



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:07 PM UTC

PDB ID : 1IOF / pdb_00001iof
Title : X-RAY CRYSTALLINE STRUCTURES OF PYRROLIDONE CARBOXYL PEPTIDASE FROM A HYPERTHERMOPHILE, PYROCOCCLUS FURIOSUS, AND ITS CYS-FREE MUTANT
Authors : Tanaka, H.; Chinami, M.; Ota, M.; Tsukihara, T.; Yutani, K.
Deposited on : 2001-03-09
Resolution : 2.20 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

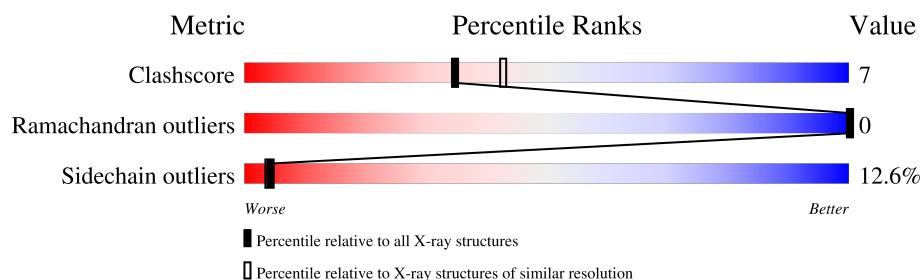
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)

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	208	
1	B	208	
1	C	208	
1	D	208	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6588 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 PYRROLIDONE CARBOXYL PEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	208	Total	C	N	O	S	0	0	0
			1605	1040	263	294	8			
1	B	208	Total	C	N	O	S	0	0	0
			1605	1040	263	294	8			
1	C	208	Total	C	N	O	S	0	0	0
			1605	1040	263	294	8			
1	D	208	Total	C	N	O	S	0	0	0
			1605	1040	263	294	8			

- Molecule 2 is water.

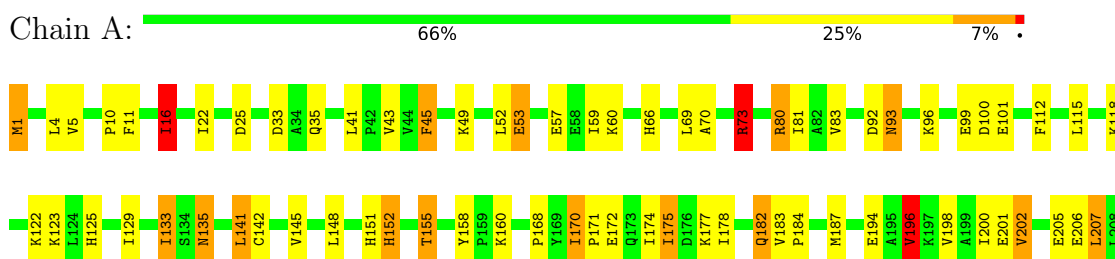
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	44	Total	O	0	0
			44	44		
2	B	42	Total	O	0	0
			42	42		
2	C	46	Total	O	0	0
			46	46		
2	D	36	Total	O	0	0
			36	36		

3 Residue-property plots

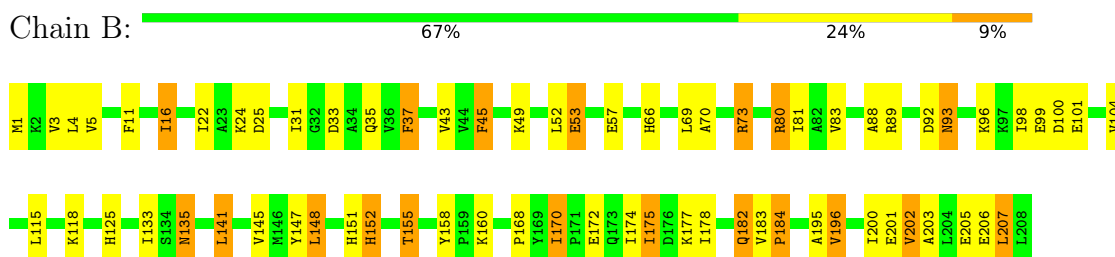
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

