



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:07 PM GMT

PDB ID : 1IU4  
Title : Crystal Structure Analysis of the Microbial Transglutaminase  
Authors : Kashiwagi, T.; Yokoyama, K.; Ishikawa, K.; Ono, K.; Ejima, D.; Matsui, H.; Suzuki, E.  
Deposited on : 2002-02-27  
Resolution : 2.40 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

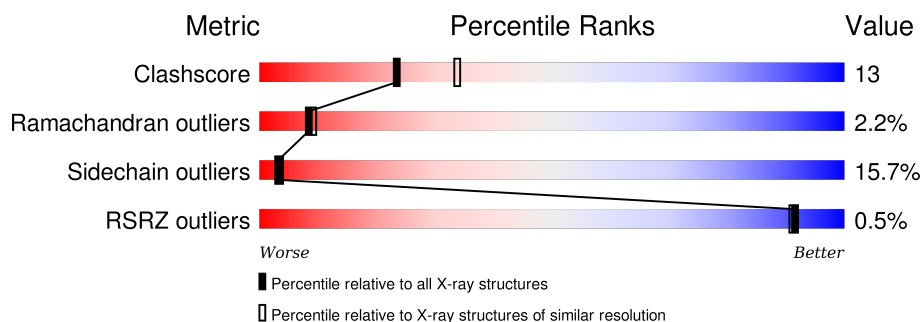
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.40 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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (2.40-2.40)
RSRZ outliers	91569	2928 (2.40-2.40)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	331	<div> <div></div> <div> <div></div> <div>53%</div> <div>35%</div> <div>11%</div> <div></div> </div> </div>
1	B	331	<div> <div>58%</div> <div>31%</div> <div>8%</div> <div></div> </div>
1	C	331	<div> <div>57%</div> <div>31%</div> <div>10%</div> <div></div> </div>
1	D	331	<div> <div></div> <div>56%</div> <div>28%</div> <div>12%</div> <div></div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11262 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 microbial transglutaminase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	331	Total	C	N	O	S	0	0	0
			2678	1659	495	517	7			
1	B	331	Total	C	N	O	S	0	0	0
			2678	1659	495	517	7			
1	C	331	Total	C	N	O	S	0	0	0
			2678	1659	495	517	7			
1	D	331	Total	C	N	O	S	0	0	0
			2678	1659	495	517	7			

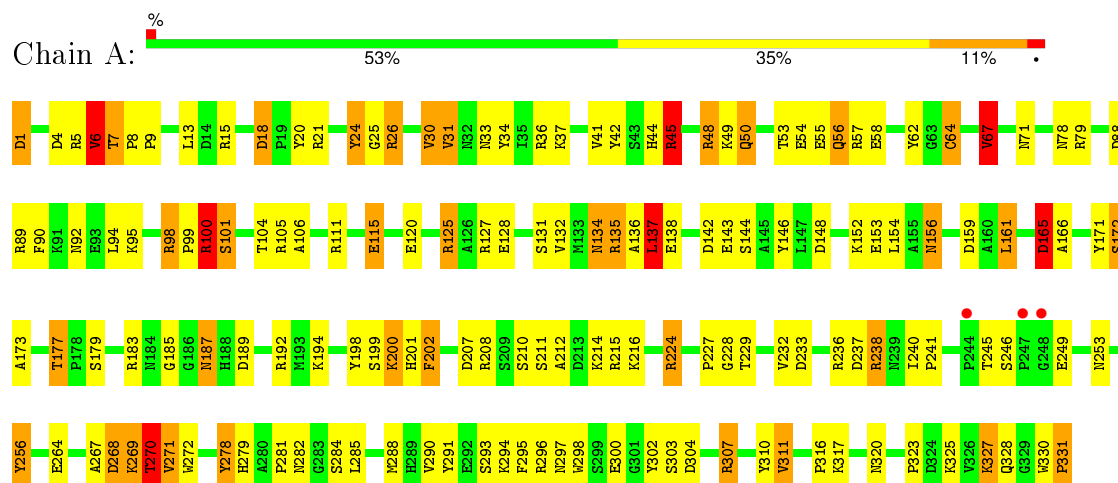
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	147	Total	O	0	0
			147	147		
2	B	157	Total	O	0	0
			157	157		
2	C	154	Total	O	0	0
			154	154		
2	D	92	Total	O	0	0
			92	92		

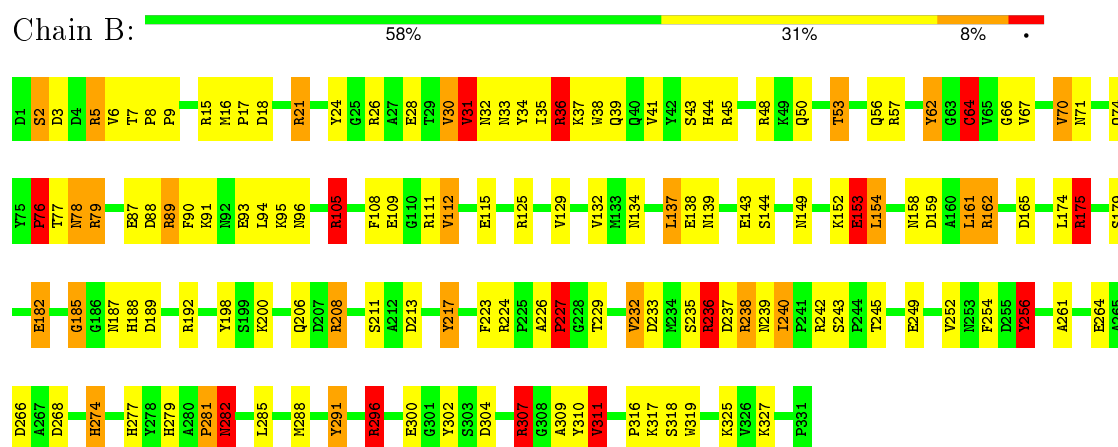
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 ( $\text{RSRZ} > 2$ ). 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.

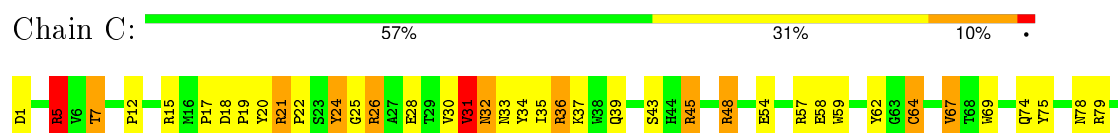
- Molecule 1: microbial transglutaminase

