



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:42 AM UTC

PDB ID : 1KIG / pdb_00001kig
Title : BOVINE FACTOR XA
Authors : Wei, A.; Alexander, R.; Chang, C.-H.
Deposited on : 1997-04-24
Resolution : 3.00 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

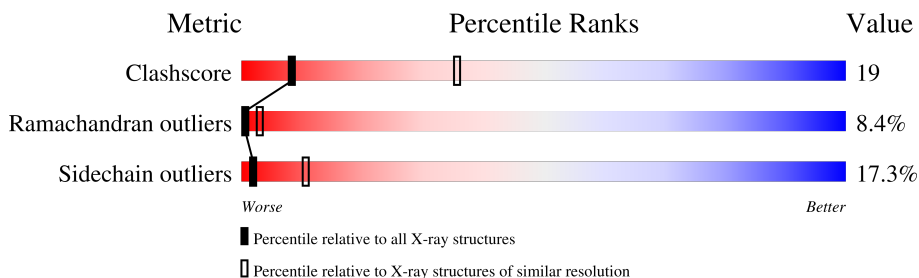
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)

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	H	241	31% 49% 17% .
2	L	51	31% 43% 20% 6%
3	I	60	27% 37% 25% 12%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2756 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 FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	241	Total	C	N	O	S	20	0	0
			1880	1179	332	354	15			

- Molecule 2 is a protein called FACTOR XA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	51	Total	C	N	O	S	14	0	0
			388	228	73	80	7			

- Molecule 3 is a protein called ANTICOAGULANT PEPTIDE.

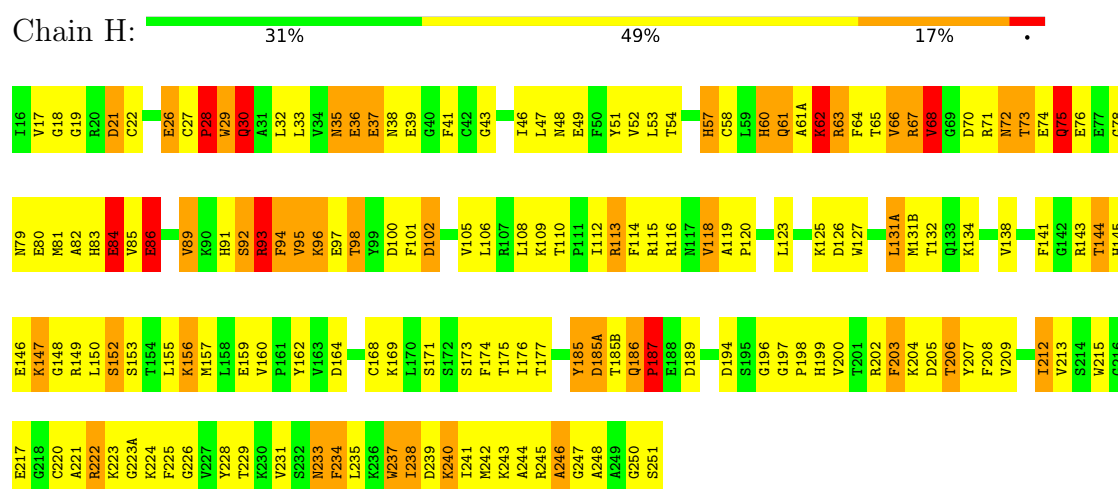
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	60	Total	C	N	O	S	0	0	0
			488	301	85	96	6			

3 Residue-property plots

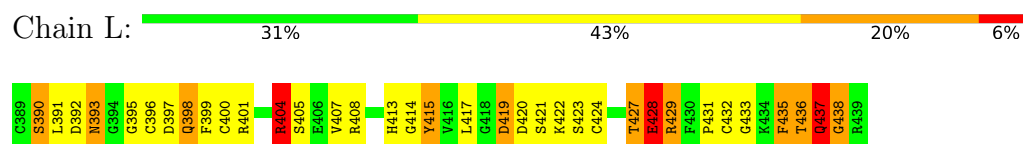
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

