



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:59 AM UTC

PDB ID : 1IBU / pdb_00001ibu
Title : STRUCTURE OF THE D53,54N MUTANT OF HISTIDINE DECARBOXY-
LASE AT 25 C
Authors : Worley, S.; Schelp, E.; Monzingo, A.F.; Ernst, S.; Robertus, J.D.
Deposited on : 2001-03-29
Resolution : 3.10 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:

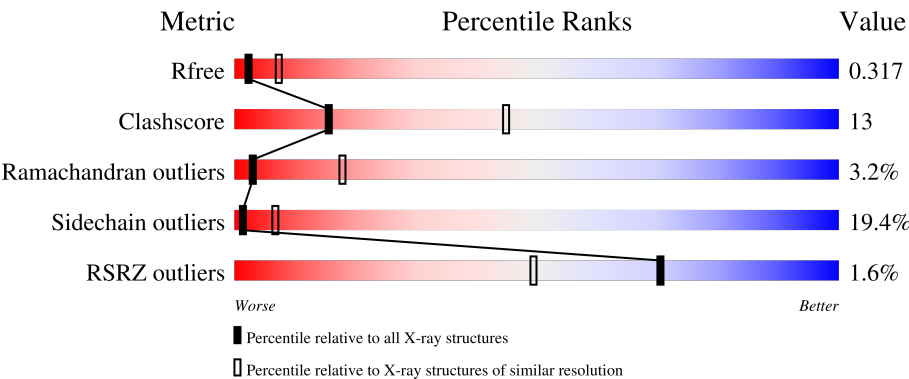
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	81	51%25%20%
1	C	81	49%30%17%
1	E	81	2% 53%22%10%14%
2	B	229	3% 49%36%13%
2	D	229	47%38%12%

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Mol	Chain	Length	Quality of chain
2	F	229	2% 46% 37% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6856 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 HISTIDINE DECARBOXYLASE BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	65	Total	C	N	O	S	0	0	0
			493	307	87	97	2			
1	C	67	Total	C	N	O	S	0	0	0
			506	314	89	101	2			
1	E	70	Total	C	N	O	S	0	0	0
			529	328	95	104	2			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	53	ASN	ASP	engineered mutation	UNP P00862
A	54	ASN	ASP	engineered mutation	UNP P00862
C	53	ASN	ASP	engineered mutation	UNP P00862
C	54	ASN	ASP	engineered mutation	UNP P00862
E	53	ASN	ASP	engineered mutation	UNP P00862
E	54	ASN	ASP	engineered mutation	UNP P00862

- Molecule 2 is a protein called HISTIDINE DECARBOXYLASE ALPHA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			
2	D	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			
2	F	229	Total	C	N	O	S	0	0	0
			1776	1127	286	352	11			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	82	PYR	SER	modified residue	UNP P00862
D	82	PYR	SER	modified residue	UNP P00862

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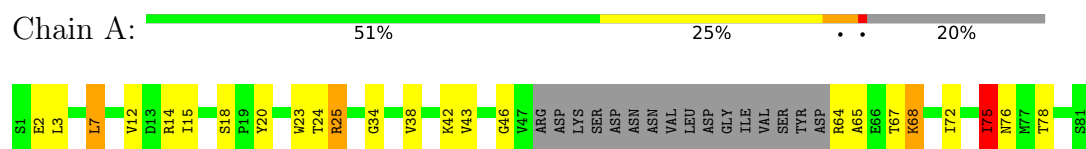
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Chain	Residue	Modelled	Actual	Comment	Reference
F	82	PYR	SER	modified residue	UNP P00862

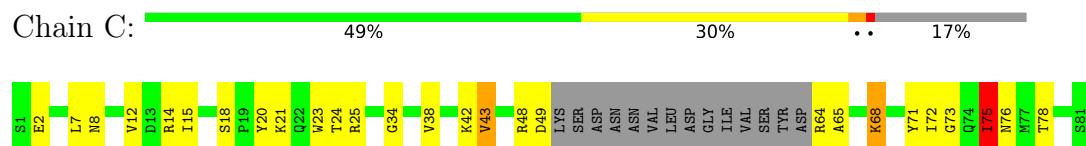
3 Residue-property plots [i](#)

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 and electron density. 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. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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.

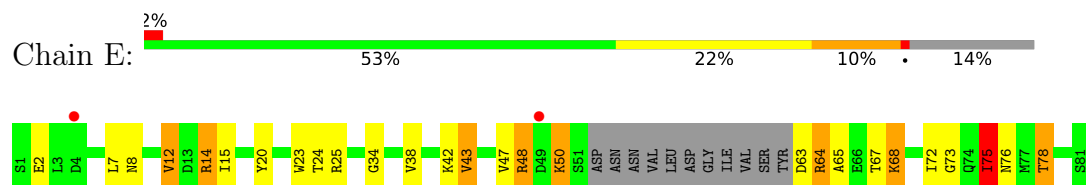
• Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN



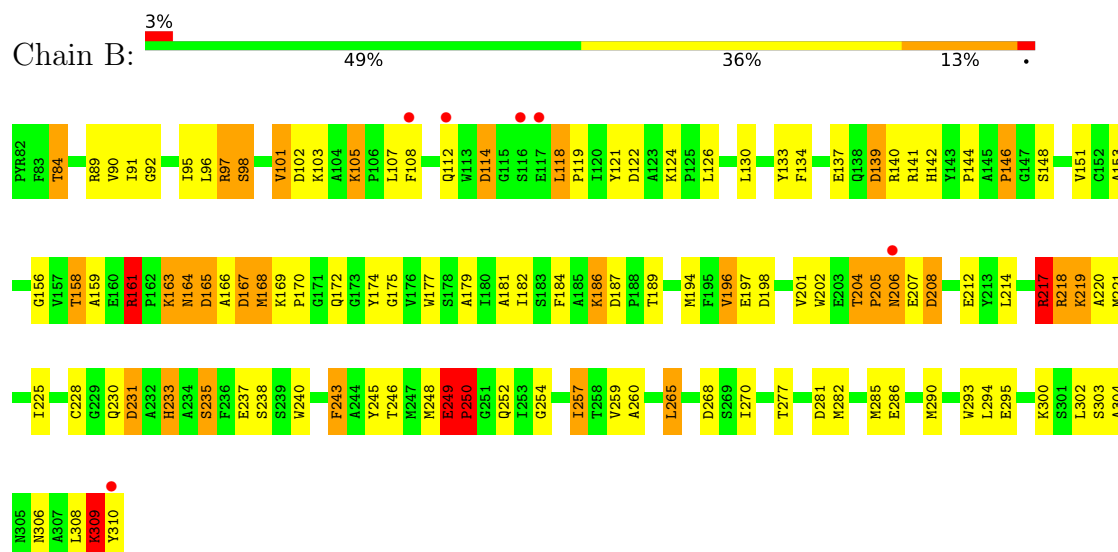
• Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN



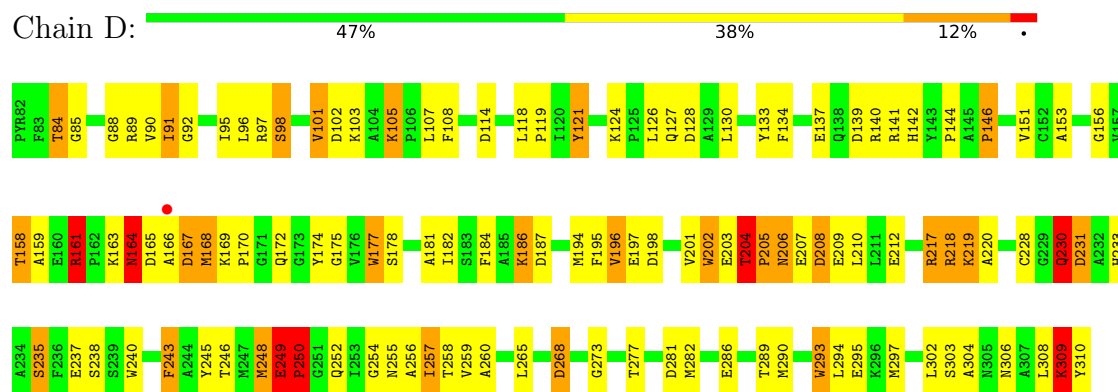
• Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN



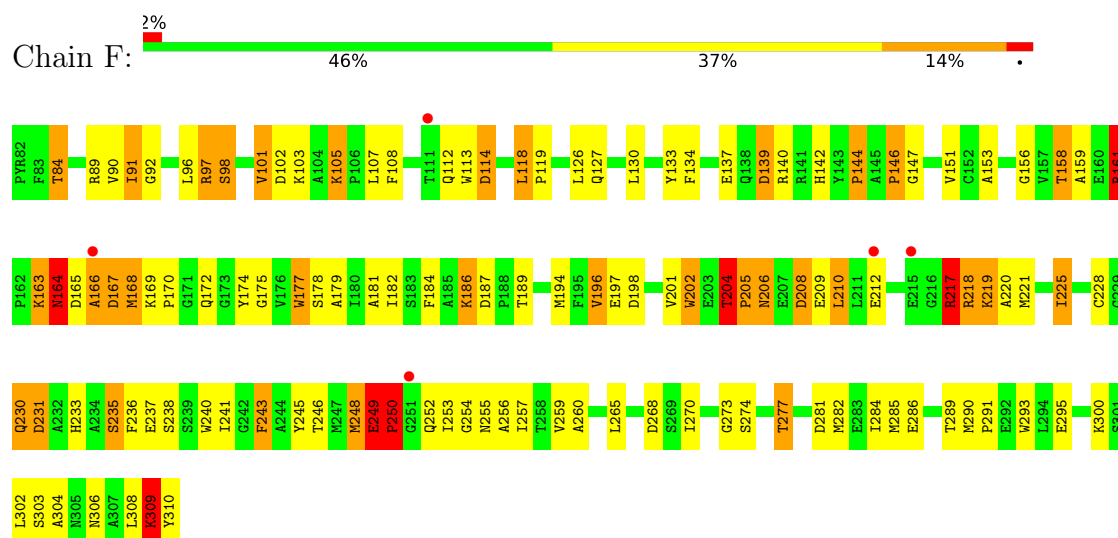
• Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN



• Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN



• Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	98.28Å 119.04Å 203.80Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 3.10 10.00 – 3.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-3.10) 79.1 (10.00-3.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.59 (at 3.10Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.270 , 0.330 0.255 , 0.317	Depositor DCC
R_{free} test set	845 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	82.7	Xtriage
Anisotropy	0.461	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 84.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6856	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.28% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PYR

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	1.12	1/499 (0.2%)	2.14	12/670 (1.8%)
1	C	1.13	1/512 (0.2%)	1.94	13/688 (1.9%)
1	E	1.22	1/535 (0.2%)	2.08	20/719 (2.8%)
2	B	1.14	3/1816 (0.2%)	1.98	59/2463 (2.4%)
2	D	1.10	2/1816 (0.1%)	2.01	55/2463 (2.2%)
2	F	1.11	3/1816 (0.2%)	1.98	59/2463 (2.4%)
All	All	1.13	11/6994 (0.2%)	2.01	218/9466 (2.3%)

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	B	0	1
2	D	0	1
2	F	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	142	HIS	CD2-NE2	-6.38	1.30	1.37
2	B	142	HIS	CD2-NE2	-6.37	1.30	1.37
2	D	233	HIS	CD2-NE2	-6.30	1.30	1.37
1	C	23	TRP	NE1-CE2	-6.25	1.30	1.37
2	F	233	HIS	CD2-NE2	-6.22	1.31	1.37
2	B	233	HIS	CD2-NE2	-6.05	1.31	1.37
2	D	142	HIS	CD2-NE2	-5.95	1.31	1.37
1	E	48	ARG	NE-CZ	5.94	1.39	1.33
1	A	25	ARG	CD-NE	-5.51	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	144	PRO	CA-CB	-5.35	1.46	1.53
2	B	233	HIS	CG-ND1	-5.08	1.32	1.38

