



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:03 AM UTC

PDB ID : 1BTH / pdb_00001bth
Title : STRUCTURE OF THROMBIN COMPLEXED WITH BOVINE PANCRE-
ATIC TRYPSIN INHIBITOR
Authors : Van De Locht, A.; Bode, W.; Stubbs, M.T.
Deposited on : 1996-12-03
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

<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

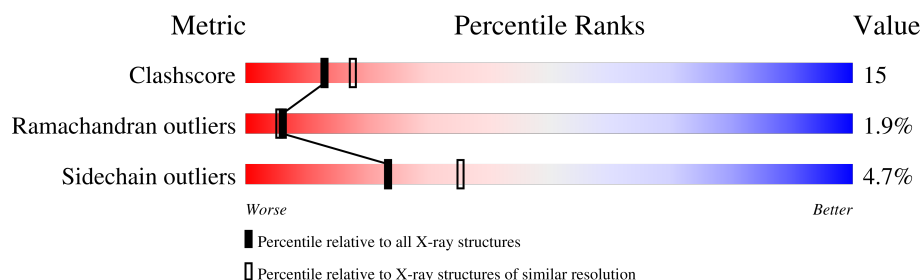
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 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	36	61% 19% 6% 14%
1	L	36	64% 19% . 14%
2	H	259	66% 27% . . .
2	K	259	66% 27% 5% .
3	P	58	64% 31% 5%
3	Q	58	59% 34% 7%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5921 atoms, of which 300 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 THROMBIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	L	31	Total	C	H	N	O	S	16	0	0
			255	153	8	40	53	1			
1	J	31	Total	C	H	N	O	S	25	0	0
			255	153	8	40	53	1			

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	H	254	Total	C	H	N	O	S	217	0	0
			2163	1310	110	365	364	14			
2	K	254	Total	C	H	N	O	S	219	0	0
			2163	1310	110	365	364	14			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	149	THR	ALA	conflict	UNP P00734
H	192	GLN	GLU	engineered mutation	UNP P00734
K	149	THR	ALA	conflict	UNP P00734
K	192	GLN	GLU	engineered mutation	UNP P00734

- Molecule 3 is a protein called BOVINE PANCREATIC TRYPSIN INHIBITOR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	P	58	Total	C	H	N	O	S	32	0	0
			486	284	32	84	79	7			
3	Q	58	Total	C	H	N	O	S	32	0	0
			486	284	32	84	79	7			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	3	Total 3	O 3	0	0
4	H	50	Total 50	O 50	0	0
4	J	5	Total 5	O 5	0	0
4	K	41	Total 41	O 41	0	0
4	P	7	Total 7	O 7	0	0
4	Q	7	Total 7	O 7	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.

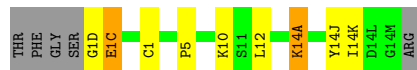
• Molecule 1: THROMBIN

Chain L: 



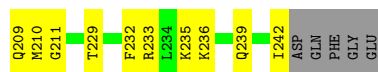
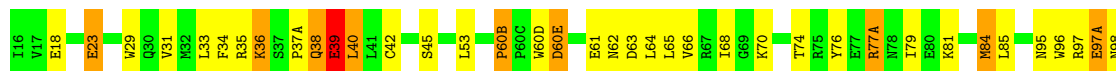
• Molecule 1: THROMBIN

Chain J: 



• Molecule 2: THROMBIN

Chain H: 



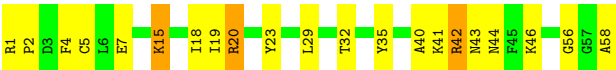
• Molecule 2: THROMBIN

Chain K: 