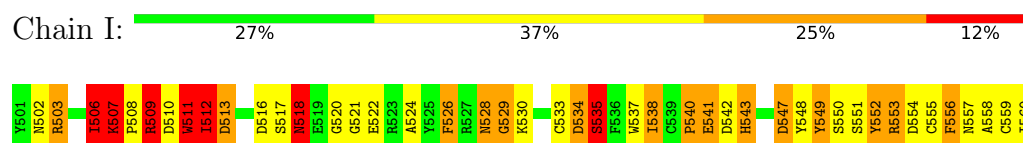
• Molecule 1: FACTOR XA



• Molecule 2: FACTOR XA



• Molecule 3: ANTICOAGULANT PEPTIDE



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 42 21 2	Depositor
Cell constants a, b, c, α , β , γ	133.10Å 133.10Å 68.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.187 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2756	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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	H	1.23	9/1920 (0.5%)	2.28	94/2588 (3.6%)
2	L	1.27	3/393 (0.8%)	2.28	28/522 (5.4%)
3	I	1.37	2/502 (0.4%)	2.49	37/677 (5.5%)
All	All	1.26	14/2815 (0.5%)	2.32	159/3787 (4.2%)

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
1	H	0	2
3	I	0	4
All	All	0	6

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	57	HIS	CD2-NE2	-7.89	1.29	1.37
3	I	512	ILE	CA-CB	7.79	1.65	1.54
2	L	427	THR	CA-CB	6.87	1.63	1.53
1	H	145	HIS	CD2-NE2	-6.80	1.30	1.37
1	H	91	HIS	CD2-NE2	-6.79	1.30	1.37
2	L	436	THR	CA-CB	6.56	1.62	1.53
1	H	83	HIS	CD2-NE2	-6.49	1.30	1.37
1	H	199	HIS	CD2-NE2	-6.39	1.30	1.37
1	H	60	HIS	CD2-NE2	-6.26	1.30	1.37
2	L	413	HIS	CD2-NE2	-6.23	1.30	1.37
3	I	547	ASP	CA-CB	5.65	1.63	1.53
1	H	57	HIS	CG-ND1	-5.34	1.32	1.38
1	H	145	HIS	CG-ND1	-5.16	1.32	1.38
1	H	160	VAL	CA-CB	5.11	1.60	1.54

