



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:12 AM UTC

PDB ID : 1HUC / pdb_00001huc
Title : THE REFINED 2.15 ANGSTROMS X-RAY CRYSTAL STRUCTURE OF
HUMAN LIVER CATHEPSIN B: THE STRUCTURAL BASIS FOR ITS
SPECIFICITY
Authors : Musil, D.; Bode, W.
Deposited on : 1993-04-21
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

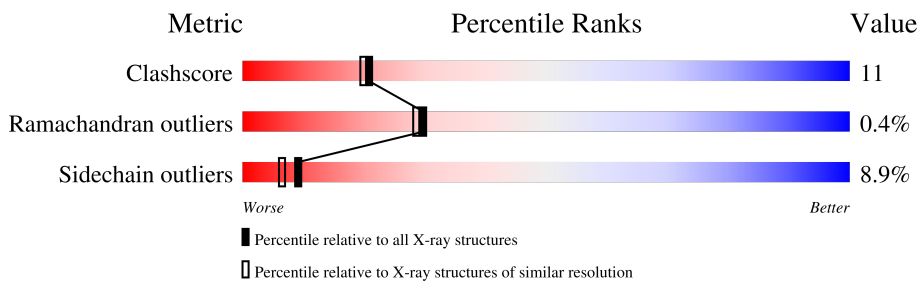
1 Overall quality at a glance

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	A	47	68% 23% 9%
1	C	47	60% 34% 6%
2	B	205	52% 37% 9% .
2	D	205	50% 42% 7% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4159 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 CATHEPSIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	47	Total	C	N	O	S	10	0	0
			364	225	65	70	4			
1	C	47	Total	C	N	O	S	12	0	0
			364	225	65	70	4			

- Molecule 2 is a protein called CATHEPSIN B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	205	Total	C	N	O	S	38	0	0
			1574	988	265	307	14			
2	D	205	Total	C	N	O	S	45	0	0
			1574	988	265	307	14			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	32	Total	O	0	0
			32	32		
3	B	121	Total	O	0	0
			121	121		
3	C	27	Total	O	0	0
			27	27		
3	D	103	Total	O	0	0
			103	103		

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.

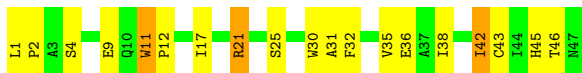
• Molecule 1: CATHEPSIN B

Chain A:  68% 23% 9%



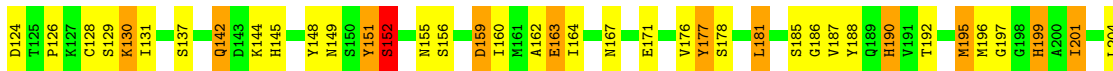
• Molecule 1: CATHEPSIN B

Chain C:  60% 34% 6%



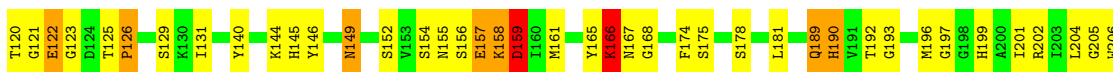
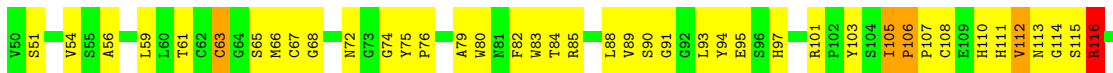
• Molecule 2: CATHEPSIN B

