



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 09:56 PM UTC

PDB ID : 1AKM / pdb_00001akm
Title : ORNITHINE TRANSCARBAMYLASE FROM ESCHERICHIA COLI
Authors : Head, J.F.; Seaton, B.; Jin, L.
Deposited on : 1997-05-23
Resolution : 2.80 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)	:	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

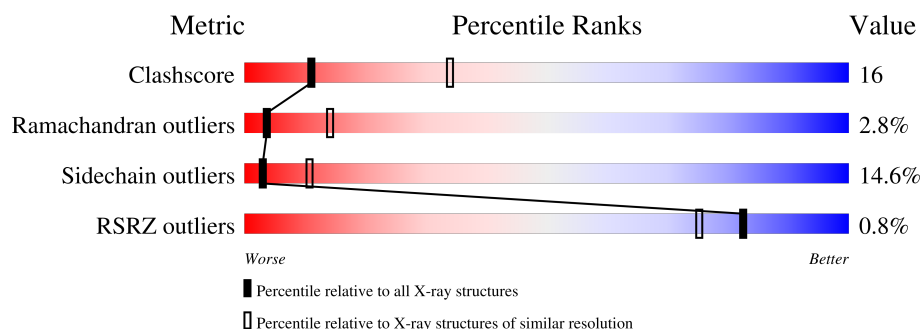
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	333	% 46% 36% 12% • •
1	B	333	% 53% 33% 8% • •
1	C	333	% 50% 34% 9% • •

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7482 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.

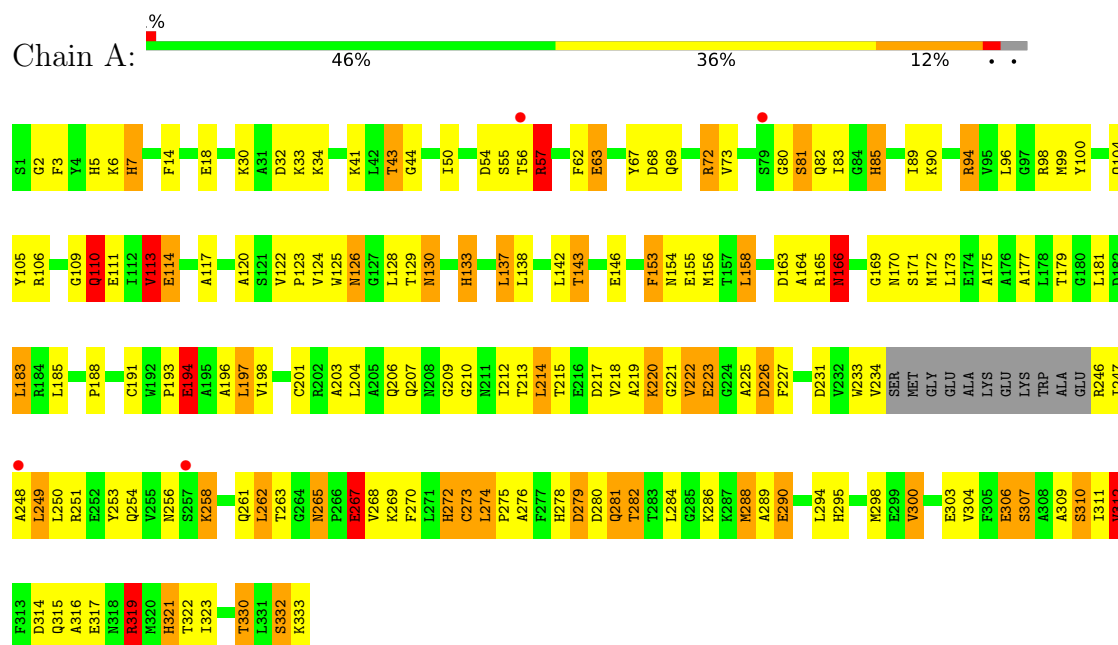
- Molecule 1 is a protein called ORNITHINE TRANSCARBAMYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	322	Total	C	N	O	S	0	0	0
			2494	1576	426	477	15			
1	B	322	Total	C	N	O	S	0	0	0
			2494	1576	426	477	15			
1	C	322	Total	C	N	O	S	0	0	0
			2494	1576	426	477	15			

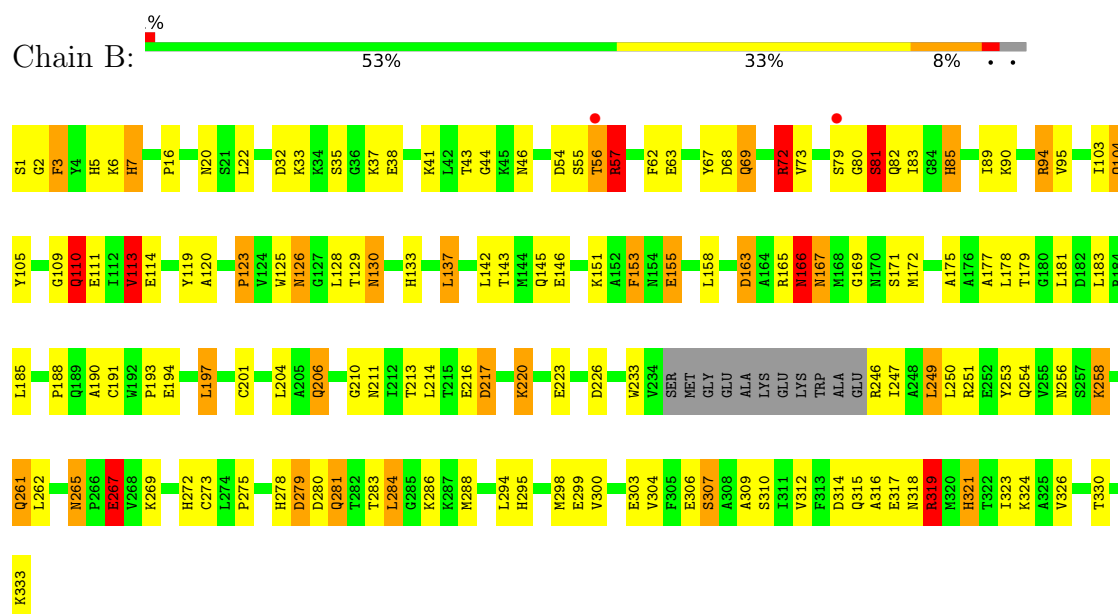
3 Residue-property plots

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.