All (218) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ARG	CD-NE-CZ	17.42	148.79	124.40
2	D	217	ARG	CD-NE-CZ	17.10	148.34	124.40
1	A	25	ARG	NE-CZ-NH2	-15.59	105.17	119.20
2	D	217	ARG	NE-CZ-NH2	-13.18	107.34	119.20
2	F	250	PRO	N-CA-C	11.76	136.69	112.47
2	B	250	PRO	N-CA-C	11.72	136.61	112.47
2	D	217	ARG	NE-CZ-NH1	11.60	133.10	121.50
2	D	250	PRO	N-CA-C	11.34	135.82	112.47
1	A	25	ARG	NE-CZ-NH1	10.61	132.11	121.50
2	B	250	PRO	CA-N-CD	-9.82	98.25	112.00
2	F	250	PRO	CA-N-CD	-9.71	98.41	112.00
2	D	250	PRO	CA-N-CD	-9.51	98.69	112.00
1	E	50	LYS	N-CA-C	9.36	130.73	110.80
2	F	208	ASP	CA-CB-CG	8.95	121.55	112.60
1	E	25	ARG	NE-CZ-NH1	-8.73	112.77	121.50
2	F	168	MET	N-CA-C	8.70	124.46	107.57
2	D	208	ASP	CA-CB-CG	8.69	121.29	112.60
2	B	217	ARG	NE-CZ-NH1	-8.42	113.08	121.50
2	B	208	ASP	CA-CB-CG	8.39	120.99	112.60
2	D	168	MET	N-CA-C	8.34	123.75	107.57
2	B	168	MET	N-CA-C	8.24	123.55	107.57
1	C	76	ASN	OD1-CG-ND2	-8.22	114.38	122.60
2	F	249	GLU	CA-C-N	8.15	130.02	119.84
2	F	249	GLU	C-N-CA	8.15	130.02	119.84
2	B	107	LEU	N-CA-C	-7.97	101.37	112.45
2	B	249	GLU	CA-C-N	7.83	129.63	119.84
2	B	249	GLU	C-N-CA	7.83	129.63	119.84
2	D	114	ASP	N-CA-C	-7.82	102.69	111.14
2	D	249	GLU	CA-C-N	7.71	129.48	119.84
2	D	249	GLU	C-N-CA	7.71	129.48	119.84
2	F	217	ARG	CD-NE-CZ	7.69	135.17	124.40
2	F	107	LEU	N-CA-C	-7.68	101.78	112.45
2	D	107	LEU	N-CA-C	-7.64	101.84	112.45
1	E	47	VAL	N-CA-C	7.58	119.26	108.42
1	C	25	ARG	NE-CZ-NH1	-7.50	114.00	121.50
2	F	252	GLN	N-CA-C	-7.38	100.58	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	204	THR	O-C-N	-7.27	112.96	121.32
2	B	114	ASP	N-CA-C	-7.25	103.31	111.14
1	A	65	ALA	N-CA-C	-7.21	99.86	111.04
2	D	166	ALA	N-CA-C	-7.20	101.58	110.65
2	B	166	ALA	N-CA-C	-7.12	101.67	110.65
2	B	204	THR	O-C-N	-7.09	113.16	121.32
2	B	196	VAL	N-CA-C	-7.05	97.27	107.78
1	C	65	ALA	N-CA-C	-7.05	100.12	111.04
2	F	114	ASP	N-CA-C	-7.03	103.55	111.14
2	D	196	VAL	N-CA-C	-7.00	97.94	108.17
2	F	196	VAL	N-CA-C	-7.00	97.94	108.17
1	E	25	ARG	NE-CZ-NH2	6.98	125.48	119.20
2	D	302	LEU	N-CA-C	-6.94	106.00	114.75
2	D	246	THR	CA-CB-OG1	-6.93	99.21	109.60
2	B	217	ARG	CD-NE-CZ	6.84	133.97	124.40
2	B	205	PRO	CA-N-CD	-6.82	102.46	112.00
2	F	220	ALA	N-CA-C	-6.82	103.46	111.03
2	F	302	LEU	N-CA-C	-6.78	106.21	114.75
2	F	204	THR	O-C-N	-6.77	113.53	121.32
2	D	220	ALA	N-CA-C	-6.76	103.52	111.03
2	B	302	LEU	N-CA-C	-6.73	106.27	114.75
2	B	220	ALA	N-CA-C	-6.70	103.60	111.03
2	F	166	ALA	N-CA-C	-6.57	102.37	110.65
1	E	76	ASN	OD1-CG-ND2	-6.55	116.05	122.60
2	B	153	ALA	N-CA-C	-6.52	98.61	109.24
2	D	153	ALA	N-CA-C	-6.51	98.11	108.73
2	F	205	PRO	CA-N-CD	-6.49	102.92	112.00
2	F	238	SER	O-C-N	-6.45	116.13	123.48
1	E	8	ASN	OD1-CG-ND2	-6.44	116.16	122.60
2	B	206	ASN	OD1-CG-ND2	-6.38	116.22	122.60
2	B	246	THR	CA-CB-OG1	-6.33	100.11	109.60
2	B	142	HIS	CA-CB-CG	-6.32	107.48	113.80
2	B	252	GLN	N-CA-C	-6.32	100.27	110.32
1	A	34	GLY	CA-C-O	-6.32	116.50	122.13
2	F	255	ASN	CA-CB-CG	-6.29	106.31	112.60
2	D	205	PRO	CA-N-CD	-6.27	103.22	112.00
2	B	141	ARG	NE-CZ-NH1	-6.26	115.24	121.50
2	D	142	HIS	CA-CB-CG	-6.26	107.54	113.80
2	D	206	ASN	CB-CG-ND2	6.24	125.76	116.40
2	F	281	ASP	CA-CB-CG	6.23	118.83	112.60
1	A	76	ASN	OD1-CG-ND2	-6.22	116.38	122.60
1	E	23	TRP	CG-CD2-CE3	6.21	140.11	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	142	HIS	CA-CB-CG	-6.21	107.59	113.80
1	E	63	ASP	CA-CB-CG	6.20	118.80	112.60
2	F	98	SER	CA-C-N	6.19	125.68	119.24
2	F	98	SER	C-N-CA	6.19	125.68	119.24
1	E	25	ARG	CD-NE-CZ	6.18	133.06	124.40
1	E	34	GLY	CA-C-O	-6.11	116.69	122.13
2	D	252	GLN	N-CA-C	-6.11	101.44	110.48
1	C	48	ARG	N-CA-C	-6.11	99.69	108.60
1	C	23	TRP	N-CA-C	6.10	119.08	110.23
2	F	187	ASP	CA-CB-CG	6.08	118.68	112.60
2	D	281	ASP	CA-CB-CG	6.06	118.66	112.60
1	E	23	TRP	N-CA-C	6.04	118.98	110.23
2	B	238	SER	O-C-N	-6.04	116.60	123.48
2	B	165	ASP	CA-CB-CG	6.02	118.62	112.60
2	F	167	ASP	N-CA-C	-6.02	98.59	108.76
2	B	260	ALA	N-CA-C	-5.98	99.17	109.15
2	D	84	THR	N-CA-C	-5.97	98.35	108.26
2	B	187	ASP	CA-CB-CG	5.93	118.53	112.60
2	D	206	ASN	OD1-CG-ND2	-5.93	116.67	122.60
2	D	303	SER	N-CA-C	-5.92	104.18	111.40
1	C	34	GLY	CA-C-O	-5.91	116.87	122.13
2	D	257	ILE	O-C-N	5.87	129.22	122.82
2	B	98	SER	CA-C-N	5.84	125.32	119.24
2	B	98	SER	C-N-CA	5.84	125.32	119.24
2	B	84	THR	CA-CB-OG1	-5.84	100.84	109.60
2	B	217	ARG	NE-CZ-NH2	5.81	124.43	119.20
2	B	206	ASN	CB-CG-ND2	5.81	125.12	116.40
2	F	303	SER	N-CA-C	-5.80	104.32	111.40
2	F	153	ALA	N-CA-C	-5.80	99.28	108.73
2	D	187	ASP	CA-CB-CG	5.79	118.39	112.60
2	D	101	VAL	N-CA-C	5.78	116.43	110.36
2	B	233	HIS	CB-CG-CD2	-5.78	123.68	131.20
