



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 09:36 PM UTC

PDB ID : 1LL6 / pdb_00001ll6
Title : STRUCTURE OF THE D169N MUTANT OF C. IMMITIS CHITINASE 1
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Deposited on : 2002-04-26
Resolution : 2.80 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
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

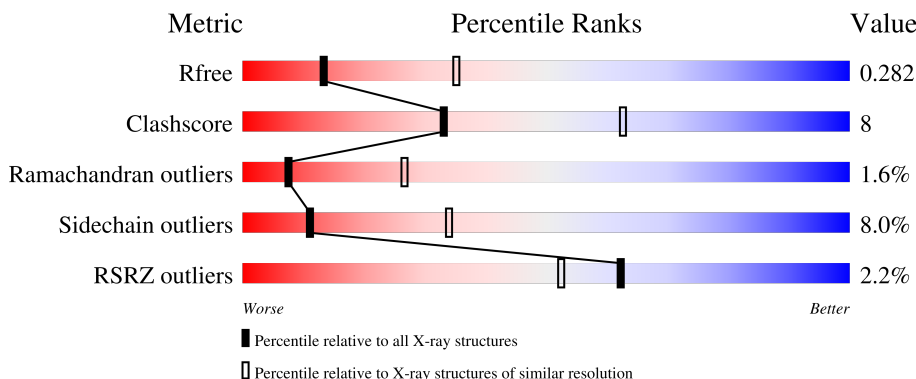
1 Overall quality at a glance

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))
R_{free}	180053	3866 (2.80-2.80)
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	392	2% 65% 30% • •
1	B	392	2% 67% 27% 5% •
1	C	392	• 65% 31% • •
1	D	392	4% 65% 31% • •

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 12375 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 CHITINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3083	1963	511	597	12			
1	B	392	Total	C	N	O	S	0	0	0
			3083	1963	511	597	12			
1	C	392	Total	C	N	O	S	0	0	0
			3083	1963	511	597	12			
1	D	392	Total	C	N	O	S	0	0	0
			3083	1963	511	597	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	169	ASN	ASP	engineered mutation	UNP P54196
B	169	ASN	ASP	engineered mutation	UNP P54196
C	169	ASN	ASP	engineered mutation	UNP P54196
D	169	ASN	ASP	engineered mutation	UNP P54196

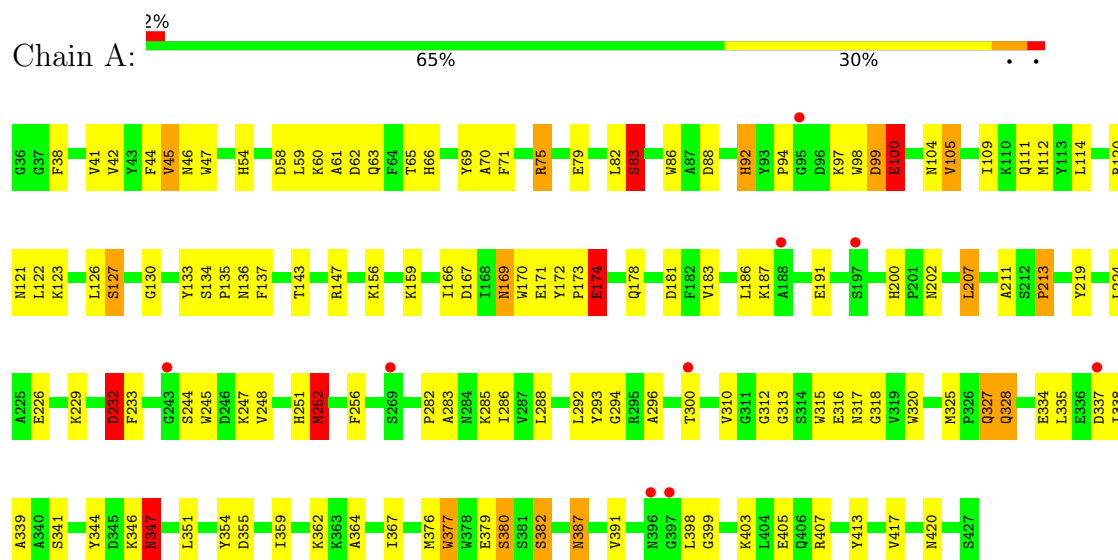
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	12	Total	O	0	0
			12	12		
2	B	12	Total	O	0	0
			12	12		
2	C	7	Total	O	0	0
			7	7		
2	D	12	Total	O	0	0
			12	12		