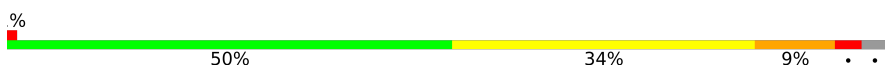
• Molecule 1: ORNITHINE TRANSCARBAMYLASE

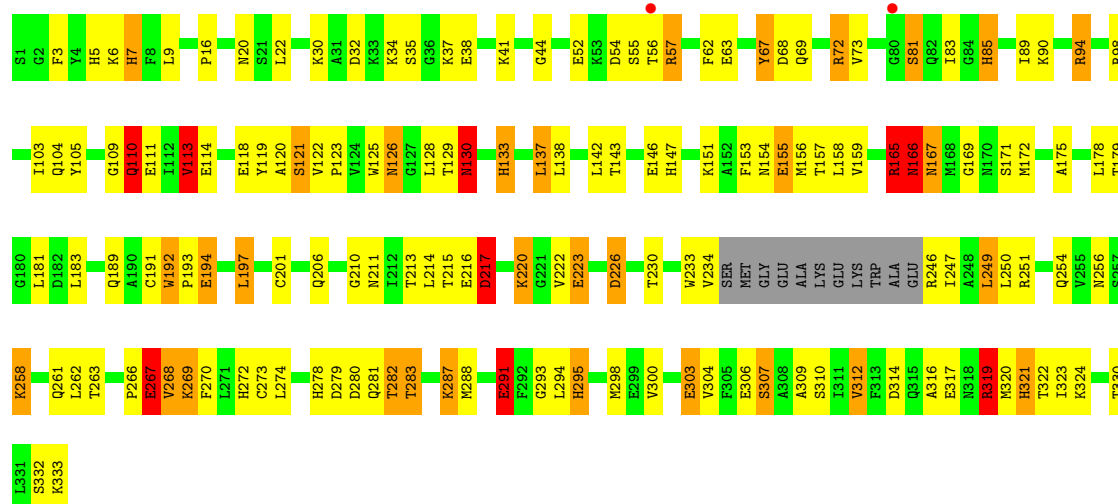


• Molecule 1: ORNITHINE TRANSCARBAMYLASE



● Molecule 1: ORNITHINE TRANSCARBAMYLASE

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	104.60Å 104.60Å 86.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.80 6.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.6 (6.00-2.80) 86.1 (6.00-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.13 (at 2.81Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.229 , 0.302 0.242 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	43.0	Xtriage
Anisotropy	0.189	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.008 for -h,-k,l 0.032 for h,-h-k,-l 0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	7482	wwPDB-VP
Average B, all atoms (Å ²)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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

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	1.25	14/2539 (0.6%)	1.92	61/3430 (1.8%)
1	B	1.27	16/2539 (0.6%)	1.97	75/3430 (2.2%)
1	C	1.23	13/2539 (0.5%)	1.95	69/3430 (2.0%)
All	All	1.25	43/7617 (0.6%)	1.95	205/10290 (2.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	278	HIS	CD2-NE2	-8.25	1.28	1.37
1	A	7	HIS	CD2-NE2	-8.02	1.29	1.37
1	C	5	HIS	CD2-NE2	-7.85	1.29	1.37
1	C	7	HIS	CD2-NE2	-7.78	1.29	1.37
1	B	7	HIS	CD2-NE2	-7.68	1.29	1.37
1	B	321	HIS	CD2-NE2	-7.58	1.29	1.37
1	B	278	HIS	CD2-NE2	-7.57	1.29	1.37
1	C	278	HIS	CD2-NE2	-7.45	1.29	1.37
1	B	272	HIS	CD2-NE2	-7.26	1.29	1.37
1	A	321	HIS	CD2-NE2	-7.24	1.29	1.37
1	A	7	HIS	CG-ND1	-6.96	1.30	1.38
1	B	5	HIS	CD2-NE2	-6.90	1.30	1.37
1	C	272	HIS	CD2-NE2	-6.84	1.30	1.37
1	A	85	HIS	CD2-NE2	-6.82	1.30	1.37
1	B	57	ARG	NE-CZ	6.79	1.40	1.33
1	C	125	TRP	CG-CD2	-6.74	1.31	1.43
1	A	57	ARG	NE-CZ	6.63	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	5	HIS	CD2-NE2	-6.56	1.30	1.37
1	A	272	HIS	CD2-NE2	-6.52	1.30	1.37
1	B	295	HIS	CD2-NE2	-6.52	1.30	1.37
1	C	321	HIS	CD2-NE2	-6.49	1.30	1.37
1	B	85	HIS	CD2-NE2	-6.30	1.30	1.37
1	B	125	TRP	CG-CD2	-6.21	1.32	1.43
1	C	5	HIS	CG-ND1	-6.02	1.31	1.38
1	C	147	HIS	CD2-NE2	-6.01	1.31	1.37
1	C	321	HIS	CG-ND1	-6.00	1.31	1.38
1	C	125	TRP	NE1-CE2	-5.96	1.30	1.37
1	A	165	ARG	NE-CZ	5.96	1.39	1.33
1	B	7	HIS	CG-ND1	-5.96	1.31	1.38
1	B	133	HIS	CD2-NE2	-5.86	1.31	1.37
1	A	133	HIS	CD2-NE2	-5.65	1.31	1.37
1	A	278	HIS	CG-ND1	-5.51	1.32	1.38
1	B	123	PRO	CA-CB	-5.50	1.46	1.53
1	B	272	HIS	CG-ND1	-5.48	1.32	1.38
1	C	268	VAL	CA-CB	5.48	1.60	1.54
1	B	278	HIS	CG-ND1	-5.46	1.32	1.38
1	C	85	HIS	CD2-NE2	-5.35	1.31	1.37
1	A	295	HIS	CD2-NE2	-5.32	1.31	1.37
1	B	321	HIS	CG-ND1	-5.26	1.32	1.38
1	A	321	HIS	CG-ND1	-5.16	1.32	1.38
1	A	125	TRP	CG-CD2	-5.16	1.34	1.43
1	C	295	HIS	CD2-NE2	-5.13	1.32	1.37
1	B	3	PHE	CA-CB	-5.08	1.44	1.53