2	F	241	ILE	CA-C-O	-5.77	115.17	121.28
2	B	303	SER	N-CA-C	-5.75	104.39	111.40
2	F	102	ASP	N-CA-C	-5.71	105.81	112.89
2	F	260	ALA	N-CA-C	-5.69	99.64	109.15
2	F	189	THR	CA-CB-OG1	-5.69	101.07	109.60
2	D	260	ALA	N-CA-C	-5.68	99.67	109.15
2	F	219	LYS	CB-CG-CD	5.68	124.36	111.30
2	B	249	GLU	O-C-N	-5.67	114.80	121.32
2	F	309	LYS	CA-C-O	-5.66	115.43	121.94
2	F	202	TRP	CG-CD2-CE3	5.63	139.53	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	167	ASP	N-CA-C	-5.63	99.25	108.76
2	F	249	GLU	O-C-N	-5.62	114.85	121.32
2	F	217	ARG	NE-CZ-NH1	-5.61	115.89	121.50
1	A	72	ILE	N-CA-C	-5.59	97.70	109.34
1	C	25	ARG	CD-NE-CZ	5.59	132.23	124.40
2	F	206	ASN	CB-CG-ND2	5.56	124.73	116.40
2	F	202	TRP	CB-CG-CD1	-5.56	118.56	126.90
1	A	23	TRP	CG-CD2-CE3	5.55	139.45	133.90
2	B	257	ILE	O-C-N	5.55	128.87	122.82
2	B	167	ASP	N-CA-C	-5.54	99.40	108.76
2	D	84	THR	CA-CB-OG1	-5.54	101.30	109.60
2	D	233	HIS	CB-CG-CD2	-5.53	124.01	131.20
1	C	72	ILE	N-CA-C	-5.51	97.88	109.34
2	D	202	TRP	CB-CG-CD1	-5.51	118.64	126.90
2	F	230	GLN	CA-CB-CG	5.51	125.12	114.10
2	F	202	TRP	CE2-CD2-CG	-5.51	100.59	107.20
2	B	189	THR	CA-CB-OG1	-5.50	101.35	109.60
2	D	98	SER	N-CA-C	-5.49	103.12	109.93
2	F	217	ARG	NE-CZ-NH2	5.49	124.14	119.20
2	B	202	TRP	CG-CD2-CE3	5.49	139.39	133.90
2	B	231	ASP	N-CA-C	-5.49	105.20	111.07
2	B	207	GLU	CA-C-O	-5.48	115.03	120.90
1	E	50	LYS	CA-C-O	5.48	128.35	120.51
1	E	78	THR	CA-CB-OG1	-5.48	101.38	109.60
2	F	84	THR	CA-CB-OG1	-5.48	101.38	109.60
2	D	127	GLN	O-C-N	5.47	127.71	122.07
2	B	265	LEU	CA-C-N	5.46	126.61	120.66
2	B	265	LEU	C-N-CA	5.46	126.61	120.66
2	B	102	ASP	N-CA-C	-5.41	106.19	112.89
2	B	141	ARG	CA-C-O	-5.40	116.69	119.77
2	D	309	LYS	CA-C-O	-5.39	115.74	121.94
1	E	72	ILE	N-CA-C	-5.39	98.12	109.34
1	C	23	TRP	CG-CD2-CE3	5.39	139.29	133.90
1	A	75	ILE	N-CA-C	5.37	117.29	108.97
1	E	75	ILE	N-CA-CB	-5.37	99.99	111.37
2	B	219	LYS	CB-CG-CD	5.37	123.64	111.30
2	F	243	PHE	CB-CA-C	-5.36	98.93	110.45
2	B	309	LYS	CA-C-O	-5.36	115.78	121.94
1	E	75	ILE	N-CA-C	5.35	117.27	108.97
2	B	250	PRO	N-CA-CB	-5.34	97.64	103.25
2	D	141	ARG	NE-CZ-NH1	-5.33	116.17	121.50
2	F	113	TRP	CB-CG-CD1	-5.33	118.91	126.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	84	THR	N-CA-C	-5.33	99.42	108.26
1	C	25	ARG	NE-CZ-NH2	5.32	123.99	119.20
2	D	202	TRP	CG-CD2-CE3	5.32	139.22	133.90
2	B	101	VAL	CA-C-O	-5.32	115.74	121.27
1	C	8	ASN	OD1-CG-ND2	-5.31	117.29	122.60
2	F	236	PHE	CA-CB-CG	-5.31	108.49	113.80
2	B	281	ASP	CA-CB-CG	5.31	117.91	112.60
1	A	23	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	E	65	ALA	N-CA-C	-5.29	100.30	110.56
2	F	164	ASN	O-C-N	5.29	129.63	122.59
2	F	177	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	A	46	GLY	O-C-N	-5.27	119.27	123.27
2	F	113	TRP	CE2-CD2-CG	-5.27	100.88	107.20
2	B	97	ARG	N-CA-C	5.27	117.86	109.96
2	F	225	ILE	O-C-N	5.25	127.04	121.89
2	D	202	TRP	CE2-CD2-CG	-5.25	100.90	107.20
2	D	230	GLN	CA-CB-CG	5.24	124.59	114.10
2	F	233	HIS	CB-CG-CD2	-5.23	124.40	131.20
2	D	238	SER	O-C-N	-5.23	117.51	123.48
2	F	250	PRO	N-CA-CB	-5.22	97.77	103.25
2	D	164	ASN	O-C-N	5.21	129.52	122.59
2	D	219	LYS	CB-CG-CD	5.21	123.29	111.30
2	B	91	ILE	N-CA-CB	5.19	116.46	110.49
2	D	249	GLU	O-C-N	-5.18	115.36	121.32
2	D	255	ASN	CA-CB-CG	-5.18	107.42	112.60
2	F	101	VAL	CA-C-O	-5.18	115.88	121.27
2	B	98	SER	N-CA-C	-5.17	103.52	109.93
2	D	207	GLU	CA-C-O	-5.17	115.37	120.90
2	B	84	THR	N-CA-C	-5.16	99.69	108.26
2	B	243	PHE	CB-CA-C	-5.16	99.36	110.45
2	D	102	ASP	N-CA-C	-5.16	106.84	113.23
1	C	75	ILE	N-CA-CB	-5.14	100.47	111.37
1	E	48	ARG	CG-CD-NE	5.13	123.29	112.00
2	B	202	TRP	CB-CG-CD1	-5.12	119.21	126.90
1	E	14	ARG	N-CA-C	-5.12	104.20	110.61
2	D	246	THR	CA-CB-CG2	5.12	119.21	110.50
2	F	210	LEU	O-C-N	5.10	127.54	122.03
2	D	273	GLY	N-CA-C	-5.09	104.84	112.89
1	E	12	VAL	CA-C-O	-5.09	115.12	120.57
1	C	75	ILE	N-CA-C	5.09	116.86	108.97
2	D	293	TRP	CE2-CD2-CG	-5.08	101.10	107.20
2	F	273	GLY	N-CA-C	-5.08	104.87	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	246	THR	CA-CB-OG1	-5.07	101.99	109.60
1	A	75	ILE	N-CA-CB	-5.07	100.62	111.37
2	F	97	ARG	N-CA-C	5.07	117.56	109.96
2	B	148	SER	N-CA-C	5.06	117.06	110.53
2	D	177	TRP	CE2-CD2-CG	-5.06	101.13	107.20
2	D	289	THR	N-CA-C	-5.06	102.28	110.32
2	B	202	TRP	CE2-CD2-CG	-5.05	101.14	107.20
2	B	214	LEU	CA-C-O	-5.05	115.51	121.07
2	B	246	THR	CA-CB-CG2	5.05	119.08	110.50
2	D	91	ILE	N-CA-CB	5.04	116.29	110.49
2	F	91	ILE	N-CA-CB	5.02	116.26	110.49
2	F	206	ASN	OD1-CG-ND2	-5.01	117.59	122.60
2	D	243	PHE	CB-CA-C	-5.00	99.70	110.45
2	F	91	ILE	N-CA-C	-5.00	102.18	108.93

