



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:59 PM UTC

PDB ID : 1IBT / pdb_00001ibt
Title : STRUCTURE OF THE D53,54N MUTANT OF HISTIDINE DECARBOXY-
LASE AT-170 C
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Deposited on : 2001-03-29
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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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

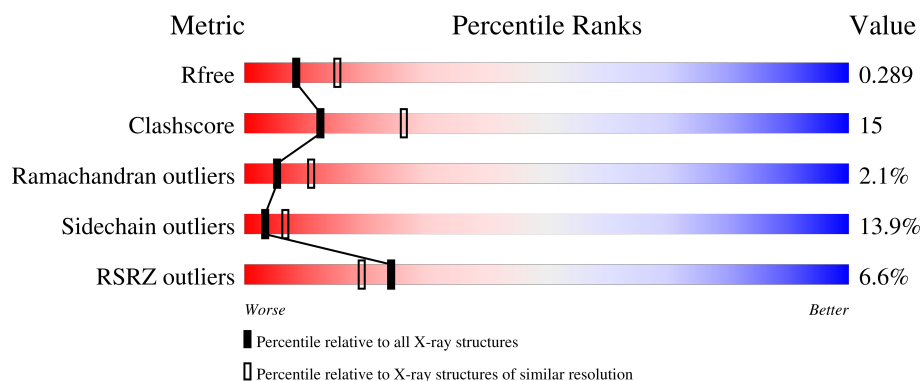
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	6% 54% 30% 14% .
1	C	81	10% 53% 30% 10% 6%
1	E	81	51% 37% 10% .
2	B	229	7% 53% 35% 9% .
2	D	229	7% 56% 33% 8% .

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Mol	Chain	Length	Quality of chain
2	F	229	7% 53% 36% 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7172 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	81	Total	C	N	O	S	0	0	0
			605	375	104	124	2			
1	C	76	Total	C	N	O	S	0	0	0
			574	358	98	116	2			
1	E	81	Total	C	N	O	S	0	0	0
			613	380	108	123	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
			1775	1127	286	351	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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Chain	Residue	Modelled	Actual	Comment	Reference
F	82	PYR	SER	modified residue	UNP P00862

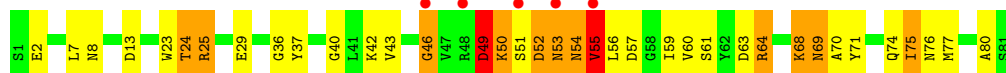
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	9	Total O 9 9	0	0
3	B	12	Total O 12 12	0	0
3	C	4	Total O 4 4	0	0
3	D	7	Total O 7 7	0	0
3	E	10	Total O 10 10	0	0
3	F	11	Total O 11 11	0	0

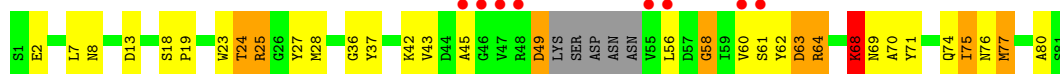
3 Residue-property plots

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 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.

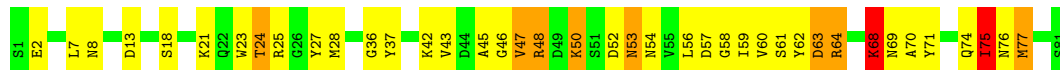
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN



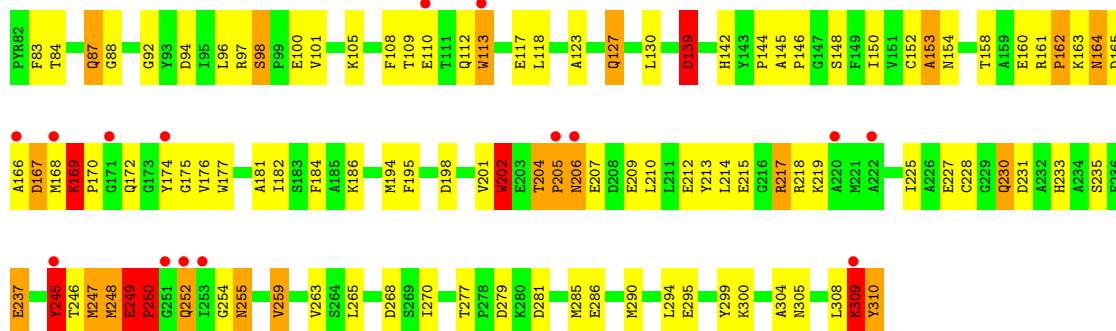
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN



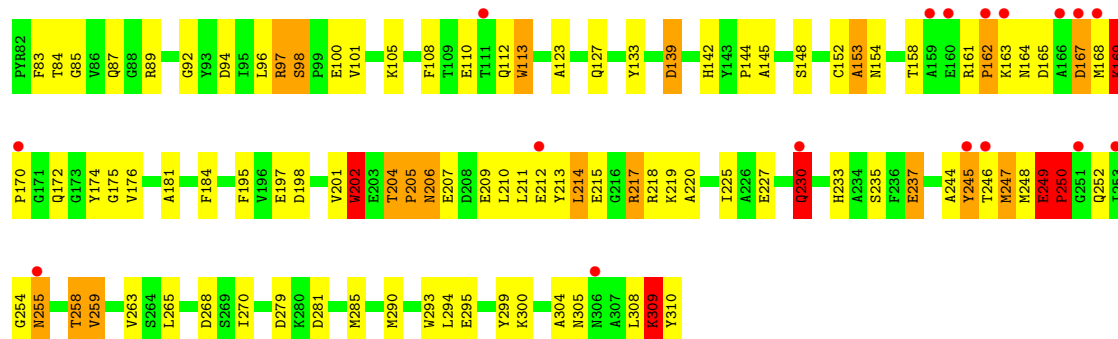
- Molecule 1: HISTIDINE DECARBOXYLASE BETA CHAIN



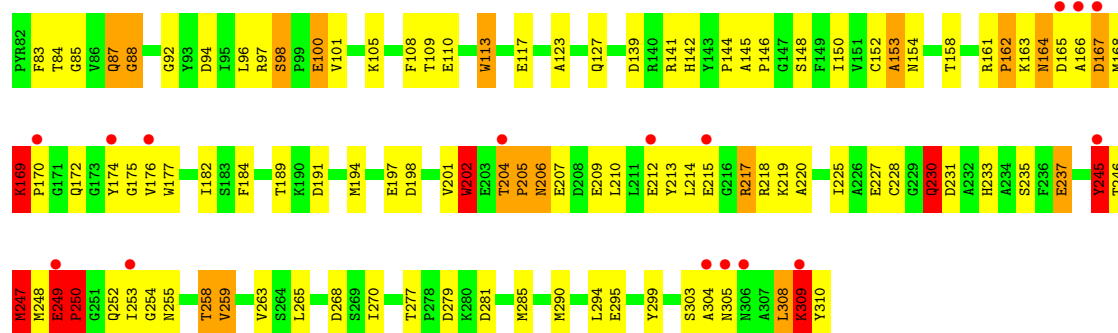
- Molecule 2: HISTIDINE DECARBOXYLASE ALPHA CHAIN