All (205) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	166	ASN	OD1-CG-ND2	-11.18	111.42	122.60
1	A	57	ARG	N-CA-C	10.01	121.95	111.14
1	C	113	VAL	CB-CA-C	-9.54	99.26	112.14
1	B	113	VAL	CB-CA-C	-9.51	99.30	112.14
1	A	82	GLN	OE1-CD-NE2	-9.47	113.12	122.60
1	B	57	ARG	NE-CZ-NH1	8.82	130.32	121.50
1	A	113	VAL	CB-CA-C	-8.79	100.28	112.14
1	B	110	GLN	OE1-CD-NE2	-8.71	113.89	122.60
1	C	167	ASN	OD1-CG-ND2	-8.67	113.93	122.60
1	C	269	LYS	CG-CD-CE	8.46	130.75	111.30
1	C	57	ARG	N-CA-C	8.36	120.17	111.14
1	B	57	ARG	N-CA-C	8.16	119.95	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	57	ARG	NE-CZ-NH2	-8.12	111.89	119.20
1	C	110	GLN	OE1-CD-NE2	-8.12	114.48	122.60
1	C	126	ASN	OD1-CG-ND2	-7.85	114.75	122.60
1	A	57	ARG	NE-CZ-NH1	7.83	129.34	121.50
1	C	314	ASP	N-CA-C	-7.81	102.08	111.69
1	B	314	ASP	N-CA-C	-7.70	102.96	111.36
1	C	5	HIS	CB-CG-CD2	-7.69	121.20	131.20
1	C	69	GLN	OE1-CD-NE2	-7.67	114.93	122.60
1	B	269	LYS	CG-CD-CE	7.63	128.85	111.30
1	A	272	HIS	CB-CG-CD2	-7.62	121.30	131.20
1	B	5	HIS	CB-CG-CD2	-7.55	121.38	131.20
1	A	69	GLN	OE1-CD-NE2	-7.54	115.06	122.60
1	A	217	ASP	N-CA-C	7.49	120.62	108.63
1	B	167	ASN	OD1-CG-ND2	-7.46	115.14	122.60
1	A	57	ARG	NE-CZ-NH2	-7.45	112.50	119.20
1	B	272	HIS	CB-CG-CD2	-7.43	121.54	131.20
1	B	126	ASN	OD1-CG-ND2	-7.43	115.17	122.60
1	C	54	ASP	N-CA-C	7.38	119.85	110.33
1	C	272	HIS	CB-CG-CD2	-7.37	121.62	131.20
1	C	113	VAL	N-CA-CB	7.32	120.50	110.54
1	A	166	ASN	OD1-CG-ND2	-7.31	115.29	122.60
1	B	273	CYS	O-C-N	-7.21	113.88	122.96
1	C	89	ILE	CB-CA-C	-7.13	102.85	111.97
1	C	330	THR	CA-CB-OG1	-7.07	98.99	109.60
1	B	68	ASP	CA-CB-CG	7.06	119.66	112.60
1	B	166	ASN	CB-CG-ND2	7.04	126.95	116.40
1	C	319	ARG	CB-CG-CD	-7.00	95.19	111.30
1	A	156	MET	CG-SD-CE	-6.98	85.55	100.90
1	B	295	HIS	CB-CG-CD2	-6.97	122.13	131.20
1	C	166	ASN	OD1-CG-ND2	-6.97	115.63	122.60
1	C	280	ASP	N-CA-C	-6.94	103.10	112.26
1	B	113	VAL	N-CA-CB	6.94	119.97	110.54
1	A	194	GLU	O-C-N	6.92	131.17	123.01
1	B	57	ARG	CB-CA-C	-6.90	100.00	110.90
1	B	217	ASP	CA-CB-CG	6.89	119.49	112.60
1	A	314	ASP	N-CA-C	-6.84	103.90	111.36
1	C	272	HIS	CB-CG-ND1	6.79	132.89	122.70
1	C	211	ASN	OD1-CG-ND2	-6.76	115.84	122.60
1	B	110	GLN	CG-CD-NE2	6.74	126.51	116.40
1	C	110	GLN	CG-CD-NE2	6.74	126.51	116.40
1	A	126	ASN	OD1-CG-ND2	-6.72	115.88	122.60
1	C	319	ARG	CD-NE-CZ	-6.67	115.07	124.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	272	HIS	CB-CG-ND1	6.62	132.62	122.70
1	A	196	ALA	CA-C-O	-6.60	113.81	121.07
1	A	5	HIS	CB-CG-CD2	-6.50	122.75	131.20
1	B	265	ASN	OD1-CG-ND2	-6.48	116.12	122.60
1	B	133	HIS	CB-CG-CD2	-6.47	122.79	131.20
1	A	57	ARG	CB-CA-C	-6.46	100.69	110.90
1	B	69	GLN	OE1-CD-NE2	-6.46	116.14	122.60
1	A	54	ASP	N-CA-C	6.43	118.63	110.33
1	A	113	VAL	N-CA-CB	6.42	119.28	110.54
1	B	89	ILE	CB-CA-C	-6.35	103.72	112.04
1	A	288	MET	CG-SD-CE	-6.32	87.00	100.90
1	B	273	CYS	N-CA-C	-6.30	100.32	109.59
1	A	300	VAL	CB-CA-C	-6.30	101.24	110.62
1	C	287	LYS	N-CA-C	-6.29	104.42	111.28
1	A	319	ARG	CB-CG-CD	-6.29	96.84	111.30
1	C	57	ARG	CB-CA-C	-6.26	101.00	110.90
1	B	119	TYR	N-CA-C	6.25	121.19	113.50
1	C	216	GLU	N-CA-C	-6.25	106.24	114.31
1	B	33	LYS	N-CA-C	-6.25	104.39	111.14
1	C	312	VAL	N-CA-C	6.25	117.74	110.62
1	C	216	GLU	N-CA-CB	6.23	119.18	110.90
1	C	54	ASP	CA-CB-CG	-6.22	106.38	112.60
1	C	321	HIS	CA-CB-CG	-6.22	107.58	113.80
1	B	272	HIS	CB-CG-ND1	6.20	132.01	122.70
1	A	273	CYS	N-CA-C	-6.20	100.22	109.15
1	B	321	HIS	CB-CG-CD2	-6.20	123.14	131.20
1	C	120	ALA	CA-C-N	-6.19	112.37	122.65
1	C	120	ALA	C-N-CA	-6.19	112.37	122.65
1	A	89	ILE	CB-CA-C	-6.18	103.80	112.14
1	A	282	THR	N-CA-C	6.17	123.93	110.80
1	B	267	GLU	O-C-N	-6.15	114.41	122.59
1	C	191	CYS	N-CA-CB	-6.14	101.09	111.17
1	A	170	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	B	82	GLN	N-CA-C	6.11	119.52	110.48
1	A	295	HIS	O-C-N	-6.11	116.22	123.06
1	B	54	ASP	N-CA-C	6.11	118.21	110.33
1	B	82	GLN	OE1-CD-NE2	-6.11	116.50	122.60
1	B	20	ASN	OD1-CG-ND2	-6.10	116.50	122.60
1	A	33	LYS	N-CA-C	-6.10	104.56	111.14
1	A	89	ILE	N-CA-C	-6.07	104.43	110.62
1	B	46	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	A	321	HIS	CA-CB-CG	-6.06	107.74	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	211	ASN	OD1-CG-ND2	-6.06	116.54	122.60
1	A	80	GLY	N-CA-C	-6.06	104.46	112.82
1	C	119	TYR	N-CA-C	6.03	120.76	113.41
1	B	279	ASP	O-C-N	6.01	129.70	122.85
1	B	80	GLY	N-CA-C	-5.98	103.99	112.37
1	B	261	GLN	OE1-CD-NE2	-5.98	116.62	122.60
1	A	280	ASP	CA-CB-CG	-5.98	106.62	112.60
1	A	267	GLU	N-CA-CB	-5.96	102.09	111.39