Chain B:  52% 37% 9%



• Molecule 2: CATHEPSIN B

Chain D:  50% 42% 7%



P213	Y214	W215	L216	S220	W221	R222	T223	D224	W225	W228	R235	G236	Q237	D238	H239	C240	G241	I242	E243	S244	E245	V246	V247	A248	R252	T253	D254
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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	86.23Å 34.16Å 85.56Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.10	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	EREF, X-PLOR	Depositor
R, R_{free}	0.164 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4159	wwPDB-VP
Average B, all atoms (Å ²)	16.0	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	A	1.55	6/373 (1.6%)	2.05	6/505 (1.2%)
1	C	1.48	4/373 (1.1%)	1.82	7/505 (1.4%)
2	B	1.62	24/1622 (1.5%)	2.02	44/2203 (2.0%)
2	D	1.55	21/1622 (1.3%)	1.96	51/2203 (2.3%)
All	All	1.57	55/3990 (1.4%)	1.98	108/5416 (2.0%)

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	A	0	1
1	C	0	1
2	B	0	10
2	D	0	15
All	All	0	27

All (55) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	199	HIS	ND1-CE1	11.74	1.44	1.32
2	D	145	HIS	CE1-NE2	10.64	1.43	1.32
2	B	190	HIS	ND1-CE1	10.18	1.42	1.32
2	B	111	HIS	CE1-NE2	9.99	1.42	1.32
2	D	239	HIS	CE1-NE2	9.93	1.42	1.32
2	D	80	TRP	NE1-CE2	-9.85	1.26	1.37
1	C	45	HIS	CE1-NE2	9.72	1.42	1.32
2	B	110	HIS	CE1-NE2	9.69	1.42	1.32
2	D	221	TRP	NE1-CE2	-9.66	1.26	1.37
2	B	239	HIS	ND1-CE1	9.58	1.42	1.32
2	B	206	TRP	NE1-CE2	-9.39	1.27	1.37
2	D	239	HIS	ND1-CE1	9.28	1.41	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	199	HIS	CE1-NE2	9.23	1.41	1.32
1	A	45	HIS	ND1-CE1	9.21	1.41	1.32
2	B	97	HIS	ND1-CE1	9.03	1.41	1.32
2	B	145	HIS	ND1-CE1	9.03	1.41	1.32
1	C	11	TRP	NE1-CE2	-8.96	1.27	1.37
2	B	83	TRP	NE1-CE2	-8.82	1.27	1.37
2	B	145	HIS	CE1-NE2	8.74	1.41	1.32
2	B	111	HIS	ND1-CE1	8.67	1.41	1.32
2	D	199	HIS	CE1-NE2	8.60	1.41	1.32
2	D	97	HIS	CE1-NE2	8.57	1.41	1.32
2	B	199	HIS	ND1-CE1	8.53	1.41	1.32
2	B	221	TRP	NE1-CE2	-8.48	1.28	1.37
2	D	83	TRP	NE1-CE2	-8.48	1.28	1.37
2	B	190	HIS	CE1-NE2	8.44	1.41	1.32
2	D	111	HIS	CE1-NE2	8.41	1.41	1.32
2	D	215	TRP	NE1-CE2	-8.41	1.28	1.37
1	A	30	TRP	NE1-CE2	-8.39	1.28	1.37
2	B	239	HIS	CE1-NE2	8.31	1.40	1.32
2	B	225	TRP	NE1-CE2	-8.28	1.28	1.37
2	D	206	TRP	NE1-CE2	-8.28	1.28	1.37
2	B	110	HIS	ND1-CE1	8.09	1.40	1.32
2	D	225	TRP	NE1-CE2	-8.07	1.28	1.37
2	D	97	HIS	ND1-CE1	8.05	1.40	1.32
1	A	11	TRP	NE1-CE2	-7.94	1.28	1.37
1	C	30	TRP	NE1-CE2	-7.94	1.28	1.37
2	B	97	HIS	CE1-NE2	7.75	1.40	1.32
2	D	110	HIS	CE1-NE2	7.66	1.40	1.32
2	D	110	HIS	ND1-CE1	7.59	1.40	1.32
2	B	80	TRP	NE1-CE2	-7.49	1.29	1.37
1	C	45	HIS	ND1-CE1	7.46	1.40	1.32
1	A	45	HIS	CD2-NE2	6.92	1.45	1.37
1	A	11	TRP	C-N	-6.79	1.28	1.33
2	D	190	HIS	CE1-NE2	6.78	1.39	1.32
2	D	111	HIS	ND1-CE1	6.58	1.39	1.32
2	B	215	TRP	NE1-CE2	-6.49	1.30	1.37
1	A	45	HIS	CE1-NE2	6.46	1.39	1.32
2	B	121	GLY	C-N	-6.31	1.25	1.33
2	D	145	HIS	ND1-CE1	6.29	1.38	1.32
2	B	85	ARG	CD-NE	6.15	1.54	1.46
2	D	190	HIS	ND1-CE1	5.92	1.38	1.32
2	D	199	HIS	CD2-NE2	5.18	1.43	1.37
2	B	190	HIS	CG-ND1	5.02	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	224	ASP	C-N	-5.01	1.26	1.33