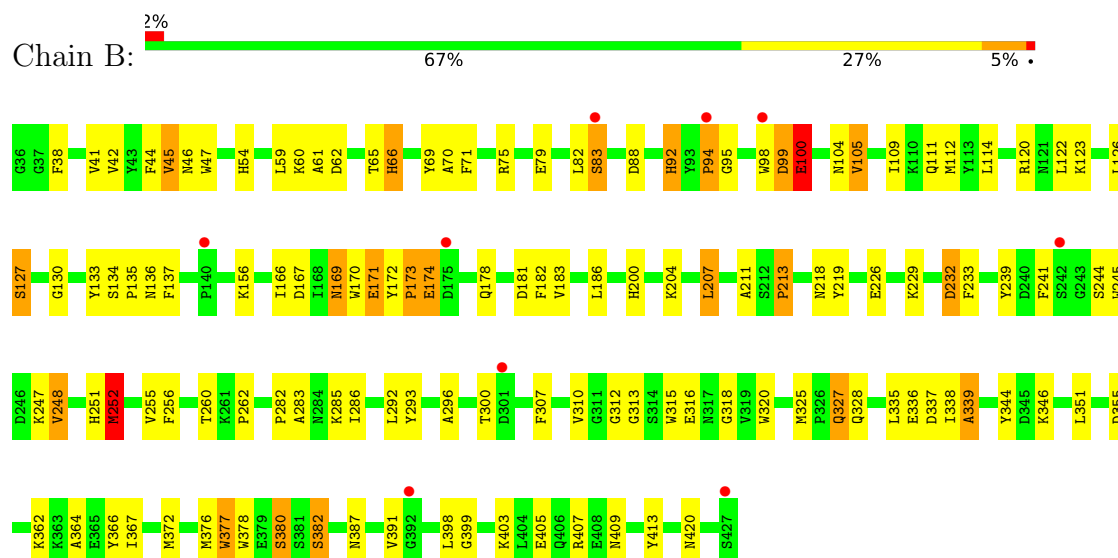
3 Residue-property plots

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: CHITINASE 1

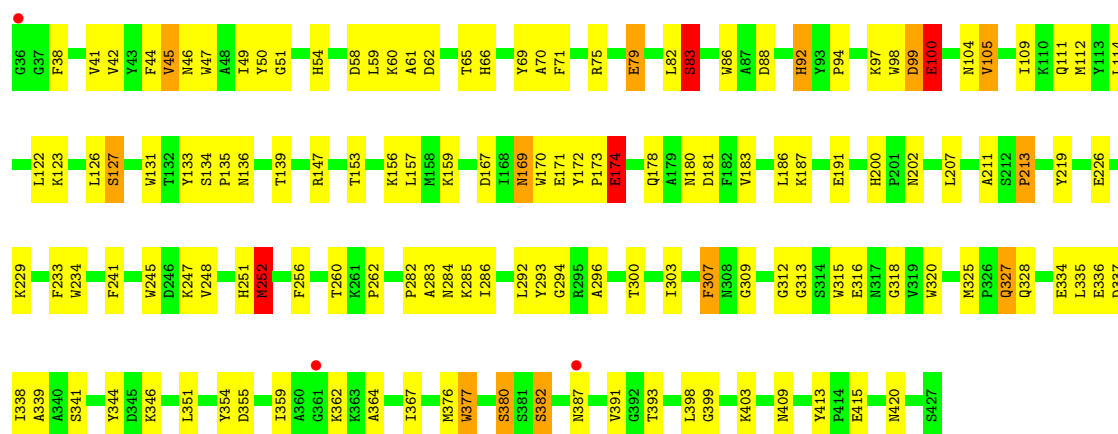


• Molecule 1: CHITINASE 1

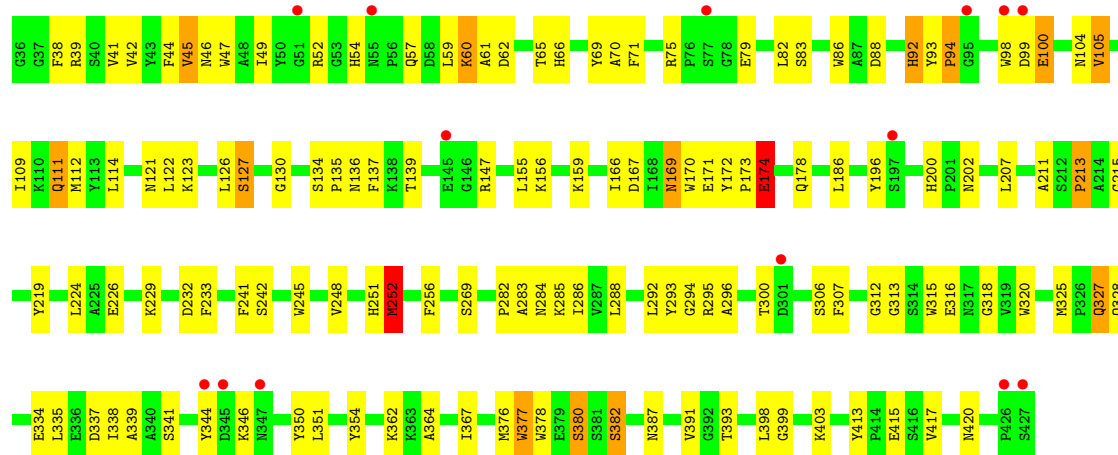


• Molecule 1: CHITINASE 1





● Molecule 1: CHITINASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.89Å 78.18Å 88.43Å 80.51° 82.13° 66.99°	Depositor
Resolution (Å)	5.00 – 2.80 5.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.80) 73.1 (5.00-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 2.79Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.182 , 0.256 0.238 , 0.282	Depositor DCC
R_{free} test set	1609 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.70 , 104.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	12375	wwPDB-VP
Average B, all atoms (Å ²)	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.08% 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	0.96	7/3165 (0.2%)	1.75	65/4282 (1.5%)
1	B	0.96	6/3165 (0.2%)	1.75	61/4282 (1.4%)
1	C	0.98	8/3165 (0.3%)	1.76	61/4282 (1.4%)
1	D	0.98	7/3165 (0.2%)	1.75	59/4282 (1.4%)
All	All	0.97	28/12660 (0.2%)	1.75	246/17128 (1.4%)

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	D	0	1

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	251	HIS	CD2-NE2	-7.81	1.29	1.37
1	B	200	HIS	CD2-NE2	-7.59	1.29	1.37
1	B	92	HIS	CD2-NE2	-7.25	1.29	1.37
1	A	251	HIS	CD2-NE2	-7.19	1.29	1.37
1	C	66	HIS	CD2-NE2	-7.16	1.29	1.37
1	C	251	HIS	CD2-NE2	-7.10	1.30	1.37
1	A	200	HIS	CD2-NE2	-6.91	1.30	1.37
1	D	66	HIS	CD2-NE2	-6.84	1.30	1.37
1	B	251	HIS	CD2-NE2	-6.77	1.30	1.37
1	A	54	HIS	CD2-NE2	-6.76	1.30	1.37
1	B	54	HIS	CD2-NE2	-6.75	1.30	1.37
1	A	92	HIS	CD2-NE2	-6.60	1.30	1.37
1	D	54	HIS	CD2-NE2	-6.57	1.30	1.37
1	D	92	HIS	CD2-NE2	-6.42	1.30	1.37
1	D	200	HIS	CD2-NE2	-6.34	1.30	1.37
1	C	200	HIS	CD2-NE2	-6.25	1.30	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	66	HIS	CD2-NE2	-5.78	1.31	1.37
1	C	303	ILE	CA-CB	5.61	1.60	1.54
1	C	54	HIS	CD2-NE2	-5.60	1.31	1.37
1	A	200	HIS	CG-ND1	-5.57	1.32	1.38
1	C	92	HIS	CD2-NE2	-5.53	1.31	1.37
1	B	166	ILE	CA-CB	5.48	1.62	1.54
1	A	66	HIS	CD2-NE2	-5.44	1.31	1.37
1	D	251	HIS	CG-ND1	-5.41	1.32	1.38
1	C	251	HIS	CG-ND1	-5.36	1.32	1.38
1	D	166	ILE	CA-CB	5.23	1.62	1.54
1	C	200	HIS	CG-ND1	-5.17	1.32	1.38
1	A	166	ILE	CA-CB	5.12	1.62	1.54