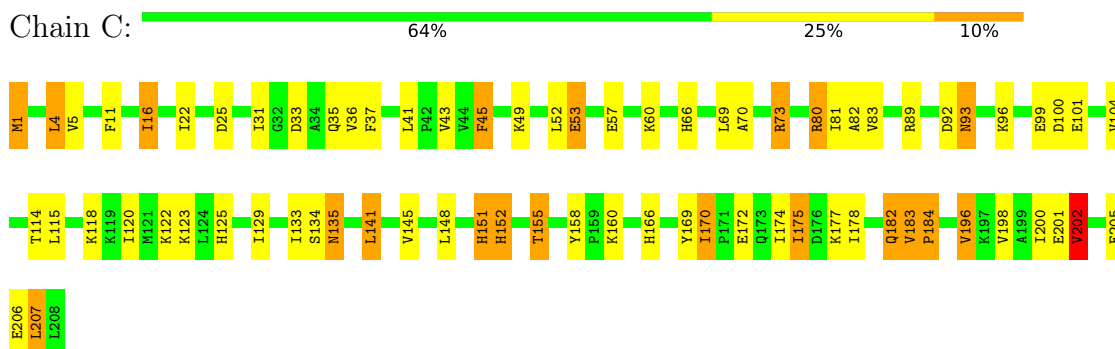
• Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE



• Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE

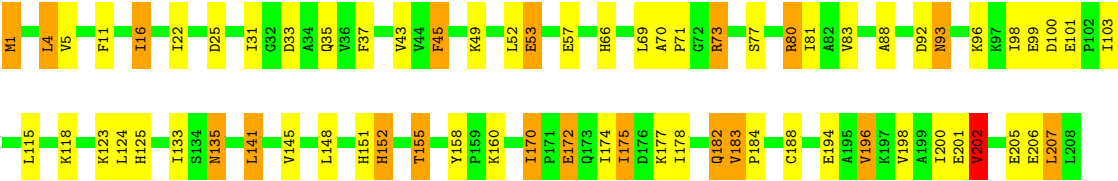


• Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE



• Molecule 1: PYRROLIDONE CARBOXYL PEPTIDASE





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	57.90Å 105.00Å 78.50Å 90.00° 90.70° 90.00°	Depositor
Resolution (Å)	10.00 – 2.20	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.20)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.195 , 0.232	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6588	wwPDB-VP
Average B, all atoms (Å ²)	41.0	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	1.37	14/1639 (0.9%)	1.88	35/2216 (1.6%)
1	B	1.35	11/1639 (0.7%)	1.88	36/2216 (1.6%)
1	C	1.37	13/1639 (0.8%)	1.89	43/2216 (1.9%)
1	D	1.32	7/1639 (0.4%)	1.90	31/2216 (1.4%)
All	All	1.35	45/6556 (0.7%)	1.89	145/8864 (1.6%)