All (108) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	197	GLY	CA-C-N	10.79	130.35	120.10
2	B	197	GLY	C-N-CA	10.79	130.35	120.10
2	D	97	HIS	CA-CB-CG	-10.07	103.73	113.80
2	D	122	GLU	N-CA-C	-8.31	96.83	109.96
2	B	159	ASP	CA-CB-CG	-8.29	104.31	112.60
2	B	122	GLU	CA-C-N	-8.26	113.09	122.42
2	B	122	GLU	C-N-CA	-8.26	113.09	122.42
2	D	105	ILE	O-C-N	8.03	128.31	120.92
2	B	58	ASP	CA-CB-CG	-7.71	104.89	112.60
2	B	237	GLN	CB-CG-CD	-7.65	99.59	112.60
2	D	189	GLN	CB-CG-CD	-7.59	99.69	112.60
2	B	98	VAL	N-CA-CB	7.42	119.89	110.99
2	D	245	GLU	CB-CG-CD	-7.37	100.06	112.60
2	D	199	HIS	CA-C-O	-7.29	112.43	120.38
2	B	151	TYR	CA-C-N	7.29	131.84	121.42
2	B	151	TYR	C-N-CA	7.29	131.84	121.42
2	D	75	TYR	CB-CA-C	-7.28	102.97	110.17
2	D	159	ASP	CA-CB-CG	-7.12	105.48	112.60
2	B	162	ALA	CA-C-O	-7.03	113.44	120.82
1	C	21	ARG	NE-CZ-NH2	-7.00	112.90	119.20
2	B	244	SER	CA-C-N	-6.99	111.44	123.25
2	B	244	SER	C-N-CA	-6.99	111.44	123.25
2	B	148	TYR	N-CA-C	-6.92	103.19	111.69
1	A	22	ASP	CA-CB-CG	-6.84	105.76	112.60
2	D	74	GLY	CA-C-O	-6.75	114.29	121.38
2	B	126	PRO	CA-C-N	-6.75	111.04	122.92
2	B	126	PRO	C-N-CA	-6.75	111.04	122.92
2	B	116	ARG	NE-CZ-NH2	-6.66	113.21	119.20
2	B	188	TYR	O-C-N	6.66	130.81	123.22
2	B	142	GLN	CB-CA-C	6.66	121.23	109.65
2	D	244	SER	CA-C-N	-6.44	113.60	122.87
2	D	244	SER	C-N-CA	-6.44	113.60	122.87
1	C	43	CYS	N-CA-C	6.42	118.07	111.14
1	A	25	SER	CB-CA-C	-6.41	101.68	112.00
1	A	6	ASP	CA-CB-CG	-6.40	106.20	112.60
2	B	81	ASN	CA-CB-CG	6.32	118.92	112.60
2	B	56	ALA	CA-C-N	6.28	128.60	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	56	ALA	C-N-CA	6.28	128.60	120.44
2	B	122	GLU	N-CA-C	-6.26	100.14	108.34
1	C	32	PHE	CA-CB-CG	-6.19	107.61	113.80
2	D	51	SER	CA-C-N	-6.14	115.58	123.19
2	D	51	SER	C-N-CA	-6.14	115.58	123.19
2	D	111	HIS	CA-CB-CG	-6.11	107.69	113.80
2	B	239	HIS	CA-CB-CG	-5.99	107.81	113.80
1	C	45	HIS	CA-C-N	-5.97	112.50	122.64
1	C	45	HIS	C-N-CA	-5.97	112.50	122.64
2	D	166	LYS	CB-CA-C	-5.95	101.50	110.90
2	D	204	LEU	CA-C-N	-5.93	114.12	121.83
2	D	204	LEU	C-N-CA	-5.93	114.12	121.83
2	B	149	ASN	N-CA-C	5.91	116.21	107.88
2	D	116	ARG	CB-CA-C	5.89	117.92	108.91
2	D	199	HIS	CA-CB-CG	-5.86	107.94	113.80
2	B	236	GLY	CA-C-N	-5.85	113.47	122.60