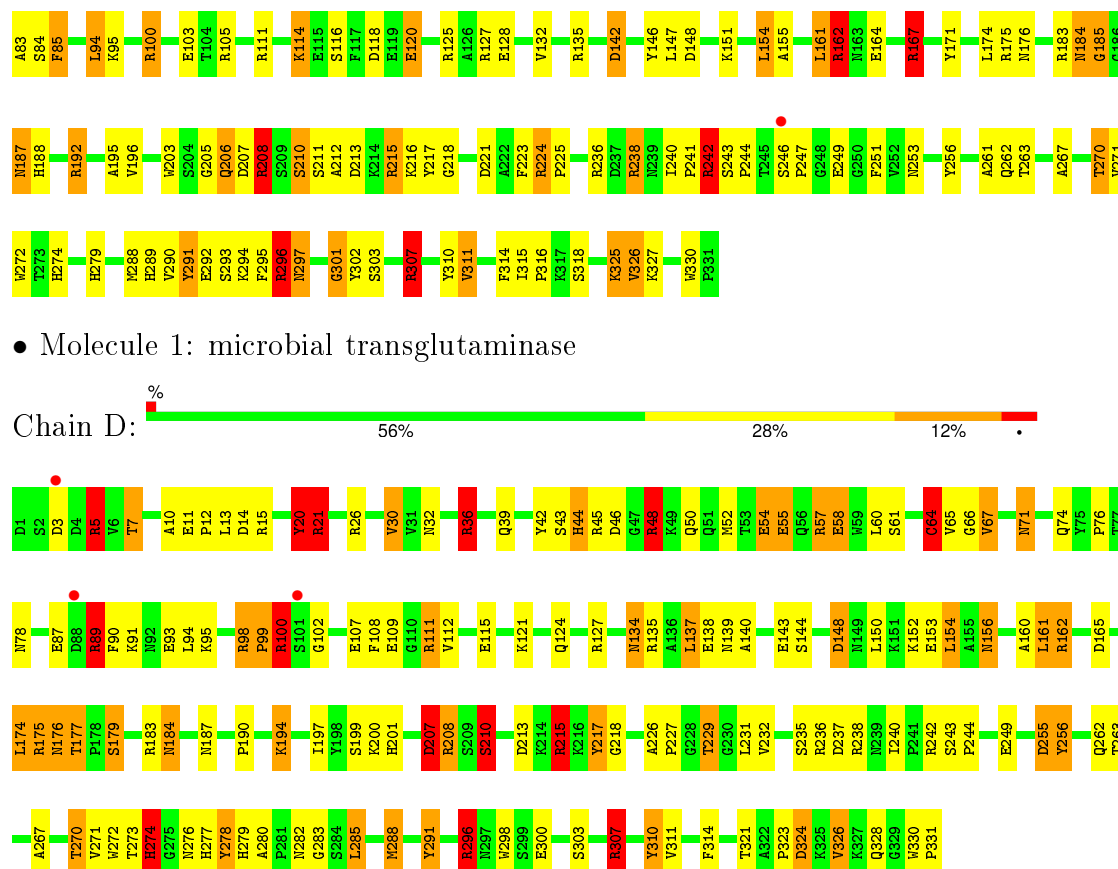


- Molecule 1: microbial transglutaminase



- Molecule 1: microbial transglutaminase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	78.41Å 117.12Å 85.74Å 90.00° 112.80° 90.00°	Depositor
Resolution (Å)	40.00 – 2.40 37.08 – 2.39	Depositor EDS
% Data completeness (in resolution range)	96.5 (40.00-2.40) 97.4 (37.08-2.39)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.08 (at 2.39Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.199 , 0.266 0.207 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.203	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 74.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 55351 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	11262	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.13% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.15	2/2755 (0.1%)	1.89	57/3726 (1.5%)
1	B	1.11	2/2755 (0.1%)	1.87	50/3726 (1.3%)
1	C	1.15	1/2755 (0.0%)	1.91	55/3726 (1.5%)
1	D	1.14	0/2755	1.89	48/3726 (1.3%)
All	All	1.14	5/11020 (0.0%)	1.89	210/14904 (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	A	0	14
1	B	0	17
1	C	0	17
1	D	0	19
All	All	0	67

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	64	CYS	CB-SG	10.82	2.00	1.82
1	B	64	CYS	CB-SG	7.09	1.94	1.82
1	B	45	ARG	NE-CZ	6.54	1.41	1.33
1	A	64	CYS	CB-SG	6.46	1.93	1.82
1	A	298	TRP	CG-CD1	5.14	1.44	1.36