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	B	0	1

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	HIS	CD2-NE2	-7.83	1.29	1.37
1	A	202	VAL	CA-CB	7.37	1.63	1.54
1	D	125	HIS	CD2-NE2	-7.28	1.29	1.37
1	B	202	VAL	CA-CB	7.20	1.63	1.54
1	D	202	VAL	CA-CB	6.93	1.63	1.54
1	D	175	ILE	CA-CB	6.86	1.63	1.54
1	B	175	ILE	CA-CB	6.86	1.63	1.54
1	C	66	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	151	HIS	CD2-NE2	-6.82	1.30	1.37
1	A	125	HIS	CD2-NE2	-6.78	1.30	1.37
1	A	175	ILE	CA-CB	6.74	1.62	1.54
1	C	125	HIS	CD2-NE2	-6.64	1.30	1.37
1	A	168	PRO	CA-CB	-6.53	1.44	1.53
1	A	66	HIS	CD2-NE2	-6.45	1.30	1.37
1	A	16	ILE	CA-CB	6.24	1.64	1.54
1	B	66	HIS	CD2-NE2	-6.18	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	169	TYR	CA-CB	-6.15	1.43	1.53
1	B	184	PRO	CA-CB	-5.84	1.49	1.54
1	C	184	PRO	CA-CB	-5.75	1.49	1.54
1	D	152	HIS	CD2-NE2	-5.73	1.31	1.37
1	C	152	HIS	CD2-NE2	-5.71	1.31	1.37
1	C	202	VAL	CA-CB	5.71	1.61	1.54
1	C	175	ILE	CA-CB	5.60	1.62	1.54
1	C	151	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	112	PHE	CA-CB	-5.58	1.44	1.53
1	A	151	HIS	CD2-NE2	-5.55	1.31	1.37
1	B	148	LEU	CA-CB	-5.53	1.44	1.53
1	A	59	ILE	CA-CB	5.50	1.62	1.54
1	C	125	HIS	CG-ND1	-5.49	1.32	1.38
1	C	120	ILE	CA-CB	-5.47	1.48	1.54
1	C	166	HIS	CG-ND1	-5.45	1.32	1.38
1	B	168	PRO	CA-CB	-5.40	1.46	1.53
1	A	133	ILE	CA-CB	-5.36	1.47	1.54
1	D	71	PRO	CA-CB	-5.33	1.46	1.53
1	B	3	VAL	CA-CB	-5.33	1.48	1.54
1	A	129	ILE	CA-CB	-5.25	1.47	1.54
1	C	134	SER	CA-CB	-5.20	1.45	1.53
1	B	152	HIS	CD2-NE2	-5.20	1.32	1.37
1	A	196	VAL	CA-CB	5.19	1.60	1.54
1	A	171	PRO	CA-CB	-5.15	1.46	1.53
1	A	152	HIS	CD2-NE2	-5.11	1.32	1.37
1	B	24	LYS	CA-CB	-5.09	1.45	1.53
1	B	125	HIS	CD2-NE2	-5.08	1.32	1.37
1	D	151	HIS	CD2-NE2	-5.03	1.32	1.37
1	C	60	LYS	CA-CB	5.02	1.57	1.52