All (246) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	202	ASN	CA-CB-CG	9.03	121.63	112.60
1	D	92	HIS	CB-CG-CD2	-8.99	119.52	131.20
1	D	104	ASN	N-CA-C	8.62	123.66	109.95
1	B	169	ASN	OD1-CG-ND2	-8.59	114.01	122.60
1	B	92	HIS	CB-CG-CD2	-8.54	120.10	131.20
1	D	45	VAL	N-CA-CB	-8.39	100.99	111.31
1	C	327	GLN	OE1-CD-NE2	-8.32	114.28	122.60
1	A	92	HIS	CB-CG-CD2	-8.30	120.41	131.20
1	C	92	HIS	CB-CG-CD2	-8.30	120.41	131.20
1	A	328	GLN	OE1-CD-NE2	-8.28	114.32	122.60
1	A	105	VAL	CB-CA-C	-8.28	99.31	110.98
1	B	104	ASN	N-CA-C	8.25	122.91	109.72
1	C	45	VAL	N-CA-CB	-8.17	101.26	111.31
1	D	327	GLN	OE1-CD-NE2	-8.17	114.43	122.60
1	A	104	ASN	N-CA-C	8.16	122.92	109.95
1	C	104	ASN	N-CA-C	8.05	122.75	109.95
1	B	252	MET	CG-SD-CE	-7.98	83.34	100.90
1	B	45	VAL	N-CA-CB	-7.96	101.52	111.31
1	D	105	VAL	CB-CA-C	-7.94	99.78	110.98
1	C	105	VAL	CB-CA-C	-7.92	99.81	110.98
1	C	169	ASN	OD1-CG-ND2	-7.91	114.69	122.60
1	B	233	PHE	CA-CB-CG	7.83	121.62	113.80
1	D	202	ASN	CA-CB-CG	7.74	120.34	112.60
1	A	45	VAL	N-CA-CB	-7.57	102.00	111.31
1	D	328	GLN	OE1-CD-NE2	-7.55	115.05	122.60
1	D	233	PHE	CA-CB-CG	7.54	121.34	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	233	PHE	CA-CB-CG	7.51	121.31	113.80
1	C	44	PHE	N-CA-C	-7.36	96.53	108.52
1	D	83	SER	N-CA-C	7.30	121.83	112.34
1	A	46	ASN	CA-CB-CG	7.19	119.79	112.60
1	D	420	ASN	CA-CB-CG	7.12	119.72	112.60
1	D	44	PHE	N-CA-C	-7.11	96.93	108.52
1	B	105	VAL	CB-CA-C	-6.97	101.15	110.98
1	B	46	ASN	CA-CB-CG	6.95	119.55	112.60
1	A	347	ASN	CB-CG-ND2	6.91	126.76	116.40
1	C	46	ASN	CA-CB-CG	6.85	119.45	112.60
1	A	44	PHE	N-CA-C	-6.79	97.44	108.52
1	B	44	PHE	N-CA-C	-6.76	97.49	108.52
1	A	181	ASP	CA-CB-CG	6.72	119.32	112.60
1	C	213	PRO	N-CA-C	6.72	121.04	110.50
1	D	62	ASP	CA-CB-CG	6.72	119.32	112.60
1	D	169	ASN	OD1-CG-ND2	-6.71	115.89	122.60
1	C	183	VAL	N-CA-C	-6.67	104.26	110.53
1	C	420	ASN	CA-CB-CG	6.67	119.27	112.60
1	C	181	ASP	CA-CB-CG	6.66	119.26	112.60
1	A	54	HIS	CB-CG-CD2	-6.59	122.64	131.20
1	C	54	HIS	CB-CG-CD2	-6.57	122.65	131.20
1	A	202	ASN	CA-CB-CG	6.56	119.16	112.60
1	D	92	HIS	CB-CG-ND1	6.55	132.53	122.70
1	B	100	GLU	N-CA-C	6.49	124.14	109.81
1	B	54	HIS	CB-CG-CD2	-6.47	122.78	131.20
1	C	252	MET	CG-SD-CE	-6.47	86.66	100.90
1	B	88	ASP	N-CA-C	6.46	118.02	110.97
1	D	45	VAL	CB-CA-C	6.46	119.45	111.25
1	C	66	HIS	CB-CG-CD2	-6.45	122.82	131.20
1	D	213	PRO	N-CA-C	6.43	120.76	110.21
1	D	46	ASN	CA-CB-CG	6.43	119.03	112.60
1	B	420	ASN	CA-CB-CG	6.43	119.03	112.60
1	C	45	VAL	CB-CA-C	6.42	119.40	111.25
1	B	62	ASP	CA-CB-CG	6.40	119.00	112.60
1	A	171	GLU	CA-CB-CG	6.38	126.85	114.10
1	A	66	HIS	CB-CG-CD2	-6.36	122.94	131.20
1	C	92	HIS	CB-CG-ND1	6.36	132.24	122.70
1	C	75	ARG	NE-CZ-NH2	6.34	124.91	119.20
1	C	62	ASP	CA-CB-CG	6.33	118.93	112.60
1	B	171	GLU	CA-CB-CG	6.32	126.74	114.10
1	D	252	MET	CG-SD-CE	-6.31	87.01	100.90
1	A	82	LEU	N-CA-C	6.31	118.24	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	HIS	CB-CG-ND1	6.30	132.15	122.70
1	C	100	GLU	N-CA-C	6.30	123.74	109.81
1	A	251	HIS	CB-CG-CD2	-6.28	123.04	131.20
1	B	247	LYS	CA-CB-CG	-6.23	101.64	114.10
1	A	169	ASN	OD1-CG-ND2	-6.23	116.37	122.60
1	B	66	HIS	CB-CG-CD2	-6.22	123.11	131.20
1	B	241	PHE	N-CA-C	-6.20	104.41	112.23
1	D	130	GLY	CA-C-O	-6.19	117.63	122.52
1	A	355	ASP	CA-CB-CG	6.17	118.77	112.60
1	D	66	HIS	CB-CG-CD2	-6.16	123.19	131.20
1	A	213	PRO	N-CA-C	6.16	120.31	110.21
1	A	45	VAL	CB-CA-C	6.14	119.05	111.25
1	D	54	HIS	CB-CG-ND1	6.14	131.90	122.70
1	A	88	ASP	N-CA-C	6.13	117.65	110.97
1	A	347	ASN	OD1-CG-ND2	-6.12	116.48	122.60
1	D	171	GLU	CA-CB-CG	6.11	126.31	114.10