All (159) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	547	ASP	CA-CB-CG	12.81	125.42	112.60
2	L	435	PHE	CA-CB-CG	11.20	125.00	113.80
1	H	205	ASP	CA-CB-CG	-10.99	101.61	112.60
3	I	543	HIS	CA-CB-CG	10.88	124.67	113.80
1	H	235	LEU	N-CA-C	10.77	122.70	110.97
1	H	30	GLN	OE1-CD-NE2	-10.74	111.86	122.60
1	H	72	ASN	CA-CB-CG	10.57	123.17	112.60
1	H	185	TYR	N-CA-C	10.44	128.63	114.12
3	I	534	ASP	CA-CB-CG	10.29	122.89	112.60
1	H	189	ASP	CA-CB-CG	10.21	122.81	112.60
1	H	149	ARG	N-CA-C	9.62	124.76	110.52
1	H	205	ASP	N-CA-C	9.58	124.76	111.92
3	I	511	TRP	CA-C-O	-9.55	110.77	120.80
2	L	419	ASP	CA-CB-CG	9.32	121.92	112.60
3	I	518	ASN	CA-CB-CG	9.25	121.85	112.60
1	H	96	LYS	N-CA-C	9.21	126.57	111.37
3	I	513	ASP	N-CA-C	9.15	122.62	109.71
3	I	528	ASN	CA-CB-CG	8.91	121.51	112.60
2	L	436	THR	N-CA-C	8.74	123.42	109.79
1	H	150	LEU	N-CA-C	8.61	122.99	110.42
1	H	102	ASP	CA-CB-CG	8.57	121.17	112.60
1	H	72	ASN	OD1-CG-ND2	-8.46	114.14	122.60
1	H	38	ASN	OD1-CG-ND2	-8.27	114.33	122.60
1	H	176	ILE	N-CA-C	-8.22	98.04	108.89
1	H	226	GLY	CA-C-O	-7.79	114.33	121.18
1	H	159	GLU	N-CA-CB	-7.71	97.44	110.16
2	L	437	GLN	O-C-N	7.65	131.80	121.78
1	H	113	ARG	N-CA-C	-7.65	96.10	108.41
1	H	70	ASP	CA-CB-CG	7.49	120.09	112.60
3	I	535	SER	N-CA-C	-7.46	94.90	110.80
1	H	119	ALA	O-C-N	-7.43	116.22	121.65
1	H	240	LYS	CA-CB-CG	7.37	128.85	114.10
1	H	91	HIS	CB-CG-CD2	-7.33	121.67	131.20
1	H	75	GLN	OE1-CD-NE2	-7.29	115.31	122.60
1	H	234	PHE	CA-CB-CG	-7.25	106.55	113.80
2	L	429	ARG	N-CA-C	-7.23	103.57	113.18
3	I	511	TRP	CG-CD2-CE3	7.22	141.12	133.90
2	L	398	GLN	OE1-CD-NE2	-7.16	115.44	122.60
1	H	30	GLN	CG-CD-NE2	7.12	127.08	116.40
1	H	159	GLU	N-CA-C	-7.11	97.66	109.46
1	H	33	LEU	N-CA-C	-7.09	97.00	108.41
1	H	96	LYS	CA-C-O	-7.07	113.00	120.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	116	ARG	N-CA-C	-7.00	99.92	110.28
3	I	552	TYR	N-CA-C	-6.99	102.23	111.24
3	I	526	PHE	N-CA-C	-6.95	99.65	110.42
2	L	397	ASP	N-CA-C	6.94	121.19	112.87
2	L	393	ASN	CA-CB-CG	6.92	119.52	112.60
1	H	240	LYS	N-CA-C	-6.91	103.44	110.97
1	H	89	VAL	O-C-N	-6.78	116.13	123.18
3	I	506	ILE	N-CA-C	6.72	118.85	108.44
2	L	435	PHE	N-CA-C	6.71	121.31	112.72
3	I	553	ARG	N-CA-C	-6.69	99.92	109.96