All (145) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	135	ASN	OD1-CG-ND2	-10.43	112.17	122.60
1	C	92	ASP	CA-CB-CG	9.72	122.32	112.60
1	A	92	ASP	CA-CB-CG	9.48	122.08	112.60
1	B	92	ASP	CA-CB-CG	9.41	122.01	112.60
1	C	100	ASP	N-CA-C	9.28	122.62	111.02
1	A	100	ASP	N-CA-C	9.24	122.58	111.02
1	B	100	ASP	N-CA-C	9.24	122.57	111.02
1	D	100	ASP	N-CA-C	9.16	122.48	111.02
1	D	155	THR	N-CA-CB	-8.89	97.00	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	155	THR	N-CA-CB	-8.72	97.25	110.07
1	D	92	ASP	CA-CB-CG	8.64	121.24	112.60
1	C	11	PHE	CA-CB-CG	8.53	122.33	113.80
1	A	155	THR	N-CA-CB	-8.51	97.56	110.07
1	D	11	PHE	CA-CB-CG	8.42	122.22	113.80
1	B	155	THR	N-CA-CB	-8.34	97.82	110.07
1	A	11	PHE	CA-CB-CG	8.32	122.12	113.80
1	B	11	PHE	CA-CB-CG	8.28	122.08	113.80
1	B	155	THR	CA-CB-OG1	-8.09	97.47	109.60
1	D	155	THR	CA-CB-OG1	-8.03	97.56	109.60
1	A	201	GLU	CA-C-O	-7.96	112.46	120.82
1	A	155	THR	CA-CB-OG1	-7.85	97.83	109.60
1	C	201	GLU	CA-C-O	-7.85	112.23	120.55
1	C	155	THR	CA-CB-OG1	-7.72	98.02	109.60
1	D	201	GLU	CA-C-O	-7.47	112.63	120.55
1	B	135	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	C	155	THR	CA-CB-CG2	7.43	123.14	110.50
1	C	53	GLU	CA-CB-CG	-7.38	99.34	114.10
1	B	155	THR	CA-CB-CG2	7.37	123.03	110.50
1	B	25	ASP	CA-CB-CG	7.36	119.96	112.60
1	A	80	ARG	CB-CG-CD	-7.18	94.78	111.30
1	A	155	THR	CA-CB-CG2	7.13	122.63	110.50
1	D	53	GLU	CA-CB-CG	-7.13	99.83	114.10
1	B	80	ARG	CB-CG-CD	-7.13	94.90	111.30
1	C	25	ASP	CA-CB-CG	7.11	119.71	112.60
1	D	155	THR	CA-CB-CG2	7.08	122.54	110.50
1	B	115	LEU	O-C-N	-7.07	113.75	121.53
1	A	53	GLU	CA-CB-CG	-7.03	100.05	114.10
1	A	135	ASN	OD1-CG-ND2	-6.96	115.64	122.60
1	B	53	GLU	CA-CB-CG	-6.89	100.32	114.10
1	C	80	ARG	CB-CG-CD	-6.84	95.56	111.30
1	C	135	ASN	OD1-CG-ND2	-6.82	115.78	122.60
1	B	201	GLU	CA-C-O	-6.80	113.34	120.55
1	B	182	GLN	OE1-CD-NE2	-6.79	115.81	122.60
1	D	25	ASP	CA-CB-CG	6.72	119.32	112.60
1	A	25	ASP	CA-CB-CG	6.63	119.23	112.60
1	D	66	HIS	CB-CG-CD2	-6.60	122.62	131.20
1	C	11	PHE	N-CA-C	-6.56	102.34	110.41
1	B	170	ILE	CA-C-N	6.52	126.02	119.24
1	B	170	ILE	C-N-CA	6.52	126.02	119.24
1	C	66	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	C	170	ILE	CA-C-N	6.50	126.72	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	170	ILE	C-N-CA	6.50	126.72	119.32
1	A	205	GLU	CA-CB-CG	6.46	127.02	114.10
1	D	205	GLU	CA-CB-CG	6.45	126.99	114.10
1	D	80	ARG	CB-CG-CD	-6.43	96.50	111.30
1	B	205	GLU	CA-CB-CG	6.43	126.97	114.10
1	A	183	VAL	N-CA-CB	-6.40	102.25	111.21
1	A	151	HIS	CA-CB-CG	-6.40	107.40	113.80
1	C	205	GLU	CA-CB-CG	6.32	126.74	114.10
1	A	182	GLN	OE1-CD-NE2	-6.23	116.37	122.60
1	B	11	PHE	N-CA-C	-6.20	102.35	110.53
1	A	66	HIS	CB-CG-CD2	-6.19	123.15	131.20
1	D	182	GLN	OE1-CD-NE2	-6.19	116.41	122.60
1	D	31	ILE	N-CA-C	-6.16	98.76	107.75
1	B	184	PRO	CA-C-O	-6.14	115.88	120.73
1	B	66	HIS	CB-CG-CD2	-6.13	123.23	131.20
1	D	183	VAL	N-CA-CB	-6.11	102.65	111.21
1	B	183	VAL	N-CA-CB	-6.11	102.66	111.21
1	D	170	ILE	CA-C-N	6.11	126.28	119.32
1	D	170	ILE	C-N-CA	6.11	126.28	119.32