2	B	236	GLY	C-N-CA	-5.85	113.47	122.60
2	D	122	GLU	CA-C-N	-5.82	115.84	122.42
2	D	122	GLU	C-N-CA	-5.82	115.84	122.42
2	D	75	TYR	CA-C-O	-5.81	114.48	119.36
2	B	124	ASP	CA-CB-CG	-5.76	106.83	112.60
2	B	177	TYR	CA-C-O	-5.75	114.72	121.44
2	D	152	SER	O-C-N	5.71	129.78	123.16
2	D	126	PRO	O-C-N	-5.69	116.02	122.91
2	D	243	GLU	CA-C-N	-5.61	113.34	122.26
2	D	243	GLU	C-N-CA	-5.61	113.34	122.26
2	D	197	GLY	CA-C-N	5.61	127.37	120.92
2	D	197	GLY	C-N-CA	5.61	127.37	120.92
2	B	53	GLU	CA-C-N	5.60	128.60	120.98
2	B	53	GLU	C-N-CA	5.60	128.60	120.98
2	B	101	ARG	NE-CZ-NH1	-5.56	115.94	121.50
2	D	239	HIS	CA-C-N	5.54	130.43	122.40
2	D	239	HIS	C-N-CA	5.54	130.43	122.40
2	D	111	HIS	CB-CA-C	-5.54	102.81	111.39
1	C	45	HIS	CA-CB-CG	-5.45	108.35	113.80
2	D	123	GLY	O-C-N	5.45	130.30	123.16
2	D	114	GLY	CA-C-N	5.44	128.32	120.38
2	D	114	GLY	C-N-CA	5.44	128.32	120.38
1	A	46	THR	CA-CB-CG2	5.43	119.73	110.50
1	A	46	THR	N-CA-C	5.38	117.01	108.67
2	B	93	LEU	N-CA-C	-5.31	103.38	110.55
1	C	31	ALA	N-CA-C	-5.27	105.20	111.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	174	PHE	N-CA-C	5.25	117.17	109.24
2	D	168	GLY	O-C-N	5.24	127.01	121.77
2	B	130	LYS	CA-CB-CG	-5.24	103.62	114.10
2	D	167	ASN	CA-CB-CG	-5.24	107.36	112.60
2	B	137	SER	O-C-N	-5.23	118.16	121.88
2	D	131	ILE	CA-C-O	-5.22	116.23	121.45
2	D	157	GLU	CA-C-N	5.19	129.46	120.58
2	D	157	GLU	C-N-CA	5.19	129.46	120.58
2	D	61	THR	CA-C-N	-5.17	114.12	122.23
2	D	61	THR	C-N-CA	-5.17	114.12	122.23
2	B	219	ASN	CA-C-O	-5.15	115.86	121.89
2	B	114	GLY	CA-C-N	5.14	129.41	120.68
2	B	114	GLY	C-N-CA	5.14	129.41	120.68
2	B	62	CYS	CA-C-N	-5.11	111.84	120.58
2	B	62	CYS	C-N-CA	-5.11	111.84	120.58
2	B	240	CYS	CA-C-O	-5.11	114.30	120.32
2	B	181	LEU	O-C-N	5.10	129.03	122.39
2	B	237	GLN	OE1-CD-NE2	5.09	127.69	122.60
2	D	126	PRO	CA-C-N	-5.09	114.14	121.42
2	D	126	PRO	C-N-CA	-5.09	114.14	121.42
2	D	67	CYS	CB-CA-C	-5.08	102.84	111.02
2	D	63	CYS	N-CA-CB	5.06	117.41	110.07
1	A	34	ALA	O-C-N	-5.06	116.67	122.08
2	D	95	GLU	CB-CG-CD	-5.04	104.04	112.60
2	B	152	SER	N-CA-CB	-5.03	102.46	110.06
2	D	112	VAL	CA-C-N	-5.01	115.80	122.72
2	D	112	VAL	C-N-CA	-5.01	115.80	122.72
2	D	106	PRO	CA-C-O	5.01	124.50	120.90
2	D	202	ARG	NE-CZ-NH1	-5.00	116.50	121.50