1	A	110	GLN	CG-CD-NE2	5.95	125.32	116.40
1	C	32	ASP	CA-CB-CG	5.94	118.54	112.60
1	B	32	ASP	CA-CB-CG	5.94	118.54	112.60
1	C	217	ASP	CA-CB-CG	5.92	118.52	112.60
1	B	280	ASP	N-CA-C	-5.92	104.44	112.26
1	C	291	GLU	N-CA-C	5.92	123.40	110.80
1	A	133	HIS	CB-CG-CD2	-5.92	123.51	131.20
1	B	153	PHE	CA-CB-CG	5.91	119.71	113.80
1	A	110	GLN	OE1-CD-NE2	-5.90	116.70	122.60
1	A	63	GLU	CA-C-O	-5.89	114.63	120.70
1	C	154	ASN	OD1-CG-ND2	-5.89	116.71	122.60
1	B	267	GLU	CA-CB-CG	5.86	125.82	114.10
1	C	217	ASP	CB-CA-C	-5.85	100.31	109.84
1	A	274	LEU	O-C-N	-5.81	115.44	121.60
1	B	319	ARG	CB-CG-CD	-5.79	97.97	111.30
1	A	321	HIS	CB-CG-CD2	-5.78	123.68	131.20
1	C	267	GLU	CA-CB-CG	5.78	125.65	114.10
1	A	330	THR	CA-CB-OG1	-5.77	100.94	109.60
1	A	32	ASP	CA-CB-CG	5.76	118.36	112.60
1	B	125	TRP	CE2-CD2-CE3	5.76	124.56	118.80
1	A	315	GLN	OE1-CD-NE2	-5.75	116.84	122.60
1	C	172	MET	N-CA-C	-5.75	104.92	111.07
1	A	114	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	172	MET	N-CA-C	-5.70	105.15	111.36
1	B	326	VAL	CA-C-O	-5.70	115.49	121.41
1	A	125	TRP	CE2-CD2-CE3	5.69	124.49	118.80
1	A	153	PHE	CA-C-N	5.69	129.79	120.63
1	A	153	PHE	C-N-CA	5.69	129.79	120.63
1	C	57	ARG	CB-CG-CD	-5.68	98.24	111.30
1	B	133	HIS	CB-CG-ND1	5.67	131.21	122.70
1	C	156	MET	N-CA-C	-5.67	100.93	109.95
1	C	282	THR	N-CA-CB	-5.65	100.93	110.49
1	B	163	ASP	CA-CB-CG	5.65	118.25	112.60
1	C	273	CYS	N-CA-C	-5.63	101.05	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	ILE	N-CA-CB	5.61	117.12	110.55
1	A	265	ASN	CA-C-O	5.55	124.84	119.62
1	A	279	ASP	O-C-N	5.54	129.47	122.65
1	C	68	ASP	CA-CB-CG	5.54	118.14	112.60
1	A	276	ALA	O-C-N	-5.54	116.42	123.24
1	B	95	VAL	N-CA-C	-5.54	105.45	110.82
1	B	216	GLU	N-CA-C	-5.52	106.54	113.72
1	B	315	GLN	OE1-CD-NE2	-5.52	117.08	122.60
1	C	167	ASN	CA-CB-CG	5.51	118.11	112.60
1	C	273	CYS	O-C-N	-5.50	115.34	122.77
1	C	122	VAL	N-CA-CB	-5.50	108.04	111.83
1	C	217	ASP	N-CA-CB	5.49	118.45	109.95
1	C	130	ASN	CA-CB-CG	5.48	118.08	112.60
1	B	281	GLN	CA-C-O	-5.48	112.67	120.51
1	C	278	HIS	CB-CG-CD2	-5.47	124.09	131.20
1	C	192	TRP	CA-C-N	5.46	125.22	119.76
1	C	192	TRP	C-N-CA	5.46	125.22	119.76
1	B	120	ALA	O-C-N	-5.46	116.65	123.04
1	A	273	CYS	CA-C-O	-5.45	114.13	120.62
1	A	332	SER	N-CA-CB	-5.45	102.87	111.05
1	C	167	ASN	CB-CG-ND2	5.45	124.58	116.40
1	B	273	CYS	CA-C-O	-5.45	114.26	120.58
1	C	133	HIS	CB-CG-CD2	-5.45	124.12	131.20
1	A	68	ASP	CA-CB-CG	5.45	118.05	112.60
1	B	56	THR	CA-C-N	5.44	127.84	120.44
1	B	56	THR	C-N-CA	5.44	127.84	120.44
1	B	104	GLN	OE1-CD-NE2	-5.42	117.17	122.60
1	C	7	HIS	CB-CG-CD2	-5.42	124.15	131.20
1	A	312	VAL	N-CA-CB	-5.39	103.73	110.47
1	B	299	GLU	CA-C-O	-5.37	114.72	120.42
1	C	303	GLU	CA-CB-CG	5.37	124.84	114.10
1	C	20	ASN	OD1-CG-ND2	-5.37	117.23	122.60
1	B	103	ILE	O-C-N	-5.36	117.47	123.26
1	A	85	HIS	CA-C-O	-5.34	115.19	120.80
1	C	121	SER	CA-CB-OG	-5.32	100.45	111.10
1	B	167	ASN	CB-CG-ND2	5.30	124.36	116.40
1	A	280	ASP	N-CA-C	-5.30	105.26	112.26
1	C	103	ILE	O-C-N	-5.29	117.48	123.20
1	C	194	GLU	CA-C-O	5.29	126.51	120.80
1	C	165	ARG	CA-CB-CG	5.28	124.66	114.10
1	C	321	HIS	CB-CG-CD2	-5.27	124.35	131.20
1	A	120	ALA	N-CA-C	-5.26	101.19	109.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ARG	CB-CG-CD	-5.26	99.19	111.30
1	B	295	HIS	CA-CB-CG	-5.26	108.54	113.80
1	A	278	HIS	CB-CG-CD2	-5.25	124.37	131.20
1	B	166	ASN	CA-CB-CG	5.25	117.84	112.60
1	C	52	GLU	CA-C-O	5.24	125.83	119.38
1	C	274	LEU	CA-C-O	-5.22	115.12	120.87
1	A	281	GLN	CA-C-O	-5.17	113.12	120.51
1	B	321	HIS	CA-CB-CG	-5.16	108.64	113.80
1	B	172	MET	N-CA-C	-5.14	105.68	111.28
1	B	330	THR	CA-CB-OG1	-5.13	101.90	109.60
1	C	118	GLU	CA-C-O	-5.11	115.13	120.55
1	B	190	ALA	O-C-N	5.10	128.18	122.22
1	B	145	GLN	CB-CA-C	-5.10	102.82	110.92
1	C	312	VAL	N-CA-CB	-5.10	104.10	110.47
1	C	233	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	B	81	SER	CA-CB-OG	5.08	121.26	111.10
1	A	289	ALA	O-C-N	5.06	127.49	122.12
1	B	206	GLN	OE1-CD-NE2	-5.05	117.55	122.60
1	B	318	ASN	CA-CB-CG	-5.04	107.56	112.60
1	A	222	VAL	CA-C-O	-5.04	113.77	119.42
1	C	330	THR	CA-CB-CG2	5.04	119.07	110.50
1	B	89	ILE	N-CA-CB	5.03	116.76	110.47
1	B	167	ASN	CA-CB-CG	5.01	117.61	112.60
1	B	319	ARG	CD-NE-CZ	-5.01	117.39	124.40
1	B	295	HIS	CB-CG-ND1	5.00	130.21	122.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	67	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	2494	0	2474	106	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2494	0	2474	71	0
1	C	2494	0	2474	76	0
All	All	7482	0	7422	245	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 16.

