



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:44 PM UTC

PDB ID : 1HXF / pdb_00001hxf
Title : HUMAN THROMBIN COMPLEX WITH HIRUDIN VARIANT
Authors : Tulinsky, A.; Zhang, E.
Deposited on : 1996-09-09
Resolution : 2.10 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

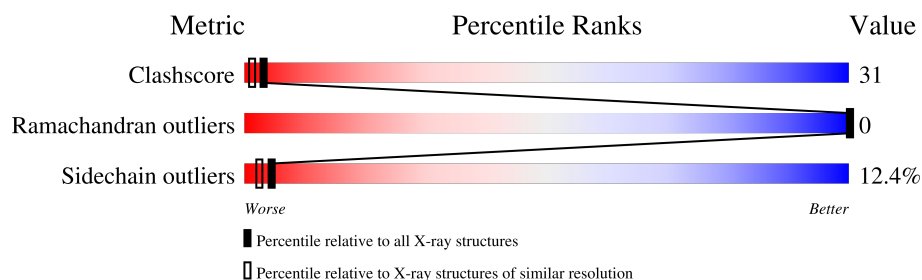
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	L	36	31% 28% 14% 28%
2	H	259	30% 44% 20% • •
3	I	10	30% 40% 10% 20%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2447 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 THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	26	Total	C	N	O	S	0	0	0
			217	137	35	44	1			

- Molecule 2 is a protein called THROMBIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	248	Total	C	N	O	S	0	0	0
			2007	1279	356	358	14			

- Molecule 3 is a protein called HIRUDIN VARIANT.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	10	Total	C	N	O	0	0	0
			85	56	10	19			

- Molecule 4 is water.

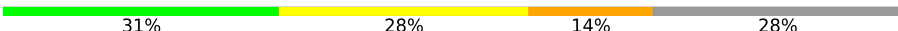
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	L	14	Total	O	0	0
			14	14		
4	H	121	Total	O	0	0
			121	121		
4	I	3	Total	O	0	0
			3	3		

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.

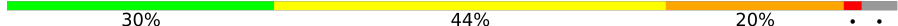
Note EDS was not executed.

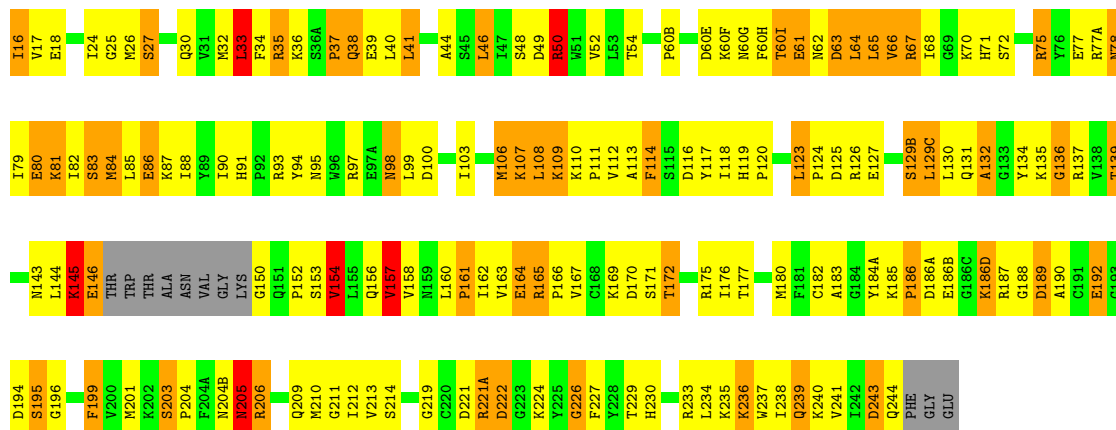
• Molecule 1: THROMBIN

Chain L: 

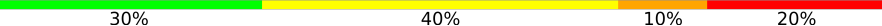


• Molecule 2: THROMBIN

Chain H: 



• Molecule 3: HIRUDIN VARIANT

Chain I: 



4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	70.66Å 72.47Å 73.09Å 90.00° 100.75° 90.00°	Depositor
Resolution (Å)	7.00 – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) (7.00-2.10)	Depositor
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.151 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2447	wwPDB-VP
Average B, all atoms (Å ²)	25.0	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	L	0.95	0/219	2.39	15/291 (5.2%)
2	H	1.13	0/2058	2.45	152/2780 (5.5%)
3	I	0.91	0/87	2.44	8/117 (6.8%)
All	All	1.11	0/2364	2.44	175/3188 (5.5%)

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	H	0	5
3	I	0	1
All	All	0	6

There are no bond length outliers.