There are no chirality outliers.

All (27) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	21	ARG	Sidechain
2	B	113	ASN	Peptide,Mainchain
2	B	142	GLN	Mainchain
2	B	151	TYR	Sidechain
2	B	187	VAL	Mainchain
2	B	192	THR	Mainchain
2	B	54	VAL	Mainchain
2	B	57	GLU	Mainchain

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Mol	Chain	Res	Type	Group
2	B	64	GLY	Mainchain
2	B	88	LEU	Mainchain
1	C	42	ILE	Mainchain
2	D	116	ARG	Mainchain
2	D	146	TYR	Mainchain
2	D	155	ASN	Mainchain
2	D	156	SER	Mainchain
2	D	158	LYS	Mainchain
2	D	159	ASP	Mainchain
2	D	165	TYR	Sidechain
2	D	166	LYS	Mainchain
2	D	192	THR	Mainchain
2	D	205	GLY	Mainchain
2	D	216	LEU	Mainchain
2	D	224	ASP	Mainchain
2	D	246	VAL	Mainchain
2	D	248	ALA	Mainchain
2	D	68	GLY	Mainchain

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	A	364	0	340	8	0
1	C	364	0	340	8	0
2	B	1574	0	1444	36	0
2	D	1574	0	1444	35	0
3	A	32	0	0	0	0
3	B	121	0	0	8	0
3	C	27	0	0	1	0
3	D	103	0	0	2	1
All	All	4159	0	3568	80	1

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 11.

