	4:H:305:HOH:O	1.92	0.68
3:K:129(C):LEU:HD21	4:K:258:HOH:O	1.93	0.68
2:H:67:ARG:CD	2:H:82:ILE:HG12	2.24	0.67
3:K:14(F):LEU:HD23	4:K:262:HOH:O	1.95	0.67
2:H:87:LYS:HD2	2:H:107:LYS:NZ	2.10	0.66
3:K:61:VAL:CG2	3:K:85:LEU:HB2	2.24	0.66
2:H:70:LYS:HB2	2:H:117:TYR:CD1	2.32	0.65
1:L:3:LEU:HD12	2:H:206:ARG:HG2	1.78	0.64
2:H:143:ASN:OD1	2:H:192:GLU:HG2	1.98	0.64
3:K:14(B):THR:CG2	3:K:159:ASN:HD21	2.10	0.64
3:K:1(C):GLU:HA	3:K:1(C):GLU:OE1	1.97	0.63
3:K:27:SER:H	3:K:71:HIS:HE1	1.46	0.63
3:K:14(B):THR:CG2	3:K:137:ARG:HH21	2.09	0.63
3:K:126:LYS:HG2	3:K:127:GLN:N	2.14	0.62
3:K:45:SER:OG	3:K:198:PRO:HG3	2.00	0.62
3:K:139:THR:HA	3:K:156:GLN:O	1.99	0.62
1:L:14(D):LYS:HE3	4:L:140:HOH:O	1.99	0.62
2:H:16:ILE:O	2:H:144:ARG:HA	1.99	0.61
3:K:216:GLY:HA2	3:K:227:PHE:H	1.66	0.61
3:K:36:LYS:HD2	4:K:314:HOH:O	1.99	0.61
2:H:95:ASN:HD21	2:H:97(A):GLU:HG2	1.66	0.61
2:H:191:CYS:SG	2:H:192:GLU:OE2	2.59	0.61
2:H:95:ASN:ND2	2:H:97(A):GLU:HG2	2.15	0.61
3:K:29:TRP:CG	3:K:121:VAL:HB	2.37	0.60
1:L:1:CYS:O	2:H:122:CYS:SG	2.59	0.60
3:K:23:GLU:HG2	3:K:26:LEU:HD13	1.84	0.59
3:K:128:THR:O	3:K:129(C):LEU:HB2	2.01	0.59
2:H:31:VAL:HB	2:H:44:ALA:HB3	1.85	0.59
3:K:237:TRP:HA	3:K:240:LYS:HE2	1.84	0.59
3:K:140:GLY:HA3	3:K:193:GLY:HA2	1.85	0.58
2:H:49:ASP:OD1	2:H:50:ARG:HD3	2.02	0.58
2:H:176:ILE:HG12	2:H:227:PHE:CE2	2.38	0.58
3:K:34:PHE:CE1	3:K:67:ARG:HD2	2.38	0.58
3:K:7:PHE:CZ	3:K:23:GLU:HG3	2.37	0.57
2:H:81:LYS:CD	2:H:112:ILE:HG23	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:129(B):LYS:HZ3	3:K:204(A):TYR:HB2	1.69	0.57
2:H:70:LYS:HB3	2:H:79:VAL:CG2	2.35	0.57
3:K:14(G):PHE:HA	3:K:14(J):TYR:CD2	2.40	0.57
2:H:60(C):PRO:HD3	2:H:96:TRP:CE3	2.40	0.57
3:K:165:ARG:NH1	4:K:292:HOH:O	2.37	0.56
2:H:107:LYS:NZ	2:H:107:LYS:HB3	2.20	0.56
2:H:174:ILE:O	2:H:176:ILE:HD12	2.06	0.56
2:H:238:ILE:O	2:H:242:ILE:HD12	2.06	0.55
2:H:204(B):ASN:OD1	2:H:206:ARG:HB2	2.05	0.55
3:K:203:SER:HB3	3:K:204(B):ASN:ND2	2.21	0.55
2:H:70:LYS:O	2:H:79:VAL:HG23	2.07	0.55
2:H:176:ILE:HG23	2:H:180:MET:HG3	1.89	0.55
2:H:71:HIS:CD2	2:H:80:GLU:OE1	2.59	0.54
3:K:32:MET:HG2	4:K:315:HOH:O	2.06	0.54
2:H:219:GLY:HA3	2:H:221(A):ARG:NE	2.21	0.54
2:H:32:MET:HE1	2:H:71:HIS:CG	2.43	0.54
3:K:158:VAL:HG11	3:K:190:ALA:HB2	1.89	0.54
3:K:173:ARG:NH1	4:K:270:HOH:O	2.41	0.53
3:K:185:LYS:HB3	3:K:186:PRO:HD2	1.91	0.53
3:K:129(B):LYS:HZ2	3:K:204(A):TYR:HB2	1.74	0.53
3:K:129(B):LYS:HE2	3:K:204:PRO:HG2	1.89	0.53
3:K:67:ARG:NH2	3:K:82:ILE:HD11	2.24	0.53
1:L:14(G):PHE:HE1	2:H:204:PRO:HB3	1.73	0.53
3:K:129(A):ALA:O	3:K:131:HIS:CE1	2.62	0.53