All (210) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	215	ARG	NE-CZ-NH1	15.72	128.16	120.30
1	C	36	ARG	NE-CZ-NH1	15.16	127.88	120.30
1	D	215	ARG	NE-CZ-NH2	-12.67	113.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	57	ARG	NE-CZ-NH2	-12.46	114.07	120.30
1	C	111	ARG	NE-CZ-NH2	-12.09	114.25	120.30
1	B	236	ARG	NE-CZ-NH2	-11.55	114.53	120.30
1	D	98	ARG	NE-CZ-NH2	-11.51	114.54	120.30
1	C	5	ARG	NE-CZ-NH2	-11.31	114.64	120.30
1	C	36	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	C	215	ARG	NE-CZ-NH1	11.14	125.87	120.30
1	D	111	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	C	296	ARG	NE-CZ-NH1	11.08	125.84	120.30
1	B	36	ARG	NE-CZ-NH2	10.77	125.69	120.30
1	C	62	TYR	CB-CG-CD1	-10.53	114.68	121.00
1	B	36	ARG	NE-CZ-NH1	-10.01	115.30	120.30
1	C	111	ARG	NE-CZ-NH1	9.99	125.30	120.30
1	C	167	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	A	34	TYR	CB-CG-CD1	-9.73	115.16	121.00
1	B	21	ARG	NE-CZ-NH1	9.71	125.15	120.30
1	A	215	ARG	NE-CZ-NH1	9.51	125.05	120.30
1	D	217	TYR	CB-CG-CD1	-9.40	115.36	121.00
1	B	224	ARG	NE-CZ-NH1	-9.30	115.65	120.30
1	D	42	TYR	CB-CG-CD1	-9.29	115.43	121.00
1	C	221	ASP	CB-CG-OD1	9.07	126.46	118.30
1	A	127	ARG	NE-CZ-NH1	8.99	124.80	120.30
1	D	310	TYR	CB-CG-CD2	-8.87	115.68	121.00
1	B	15	ARG	NE-CZ-NH2	-8.79	115.90	120.30
1	B	162	ARG	NE-CZ-NH1	8.61	124.61	120.30
1	B	310	TYR	CB-CG-CD2	-8.34	116.00	121.00
1	B	57	ARG	NE-CZ-NH2	-8.30	116.15	120.30
1	A	31	VAL	CB-CA-C	-8.21	95.81	111.40
1	A	30	VAL	CG1-CB-CG2	8.18	123.99	110.90
1	D	127	ARG	NE-CZ-NH2	-8.18	116.21	120.30
1	D	30	VAL	CG1-CB-CG2	8.17	123.98	110.90
1	C	146	TYR	CB-CG-CD2	-8.09	116.14	121.00
1	B	45	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	D	111	ARG	NE-CZ-NH1	8.07	124.34	120.30
1	A	127	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	A	125	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	C	127	ARG	NE-CZ-NH2	7.95	124.27	120.30
1	B	256	TYR	CB-CG-CD1	-7.94	116.24	121.00
1	B	111	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	5	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	31	VAL	CG1-CB-CG2	7.81	123.40	110.90
1	D	36	ARG	NE-CZ-NH1	7.80	124.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	89	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	A	135	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	C	238	ARG	CD-NE-CZ	7.65	134.31	123.60
1	B	31	VAL	CG1-CB-CG2	7.58	123.03	110.90
1	A	224	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	C	242	ARG	CD-NE-CZ	-7.45	113.17	123.60
1	D	296	ARG	CD-NE-CZ	7.41	133.97	123.60
1	A	106	ALA	CB-CA-C	-7.37	99.05	110.10
1	D	98	ARG	CD-NE-CZ	-7.37	113.29	123.60
1	A	24	TYR	CB-CG-CD2	-7.33	116.61	121.00
1	B	175	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	208	ARG	NE-CZ-NH2	-7.25	116.68	120.30
1	A	45	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	C	31	VAL	CG1-CB-CG2	7.17	122.36	110.90
1	C	238	ARG	NE-CZ-NH2	7.17	123.88	120.30
1	D	175	ARG	NE-CZ-NH1	7.10	123.85	120.30
1	C	236	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	C	34	TYR	CB-CG-CD1	-7.06	116.77	121.00
1	B	94	LEU	C-N-CA	-7.03	104.12	121.70
1	C	307	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	236	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	C	114	LYS	CA-CB-CG	6.95	128.68	113.40
1	D	98	ARG	NE-CZ-NH1	6.95	123.77	120.30
1	A	269	LYS	CB-CA-C	-6.87	96.65	110.40
1	D	21	ARG	NE-CZ-NH1	6.86	123.73	120.30
1	D	183	ARG	NE-CZ-NH1	-6.82	116.89	120.30
1	B	62	TYR	CB-CG-CD1	-6.82	116.91	121.00
1	A	270	THR	N-CA-CB	-6.81	97.36	110.30
1	B	291	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	B	111	ARG	NE-CZ-NH2	-6.69	116.95	120.30
1	D	285	LEU	C-N-CA	-6.66	108.32	122.30
1	B	24	TYR	CB-CG-CD1	-6.61	117.03	121.00
1	A	270	THR	CA-CB-CG2	6.57	121.59	112.40
1	D	274	HIS	C-N-CA	-6.55	108.55	122.30
1	A	200	LYS	CB-CA-C	-6.54	97.33	110.40
1	D	183	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	A	115	GLU	CB-CA-C	-6.45	97.51	110.40
1	D	127	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	A	146	TYR	CB-CG-CD2	-6.40	117.16	121.00
1	B	3	ASP	CA-CB-CG	-6.39	99.33	113.40
1	A	127	ARG	CD-NE-CZ	6.38	132.53	123.60
1	A	189	ASP	CB-CG-OD2	6.38	124.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	310	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	B	15	ARG	NE-CZ-NH1	6.35	123.47	120.30
1	C	162	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	D	288	MET	CG-SD-CE	-6.25	90.19	100.20
1	C	48	ARG	CD-NE-CZ	-6.23	114.88	123.60
1	B	311	VAL	CA-CB-CG2	6.19	120.19	110.90
1	A	45	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	B	153	GLU	CA-CB-CG	6.15	126.94	113.40
1	A	302	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	A	20	TYR	CB-CG-CD1	-6.11	117.33	121.00
1	C	311	VAL	CA-CB-CG2	6.10	120.06	110.90
1	A	1	ASP	CA-CB-CG	-6.10	99.98	113.40
1	B	282	ASN	N-CA-C	6.09	127.46	111.00
1	D	255	ASP	CB-CA-C	6.09	122.58	110.40
1	C	45	ARG	C-N-CA	-6.08	106.49	121.70
1	A	256	TYR	CB-CG-CD2	-6.08	117.35	121.00
1	D	67	VAL	CA-CB-CG2	6.07	120.01	110.90
1	C	135	ARG	NE-CZ-NH2	6.07	123.33	120.30
1	B	137	LEU	CA-CB-CG	6.06	129.24	115.30
1	B	309	ALA	CB-CA-C	-6.04	101.04	110.10
1	A	172	SER	CB-CA-C	-5.94	98.81	110.10
1	C	26	ARG	CD-NE-CZ	-5.94	115.28	123.60
1	A	328	GLN	C-N-CA	-5.93	109.84	122.30
1	A	227	PRO	C-N-CA	-5.93	109.85	122.30
1	B	227	PRO	N-CA-C	5.90	127.45	112.10
1	D	307	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	C	31	VAL	CB-CA-C	-5.86	100.26	111.40
1	A	18	ASP	CB-CG-OD2	5.84	123.56	118.30
1	B	185	GLY	C-N-CA	-5.84	110.03	122.30
1	B	224	ARG	NE-CZ-NH2	5.82	123.21	120.30
1	C	43	SER	CB-CA-C	-5.82	99.05	110.10
1	A	48	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	D	307	ARG	CD-NE-CZ	-5.80	115.48	123.60
1	A	100	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	A	137	LEU	CB-CA-C	5.80	121.21	110.20
1	D	236	ARG	NE-CZ-NH2	5.78	123.19	120.30
1	A	317	LYS	CA-CB-CG	5.72	125.98	113.40
1	D	65	VAL	N-CA-C	5.71	126.43	111.00
