



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 11:56 PM GMT

PDB ID : 5TLN  
Title : BINDING OF HYDROXAMIC ACID INHIBITORS TO CRYSTALLINE  
THERMOLYSIN SUGGESTS A PENTACOORDINATE ZINC INTERME-  
DIATE IN CATALYSIS  
Authors : Matthews, B.W.; Holmes, M.A.  
Deposited on : 1982-02-08  
Resolution : 2.30 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

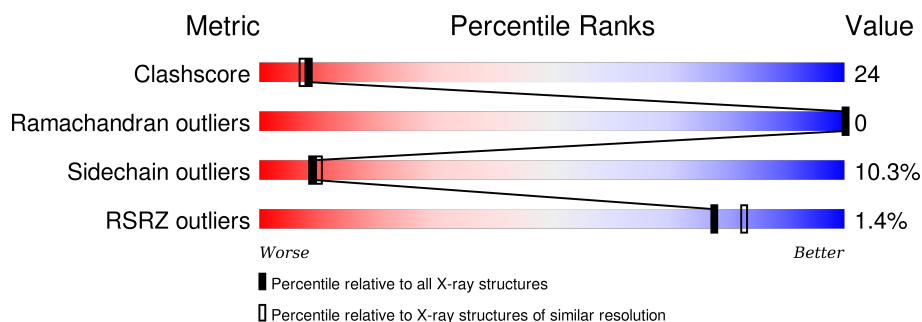
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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	4452 (2.30-2.30)
Ramachandran outliers	100387	4410 (2.30-2.30)
Sidechain outliers	100360	4409 (2.30-2.30)
RSRZ outliers	91569	3857 (2.30-2.30)

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	316	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BAN	A	322	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 2606 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 THERMOLYSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	316	Total	C	N	O	S	0	0	0
			2432	1528	408	494	2			

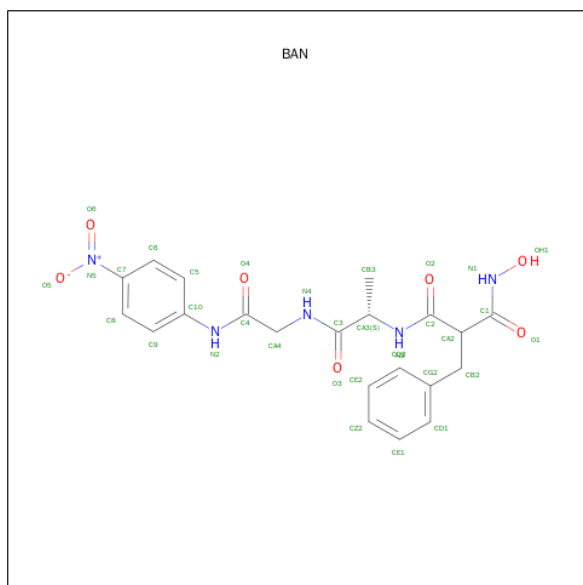
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	4	Total	Ca	0	0
			4	4		

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		

- Molecule 4 is HONH-BENZYL MALONYL-L-ALANYLGLYCINE-P-NITROANILIDE (three-letter code: BAN) (formula: C<sub>21</sub>H<sub>23</sub>N<sub>5</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			23	15	3	5		

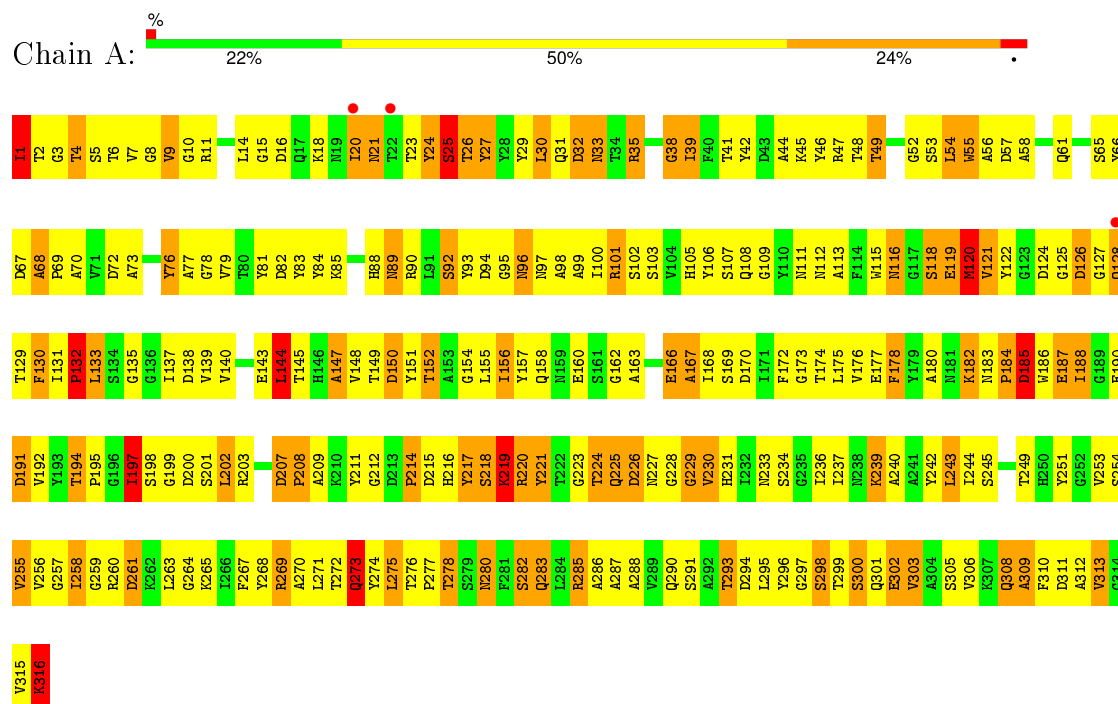
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	146	Total O 146 146	0	0