1	A	141	LEU	N-CA-C	6.10	118.73	111.71
1	D	11	PHE	N-CA-C	-6.09	102.92	110.41
1	A	11	PHE	N-CA-C	-5.99	103.05	110.41
1	A	170	ILE	CA-C-N	5.99	126.14	119.32
1	A	170	ILE	C-N-CA	5.99	126.14	119.32
1	C	182	GLN	OE1-CD-NE2	-5.94	116.66	122.60
1	C	183	VAL	N-CA-CB	-5.92	102.92	111.21
1	B	183	VAL	CA-C-N	5.91	123.91	119.66
1	B	183	VAL	C-N-CA	5.91	123.91	119.66
1	B	37	PHE	CA-CB-CG	-5.87	107.93	113.80
1	D	115	LEU	O-C-N	-5.83	115.11	121.53
1	D	141	LEU	N-CA-C	5.81	118.39	111.71
1	D	151	HIS	CA-CB-CG	-5.79	108.01	113.80
1	C	177	LYS	N-CA-C	-5.75	104.98	112.23
1	A	45	PHE	CA-CB-CG	5.74	119.54	113.80
1	B	182	GLN	N-CA-C	5.66	118.68	109.06
1	D	93	ASN	N-CA-C	5.65	119.65	112.87
1	C	31	ILE	N-CA-C	-5.64	98.31	107.28
1	C	184	PRO	CA-C-O	-5.61	116.30	120.73
1	D	182	GLN	N-CA-C	5.59	118.57	109.06
1	A	177	LYS	N-CA-C	-5.55	105.23	112.23
1	A	182	GLN	N-CA-C	5.55	118.49	109.06
1	C	183	VAL	CA-C-N	5.54	123.65	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	183	VAL	C-N-CA	5.54	123.65	119.66
1	C	129	ILE	N-CA-C	-5.54	101.57	107.77
1	C	182	GLN	N-CA-C	5.48	118.37	109.06
1	B	177	LYS	N-CA-C	-5.47	105.33	112.23
1	D	155	THR	CB-CA-C	5.41	119.79	110.86
1	C	45	PHE	CA-CB-CG	5.39	119.19	113.80
1	C	4	LEU	N-CA-C	-5.36	100.97	109.76
1	C	89	ARG	CA-C-O	5.36	126.28	120.55
1	A	93	ASN	N-CA-C	5.35	119.29	112.87
1	D	177	LYS	N-CA-C	-5.34	105.50	112.23
1	C	82	ALA	CA-C-O	-5.34	115.05	120.71
1	C	115	LEU	O-C-N	-5.33	115.95	121.60
1	C	122	LYS	CA-CB-CG	5.32	124.74	114.10
1	D	103	ILE	N-CA-C	-5.31	105.67	110.82
1	B	93	ASN	OD1-CG-ND2	-5.30	117.30	122.60
1	B	93	ASN	N-CA-C	5.27	119.20	112.87
1	D	4	LEU	CB-CA-C	-5.27	100.63	109.48
1	A	155	THR	CB-CA-C	5.26	119.55	110.86
1	C	151	HIS	CA-CB-CG	-5.26	108.54	113.80
1	C	155	THR	CB-CA-C	5.26	119.54	110.86
1	B	141	LEU	N-CA-C	5.26	117.75	111.71
1	C	93	ASN	N-CA-C	5.25	119.17	112.87
1	D	45	PHE	CA-CB-CG	5.25	119.05	113.80
1	C	184	PRO	CA-C-N	5.23	125.51	119.92
1	C	184	PRO	C-N-CA	5.23	125.51	119.92
1	B	104	VAL	CA-C-N	5.20	126.33	119.84
1	B	104	VAL	C-N-CA	5.20	126.33	119.84
1	A	41	LEU	CA-C-N	5.18	125.08	119.85
1	A	41	LEU	C-N-CA	5.18	125.08	119.85
1	C	11	PHE	N-CA-CB	5.18	117.47	110.38
1	C	104	VAL	CA-C-N	5.17	125.98	119.98
1	C	104	VAL	C-N-CA	5.17	125.98	119.98
1	B	31	ILE	N-CA-C	-5.17	99.06	107.28
1	B	151	HIS	CA-CB-CG	-5.16	108.64	113.80
1	A	129	ILE	N-CA-C	-5.13	102.02	107.77
1	B	195	ALA	CA-C-O	-5.12	115.42	120.70
1	D	77	SER	CA-C-O	5.12	125.89	120.36
1	C	41	LEU	CA-C-N	5.11	125.09	120.03
1	C	41	LEU	C-N-CA	5.11	125.09	120.03
1	D	11	PHE	N-CA-CB	5.11	117.38	110.38
1	A	60	LYS	CA-C-O	5.10	124.34	120.26
1	A	187	MET	CA-C-N	-5.10	114.12	121.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	MET	C-N-CA	-5.10	114.12	121.42
1	A	115	LEU	O-C-N	-5.09	115.93	121.53
1	A	122	LYS	CA-CB-CG	5.09	124.28	114.10
1	B	89	ARG	CA-C-O	5.09	125.99	120.55
1	C	36	VAL	O-C-N	-5.05	117.99	123.14
1	B	203	ALA	N-CA-C	-5.05	105.69	111.14
1	C	141	LEU	N-CA-C	5.04	117.51	111.71
1	B	45	PHE	CA-CB-CG	5.02	118.82	113.80
1	A	151	HIS	CB-CG-CD2	-5.01	124.68	131.20
1	A	73	ARG	N-CA-C	-5.00	102.37	110.32