1	B	377	TRP	CE2-CD2-CG	-6.10	99.88	107.20
1	B	54	HIS	CB-CG-ND1	6.09	131.84	122.70
1	B	245	TRP	CG-CD2-CE3	6.08	139.98	133.90
1	A	420	ASN	CA-CB-CG	6.07	118.67	112.60
1	B	213	PRO	N-CA-C	6.04	120.12	110.21
1	C	171	GLU	CA-CB-CG	6.04	126.18	114.10
1	C	245	TRP	CG-CD2-CE3	6.04	139.94	133.90
1	A	100	GLU	N-CA-C	6.00	123.08	109.81
1	B	328	GLN	OE1-CD-NE2	-5.99	116.61	122.60
1	B	413	TYR	CA-C-N	5.98	125.69	119.05
1	B	413	TYR	C-N-CA	5.98	125.69	119.05
1	A	136	ASN	N-CA-C	5.98	118.14	109.71
1	A	413	TYR	CA-C-N	5.97	125.68	119.05
1	A	413	TYR	C-N-CA	5.97	125.68	119.05
1	D	169	ASN	CB-CG-ND2	5.96	125.33	116.40
1	D	54	HIS	CB-CG-CD2	-5.95	123.46	131.20
1	A	245	TRP	CG-CD2-CE3	5.93	139.83	133.90
1	A	315	TRP	CE2-CD2-CG	-5.92	100.09	107.20
1	A	380	SER	N-CA-C	5.92	123.41	110.80
1	B	251	HIS	CB-CG-CD2	-5.91	123.52	131.20
1	D	136	ASN	N-CA-C	5.90	118.03	109.71
1	C	413	TYR	CA-C-N	5.89	125.59	119.05
1	C	413	TYR	C-N-CA	5.89	125.59	119.05
1	D	380	SER	N-CA-C	5.88	123.33	110.80
1	A	233	PHE	CA-CB-CG	5.87	119.67	113.80
1	B	130	GLY	CA-C-O	-5.86	117.89	122.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	45	VAL	CB-CA-C	5.85	118.68	111.25
1	A	130	GLY	CA-C-O	-5.84	118.20	122.23
1	A	174	GLU	N-CA-C	5.84	123.24	110.80
1	C	88	ASP	N-CA-C	5.84	117.33	110.97
1	C	247	LYS	CA-CB-CG	-5.83	102.44	114.10
1	A	147	ARG	CB-CG-CD	-5.82	97.91	111.30
1	B	82	LEU	N-CA-C	5.82	117.68	108.67
1	C	54	HIS	CA-CB-CG	5.81	119.61	113.80
1	A	54	HIS	CB-CG-ND1	5.80	131.40	122.70
1	B	83	SER	N-CA-C	5.78	123.12	110.80
1	D	82	LEU	N-CA-C	5.78	117.63	108.67
1	B	380	SER	N-CA-C	5.77	123.10	110.80
1	B	47	TRP	CE2-CD2-CG	-5.77	100.28	107.20
1	D	100	GLU	N-CA-C	5.77	122.56	109.81
1	C	54	HIS	CB-CG-ND1	5.76	131.34	122.70
1	B	38	PHE	N-CA-C	5.75	118.99	110.48
1	B	181	ASP	CA-CB-CG	5.75	118.35	112.60
1	D	75	ARG	CA-C-N	5.72	125.57	119.28
1	D	75	ARG	C-N-CA	5.72	125.57	119.28
1	C	38	PHE	N-CA-C	5.71	119.22	110.20
1	D	88	ASP	N-CA-C	5.71	117.19	110.97
1	B	174	GLU	N-CA-C	5.70	122.94	110.80
1	B	245	TRP	CB-CG-CD1	-5.70	118.35	126.90
1	B	183	VAL	N-CA-C	-5.67	105.19	110.53
1	D	137	PHE	N-CA-C	-5.67	104.52	112.12
1	A	377	TRP	CE2-CD2-CG	-5.66	100.41	107.20
1	C	377	TRP	CE2-CD2-CG	-5.66	100.41	107.20
1	D	121	ASN	OD1-CG-ND2	-5.65	116.95	122.60
1	D	251	HIS	CB-CG-CD2	-5.65	123.86	131.20
1	D	174	GLU	N-CA-C	5.64	122.81	110.80
1	B	66	HIS	CB-CG-ND1	5.63	131.15	122.70
1	A	252	MET	CG-SD-CE	-5.63	88.52	100.90
1	A	327	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	D	170	TRP	CG-CD2-CE3	5.61	139.51	133.90
1	C	58	ASP	CA-CB-CG	5.60	118.20	112.60
1	D	105	VAL	N-CA-CB	5.58	119.79	110.86
1	D	413	TYR	CA-C-N	5.58	125.25	119.05
1	D	413	TYR	C-N-CA	5.58	125.25	119.05
1	A	54	HIS	CA-CB-CG	5.58	119.38	113.80
1	C	241	PHE	N-CA-C	-5.57	105.21	112.23
1	D	224	LEU	N-CA-C	5.56	117.80	111.02
1	A	38	PHE	N-CA-C	5.55	118.97	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	307	PHE	N-CA-C	-5.54	100.87	109.24
1	C	170	TRP	CG-CD2-CE3	5.53	139.43	133.90
1	C	174	GLU	N-CA-C	5.53	122.59	110.80
1	B	136	ASN	N-CA-C	5.51	117.47	109.71
1	B	170	TRP	CG-CD2-CE3	5.51	139.41	133.90
1	B	54	HIS	CA-CB-CG	5.50	119.30	113.80
1	A	83	SER	N-CA-C	5.50	122.51	110.80
1	A	183	VAL	N-CA-C	-5.48	105.38	110.53
1	C	169	ASN	CB-CG-ND2	5.48	124.62	116.40
1	B	245	TRP	CE2-CD2-CG	-5.45	100.66	107.20
1	B	315	TRP	CE2-CD2-CG	-5.42	100.69	107.20
1	A	105	VAL	N-CA-CB	5.42	119.53	110.86
1	B	307	PHE	N-CA-C	-5.42	101.06	109.24
1	C	380	SER	N-CA-C	5.42	122.33	110.80
1	A	58	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	245	TRP	CE2-CD2-CG	-5.40	100.72	107.20