1	H	126	ASP	N-CA-C	6.64	118.59	111.36
2	L	438	GLY	O-C-N	6.61	131.29	122.70
1	H	246	ALA	CB-CA-C	-6.58	108.97	116.54
1	H	66	VAL	N-CA-C	6.54	116.66	107.37
2	L	438	GLY	CA-C-N	6.52	133.43	121.70
2	L	438	GLY	C-N-CA	6.52	133.43	121.70
1	H	29	TRP	CG-CD2-CE3	6.50	140.40	133.90
1	H	92	SER	CA-C-O	6.49	128.48	121.02
1	H	115	ARG	O-C-N	-6.46	118.26	123.11
3	I	518	ASN	OD1-CG-ND2	-6.45	116.15	122.60
3	I	511	TRP	CA-CB-CG	6.41	125.78	113.60
3	I	549	TYR	N-CA-C	6.29	118.69	108.63
2	L	397	ASP	CA-CB-CG	-6.25	106.35	112.60
1	H	91	HIS	CB-CG-ND1	6.24	132.06	122.70
1	H	57	HIS	CB-CG-CD2	-6.21	123.12	131.20
1	H	131(A)	LEU	N-CA-C	6.21	117.85	111.14
1	H	35	ASN	CB-CG-ND2	-6.18	107.12	116.40
3	I	507	LYS	CG-CD-CE	6.15	125.44	111.30
1	H	159	GLU	CB-CA-C	6.12	119.84	109.80
1	H	39	GLU	CA-CB-CG	-6.08	101.93	114.10
1	H	68	VAL	N-CA-CB	-6.05	104.14	111.21
1	H	35	ASN	N-CA-C	6.02	123.63	110.80
1	H	173	SER	N-CA-C	-5.99	106.11	113.41
2	L	427	THR	CA-C-O	5.96	126.65	120.40
1	H	152	SER	CA-C-O	5.93	127.37	120.49
1	H	203	PHE	N-CA-C	-5.90	98.79	108.41
1	H	194	ASP	CA-CB-CG	5.89	118.49	112.60
3	I	549	TYR	CA-C-O	5.87	127.77	121.02
1	H	168	CYS	CA-CB-SG	5.86	127.88	114.40
1	H	222	ARG	CG-CD-NE	-5.85	99.13	112.00
3	I	507	LYS	CA-C-O	5.83	128.15	120.16
3	I	534	ASP	CA-C-N	5.82	132.66	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	534	ASP	C-N-CA	5.82	132.66	121.54
1	H	17	VAL	O-C-N	-5.82	115.84	122.94
1	H	78	GLY	O-C-N	5.80	130.24	122.70
1	H	186	GLN	N-CA-C	5.80	117.83	109.48
1	H	123	LEU	N-CA-C	-5.77	102.34	110.31
1	H	84	GLU	N-CA-C	-5.72	101.74	110.14
1	H	28	PRO	CA-C-O	5.69	125.17	118.68
3	I	516	ASP	O-C-N	-5.67	116.33	122.79
1	H	83	HIS	CB-CG-CD2	-5.67	123.83	131.20
1	H	144	THR	N-CA-CB	-5.66	101.25	110.42
3	I	509	ARG	CA-C-N	5.62	132.27	121.54
3	I	509	ARG	C-N-CA	5.62	132.27	121.54
2	L	420	ASP	CA-CB-CG	5.61	118.21	112.60
3	I	513	ASP	CA-CB-CG	5.58	118.18	112.60
1	H	57	HIS	CA-CB-CG	5.58	119.38	113.80
1	H	212	ILE	O-C-N	-5.55	117.21	122.98
2	L	413	HIS	O-C-N	5.53	130.37	123.01
3	I	540	PRO	O-C-N	5.52	128.14	122.18
1	H	112	ILE	N-CA-CB	-5.52	104.52	111.31
1	H	187	PRO	N-CA-C	5.50	123.80	112.47
1	H	21	ASP	CA-CB-CG	5.50	118.10	112.60
1	H	206	THR	N-CA-C	-5.50	99.47	108.76