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	147	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	A	1605	0	1671	22	0
1	B	1605	0	1671	22	0
1	C	1605	0	1671	25	0
1	D	1605	0	1671	29	0
2	A	44	0	0	2	0
2	B	42	0	0	2	0
2	C	46	0	0	1	0
2	D	36	0	0	2	0
All	All	6588	0	6684	98	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 7.

All (98) 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:C:70:ALA:HB1	1:C:73:ARG:HD3	1.63	0.80
1:C:160:LYS:HD2	1:C:207:LEU:HD21	1.64	0.79
1:D:70:ALA:HB1	1:D:73:ARG:HD3	1.63	0.79
1:B:70:ALA:HB1	1:B:73:ARG:HD3	1.63	0.79
1:A:70:ALA:HB1	1:A:73:ARG:HD3	1.65	0.78
1:B:80:ARG:HH11	1:B:135:ASN:HD21	1.33	0.77
1:C:80:ARG:HH11	1:C:135:ASN:HD21	1.32	0.76
1:A:80:ARG:HH11	1:A:135:ASN:HD21	1.35	0.75
1:D:80:ARG:HH11	1:D:135:ASN:HD21	1.35	0.75
1:B:16:ILE:HD11	1:B:170:ILE:HD11	1.71	0.73
1:D:160:LYS:HD2	1:D:207:LEU:HD21	1.69	0.73
1:A:160:LYS:HD2	1:A:207:LEU:HD21	1.69	0.73
1:B:160:LYS:HD2	1:B:207:LEU:HD21	1.72	0.72
1:D:16:ILE:HD11	1:D:170:ILE:HD11	1.70	0.72
1:C:80:ARG:HD2	1:C:135:ASN:ND2	2.06	0.70
1:B:80:ARG:HD2	1:B:135:ASN:ND2	2.07	0.69
1:A:142:CYS:SG	2:A:218:HOH:O	2.51	0.69
1:A:80:ARG:HD2	1:A:135:ASN:ND2	2.08	0.68
1:D:80:ARG:HD2	1:D:135:ASN:ND2	2.09	0.68
1:C:16:ILE:HD11	1:C:170:ILE:HD11	1.76	0.67
1:C:174:ILE:HD12	1:C:184:PRO:HG2	1.77	0.66
1:B:174:ILE:HD12	1:B:184:PRO:HG2	1.77	0.66
1:A:16:ILE:HD11	1:A:170:ILE:HD11	1.79	0.65
1:A:174:ILE:HD12	1:A:184:PRO:HG2	1.78	0.64
1:D:174:ILE:HD12	1:D:184:PRO:HG2	1.80	0.64
1:A:152:HIS:HD2	1:A:158:TYR:O	1.85	0.60
1:C:152:HIS:HD2	1:C:158:TYR:O	1.85	0.58
1:D:152:HIS:HD2	1:D:158:TYR:O	1.87	0.58
1:B:152:HIS:HD2	1:B:158:TYR:O	1.87	0.57
1:C:45:PHE:HB2	1:C:96:LYS:HE3	1.88	0.56
1:D:172:GLU:HG2	2:D:220:HOH:O	2.06	0.56
1:A:5:VAL:HG21	1:A:200:ILE:HD11	1.89	0.55
1:C:80:ARG:HD2	1:C:135:ASN:HD22	1.71	0.55
1:B:80:ARG:HD2	1:B:135:ASN:HD22	1.71	0.55
1:D:5:VAL:HG21	1:D:200:ILE:HD11	1.87	0.55
1:D:175:ILE:HA	1:D:178:ILE:HD12	1.87	0.54
1:A:45:PHE:HB2	1:A:96:LYS:HE3	1.89	0.54
1:A:175:ILE:HA	1:A:178:ILE:HD12	1.90	0.54
1:B:5:VAL:HG21	1:B:200:ILE:HD11	1.90	0.53
1:C:5:VAL:HG21	1:C:200:ILE:HD11	1.90	0.53
1:D:80:ARG:HD2	1:D:135:ASN:HD22	1.74	0.53
1:A:80:ARG:HD2	1:A:135:ASN:HD22	1.74	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:PHE:HB2	1:B:96:LYS:HE3	1.91	0.53
1:B:175:ILE:HA	1:B:178:ILE:HD12	1.92	0.52
1:D:45:PHE:HB2	1:D:96:LYS:HE3	1.92	0.51
1:C:175:ILE:HA	1:C:178:ILE:HD12	1.94	0.50
1:D:45:PHE:HE1	2:D:221:HOH:O	1.94	0.50