1	D	38	PHE	N-CA-C	5.39	118.72	110.20
1	C	355	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	83	SER	N-CA-C	5.38	122.26	110.80
1	B	44	PHE	CA-C-O	5.37	126.23	120.32
1	B	327	GLN	OE1-CD-NE2	-5.37	117.23	122.60
1	C	336	GLU	N-CA-C	5.36	117.82	111.33
1	D	377	TRP	CE2-CD2-CG	-5.36	100.77	107.20
1	A	170	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	A	66	HIS	CB-CG-ND1	5.34	130.71	122.70
1	B	137	PHE	N-CA-C	-5.34	105.89	112.72
1	A	224	LEU	N-CA-C	5.33	117.52	111.02
1	A	247	LYS	CA-CB-CG	-5.33	103.44	114.10
1	A	317	ASN	OD1-CG-ND2	-5.33	117.27	122.60
1	B	248	VAL	N-CA-CB	-5.32	102.13	111.39
1	D	54	HIS	CA-CB-CG	5.32	119.12	113.80
1	D	62	ASP	N-CA-C	5.32	118.87	112.38
1	D	320	TRP	CE2-CD2-CG	-5.32	100.81	107.20
1	B	62	ASP	N-CA-C	5.32	118.87	112.38
1	A	328	GLN	CG-CD-NE2	5.31	124.36	116.40
1	A	245	TRP	CB-CG-CD1	-5.30	118.94	126.90
1	D	111	GLN	OE1-CD-NE2	-5.30	117.30	122.60
1	D	147	ARG	CB-CG-CD	-5.29	99.12	111.30
1	B	120	ARG	N-CA-C	5.29	119.22	112.87
1	D	378	TRP	CE2-CD2-CG	-5.28	100.86	107.20
1	A	75	ARG	CA-C-N	5.28	125.59	119.47
1	A	75	ARG	C-N-CA	5.28	125.59	119.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	251	HIS	CB-CG-CD2	-5.28	124.34	131.20
1	C	328	GLN	OE1-CD-NE2	-5.28	117.33	122.60
1	B	218	ASN	OD1-CG-ND2	-5.27	117.33	122.60
1	C	315	TRP	CG-CD2-CE3	5.26	139.16	133.90
1	D	241	PHE	N-CA-C	-5.26	105.60	112.23
1	A	121	ASN	OD1-CG-ND2	-5.25	117.35	122.60
1	C	147	ARG	CB-CG-CD	-5.25	99.23	111.30
1	C	131	TRP	CE2-CD2-CG	-5.25	100.90	107.20
1	D	215	GLY	CA-C-N	5.22	124.67	119.24
1	D	215	GLY	C-N-CA	5.22	124.67	119.24
1	D	315	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	C	307	PHE	N-CA-C	-5.20	101.39	109.24
1	A	120	ARG	N-CA-C	5.19	119.10	112.87
1	B	336	GLU	N-CA-C	5.19	117.61	111.33
1	C	82	LEU	N-CA-C	5.19	116.71	108.67
1	C	66	HIS	CB-CG-ND1	5.16	130.44	122.70
1	C	245	TRP	CE2-CD2-CG	-5.16	101.01	107.20
1	A	86	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	C	75	ARG	CA-C-N	5.15	125.44	119.47
1	C	75	ARG	C-N-CA	5.15	125.44	119.47
1	A	137	PHE	N-CA-C	-5.15	105.22	112.12
1	B	320	TRP	CE2-CD2-CG	-5.14	101.03	107.20
1	C	284	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	B	409	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	D	245	TRP	CG-CD2-CE3	5.13	139.03	133.90
1	A	379	GLU	CA-CB-CG	5.12	124.35	114.10
1	B	204	LYS	CA-CB-CG	-5.11	103.87	114.10
1	C	136	ASN	N-CA-C	5.11	117.09	110.65
1	A	47	TRP	CE2-CD2-CG	-5.11	101.07	107.20
1	A	232	ASP	CA-CB-CG	-5.11	107.49	112.60
1	B	377	TRP	CD1-CG-CD2	5.11	114.48	106.30
1	C	234	TRP	CE2-CD2-CG	-5.10	101.08	107.20
1	D	245	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	A	320	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	B	75	ARG	NE-CZ-NH2	5.09	123.78	119.20
1	A	159	LYS	CA-CB-CG	5.08	124.26	114.10
1	A	63	GLN	OE1-CD-NE2	-5.08	117.52	122.60
1	B	315	TRP	CG-CD2-CE3	5.07	138.97	133.90
1	D	378	TRP	CG-CD2-CE3	5.06	138.96	133.90
1	D	86	TRP	CE2-CD2-CG	-5.06	101.13	107.20
1	C	47	TRP	CE2-CD2-CG	-5.05	101.14	107.20
1	D	269	SER	CA-CB-OG	5.05	121.20	111.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	ASP	CA-CB-CG	5.04	117.64	112.60
1	D	47	TRP	CE2-CD2-CG	-5.04	101.15	107.20
1	C	409	ASN	CA-CB-CG	5.04	117.64	112.60
1	C	86	TRP	CE2-CD2-CG	-5.03	101.17	107.20
1	B	378	TRP	CG-CD2-CE3	5.02	138.92	133.90
1	C	62	ASP	N-CA-C	5.02	118.50	112.38
1	C	105	VAL	N-CA-CB	5.02	118.89	110.86
1	A	387	ASN	OD1-CG-ND2	-5.01	117.59	122.60
1	C	245	TRP	CB-CG-CD1	-5.01	119.38	126.90
1	B	355	ASP	CA-CB-CG	5.01	117.61	112.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	350	TYR	Sidechain