● Molecule 3: BOVINE PANCREATIC TRYPSIN INHIBITOR



● Molecule 3: BOVINE PANCREATIC TRYPSIN INHIBITOR



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	71.20Å 74.50Å 83.40Å 90.00° 92.50° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (6.00-2.30)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.196 , 0.271	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5921	wwPDB-VP
Average B, all atoms (Å ²)	35.0	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	0.67	1/249 (0.4%)	1.02	1/331 (0.3%)
1	L	0.60	0/249	1.01	1/331 (0.3%)
2	H	0.68	0/2107	1.08	13/2850 (0.5%)
2	K	0.68	0/2107	1.06	15/2850 (0.5%)
3	P	0.63	0/465	1.16	3/622 (0.5%)
3	Q	0.63	0/465	1.05	3/622 (0.5%)
All	All	0.67	1/5642 (0.0%)	1.07	36/7606 (0.5%)

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
2	K	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	1(C)	GLU	C-N	6.13	1.48	1.34

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	129(C)	LEU	N-CA-C	9.59	125.46	112.90
1	J	14(A)	LYS	N-CA-C	9.24	123.96	112.87
1	L	14(A)	LYS	N-CA-C	8.34	122.55	112.38
2	H	121	VAL	CB-CA-C	-8.21	100.16	111.49
3	P	42	ARG	N-CA-C	8.01	120.92	111.71
2	H	40	LEU	N-CA-C	7.75	121.53	108.90
2	K	98	ASN	N-CA-C	7.66	122.63	113.28
3	P	41	LYS	N-CA-C	-7.49	99.43	110.52
3	P	15	LYS	N-CA-C	7.44	121.20	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	121	VAL	CB-CA-C	-7.19	101.57	111.49
2	K	41	LEU	N-CA-C	-6.41	96.95	108.48
3	Q	15	LYS	N-CA-C	6.33	119.72	112.57
2	K	86	GLU	N-CA-C	-6.30	104.33	111.14
2	K	129(C)	LEU	N-CA-C	6.17	121.03	112.45
2	K	70	LYS	N-CA-C	5.96	118.59	110.55
2	H	97	ARG	NE-CZ-NH2	5.78	124.40	119.20
2	K	97	ARG	NE-CZ-NH2	5.77	124.39	119.20
2	K	44	ALA	N-CA-C	-5.70	100.68	108.38
2	H	60(E)	ASP	N-CA-C	-5.64	105.51	112.90
2	H	79	ILE	N-CA-C	5.62	116.06	111.62
2	K	43	GLY	N-CA-C	-5.59	101.92	112.10
2	K	190	ALA	N-CA-C	-5.56	102.30	110.52
2	K	76	TYR	N-CA-C	-5.51	101.69	109.96
3	Q	41	LYS	N-CA-C	-5.48	101.89	110.17
2	H	23	GLU	N-CA-C	-5.41	102.45	110.46
2	H	74	THR	N-CA-C	5.39	119.94	112.45
2	H	39	GLU	CA-C-N	-5.32	115.50	122.99
2	H	39	GLU	C-N-CA	-5.32	115.50	122.99
2	H	70	LYS	N-CA-C	5.28	117.68	110.55
2	K	198	PRO	N-CA-C	5.26	120.46	111.68
2	H	190	ALA	N-CA-C	-5.22	102.02	110.32
3	Q	42	ARG	N-CA-C	5.20	117.03	111.36
2	K	167	VAL	N-CA-C	-5.19	105.48	110.72
2	K	85	LEU	N-CA-C	5.04	116.97	109.25
2	K	79	ILE	N-CA-C	-5.04	106.74	111.48
2	H	60(B)	PRO	N-CA-C	-5.02	105.65	110.47

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	K	60(A)	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	J	247	8	241	10	0
1	L	247	8	241	6	0
2	H	2053	110	2038	60	0
2	K	2053	110	2038	60	0
3	P	454	32	438	18	0
3	Q	454	32	438	22	0
4	H	50	0	0	2	0
4	J	5	0	0	2	0
4	K	41	0	0	0	0
4	L	3	0	0	0	0
4	P	7	0	0	0	0
4	Q	7	0	0	0	0
All	All	5621	300	5434	156	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 15.