All (245) 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:197:LEU:HD22	1:C:201:CYS:SG	2.21	0.80
1:A:72:ARG:HD3	1:C:67:TYR:HB3	1.62	0.79
1:A:137:LEU:HD13	1:A:171:SER:HB3	1.66	0.77
1:B:137:LEU:HD13	1:B:171:SER:HB3	1.67	0.76
1:C:7:HIS:HD2	1:C:123:PRO:HA	1.50	0.75
1:C:137:LEU:HD13	1:C:171:SER:HB3	1.67	0.75
1:A:304:VAL:O	1:A:307:SER:HB2	1.88	0.73
1:B:304:VAL:O	1:B:307:SER:HB2	1.89	0.73
1:A:3:PHE:HA	1:A:6:LYS:HE2	1.70	0.72
1:B:197:LEU:HD22	1:B:201:CYS:SG	2.29	0.71
1:A:197:LEU:HD22	1:A:201:CYS:SG	2.31	0.71
1:A:109:GLY:HA2	1:A:130:ASN:ND2	2.06	0.70
1:C:304:VAL:O	1:C:307:SER:HB2	1.92	0.69
1:A:206:GLN:HA	1:A:210:GLY:O	1.92	0.69
1:A:90:LYS:O	1:A:94:ARG:HD3	1.95	0.67
1:C:166:ASN:ND2	1:C:169:GLY:H	1.92	0.67
1:B:7:HIS:HD2	1:B:123:PRO:HA	1.57	0.67
1:C:206:GLN:HA	1:C:210:GLY:O	1.95	0.66
1:C:7:HIS:CD2	1:C:123:PRO:HA	2.31	0.66
1:C:90:LYS:O	1:C:94:ARG:HD3	1.97	0.65
1:A:215:THR:HG21	1:A:221:GLY:HA3	1.77	0.65
1:B:3:PHE:HA	1:B:6:LYS:HE2	1.79	0.65
1:B:126:ASN:HD21	1:B:129:THR:HG23	1.62	0.65
1:A:62:PHE:CZ	1:A:104:GLN:HG3	2.32	0.64
1:B:206:GLN:HA	1:B:210:GLY:O	1.97	0.64
1:B:62:PHE:CZ	1:B:104:GLN:HG3	2.33	0.64
1:A:234:VAL:HG21	1:A:288:MET:HE1	1.79	0.64
1:B:44:GLY:HA2	1:B:72:ARG:NH2	2.14	0.63
1:A:44:GLY:HA2	1:A:72:ARG:NH2	2.14	0.63
1:C:44:GLY:HA2	1:C:72:ARG:NH2	2.14	0.63
1:B:90:LYS:O	1:B:94:ARG:HD3	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:63:GLU:HG2	1:C:73:VAL:HG11	1.82	0.62
1:C:189:GLN:HA	1:C:192:TRP:CE2	2.34	0.62
1:A:6:LYS:HE3	1:A:14:PHE:HE1	1.65	0.62
1:C:3:PHE:HA	1:C:6:LYS:HE2	1.82	0.62
1:A:163:ASP:HA	1:A:191:CYS:HB3	1.82	0.62
1:C:126:ASN:HD21	1:C:129:THR:HG23	1.65	0.61
1:B:63:GLU:HG2	1:B:73:VAL:HG11	1.82	0.61
1:A:166:ASN:ND2	1:A:169:GLY:H	1.99	0.61
1:C:109:GLY:HA2	1:C:130:ASN:ND2	2.16	0.61
1:A:153:PHE:HB3	1:A:179:THR:HG23	1.83	0.61
1:C:126:ASN:ND2	1:C:129:THR:HG23	2.16	0.61
1:C:307:SER:HB3	1:C:309:ALA:H	1.65	0.60
1:A:63:GLU:HG2	1:A:73:VAL:HG11	1.83	0.60
1:A:265:ASN:OD1	1:A:267:GLU:HG3	2.02	0.60
1:A:3:PHE:CZ	1:A:18:GLU:HB3	2.37	0.60
1:A:100:TYR:O	1:A:122:VAL:HG11	2.02	0.60
1:A:137:LEU:HD22	1:A:175:ALA:HB2	1.83	0.60
1:A:270:PHE:HD2	1:A:310:SER:HB3	1.67	0.60
1:A:226:ASP:O	1:A:269:LYS:HD2	2.01	0.59
1:C:288:MET:SD	1:C:288:MET:N	2.75	0.59
1:B:166:ASN:ND2	1:B:169:GLY:H	2.01	0.59
1:B:217:ASP:CG	1:B:220:LYS:HB3	2.28	0.59
1:C:153:PHE:HB3	1:C:179:THR:HG23	1.84	0.59
1:B:185:LEU:HB2	1:B:214:LEU:HD13	1.84	0.59
1:A:164:ALA:O	1:A:169:GLY:HA3	2.02	0.58
1:A:263:THR:HG21	1:A:268:VAL:HG21	1.85	0.58
1:B:126:ASN:ND2	1:B:129:THR:HG23	2.18	0.58
1:C:81:SER:OG	1:C:85:HIS:HB3	2.04	0.57
1:A:225:ALA:HB3	1:A:263:THR:HG22	1.86	0.57
1:B:67:TYR:HB3	1:C:72:ARG:HD3	1.87	0.57
1:B:188:PRO:HD3	1:B:253:TYR:CE2	2.39	0.57
1:C:142:LEU:O	1:C:146:GLU:HG3	2.04	0.57
1:C:3:PHE:CZ	1:C:22:LEU:HG	2.39	0.57
1:C:279:ASP:HB3	1:C:281:GLN:H	1.70	0.57
1:A:7:HIS:HD2	1:A:124:VAL:H	1.50	0.57
1:C:3:PHE:HA	1:C:6:LYS:CE	2.35	0.57
1:B:109:GLY:HA2	1:B:130:ASN:ND2	2.20	0.56
1:B:284:LEU:O	1:B:288:MET:HG2	2.05	0.56
1:B:35:SER:OG	1:B:37:LYS:NZ	2.39	0.56
1:B:113:VAL:HG22	1:B:129:THR:HG21	1.87	0.56
1:A:142:LEU:O	1:A:146:GLU:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:SER:HB3	1:A:309:ALA:H	1.68	0.56
1:A:44:GLY:HA2	1:A:72:ARG:HH22	1.70	0.56
1:A:273:CYS:O	1:A:273:CYS:SG	2.63	0.56
1:C:62:PHE:CZ	1:C:104:GLN:HG3	2.41	0.56
1:B:188:PRO:HG2	1:B:191:CYS:SG	2.46	0.55
1:C:44:GLY:HA2	1:C:72:ARG:HH22	1.72	0.55
1:C:293:GLY:HA2	1:C:295:HIS:CE1	2.41	0.55
1:A:113:VAL:HG22	1:A:129:THR:HG21	1.88	0.55
1:B:137:LEU:HD22	1:B:175:ALA:HB2	1.88	0.55
1:B:294:LEU:HD13	1:B:298:MET:HG2	1.89	0.55
1:B:7:HIS:CD2	1:B:123:PRO:HA	2.41	0.54