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	3083	0	2963	49	0
1	B	3083	0	2963	51	0
1	C	3083	0	2963	54	0
1	D	3083	0	2963	46	0
2	A	12	0	0	1	0
2	B	12	0	0	0	0
2	C	7	0	0	1	0
2	D	12	0	0	0	0
All	All	12375	0	11852	188	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 8.

All (188) 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:B:95:GLY:H	1:C:51:GLY:HA2	1.33	0.92
1:A:69:TYR:HB2	1:A:112:MET:HE1	1.64	0.80
1:A:347:ASN:HA	1:D:94:PRO:HG2	1.63	0.80
1:C:69:TYR:HB2	1:C:112:MET:HE1	1.70	0.74
1:D:69:TYR:HB2	1:D:112:MET:HE1	1.74	0.69
1:D:282:PRO:HG2	1:D:285:LYS:HD3	1.75	0.68
1:A:325:MET:HE1	1:A:327:GLN:HE21	1.58	0.68
1:C:325:MET:HE1	1:C:327:GLN:HE21	1.59	0.67
1:D:169:ASN:ND2	1:D:211:ALA:HB3	2.09	0.67
1:A:282:PRO:HG2	1:A:285:LYS:HD3	1.75	0.66
1:B:69:TYR:HB2	1:B:112:MET:HE1	1.76	0.66
1:A:169:ASN:ND2	1:A:211:ALA:HB3	2.10	0.66
1:A:328:GLN:HE21	1:D:60:LYS:N	1.94	0.65
1:C:282:PRO:HG2	1:C:285:LYS:HD3	1.78	0.64
1:B:325:MET:HE1	1:B:327:GLN:HE21	1.62	0.64
1:B:282:PRO:HG2	1:B:285:LYS:HD3	1.80	0.63
1:C:169:ASN:ND2	1:C:211:ALA:HB3	2.14	0.62
1:B:95:GLY:HA2	1:C:51:GLY:O	1.99	0.62
1:A:75:ARG:NH2	1:B:244:SER:O	2.34	0.61
1:B:95:GLY:N	1:C:51:GLY:HA2	2.11	0.61
1:A:325:MET:HE1	1:A:327:GLN:NE2	2.15	0.60
1:D:42:VAL:HG23	1:D:377:TRP:HB2	1.84	0.59
1:B:325:MET:HE1	1:B:327:GLN:NE2	2.17	0.59
1:A:172:TYR:CE2	1:A:213:PRO:HB3	2.39	0.58
1:B:169:ASN:ND2	1:B:211:ALA:HB3	2.18	0.58
1:B:42:VAL:HG23	1:B:377:TRP:HB2	1.86	0.57
1:C:172:TYR:CE2	1:C:213:PRO:HB3	2.40	0.57
1:C:325:MET:HE1	1:C:327:GLN:NE2	2.18	0.57
1:C:226:GLU:HA	1:C:229:LYS:HZ2	1.69	0.57
1:D:69:TYR:CD1	1:D:112:MET:SD	2.98	0.56
1:D:283:ALA:HA	1:D:286:ILE:HD12	1.87	0.56
1:A:42:VAL:HG23	1:A:377:TRP:HB2	1.87	0.56
1:A:92:HIS:NE2	1:A:98:TRP:HA	2.20	0.56
1:C:252:MET:HE1	1:C:293:TYR:CE2	2.41	0.56
1:D:325:MET:HE1	1:D:327:GLN:HE21	1.71	0.56
1:C:83:SER:HG	1:C:133:TYR:HE1	1.52	0.55
1:D:172:TYR:CE2	1:D:213:PRO:HB3	2.42	0.55
1:C:256:PHE:HB2	1:C:338:ILE:HA	1.88	0.55
1:C:313:GLY:HA3	1:C:316:GLU:O	2.07	0.55
1:B:292:LEU:O	1:B:382:SER:HB2	2.07	0.55
1:B:174:GLU:HG2	1:B:178:GLN:CD	2.32	0.54
1:A:111:GLN:HA	1:A:114:LEU:HD12	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLY:HA3	1:A:316:GLU:O	2.08	0.54
1:B:226:GLU:HA	1:B:229:LYS:HZ2	1.73	0.54
1:A:347:ASN:OD1	1:D:93:TYR:HD2	1.90	0.54
1:D:292:LEU:O	1:D:382:SER:HB2	2.08	0.54
1:B:172:TYR:CE2	1:B:213:PRO:HB3	2.43	0.54
1:A:256:PHE:HB2	1:A:338:ILE:HA	1.89	0.53
1:B:95:GLY:CA	1:C:51:GLY:O	2.56	0.53
1:D:70:ALA:HB1	1:D:71:PHE:CD2	2.43	0.53
1:D:226:GLU:HA	1:D:229:LYS:HZ2	1.73	0.53
1:C:42:VAL:HG23	1:C:377:TRP:HB2	1.89	0.53
1:A:226:GLU:HA	1:A:229:LYS:HZ2	1.72	0.53
1:D:252:MET:HE1	1:D:293:TYR:CE2	2.44	0.53
1:A:174:GLU:HG2	1:A:178:GLN:NE2	2.23	0.53
1:A:328:GLN:HE21	1:D:60:LYS:H	1.56	0.52
1:B:283:ALA:HA	1:B:286:ILE:HD12	1.92	0.52
1:D:174:GLU:HG2	1:D:178:GLN:CD	2.34	0.52
1:C:283:ALA:HA	1:C:286:ILE:HD12	1.90	0.52
1:B:256:PHE:HB2	1:B:338:ILE:HA	1.89	0.52
1:C:92:HIS:NE2	1:C:98:TRP:HA	2.25	0.52
1:A:69:TYR:CD1	1:A:112:MET:SD	3.03	0.52
1:C:292:LEU:O	1:C:382:SER:HB2	2.09	0.52
1:A:174:GLU:HG2	1:A:178:GLN:CD	2.35	0.52
1:A:292:LEU:O	1:A:382:SER:HB2	2.10	0.52
1:B:313:GLY:HA3	1:B:316:GLU:O	2.10	0.52
1:A:283:ALA:HA	1:A:286:ILE:HD12	1.91	0.51
1:C:111:GLN:HA	1:C:114:LEU:HD12	1.91	0.51
1:D:92:HIS:NE2	1:D:98:TRP:HA	2.25	0.51
1:A:83:SER:HG	1:A:133:TYR:HE1	1.58	0.51
1:B:174:GLU:HG2	1:B:178:GLN:NE2	2.26	0.51
1:D:111:GLN:HA	1:D:114:LEU:HD12	1.92	0.51
1:B:377:TRP:CE2	1:B:391:VAL:HG22	2.46	0.51
1:D:325:MET:HE1	1:D:327:GLN:NE2	2.26	0.51
1:B:70:ALA:HB1	1:B:71:PHE:CD2	2.46	0.51
1:D:213:PRO:O	1:D:219:TYR:HD1	1.94	0.51
1:D:256:PHE:HB2	1:D:338:ILE:HA	1.92	0.51
1:D:313:GLY:HA3	1:D:316:GLU:O	2.11	0.51
1:D:296:ALA:HA	1:D:351:LEU:O	2.11	0.50
1:A:65:THR:O	1:A:123:LYS:HE3	2.11	0.50
1:A:377:TRP:CE2	1:A:391:VAL:HG22	2.45	0.50
1:C:377:TRP:CE2	1:C:391:VAL:HG22	2.46	0.50
1:A:213:PRO:O	1:A:219:TYR:HD1	1.95	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:65:THR:O	1:B:123:LYS:HE3	2.12	0.49
1:C:174:GLU:HG2	1:C:178:GLN:CD	2.37	0.49
1:C:213:PRO:O	1:C:219:TYR:HD1	1.95	0.49
1:D:377:TRP:CE2	1:D:391:VAL:HG22	2.47	0.49
1:C:174:GLU:HG2	1:C:178:GLN:NE2	2.27	0.49
1:B:213:PRO:O	1:B:219:TYR:HD1	1.96	0.49
1:A:344:TYR:HE2	1:A:346:LYS:HD2	1.78	0.49
1:D:174:GLU:HG2	1:D:178:GLN:NE2	2.28	0.49
1:C:70:ALA:HB1	1:C:71:PHE:CD2	2.47	0.48
1:A:296:ALA:HA	1:A:351:LEU:O	2.13	0.48