1	C	290	VAL	CG1-CB-CG2	5.71	120.03	110.90
1	B	162	ARG	CD-NE-CZ	5.70	131.58	123.60
1	A	303	SER	CA-C-N	-5.70	104.66	117.20
1	C	238	ARG	CA-CB-CG	5.69	125.92	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	13	LEU	C-N-CA	5.67	135.87	121.70
1	D	5	ARG	CA-CB-CG	5.66	125.85	113.40
1	C	57	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	165	ASP	CB-CG-OD1	5.65	123.39	118.30
1	A	67	VAL	CA-CB-CG2	5.64	119.36	110.90
1	A	165	ASP	N-CA-CB	-5.63	100.46	110.60
1	B	162	ARG	CA-CB-CG	5.63	125.79	113.40
1	C	5	ARG	CG-CD-NE	-5.63	99.98	111.80
1	C	256	TYR	CB-CA-C	-5.60	99.19	110.40
1	A	6	VAL	CA-CB-CG2	5.58	119.27	110.90
1	D	208	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	D	207	ASP	CA-CB-CG	-5.55	101.18	113.40
1	B	31	VAL	CB-CA-C	-5.55	100.85	111.40
1	D	217	TYR	CB-CG-CD2	5.53	124.32	121.00
1	A	271	VAL	CA-CB-CG2	5.53	119.19	110.90
1	D	194	LYS	CA-CB-CG	5.52	125.55	113.40
1	C	79	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	285	LEU	CA-CB-CG	-5.50	102.65	115.30
1	C	142	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	B	105	ARG	CG-CD-NE	5.50	123.34	111.80
1	A	233	ASP	CB-CA-C	5.48	121.37	110.40
1	C	208	ARG	CA-CB-CG	5.47	125.43	113.40
1	B	182	GLU	CA-CB-CG	5.46	125.40	113.40
1	A	1	ASP	CB-CA-C	5.44	121.29	110.40
1	D	13	LEU	N-CA-C	5.42	125.62	111.00
1	B	5	ARG	NE-CZ-NH1	-5.41	117.59	120.30
1	C	36	ARG	CB-CG-CD	5.41	125.66	111.60
1	A	56	GLN	N-CA-CB	-5.41	100.87	110.60
1	D	48	ARG	CA-CB-CG	5.41	125.29	113.40
1	C	221	ASP	CB-CA-C	5.40	121.19	110.40
1	C	85	PHE	N-CA-CB	-5.40	100.89	110.60
1	C	192	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	A	15	ARG	CD-NE-CZ	-5.35	116.11	123.60
1	B	30	VAL	CA-CB-CG1	5.33	118.90	110.90
1	A	228	GLY	CA-C-O	5.33	130.19	120.60
1	A	311	VAL	CA-CB-CG2	5.33	118.89	110.90
1	B	15	ARG	CA-C-N	-5.32	105.49	117.20
1	D	161	LEU	N-CA-CB	-5.31	99.78	110.40
1	A	293	SER	CB-CA-C	-5.31	100.02	110.10
1	C	301	GLY	CA-C-O	5.28	130.11	120.60
1	A	310	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	A	136	ALA	CB-CA-C	-5.27	102.19	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	TYR	CG-CD1-CE1	-5.27	117.09	121.30
1	C	256	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	C	64	CYS	CA-C-O	5.26	131.14	120.10
1	D	98	ARG	CA-CB-CG	5.25	124.96	113.40
1	D	30	VAL	CB-CA-C	-5.25	101.42	111.40
1	B	242	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	235	SER	CB-CA-C	-5.25	100.13	110.10
1	D	107	GLU	CB-CA-C	5.24	120.89	110.40
1	D	229	THR	CA-CB-CG2	5.22	119.71	112.40
1	A	238	ARG	CA-CB-CG	5.21	124.87	113.40
1	B	245	THR	CA-CB-CG2	-5.21	105.10	112.40
1	C	184	ASN	C-N-CA	-5.21	111.36	122.30
1	C	297	ASN	CB-CA-C	-5.21	99.98	110.40
1	B	229	THR	CA-CB-CG2	-5.20	105.13	112.40
1	A	237	ASP	CB-CG-OD2	5.19	122.97	118.30
1	C	64	CYS	CB-CA-C	5.19	120.78	110.40
1	B	162	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	D	21	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	B	88	ASP	CB-CA-C	5.17	120.75	110.40
1	C	192	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	175	ARG	CA-CB-CG	5.17	124.77	113.40
1	B	95	LYS	N-CA-CB	5.16	119.89	110.60
1	D	256	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	D	20	TYR	CG-CD2-CE2	-5.13	117.19	121.30
1	C	211	SER	C-N-CA	-5.13	108.88	121.70
1	C	224	ARG	CA-CB-CG	-5.13	102.12	113.40
1	D	5	ARG	N-CA-CB	5.11	119.80	110.60
1	A	307	ARG	CA-CB-CG	5.10	124.62	113.40
1	A	331	PRO	N-CA-C	5.09	125.34	112.10
1	A	268	ASP	N-CA-C	5.09	124.75	111.00
1	A	98	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	B	227	PRO	N-CA-CB	-5.08	97.01	102.60
1	D	291	TYR	CB-CG-CD2	-5.05	117.97	121.00
1	B	232	VAL	CA-CB-CG2	5.04	118.46	110.90
1	C	247	PRO	C-N-CA	-5.03	111.74	122.30
1	B	79	ARG	NE-CZ-NH2	5.03	122.81	120.30
1	A	148	ASP	CB-CG-OD2	5.03	122.83	118.30
1	A	49	LYS	CA-CB-CG	5.02	124.44	113.40
1	C	95	LYS	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (67) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	105	ARG	Sidechain
1	A	166	ALA	Peptide
1	A	183	ARG	Sidechain
1	A	202	PHE	Sidechain
1	A	224	ARG	Sidechain
1	A	238	ARG	Sidechain
1	A	26	ARG	Sidechain
1	A	278	TYR	Sidechain
1	A	282	ASN	Peptide
1	A	300	GLU	Peptide
1	A	36	ARG	Sidechain
1	A	42	TYR	Sidechain
1	A	45	ARG	Sidechain
1	A	62	TYR	Sidechain
1	B	105	ARG	Sidechain
1	B	175	ARG	Sidechain
1	B	198	TYR	Sidechain
1	B	208	ARG	Sidechain
1	B	217	TYR	Sidechain
1	B	226	ALA	Peptide
1	B	254	PHE	Sidechain
1	B	256	TYR	Sidechain
1	B	281	PRO	Peptide
1	B	296	ARG	Sidechain
1	B	307	ARG	Sidechain
1	B	34	TYR	Sidechain
1	B	36	ARG	Sidechain
1	B	5	ARG	Sidechain
1	B	62	TYR	Sidechain
1	B	76	PRO	Peptide
1	B	89	ARG	Sidechain
1	C	100	ARG	Peptide
1	C	105	ARG	Sidechain
1	C	162	ARG	Sidechain
1	C	175	ARG	Sidechain
1	C	192	ARG	Sidechain
1	C	20	TYR	Peptide
1	C	206	GLN	Peptide
1	C	208	ARG	Peptide
1	C	21	ARG	Sidechain
1	C	217	TYR	Sidechain
1	C	24	TYR	Sidechain
1	C	242	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	291	TYR	Sidechain
1	C	302	TYR	Sidechain
1	C	307	ARG	Sidechain
1	C	48	ARG	Sidechain
1	C	75	TYR	Sidechain
1	D	100	ARG	Peptide
1	D	102	GLY	Peptide
1	D	111	ARG	Sidechain
1	D	156	ASN	Peptide
1	D	20	TYR	Peptide
1	D	21	ARG	Sidechain
1	D	215	ARG	Sidechain
1	D	218	GLY	Peptide
1	D	238	ARG	Sidechain
1	D	274	HIS	Peptide
1	D	278	TYR	Sidechain
1	D	282	ASN	Peptide
1	D	307	ARG	Sidechain
1	D	310	TYR	Sidechain
1	D	324	ASP	Peptide
1	D	45	ARG	Peptide
1	D	57	ARG	Sidechain
1	D	95	LYS	Peptide
1	D	98	ARG	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	2678	0	2486	70	0
1	B	2678	0	2486	57	0
1	C	2678	0	2486	79	0
1	D	2678	0	2486	75	0
2	A	147	0	0	3	0
2	B	157	0	0	0	0
2	C	154	0	0	3	0
2	D	92	0	0	1	0
All	All	11262	0	9944	274	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (274) 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:D:177:THR:HG21	1:D:314:PHE:HB2	1.64	0.79
1:D:207:ASP:HB3	1:D:210:SER:HB3	1.66	0.78
1:C:242:ARG:HD2	1:C:251:PHE:CE1	2.21	0.75
1:D:5:ARG:HB3	1:D:278:TYR:HD1	1.53	0.74