- 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	96.20Å 115.31Å 202.39Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.60 20.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.60) 91.7 (20.00-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.59Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.260 , 0.316 0.250 , 0.289	Depositor DCC
R_{free} test set	3399 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	42.8	Xtriage
Anisotropy	0.861	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	7172	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.62% 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

5.1 Standard geometry

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	1.22	1/613 (0.2%)	2.35	25/829 (3.0%)
1	C	1.10	0/581	1.89	20/783 (2.6%)
1	E	1.15	0/621	2.16	31/839 (3.7%)
2	B	1.08	2/1816 (0.1%)	1.93	56/2463 (2.3%)
2	D	1.06	3/1816 (0.2%)	1.98	56/2463 (2.3%)
2	F	1.07	2/1815 (0.1%)	1.92	62/2463 (2.5%)
All	All	1.09	8/7262 (0.1%)	2.00	250/9840 (2.5%)

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	B	0	3
2	D	0	1
2	F	0	2
All	All	0	6

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	233	HIS	CD2-NE2	-6.89	1.30	1.37
2	D	142	HIS	CD2-NE2	-6.89	1.30	1.37
2	B	142	HIS	CD2-NE2	-6.44	1.30	1.37
1	A	55	VAL	CA-CB	6.32	1.63	1.54
2	F	142	HIS	CD2-NE2	-6.14	1.31	1.37
2	F	233	HIS	CD2-NE2	-5.69	1.31	1.37
2	B	233	HIS	CD2-NE2	-5.10	1.32	1.37
2	D	142	HIS	CG-ND1	-5.06	1.32	1.38