All (156) 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:J:1(D):GLY:HA2	4:J:56:HOH:O	1.42	1.17
2:K:35:ARG:HH21	2:K:39:GLU:HG3	1.37	0.87
2:K:18:GLU:HG3	2:K:187:ARG:HB2	1.53	0.86
2:K:37(A):PRO:HB2	2:K:39:GLU:HG2	1.59	0.83
2:H:33:LEU:HD21	2:H:106:MET:HE1	1.62	0.81
2:H:39:GLU:O	3:P:18:ILE:HA	1.80	0.81
3:Q:1:ARG:HB3	3:Q:58:ALA:HA	1.63	0.80
2:K:39:GLU:HB2	3:Q:18:ILE:HG23	1.64	0.79
2:H:18:GLU:HG3	2:H:187:ARG:HB2	1.67	0.76
2:K:39:GLU:HA	3:Q:19:ILE:H	1.51	0.75
2:K:50:ARG:HH11	2:K:107:LYS:HE2	1.51	0.75
2:H:62:ASN:O	2:H:63:ASP:HB3	1.87	0.74
2:H:35:ARG:HH21	2:H:39:GLU:HG3	1.55	0.71
2:K:29:TRP:CD2	2:K:121:VAL:HG13	2.28	0.69
1:J:1(C):GLU:HA	1:J:1:CYS:HB3	1.75	0.68
3:P:1:ARG:HB3	3:P:58:ALA:HA	1.75	0.68
1:J:1:CYS:O	2:K:122:CYS:SG	2.53	0.67
2:H:81:LYS:NZ	2:H:113:ALA:H	1.94	0.66
2:K:39:GLU:HB2	3:Q:18:ILE:CG2	2.27	0.65
2:H:29:TRP:CD2	2:H:121:VAL:HG13	2.32	0.65
2:K:17:VAL:O	2:K:188:GLY:HA2	1.96	0.65
1:J:1:CYS:C	2:K:122:CYS:SG	2.81	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:1(A):ASP:HA	2:H:206:ARG:HH12	1.63	0.64
2:H:29:TRP:CG	2:H:121:VAL:HG13	2.33	0.63
2:H:38:GLN:O	2:H:40:LEU:N	2.32	0.62
3:Q:20:ARG:HD2	3:Q:44:ASN:OD1	1.99	0.62
3:Q:4:PHE:O	3:Q:7:GLU:HG2	1.99	0.62
2:H:76:TYR:HE2	2:H:77(A):ARG:HG2	1.62	0.61
3:P:1:ARG:H2	3:P:2:PRO:HD3	1.66	0.61
2:K:50:ARG:NH1	2:K:107:LYS:HE2	2.14	0.60
2:H:66:VAL:HG21	2:H:85:LEU:HD21	1.84	0.60
2:K:18:GLU:HB2	2:K:188:GLY:HA2	1.85	0.59
2:H:95:ASN:HB3	2:H:97(A):GLU:HB3	1.84	0.58
2:K:95:ASN:HB3	2:K:97(A):GLU:HB3	1.83	0.58
2:H:165:ARG:HB3	2:H:166:PRO:HD3	1.84	0.58
2:K:86:GLU:HB2	2:K:109:LYS:HA	1.84	0.58
2:H:126:ARG:HD2	2:H:232:PHE:HZ	1.68	0.58
2:K:49:ASP:O	2:K:112:VAL:HG12	2.04	0.58
3:Q:1:ARG:H2	3:Q:2:PRO:HD3	1.69	0.57
2:K:60(B):PRO:O	2:K:60(E):ASP:HB2	2.05	0.57
2:H:84:MET:HB2	2:H:109:LYS:CG	2.34	0.57
3:Q:35:TYR:CZ	3:Q:40:ALA:HB2	2.40	0.57
3:P:20:ARG:O	3:P:32:THR:HA	2.05	0.57
2:K:64:LEU:H	2:K:64:LEU:HD23	1.70	0.57
2:H:124:PRO:HD3	2:H:209:GLN:O	2.05	0.56
2:K:37(A):PRO:C	2:K:39:GLU:H	2.12	0.56
2:H:39:GLU:HB2	3:P:18:ILE:HG23	1.86	0.56
3:P:4:PHE:O	3:P:7:GLU:HG2	2.06	0.56
3:Q:1:ARG:CB	3:Q:58:ALA:HA	2.34	0.56
2:H:84:MET:HB2	2:H:109:LYS:HG3	1.87	0.56
2:H:236:LYS:HD3	2:H:239:GLN:NE2	2.21	0.56
2:K:130:LEU:HG	2:K:210:MET:HE2	1.88	0.56
2:K:85:LEU:HD22	2:K:106:MET:HB3	1.88	0.56
3:P:1:ARG:N	3:P:2:PRO:HD3	2.21	0.56
1:J:5:PRO:HB2	2:K:116:ASP:HA	1.87	0.55