1	H	21	ASP	O-C-N	-5.49	116.33	122.75
1	H	48	ASN	CA-CB-CG	5.48	118.08	112.60
2	L	415	TYR	N-CA-C	-5.44	100.03	108.90
3	I	540	PRO	CA-C-N	5.44	127.57	120.28
3	I	540	PRO	C-N-CA	5.44	127.57	120.28
1	H	132	THR	N-CA-C	-5.41	106.26	112.92
2	L	390	SER	CA-C-O	-5.41	112.78	120.51
1	H	62	LYS	N-CA-C	-5.40	99.30	110.80
1	H	48	ASN	OD1-CG-ND2	-5.39	117.21	122.60
2	L	408	ARG	CA-C-O	5.37	127.72	121.11
3	I	516	ASP	CA-CB-CG	5.37	117.97	112.60
1	H	93	ARG	NE-CZ-NH2	-5.35	114.38	119.20
2	L	438	GLY	N-CA-C	5.35	125.86	113.18
3	I	509	ARG	O-C-N	5.35	129.70	122.59
1	H	118	VAL	CA-C-O	-5.34	115.46	120.22
2	L	399	PHE	N-CA-C	5.29	117.52	110.53
1	H	209	VAL	CA-CB-CG2	-5.28	101.42	110.40
1	H	221	ALA	CA-C-O	5.26	128.03	120.51
1	H	91	HIS	CA-C-O	-5.25	113.00	120.51
2	L	428	GLU	N-CA-C	-5.25	99.62	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	177	THR	CA-CB-OG1	-5.25	101.73	109.60
1	H	38	ASN	CB-CG-ND2	5.24	124.25	116.40
2	L	431	PRO	N-CD-CG	-5.22	95.37	103.20
3	I	502	ASN	OD1-CG-ND2	5.22	127.82	122.60
3	I	548	TYR	N-CA-C	5.22	117.86	110.50
1	H	237	TRP	CG-CD2-CE3	5.21	139.11	133.90
1	H	28	PRO	CB-CA-C	5.21	115.83	110.00
1	H	177	THR	CA-C-N	5.21	125.26	119.32
1	H	177	THR	C-N-CA	5.21	125.26	119.32
1	H	237	TRP	CE2-CD2-CG	-5.21	100.95	107.20
1	H	243	LYS	CG-CD-CE	5.21	123.27	111.30
1	H	238	ILE	CA-C-N	5.18	128.18	120.31
1	H	238	ILE	C-N-CA	5.18	128.18	120.31
1	H	127	TRP	CE2-CD2-CG	-5.17	101.00	107.20
3	I	537	TRP	CG-CD2-CE3	5.17	139.07	133.90
1	H	215	TRP	CE2-CD2-CG	-5.14	101.04	107.20
1	H	29	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	H	67	ARG	CA-CB-CG	5.12	124.33	114.10
1	H	83	HIS	CB-CG-ND1	5.11	130.37	122.70
2	L	398	GLN	CA-CB-CG	5.10	124.30	114.10
1	H	83	HIS	N-CA-C	-5.10	102.24	110.14
1	H	86	GLU	N-CA-C	-5.09	107.62	113.88
3	I	533	CYS	CA-C-O	-5.09	115.94	121.89
3	I	517	SER	CA-C-N	5.09	128.04	120.31
3	I	517	SER	C-N-CA	5.09	128.04	120.31
1	H	63	ARG	CD-NE-CZ	-5.08	117.29	124.40
2	L	393	ASN	OD1-CG-ND2	-5.07	117.53	122.60
2	L	437	GLN	CA-C-N	5.07	131.34	121.41
2	L	437	GLN	C-N-CA	5.07	131.34	121.41
2	L	404	ARG	CD-NE-CZ	-5.07	117.31	124.40
3	I	556	PHE	O-C-N	-5.02	116.61	122.03
1	H	237	TRP	CB-CG-CD1	-5.02	119.37	126.90
1	H	57	HIS	CB-CG-ND1	5.01	130.22	122.70