1:D:43:VAL:HB	1:D:93:ASN:OD1	2.12	0.50
1:C:49:LYS:HG3	1:C:148:LEU:HD13	1.95	0.48
1:C:118:LYS:HD3	1:C:133:ILE:CD1	2.43	0.48
1:A:118:LYS:HD3	1:A:133:ILE:CD1	2.44	0.48
1:D:118:LYS:HD3	1:D:133:ILE:CD1	2.43	0.48
1:D:49:LYS:HG3	1:D:148:LEU:HD13	1.94	0.48
1:C:22:ILE:HG21	1:C:196:VAL:HG11	1.97	0.47
1:D:1:MET:HE1	1:D:207:LEU:O	2.14	0.47
1:B:1:MET:HE1	1:B:207:LEU:O	2.14	0.47
1:B:81:ILE:HD12	1:B:135:ASN:O	2.14	0.47
1:B:118:LYS:HD3	1:B:133:ILE:CD1	2.45	0.47
1:C:1:MET:HE1	1:C:207:LEU:O	2.15	0.47
1:B:43:VAL:HB	1:B:93:ASN:OD1	2.15	0.47
1:A:43:VAL:HB	1:A:93:ASN:OD1	2.15	0.47
1:D:22:ILE:HG21	1:D:196:VAL:HG11	1.98	0.46
1:A:49:LYS:HG3	1:A:148:LEU:HD13	1.96	0.46
1:A:1:MET:HE1	1:A:207:LEU:O	2.16	0.45
1:C:43:VAL:HB	1:C:93:ASN:OD1	2.16	0.45
1:D:88:ALA:HB3	1:D:98:ILE:H	1.82	0.45
1:D:124:LEU:HD23	1:D:124:LEU:HA	1.77	0.45
1:D:81:ILE:HD12	1:D:135:ASN:O	2.17	0.45
1:B:175:ILE:HG13	2:B:217:HOH:O	2.16	0.45
1:D:37:PHE:CD1	1:D:37:PHE:N	2.85	0.43
1:B:207:LEU:O	1:B:207:LEU:HD13	2.19	0.43
1:C:151:HIS:HE1	2:C:240:HOH:O	2.02	0.43
1:D:194:GLU:O	1:D:198:VAL:HG23	2.18	0.43
1:C:37:PHE:CD1	1:C:37:PHE:N	2.86	0.43
1:A:22:ILE:HG21	1:A:196:VAL:HG11	2.00	0.43
1:C:123:LYS:HD2	1:C:123:LYS:HA	1.85	0.43
1:B:88:ALA:HB3	1:B:98:ILE:H	1.84	0.43
1:B:37:PHE:CD1	1:B:37:PHE:N	2.87	0.43
1:C:45:PHE:HB2	1:C:96:LYS:CE	2.49	0.43
1:A:194:GLU:O	1:A:198:VAL:HG23	2.19	0.42
1:B:22:ILE:HG21	1:B:196:VAL:HG11	2.01	0.42
1:A:81:ILE:HD12	1:A:135:ASN:O	2.19	0.42
1:B:49:LYS:HG3	1:B:148:LEU:HD13	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:207:LEU:O	1:D:207:LEU:HD13	2.20	0.42
1:C:16:ILE:HD13	1:C:16:ILE:HG21	1.87	0.42
1:D:118:LYS:HD3	1:D:133:ILE:HD11	2.00	0.42
1:D:183:VAL:HA	1:D:184:PRO:HD2	1.93	0.42
1:A:118:LYS:HD3	1:A:133:ILE:HD11	2.01	0.41
1:C:81:ILE:HD12	1:C:135:ASN:O	2.20	0.41
1:C:118:LYS:HD3	1:C:133:ILE:HD11	2.01	0.41
1:A:10:PRO:HA	2:A:220:HOH:O	2.20	0.41
1:A:123:LYS:HA	1:A:123:LYS:HD2	1.86	0.41
1:C:198:VAL:O	1:C:202:VAL:HG13	2.21	0.41
1:C:183:VAL:HA	1:C:184:PRO:HD2	1.92	0.41
1:D:123:LYS:HD2	1:D:123:LYS:HA	1.87	0.41
1:D:198:VAL:O	1:D:202:VAL:HG13	2.21	0.40
2:B:211:HOH:O	1:D:188:CYS:HB3	2.22	0.40
1:B:118:LYS:HD3	1:B:133:ILE:HD11	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
1	B	206/208 (99%)	193 (94%)	13 (6%)	0	100	100
1	C	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
1	D	206/208 (99%)	194 (94%)	12 (6%)	0	100	100
All	All	824/832 (99%)	775 (94%)	49 (6%)	0	100	100