All (80) 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:D:120:THR:HG22	2:D:121:GLY:H	1.37	0.87
2:B:190:HIS:H	2:B:239:HIS:HE1	1.29	0.81
1:A:43:CYS:O	1:A:46:THR:HG22	1.88	0.73
2:B:96:SER:HB2	2:B:98:VAL:HG13	1.72	0.72
2:D:242:ILE:HG23	2:D:243:GLU:HG3	1.76	0.66
2:B:84:THR:HG21	3:B:765:HOH:O	1.95	0.65
2:D:175:SER:HB2	2:D:240:CYS:HB3	1.80	0.64
2:D:59:LEU:HD21	2:D:79:ALA:HB1	1.80	0.63
2:D:120:THR:CG2	2:D:121:GLY:H	2.08	0.62
2:B:72:ASN:HB3	3:B:688:HOH:O	2.00	0.61
2:D:158:LYS:HA	2:D:161:MET:HE3	1.83	0.60
2:B:76:PRO:HB3	2:B:171:GLU:OE1	2.03	0.59
1:A:42:ILE:O	1:A:46:THR:HB	2.03	0.58
2:B:103:TYR:CE2	2:B:105:ILE:HB	2.39	0.57
1:C:21:ARG:HD3	1:C:36:GLU:HG2	1.87	0.56
2:B:107:PRO:HB2	2:B:116:ARG:HD3	1.87	0.56
2:B:181:LEU:HD11	2:B:196:MET:HE1	1.88	0.56
2:B:81:ASN:O	2:B:84:THR:HG22	2.06	0.55
1:A:25:SER:HB3	2:B:120:THR:HB	1.89	0.55
2:D:103:TYR:CE2	2:D:105:ILE:HB	2.41	0.55
2:D:108:CYS:HA	2:D:116:ARG:CG	2.37	0.55
1:C:21:ARG:HD2	3:C:737:HOH:O	2.05	0.54
2:D:166:LYS:HG3	3:D:840:HOH:O	2.07	0.54
2:B:190:HIS:H	2:B:239:HIS:CE1	2.19	0.54
1:A:45:HIS:HE1	2:B:167:ASN:O	1.90	0.54
2:B:186:GLY:O	2:B:232:LYS:HB2	2.09	0.53
1:C:38:ILE:HG22	2:D:54:VAL:HG21	1.90	0.53
2:D:190:HIS:H	2:D:239:HIS:CE1	2.26	0.53
2:D:108:CYS:HA	2:D:116:ARG:HG3	1.91	0.52
2:D:158:LYS:HA	2:D:161:MET:CE	2.40	0.52
2:D:178:SER:HB2	2:D:193:GLY:HA3	1.92	0.52
2:B:81:ASN:HA	2:B:84:THR:HG22	1.90	0.52
2:B:59:LEU:HD21	2:B:79:ALA:HB1	1.93	0.49
2:D:101:ARG:NH2	2:D:129:SER:H	2.11	0.49
2:D:213:PRO:HB2	2:D:235:ARG:HB3	1.93	0.49
2:B:93:LEU:HB2	3:B:614:HOH:O	2.13	0.49
2:D:223:THR:O	2:D:228:ASN:HA	2.13	0.48
2:D:189:GLN:HG2	3:D:815:HOH:O	2.12	0.48
2:D:94:TYR:CD2	2:D:107:PRO:HD3	2.49	0.48
2:D:181:LEU:HD11	2:D:196:MET:SD	2.54	0.48
1:A:42:ILE:HG21	2:B:52:VAL:HG12	1.96	0.48
2:D:149:ASN:C	2:D:149:ASN:HD22	2.21	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:177:TYR:CE2	2:B:195:MET:HG2	2.50	0.47
2:B:89:VAL:HG13	2:B:144:LYS:HD3	1.97	0.47
1:C:9:GLU:O	1:C:12:PRO:HD3	2.15	0.47
2:D:154:SER:HB2	2:D:159:ASP:OD2	2.14	0.47
2:B:108:CYS:HB3	3:B:676:HOH:O	2.14	0.47
1:C:35:VAL:HG21	2:D:56:ALA:HB2	1.97	0.46
2:B:219:ASN:HB3	3:B:651:HOH:O	2.15	0.46
2:D:89:VAL:HG11	2:D:140:TYR:CE1	2.51	0.46
1:C:11:TRP:HB2	1:C:17:ILE:HD12	1.98	0.45
2:B:155:ASN:HA	2:B:243:GLU:O	2.16	0.45
2:B:163:GLU:HG2	3:B:793:HOH:O	2.17	0.45
2:D:106:PRO:HA	2:D:107:PRO:HD3	1.91	0.45
2:D:89:VAL:HG11	2:D:140:TYR:CD1	2.53	0.44
2:D:91:GLY:HA3	2:D:101:ARG:O	2.18	0.44
2:D:72:ASN:HA	2:D:122:GLU:OE2	2.18	0.44
2:B:120:THR:HG21	3:B:686:HOH:O	2.17	0.43
2:D:63:CYS:HA	2:D:82:PHE:CE1	2.53	0.43
1:A:18:LYS:H	1:A:18:LYS:HG3	1.63	0.43
2:B:176:VAL:HG23	2:B:199:HIS:HB2	1.99	0.43
2:B:152:SER:HB2	3:B:633:HOH:O	2.19	0.43
2:D:89:VAL:HG23	2:D:90:SER:O	2.18	0.43
1:C:1:LEU:HB3	1:C:2:PRO:HD2	2.01	0.42
2:B:156:SER:HB3	2:B:159:ASP:HB2	2.01	0.42
2:B:160:ILE:O	2:B:164:ILE:HG13	2.18	0.42
2:D:157:GLU:O	2:D:161:MET:HG3	2.19	0.42
1:A:33:GLY:HA3	2:B:171:GLU:OE2	2.20	0.42
2:B:94:TYR:CZ	2:B:106:PRO:HB3	2.55	0.42
2:B:201:ILE:HG12	2:B:217:VAL:HG11	2.01	0.42
2:B:96:SER:CB	2:B:98:VAL:HG13	2.46	0.41
2:D:89:VAL:HG12	2:D:144:LYS:HD2	2.01	0.41
1:A:30:TRP:CZ3	2:B:67:CYS:HB3	2.56	0.41
2:B:228:ASN:HD22	2:B:228:ASN:HA	1.74	0.41
2:B:250:ILE:HA	2:B:251:PRO:HD3	1.92	0.41
1:C:42:ILE:O	1:C:46:THR:HG23	2.21	0.41
2:D:66:MET:HE1	2:D:82:PHE:HB2	2.03	0.41
2:D:125:THR:HA	2:D:126:PRO:HD3	1.76	0.41
2:B:128:CYS:SG	2:B:130:LYS:HE2	2.61	0.40
2:D:108:CYS:C	2:D:116:ARG:HH11	2.29	0.40