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	H	228	TYR	Sidechain
1	H	247	GLY	Peptide
3	I	506	ILE	Peptide
3	I	507	LYS	Peptide

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Mol	Chain	Res	Type	Group
3	I	529	GLY	Mainchain
3	I	552	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	H	1880	0	1828	75	4
2	L	388	0	346	12	2
3	I	488	0	418	19	6
All	All	2756	0	2592	101	6

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 (101) 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:H:94:PHE:HE2	1:H:96:LYS:HZ2	1.04	1.00
1:H:35:ASN:HD21	1:H:61(A):ALA:HA	1.47	0.79
2:L:415:TYR:HB3	2:L:424:CYS:HB3	1.65	0.79
1:H:185(B):THR:HA	1:H:223:LYS:HD2	1.65	0.78
2:L:400:CYS:SG	2:L:407:VAL:HB	2.24	0.77
1:H:185:TYR:HB3	1:H:186:GLN:HB3	1.68	0.75
1:H:41:PHE:CZ	1:H:61(A):ALA:HB2	2.22	0.74
1:H:239:ASP:HA	1:H:242:MET:HB2	1.71	0.72
3:I:509:ARG:NH1	3:I:511:TRP:HA	2.04	0.71
1:H:30:GLN:HG3	1:H:155:LEU:HD11	1.72	0.71
1:H:237:TRP:HA	1:H:240:LYS:HE2	1.73	0.69
1:H:67:ARG:HA	1:H:82:ALA:HA	1.75	0.69
3:I:540:PRO:HA	3:I:543:HIS:ND1	2.09	0.68
1:H:86:GLU:HB2	1:H:109:LYS:HG2	1.76	0.67
1:H:212:ILE:HB	1:H:229:THR:HB	1.75	0.67
1:H:26:GLU:O	1:H:28:PRO:HD3	1.94	0.66
2:L:437:GLN:NE2	2:L:438:GLY:H	1.93	0.65
1:H:73:THR:O	1:H:76:GLU:HG2	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:147:LYS:HG3	3:I:558:ALA:HB2	1.79	0.65
3:I:524:ALA:HB3	3:I:526:PHE:CE1	2.32	0.65
3:I:556:PHE:HA	3:I:560:ILE:HD13	1.79	0.64
1:H:27:CYS:HB2	1:H:155:LEU:HD21	1.83	0.60
1:H:202:ARG:NH2	1:H:204:LYS:HA	2.17	0.60
3:I:556:PHE:HA	3:I:560:ILE:CD1	2.33	0.59
3:I:506:ILE:HB	3:I:508:PRO:HG3	1.85	0.58
1:H:62:LYS:HE3	1:H:62:LYS:HA	1.85	0.58
1:H:147:LYS:HZ3	3:I:554:ASP:CG	2.11	0.58
1:H:202:ARG:HB3	1:H:207:TYR:CE1	2.38	0.58
3:I:528:ASN:HB3	3:I:534:ASP:HB3	1.87	0.57
1:H:202:ARG:HH21	1:H:204:LYS:HA	1.70	0.56
1:H:206:THR:HA	2:L:433:GLY:O	2.05	0.55
2:L:437:GLN:HE21	2:L:438:GLY:H	1.53	0.55
1:H:73:THR:HB	1:H:153:SER:OG	2.07	0.55
1:H:241:ILE:HA	1:H:244:ALA:O	2.07	0.55
1:H:84:GLU:CD	1:H:109:LYS:HZ3	2.16	0.54
1:H:185(B):THR:HA	1:H:223:LYS:CD	2.34	0.54
1:H:22:CYS:SG	1:H:157:MET:HB3	2.48	0.53
1:H:51:TYR:HB3	1:H:105:VAL:HG12	1.90	0.53
1:H:197:GLY:O	1:H:213:VAL:HG23	2.07	0.53
1:H:120:PRO:O	2:L:432:CYS:HA	2.08	0.52
3:I:521:GLY:HA2	3:I:538:ILE:O	2.08	0.52
1:H:95:VAL:HB	1:H:98:THR:HB	1.92	0.52
3:I:511:TRP:O	3:I:512:ILE:HB	2.09	0.52
1:H:35:ASN:HA	1:H:63:ARG:O	2.10	0.51
3:I:511:TRP:CE3	3:I:542:ASP:HB3	2.45	0.51