2:H:21:ASP:HB2	4:H:296:HOH:O	2.07	0.52
1:L:3:LEU:CD1	2:H:206:ARG:HG2	2.39	0.52
2:H:81:LYS:HD3	2:H:112:ILE:HD12	1.92	0.51
1:L:14(B):THR:HB	2:H:159:ASN:HD21	1.74	0.51
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.93	0.51
3:K:160:LEU:CD1	3:K:199:PHE:HE1	2.24	0.51
2:H:143:ASN:OD1	2:H:192:GLU:CG	2.58	0.51
3:K:14(J):TYR:CD2	4:K:302:HOH:O	2.64	0.50
2:H:143:ASN:HB2	2:H:192:GLU:OE2	2.10	0.50
2:H:32:MET:HE3	2:H:71:HIS:CD2	2.46	0.50
3:K:114:LEU:O	3:K:115:SER:HB3	2.11	0.50
3:K:35:ARG:O	3:K:38:GLN:HA	2.12	0.49
2:H:165:ARG:O	2:H:169:LYS:HG3	2.12	0.49
3:K:105:LEU:HD11	3:K:238:ILE:HG23	1.94	0.49
1:L:14(G):PHE:HA	1:L:14(J):TYR:CD2	2.47	0.49
2:H:103:ILE:HD11	2:H:238:ILE:HD11	1.93	0.49
3:K:163:VAL:HG13	3:K:185:LYS:HE2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:70:LYS:HD2	2:H:117:TYR:CE1	2.48	0.49
1:L:14(D):LYS:O	1:L:14(H):GLU:HG3	2.12	0.49
3:K:204(B):ASN:HD22	3:K:206:ARG:H	1.61	0.48
3:K:14(J):TYR:CG	4:K:302:HOH:O	2.55	0.48
3:K:35:ARG:NH2	3:K:60(H):PHE:HE1	2.12	0.48
3:K:211:GLY:HA2	3:K:229:THR:O	2.14	0.48
3:K:139:THR:HG22	3:K:156:GLN:O	2.14	0.47
2:H:213:VAL:HG13	4:H:293:HOH:O	2.14	0.47
2:H:22:ALA:HB1	2:H:26:LEU:HD22	1.96	0.47
3:K:129(A):ALA:O	3:K:131:HIS:HE1	1.97	0.47
3:K:46:LEU:HD22	3:K:48:SER:O	2.15	0.47
2:H:70:LYS:HB3	2:H:79:VAL:HB	1.97	0.47
3:K:216:GLY:HA2	3:K:226:GLY:CA	2.39	0.46
3:K:190:ALA:C	3:K:192:GLU:H	2.15	0.46
3:K:101:ARG:HG2	3:K:234:LEU:HD21	1.96	0.46
2:H:236:LYS:N	2:H:236:LYS:HD2	2.31	0.46
2:H:123:LEU:HA	2:H:123:LEU:HD12	1.59	0.45
3:K:46:LEU:HD11	3:K:112:ILE:HD11	1.99	0.45
3:K:236:LYS:O	3:K:240:LYS:HB2	2.17	0.44
2:H:165:ARG:NH2	2:H:180:MET:O	2.48	0.44
2:H:60(C):PRO:HG3	2:H:96:TRP:CZ3	2.53	0.44
3:K:240:LYS:NZ	4:K:316:HOH:O	2.41	0.43
2:H:185:LYS:HB2	2:H:186(B):GLU:HG3	2.00	0.43
3:K:67:ARG:HH21	3:K:82:ILE:HD11	1.83	0.43
3:K:204(B):ASN:ND2	3:K:206:ARG:H	2.16	0.43
2:H:242:ILE:HG22	2:H:242:ILE:O	2.19	0.43
2:H:24:VAL:HG13	2:H:117:TYR:HE1	1.84	0.43
3:K:14(A):GLN:HE21	3:K:14(A):GLN:HB2	1.61	0.43
2:H:110:ARG:HG2	2:H:111:PRO:O	2.18	0.43
2:H:70:LYS:HB2	2:H:117:TYR:CG	2.54	0.43
1:L:6:LEU:HA	1:L:6:LEU:HD23	1.75	0.43
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.65	0.43
3:K:36:LYS:O	3:K:38:GLN:HG2	2.19	0.43
3:K:32:MET:HB2	3:K:67:ARG:HB2	2.01	0.43
3:K:35:ARG:NH2	3:K:60(H):PHE:CE1	2.87	0.42
3:K:194:ASP:OD1	3:K:197:GLY:HA3	2.18	0.42
3:K:96:TRP:HA	3:K:99:LEU:HD23	2.01	0.42
3:K:85:LEU:N	3:K:85:LEU:HD13	2.33	0.42
2:H:67:ARG:HD2	2:H:82:ILE:CG1	2.42	0.42
3:K:49:ASP:HA	3:K:112:ILE:HD11	2.01	0.42