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	161	ARG	Peptide
2	D	161	ARG	Peptide
2	F	161	ARG	Peptide

5.2 Too-close contacts [i](#)

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	493	0	491	13	0
1	C	506	0	497	18	0
1	E	529	0	521	20	0
2	B	1776	0	1704	49	0
2	D	1776	0	1704	58	0
2	F	1776	0	1704	61	0
All	All	6856	0	6621	181	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 13.

All (181) 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:F:218:ARG:HG2	2:F:243:PHE:HZ	1.44	0.82
2:D:218:ARG:HG2	2:D:243:PHE:HZ	1.46	0.81
2:B:218:ARG:HG2	2:B:243:PHE:HZ	1.46	0.78
2:D:161:ARG:NE	2:D:249:GLU:HA	2.00	0.77
2:F:249:GLU:HB2	2:F:250:PRO:HD2	1.66	0.77
2:B:161:ARG:NE	2:B:249:GLU:HA	2.02	0.75
2:D:249:GLU:HB2	2:D:250:PRO:HD2	1.68	0.75
2:D:175:GLY:HA2	2:D:248:MET:SD	2.27	0.74
2:B:249:GLU:HB2	2:B:250:PRO:HD2	1.70	0.74
2:F:161:ARG:HG3	2:F:174:TYR:HA	1.70	0.73
2:D:161:ARG:HG3	2:D:174:TYR:HA	1.71	0.73
2:D:194:MET:HE1	2:D:228:CYS:SG	2.31	0.70
2:F:175:GLY:HA2	2:F:248:MET:SD	2.31	0.70
2:F:161:ARG:NE	2:F:249:GLU:HA	2.05	0.70
2:F:194:MET:HE1	2:F:228:CYS:SG	2.33	0.68
1:E:38:VAL:HG11	2:F:265:LEU:HD21	1.77	0.67
2:B:194:MET:HE1	2:B:228:CYS:SG	2.35	0.66
2:B:161:ARG:HG3	2:B:174:TYR:HA	1.78	0.65
2:D:156:GLY:HA2	2:D:257:ILE:HG22	1.81	0.63
2:F:156:GLY:HA2	2:F:257:ILE:HG22	1.79	0.63
2:D:231:ASP:HB3	1:E:67:THR:HG21	1.82	0.62
2:B:156:GLY:HA2	2:B:257:ILE:HG22	1.83	0.60
2:B:175:GLY:HA2	2:B:248:MET:SD	2.43	0.59
1:A:68:LYS:HZ2	1:A:68:LYS:HB2	1.68	0.59
1:E:68:LYS:HZ2	1:E:68:LYS:HB2	1.69	0.58
1:C:68:LYS:HZ2	1:C:68:LYS:HB2	1.68	0.58
1:E:42:LYS:HB3	2:F:259:VAL:HG13	1.86	0.58
2:D:161:ARG:HE	2:D:249:GLU:HA	1.68	0.58
1:A:67:THR:HG21	2:F:231:ASP:HB3	1.86	0.57
1:C:38:VAL:HG11	2:D:265:LEU:HD21	1.86	0.57
1:E:75:ILE:HD11	2:F:144:PRO:HB2	1.87	0.56
2:F:218:ARG:HG2	2:F:243:PHE:CZ	2.33	0.56
1:C:14:ARG:HB2	2:D:89:ARG:NH1	2.21	0.56
1:C:42:LYS:HB3	2:D:259:VAL:HG13	1.88	0.55
2:D:218:ARG:HG2	2:D:243:PHE:CZ	2.34	0.55
1:A:14:ARG:HB2	2:B:89:ARG:NH1	2.21	0.55
1:C:75:ILE:HD11	2:D:144:PRO:HB2	1.89	0.55
1:A:38:VAL:HG11	2:B:265:LEU:HD21	1.88	0.54
1:A:42:LYS:HB3	2:B:259:VAL:HG13	1.89	0.54
2:D:92:GLY:O	2:D:97:ARG:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:218:ARG:HG2	2:B:243:PHE:CZ	2.36	0.54
1:A:75:ILE:HD11	2:B:144:PRO:HB2	1.90	0.53
2:B:92:GLY:O	2:B:97:ARG:HA	2.09	0.53
2:D:101:VAL:HG13	2:D:240:TRP:CH2	2.44	0.53
1:E:48:ARG:HB3	2:F:253:ILE:HG23	1.91	0.53
2:B:177:TRP:HH2	2:B:217:ARG:HH11	1.58	0.52
2:F:92:GLY:O	2:F:97:ARG:HA	2.08	0.52
2:F:161:ARG:HE	2:F:249:GLU:HA	1.72	0.52
2:F:182:ILE:HG23	2:F:240:TRP:HB2	1.92	0.52
2:B:108:PHE:CZ	2:B:219:LYS:HG2	2.46	0.51
2:F:179:ALA:HB3	2:F:221:MET:HE1	1.91	0.51
2:B:161:ARG:HE	2:B:249:GLU:HA	1.74	0.51
2:D:85:GLY:HA3	2:F:147:GLY:HA3	1.92	0.51
2:F:309:LYS:NZ	2:F:310:TYR:HA	2.25	0.51
2:F:103:LYS:O	2:F:105:LYS:NZ	2.44	0.51
1:C:12:VAL:HG22	1:E:20:TYR:CE1	2.47	0.50