1:D:39:GLN:HA	1:D:43:SER:HB3	1.69	0.73
1:C:31:VAL:HG22	1:C:288:MET:O	1.90	0.72
1:C:22:PRO:HA	1:C:26:ARG:O	1.90	0.71
1:D:262:GLN:HG2	1:D:326:VAL:HG13	1.73	0.71
1:D:280:ALA:O	1:D:283:GLY:HA2	1.89	0.70
1:C:25:GLY:HA2	1:C:294:LYS:HE3	1.73	0.70
1:C:155:ALA:HB2	1:C:162:ARG:HD3	1.74	0.69
1:D:267:ALA:O	1:D:270:THR:HB	1.93	0.69
1:C:148:ASP:HA	1:C:151:LYS:NZ	2.07	0.69
1:C:242:ARG:HB3	1:C:251:PHE:CD1	2.29	0.68
1:C:325:LYS:HE2	1:C:325:LYS:HA	1.75	0.67
1:A:90:PHE:O	1:A:94:LEU:HB2	1.95	0.67
1:C:148:ASP:HA	1:C:151:LYS:HZ3	1.60	0.66
1:D:20:TYR:HB2	1:D:21:ARG:HD3	1.78	0.66
1:D:64:CYS:HB3	1:D:255:ASP:HA	1.78	0.65
1:A:207:ASP:HB3	1:A:210:SER:HB2	1.79	0.65
1:A:67:VAL:O	1:A:71:ASN:HB2	1.97	0.65
1:C:167:ARG:HH11	1:C:167:ARG:HB3	1.61	0.64
1:C:212:ALA:O	1:C:216:LYS:HG2	1.97	0.64
1:D:44:HIS:HA	1:D:48:ARG:O	1.97	0.64
1:B:159:ASP:OD1	1:B:161:LEU:HB2	1.97	0.64
1:A:267:ALA:O	1:A:270:THR:HB	1.98	0.63
1:D:199:SER:HB3	1:D:298:TRP:CZ2	2.33	0.63
1:B:279:HIS:HD2	1:B:288:MET:H	1.45	0.63
1:B:134:ASN:O	1:B:138:GLU:HG2	1.98	0.63
1:A:18:ASP:H	1:A:33:ASN:HD21	1.47	0.62
1:B:37:LYS:O	1:B:41:VAL:HG22	2.00	0.62
1:B:78:ASN:HA	1:B:311:VAL:HG21	1.82	0.62
1:D:154:LEU:HB3	1:D:162:ARG:HG2	1.82	0.61
1:C:5:ARG:HH22	1:C:7:THR:HG22	1.65	0.61
1:C:267:ALA:O	1:C:270:THR:HB	2.00	0.61
1:C:185:GLY:HA3	1:C:316:PRO:HB3	1.83	0.61
1:A:53:THR:HB	1:A:56:GLN:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:HIS:HD2	1:A:288:MET:H	1.47	0.60
1:C:15:ARG:HG2	1:C:36:ARG:HD2	1.83	0.60
1:D:201:HIS:HE1	1:D:298:TRP:O	1.85	0.60
1:C:83:ALA:HB3	1:C:225:PRO:HG3	1.83	0.60
1:A:159:ASP:OD1	1:A:161:LEU:HB2	2.02	0.60
1:A:330:TRP:HA	1:A:331:PRO:C	2.21	0.59
1:B:39:GLN:HA	1:B:43:SER:HB3	1.84	0.59
1:A:278:TYR:CE2	1:A:285:LEU:HD12	2.37	0.59
1:D:134:ASN:O	1:D:137:LEU:HB2	2.03	0.58
1:A:54:GLU:O	1:A:58:GLU:HG3	2.03	0.58
1:C:154:LEU:HB3	1:C:162:ARG:HB2	1.85	0.58
1:C:205:GLY:O	1:C:215:ARG:HD2	2.03	0.58
1:D:213:ASP:HB2	1:D:217:TYR:HD1	1.67	0.58
1:B:238:ARG:HB2	1:B:240:ILE:HG23	1.86	0.58
1:B:125:ARG:NH2	1:B:161:LEU:HD22	2.19	0.57
1:A:179:SER:OG	1:A:316:PRO:HD3	2.05	0.57
1:C:5:ARG:NH2	1:C:7:THR:HG22	2.19	0.57
1:D:135:ARG:HB2	1:D:153:GLU:OE1	2.04	0.57
1:B:87:GLU:HG3	1:B:91:LYS:HE3	1.87	0.57
1:B:277:HIS:O	1:B:288:MET:HG3	2.05	0.56
1:A:111:ARG:O	1:A:115:GLU:HG3	2.05	0.56
1:A:210:SER:OG	1:A:214:LYS:HB2	2.04	0.56
1:C:37:LYS:HG3	1:C:330:TRP:CE3	2.40	0.56
1:C:244:PRO:HB3	1:C:249:GLU:O	2.06	0.56
1:D:60:LEU:O	1:D:288:MET:HE1	2.05	0.56
1:A:270:THR:CG2	1:A:272:TRP:HE1	2.17	0.56
1:C:293:SER:HB3	1:C:297:ASN:HB2	1.88	0.55
1:D:93:GLU:HB3	1:D:112:VAL:HG11	1.88	0.55
1:D:307:ARG:HG2	2:D:334:HOH:O	2.07	0.55
1:C:85:PHE:CZ	1:C:224:ARG:HD3	2.42	0.54
1:A:327:LYS:HE2	1:A:331:PRO:OXT	2.06	0.54
1:D:256:TYR:O	1:D:274:HIS:HB3	2.08	0.54
1:A:152:LYS:O	1:A:156:ASN:HB2	2.07	0.54
1:A:269:LYS:HE2	1:B:115:GLU:O	2.08	0.54
1:C:279:HIS:HD2	1:C:288:MET:H	1.56	0.54
1:D:90:PHE:CZ	1:D:94:LEU:HD11	2.43	0.54
1:D:161:LEU:CD1	1:D:231:LEU:HD21	2.38	0.54
1:A:94:LEU:O	1:A:95:LYS:HD2	2.08	0.53
1:D:279:HIS:HD2	1:D:288:MET:H	1.55	0.53
1:A:173:ALA:O	1:A:177:THR:HG22	2.09	0.53
1:D:161:LEU:HD13	1:D:231:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:HH11	1:A:100:ARG:HG2	1.73	0.53
1:B:35:ILE:O	1:B:39:GLN:HG3	2.09	0.53
1:C:18:ASP:H	1:C:33:ASN:HD21	1.57	0.53
1:B:31:VAL:HG22	1:B:288:MET:O	2.09	0.53
1:A:330:TRP:HA	1:A:331:PRO:O	2.08	0.53
1:C:206:GLN:HB2	1:C:238:ARG:NH1	2.23	0.53
1:C:12:PRO:HD2	1:C:15:ARG:CZ	2.39	0.53
1:C:241:PRO:HB3	1:C:253:ASN:HA	1.92	0.52
1:D:277:HIS:ND1	1:D:285:LEU:HD13	2.24	0.52
1:C:270:THR:HG22	1:C:295:PHE:HB2	1.92	0.52
1:D:99:PRO:HA	1:D:108:PHE:CD2	2.43	0.52
1:A:53:THR:HG22	1:A:55:GLU:H	1.74	0.52
1:D:150:LEU:O	1:D:154:LEU:HB2	2.10	0.52
1:C:206:GLN:O	1:C:240:ILE:HD11	2.09	0.51
1:A:270:THR:HG22	1:A:295:PHE:HB2	1.92	0.51
1:A:125:ARG:NH2	1:A:161:LEU:HD22	2.25	0.51
1:A:44:HIS:H	1:A:44:HIS:CD2	2.27	0.51
1:C:296:ARG:HB3	1:D:296:ARG:CZ	2.39	0.51
1:D:5:ARG:HH22	1:D:7:THR:HG22	1.75	0.51
1:C:31:VAL:O	1:C:35:ILE:HG13	2.10	0.51
1:B:159:ASP:O	1:B:162:ARG:HB3	2.11	0.51
1:B:233:ASP:OD1	1:B:236:ARG:HD2	2.10	0.51
1:C:24:TYR:HA	1:D:300:GLU:HG2	1.92	0.51
1:C:28:GLU:OE1	1:C:289:HIS:HD2	1.93	0.51
1:B:256:TYR:O	1:B:274:HIS:HB3	2.11	0.51
1:D:90:PHE:CE1	1:D:94:LEU:HD11	2.45	0.51
1:A:187:ASN:HB2	1:A:192:ARG:HH21	1.75	0.51
1:D:270:THR:HG22	1:D:272:TRP:HE1	1.76	0.50
1:D:134:ASN:HA	1:D:137:LEU:HD22	1.92	0.50
1:C:128:GLU:O	1:C:132:VAL:HG23	2.11	0.50
1:C:223:PHE:HB2	1:C:307:ARG:HD3	1.93	0.50
2:A:439:HOH:O	1:B:268:ASP:HB2	2.10	0.50
1:A:241:PRO:HD3	1:A:253:ASN:HB3	1.94	0.50
1:B:44:HIS:CD2	1:B:44:HIS:H	2.29	0.50
1:D:270:THR:CG2	1:D:272:TRP:HE1	2.24	0.50
1:C:7:THR:HG21	1:C:58:GLU:HG2	1.93	0.50
1:B:206:GLN:NE2	1:B:238:ARG:H	2.10	0.50
1:C:45:ARG:O	1:C:318:SER:O	2.29	0.50
1:D:323:PRO:HG2	1:D:326:VAL:HG12	1.94	0.50
1:D:330:TRP:HA	1:D:331:PRO:C	2.31	0.50
1:A:37:LYS:O	1:A:41:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:HIS:HD2	1:A:288:MET:N	2.11	0.49
1:C:206:GLN:HB2	1:C:238:ARG:HH11	1.76	0.49
1:B:316:PRO:HD2	1:B:319:TRP:CE2	2.48	0.49
1:A:25:GLY:HA2	1:A:294:LYS:HZ1	1.77	0.49
1:A:330:TRP:CG	1:A:331:PRO:HA	2.48	0.49
1:C:67:VAL:HG13	2:C:338:HOH:O	2.11	0.49
1:A:53:THR:HG22	1:A:55:GLU:N	2.28	0.48
1:B:189:ASP:HB3	1:B:192:ARG:HG3	1.95	0.48
1:B:105:ARG:NH1	1:B:109:GLU:OE2	2.45	0.48
1:B:18:ASP:H	1:B:33:ASN:HD21	1.60	0.48
1:C:303:SER:HB3	2:C:471:HOH:O	2.12	0.48
1:D:100:ARG:HE	1:D:100:ARG:HB3	1.54	0.48
1:B:6:VAL:HG21	1:B:281:PRO:HD2	1.95	0.48
1:B:200:LYS:NZ	1:B:237:ASP:OD1	2.45	0.48
1:D:213:ASP:HB2	1:D:217:TYR:CD1	2.47	0.48
1:D:60:LEU:HA	1:D:66:GLY:HA3	1.96	0.48
1:A:26:ARG:HG3	1:A:297:ASN:HD22	1.79	0.47
1:B:213:ASP:O	1:B:217:TYR:HB2	2.14	0.47
1:D:94:LEU:HD22	1:D:109:GLU:HG2	1.96	0.47
1:A:200:LYS:HE3	1:A:256:TYR:CZ	2.49	0.47
1:C:100:ARG:O	1:C:103:GLU:HB2	2.13	0.47
1:B:132:VAL:HG11	1:B:154:LEU:HD13	1.97	0.47
1:B:235:SER:OG	1:B:236:ARG:HG3	2.15	0.47