3:K:216:GLY:HA2	3:K:227:PHE:N	2.32	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:84:MET:O	3:K:109:LYS:HB2	2.19	0.42
3:K:22:ALA:HB3	3:K:155:LEU:O	2.19	0.42
1:L:14(D):LYS:HG3	1:L:14(H):GLU:OE2	2.20	0.41
3:K:115:SER:C	3:K:117:TYR:N	2.73	0.41
2:H:17:VAL:HG12	2:H:18:GLU:HG2	2.03	0.41
3:K:140:GLY:HA3	3:K:194:ASP:H	1.85	0.41
2:H:152:PRO:HG2	4:H:271:HOH:O	2.20	0.41
2:H:97(A):GLU:CD	2:H:175:ARG:HH21	2.22	0.41
2:H:91:HIS:HA	2:H:92:PRO:HD2	1.78	0.41
2:H:182:CYS:HB3	2:H:227:PHE:CE2	2.56	0.41
3:K:206:ARG:HG2	3:K:206:ARG:HH11	1.85	0.41
3:K:68:ILE:HG22	3:K:118:ILE:HG12	2.02	0.41
3:K:138:VAL:HG23	3:K:158:VAL:HG12	2.03	0.41
3:K:172:THR:OG1	3:K:174:ILE:HG12	2.20	0.41
2:H:31:VAL:CG1	2:H:66:VAL:HG13	2.51	0.41
1:L:13:GLN:HA	4:L:75:HOH:O	2.20	0.41
3:K:14(B):THR:HG23	3:K:159:ASN:ND2	2.29	0.40
2:H:211:GLY:HA2	2:H:229:THR:O	2.22	0.40
3:K:129(C):LEU:HD23	3:K:129(C):LEU:HA	1.84	0.40
3:K:3:LEU:O	3:K:9:LYS:NZ	2.49	0.40
3:K:101:ARG:HG2	3:K:234:LEU:CD2	2.50	0.40

There are no symmetry-related clashes.

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	L	27/49 (55%)	23 (85%)	2 (7%)	2 (7%)	1	0
2	H	253/259 (98%)	227 (90%)	20 (8%)	6 (2%)	7	5
3	K	285/308 (92%)	236 (83%)	32 (11%)	17 (6%)	2	1
All	All	565/616 (92%)	486 (86%)	54 (10%)	25 (4%)	3	1

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	73	ARG
2	H	74	THR
2	H	77(A)	ARG
3	K	1(C)	GLU
3	K	17	VAL
3	K	149(C)	VAL
3	K	150	VAL
3	K	186(B)	GLU
3	K	221(A)	ARG
2	H	149(A)	THR
3	K	14(L)	GLU
3	K	16	ILE
3	K	149(E)	GLU
3	K	216	GLY
3	K	14(M)	GLY
1	L	1(B)	ALA
3	K	149(D)	ALA
3	K	186(A)	GLY
2	H	60(G)	ASN
2	H	150	VAL
3	K	18	GLU
3	K	145	ARG
3	K	152	PRO
1	L	14(K)	ILE
3	K	79	VAL

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	L	27/43 (63%)	23 (85%)	4 (15%)	4 3
2	H	223/226 (99%)	193 (86%)	30 (14%)	5 4
3	K	251/269 (93%)	210 (84%)	41 (16%)	3 3
All	All	501/538 (93%)	426 (85%)	75 (15%)	3 3

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	1(C)	GLU
1	L	13	GLN
1	L	14	ASP
1	L	14(K)	ILE
2	H	20	GLN
2	H	33	LEU
2	H	38	GLN
2	H	46	LEU
2	H	50	ARG
2	H	60(C)	PRO
2	H	63	ASP
2	H	67	ARG
2	H	73	ARG
2	H	75	ARG
2	H	78	LYS
2	H	97	LYS
2	H	110	ARG
2	H	123	LEU
2	H	125	ASP
2	H	127	GLN
2	H	141	TRP
2	H	146	GLU
2	H	148	TRP
2	H	149(A)	THR
2	H	153	SER
2	H	157	VAL
2	H	180	MET
2	H	182	CYS
2	H	192	GLU
2	H	233	ARG
2	H	234	LEU
2	H	236	LYS
2	H	240	LYS
2	H	243	ASP
3	K	1(C)	GLU
3	K	1(A)	ASP
3	K	14(A)	GLN
3	K	14(B)	THR
3	K	16	ILE
3	K	17	VAL
3	K	20	GLN
3	K	33	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	K	35	ARG
3	K	41	LEU
3	K	45	SER
3	K	46	LEU