All (250) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	ARG	CD-NE-CZ	19.07	151.10	124.40
2	D	217	ARG	CD-NE-CZ	17.84	149.37	124.40
2	D	217	ARG	NE-CZ-NH2	-15.88	104.91	119.20
1	A	25	ARG	NE-CZ-NH2	-15.22	105.50	119.20
1	A	25	ARG	NE-CZ-NH1	14.67	136.17	121.50
1	A	51	SER	N-CA-C	14.66	128.46	108.23
1	A	57	ASP	CA-CB-CG	13.89	126.49	112.60
1	E	76	ASN	OD1-CG-ND2	-11.33	111.27	122.60
2	B	217	ARG	NE-CZ-NH2	10.90	129.01	119.20
2	D	217	ARG	NE-CZ-NH1	10.63	132.13	121.50
2	B	217	ARG	NE-CZ-NH1	-10.62	110.88	121.50
1	E	53	ASN	CA-CB-CG	-10.55	102.05	112.60
2	F	217	ARG	CD-NE-CZ	10.34	138.87	124.40
1	A	50	LYS	N-CA-C	10.26	132.64	110.80
1	E	53	ASN	N-CA-C	9.88	125.60	108.02
1	E	45	ALA	O-C-N	9.49	135.11	123.44
2	F	217	ARG	NE-CZ-NH1	-9.30	112.20	121.50
2	B	206	ASN	CA-CB-CG	-9.29	103.31	112.60
2	D	233	HIS	CB-CG-CD2	-8.99	119.52	131.20
2	F	268	ASP	CA-CB-CG	8.88	121.48	112.60
2	B	217	ARG	CD-NE-CZ	8.74	136.64	124.40
2	F	233	HIS	CB-CG-CD2	-8.58	120.04	131.20
1	C	25	ARG	NE-CZ-NH2	8.50	126.85	119.20
2	F	250	PRO	N-CA-C	8.39	129.75	112.47
2	D	250	PRO	N-CA-C	8.39	129.75	112.47
2	B	154	ASN	OD1-CG-ND2	-8.27	114.33	122.60
2	F	217	ARG	NE-CZ-NH2	8.24	126.62	119.20
1	A	52	ASP	CA-C-O	8.18	129.04	120.54
2	B	250	PRO	CA-N-CD	-8.18	100.55	112.00
2	B	268	ASP	CA-CB-CG	8.12	120.72	112.60
2	B	250	PRO	N-CA-C	8.12	129.19	112.47
1	E	54	ASN	CA-CB-CG	-8.06	104.54	112.60
2	B	233	HIS	CB-CG-CD2	-8.06	120.73	131.20
2	D	154	ASN	OD1-CG-ND2	-7.99	114.61	122.60
2	F	279	ASP	CA-CB-CG	7.93	120.53	112.60
2	D	206	ASN	CA-CB-CG	-7.92	104.68	112.60
2	F	198	ASP	CA-CB-CG	7.89	120.49	112.60
1	A	53	ASN	N-CA-C	7.81	127.43	110.80
2	F	250	PRO	CA-N-CD	-7.80	101.08	112.00
2	D	198	ASP	CA-CB-CG	7.69	120.29	112.60
2	D	250	PRO	CA-N-CD	-7.68	101.25	112.00
2	D	268	ASP	CA-CB-CG	7.61	120.21	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	25	ARG	NE-CZ-NH2	7.49	125.94	119.20
1	A	51	SER	CA-C-O	7.48	127.82	120.56
2	D	233	HIS	CB-CG-ND1	7.48	133.92	122.70
2	F	233	HIS	CB-CG-ND1	7.40	133.81	122.70
2	D	167	ASP	CA-C-O	7.39	128.08	120.24
2	F	305	ASN	CA-CB-CG	-7.38	105.22	112.60
2	D	249	GLU	CA-CB-CG	7.29	128.68	114.10
2	B	198	ASP	CA-CB-CG	7.28	119.88	112.60
2	B	164	ASN	OD1-CG-ND2	-7.26	115.34	122.60
2	F	249	GLU	CA-CB-CG	7.20	128.49	114.10
1	A	71	TYR	N-CA-C	7.17	119.47	109.15
1	C	71	TYR	N-CA-C	7.14	119.44	109.15
1	A	49	ASP	N-CA-C	7.10	125.92	110.80
2	F	167	ASP	CA-C-O	7.04	127.70	120.24
1	A	13	ASP	CA-CB-CG	7.03	119.63	112.60
1	A	52	ASP	CA-CB-CG	7.01	119.61	112.60
2	B	279	ASP	CA-CB-CG	6.92	119.52	112.60
1	E	45	ALA	CA-C-N	6.92	128.62	122.47
1	E	45	ALA	C-N-CA	6.92	128.62	122.47
2	F	94	ASP	CA-CB-CG	6.91	119.51	112.60
1	E	25	ARG	NE-CZ-NH1	-6.90	114.60	121.50
1	C	25	ARG	NE-CZ-NH1	-6.88	114.62	121.50
2	F	113	TRP	N-CA-C	6.87	121.27	112.34
1	C	25	ARG	CD-NE-CZ	6.81	133.93	124.40
1	E	25	ARG	CD-NE-CZ	6.80	133.93	124.40
1	E	71	TYR	N-CA-C	6.80	118.94	109.15
2	F	141	ARG	NE-CZ-NH2	6.76	125.28	119.20
2	D	279	ASP	CA-CB-CG	6.76	119.36	112.60
2	F	206	ASN	CA-CB-CG	-6.74	105.86	112.60
2	B	255	ASN	OD1-CG-ND2	-6.73	115.87	122.60
2	B	127	GLN	OE1-CD-NE2	-6.72	115.88	122.60
1	A	53	ASN	O-C-N	6.70	131.50	122.59
2	B	305	ASN	CA-CB-CG	-6.68	105.92	112.60
2	B	94	ASP	CA-CB-CG	6.65	119.25	112.60
2	B	167	ASP	CA-C-O	6.60	127.24	120.24
2	F	154	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	A	76	ASN	OD1-CG-ND2	-6.59	116.01	122.60
2	B	233	HIS	CB-CG-ND1	6.57	132.55	122.70
2	B	153	ALA	N-CA-C	-6.51	98.61	108.96
2	D	305	ASN	CA-CB-CG	-6.50	106.10	112.60
2	B	237	GLU	CA-CB-CG	6.48	127.06	114.10
2	D	217	ARG	CG-CD-NE	6.45	126.19	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	57	ASP	N-CA-C	-6.43	105.25	113.23
2	F	164	ASN	OD1-CG-ND2	-6.43	116.17	122.60
2	F	169	LYS	CA-C-N	6.41	126.10	119.82
2	F	169	LYS	C-N-CA	6.41	126.10	119.82
2	B	113	TRP	N-CA-C	6.38	120.63	112.34
1	E	50	LYS	N-CA-C	6.36	124.35	110.80
2	D	113	TRP	N-CA-C	6.29	120.52	112.34
1	E	24	THR	N-CA-C	-6.28	101.49	110.59
2	F	205	PRO	CA-C-N	-6.25	114.11	122.42
2	F	205	PRO	C-N-CA	-6.25	114.11	122.42
2	D	94	ASP	CA-CB-CG	6.24	118.84	112.60
2	F	237	GLU	CA-CB-CG	6.24	126.57	114.10
2	F	252	GLN	N-CA-C	-6.21	99.89	109.76
2	F	141	ARG	NE-CZ-NH1	-6.19	115.31	121.50
2	D	227	GLU	N-CA-C	-6.16	104.26	110.97
2	F	225	ILE	N-CA-C	-6.14	104.64	110.42
2	B	249	GLU	CA-CB-CG	6.14	126.38	114.10
2	D	164	ASN	OD1-CG-ND2	-6.13	116.47	122.60
2	B	184	PHE	CA-CB-CG	-6.13	107.67	113.80
2	B	110	GLU	CB-CG-CD	6.11	122.99	112.60
2	F	309	LYS	CA-C-O	-6.08	114.27	120.71
2	B	227	GLU	N-CA-C	-6.07	104.36	110.97
2	B	250	PRO	N-CA-CB	-6.02	96.92	103.25
2	D	205	PRO	CA-C-N	-6.02	114.42	122.42
2	D	205	PRO	C-N-CA	-6.02	114.42	122.42
2	D	225	ILE	N-CA-C	-6.00	104.78	110.42
2	D	169	LYS	CA-C-N	5.99	125.69	119.82
2	D	169	LYS	C-N-CA	5.99	125.69	119.82
2	B	309	LYS	O-C-N	-5.96	116.21	123.19
1	E	8	ASN	OD1-CG-ND2	-5.96	116.64	122.60
2	D	184	PHE	CA-CB-CG	-5.95	107.85	113.80
2	D	250	PRO	N-CA-CB	-5.92	97.03	103.25
2	D	98	SER	CA-CB-OG	5.92	122.95	111.10
2	B	263	VAL	N-CA-C	5.91	117.68	109.29
2	F	191	ASP	CA-CB-CG	5.90	118.50	112.60
1	E	47	VAL	N-CA-C	5.89	117.57	108.44
1	C	58	GLY	O-C-N	5.88	127.83	122.19
2	D	164	ASN	N-CA-C	-5.83	98.39	110.80
2	D	263	VAL	N-CA-C	5.80	117.53	109.29
2	B	225	ILE	N-CA-C	-5.79	104.98	110.42