1:A:320:ASN:O	1:A:323:PRO:HD3	2.14	0.47
1:D:11:GLU:HA	1:D:12:PRO:HD3	1.78	0.47
1:D:10:ALA:O	1:D:12:PRO:HD3	2.14	0.47
1:C:18:ASP:N	1:C:33:ASN:HD21	2.12	0.47
1:D:87:GLU:O	1:D:91:LYS:HG2	2.15	0.47
1:B:206:GLN:HE22	1:B:238:ARG:H	1.64	0.46
1:A:240:ILE:HG21	1:A:240:ILE:HD13	1.64	0.46
1:C:184:ASN:O	1:C:185:GLY:O	2.34	0.46
1:A:128:GLU:O	1:A:132:VAL:HG23	2.15	0.46
1:A:100:ARG:CG	1:A:100:ARG:HH11	2.29	0.46
1:B:264:GLU:HG3	1:B:266:ASP:H	1.79	0.46
1:B:16:MET:HA	1:B:17:PRO:HD3	1.87	0.46
1:C:85:PHE:CE2	1:C:116:SER:HB2	2.50	0.46
1:C:296:ARG:HB3	1:D:296:ARG:NE	2.30	0.46
1:D:10:ALA:HB2	1:D:57:ARG:CZ	2.45	0.46
1:B:179:SER:O	1:B:185:GLY:O	2.34	0.46
1:D:244:PRO:HB3	1:D:249:GLU:O	2.15	0.46
1:D:213:ASP:O	1:D:217:TYR:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:32:ASN:H	1:C:32:ASN:ND2	2.13	0.46
1:C:120:GLU:HG3	1:C:295:PHE:HE1	1.81	0.46
1:C:196:VAL:HG11	1:C:315:ILE:HG12	1.98	0.46
1:B:90:PHE:CD2	1:B:112:VAL:HG23	2.51	0.45
1:B:8:PRO:HA	1:B:9:PRO:HD3	1.72	0.45
1:A:179:SER:O	1:A:185:GLY:O	2.34	0.45
1:A:24:TYR:HH	1:B:302:TYR:HD2	1.63	0.45
1:C:195:ALA:HB2	1:C:314:PHE:CE2	2.52	0.45
1:C:243:SER:HA	1:C:244:PRO:HD3	1.80	0.45
1:C:30:VAL:HG22	1:C:289:HIS:CE1	2.52	0.45
1:A:199:SER:HB2	1:A:272:TRP:CZ3	2.52	0.45
1:D:330:TRP:HA	1:D:331:PRO:O	2.16	0.45
1:D:176:ASN:HD22	1:D:176:ASN:C	2.19	0.45
1:A:78:ASN:HA	1:A:311:VAL:HG21	1.98	0.45
1:D:10:ALA:HB2	1:D:57:ARG:NH2	2.32	0.45
1:D:148:ASP:CG	1:D:152:LYS:HZ2	2.20	0.45
1:B:187:ASN:O	1:B:188:HIS:HB2	2.17	0.45
1:C:147:LEU:O	1:C:151:LYS:HG3	2.17	0.45
1:C:15:ARG:HD2	2:C:454:HOH:O	2.16	0.45
1:B:143:GLU:OE2	1:B:175:ARG:HB2	2.17	0.45
1:B:132:VAL:HG13	1:B:153:GLU:HG3	1.98	0.45
1:A:8:PRO:O	1:A:57:ARG:HD2	2.17	0.45
1:D:197:ILE:HG23	1:D:311:VAL:O	2.17	0.44
1:A:165:ASP:O	1:A:171:TYR:HD1	1.99	0.44
1:B:125:ARG:O	1:B:129:VAL:HG23	2.16	0.44
1:A:142:ASP:OD2	1:A:144:SER:HB2	2.18	0.44
1:A:8:PRO:HA	1:A:9:PRO:HD2	1.78	0.44
1:A:291:TYR:CD1	1:A:291:TYR:N	2.86	0.44
1:D:55:GLU:O	1:D:58:GLU:HB3	2.17	0.44
1:C:187:ASN:O	1:C:188:HIS:HB2	2.17	0.44
1:A:270:THR:HG23	1:A:272:TRP:HE1	1.82	0.44
1:D:243:SER:HA	1:D:244:PRO:HD3	1.87	0.44
1:A:98:ARG:HA	1:A:99:PRO:HD3	1.70	0.44
1:C:270:THR:CG2	1:C:272:TRP:HE1	2.30	0.44
1:C:216:LYS:NZ	1:C:244:PRO:O	2.43	0.43
1:A:279:HIS:CD2	1:A:288:MET:H	2.32	0.43
1:B:66:GLY:O	1:B:70:VAL:HG13	2.17	0.43
1:D:89:ARG:HH21	1:D:115:GLU:HB3	1.83	0.43
1:D:11:GLU:OE2	1:D:15:ARG:HD2	2.19	0.43
1:D:226:ALA:HA	1:D:227:PRO:HD3	1.80	0.43
1:A:198:TYR:CZ	1:A:311:VAL:HG22	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:200:LYS:HE3	1:A:256:TYR:OH	2.18	0.43
1:C:32:ASN:H	1:C:32:ASN:HD22	1.66	0.43
1:B:74:GLN:HB3	1:B:74:GLN:HE21	1.68	0.43
1:A:294:LYS:NZ	1:B:300:GLU:OE2	2.50	0.43
1:A:296:ARG:HB2	1:B:296:ARG:HB3	2.00	0.43
1:C:203:TRP:CZ2	1:C:218:GLY:N	2.87	0.43
1:A:161:LEU:HD13	1:A:229:THR:HG22	2.00	0.43
1:C:19:PRO:HA	1:C:330:TRP:O	2.19	0.43
1:D:148:ASP:OD1	1:D:152:LYS:NZ	2.52	0.43
1:B:32:ASN:O	1:B:36:ARG:HG3	2.18	0.43
1:A:79:ARG:HD3	2:A:435:HOH:O	2.17	0.43
1:A:199:SER:HB2	1:A:272:TRP:HZ3	1.84	0.43
1:C:205:GLY:O	1:C:215:ARG:NH1	2.50	0.42
1:C:26:ARG:HD3	1:C:291:TYR:CD2	2.53	0.42
1:D:54:GLU:OE1	1:D:57:ARG:NH1	2.51	0.42
1:D:194:LYS:NZ	1:D:324:ASP:OD2	2.52	0.42
1:A:45:ARG:HD2	1:A:50:GLN:OE1	2.19	0.42
1:C:125:ARG:NH2	1:C:161:LEU:HD22	2.34	0.42
1:A:201:HIS:O	1:A:202:PHE:HB3	2.18	0.42
1:A:134:ASN:HA	1:A:137:LEU:HD22	2.00	0.42
1:D:5:ARG:HH11	1:D:5:ARG:HD3	1.71	0.42
1:C:176:ASN:HD22	1:C:176:ASN:HA	1.69	0.42
1:C:25:GLY:HA2	1:C:294:LYS:CE	2.45	0.42
1:A:18:ASP:H	1:A:33:ASN:ND2	2.14	0.42
1:B:53:THR:H	1:B:56:GLN:HE21	1.67	0.42
1:C:223:PHE:HB2	1:C:307:ARG:CD	2.49	0.42
1:A:327:LYS:HD2	1:A:327:LYS:O	2.20	0.42
1:D:138:GLU:C	1:D:140:ALA:H	2.22	0.42
1:C:59:TRP:CE3	1:C:69:TRP:CD1	3.08	0.42
1:C:216:LYS:O	1:C:242:ARG:NH2	2.49	0.42
1:C:206:GLN:HB3	1:C:240:ILE:HG12	2.02	0.42
1:A:6:VAL:HG13	1:A:281:PRO:HD2	2.02	0.42
1:C:17:PRO:HG3	1:C:37:LYS:N	2.35	0.42
1:D:39:GLN:HG2	1:D:52:MET:H	1.84	0.41
1:C:35:ILE:O	1:C:39:GLN:HG3	2.20	0.41
1:B:26:ARG:HD3	1:B:291:TYR:CD2	2.55	0.41
1:C:84:SER:OG	1:C:118:ASP:HB3	2.19	0.41
1:C:262:GLN:CD	1:C:326:VAL:HG13	2.40	0.41
1:C:240:ILE:HA	1:C:241:PRO:HD3	1.93	0.41
1:B:108:PHE:O	1:B:112:VAL:HG13	2.20	0.41
1:D:200:LYS:NZ	1:D:237:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:GLU:O	1:C:171:TYR:HE1	2.04	0.41
1:D:184:ASN:OD1	1:D:184:ASN:N	2.53	0.41
1:A:5:ARG:HA	1:A:279:HIS:O	2.20	0.41
1:B:138:GLU:CD	1:B:317:LYS:HZ1	2.23	0.41
1:C:37:LYS:NZ	1:C:292:GLU:OE1	2.50	0.41
1:A:135:ARG:HH12	1:A:153:GLU:CD	2.23	0.41
1:D:39:GLN:HB2	1:D:39:GLN:HE21	1.71	0.41
1:B:38:TRP:HE1	1:B:71:ASN:HD21	1.67	0.41
2:A:439:HOH:O	1:B:266:ASP:HB3	2.20	0.41
1:B:105:ARG:O	1:B:109:GLU:HG3	2.21	0.41
1:D:143:GLU:OE2	1:D:175:ARG:NH1	2.53	0.41
1:C:94:LEU:HA	1:C:94:LEU:HD12	1.73	0.41
1:D:197:ILE:HG21	1:D:197:ILE:HD13	1.82	0.41
1:B:2:SER:O	1:B:282:ASN:HB2	2.20	0.41
1:B:18:ASP:N	1:B:33:ASN:HD21	2.18	0.41
1:B:90:PHE:HD2	1:B:112:VAL:HG23	1.84	0.41
1:D:276:ASN:HB3	1:D:291:TYR:HE1	1.85	0.41
1:C:207:ASP:HA	1:C:238:ARG:NH2	2.36	0.41
1:A:1:ASP:HB3	1:A:4:ASP:OD2	2.21	0.41
1:A:307:ARG:HD2	1:A:307:ARG:HH11	1.70	0.41
1:B:223:PHE:HB2	1:B:307:ARG:CD	2.51	0.41
1:D:215:ARG:HH22	1:D:240:ILE:CG2	2.33	0.41
1:B:53:THR:H	1:B:56:GLN:NE2	2.18	0.41
1:D:174:LEU:HD11	1:D:190:PRO:HG3	2.02	0.41
1:A:5:ARG:HH22	1:A:7:THR:HG22	1.86	0.40
1:B:18:ASP:H	1:B:33:ASN:ND2	2.18	0.40
1:C:208:ARG:N	1:C:210:SER:H	2.19	0.40
1:D:71:ASN:HA	1:D:321:THR:HG21	2.02	0.40
1:D:276:ASN:HB3	1:D:291:TYR:CE1	2.56	0.40
1:A:211:SER:O	1:A:212:ALA:C	2.59	0.40
1:D:26:ARG:HH11	1:D:26:ARG:HD2	1.77	0.40
1:D:242:ARG:NH1	1:D:303:SER:O	2.54	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	329/331 (99%)	298 (91%)	26 (8%)	5 (2%)	13	17
1	B	329/331 (99%)	294 (89%)	26 (8%)	9 (3%)	6	6
1	C	329/331 (99%)	300 (91%)	26 (8%)	3 (1%)	21	30
1	D	329/331 (99%)	281 (85%)	36 (11%)	12 (4%)	4	3
All	All	1316/1324 (99%)	1173 (89%)	114 (9%)	29 (2%)	8	9