All (1) 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)
3:D:747:HOH:O	3:D:776:HOH:O[1_565]	2.17	0.03

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	A	45/47 (96%)	44 (98%)	1 (2%)	0	100	100
1	C	45/47 (96%)	45 (100%)	0	0	100	100
2	B	203/205 (99%)	193 (95%)	9 (4%)	1 (0%)	24	22
2	D	203/205 (99%)	185 (91%)	17 (8%)	1 (0%)	24	22
All	All	496/504 (98%)	467 (94%)	27 (5%)	2 (0%)	30	28

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	121	GLY
2	D	65	SER

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	A	39/39 (100%)	37 (95%)	2 (5%)	21	21
1	C	39/39 (100%)	37 (95%)	2 (5%)	21	21
2	B	169/169 (100%)	152 (90%)	17 (10%)	7	5

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	169/169 (100%)	153 (90%)	16 (10%)	8	5
All	All	416/416 (100%)	379 (91%)	37 (9%)	9	6

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	GLU
1	A	47	ASN
2	B	85	ARG
2	B	93	LEU
2	B	95	GLU
2	B	98	VAL
2	B	122	GLU
2	B	129	SER
2	B	131	ILE
2	B	152	SER
2	B	163	GLU
2	B	178	SER
2	B	185	SER
2	B	195	MET
2	B	201	ILE
2	B	204	LEU
2	B	220	SER
2	B	237	GLN
2	B	247	VAL
1	C	4	SER
1	C	25	SER
2	D	76	PRO
2	D	84	THR
2	D	85	ARG
2	D	88	LEU
2	D	93	LEU
2	D	112	VAL
2	D	113	ASN
2	D	115	SER
2	D	116	ARG
2	D	149	ASN
2	D	201	ILE
2	D	220	SER
2	D	237	GLN
2	D	245	GLU
2	D	247	VAL

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Mol	Chain	Res	Type
2	D	252	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	81	ASN
2	B	97	HIS
2	B	155	ASN
2	B	189	GLN
2	B	228	ASN
2	B	239	HIS
1	C	23	GLN
2	D	149	ASN
2	D	237	GLN
2	D	239	HIS

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.