1	E	23	TRP	CG-CD2-CE3	5.78	139.68	133.90
2	F	164	ASN	N-CA-C	-5.77	98.51	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	GLY	O-C-N	5.74	129.37	123.29
2	D	309	LYS	CA-C-O	-5.72	114.45	120.80
2	B	164	ASN	N-CA-C	-5.72	98.62	110.80
2	B	205	PRO	CA-C-N	-5.71	114.83	122.42
2	B	205	PRO	C-N-CA	-5.71	114.83	122.42
2	B	252	GLN	N-CA-C	-5.69	100.71	109.76
1	C	63	ASP	CA-CB-CG	5.68	118.28	112.60
2	F	250	PRO	N-CA-CB	-5.68	97.28	103.25
2	F	227	GLU	CA-CB-CG	5.67	125.44	114.10
1	C	24	THR	N-CA-C	-5.66	102.38	110.59
2	D	258	THR	N-CA-C	-5.65	100.19	109.40
2	F	153	ALA	N-CA-C	-5.64	99.99	108.96
2	F	142	HIS	CA-CB-CG	-5.64	108.16	113.80
2	B	98	SER	CA-CB-OG	5.63	122.37	111.10
2	B	309	LYS	CA-C-O	-5.63	114.55	120.80
2	D	237	GLU	CA-CB-CG	5.63	125.35	114.10
2	F	202	TRP	CE2-CD2-CG	-5.62	100.45	107.20
2	D	153	ALA	N-CA-C	-5.62	100.02	108.96
2	B	162	PRO	N-CA-C	5.62	120.05	111.34
2	B	202	TRP	CE2-CD2-CG	-5.62	100.46	107.20
1	C	56	LEU	CA-C-N	5.61	129.24	120.82
1	C	56	LEU	C-N-CA	5.61	129.24	120.82
1	A	24	THR	N-CA-C	-5.61	102.46	110.59
2	F	110	GLU	CB-CG-CD	5.61	122.13	112.60
1	E	68	LYS	CG-CD-CE	5.57	124.11	111.30
2	F	220	ALA	N-CA-C	-5.57	105.13	111.14
2	F	184	PHE	CA-CB-CG	-5.55	108.25	113.80
1	E	69	ASN	CB-CA-C	-5.54	110.20	116.63
1	A	23	TRP	CG-CD2-CE3	5.54	139.44	133.90
1	C	23	TRP	CG-CD2-CE3	5.54	139.44	133.90
1	A	8	ASN	OD1-CG-ND2	-5.54	117.06	122.60
2	D	293	TRP	CG-CD2-CE3	5.54	139.44	133.90
2	F	265	LEU	CA-C-N	5.53	125.44	119.85
2	F	265	LEU	C-N-CA	5.53	125.44	119.85
2	D	89	ARG	NE-CZ-NH2	-5.53	114.23	119.20
2	D	110	GLU	CA-CB-CG	-5.51	103.07	114.10
2	D	230	GLN	OE1-CD-NE2	-5.51	117.09	122.60
2	D	265	LEU	N-CA-C	5.50	116.58	109.65
2	D	252	GLN	N-CA-C	-5.50	101.02	109.76
2	B	169	LYS	CA-C-N	5.50	125.21	119.82
2	B	169	LYS	C-N-CA	5.50	125.21	119.82
2	F	177	TRP	CG-CD2-CE3	5.49	139.39	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	202	TRP	CE2-CD2-CG	-5.48	100.62	107.20
1	E	46	GLY	CA-C-N	5.46	129.67	122.51
1	E	46	GLY	C-N-CA	5.46	129.67	122.51
2	F	265	LEU	N-CA-C	5.46	116.71	109.93
2	D	230	GLN	CA-CB-CG	5.46	125.03	114.10
1	C	8	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	C	13	ASP	CA-CB-CG	5.45	118.05	112.60
2	D	255	ASN	OD1-CG-ND2	-5.45	117.15	122.60
1	C	23	TRP	N-CA-C	5.44	118.33	110.28
2	D	202	TRP	CG-CD2-CE3	5.44	139.34	133.90
2	B	110	GLU	CA-CB-CG	-5.42	103.26	114.10
2	B	139	ASP	N-CA-C	-5.42	99.56	108.49
1	A	2	GLU	N-CA-CB	-5.41	101.12	110.32
1	C	23	TRP	CE2-CD2-CG	-5.41	100.71	107.20
1	E	2	GLU	N-CA-CB	-5.41	101.13	110.32
2	F	98	SER	CA-CB-OG	5.39	121.88	111.10
2	F	263	VAL	N-CA-C	5.38	116.93	109.29
2	D	309	LYS	O-C-N	-5.37	116.91	123.19
1	A	69	ASN	CB-CA-C	-5.35	110.42	116.63
2	F	309	LYS	CB-CG-CD	5.33	123.55	111.30
1	C	2	GLU	N-CA-CB	-5.32	101.27	110.32
1	C	68	LYS	CG-CD-CE	5.32	123.54	111.30
2	B	265	LEU	CA-C-N	5.31	125.22	119.85
2	B	265	LEU	C-N-CA	5.31	125.22	119.85
1	E	21	LYS	CB-CG-CD	5.29	123.48	111.30
1	A	29	GLU	CA-C-N	5.29	125.05	119.76
1	A	29	GLU	C-N-CA	5.29	125.05	119.76
2	B	202	TRP	CG-CD2-CE3	5.29	139.19	133.90
1	E	13	ASP	CA-CB-CG	5.28	117.88	112.60
2	F	110	GLU	CA-CB-CG	-5.27	103.56	114.10
2	B	177	TRP	CG-CD2-CE3	5.27	139.17	133.90
2	D	265	LEU	CA-C-N	5.26	125.16	119.85
2	D	265	LEU	C-N-CA	5.26	125.16	119.85
1	C	69	ASN	CB-CA-C	-5.26	110.53	116.63
1	C	45	ALA	O-C-N	-5.24	116.99	123.44
1	E	75	ILE	O-C-N	-5.24	117.53	122.98
1	C	49	ASP	CA-CB-CG	5.23	117.83	112.60
2	F	247	MET	CA-CB-CG	-5.23	103.65	114.10
2	F	162	PRO	N-CA-C	5.22	119.42	111.34
2	D	154	ASN	CB-CG-ND2	5.21	124.22	116.40
2	F	189	THR	N-CA-CB	-5.21	102.50	110.26
2	B	164	ASN	O-C-N	5.21	129.52	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	142	HIS	CB-CG-CD2	-5.21	124.43	131.20
2	B	88	GLY	N-CA-C	5.20	119.19	111.18
2	F	87	GLN	CA-C-N	-5.20	117.11	121.58
2	F	87	GLN	C-N-CA	-5.20	117.11	121.58
2	F	202	TRP	CG-CD2-CE3	5.19	139.09	133.90
1	E	76	ASN	CB-CG-ND2	5.18	124.18	116.40
2	F	177	TRP	CE2-CD2-CG	-5.18	100.98	107.20
2	F	277	THR	CA-C-N	5.18	124.63	119.24
2	F	277	THR	C-N-CA	5.18	124.63	119.24
2	B	227	GLU	CA-CB-CG	5.17	124.45	114.10
1	E	18	SER	CA-C-N	5.17	125.25	119.87
1	E	18	SER	C-N-CA	5.17	125.25	119.87
2	D	164	ASN	O-C-N	5.16	129.45	122.59
1	C	76	ASN	OD1-CG-ND2	-5.16	117.44	122.60
2	D	142	HIS	CB-CG-CD2	-5.14	124.51	131.20
1	E	63	ASP	CA-CB-CG	5.14	117.74	112.60
2	D	133	TYR	CA-C-O	-5.13	115.61	120.90
2	D	110	GLU	CB-CG-CD	5.11	121.28	112.60
2	F	177	TRP	CB-CG-CD1	-5.11	119.24	126.90
2	F	230	GLN	OE1-CD-NE2	-5.10	117.50	122.60
2	F	309	LYS	O-C-N	-5.10	116.74	123.21
1	A	54	ASN	CA-C-O	-5.09	113.23	120.51
2	F	164	ASN	O-C-N	5.09	129.36	122.59
2	B	286	GLU	CA-CB-CG	5.07	124.24	114.10
2	D	97	ARG	N-CA-C	5.05	117.37	110.24
2	D	220	ALA	N-CA-C	-5.05	105.69	111.14
2	B	265	LEU	N-CA-C	5.05	116.19	109.93
2	B	277	THR	CA-C-N	5.05	124.49	119.24
2	B	277	THR	C-N-CA	5.05	124.49	119.24
2	F	88	GLY	N-CA-C	5.05	118.95	111.18
2	F	258	THR	N-CA-C	-5.04	100.69	108.90
2	D	244	ALA	N-CA-C	-5.03	101.46	108.96
1	E	23	TRP	CE2-CD2-CG	-5.03	101.17	107.20
2	B	142	HIS	CA-CB-CG	-5.02	108.78	113.80
1	A	23	TRP	CE2-CD2-CG	-5.02	101.18	107.20
2	B	160	GLU	CA-CB-CG	5.02	124.13	114.10
1	E	23	TRP	N-CA-C	5.02	117.70	110.28
2	B	87	GLN	CA-C-N	-5.01	117.27	121.58
2	B	87	GLN	C-N-CA	-5.01	117.27	121.58
2	D	162	PRO	N-CA-C	5.00	119.09	111.34