1:B:69:TYR:CD1	1:B:112:MET:SD	3.06	0.48
1:A:134:SER:N	1:A:135:PRO:HD2	2.28	0.48
1:A:252:MET:HE1	1:A:293:TYR:CE2	2.48	0.48
1:A:41:VAL:O	1:A:376:MET:HA	2.13	0.48
1:B:92:HIS:NE2	1:B:98:TRP:HA	2.27	0.48
1:B:296:ALA:HA	1:B:351:LEU:O	2.13	0.48
1:C:296:ALA:HA	1:C:351:LEU:O	2.13	0.47
1:D:41:VAL:O	1:D:376:MET:HA	2.14	0.47
1:B:95:GLY:H	1:C:51:GLY:CA	2.15	0.47
1:C:312:GLY:O	1:C:318:GLY:N	2.47	0.47
1:C:344:TYR:HE2	1:C:346:LYS:HD2	1.80	0.47
1:B:41:VAL:O	1:B:376:MET:HA	2.15	0.47
1:C:97:LYS:HD3	1:C:100:GLU:HG3	1.97	0.47
1:A:328:GLN:NE2	2:A:434:HOH:O	2.47	0.47
1:C:399:GLY:O	1:C:403:LYS:HD3	2.14	0.47
1:A:70:ALA:HB1	1:A:71:PHE:CD2	2.48	0.47
1:A:207:LEU:HD12	1:A:232:ASP:OD2	2.14	0.47
1:A:399:GLY:O	1:A:403:LYS:HD3	2.15	0.47
1:B:134:SER:N	1:B:135:PRO:HD2	2.30	0.47
1:B:252:MET:HE1	1:B:293:TYR:CE2	2.50	0.47
1:B:344:TYR:HE2	1:B:346:LYS:HD2	1.79	0.47
1:C:70:ALA:HA	1:C:71:PHE:HA	1.66	0.46
1:C:127:SER:HA	1:C:167:ASP:O	2.15	0.46
1:C:341:SER:OG	1:C:359:ILE:HG13	2.15	0.46
1:B:94:PRO:HB3	1:C:50:TYR:C	2.40	0.46
1:B:61:ALA:HB1	1:B:122:LEU:HD22	1.97	0.46
1:A:312:GLY:O	1:A:318:GLY:N	2.49	0.46
1:C:41:VAL:O	1:C:376:MET:HA	2.16	0.45
1:B:364:ALA:O	1:B:367:ILE:HB	2.16	0.45
1:B:111:GLN:HA	1:B:114:LEU:HD12	1.96	0.45
1:B:399:GLY:O	1:B:403:LYS:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ALA:O	1:A:367:ILE:HB	2.16	0.45
1:A:127:SER:HA	1:A:167:ASP:O	2.17	0.45
1:A:97:LYS:HD3	1:A:100:GLU:HG3	2.00	0.44
1:B:244:SER:HB3	1:B:310:VAL:HG11	1.99	0.44
1:B:312:GLY:O	1:B:318:GLY:N	2.49	0.44
1:C:364:ALA:O	1:C:367:ILE:HB	2.16	0.44
1:C:65:THR:O	1:C:123:LYS:HE3	2.18	0.44
1:D:39:ARG:NH2	1:D:284:ASN:O	2.50	0.44
1:D:312:GLY:O	1:D:318:GLY:N	2.50	0.44
1:A:70:ALA:HA	1:A:71:PHE:HA	1.67	0.44
1:C:69:TYR:CD1	1:C:112:MET:SD	3.11	0.44
1:D:61:ALA:HB1	1:D:122:LEU:HD22	2.00	0.44
1:B:99:ASP:CG	1:B:100:GLU:H	2.26	0.43
1:B:83:SER:HG	1:B:133:TYR:HE1	1.63	0.43
1:C:187:LYS:O	1:C:191:GLU:HG3	2.17	0.43
1:D:242:SER:O	1:D:295:ARG:HD2	2.19	0.43
1:B:127:SER:HA	1:B:167:ASP:O	2.18	0.43
1:C:320:TRP:HB3	1:C:325:MET:HE3	2.00	0.43
1:A:61:ALA:HB1	1:A:122:LEU:HD22	2.00	0.43
1:B:260:THR:C	1:B:262:PRO:HD3	2.44	0.43
1:D:127:SER:HA	1:D:167:ASP:O	2.19	0.43
1:A:92:HIS:CD2	1:A:98:TRP:HA	2.54	0.42
1:B:174:GLU:HG2	1:B:178:GLN:OE1	2.19	0.42
1:C:159:LYS:HD3	1:C:415:GLU:HB2	2.00	0.42
1:D:159:LYS:HD3	1:D:415:GLU:HB2	2.00	0.42
1:D:226:GLU:HA	1:D:229:LYS:NZ	2.34	0.42
1:D:65:THR:O	1:D:123:LYS:HE3	2.19	0.42
1:C:61:ALA:HB1	1:C:122:LEU:HD22	2.01	0.42
1:A:334:GLU:HA	1:A:341:SER:HB3	2.01	0.42
1:A:341:SER:OG	1:A:359:ILE:HG13	2.19	0.42
1:B:41:VAL:HG22	1:B:66:HIS:HB2	2.02	0.42
1:C:92:HIS:CD2	1:C:98:TRP:HA	2.54	0.42
1:A:244:SER:HB3	1:A:310:VAL:HG11	2.02	0.42
1:D:344:TYR:HE2	1:D:346:LYS:HD2	1.84	0.42
1:B:255:VAL:CG2	1:B:339:ALA:HB3	2.50	0.42
1:B:366:TYR:CE2	1:B:372:MET:SD	3.13	0.42
1:D:92:HIS:CD2	1:D:98:TRP:HA	2.55	0.42
1:B:92:HIS:CD2	1:B:98:TRP:HA	2.55	0.42
1:D:399:GLY:O	1:D:403:LYS:HD3	2.19	0.42
1:C:153:THR:O	1:C:157:LEU:HB2	2.20	0.41
1:D:39:ARG:HH11	1:D:39:ARG:HD3	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:ASP:CG	1:A:100:GLU:H	2.28	0.41
1:C:226:GLU:HA	1:C:229:LYS:NZ	2.34	0.41
1:A:347:ASN:OD1	1:D:57:GLN:NE2	2.53	0.41
1:C:294:GLY:HA3	1:C:354:TYR:HB3	2.02	0.41
1:D:52:ARG:HH11	1:D:52:ARG:HG3	1.85	0.41
1:C:180:ASN:HB3	2:C:434:HOH:O	2.20	0.41
1:B:207:LEU:HD12	1:B:232:ASP:OD2	2.21	0.41
1:C:99:ASP:CG	1:C:100:GLU:H	2.29	0.41
1:D:134:SER:N	1:D:135:PRO:HD2	2.36	0.41
1:D:364:ALA:O	1:D:367:ILE:HB	2.20	0.41
1:A:294:GLY:HA3	1:A:354:TYR:HB3	2.03	0.41
1:B:171:GLU:HA	1:B:172:TYR:CD2	2.55	0.41
1:A:187:LYS:O	1:A:191:GLU:HG3	2.20	0.41
1:B:173:PRO:HG2	1:B:182:PHE:CD2	2.56	0.41
1:C:134:SER:N	1:C:135:PRO:HD2	2.36	0.41
1:C:260:THR:C	1:C:262:PRO:HD3	2.46	0.41
1:C:307:PHE:HD1	1:C:309:GLY:O	2.04	0.41
1:D:155:LEU:HD21	1:D:196:TYR:HB2	2.03	0.41
1:C:334:GLU:HA	1:C:341:SER:HB3	2.02	0.40
1:D:294:GLY:HA3	1:D:354:TYR:HB3	2.03	0.40
1:D:334:GLU:HA	1:D:341:SER:HB3	2.04	0.40
1:B:239:TYR:OH	1:B:376:MET:HE1	2.21	0.40
1:C:79:GLU:HG2	1:C:153:THR:HG21	2.04	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	390/392 (100%)	367 (94%)	16 (4%)	7 (2%)	6	23
1	B	390/392 (100%)	369 (95%)	16 (4%)	5 (1%)	9	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	390/392 (100%)	368 (94%)	15 (4%)	7 (2%)	6	23
1	D	390/392 (100%)	367 (94%)	17 (4%)	6 (2%)	8	28
All	All	1560/1568 (100%)	1471 (94%)	64 (4%)	25 (2%)	7	27