1:H:36:GLU:HG3	1:H:63:ARG:H	1.75	0.51
1:H:101:PHE:HA	1:H:234:PHE:CZ	2.47	0.50
2:L:395:GLY:O	2:L:422:LYS:HB3	2.11	0.50
1:H:202:ARG:HB3	1:H:207:TYR:CZ	2.47	0.50
1:H:18:GLY:O	1:H:156:LYS:NZ	2.45	0.50
1:H:85:VAL:HG22	1:H:108:LEU:HD23	1.94	0.50
1:H:143:ARG:HD3	1:H:148:GLY:O	2.12	0.49
1:H:58:CYS:HA	1:H:61:GLN:HE21	1.78	0.49
1:H:46:ILE:HD11	1:H:68:VAL:HG13	1.93	0.49
1:H:51:TYR:HB3	1:H:105:VAL:CG1	2.43	0.49
1:H:74:GLU:N	1:H:153:SER:OG	2.42	0.49
1:H:47:LEU:HD11	1:H:53:LEU:HG	1.93	0.48
1:H:185(A):ASP:OD1	1:H:223(A):GLY:HA2	2.12	0.48
1:H:174:PHE:HE1	1:H:217:GLU:HG2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:146:GLU:HB2	1:H:220:CYS:HB2	1.95	0.48
2:L:417:LEU:HA	2:L:423:SER:O	2.14	0.48
1:H:28:PRO:HD2	1:H:29:TRP:CD2	2.49	0.47
1:H:92:SER:HB2	1:H:251:SER:OXT	2.14	0.47
3:I:520:GLY:O	3:I:540:PRO:HG3	2.14	0.47
3:I:541:GLU:H	3:I:541:GLU:CD	2.23	0.47
1:H:72:ASN:HB2	1:H:75:GLN:NE2	2.30	0.47
1:H:94:PHE:HA	1:H:100:ASP:O	2.14	0.47
2:L:437:GLN:NE2	2:L:438:GLY:N	2.61	0.47
3:I:511:TRP:HB2	3:I:513:ASP:OD1	2.15	0.47
3:I:549:TYR:CE2	3:I:559:CYS:SG	3.08	0.47
1:H:223:LYS:HD3	1:H:223:LYS:HA	1.86	0.45
1:H:93:ARG:NH2	1:H:250:GLY:O	2.50	0.45
1:H:185(A):ASP:HB2	1:H:225:PHE:CE1	2.52	0.44
1:H:131(A):LEU:HD21	1:H:203:PHE:HB2	1.99	0.44
2:L:437:GLN:HE21	2:L:437:GLN:HB2	1.32	0.44
1:H:52:VAL:HG21	1:H:66:VAL:HG11	2.00	0.44
1:H:97:GLU:O	3:I:503:ARG:NH2	2.51	0.43
1:H:186:GLN:HA	1:H:187:PRO:HD3	1.79	0.43
1:H:37:GLU:CD	1:H:37:GLU:N	2.77	0.43
1:H:57:HIS:HD2	1:H:102:ASP:OD2	2.00	0.43
1:H:114:PHE:HA	1:H:118:VAL:HB	1.99	0.43
1:H:94:PHE:CD1	1:H:102:ASP:HA	2.54	0.43
1:H:234:PHE:O	1:H:238:ILE:HG13	2.17	0.43
3:I:520:GLY:O	3:I:543:HIS:CE1	2.72	0.43
1:H:138:VAL:HA	1:H:198:PRO:O	2.19	0.43
2:L:414:GLY:O	2:L:427:THR:HB	2.19	0.42
1:H:43:GLY:O	1:H:196:GLY:HA3	2.19	0.42
1:H:89:VAL:HG22	1:H:246:ALA:O	2.19	0.42
1:H:57:HIS:O	1:H:61:GLN:NE2	2.53	0.42
1:H:202:ARG:HA	1:H:207:TYR:HA	2.00	0.42
1:H:141:PHE:HB3	1:H:152:SER:O	2.20	0.42
1:H:171:SER:O	1:H:224:LYS:HE2	2.19	0.42
1:H:200:VAL:HA	1:H:208:PHE:O	2.20	0.42
1:H:74:GLU:N	1:H:153:SER:HG	2.18	0.41
1:H:222:ARG:HB3	1:H:224:LYS:HB2	2.01	0.41
2:L:401:ARG:O	2:L:407:VAL:HA	2.19	0.41
1:H:84:GLU:OE1	1:H:109:LYS:NZ	2.53	0.41
1:H:94:PHE:HE2	1:H:96:LYS:NZ	1.92	0.41
1:H:101:PHE:HA	1:H:234:PHE:HZ	1.85	0.41
1:H:131(B):MET:HG2	1:H:162:TYR:CE2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:509:ARG:CZ	3:I:511:TRP:HA	2.51	0.41