1:B:254:GLN:HG3	1:B:298:MET:O	2.08	0.54
1:B:3:PHE:CZ	1:B:22:LEU:HG	2.43	0.54
1:B:265:ASN:OD1	1:B:267:GLU:HG3	2.07	0.53
1:B:153:PHE:HB3	1:B:179:THR:HG23	1.89	0.53
1:C:137:LEU:HD22	1:C:175:ALA:HB2	1.89	0.53
1:C:113:VAL:HG22	1:C:129:THR:HG21	1.90	0.53
1:C:230:THR:HG22	1:C:270:PHE:HE1	1.74	0.53
1:A:7:HIS:CE1	1:A:117:ALA:HB1	2.44	0.53
1:A:188:PRO:HG3	1:A:249:LEU:HD22	1.91	0.53
1:A:212:ILE:HG22	1:A:214:LEU:CD2	2.38	0.53
1:B:105:TYR:CD2	1:B:113:VAL:HG13	2.43	0.53
1:A:105:TYR:CD2	1:A:113:VAL:HG13	2.44	0.52
1:A:126:ASN:ND2	1:A:129:THR:HG23	2.24	0.52
1:A:67:TYR:HB3	1:B:72:ARG:HD3	1.92	0.52
1:C:105:TYR:CD2	1:C:113:VAL:HG13	2.45	0.52
1:A:215:THR:HG21	1:A:221:GLY:CA	2.40	0.51
1:B:153:PHE:CB	1:B:179:THR:HG23	2.40	0.51
1:A:219:ALA:HB2	1:A:262:LEU:HD22	1.92	0.51
1:A:153:PHE:HB3	1:A:179:THR:CG2	2.40	0.51
1:C:3:PHE:CE2	1:C:22:LEU:HG	2.46	0.51
1:B:288:MET:HE3	1:B:298:MET:HE1	1.92	0.51
1:B:217:ASP:HB3	1:B:220:LYS:HB3	1.93	0.51
1:A:227:PHE:HA	1:A:269:LYS:O	2.11	0.51
1:A:126:ASN:HD21	1:A:129:THR:HG23	1.76	0.50
1:A:188:PRO:HG2	1:A:191:CYS:SG	2.52	0.50
1:B:179:THR:CG2	1:B:181:LEU:HG	2.42	0.50
1:A:279:ASP:HB3	1:A:281:GLN:H	1.75	0.50
1:B:62:PHE:CE2	1:B:104:GLN:HG3	2.47	0.50
1:B:81:SER:OG	1:B:85:HIS:HB3	2.11	0.50
1:C:165:ARG:HB2	1:C:192:TRP:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:173:LEU:HD11	1:A:193:PRO:HB2	1.94	0.50
1:B:166:ASN:HD22	1:B:169:GLY:H	1.59	0.49
1:A:212:ILE:HG22	1:A:214:LEU:HD21	1.95	0.49
1:B:316:ALA:O	1:B:319:ARG:HB2	2.11	0.49
1:A:256:ASN:OD1	1:A:258:LYS:HB3	2.12	0.49
1:B:110:GLN:O	1:B:113:VAL:HG23	2.13	0.49
1:A:194:GLU:OE1	1:A:197:LEU:HB2	2.13	0.49
1:A:179:THR:CG2	1:A:181:LEU:HG	2.43	0.49
1:B:249:LEU:HD13	1:B:250:LEU:HG	1.94	0.49
1:C:16:PRO:HB3	1:C:178:LEU:O	2.12	0.49
1:C:153:PHE:HB3	1:C:179:THR:CG2	2.42	0.49
1:A:81:SER:OG	1:A:85:HIS:HB3	2.14	0.48
1:A:281:GLN:O	1:A:286:LYS:HB2	2.13	0.48
1:A:153:PHE:CB	1:A:179:THR:HG23	2.43	0.48
1:B:307:SER:HB3	1:B:309:ALA:H	1.78	0.48
1:C:247:ILE:HG23	1:C:294:LEU:HD11	1.95	0.48
1:A:317:GLU:OE2	1:A:321:HIS:HE1	1.96	0.48
1:B:317:GLU:OE2	1:B:321:HIS:HE1	1.97	0.48
1:C:179:THR:CG2	1:C:181:LEU:HG	2.44	0.48
1:C:234:VAL:HG12	1:C:246:ARG:HB3	1.96	0.48
1:A:188:PRO:CG	1:A:249:LEU:HD22	2.43	0.48
1:C:317:GLU:OE2	1:C:321:HIS:HE1	1.97	0.48
1:C:291:GLU:CD	1:C:291:GLU:H	2.22	0.48
1:C:9:LEU:HD22	1:C:113:VAL:HB	1.96	0.47
1:A:62:PHE:CE2	1:A:104:GLN:HG3	2.49	0.47
1:B:41:LYS:NZ	1:B:333:LYS:O	2.47	0.47
1:C:30:LYS:O	1:C:34:LYS:HG3	2.14	0.47
1:A:231:ASP:HA	1:A:272:HIS:CE1	2.49	0.47
1:C:151:LYS:NZ	1:C:155:GLU:HB2	2.30	0.47
1:C:153:PHE:CB	1:C:179:THR:HG23	2.44	0.47
1:C:222:VAL:HG13	1:C:263:THR:HG22	1.97	0.47
1:A:133:HIS:CE1	1:A:319:ARG:NH2	2.83	0.47
1:B:16:PRO:HB3	1:B:178:LEU:O	2.15	0.47
1:B:142:LEU:O	1:B:146:GLU:HG3	2.15	0.47
1:A:3:PHE:HZ	1:A:18:GLU:HB3	1.80	0.47
1:A:254:GLN:HG3	1:A:298:MET:O	2.15	0.46
1:A:6:LYS:O	1:A:123:PRO:HB3	2.15	0.46
1:B:44:GLY:HA2	1:B:72:ARG:HH22	1.78	0.46
1:A:185:LEU:HB2	1:A:214:LEU:HD13	1.96	0.46
1:B:153:PHE:HB3	1:B:179:THR:CG2	2.45	0.46
1:C:151:LYS:HZ2	1:C:155:GLU:HB2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:PHE:HE1	1:A:14:PHE:CD1	2.33	0.46
1:B:279:ASP:HB3	1:B:281:GLN:H	1.80	0.46
1:C:249:LEU:HD12	1:C:249:LEU:H	1.80	0.46
1:A:188:PRO:HD3	1:A:253:TYR:CE2	2.51	0.46
1:C:110:GLN:O	1:C:113:VAL:HG23	2.16	0.46
1:C:217:ASP:HB2	1:C:220:LYS:HB3	1.98	0.46
1:A:137:LEU:CD1	1:A:171:SER:HB3	2.40	0.46
1:A:234:VAL:HG21	1:A:288:MET:CE	2.46	0.46
1:B:151:LYS:NZ	1:B:155:GLU:HB2	2.30	0.46
1:C:175:ALA:O	1:C:179:THR:HB	2.16	0.46
1:C:256:ASN:OD1	1:C:258:LYS:HB3	2.15	0.46
1:C:41:LYS:NZ	1:C:333:LYS:O	2.49	0.45
1:C:159:VAL:HG21	1:C:222:VAL:HA	1.98	0.45