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	169	LYS	Peptide
2	B	245	TYR	Sidechain
2	B	310	TYR	Sidechain
2	D	169	LYS	Peptide
2	F	169	LYS	Peptide
2	F	245	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	605	0	579	19	0
1	C	574	0	562	20	0
1	E	613	0	599	28	0
2	B	1776	0	1704	63	0
2	D	1776	0	1704	61	0
2	F	1775	0	1704	62	0
3	A	9	0	0	0	0
3	B	12	0	0	0	0
3	C	4	0	0	0	0
3	D	7	0	0	2	0
3	E	10	0	0	0	0
3	F	11	0	0	1	0
All	All	7172	0	6852	214	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 15.

All (214) 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:217:ARG:HH22	1:E:53:ASN:HB2	1.33	0.92
2:D:213:TYR:CZ	2:D:217:ARG:HD3	2.18	0.78
2:B:161:ARG:HG2	2:B:174:TYR:HA	1.67	0.77
2:F:204:THR:HG23	2:F:206:ASN:H	1.49	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:49:ASP:HA	2:B:252:GLN:HA	1.67	0.76
2:F:161:ARG:HG2	2:F:174:TYR:HA	1.68	0.76
2:D:161:ARG:HG2	2:D:174:TYR:HA	1.68	0.75
2:D:204:THR:HG23	2:D:206:ASN:H	1.54	0.72
2:D:217:ARG:HH22	1:E:53:ASN:CB	2.04	0.70
2:D:113:TRP:HB3	2:D:230:GLN:HB2	1.73	0.70
2:B:113:TRP:HB3	2:B:230:GLN:HB2	1.74	0.69
2:B:176:VAL:HG12	2:B:246:THR:HG22	1.75	0.68
2:B:204:THR:HG23	2:B:206:ASN:H	1.58	0.68
2:F:113:TRP:HB3	2:F:230:GLN:HB2	1.75	0.68
2:F:176:VAL:HG12	2:F:246:THR:HG22	1.75	0.67
2:D:176:VAL:HG12	2:D:246:THR:HG22	1.75	0.67
2:F:207:GLU:HA	2:F:247:MET:HE2	1.77	0.67
2:D:217:ARG:NH2	1:E:53:ASN:HB2	2.10	0.64
2:F:270:ILE:HG12	2:F:285:MET:HE2	1.79	0.64
2:D:207:GLU:HA	2:D:247:MET:HE2	1.80	0.63
2:D:249:GLU:HB2	2:D:250:PRO:HD2	1.80	0.62
2:B:98:SER:HB3	2:B:101:VAL:HG23	1.80	0.62
2:F:98:SER:HB3	2:F:101:VAL:HG23	1.82	0.61
1:A:55:VAL:HG12	1:A:56:LEU:HD23	1.82	0.61
2:F:249:GLU:HB2	2:F:250:PRO:HD2	1.81	0.61
1:A:46:GLY:O	2:B:246:THR:HG21	2.00	0.61
2:B:207:GLU:HA	2:B:247:MET:HE2	1.84	0.60
2:F:162:PRO:HD2	2:F:168:MET:SD	2.42	0.59
2:B:92:GLY:O	2:B:97:ARG:HA	2.03	0.58
2:D:108:PHE:CZ	2:D:219:LYS:HG2	2.39	0.58
2:B:249:GLU:HB2	2:B:250:PRO:HD2	1.85	0.58
2:D:85:GLY:HA3	2:F:146:PRO:O	2.03	0.58
1:C:75:ILE:HD11	2:D:144:PRO:HB2	1.85	0.58
2:F:123:ALA:O	2:F:127:GLN:HG3	2.04	0.57
1:A:60:VAL:O	1:A:64:ARG:HG2	2.04	0.57
2:B:270:ILE:HG12	2:B:285:MET:HE2	1.86	0.57
2:D:98:SER:HB3	2:D:101:VAL:HG23	1.85	0.57
1:C:60:VAL:O	1:C:64:ARG:HG2	2.04	0.56
2:D:270:ILE:HG12	2:D:285:MET:HE2	1.87	0.56
2:F:161:ARG:NE	2:F:249:GLU:HA	2.20	0.56
2:D:92:GLY:O	2:D:97:ARG:HA	2.04	0.56
2:F:108:PHE:CZ	2:F:219:LYS:HG2	2.41	0.56
2:D:152:CYS:HB3	2:D:259:VAL:HG23	1.87	0.56
1:C:42:LYS:HE2	1:C:70:ALA:O	2.06	0.56
2:D:161:ARG:NE	2:D:249:GLU:HA	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:SER:HA	1:C:64:ARG:HG3	1.87	0.55
1:A:75:ILE:HD11	2:B:144:PRO:HB2	1.87	0.55
1:A:42:LYS:HE2	1:A:70:ALA:O	2.06	0.55
2:F:92:GLY:O	2:F:97:ARG:HA	2.06	0.55
1:E:75:ILE:HD11	2:F:144:PRO:HB2	1.88	0.54
1:C:42:LYS:HB3	2:D:259:VAL:HG13	1.90	0.54
2:D:217:ARG:HH12	1:E:53:ASN:CG	2.14	0.54
2:B:108:PHE:CZ	2:B:219:LYS:HG2	2.43	0.54
1:C:61:SER:HB2	2:D:255:ASN:HB2	1.89	0.53
2:B:161:ARG:CG	2:B:174:TYR:HA	2.38	0.53
2:B:161:ARG:NE	2:B:249:GLU:HA	2.23	0.53
2:B:202:TRP:NE1	2:B:204:THR:HG22	2.24	0.53
2:D:123:ALA:O	2:D:127:GLN:HG3	2.08	0.53
1:E:60:VAL:O	1:E:64:ARG:HG2	2.08	0.53
1:A:61:SER:HA	1:A:64:ARG:HG3	1.91	0.53
2:B:152:CYS:HB3	2:B:259:VAL:HG23	1.91	0.53
1:C:19:PRO:HD2	1:C:25:ARG:HD3	1.90	0.53
2:F:309:LYS:HZ2	2:F:310:TYR:HA	1.73	0.52
2:D:202:TRP:NE1	2:D:204:THR:HG22	2.24	0.52
1:E:61:SER:HB2	2:F:255:ASN:HB2	1.91	0.52