All (6) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:233:ASN:O	3:I:518:ASN:ND2[3_655]	1.32	0.88
1:H:233:ASN:O	3:I:518:ASN:CG[3_655]	1.85	0.35
2:L:401:ARG:NH2	3:I:535:SER:OG[3_655]	1.97	0.23
1:H:233:ASN:C	3:I:518:ASN:ND2[3_655]	2.06	0.14
1:H:233:ASN:O	3:I:518:ASN:OD1[3_655]	2.17	0.03
2:L:404:ARG:NH1	3:I:556:PHE:CD2[3_655]	2.18	0.02

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	H	239/241 (99%)	190 (80%)	36 (15%)	13 (5%)	1	9
2	L	49/51 (96%)	32 (65%)	9 (18%)	8 (16%)	0	0
3	I	58/60 (97%)	37 (64%)	13 (22%)	8 (14%)	0	1
All	All	346/352 (98%)	259 (75%)	58 (17%)	29 (8%)	0	3

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	60	HIS
1	H	73	THR
1	H	79	ASN
1	H	93	ARG
2	L	421	SER
2	L	428	GLU

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Mol	Chain	Res	Type
3	I	512	ILE
3	I	529	GLY
3	I	535	SER
3	I	555	CYS
1	H	19	GLY
1	H	26	GLU
1	H	81	MET
2	L	392	ASP
2	L	405	SER
3	I	510	ASP
1	H	185(A)	ASP
1	H	245	ARG
1	H	248	ALA
2	L	404	ARG
3	I	509	ARG
1	H	94	PHE
2	L	390	SER
2	L	398	GLN
3	I	547	ASP
1	H	80	GLU
3	I	530	LYS
1	H	187	PRO
2	L	393	ASN

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	H	200/200 (100%)	168 (84%)	32 (16%)	2	12
2	L	44/44 (100%)	36 (82%)	8 (18%)	2	9
3	I	51/51 (100%)	40 (78%)	11 (22%)	1	6
All	All	295/295 (100%)	244 (83%)	51 (17%)	2	10

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	21	ASP
1	H	28	PRO
1	H	30	GLN
1	H	32	LEU
1	H	36	GLU
1	H	37	GLU
1	H	49	GLU
1	H	54	THR
1	H	61	GLN
1	H	62	LYS
1	H	64	PHE
1	H	65	THR
1	H	68	VAL
1	H	71	ARG
1	H	75	GLN
1	H	84	GLU
1	H	86	GLU
1	H	95	VAL
1	H	98	THR
1	H	106	LEU
1	H	110	THR
1	H	113	ARG
1	H	125	LYS
1	H	134	LYS
1	H	144	THR
1	H	147	LYS
1	H	156	LYS
1	H	164	ASP
1	H	169	LYS
1	H	175	THR
1	H	231	VAL
1	H	233	ASN
2	L	391	LEU
2	L	396	CYS
2	L	419	ASP
2	L	428	GLU
2	L	429	ARG
2	L	435	PHE
2	L	436	THR
2	L	437	GLN
3	I	503	ARG
3	I	507	LYS
3	I	511	TRP

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Mol	Chain	Res	Type
3	I	518	ASN
3	I	522	GLU
3	I	538	ILE
3	I	541	GLU
3	I	550	SER
3	I	551	SER
3	I	553	ARG
3	I	557	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	57	HIS
1	H	83	HIS
1	H	145	HIS
2	L	437	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 ⓘ

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.