3	K	65	LEU
3	K	71	HIS
3	K	79	VAL
3	K	80	GLU
3	K	85	LEU
3	K	97(A)	GLU
3	K	101	ARG
3	K	109	LYS
3	K	110	ARG
3	K	126	LYS
3	K	127	GLN
3	K	129(B)	LYS
3	K	138	VAL
3	K	141	TRP
3	K	145	ARG
3	K	148	TRP
3	K	149	THR
3	K	149(C)	VAL
3	K	158	VAL
3	K	160	LEU
3	K	176	ILE
3	K	180	MET
3	K	186(B)	GLU
3	K	204(B)	ASN
3	K	221	ASP
3	K	222	ASP
3	K	224	LYS
3	K	235	LYS
3	K	243	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	13	GLN
1	L	14(A)	GLN
2	H	20	GLN
2	H	38	GLN
2	H	71	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	95	ASN
3	K	14(A)	GLN
3	K	38	GLN
3	K	71	HIS
3	K	131	HIS
3	K	204(B)	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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%)	-0.60	0 100 100	13, 25, 55, 70	0
2	H	255/259 (98%)	0.19	18 (7%) 19 26	3, 18, 68, 84	18 (7%)
3	K	287/308 (93%)	1.94	58 (20%) 1 2	4, 22, 59, 74	51 (17%)
All	All	571/616 (92%)	1.03	76 (13%) 4 7	3, 20, 61, 84	69 (12%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	H	150	VAL	30.8
3	K	152	PRO	25.3
2	H	149(A)	THR	24.2
3	K	21	ASP	23.1
3	K	149(D)	ALA	23.0
3	K	141	TRP	22.8
3	K	72	SER	22.4
3	K	76	TYR	22.2
2	H	76	TYR	21.9
3	K	149(C)	VAL	21.9
3	K	154	VAL	21.5
2	H	149(C)	VAL	21.4
3	K	148	TRP	20.8
3	K	77	GLU	19.2
3	K	186(D)	LYS	19.0
3	K	151	GLN	17.8
3	K	223	GLY	17.5
2	H	149(B)	SER	17.5
2	H	151	GLN	17.2
3	K	221	ASP	16.8
3	K	73	ARG	15.7
2	H	75	ARG	15.5
3	K	149	THR	15.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	187	ARG	15.3
3	K	145	ARG	15.2
3	K	221(A)	ARG	14.8
3	K	74	THR	14.7
2	H	149	THR	14.5
3	K	150	VAL	14.4
3	K	186(C)	GLY	14.3
3	K	20	GLN	14.2
3	K	149(E)	GLU	14.1
3	K	153	SER	13.8
3	K	149(B)	SER	13.7
3	K	144	ARG	13.4
3	K	186(B)	GLU	13.0
3	K	143	ASN	12.8
3	K	149(A)	THR	12.7
3	K	78	LYS	12.7
3	K	19	GLY	12.7
3	K	222	ASP	12.6
3	K	142	GLY	12.5
2	H	74	THR	12.4
2	H	149(D)	ALA	12.0
3	K	186(A)	GLY	11.3
2	H	78	LYS	11.1
3	K	147	THR	11.0
3	K	220	CYS	10.9
3	K	188	GLY	10.6
3	K	77(A)	ARG	10.5
2	H	77(A)	ARG	10.4
3	K	15	ARG	10.3
3	K	224	LYS	9.8
3	K	16	ILE	9.7
3	K	75	ARG	9.5
3	K	14(L)	GLU	8.9
3	K	146	GLU	8.8
2	H	77	GLU	8.4
2	H	72	SER	7.9
3	K	17	VAL	7.6
2	H	149(E)	GLU	7.6
2	H	148	TRP	7.5
3	K	79	VAL	7.3
2	H	73	ARG	7.1
3	K	14(M)	GLY	6.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	K	217	GLU	6.5
2	H	147	THR	5.7
3	K	191	CYS	5.6
3	K	18	GLU	5.6
3	K	219	GLY	5.5
3	K	193	GLY	3.9
3	K	1(D)	GLY	3.7
3	K	216	GLY	3.6
3	K	71	HIS	3.5
3	K	186	PRO	2.6
3	K	155	LEU	2.3

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 carbohydrates 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.