2:D:108:PHE:CZ	2:D:219:LYS:HG2	2.46	0.50
2:D:309:LYS:NZ	2:D:310:TYR:HA	2.27	0.50
2:D:103:LYS:O	2:D:105:LYS:NZ	2.45	0.49
2:B:103:LYS:O	2:B:105:LYS:NZ	2.45	0.49
2:F:108:PHE:CZ	2:F:219:LYS:HG2	2.47	0.49
2:F:178:SER:OG	2:F:256:ALA:HB1	2.13	0.49
2:D:133:TYR:HD1	2:D:293:TRP:CH2	2.31	0.49
2:B:182:ILE:HG23	2:B:240:TRP:HB2	1.94	0.49
2:B:89:ARG:HH21	2:B:286:GLU:CD	2.21	0.49
1:A:15:ILE:HA	2:B:282:MET:HG3	1.95	0.48
1:C:15:ILE:HA	2:D:282:MET:HG3	1.94	0.48
1:A:75:ILE:CD1	2:B:144:PRO:HB2	2.43	0.48
2:D:124:LYS:HZ2	2:D:128:ASP:CG	2.21	0.48
2:D:182:ILE:HG23	2:D:240:TRP:HB2	1.95	0.48
2:D:186:LYS:NZ	2:D:235:SER:OG	2.47	0.48
1:E:75:ILE:CD1	2:F:144:PRO:HB2	2.44	0.48
2:B:309:LYS:NZ	2:B:310:TYR:HA	2.29	0.48
2:F:91:ILE:HD12	2:F:130:LEU:HD13	1.95	0.48
2:B:101:VAL:HG13	2:B:240:TRP:CH2	2.49	0.47
2:F:177:TRP:HH2	2:F:217:ARG:HH11	1.61	0.47
2:B:137:GLU:O	2:B:140:ARG:NH1	2.47	0.47
1:E:78:THR:HB	2:F:151:VAL:HA	1.97	0.47
2:F:89:ARG:HH21	2:F:286:GLU:CD	2.22	0.47
2:F:225:ILE:O	2:F:228:CYS:HB3	2.14	0.47
2:B:90:VAL:HG21	2:B:184:PHE:HE1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:15:ILE:HA	2:F:282:MET:HG3	1.96	0.47
2:B:179:ALA:HB3	2:B:221:MET:HE1	1.97	0.47
2:D:89:ARG:HH21	2:D:286:GLU:CD	2.22	0.47
1:A:78:THR:HB	2:B:151:VAL:HA	1.97	0.46
1:E:73:GLY:O	1:E:75:ILE:HD13	2.15	0.46
2:F:156:GLY:CA	2:F:257:ILE:HG22	2.45	0.46
2:F:202:TRP:CD1	2:F:210:LEU:HD13	2.50	0.46
2:B:270:ILE:HG12	2:B:285:MET:HE2	1.98	0.46
2:F:101:VAL:HG13	2:F:240:TRP:CH2	2.50	0.46
2:D:177:TRP:HH2	2:D:217:ARG:NH1	2.13	0.46
1:C:75:ILE:CD1	2:D:144:PRO:HB2	2.45	0.46
1:E:14:ARG:HB2	2:F:89:ARG:NH1	2.31	0.46
2:D:290:MET:O	2:D:294:LEU:HD12	2.16	0.46
1:C:78:THR:HB	2:D:151:VAL:HA	1.98	0.46
2:D:90:VAL:HG21	2:D:184:PHE:HE1	1.81	0.46
2:B:95:ILE:HD12	2:B:96:LEU:HD13	1.98	0.45
2:D:181:ALA:N	2:D:196:VAL:O	2.49	0.45
2:D:96:LEU:O	2:D:290:MET:HB2	2.16	0.45
2:B:290:MET:O	2:B:294:LEU:HD12	2.17	0.45
2:B:96:LEU:O	2:B:290:MET:HB2	2.18	0.44
2:B:139:ASP:OD2	2:B:300:LYS:NZ	2.51	0.44
2:B:177:TRP:HH2	2:B:217:ARG:NH1	2.16	0.44
2:D:202:TRP:CD1	2:D:210:LEU:HD13	2.53	0.44
2:B:118:LEU:HA	2:B:119:PRO:HD2	1.88	0.44
2:F:139:ASP:OD2	2:F:300:LYS:NZ	2.51	0.44
2:B:156:GLY:CA	2:B:257:ILE:HG22	2.47	0.43
2:F:174:TYR:O	2:F:248:MET:SD	2.76	0.43
2:D:249:GLU:HB2	2:D:250:PRO:CD	2.44	0.43
2:B:159:ALA:HB1	2:B:172:GLN:HA	2.00	0.43
2:B:186:LYS:NZ	2:B:235:SER:OG	2.50	0.43
1:C:43:VAL:HA	2:D:257:ILE:O	2.18	0.43
2:F:159:ALA:HB1	2:F:172:GLN:HA	2.00	0.43
2:B:130:LEU:HD11	2:B:134:PHE:CE1	2.54	0.43
2:B:163:LYS:NZ	2:B:250:PRO:O	2.50	0.43
2:D:137:GLU:O	2:D:140:ARG:NH1	2.50	0.43
2:B:133:TYR:HD1	2:B:293:TRP:CH2	2.36	0.43
2:D:158:THR:HA	2:D:254:GLY:O	2.18	0.43
1:E:68:LYS:HZ2	1:E:68:LYS:CB	2.31	0.43
1:C:73:GLY:O	1:C:75:ILE:HD13	2.18	0.43
2:D:156:GLY:CA	2:D:257:ILE:HG22	2.45	0.43
2:D:309:LYS:HZ2	2:D:310:TYR:HA	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:186:LYS:NZ	2:F:235:SER:OG	2.52	0.43