All (175) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	132	ALA	CA-C-O	-12.39	106.80	120.92
2	H	205	ASN	OD1-CG-ND2	12.16	134.76	122.60
2	H	34	PHE	CA-CB-CG	11.03	124.83	113.80
2	H	132	ALA	O-C-N	10.84	136.39	122.95
2	H	109	LYS	CA-CB-CG	10.34	134.78	114.10
2	H	95	ASN	OD1-CG-ND2	-10.22	112.38	122.60
2	H	233	ARG	NE-CZ-NH1	10.18	131.68	121.50
1	L	3	LEU	CA-C-O	-9.01	111.17	120.54
2	H	233	ARG	NE-CZ-NH2	-8.88	111.21	119.20
2	H	114	PHE	CA-CB-CG	-8.87	104.93	113.80
3	I	64	LEU	CA-C-O	8.68	135.56	120.80
2	H	205	ASN	CB-CG-ND2	-8.62	103.47	116.40
2	H	205	ASN	CA-CB-CG	-8.50	104.10	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	192	GLU	CA-C-O	-8.37	113.01	120.88
2	H	60(E)	ASP	CA-CB-CG	-8.30	104.30	112.60
2	H	129(B)	SER	CA-C-O	-8.25	111.68	120.42
2	H	66	VAL	N-CA-CB	-8.22	101.10	111.46
3	I	63	TYR	CB-CA-C	8.04	126.80	109.99
2	H	111	PRO	N-CA-CB	7.89	110.21	103.35
2	H	163	VAL	CA-C-N	7.82	131.85	120.82
2	H	163	VAL	C-N-CA	7.82	131.85	120.82
2	H	118	ILE	O-C-N	7.81	130.61	123.03
2	H	100	ASP	CA-C-O	-7.76	112.47	121.16
2	H	77	GLU	CB-CG-CD	7.70	125.69	112.60
2	H	226	GLY	CA-C-O	-7.68	114.42	121.18
1	L	14(G)	LEU	CA-C-O	7.67	128.76	120.10
2	H	226	GLY	O-C-N	7.46	130.81	123.35
2	H	165	ARG	NE-CZ-NH1	7.43	128.93	121.50
1	L	13	GLU	CB-CG-CD	7.38	125.15	112.60
2	H	135	LYS	CA-C-O	-7.34	112.68	121.05
2	H	117	TYR	O-C-N	7.33	131.11	122.24
2	H	190	ALA	N-CA-C	-7.31	101.13	110.19
2	H	100	ASP	O-C-N	7.19	131.66	122.89
2	H	154	VAL	N-CA-CB	-7.19	99.06	112.36
2	H	221(A)	ARG	NE-CZ-NH1	-7.15	114.35	121.50
2	H	164	GLU	CB-CG-CD	7.13	124.73	112.60
2	H	98	ASN	OD1-CG-ND2	-7.08	115.52	122.60
2	H	49	ASP	CA-CB-CG	7.05	119.65	112.60
2	H	158	VAL	CA-C-O	-7.04	113.37	120.90
2	H	82	ILE	CA-C-O	-7.00	113.07	120.48
2	H	161	PRO	CA-C-O	-6.98	113.11	121.48
2	H	157	VAL	CA-C-O	-6.97	114.73	121.63
2	H	237	TRP	N-CA-C	-6.93	103.81	111.36
2	H	235	LYS	N-CA-C	6.82	119.56	111.71
2	H	38	GLN	CA-C-O	-6.79	113.46	120.80
2	H	169	LYS	CA-C-N	6.78	134.61	121.18
2	H	169	LYS	C-N-CA	6.78	134.61	121.18
2	H	110	LYS	CA-CB-CG	6.73	127.56	114.10
2	H	154	VAL	CA-C-O	-6.70	115.00	121.63
2	H	107	LYS	O-C-N	6.63	130.76	123.13
2	H	212	ILE	CA-C-O	-6.62	113.35	120.36
2	H	80	GLU	CA-CB-CG	6.60	127.30	114.10
1	L	14(J)	TYR	N-CA-C	-6.58	102.34	111.81
2	H	107	LYS	CA-C-O	-6.57	113.07	120.43
2	H	114	PHE	O-C-N	6.56	130.43	122.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	97	ARG	CD-NE-CZ	-6.54	115.25	124.40