1:C:223:GLU:O	1:C:263:THR:HA	2.16	0.45
1:A:233:TRP:O	1:A:246:ARG:HD2	2.16	0.45
1:B:177:ALA:HB1	1:B:204:LEU:HD22	1.99	0.45
1:A:6:LYS:HE3	1:A:14:PHE:CE1	2.50	0.45
1:B:193:PRO:HD2	1:B:214:LEU:HD11	1.97	0.45
1:A:7:HIS:HD2	1:A:123:PRO:HA	1.81	0.45
1:B:286:LYS:HE3	1:B:286:LYS:HB2	1.66	0.45
1:B:151:LYS:HZ2	1:B:155:GLU:HB2	1.81	0.45
1:C:38:GLU:OE2	1:C:324:LYS:NZ	2.50	0.45
1:C:130:ASN:O	1:C:167:ASN:HB3	2.17	0.45
1:B:57:ARG:NH2	1:B:275:PRO:HG3	2.32	0.45
1:B:217:ASP:CB	1:B:220:LYS:HB3	2.47	0.45
1:C:62:PHE:CE2	1:C:104:GLN:HG3	2.52	0.45
1:A:30:LYS:O	1:A:34:LYS:HG3	2.17	0.45
1:B:163:ASP:HA	1:B:191:CYS:HB3	1.98	0.45
1:A:98:ARG:NH1	1:C:317:GLU:OE1	2.50	0.45
1:B:113:VAL:CG2	1:B:129:THR:HG21	2.47	0.44
1:C:287:LYS:O	1:C:291:GLU:HB2	2.17	0.44
1:A:247:ILE:O	1:A:251:ARG:HB2	2.16	0.44
1:C:35:SER:OG	1:C:37:LYS:NZ	2.48	0.44
1:A:113:VAL:CG2	1:A:129:THR:HG21	2.47	0.44
1:B:105:TYR:HD2	1:B:113:VAL:HG13	1.82	0.44
1:B:249:LEU:HD12	1:B:249:LEU:H	1.82	0.44
1:A:3:PHE:O	1:A:330:THR:HG22	2.17	0.44
1:A:194:GLU:O	1:A:198:VAL:HG23	2.18	0.44
1:C:316:ALA:O	1:C:319:ARG:HB2	2.18	0.44
1:A:179:THR:HG22	1:A:181:LEU:HG	1.99	0.44
1:A:225:ALA:HB3	1:A:263:THR:CG2	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ALA:O	1:A:319:ARG:HB2	2.17	0.44
1:B:38:GLU:OE2	1:B:324:LYS:NZ	2.51	0.43
1:A:7:HIS:CD2	1:A:123:PRO:HA	2.53	0.43
1:A:177:ALA:HB1	1:A:204:LEU:HD22	2.01	0.43
1:C:138:LEU:HB3	1:C:322:THR:HB	2.00	0.43
1:C:133:HIS:HE1	1:C:319:ARG:HH22	1.66	0.43
1:C:249:LEU:HD13	1:C:250:LEU:HG	2.00	0.43
1:B:2:GLY:O	1:B:6:LYS:HE2	2.19	0.43
1:A:110:GLN:O	1:A:113:VAL:HG23	2.18	0.43
1:A:219:ALA:CB	1:A:262:LEU:HD22	2.49	0.43
1:C:113:VAL:CG2	1:C:129:THR:HG21	2.47	0.43
1:A:203:ALA:O	1:A:207:GLN:HB2	2.18	0.43
1:A:99:MET:HE2	1:C:320:MET:HB2	2.01	0.43
1:A:222:VAL:HG13	1:A:263:THR:HG22	2.01	0.43
1:C:254:GLN:HG3	1:C:298:MET:O	2.19	0.42
1:B:41:LYS:H	1:B:69:GLN:NE2	2.17	0.42
1:A:98:ARG:HH11	1:A:98:ARG:HD2	1.71	0.42
1:A:249:LEU:HD13	1:A:250:LEU:HG	2.00	0.42
1:B:130:ASN:O	1:B:167:ASN:HB3	2.19	0.42
1:B:233:TRP:O	1:B:246:ARG:HD2	2.19	0.42
1:A:7:HIS:CD2	1:A:124:VAL:H	2.35	0.42
1:A:220:LYS:O	1:A:223:GLU:HB2	2.20	0.42
1:B:179:THR:HG22	1:B:181:LEU:HG	2.01	0.42
1:C:193:PRO:HD2	1:C:214:LEU:HD11	2.00	0.42
1:A:143:THR:HG22	1:A:311:ILE:HD12	2.01	0.42
1:B:247:ILE:O	1:B:251:ARG:HB2	2.19	0.42
1:C:230:THR:HG22	1:C:270:PHE:CE1	2.54	0.41
1:A:306:GLU:OE1	1:B:94:ARG:NH2	2.51	0.41
1:A:306:GLU:CD	1:B:94:ARG:HH22	2.28	0.41
1:A:41:LYS:NZ	1:A:333:LYS:O	2.53	0.41
1:A:233:TRP:CE3	1:A:247:ILE:HG12	2.56	0.41
1:B:256:ASN:OD1	1:B:258:LYS:HB3	2.21	0.41
1:A:105:TYR:HD2	1:A:113:VAL:HG13	1.84	0.41
1:A:154:ASN:OD1	1:A:209:GLY:HA3	2.21	0.41
1:A:158:LEU:HB3	1:A:183:LEU:HD23	2.01	0.41
1:C:247:ILE:O	1:C:251:ARG:HB2	2.21	0.41
1:A:133:HIS:HE1	1:A:319:ARG:NH2	2.18	0.41
1:A:290:GLU:OE1	1:A:290:GLU:HA	2.21	0.41
1:C:267:GLU:CD	1:C:269:LYS:HZ1	2.29	0.41
1:C:319:ARG:HH11	1:C:319:ARG:HD2	1.61	0.41
1:C:133:HIS:CE1	1:C:319:ARG:NH2	2.90	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:THR:HG22	1:A:43:THR:O	2.21	0.40
1:A:106:ARG:HH11	1:A:106:ARG:HD2	1.74	0.40
1:A:219:ALA:O	1:A:223:GLU:N	2.53	0.40
1:A:274:LEU:HD11	1:A:312:VAL:HG13	2.04	0.40
1:A:50:ILE:HD11	1:A:96:LEU:HD11	2.02	0.40
1:A:138:LEU:HB3	1:A:322:THR:HB	2.02	0.40
1:B:317:GLU:OE1	1:C:98:ARG:NH1	2.55	0.40
1:C:157:THR:H	1:C:226:ASP:HB2	1.85	0.40
1:A:57:ARG:NH2	1:A:275:PRO:HG3	2.37	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	318/333 (96%)	282 (89%)	24 (8%)	12 (4%)	2	9
1	B	318/333 (96%)	289 (91%)	22 (7%)	7 (2%)	5	19
1	C	318/333 (96%)	287 (90%)	23 (7%)	8 (2%)	4	16
All	All	954/999 (96%)	858 (90%)	69 (7%)	27 (3%)	4	14