1:E:47:VAL:HG12	2:F:254:GLY:HA2	1.91	0.52
2:B:162:PRO:HD2	2:B:168:MET:SD	2.50	0.52
2:D:162:PRO:HD2	2:D:168:MET:SD	2.49	0.52
1:E:42:LYS:HE2	1:E:70:ALA:O	2.10	0.52
1:E:61:SER:HA	1:E:64:ARG:HG3	1.92	0.50
2:F:202:TRP:HA	2:F:202:TRP:CE3	2.46	0.50
2:D:245:TYR:C	2:D:245:TYR:CD2	2.90	0.50
2:F:245:TYR:C	2:F:245:TYR:CD2	2.90	0.49
1:A:61:SER:HB2	2:B:255:ASN:HB2	1.93	0.49
2:B:245:TYR:C	2:B:245:TYR:CD2	2.89	0.49
2:D:113:TRP:HD1	3:D:48:HOH:O	1.95	0.49
2:D:249:GLU:HB2	2:D:250:PRO:CD	2.42	0.49
2:B:174:TYR:HB2	2:B:204:THR:O	2.13	0.49
2:D:217:ARG:NH1	1:E:53:ASN:ND2	2.61	0.49
2:D:230:GLN:HE22	1:E:64:ARG:HH22	1.61	0.49
1:E:48:ARG:O	2:F:253:ILE:HG22	2.13	0.49
2:F:152:CYS:HB3	2:F:259:VAL:HG23	1.95	0.49
2:F:202:TRP:NE1	2:F:204:THR:HG22	2.28	0.48
2:F:206:ASN:HB3	2:F:209:GLU:HB2	1.95	0.48
2:F:249:GLU:HB2	2:F:250:PRO:CD	2.43	0.48
2:F:161:ARG:CG	2:F:174:TYR:HA	2.41	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:158:THR:HA	2:B:254:GLY:O	2.14	0.48
2:F:294:LEU:HD23	2:F:299:TYR:HB2	1.94	0.48
2:B:270:ILE:HD13	2:B:281:ASP:HB3	1.95	0.48
2:D:202:TRP:HA	2:D:202:TRP:CE3	2.48	0.48
2:B:309:LYS:HZ2	2:B:310:TYR:HA	1.79	0.48
2:B:96:LEU:O	2:B:290:MET:HB2	2.13	0.48
1:C:27:TYR:CD1	1:C:37:TYR:HB3	2.49	0.47
2:F:213:TYR:CE1	2:F:217:ARG:HD3	2.49	0.47
2:B:202:TRP:HA	2:B:202:TRP:CE3	2.49	0.47
1:A:37:TYR:HE1	2:B:84:THR:HG23	1.79	0.47
1:A:68:LYS:HE3	1:A:68:LYS:HA	1.96	0.47
1:C:80:ALA:HA	1:E:77:MET:O	2.15	0.47
2:D:83:PHE:CE2	1:E:74:GLN:HA	2.49	0.47
2:B:249:GLU:HB2	2:B:250:PRO:CD	2.45	0.47
1:E:37:TYR:HE1	2:F:84:THR:HG23	1.79	0.47
2:F:174:TYR:HB2	2:F:204:THR:O	2.15	0.47
2:B:83:PHE:CE2	1:C:74:GLN:HA	2.50	0.46
2:D:170:PRO:C	2:D:172:GLN:H	2.23	0.46
2:F:158:THR:HA	2:F:254:GLY:O	2.15	0.46
2:B:83:PHE:CZ	1:C:74:GLN:HA	2.50	0.46
2:D:174:TYR:HB2	2:D:204:THR:O	2.15	0.46
2:B:228:CYS:O	2:B:231:ASP:HB2	2.16	0.46
1:C:27:TYR:CD2	1:C:28:MET:HG3	2.51	0.46
2:F:204:THR:HG23	2:F:206:ASN:N	2.25	0.46
2:D:217:ARG:HH12	1:E:53:ASN:ND2	2.14	0.46
2:D:309:LYS:HZ2	2:D:310:TYR:HA	1.81	0.46
1:A:42:LYS:HB3	2:B:259:VAL:HG13	1.97	0.46
1:A:68:LYS:HA	1:A:68:LYS:CE	2.46	0.46
2:B:145:ALA:HB3	2:B:148:SER:HB3	1.97	0.46
2:D:83:PHE:CZ	1:E:74:GLN:HA	2.51	0.46
2:D:112:GLN:HB2	3:D:48:HOH:O	2.16	0.46
2:F:202:TRP:HD1	2:F:247:MET:HE1	1.80	0.46
2:D:153:ALA:O	2:D:259:VAL:HA	2.15	0.46
2:F:210:LEU:O	2:F:213:TYR:HB3	2.16	0.46
2:D:202:TRP:NE1	2:D:210:LEU:HB2	2.30	0.45
2:F:153:ALA:O	2:F:259:VAL:HA	2.16	0.45
2:F:202:TRP:NE1	2:F:210:LEU:HB2	2.31	0.45
1:A:69:ASN:HB3	1:A:70:ALA:H	1.66	0.45
2:F:202:TRP:CD1	2:F:210:LEU:HB2	2.51	0.45
2:F:309:LYS:NZ	2:F:310:TYR:HA	2.31	0.45
2:B:294:LEU:HD23	2:B:299:TYR:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:42:LYS:HB3	2:F:259:VAL:HG13	1.98	0.45
2:B:202:TRP:CD1	2:B:210:LEU:HB2	2.51	0.45
2:B:210:LEU:O	2:B:213:TYR:HB3	2.16	0.45
2:D:96:LEU:O	2:D:290:MET:HB2	2.16	0.45
1:E:42:LYS:NZ	1:E:68:LYS:O	2.49	0.45
2:B:153:ALA:O	2:B:259:VAL:HA	2.16	0.45
2:B:175:GLY:HA3	2:B:247:MET:SD	2.57	0.45
2:B:123:ALA:O	2:B:127:GLN:HG3	2.16	0.45
1:E:58:GLY:O	1:E:62:TYR:HB2	2.17	0.45
2:B:213:TYR:CE1	2:B:217:ARG:HD3	2.52	0.44
2:D:145:ALA:HB3	2:D:148:SER:HB3	1.98	0.44
2:F:145:ALA:HB3	2:F:148:SER:HB3	1.98	0.44
2:F:96:LEU:O	2:F:290:MET:HB2	2.18	0.44
2:B:170:PRO:C	2:B:172:GLN:H	2.25	0.44
2:B:175:GLY:HA2	2:B:248:MET:SD	2.57	0.44
2:B:112:GLN:NE2	2:B:118:LEU:HB2	2.31	0.44
2:B:202:TRP:HD1	2:B:247:MET:HE1	1.83	0.44