2	H	160	LEU	O-C-N	6.42	126.44	121.88
2	H	139	THR	CA-C-O	-6.34	113.69	121.11
2	H	60(I)	THR	O-C-N	-6.33	115.50	122.84
2	H	35	ARG	NE-CZ-NH2	-6.33	113.51	119.20
2	H	112	VAL	CB-CA-C	6.32	120.85	111.31
2	H	154	VAL	CB-CA-C	6.31	120.96	110.30
2	H	34	PHE	CA-C-O	6.29	127.31	120.32
2	H	78	ASN	N-CA-CB	-6.28	107.01	114.17
2	H	169	LYS	N-CA-C	6.23	118.07	111.28
2	H	180	MET	CA-C-O	-6.23	114.15	121.44
2	H	209	GLN	O-C-N	-6.17	114.80	122.82
3	I	57	GLU	CA-C-N	6.17	129.47	120.71
3	I	57	GLU	C-N-CA	6.17	129.47	120.71
2	H	203	SER	CA-C-O	6.16	125.59	119.49
2	H	67	ARG	NE-CZ-NH1	6.14	127.64	121.50
1	L	14	ASP	CA-C-O	6.13	129.00	121.94
2	H	146	GLU	N-CA-CB	6.13	120.91	110.50
2	H	175	ARG	NE-CZ-NH2	6.13	124.72	119.20
2	H	93	ARG	CD-NE-CZ	-6.09	115.87	124.40
2	H	66	VAL	CB-CA-C	6.08	119.84	110.96
2	H	214	SER	CA-C-O	-6.08	112.62	119.98
2	H	27	SER	CB-CA-C	-6.07	101.67	111.14
2	H	189	ASP	CA-CB-CG	6.07	118.67	112.60
2	H	84	MET	O-C-N	6.05	130.89	123.21
2	H	153	SER	N-CA-C	-6.02	106.07	113.41
2	H	123	LEU	N-CA-CB	6.01	119.15	109.90
2	H	93	ARG	NE-CZ-NH2	6.00	124.60	119.20
1	L	14(H)	GLU	CA-C-O	-5.98	113.09	119.97
2	H	60(I)	THR	N-CA-CB	-5.94	101.25	110.46
2	H	171	SER	O-C-N	5.89	130.53	122.46
2	H	201	MET	CA-C-O	-5.86	114.58	121.44
1	L	13	GLU	CA-C-O	-5.86	114.37	121.28
1	L	3	LEU	O-C-N	5.80	129.95	123.05
2	H	154	VAL	CA-C-N	5.79	130.47	121.26
2	H	154	VAL	C-N-CA	5.79	130.47	121.26
2	H	37	PRO	CA-C-N	5.79	130.46	121.26
2	H	37	PRO	C-N-CA	5.79	130.46	121.26
2	H	30	GLN	OE1-CD-NE2	-5.78	116.82	122.60
2	H	94	TYR	CA-C-O	-5.76	114.81	121.15
2	H	110	LYS	O-C-N	5.76	126.33	121.83
2	H	60(B)	PRO	N-CA-C	5.76	117.73	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	205	ASN	N-CA-CB	-5.75	103.78	113.15
2	H	206	ARG	CD-NE-CZ	-5.70	116.42	124.40
2	H	175	ARG	CA-C-N	5.68	129.50	121.66
2	H	175	ARG	C-N-CA	5.68	129.50	121.66
2	H	16	ILE	CA-C-N	5.68	130.50	123.12
2	H	16	ILE	C-N-CA	5.68	130.50	123.12
2	H	60(I)	THR	CA-C-N	5.68	128.21	120.54
2	H	60(I)	THR	C-N-CA	5.68	128.21	120.54
2	H	129(B)	SER	N-CA-C	5.68	117.55	111.36
2	H	91	HIS	CA-CB-CG	-5.67	108.14	113.80
2	H	50	ARG	CB-CA-C	-5.66	99.88	109.38
2	H	196	GLY	O-C-N	-5.63	115.19	122.34
2	H	192	GLU	O-C-N	5.63	129.87	122.89
2	H	186(D)	LYS	CA-C-O	-5.60	114.72	120.99
2	H	170	ASP	CA-CB-CG	-5.55	107.05	112.60
1	L	14(D)	ARG	CG-CD-NE	5.54	124.18	112.00
2	H	165	ARG	CA-C-N	5.51	124.70	118.97
2	H	165	ARG	C-N-CA	5.51	124.70	118.97
2	H	81	LYS	CA-C-N	5.49	129.99	123.19