1:C:43:VAL:HG12	2:D:258:THR:HA	2.01	0.43
2:F:90:VAL:HG21	2:F:184:PHE:HE1	1.83	0.43
2:F:249:GLU:HB2	2:F:250:PRO:CD	2.43	0.43
2:D:175:GLY:CA	2:D:248:MET:SD	3.03	0.43
1:A:12:VAL:HG22	1:C:20:TYR:CE1	2.54	0.42
1:A:20:TYR:CD1	1:E:12:VAL:HG22	2.54	0.42
1:C:21:LYS:NZ	2:D:268:ASP:CG	2.77	0.42
2:D:119:PRO:HB2	2:D:121:TYR:CE1	2.54	0.42
2:F:161:ARG:CZ	2:F:174:TYR:HD1	2.32	0.42
2:B:122:ASP:OD2	2:B:124:LYS:HB2	2.19	0.42
2:B:158:THR:HA	2:B:254:GLY:O	2.19	0.42
2:D:159:ALA:HB1	2:D:172:GLN:HA	2.01	0.42
2:D:174:TYR:O	2:D:248:MET:SD	2.77	0.42
2:F:181:ALA:N	2:F:196:VAL:O	2.52	0.42
2:D:88:GLY:O	2:D:89:ARG:HG3	2.19	0.42
2:F:130:LEU:HD11	2:F:134:PHE:CE1	2.54	0.42
2:F:137:GLU:O	2:F:140:ARG:NH1	2.52	0.42
2:F:270:ILE:HG12	2:F:285:MET:HE2	2.01	0.42
2:F:204:THR:HG21	2:F:209:GLU:HB2	2.02	0.42
1:E:42:LYS:HB3	2:F:259:VAL:CG1	2.48	0.42
2:F:118:LEU:HA	2:F:119:PRO:HD2	1.95	0.42
2:F:289:THR:CB	2:F:291:PRO:HD2	2.50	0.42
2:B:181:ALA:N	2:B:196:VAL:O	2.53	0.42
2:D:95:ILE:HD12	2:D:96:LEU:HD13	2.02	0.42
2:D:161:ARG:CZ	2:D:174:TYR:HD1	2.33	0.41
2:F:177:TRP:HH2	2:F:217:ARG:NH1	2.18	0.41
2:F:309:LYS:HZ2	2:F:310:TYR:HA	1.84	0.41
2:B:179:ALA:HB2	2:B:243:PHE:CD1	2.55	0.41
2:D:91:ILE:HD12	2:D:130:LEU:HD13	2.02	0.41
1:A:42:LYS:HB3	2:B:259:VAL:CG1	2.51	0.41
2:D:230:GLN:OE1	1:E:64:ARG:NH1	2.53	0.41
1:E:43:VAL:HA	2:F:257:ILE:O	2.20	0.41
2:F:133:TYR:HD1	2:F:293:TRP:CH2	2.38	0.41
1:E:48:ARG:HB3	2:F:253:ILE:CG2	2.50	0.41
2:B:112:GLN:HB2	2:B:114:ASP:OD2	2.20	0.41
1:E:64:ARG:HH11	1:E:64:ARG:HD2	1.68	0.41
2:F:127:GLN:HB3	2:F:310:TYR:OH	2.20	0.41
2:F:163:LYS:NZ	2:F:250:PRO:O	2.53	0.41
1:C:12:VAL:HG22	1:E:20:TYR:CD1	2.56	0.41
2:D:204:THR:HG21	2:D:209:GLU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:158:THR:HA	2:F:254:GLY:O	2.21	0.41
2:B:225:ILE:O	2:B:228:CYS:HB3	2.21	0.41
1:C:71:TYR:CZ	1:C:73:GLY:HA3	2.56	0.41
2:D:97:ARG:HH21	2:D:97:ARG:HD3	1.75	0.41
2:F:274:SER:HB3	2:F:277:THR:OG1	2.21	0.41
1:C:42:LYS:HB3	2:D:259:VAL:CG1	2.49	0.41
1:C:68:LYS:HZ2	1:C:68:LYS:CB	2.32	0.41
2:D:130:LEU:HD11	2:D:134:PHE:CE1	2.55	0.41
2:D:181:ALA:O	2:D:195:PHE:HA	2.21	0.41
2:F:112:GLN:HB2	2:F:114:ASP:OD2	2.21	0.41
2:F:164:ASN:O	2:F:166:ALA:N	2.54	0.41
2:F:96:LEU:O	2:F:290:MET:HB2	2.21	0.40
1:A:3:LEU:O	1:A:7:LEU:HB2	2.21	0.40
2:B:108:PHE:CE1	2:B:219:LYS:HE3	2.57	0.40
2:F:284:ILE:HD13	2:F:284:ILE:HG21	1.91	0.40
2:D:124:LYS:HG3	2:D:128:ASP:OD1	2.22	0.40
2:B:161:ARG:HH11	2:B:161:ARG:HD3	1.74	0.40
2:D:178:SER:OG	2:D:256:ALA:HB1	2.22	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	61/81 (75%)	51 (84%)	10 (16%)	0	100	100
1	C	63/81 (78%)	52 (82%)	11 (18%)	0	100	100
1	E	66/81 (82%)	55 (83%)	10 (15%)	1 (2%)	8	32
2	B	227/229 (99%)	195 (86%)	23 (10%)	9 (4%)	2	13
2	D	227/229 (99%)	195 (86%)	23 (10%)	9 (4%)	2	13
2	F	227/229 (99%)	195 (86%)	23 (10%)	9 (4%)	2	13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	871/930 (94%)	743 (85%)	100 (12%)	28 (3%)	3 18