2:K:66:VAL:HG21	2:K:85:LEU:HD21	1.88	0.55
3:Q:1:ARG:N	3:Q:2:PRO:HD3	2.21	0.55
2:H:38:GLN:O	2:H:38:GLN:HG2	2.07	0.55
1:L:14(A):LYS:HG2	2:H:23:GLU:OE2	2.08	0.54
2:H:31:VAL:HG22	2:H:68:ILE:HG23	1.89	0.54
2:H:31:VAL:CG1	2:H:66:VAL:HG13	2.39	0.53
2:H:147:THR:HG22	2:H:149:THR:H	1.72	0.53
2:H:34:PHE:CE2	2:H:65:LEU:HD12	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:4:PHE:O	3:P:43:ASN:HB2	2.09	0.53
3:Q:9:PRO:HB2	3:Q:33:PHE:CD2	2.43	0.53
2:H:95:ASN:HB2	2:H:98:ASN:OD1	2.10	0.52
2:H:18:GLU:HG3	2:H:187:ARG:CB	2.36	0.52
2:K:73:ARG:HD3	2:K:152:PRO:O	2.10	0.52
2:H:126:ARG:HD2	2:H:232:PHE:CZ	2.46	0.51
2:H:195:SER:OG	3:P:15:LYS:HB2	2.10	0.51
2:H:203:SER:HB3	2:H:204(B):ASN:OD1	2.10	0.51
2:K:91:HIS:CE1	2:K:93:ARG:HB2	2.46	0.51
2:K:29:TRP:CG	2:K:121:VAL:HG13	2.45	0.50
2:H:140:GLY:HA3	2:H:194:ASP:OD1	2.11	0.50
2:K:39:GLU:HA	3:Q:19:ILE:N	2.25	0.50
2:K:178:ASP:O	2:K:233:ARG:HD2	2.12	0.50
3:P:35:TYR:CZ	3:P:40:ALA:HB2	2.47	0.50
2:H:36:LYS:H	2:H:36:LYS:CE	2.24	0.49
2:H:81:LYS:HZ3	2:H:113:ALA:H	1.61	0.49
2:K:31:VAL:HG22	2:K:68:ILE:HG23	1.94	0.49
2:K:165:ARG:NH2	2:K:177:THR:O	2.46	0.49
2:H:76:TYR:CE2	2:H:77(A):ARG:HG2	2.46	0.49
2:H:34:PHE:HE2	2:H:65:LEU:HD12	1.78	0.48
2:K:37(A):PRO:C	2:K:39:GLU:N	2.71	0.48
2:K:195:SER:OG	3:Q:15:LYS:HB2	2.13	0.48
3:Q:2:PRO:HD2	3:Q:5:CYS:SG	2.52	0.48
2:H:81:LYS:HZ2	2:H:113:ALA:H	1.62	0.48
2:H:151:GLN:HG2	4:H:276:HOH:O	2.14	0.48
2:K:61:GLU:O	2:K:62:ASN:HB2	2.13	0.48
3:P:23:TYR:HE2	3:P:58:ALA:HB3	1.77	0.48
1:J:1(D):GLY:CA	4:J:56:HOH:O	2.24	0.48
3:Q:35:TYR:OH	3:Q:40:ALA:HB2	2.14	0.48
2:K:95:ASN:CB	2:K:97(A):GLU:HB3	2.43	0.47
3:Q:1:ARG:HA	3:Q:58:ALA:HA	1.96	0.47
3:P:35:TYR:OH	3:P:40:ALA:HB2	2.14	0.47
2:H:76:TYR:CE2	2:H:77(A):ARG:HA	2.49	0.47
2:K:87:LYS:HD2	2:K:87:LYS:HA	1.62	0.47
2:H:36:LYS:H	2:H:36:LYS:NZ	2.13	0.47
2:K:95:ASN:HB2	2:K:98:ASN:OD1	2.13	0.47
2:H:60(B):PRO:HB3	2:H:60(D):TRP:CZ2	2.50	0.47
2:K:81:LYS:HD2	2:K:118:ILE:HD12	1.97	0.47
3:Q:20:ARG:O	3:Q:32:THR:HA	2.15	0.47
3:P:23:TYR:CE2	3:P:58:ALA:HB3	2.50	0.47
3:P:2:PRO:HD2	3:P:5:CYS:SG	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:201:MET:SD	2:K:210:MET:HG3	2.56	0.46
2:H:165:ARG:NH2	2:H:177:THR:O	2.48	0.46
2:H:39:GLU:HA	3:P:19:ILE:H	1.81	0.46
2:K:93:ARG:O	2:K:95:ASN:ND2	2.48	0.46
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.97	0.45