2	H	81	LYS	C-N-CA	5.49	129.99	123.19
1	L	13	GLU	CA-CB-CG	5.45	125.01	114.10
2	H	108	LEU	CB-CA-C	5.45	118.73	109.53
1	L	14(H)	GLU	N-CA-C	-5.44	105.51	111.82
2	H	113	ALA	CA-C-N	5.43	130.04	120.87
2	H	113	ALA	C-N-CA	5.43	130.04	120.87
2	H	221(A)	ARG	CA-C-O	-5.43	114.86	121.05
3	I	58	GLU	CB-CG-CD	5.42	121.82	112.60
2	H	136	GLY	CA-C-O	-5.42	116.54	121.47
2	H	86	GLU	N-CA-C	-5.40	104.94	112.45
2	H	63	ASP	CA-C-O	-5.40	112.20	119.11
2	H	199	PHE	O-C-N	-5.40	115.99	123.12
3	I	63	TYR	CA-CB-CG	5.39	123.61	113.90
2	H	235	LYS	CA-CB-CG	-5.38	103.34	114.10
2	H	186	PRO	N-CA-C	-5.38	107.14	113.86
2	H	33	LEU	CA-C-N	-5.36	114.48	122.74
2	H	33	LEU	C-N-CA	-5.36	114.48	122.74
2	H	95	ASN	CB-CG-OD1	5.35	131.51	120.80
2	H	25	GLY	CA-C-N	5.35	128.44	120.31
2	H	25	GLY	C-N-CA	5.35	128.44	120.31
2	H	67	ARG	NH1-CZ-NH2	-5.35	112.35	119.30
2	H	186	PRO	N-CA-CB	5.34	108.64	103.51
2	H	66	VAL	O-C-N	-5.34	116.86	123.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	60(G)	ASN	CA-CB-CG	-5.33	107.27	112.60
2	H	222	ASP	N-CA-CB	5.32	117.79	109.97
2	H	26	MET	CA-C-N	5.30	129.56	123.15
2	H	26	MET	C-N-CA	5.30	129.56	123.15
1	L	14(D)	ARG	CD-NE-CZ	5.29	131.81	124.40
2	H	114	PHE	CA-C-O	-5.29	116.05	121.87
2	H	164	GLU	CG-CD-OE2	5.29	130.58	118.40
2	H	164	GLU	CA-CB-CG	5.29	124.68	114.10
2	H	135	LYS	O-C-N	5.28	129.24	123.01
2	H	116	ASP	O-C-N	5.27	128.38	122.22
2	H	35	ARG	NH1-CZ-NH2	5.26	126.14	119.30
2	H	199	PHE	CB-CA-C	5.25	119.20	110.74
2	H	44	ALA	CA-C-O	-5.22	115.56	121.25
2	H	145	LYS	CA-C-O	-5.21	114.13	120.54
2	H	125	ASP	N-CA-C	-5.21	102.07	110.14
2	H	106	MET	CA-C-O	-5.19	114.76	120.36
2	H	230	HIS	CG-CD2-NE2	-5.17	102.03	107.20
2	H	132	ALA	N-CA-C	-5.17	102.40	110.10
2	H	233	ARG	CD-NE-CZ	5.16	131.62	124.40
2	H	183	ALA	CA-C-N	5.15	129.60	121.62
2	H	183	ALA	C-N-CA	5.15	129.60	121.62
2	H	137	ARG	NE-CZ-NH2	5.14	123.82	119.20
2	H	172	THR	N-CA-CB	-5.13	102.75	111.31
3	I	63	TYR	CB-CG-CD1	5.12	128.49	120.80
2	H	83	SER	N-CA-CB	5.12	119.57	111.43
2	H	233	ARG	CA-C-O	-5.11	113.30	119.49
2	H	123	LEU	N-CA-C	-5.10	102.22	109.62
1	L	14(E)	GLU	CB-CG-CD	5.06	121.20	112.60
1	L	14(C)	GLU	N-CA-CB	5.05	117.64	110.06
2	H	50	ARG	CA-CB-CG	5.05	124.20	114.10
2	H	169	LYS	CA-C-O	5.05	125.90	120.55
2	H	94	TYR	N-CA-CB	-5.03	101.69	109.69
3	I	57	GLU	N-CA-C	-5.03	103.76	110.55
2	H	97	ARG	NE-CZ-NH2	-5.01	114.69	119.20
1	L	14(K)	ILE	CB-CA-C	5.00	121.61	111.60
2	H	243	ASP	CA-CB-CG	5.00	117.61	112.60