2:F:109:THR:HB	2:F:117:GLU:HB3	1.99	0.44
2:F:270:ILE:HD13	2:F:281:ASP:HB3	2.00	0.44
1:C:37:TYR:HE1	2:D:84:THR:HG23	1.83	0.44
2:D:270:ILE:HD13	2:D:281:ASP:HB3	1.99	0.44
2:F:245:TYR:C	2:F:245:TYR:HD2	2.26	0.44
2:D:161:ARG:CG	2:D:174:TYR:HA	2.42	0.44
2:F:182:ILE:HD12	2:F:194:MET:O	2.18	0.44
2:D:206:ASN:HB3	2:D:209:GLU:HB2	1.98	0.43
2:B:217:ARG:HA	2:B:217:ARG:HD2	1.64	0.43
2:D:309:LYS:NZ	2:D:310:TYR:HA	2.33	0.43
2:F:170:PRO:C	2:F:172:GLN:H	2.25	0.43
2:B:202:TRP:NE1	2:B:210:LEU:HB2	2.33	0.43
2:B:96:LEU:HB3	2:B:290:MET:HE2	2.00	0.43
2:B:146:PRO:O	2:F:85:GLY:HA3	2.18	0.43
2:B:245:TYR:C	2:B:245:TYR:HD2	2.25	0.43
2:D:294:LEU:HD23	2:D:299:TYR:HB2	2.00	0.43
2:D:202:TRP:CD1	2:D:210:LEU:HB2	2.54	0.43
2:F:197:GLU:HB3	2:F:258:THR:HG21	2.01	0.43
1:A:42:LYS:NZ	1:A:68:LYS:O	2.51	0.43
2:B:186:LYS:HE2	2:B:186:LYS:HB3	1.76	0.43
1:C:36:GLY:HA2	2:D:87:GLN:HB3	2.01	0.43
2:D:181:ALA:O	2:D:195:PHE:HA	2.19	0.43
1:A:74:GLN:HA	2:F:83:PHE:CZ	2.54	0.43
2:B:109:THR:HB	2:B:117:GLU:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:36:GLY:HA2	2:F:87:GLN:HB3	2.01	0.43
2:B:182:ILE:HD12	2:B:194:MET:O	2.19	0.43
2:B:206:ASN:HB3	2:B:209:GLU:HB2	1.99	0.43
2:B:207:GLU:O	2:B:210:LEU:HB3	2.19	0.43
1:C:58:GLY:O	1:C:62:TYR:HB2	2.19	0.43
2:D:230:GLN:NE2	1:E:64:ARG:HH22	2.17	0.42
2:F:85:GLY:HA2	3:F:11:HOH:O	2.18	0.42
2:F:228:CYS:O	2:F:231:ASP:HB2	2.19	0.42
2:D:158:THR:HA	2:D:254:GLY:O	2.19	0.42
2:B:164:ASN:O	2:B:166:ALA:N	2.53	0.42
2:B:181:ALA:O	2:B:195:PHE:HA	2.19	0.42
2:D:210:LEU:O	2:D:213:TYR:HB3	2.20	0.42
2:D:214:LEU:HD12	2:D:214:LEU:HA	1.82	0.42
2:D:245:TYR:C	2:D:245:TYR:HD2	2.26	0.42
2:F:100:GLU:CD	2:F:100:GLU:H	2.28	0.42
2:F:164:ASN:O	2:F:166:ALA:N	2.53	0.42
2:B:139:ASP:OD2	2:B:300:LYS:NZ	2.53	0.42
1:E:27:TYR:CD2	1:E:28:MET:HG3	2.55	0.42
2:D:211:LEU:HD13	2:D:211:LEU:HA	1.93	0.42
1:E:77:MET:HE2	1:E:77:MET:HB2	1.78	0.42
2:B:309:LYS:NZ	2:B:310:TYR:HA	2.35	0.41
2:D:139:ASP:OD2	2:D:300:LYS:NZ	2.53	0.41
2:F:207:GLU:O	2:F:210:LEU:HB3	2.20	0.41
2:F:217:ARG:HA	2:F:217:ARG:HD2	1.67	0.41
2:F:202:TRP:HA	2:F:202:TRP:HE3	1.85	0.41
2:F:144:PRO:HB3	2:F:150:ILE:HD11	2.03	0.41
1:A:40:GLY:HA3	2:B:130:LEU:HD13	2.01	0.41
2:F:303:SER:HB3	2:F:308:LEU:HD22	2.02	0.41
1:E:37:TYR:O	2:F:88:GLY:HA2	2.21	0.41
1:E:56:LEU:HD23	1:E:59:ILE:HD12	2.02	0.41
2:B:248:MET:SD	2:B:248:MET:N	2.93	0.41
1:C:18:SER:HA	1:C:19:PRO:HD2	1.91	0.41
1:E:68:LYS:HA	1:E:68:LYS:HE3	2.03	0.41
1:A:80:ALA:HA	1:C:77:MET:O	2.19	0.41
2:D:197:GLU:HB3	2:D:258:THR:HG21	2.03	0.41
2:D:207:GLU:O	2:D:210:LEU:HB3	2.20	0.41
1:A:36:GLY:HA2	2:B:87:GLN:HB3	2.02	0.41
1:A:74:GLN:HA	2:F:83:PHE:CE2	2.56	0.41
2:B:174:TYR:O	2:B:248:MET:SD	2.79	0.40
1:C:68:LYS:HE3	1:C:68:LYS:HA	2.04	0.40
1:C:77:MET:HE2	1:C:77:MET:HB2	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:175:GLY:HA3	2:D:247:MET:SD	2.62	0.40
2:F:175:GLY:HA3	2:F:247:MET:SD	2.62	0.40
2:B:144:PRO:HB3	2:B:150:ILE:HD11	2.04	0.40
1:C:68:LYS:HA	1:C:68:LYS:CE	2.51	0.40
2:D:213:TYR:CE1	2:D:217:ARG:HD3	2.54	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	A	79/81 (98%)	66 (84%)	7 (9%)	6 (8%)	1	1
1	C	72/81 (89%)	67 (93%)	5 (7%)	0	100	100
1	E	79/81 (98%)	71 (90%)	7 (9%)	1 (1%)	9	21
2	B	227/229 (99%)	199 (88%)	24 (11%)	4 (2%)	6	14
2	D	227/229 (99%)	199 (88%)	24 (11%)	4 (2%)	6	14
2	F	227/229 (99%)	199 (88%)	24 (11%)	4 (2%)	6	14
All	All	911/930 (98%)	801 (88%)	91 (10%)	19 (2%)	5	11