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	165	ASP
2	B	205	PRO
2	B	250	PRO
2	D	165	ASP
2	D	205	PRO
2	D	250	PRO
1	E	50	LYS
2	F	165	ASP
2	F	205	PRO
2	F	250	PRO
2	B	304	ALA
2	D	249	GLU
2	D	304	ALA
2	F	249	GLU
2	F	304	ALA
2	B	164	ASN
2	B	249	GLU
2	F	164	ASN
2	F	306	ASN
2	D	164	ASN
2	D	306	ASN
2	B	146	PRO
2	B	306	ASN
2	D	146	PRO
2	F	146	PRO
2	F	170	PRO
2	B	170	PRO
2	D	170	PRO

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	50/66 (76%)	41 (82%)	9 (18%)	2	8
1	C	51/66 (77%)	42 (82%)	9 (18%)	2	9
1	E	53/66 (80%)	46 (87%)	7 (13%)	4	17
2	B	188/188 (100%)	150 (80%)	38 (20%)	1	5
2	D	188/188 (100%)	149 (79%)	39 (21%)	1	5
2	F	188/188 (100%)	151 (80%)	37 (20%)	1	6
All	All	718/762 (94%)	579 (81%)	139 (19%)	1	7

All (139) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	GLU
1	A	7	LEU
1	A	18	SER
1	A	24	THR
1	A	25	ARG
1	A	43	VAL
1	A	64	ARG
1	A	68	LYS
1	A	75	ILE
2	B	84	THR
2	B	98	SER
2	B	105	LYS
2	B	118	LEU
2	B	121	TYR
2	B	126	LEU
2	B	139	ASP
2	B	146	PRO
2	B	158	THR
2	B	161	ARG
2	B	163	LYS
2	B	164	ASN
2	B	167	ASP
2	B	168	MET
2	B	169	LYS
2	B	186	LYS
2	B	197	GLU
2	B	198	ASP
2	B	201	VAL
2	B	204	THR
2	B	206	ASN

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Mol	Chain	Res	Type
2	B	208	ASP
2	B	212	GLU
2	B	217	ARG
2	B	218	ARG
2	B	230	GLN
2	B	231	ASP
2	B	233	HIS
2	B	235	SER
2	B	237	GLU
2	B	245	TYR
2	B	249	GLU
2	B	250	PRO
2	B	268	ASP
2	B	277	THR
2	B	295	GLU
2	B	308	LEU
2	B	309	LYS
1	C	2	GLU
1	C	7	LEU
1	C	18	SER
1	C	24	THR
1	C	43	VAL
1	C	49	ASP
1	C	64	ARG
1	C	68	LYS
1	C	75	ILE
2	D	84	THR
2	D	98	SER
2	D	105	LYS
2	D	118	LEU
2	D	121	TYR
2	D	126	LEU
2	D	139	ASP
2	D	146	PRO
2	D	158	THR
2	D	161	ARG
2	D	163	LYS
2	D	164	ASN
2	D	167	ASP
2	D	168	MET
2	D	169	LYS
2	D	186	LYS

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Mol	Chain	Res	Type
2	D	197	GLU
2	D	198	ASP
2	D	201	VAL
2	D	203	GLU
2	D	204	THR
2	D	206	ASN
2	D	208	ASP
2	D	212	GLU
2	D	218	ARG
2	D	230	GLN
2	D	231	ASP
2	D	235	SER
2	D	237	GLU
2	D	245	TYR
2	D	248	MET
2	D	249	GLU
2	D	250	PRO
2	D	268	ASP
2	D	277	THR
2	D	295	GLU
2	D	297	MET
2	D	308	LEU
2	D	309	LYS
1	E	2	GLU
1	E	7	LEU
1	E	24	THR
1	E	43	VAL
1	E	64	ARG
1	E	68	LYS
1	E	75	ILE
2	F	84	THR
2	F	98	SER
2	F	105	LYS
2	F	118	LEU
2	F	126	LEU
2	F	139	ASP
2	F	146	PRO
2	F	158	THR
2	F	161	ARG
2	F	163	LYS
2	F	164	ASN
2	F	167	ASP

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Mol	Chain	Res	Type
2	F	168	MET
2	F	169	LYS
2	F	186	LYS
2	F	197	GLU
2	F	198	ASP
2	F	201	VAL
2	F	204	THR
2	F	206	ASN
2	F	208	ASP
2	F	212	GLU
2	F	217	ARG
2	F	218	ARG
2	F	230	GLN
2	F	231	ASP
2	F	235	SER
2	F	237	GLU
2	F	245	TYR
2	F	248	MET
2	F	249	GLU
2	F	250	PRO
2	F	268	ASP
2	F	277	THR
2	F	295	GLU
2	F	308	LEU
2	F	309	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
2	B	87	GLN
2	B	306	ASN
1	C	69	ASN
2	D	138	GLN
2	D	306	ASN
1	E	69	ASN
2	F	87	GLN
2	F	138	GLN
2	F	164	ASN
2	F	305	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	65/81 (80%)	-0.27	0 100 100	27, 44, 78, 93	0
1	C	67/81 (82%)	-0.27	0 100 100	27, 44, 91, 100	0
1	E	70/81 (86%)	-0.11	2 (2%) 53 32	26, 45, 94, 100	0
2	B	228/229 (99%)	0.15	6 (2%) 57 36	24, 59, 94, 100	0
2	D	228/229 (99%)	0.03	1 (0%) 88 76	22, 61, 94, 100	0
2	F	228/229 (99%)	0.06	5 (2%) 62 41	24, 61, 93, 100	0
All	All	886/930 (95%)	0.01	14 (1%) 70 49	22, 58, 94, 100	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	206	ASN	4.8
1	E	49	ASP	3.4
2	F	212	GLU	2.8
2	F	166	ALA	2.4
2	B	310	TYR	2.4
2	B	112	GLN	2.4
2	B	116	SER	2.3
2	F	251	GLY	2.3
2	F	215	GLU	2.2
2	B	108	PHE	2.2
2	F	111	THR	2.2
2	B	117	GLU	2.2
2	D	166	ALA	2.1
1	E	4	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.