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	H	157	VAL	Mainchain

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Mol	Chain	Res	Type	Group
2	H	172	THR	Mainchain
2	H	210	MET	Mainchain
2	H	54	THR	Mainchain
2	H	60(H)	PHE	Mainchain
3	I	63	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	217	0	220	6	0
2	H	2007	0	1985	131	0
3	I	85	0	71	7	0
4	H	121	0	0	22	0
4	I	3	0	0	0	0
4	L	14	0	0	0	0
All	All	2447	0	2276	143	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 31.

All (143) 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:236:LYS:N	2:H:236:LYS:HD2	1.36	1.24
2:H:224:LYS:HG3	4:H:514:HOH:O	1.43	1.19
2:H:236:LYS:H	2:H:236:LYS:CD	1.51	1.15
2:H:187:ARG:HG2	4:H:532:HOH:O	1.54	1.06
2:H:50:ARG:HH11	2:H:50:ARG:HG2	1.11	1.06
2:H:85:LEU:HD13	2:H:106:MET:HE2	1.37	1.03
2:H:50:ARG:HD2	4:H:476:HOH:O	1.61	0.97
2:H:17:VAL:O	2:H:188:GLY:HA2	1.71	0.89
2:H:50:ARG:HH11	2:H:50:ARG:CG	1.85	0.89
2:H:75:ARG:HH11	2:H:75:ARG:HG3	1.36	0.88
2:H:176:ILE:HD12	2:H:227:PHE:CE2	2.11	0.85
2:H:46:LEU:HD22	2:H:48:SER:O	1.76	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:35:ARG:O	2:H:38:GLN:HA	1.80	0.80
2:H:85:LEU:CD1	2:H:106:MET:HE2	2.12	0.79
2:H:50:ARG:HG2	2:H:50:ARG:NH1	1.94	0.78
2:H:61:GLU:OE1	2:H:87:LYS:HA	1.85	0.77
2:H:75:ARG:NH2	4:H:469:HOH:O	2.18	0.76
2:H:50:ARG:NE	2:H:107:LYS:NZ	2.34	0.76
2:H:50:ARG:HE	2:H:107:LYS:NZ	1.84	0.75
2:H:139:THR:HG22	2:H:157:VAL:HG22	1.67	0.74
2:H:18:GLU:HG3	2:H:187:ARG:HB2	1.67	0.73
2:H:50:ARG:HE	2:H:107:LYS:HZ1	1.35	0.73
2:H:236:LYS:HD2	2:H:236:LYS:H	0.64	0.73
2:H:60(F):LYS:HE2	4:H:527:HOH:O	1.88	0.73
2:H:75:ARG:HG3	2:H:75:ARG:NH1	2.03	0.71
2:H:146:GLU:HB2	4:H:519:HOH:O	1.89	0.71
2:H:72:SER:OG	2:H:75:ARG:HG2	1.91	0.71
2:H:60(F):LYS:CE	4:H:527:HOH:O	2.38	0.70
2:H:50:ARG:NE	2:H:107:LYS:HZ2	1.90	0.70
2:H:36:LYS:HE2	4:H:513:HOH:O	1.91	0.70
2:H:224:LYS:HE3	4:H:514:HOH:O	1.94	0.67
2:H:185:LYS:H	2:H:186(B):GLU:HG3	1.59	0.66