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	B	99	ASP
1	C	99	ASP
1	D	99	ASP
1	A	83	SER
1	A	380	SER
1	C	380	SER
1	D	380	SER
1	A	100	GLU
1	A	173	PRO
1	A	174	GLU
1	A	339	ALA
1	B	100	GLU
1	B	380	SER
1	C	100	GLU
1	D	100	GLU
1	D	339	ALA
1	B	173	PRO
1	B	339	ALA
1	C	83	SER
1	C	173	PRO
1	C	174	GLU
1	C	339	ALA
1	D	173	PRO
1	D	174	GLU

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	326/326 (100%)	298 (91%)	28 (9%)	10	31
1	B	326/326 (100%)	302 (93%)	24 (7%)	13	37
1	C	326/326 (100%)	302 (93%)	24 (7%)	13	37
1	D	326/326 (100%)	298 (91%)	28 (9%)	10	31
All	All	1304/1304 (100%)	1200 (92%)	104 (8%)	11	34

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

Mol	Chain	Res	Type
1	A	45	VAL
1	A	59	LEU
1	A	60	LYS
1	A	79	GLU
1	A	94	PRO
1	A	105	VAL
1	A	109	ILE
1	A	126	LEU
1	A	127	SER
1	A	143	THR
1	A	156	LYS
1	A	186	LEU
1	A	207	LEU
1	A	232	ASP
1	A	248	VAL
1	A	252	MET
1	A	288	LEU
1	A	300	THR
1	A	335	LEU
1	A	337	ASP
1	A	347	ASN
1	A	362	LYS
1	A	382	SER
1	A	387	ASN
1	A	398	LEU
1	A	405	GLU
1	A	407	ARG
1	A	417	VAL
1	B	45	VAL
1	B	59	LEU
1	B	60	LYS
1	B	79	GLU
1	B	94	PRO

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Mol	Chain	Res	Type
1	B	105	VAL
1	B	109	ILE
1	B	126	LEU
1	B	127	SER
1	B	156	LYS
1	B	186	LEU
1	B	207	LEU
1	B	232	ASP
1	B	248	VAL
1	B	252	MET
1	B	300	THR
1	B	335	LEU
1	B	337	ASP
1	B	362	LYS
1	B	382	SER
1	B	387	ASN
1	B	398	LEU
1	B	405	GLU
1	B	407	ARG
1	C	45	VAL
1	C	49	ILE
1	C	59	LEU
1	C	60	LYS
1	C	79	GLU
1	C	94	PRO
1	C	105	VAL
1	C	109	ILE
1	C	126	LEU
1	C	127	SER
1	C	139	THR
1	C	156	LYS
1	C	186	LEU
1	C	207	LEU
1	C	248	VAL
1	C	252	MET
1	C	300	THR
1	C	335	LEU
1	C	337	ASP
1	C	362	LYS
1	C	382	SER
1	C	387	ASN
1	C	393	THR

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Mol	Chain	Res	Type
1	C	398	LEU
1	D	45	VAL
1	D	49	ILE
1	D	59	LEU
1	D	60	LYS
1	D	79	GLU
1	D	94	PRO
1	D	105	VAL
1	D	109	ILE
1	D	126	LEU
1	D	127	SER
1	D	139	THR
1	D	156	LYS
1	D	186	LEU
1	D	207	LEU
1	D	232	ASP
1	D	248	VAL
1	D	252	MET
1	D	288	LEU
1	D	300	THR
1	D	306	SER
1	D	335	LEU
1	D	337	ASP
1	D	362	LYS
1	D	382	SER
1	D	387	ASN
1	D	393	THR
1	D	398	LEU
1	D	417	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	169	ASN
1	A	218	ASN
1	A	251	HIS
1	A	327	GLN
1	A	328	GLN
1	B	66	HIS
1	B	169	ASN
1	B	178	GLN

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Mol	Chain	Res	Type
1	B	218	ASN
1	B	251	HIS
1	B	327	GLN
1	C	66	HIS
1	C	169	ASN
1	C	218	ASN
1	C	251	HIS
1	C	327	GLN
1	D	66	HIS
1	D	169	ASN
1	D	218	ASN
1	D	251	HIS
1	D	327	GLN

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 ⓘ

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	392/392 (100%)	0.35	9 (2%) 61 51	3, 15, 23, 30	0
1	B	392/392 (100%)	0.37	9 (2%) 61 51	4, 16, 25, 31	0
1	C	392/392 (100%)	0.32	3 (0%) 82 75	3, 16, 24, 37	0
1	D	392/392 (100%)	0.40	14 (3%) 46 37	5, 16, 25, 33	0
All	All	1568/1568 (100%)	0.36	35 (2%) 62 52	3, 16, 24, 37	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	427	SER	4.1
1	D	95	GLY	3.5
1	B	94	PRO	3.3
1	D	98	TRP	3.1
1	A	269	SER	2.9
1	A	197	SER	2.9
1	B	83	SER	2.9
1	C	361	GLY	2.8
1	B	301	ASP	2.7
1	A	397	GLY	2.7
1	D	301	ASP	2.6
1	B	140	PRO	2.6
1	D	145	GLU	2.6
1	A	243	GLY	2.5
1	C	387	ASN	2.4
1	D	347	ASN	2.4
1	A	337	ASP	2.4
1	D	426	PRO	2.4
1	C	36	GLY	2.3
1	D	55	ASN	2.3
1	D	344	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	197	SER	2.2
1	B	175	ASP	2.2
1	D	345	ASP	2.2
1	B	392	GLY	2.2
1	D	99	ASP	2.1
1	D	427	SER	2.1
1	D	77	SER	2.1
1	A	188	ALA	2.1
1	B	242	SER	2.1
1	A	95	GLY	2.1
1	D	51	GLY	2.1
1	B	98	TRP	2.1
1	A	396	ASN	2.0
1	A	300	THR	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.