There are no Ramachandran outliers to report.

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	A	174/174 (100%)	152 (87%)	22 (13%)	4	4
1	B	174/174 (100%)	153 (88%)	21 (12%)	5	4
1	C	174/174 (100%)	151 (87%)	23 (13%)	4	3
1	D	174/174 (100%)	152 (87%)	22 (13%)	4	4
All	All	696/696 (100%)	608 (87%)	88 (13%)	4	4

All (88) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	LEU
1	A	16	ILE
1	A	33	ASP
1	A	35	GLN
1	A	52	LEU
1	A	53	GLU
1	A	57	GLU
1	A	69	LEU
1	A	73	ARG
1	A	83	VAL
1	A	99	GLU
1	A	101	GLU
1	A	141	LEU
1	A	145	VAL
1	A	155	THR
1	A	172	GLU
1	A	182	GLN
1	A	196	VAL
1	A	202	VAL
1	A	206	GLU
1	A	207	LEU
1	B	4	LEU
1	B	16	ILE

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Mol	Chain	Res	Type
1	B	33	ASP
1	B	35	GLN
1	B	52	LEU
1	B	53	GLU
1	B	57	GLU
1	B	69	LEU
1	B	73	ARG
1	B	83	VAL
1	B	99	GLU
1	B	101	GLU
1	B	141	LEU
1	B	145	VAL
1	B	155	THR
1	B	172	GLU
1	B	182	GLN
1	B	196	VAL
1	B	202	VAL
1	B	206	GLU
1	B	207	LEU
1	C	1	MET
1	C	4	LEU
1	C	16	ILE
1	C	33	ASP
1	C	35	GLN
1	C	52	LEU
1	C	53	GLU
1	C	57	GLU
1	C	69	LEU
1	C	73	ARG
1	C	83	VAL
1	C	99	GLU
1	C	101	GLU
1	C	114	THR
1	C	141	LEU
1	C	145	VAL
1	C	155	THR
1	C	172	GLU
1	C	182	GLN
1	C	196	VAL
1	C	202	VAL
1	C	206	GLU
1	C	207	LEU

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Mol	Chain	Res	Type
1	D	1	MET
1	D	4	LEU
1	D	16	ILE
1	D	33	ASP
1	D	35	GLN
1	D	52	LEU
1	D	53	GLU
1	D	57	GLU
1	D	69	LEU
1	D	73	ARG
1	D	83	VAL
1	D	99	GLU
1	D	101	GLU
1	D	141	LEU
1	D	145	VAL
1	D	155	THR
1	D	172	GLU
1	D	182	GLN
1	D	196	VAL
1	D	202	VAL
1	D	206	GLU
1	D	207	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	ASN
1	A	152	HIS
1	B	135	ASN
1	B	152	HIS
1	C	135	ASN
1	C	152	HIS
1	D	135	ASN
1	D	152	HIS

5.3.3 RNA ⓘ

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.