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	128	LEU
1	A	223	GLU
1	B	128	LEU
1	B	223	GLU
1	C	128	LEU
1	C	223	GLU
1	C	291	GLU
1	A	294	LEU

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Mol	Chain	Res	Type
1	A	2	GLY
1	A	218	VAL
1	A	282	THR
1	C	83	ILE
1	C	262	LEU
1	C	282	THR
1	C	283	THR
1	A	248	ALA
1	A	262	LEU
1	B	55	SER
1	C	55	SER
1	A	290	GLU
1	B	43	THR
1	B	79	SER
1	B	262	LEU
1	A	43	THR
1	A	55	SER
1	A	83	ILE
1	B	83	ILE

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	262/270 (97%)	226 (86%)	36 (14%)	3	13
1	B	262/270 (97%)	225 (86%)	37 (14%)	3	12
1	C	262/270 (97%)	220 (84%)	42 (16%)	2	9
All	All	786/810 (97%)	671 (85%)	115 (15%)	3	11

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	THR
1	A	57	ARG
1	A	72	ARG

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Mol	Chain	Res	Type
1	A	81	SER
1	A	94	ARG
1	A	110	GLN
1	A	111	GLU
1	A	113	VAL
1	A	114	GLU
1	A	130	ASN
1	A	137	LEU
1	A	143	THR
1	A	155	GLU
1	A	158	LEU
1	A	166	ASN
1	A	183	LEU
1	A	194	GLU
1	A	197	LEU
1	A	213	THR
1	A	214	LEU
1	A	220	LYS
1	A	226	ASP
1	A	249	LEU
1	A	258	LYS
1	A	261	GLN
1	A	267	GLU
1	A	284	LEU
1	A	300	VAL
1	A	303	GLU
1	A	306	GLU
1	A	307	SER
1	A	310	SER
1	A	312	VAL
1	A	319	ARG
1	A	323	ILE
1	A	332	SER
1	B	1	SER
1	B	56	THR
1	B	57	ARG
1	B	72	ARG
1	B	81	SER
1	B	94	ARG
1	B	110	GLN
1	B	111	GLU
1	B	113	VAL

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Mol	Chain	Res	Type
1	B	114	GLU
1	B	130	ASN
1	B	137	LEU
1	B	143	THR
1	B	155	GLU
1	B	158	LEU
1	B	165	ARG
1	B	166	ASN
1	B	183	LEU
1	B	194	GLU
1	B	197	LEU
1	B	213	THR
1	B	220	LYS
1	B	226	ASP
1	B	249	LEU
1	B	258	LYS
1	B	261	GLN
1	B	267	GLU
1	B	283	THR
1	B	284	LEU
1	B	300	VAL
1	B	303	GLU
1	B	306	GLU
1	B	307	SER
1	B	310	SER
1	B	312	VAL
1	B	319	ARG
1	B	323	ILE
1	C	56	THR
1	C	57	ARG
1	C	72	ARG
1	C	81	SER
1	C	94	ARG
1	C	110	GLN
1	C	111	GLU
1	C	113	VAL
1	C	114	GLU
1	C	121	SER
1	C	130	ASN
1	C	137	LEU
1	C	143	THR
1	C	155	GLU

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Mol	Chain	Res	Type
1	C	158	LEU
1	C	165	ARG
1	C	166	ASN
1	C	183	LEU
1	C	194	GLU
1	C	197	LEU
1	C	213	THR
1	C	215	THR
1	C	217	ASP
1	C	220	LYS
1	C	226	ASP
1	C	249	LEU
1	C	258	LYS
1	C	261	GLN
1	C	266	PRO
1	C	267	GLU
1	C	268	VAL
1	C	283	THR
1	C	291	GLU
1	C	300	VAL
1	C	303	GLU
1	C	306	GLU
1	C	307	SER
1	C	310	SER
1	C	312	VAL
1	C	319	ARG
1	C	323	ILE
1	C	332	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	HIS
1	A	46	ASN
1	A	69	GLN
1	A	85	HIS
1	A	110	GLN
1	A	126	ASN
1	A	130	ASN
1	A	133	HIS
1	A	166	ASN
1	A	295	HIS

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Mol	Chain	Res	Type
1	A	321	HIS
1	B	7	HIS
1	B	46	ASN
1	B	69	GLN
1	B	85	HIS
1	B	110	GLN
1	B	126	ASN
1	B	130	ASN
1	B	166	ASN
1	B	321	HIS
1	C	7	HIS
1	C	46	ASN
1	C	69	GLN
1	C	85	HIS
1	C	110	GLN
1	C	126	ASN
1	C	130	ASN
1	C	133	HIS
1	C	321	HIS

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 [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	322/333 (96%)	-0.09	4 (1%) 76 68	2, 36, 67, 106	0
1	B	322/333 (96%)	-0.46	2 (0%) 85 80	2, 19, 47, 81	0
1	C	322/333 (96%)	-0.31	2 (0%) 85 80	3, 27, 58, 93	0
All	All	966/999 (96%)	-0.29	8 (0%) 82 75	2, 26, 61, 106	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	79	SER	4.4
1	C	56	THR	4.3
1	A	56	THR	4.1
1	B	56	THR	3.5
1	A	248	ALA	3.2
1	A	79	SER	2.4
1	C	80	GLY	2.2
1	A	257	SER	2.1

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.