1:L:14(J):TYR:HE2	2:H:202:LYS:O	1.98	0.45
2:H:38:GLN:C	2:H:40:LEU:H	2.24	0.45
2:K:41:LEU:HB3	3:Q:17:ARG:HB3	1.99	0.45
2:K:101:ARG:HG2	2:K:234:LEU:HD11	1.99	0.45
2:H:60(B):PRO:O	2:H:60(E):ASP:HB2	2.16	0.45
2:H:211:GLY:HA2	2:H:229:THR:O	2.16	0.45
2:H:144:LEU:HD21	2:H:152:PRO:HB3	1.99	0.45
2:K:165:ARG:HB3	2:K:166:PRO:HD3	1.99	0.45
2:K:203:SER:HB3	2:K:204(B):ASN:OD1	2.17	0.45
2:H:53:LEU:HD11	2:H:103:ILE:HD11	1.98	0.44
1:L:1:CYS:C	2:H:122:CYS:SG	3.00	0.44
1:J:10:LYS:HB3	1:J:12:LEU:HD23	1.99	0.44
2:K:128:THR:HG23	2:K:129(C):LEU:HD12	2.00	0.44
3:Q:7:GLU:HA	3:Q:8:PRO:HD3	1.90	0.44
2:K:75:ARG:NH1	2:K:77:GLU:HG2	2.32	0.44
2:H:242:ILE:O	2:H:242:ILE:HG22	2.18	0.43
3:P:1:ARG:CB	3:P:58:ALA:HA	2.44	0.43
2:K:39:GLU:HB3	3:Q:19:ILE:O	2.18	0.43
2:K:39:GLU:HG3	2:K:39:GLU:O	2.18	0.43
2:H:197:GLY:HA3	4:H:272:HOH:O	2.18	0.43
2:H:36:LYS:H	2:H:36:LYS:CD	2.32	0.43
2:H:37(A):PRO:C	2:H:39:GLU:N	2.77	0.43
2:K:38:GLN:O	2:K:38:GLN:HG2	2.19	0.43
1:J:14(J):TYR:HE2	2:K:202:LYS:O	2.02	0.42
2:K:25:GLY:O	2:K:28:PRO:HD3	2.19	0.42
2:H:130:LEU:HG	2:H:210:MET:HE2	2.01	0.42
2:H:33:LEU:CD2	2:H:106:MET:HE1	2.40	0.42
3:P:20:ARG:HD2	3:P:44:ASN:OD1	2.19	0.42
2:H:85:LEU:HD22	2:H:106:MET:HB3	2.01	0.41
3:Q:46:LYS:NZ	3:Q:46:LYS:CB	2.83	0.41
2:H:84:MET:HB2	2:H:109:LYS:HG2	2.02	0.41
1:J:14(K):ILE:O	1:J:14(K):ILE:HG22	2.18	0.41
2:K:70:LYS:HB3	2:K:70:LYS:HE2	1.61	0.41
2:H:178:ASP:HB3	2:H:233:ARG:CZ	2.51	0.41
2:K:197:GLY:O	2:K:213:VAL:HG23	2.20	0.41
3:P:20:ARG:CD	3:P:44:ASN:OD1	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:105:LEU:HD11	2:K:238:ILE:HG23	2.03	0.41
1:L:10:LYS:HB3	1:L:12:LEU:HD23	2.03	0.41
2:K:242:ILE:O	2:K:242:ILE:HG22	2.20	0.41
2:K:81:LYS:HD2	2:K:118:ILE:CD1	2.51	0.40
1:J:14(A):LYS:HG2	2:K:23:GLU:OE2	2.22	0.40
2:K:56:ALA:HB1	2:K:90:ILE:HG23	2.04	0.40
2:K:224:LYS:HA	2:K:224:LYS:HD3	1.83	0.40
3:Q:1:ARG:CA	3:Q:58:ALA:HA	2.51	0.40
1:L:14:ASP:OD1	1:L:14(C):GLU:HB2	2.21	0.40
2:K:98:ASN:O	2:K:99:LEU:HB2	2.21	0.40
2:K:136:GLY:O	2:K:159:ASN:HA	2.21	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	J	29/36 (81%)	25 (86%)	4 (14%)	0	100	100
1	L	29/36 (81%)	25 (86%)	4 (14%)	0	100	100
2	H	252/259 (97%)	237 (94%)	9 (4%)	6 (2%)	4	4
2	K	252/259 (97%)	233 (92%)	14 (6%)	5 (2%)	6	5
3	P	56/58 (97%)	55 (98%)	0	1 (2%)	6	6
3	Q	56/58 (97%)	52 (93%)	3 (5%)	1 (2%)	6	6
All	All	674/706 (96%)	627 (93%)	34 (5%)	13 (2%)	6	5