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	165	ASP
1	B	227	PRO
1	B	249	GLU
1	C	185	GLY
1	D	44	HIS
1	D	100	ARG
1	A	101	SER
1	A	304	ASP
1	B	76	PRO
1	B	96	ASN
1	B	261	ALA
1	B	282	ASN
1	D	160	ALA
1	D	179	SER
1	D	210	SER
1	A	264	GLU
1	D	165	ASP
1	D	296	ARG
1	A	268	ASP
1	B	64	CYS
1	B	77	THR
1	D	36	ARG
1	C	261	ALA
1	D	46	ASP
1	D	76	PRO
1	D	99	PRO
1	B	78	ASN
1	C	301	GLY

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Mol	Chain	Res	Type
1	D	64	CYS

### 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	279/279 (100%)	237 (85%)	42 (15%)	3	4
1	B	279/279 (100%)	232 (83%)	47 (17%)	2	3
1	C	279/279 (100%)	244 (88%)	35 (12%)	6	7
1	D	279/279 (100%)	228 (82%)	51 (18%)	2	2
All	All	1116/1116 (100%)	941 (84%)	175 (16%)	3	3

All (175) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	VAL
1	A	7	THR
1	A	13	LEU
1	A	21	ARG
1	A	30	VAL
1	A	31	VAL
1	A	48	ARG
1	A	50	GLN
1	A	64	CYS
1	A	67	VAL
1	A	88	ASP
1	A	89	ARG
1	A	92	ASN
1	A	100	ARG
1	A	101	SER
1	A	104	THR
1	A	120	GLU
1	A	131	SER
1	A	134	ASN
1	A	137	LEU