2:H:236:LYS:N	2:H:236:LYS:CD	2.21	0.66
2:H:185:LYS:N	2:H:186(B):GLU:HG3	2.11	0.65
2:H:46:LEU:CD2	2:H:48:SER:O	2.44	0.65
2:H:146:GLU:CD	2:H:221(A):ARG:HE	2.05	0.65
2:H:87:LYS:HD3	2:H:88:ILE:H	1.64	0.63
2:H:75:ARG:NH1	2:H:75:ARG:CG	2.62	0.62
2:H:36:LYS:HD3	3:I:64:LEU:HD23	1.82	0.61
1:L:14(J):TYR:C	1:L:14(K):ILE:HG12	2.26	0.61
2:H:165:ARG:CD	4:H:422:HOH:O	2.50	0.60
2:H:204(B):ASN:O	2:H:205:ASN:HB2	2.03	0.58
2:H:146:GLU:OE1	2:H:221(A):ARG:NE	2.37	0.57
2:H:80:GLU:O	2:H:81:LYS:HD2	2.04	0.57
2:H:50:ARG:HH21	2:H:107:LYS:HE3	1.69	0.57
2:H:77(A):ARG:O	4:H:404:HOH:O	2.17	0.57
2:H:239:GLN:HG3	4:H:496:HOH:O	2.04	0.57
3:I:60:PRO:HB2	3:I:62:GLU:CD	2.29	0.57
2:H:87:LYS:HD3	2:H:88:ILE:N	2.20	0.56
2:H:75:ARG:CZ	4:H:469:HOH:O	2.52	0.56
2:H:70:LYS:HE3	2:H:72:SER:O	2.05	0.55
1:L:5:PRO:HA	1:L:9:LYS:HG3	1.89	0.54
1:L:14(I):SER:C	1:L:14(K):ILE:H	2.13	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:165:ARG:HD3	4:H:422:HOH:O	2.05	0.54
2:H:146:GLU:CB	4:H:519:HOH:O	2.53	0.54
2:H:165:ARG:NH2	2:H:177:THR:O	2.40	0.54
2:H:165:ARG:HB3	2:H:166:PRO:HD3	1.90	0.53
2:H:37:PRO:O	2:H:39:GLU:HG2	2.08	0.53
2:H:35:ARG:HD3	2:H:39:GLU:OE2	2.09	0.52
2:H:165:ARG:NE	4:H:422:HOH:O	2.43	0.52
3:I:58:GLU:H	3:I:58:GLU:CD	2.18	0.51
2:H:85:LEU:HD13	2:H:106:MET:CE	2.26	0.51
2:H:187:ARG:NH2	2:H:221:ASP:O	2.44	0.51
2:H:84:MET:HE2	4:H:513:HOH:O	2.09	0.51
2:H:188:GLY:O	2:H:189:ASP:HB2	2.09	0.51
2:H:36:LYS:HG2	2:H:65:LEU:HD22	1.92	0.51
2:H:167:VAL:HG11	2:H:185:LYS:HE2	1.93	0.51
2:H:52:VAL:HG21	2:H:108:LEU:HD21	1.92	0.51
2:H:52:VAL:CG2	2:H:108:LEU:HD21	2.41	0.50
2:H:204(B):ASN:C	2:H:204(B):ASN:HD22	2.19	0.50
2:H:187:ARG:HB3	2:H:221:ASP:OD1	2.11	0.50
1:L:14(D):ARG:CZ	1:L:14(H):GLU:OE2	2.60	0.50
2:H:103:ILE:HD11	2:H:238:ILE:HD11	1.94	0.50
2:H:156:GLN:C	2:H:157:VAL:HG23	2.35	0.50
2:H:36:LYS:HE3	2:H:62:ASN:O	2.12	0.49
2:H:16:ILE:HA	2:H:189:ASP:O	2.13	0.49
2:H:203:SER:HB3	2:H:204(B):ASN:ND2	2.28	0.49
2:H:18:GLU:HB2	2:H:188:GLY:HA2	1.95	0.48