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	H	39	GLU

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Mol	Chain	Res	Type
2	K	97(A)	GLU
2	H	38	GLN
2	H	77(A)	ARG
2	H	97(A)	GLU
2	K	62	ASN
3	P	56	GLY
2	K	39	GLU
2	K	61	GLU
2	K	63	ASP
2	H	61	GLU
2	H	149	THR
3	Q	56	GLY

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	27/31 (87%)	27 (100%)	0	100	100
1	L	27/31 (87%)	27 (100%)	0	100	100
2	H	222/226 (98%)	208 (94%)	14 (6%)	16	23
2	K	222/226 (98%)	217 (98%)	5 (2%)	44	63
3	P	46/46 (100%)	42 (91%)	4 (9%)	9	12
3	Q	46/46 (100%)	41 (89%)	5 (11%)	6	7
All	All	590/606 (97%)	562 (95%)	28 (5%)	23	35

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	H	36	LYS
2	H	42	CYS
2	H	45	SER
2	H	64	LEU
2	H	84	MET
2	H	96	TRP

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Mol	Chain	Res	Type
2	H	121	VAL
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	139	THR
2	H	153	SER
2	H	172	THR
2	H	180	MET
2	H	235	LYS
2	K	63	ASP
2	K	95	ASN
2	K	96	TRP
2	K	99	LEU
2	K	121	VAL
3	P	20	ARG
3	P	29	LEU
3	P	42	ARG
3	P	46	LYS
3	Q	1	ARG
3	Q	3	ASP
3	Q	29	LEU
3	Q	42	ARG
3	Q	46	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
2	H	71	HIS
2	H	95	ASN
2	H	179	ASN
2	H	239	GLN
2	K	95	ASN
2	K	179	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 [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.