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Mol	Chain	Res	Type
1	A	138	GLU
1	A	143	GLU
1	A	154	LEU
1	A	156	ASN
1	A	161	LEU
1	A	165	ASP
1	A	172	SER
1	A	177	THR
1	A	187	ASN
1	A	194	LYS
1	A	208	ARG
1	A	216	LYS
1	A	232	VAL
1	A	245	THR
1	A	246	SER
1	A	249	GLU
1	A	270	THR
1	A	271	VAL
1	A	284	SER
1	A	290	VAL
1	A	325	LYS
1	A	327	LYS
1	B	2	SER
1	B	7	THR
1	B	21	ARG
1	B	28	GLU
1	B	30	VAL
1	B	31	VAL
1	B	48	ARG
1	B	50	GLN
1	B	53	THR
1	B	64	CYS
1	B	67	VAL
1	B	70	VAL
1	B	76	PRO
1	B	79	ARG
1	B	89	ARG
1	B	93	GLU
1	B	105	ARG
1	B	112	VAL
1	B	137	LEU
1	B	139	ASN

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Mol	Chain	Res	Type
1	B	144	SER
1	B	149	ASN
1	B	152	LYS
1	B	153	GLU
1	B	154	LEU
1	B	158	ASN
1	B	161	LEU
1	B	174	LEU
1	B	182	GLU
1	B	211	SER
1	B	227	PRO
1	B	232	VAL
1	B	236	ARG
1	B	238	ARG
1	B	239	ASN
1	B	240	ILE
1	B	243	SER
1	B	252	VAL
1	B	274	HIS
1	B	282	ASN
1	B	296	ARG
1	B	304	ASP
1	B	307	ARG
1	B	311	VAL
1	B	318	SER
1	B	325	LYS
1	B	327	LYS
1	C	1	ASP
1	C	5	ARG
1	C	7	THR
1	C	21	ARG
1	C	31	VAL
1	C	32	ASN
1	C	54	GLU
1	C	64	CYS
1	C	67	VAL
1	C	74	GLN
1	C	78	ASN
1	C	94	LEU
1	C	114	LYS
1	C	120	GLU
1	C	142	ASP

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Mol	Chain	Res	Type
1	C	154	LEU
1	C	161	LEU
1	C	167	ARG
1	C	174	LEU
1	C	183	ARG
1	C	187	ASN
1	C	208	ARG
1	C	210	SER
1	C	213	ASP
1	C	246	SER
1	C	263	THR
1	C	270	THR
1	C	271	VAL
1	C	274	HIS
1	C	296	ARG
1	C	307	ARG
1	C	311	VAL
1	C	325	LYS
1	C	326	VAL
1	C	327	LYS
1	D	3	ASP
1	D	5	ARG
1	D	7	THR
1	D	14	ASP
1	D	21	ARG
1	D	30	VAL
1	D	32	ASN
1	D	36	ARG
1	D	48	ARG
1	D	50	GLN
1	D	54	GLU
1	D	55	GLU
1	D	58	GLU
1	D	61	SER
1	D	64	CYS
1	D	67	VAL
1	D	71	ASN
1	D	74	GLN
1	D	78	ASN
1	D	89	ARG
1	D	121	LYS
1	D	124	GLN

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Mol	Chain	Res	Type
1	D	134	ASN
1	D	137	LEU
1	D	139	ASN
1	D	144	SER
1	D	148	ASP
1	D	154	LEU
1	D	156	ASN
1	D	162	ARG
1	D	174	LEU
1	D	176	ASN
1	D	177	THR
1	D	179	SER
1	D	184	ASN
1	D	187	ASN
1	D	207	ASP
1	D	208	ARG
1	D	210	SER
1	D	215	ARG
1	D	229	THR
1	D	232	VAL
1	D	263	THR
1	D	270	THR
1	D	271	VAL
1	D	273	THR
1	D	274	HIS
1	D	296	ARG
1	D	307	ARG
1	D	326	VAL
1	D	328	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	33	ASN
1	A	44	HIS
1	A	92	ASN
1	A	156	ASN
1	A	201	HIS
1	A	279	HIS
1	A	297	ASN
1	B	33	ASN

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Mol	Chain	Res	Type
1	B	44	HIS
1	B	50	GLN
1	B	56	GLN
1	B	71	ASN
1	B	74	GLN
1	B	78	ASN
1	B	124	GLN
1	B	134	ASN
1	B	206	GLN
1	B	279	HIS
1	C	32	ASN
1	C	33	ASN
1	C	44	HIS
1	C	78	ASN
1	C	96	ASN
1	C	124	GLN
1	C	176	ASN
1	C	187	ASN
1	C	279	HIS
1	C	328	GLN
1	D	71	ASN
1	D	78	ASN
1	D	96	ASN
1	D	158	ASN
1	D	176	ASN
1	D	201	HIS
1	D	279	HIS
1	D	320	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 carbohydrates 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	331/331 (100%)	-0.43	3 (0%) 85 85	7, 24, 48, 67	0
1	B	331/331 (100%)	-0.68	0 100 100	5, 19, 38, 60	0
1	C	331/331 (100%)	-0.59	1 (0%) 94 94	7, 20, 41, 63	0
1	D	331/331 (100%)	-0.31	3 (0%) 85 85	10, 31, 53, 71	0
All	All	1324/1324 (100%)	-0.50	7 (0%) 91 91	5, 23, 48, 71	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	101	SER	3.1
1	A	247	PRO	2.5
1	A	248	GLY	2.4
1	A	244	PRO	2.3
1	D	88	ASP	2.3
1	C	246	SER	2.1
1	D	3	ASP	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 carbohydrates 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.