2:H:182:CYS:HA	2:H:226:GLY:O	2.13	0.48
2:H:17:VAL:HG11	2:H:221:ASP:CB	2.44	0.47
2:H:129(C):LEU:HD21	2:H:204:PRO:CD	2.44	0.47
2:H:186(D):LYS:O	4:H:532:HOH:O	2.20	0.47
2:H:50:ARG:CG	2:H:50:ARG:NH1	2.56	0.47
2:H:70:LYS:NZ	2:H:80:GLU:OE2	2.41	0.47
2:H:156:GLN:C	2:H:157:VAL:CG2	2.88	0.47
2:H:60(I):THR:HB	2:H:63:ASP:OD2	2.15	0.47
2:H:211:GLY:HA2	2:H:229:THR:O	2.15	0.47
2:H:85:LEU:CD1	2:H:106:MET:CE	2.87	0.46
3:I:61:GLY:C	3:I:63:TYR:N	2.72	0.46
1:L:14(C):GLU:O	1:L:14(F):LEU:HB2	2.15	0.46
2:H:67:ARG:HH21	2:H:80:GLU:CD	2.24	0.46
2:H:114:PHE:HD1	2:H:114:PHE:HA	1.43	0.46
2:H:204(B):ASN:O	2:H:205:ASN:CB	2.64	0.46
2:H:35:ARG:NH2	4:H:486:HOH:O	2.47	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77(A):ARG:O	2:H:78:ASN:HB2	2.16	0.46
2:H:50:ARG:NH2	2:H:86:GLU:OE1	2.49	0.45
2:H:136:GLY:HA3	2:H:199:PHE:CZ	2.51	0.45
2:H:203:SER:HB3	2:H:204(B):ASN:HD21	1.81	0.45
2:H:86:GLU:HB2	2:H:109:LYS:HA	1.97	0.45
2:H:229:THR:HG22	2:H:234:LEU:HD12	1.98	0.45
2:H:98:ASN:O	2:H:99:LEU:HB2	2.17	0.45
2:H:123:LEU:HA	2:H:124:PRO:HD3	1.86	0.45
2:H:17:VAL:O	2:H:18:GLU:HB2	2.17	0.45
2:H:144:LEU:HD11	2:H:152:PRO:HA	2.00	0.44
2:H:186(A):ASP:OD1	2:H:186(A):ASP:C	2.60	0.44
3:I:60:PRO:HG2	3:I:63:TYR:CD2	2.52	0.44
2:H:186:PRO:HB3	2:H:222:ASP:HB3	2.00	0.44
1:L:14(I):SER:C	1:L:14(K):ILE:N	2.76	0.44
2:H:134:TYR:O	2:H:162:ILE:HG13	2.18	0.44
2:H:70:LYS:NZ	2:H:75:ARG:O	2.45	0.43
2:H:176:ILE:HD12	2:H:227:PHE:HE2	1.78	0.43
2:H:70:LYS:HE3	2:H:70:LYS:HB3	1.76	0.43
2:H:204(B):ASN:ND2	2:H:204(B):ASN:H	2.16	0.43
2:H:131:GLN:O	2:H:132:ALA:C	2.62	0.43
2:H:114:PHE:N	2:H:114:PHE:CD1	2.85	0.43
2:H:145:LYS:O	2:H:146:GLU:C	2.62	0.42
2:H:204(B):ASN:HD22	2:H:204(B):ASN:N	2.17	0.42
2:H:204(B):ASN:ND2	2:H:204(B):ASN:N	2.67	0.42
2:H:41:LEU:HD23	2:H:64:LEU:HD22	2.02	0.42
2:H:176:ILE:CD1	2:H:227:PHE:CE2	2.93	0.42
2:H:164:GLU:H	2:H:164:GLU:CD	2.28	0.42
2:H:60(I):THR:O	2:H:63:ASP:HB2	2.20	0.42