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	LYS
1	A	53	ASN
1	A	54	ASN
1	A	55	VAL
2	B	165	ASP
2	B	250	PRO
2	D	165	ASP

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Mol	Chain	Res	Type
2	D	250	PRO
2	D	304	ALA
1	E	50	LYS
2	F	165	ASP
2	F	250	PRO
2	B	304	ALA
2	F	304	ALA
1	A	49	ASP
1	A	59	ILE
2	F	205	PRO
2	B	205	PRO
2	D	205	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	61/66 (92%)	51 (84%)	10 (16%)	2	4
1	C	59/66 (89%)	50 (85%)	9 (15%)	3	5
1	E	63/66 (96%)	53 (84%)	10 (16%)	2	4
2	B	188/188 (100%)	163 (87%)	25 (13%)	4	8
2	D	188/188 (100%)	163 (87%)	25 (13%)	4	8
2	F	188/188 (100%)	163 (87%)	25 (13%)	4	8
All	All	747/762 (98%)	643 (86%)	104 (14%)	3	7

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LEU
1	A	24	THR
1	A	25	ARG
1	A	43	VAL
1	A	52	ASP
1	A	63	ASP

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Mol	Chain	Res	Type
1	A	64	ARG
1	A	68	LYS
1	A	75	ILE
1	A	77	MET
2	B	100	GLU
2	B	105	LYS
2	B	139	ASP
2	B	163	LYS
2	B	167	ASP
2	B	169	LYS
2	B	201	VAL
2	B	202	TRP
2	B	204	THR
2	B	212	GLU
2	B	214	LEU
2	B	215	GLU
2	B	218	ARG
2	B	230	GLN
2	B	235	SER
2	B	237	GLU
2	B	245	TYR
2	B	247	MET
2	B	248	MET
2	B	249	GLU
2	B	250	PRO
2	B	259	VAL
2	B	295	GLU
2	B	308	LEU
2	B	309	LYS
1	C	7	LEU
1	C	24	THR
1	C	43	VAL
1	C	49	ASP
1	C	63	ASP
1	C	64	ARG
1	C	68	LYS
1	C	75	ILE
1	C	77	MET
2	D	100	GLU
2	D	105	LYS
2	D	139	ASP
2	D	163	LYS

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Mol	Chain	Res	Type
2	D	167	ASP
2	D	169	LYS
2	D	201	VAL
2	D	202	TRP
2	D	204	THR
2	D	212	GLU
2	D	214	LEU
2	D	215	GLU
2	D	218	ARG
2	D	230	GLN
2	D	235	SER
2	D	237	GLU
2	D	245	TYR
2	D	247	MET
2	D	248	MET
2	D	249	GLU
2	D	250	PRO
2	D	259	VAL
2	D	295	GLU
2	D	308	LEU
2	D	309	LYS
1	E	7	LEU
1	E	24	THR
1	E	43	VAL
1	E	48	ARG
1	E	52	ASP
1	E	63	ASP
1	E	64	ARG
1	E	68	LYS
1	E	75	ILE
1	E	77	MET
2	F	100	GLU
2	F	105	LYS
2	F	139	ASP
2	F	163	LYS
2	F	167	ASP
2	F	169	LYS
2	F	201	VAL
2	F	202	TRP
2	F	204	THR
2	F	212	GLU
2	F	214	LEU

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Mol	Chain	Res	Type
2	F	215	GLU
2	F	218	ARG
2	F	230	GLN
2	F	235	SER
2	F	237	GLU
2	F	245	TYR
2	F	247	MET
2	F	248	MET
2	F	249	GLU
2	F	250	PRO
2	F	259	VAL
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 (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	ASN
2	B	138	GLN
2	B	287	ASN
1	C	35	ASN
2	D	138	GLN
2	D	287	ASN
1	E	35	ASN
1	E	54	ASN
2	F	255	ASN
2	F	287	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

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

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	81/81 (100%)	0.15	5 (6%) 26 21	14, 29, 85, 91	0
1	C	76/81 (93%)	0.18	8 (10%) 11 9	13, 28, 78, 83	0
1	E	81/81 (100%)	0.09	0 100 100	14, 29, 71, 82	0
2	B	228/229 (99%)	0.49	15 (6%) 24 19	13, 41, 74, 84	0
2	D	228/229 (99%)	0.42	17 (7%) 20 16	12, 40, 74, 84	0
2	F	228/229 (99%)	0.43	16 (7%) 22 18	13, 40, 74, 84	0
All	All	922/930 (99%)	0.37	61 (6%) 24 19	12, 38, 75, 91	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	245	TYR	3.7
2	D	168	MET	3.6
2	B	220	ALA	3.6
2	F	305	ASN	3.5
1	A	55	VAL	3.5
2	B	206	ASN	3.4
2	F	167	ASP	3.4
1	C	48	ARG	3.4
2	D	253	ILE	3.4
1	C	46	GLY	3.2
2	D	166	ALA	3.2
2	D	251	GLY	3.2
2	B	245	TYR	3.1
1	C	61	SER	3.1
2	D	160	GLU	3.1
2	D	162	PRO	2.9
2	D	170	PRO	2.9
2	B	253	ILE	2.9
2	F	306	ASN	2.9

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Mol	Chain	Res	Type	RSRZ
2	D	167	ASP	2.7
2	D	159	ALA	2.6
2	F	166	ALA	2.6
2	D	230	GLN	2.6
2	F	215	GLU	2.6
2	D	255	ASN	2.6
2	B	113	TRP	2.5
1	A	48	ARG	2.5
2	D	246	THR	2.5
2	F	309	LYS	2.5
1	C	60	VAL	2.5
1	A	51	SER	2.5
2	D	245	TYR	2.5
2	D	111	THR	2.4
1	A	46	GLY	2.4
2	D	163	LYS	2.4
1	C	56	LEU	2.4
2	F	249	GLU	2.4
2	B	205	PRO	2.4
1	C	55	VAL	2.3
2	F	253	ILE	2.3
2	F	204	THR	2.3
2	B	168	MET	2.2
2	B	110	GLU	2.2
2	B	174	TYR	2.2
2	F	176	VAL	2.2
2	F	170	PRO	2.2
1	C	47	VAL	2.2
2	F	212	GLU	2.2
2	F	304	ALA	2.1
2	B	309	LYS	2.1
2	B	252	GLN	2.1
2	B	166	ALA	2.1
2	B	222	ALA	2.1
2	D	212	GLU	2.1
1	A	53	ASN	2.1
2	F	174	TYR	2.1
2	F	165	ASP	2.0
1	C	45	ALA	2.0
2	D	306	ASN	2.0
2	B	251	GLY	2.0
2	B	171	GLY	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.