2:H:167:VAL:H	2:H:167:VAL:HG23	1.59	0.42
2:H:213:VAL:HG13	4:H:429:HOH:O	2.19	0.42
2:H:35:ARG:HD2	2:H:41:LEU:HD11	2.01	0.42
2:H:206:ARG:HH11	2:H:206:ARG:HD3	1.47	0.41
2:H:219:GLY:HA3	2:H:221(A):ARG:NE	2.35	0.41
2:H:194:ASP:O	2:H:195:SER:C	2.63	0.41
3:I:60:PRO:HB2	3:I:62:GLU:OE2	2.20	0.41
2:H:71:HIS:CD2	2:H:154:VAL:HG22	2.56	0.41
2:H:32:MET:HB3	2:H:67:ARG:HB2	2.02	0.41
2:H:32:MET:HG3	2:H:40:LEU:HD12	2.03	0.41
2:H:161:PRO:HD3	2:H:184(A):TYR:CZ	2.56	0.41
2:H:126:ARG:NE	4:H:466:HOH:O	2.53	0.41
2:H:236:LYS:O	2:H:240:LYS:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:17:VAL:HG11	2:H:221:ASP:HB3	2.03	0.41
2:H:61:GLU:OE1	2:H:87:LYS:CA	2.62	0.41
2:H:119:HIS:HA	2:H:120:PRO:HD3	1.88	0.41
2:H:33:LEU:HD23	2:H:33:LEU:HA	1.85	0.40
2:H:129(C):LEU:HD21	2:H:204:PRO:HD3	2.03	0.40
2:H:146:GLU:N	4:H:509:HOH:O	2.15	0.40
2:H:143:ASN:HA	2:H:150:GLY:O	2.22	0.40
3:I:60:PRO:HG2	3:I:63:TYR:CE2	2.56	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	24/36 (67%)	22 (92%)	2 (8%)	0	100	100
2	H	244/259 (94%)	227 (93%)	17 (7%)	0	100	100
3	I	8/10 (80%)	8 (100%)	0	0	100	100
All	All	276/305 (90%)	257 (93%)	19 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	25/31 (81%)	24 (96%)	1 (4%)	28	29
2	H	217/225 (96%)	188 (87%)	29 (13%)	4	2
3	I	9/9 (100%)	8 (89%)	1 (11%)	6	3
All	All	251/265 (95%)	220 (88%)	31 (12%)	4	2

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	6	LEU
2	H	24	ILE
2	H	27	SER
2	H	33	LEU
2	H	41	LEU
2	H	46	LEU
2	H	50	ARG
2	H	61	GLU
2	H	64	LEU
2	H	65	LEU
2	H	66	VAL
2	H	68	ILE
2	H	75	ARG
2	H	79	ILE
2	H	83	SER
2	H	90	ILE
2	H	127	GLU
2	H	129(B)	SER
2	H	129(C)	LEU
2	H	130	LEU
2	H	145	LYS
2	H	154	VAL
2	H	192	GLU
2	H	195	SER
2	H	205	ASN
2	H	236	LYS
2	H	239	GLN
2	H	241	VAL
2	H	243	ASP
2	H	244	GLN
3	I	58	GLU

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

Mol	Chain	Res	Type
2	H	78	ASN
2	H	156	GLN
2	H	204(B)	ASN
2	H	205	ASN

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.