### 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 ( $RSRZ > 2$ ). 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: THERMOLYSIN



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.20 Å 94.20 Å 131.40 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 22.63 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 76.6 (22.63-2.31)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	88777.78 (at 2.31 Å)	Xtriage
Refinement program	TNT	Depositor
R, $R_{free}$	0.179 , (Not available) 0.162 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	18.6	Xtriage
Anisotropy	0.037	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 59.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 11989 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	2606	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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 ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BAN, ZN, CA

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	2.29	107/2491 (4.3%)	3.28	332/3391 (9.8%)

All (107) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ARG	CG-CD	12.22	1.82	1.51
1	A	35	ARG	C-N	-9.76	1.15	1.33
1	A	102	SER	CA-CB	9.60	1.67	1.52
1	A	25	SER	CB-OG	9.05	1.54	1.42
1	A	166	GLU	CD-OE1	-8.95	1.15	1.25
1	A	144	LEU	C-O	8.68	1.39	1.23
1	A	302	GLU	CD-OE2	-8.64	1.16	1.25
1	A	186	TRP	CG-CD2	8.60	1.58	1.43
1	A	119	GLU	CD-OE1	-8.56	1.16	1.25
1	A	265	LYS	CA-CB	-8.30	1.35	1.53
1	A	95	GLY	C-O	7.91	1.36	1.23
1	A	65	SER	C-O	7.80	1.38	1.23
1	A	20	ILE	C-O	7.76	1.38	1.23
1	A	190	GLU	CD-OE1	-7.66	1.17	1.25
1	A	187	GLU	CD-OE2	7.64	1.34	1.25
1	A	8	GLY	N-CA	7.61	1.57	1.46
1	A	44	ALA	C-O	7.53	1.37	1.23
1	A	10	GLY	C-N	-7.46	1.16	1.34
1	A	38	GLY	CA-C	-7.43	1.40	1.51
1	A	282	SER	CA-CB	-7.43	1.41	1.52
1	A	278	THR	CB-OG1	7.40	1.58	1.43
1	A	53	SER	CA-CB	7.28	1.63	1.52
1	A	11	ARG	NE-CZ	7.23	1.42	1.33
1	A	108	GLN	C-O	7.13	1.36	1.23
1	A	267	PHE	C-O	6.97	1.36	1.23
1	A	260	ARG	C-N	-6.88	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ARG	NE-CZ	-6.88	1.24	1.33
1	A	115	TRP	CD2-CE2	-6.84	1.33	1.41
1	A	118	SER	CB-OG	-6.71	1.33	1.42
1	A	101	ARG	CZ-NH2	6.60	1.41	1.33
1	A	118	SER	CA-CB	-6.47	1.43	1.52
1	A	194	THR	CB-OG1	6.47	1.56	1.43
1	A	297	GLY	N-CA	-6.47	1.36	1.46
1	A	98	ALA	C-O	6.39	1.35	1.23
1	A	119	GLU	CB-CG	-6.30	1.40	1.52
1	A	214	PRO	CA-CB	-6.29	1.41	1.53
1	A	230	VAL	CB-CG1	-6.27	1.39	1.52
1	A	93	TYR	CG-CD1	-6.26	1.31	1.39
1	A	9	VAL	C-O	6.20	1.35	1.23
1	A	52	GLY	C-O	6.17	1.33	1.23
1	A	152	THR	N-CA	6.17	1.58	1.46
1	A	242	TYR	CZ-OH	6.05	1.48	1.37
1	A	116	ASN	CG-ND2	-6.04	1.17	1.32
1	A	96	ASN	CG-OD1	6.04	1.37	1.24
1	A	160	GLU	CG-CD	-6.04	1.42	1.51
1	A	265	LYS	CB-CG	-6.01	1.36	1.52
1	A	10	GLY	C-O	5.98	1.33	1.23
1	A	199	GLY	CA-C	-5.98	1.42	1.51
1	A	305	SER	CB-OG	-5.88	1.34	1.42
1	A	245	SER	CB-OG	5.84	1.49	1.42
1	A	88	HIS	CA-C	-5.83	1.37	1.52
1	A	308	GLN	CD-NE2	5.83	1.47	1.32
1	A	127	GLY	C-O	5.80	1.32	1.23
1	A	225	GLN	C-O	5.74	1.34	1.23
1	A	173	GLY	CA-C	-5.74	1.42	1.51
1	A	264	GLY	CA-C	-5.72	1.42	1.51
1	A	297	GLY	C-N	-5.72	1.20	1.34
1	A	11	ARG	CZ-NH2	5.71	1.40	1.33
1	A	212	GLY	C-O	5.70	1.32	1.23
1	A	160	GLU	CD-OE1	-5.68	1.19	1.25
1	A	316	LYS	C-OXT	5.68	1.34	1.23
1	A	198	SER	N-CA	5.66	1.57	1.46
1	A	92	SER	CB-OG	5.65	1.49	1.42
1	A	46	TYR	CB-CG	-5.65	1.43	1.51
1	A	4	THR	N-CA	5.64	1.57	1.46
1	A	81	TYR	CG-CD1	-5.64	1.31	1.39
1	A	297	GLY	C-O	-5.62	1.14	1.23
1	A	255	VAL	CB-CG1	-5.61	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	208	PRO	N-CA	-5.58	1.37	1.47
1	A	273	GLN	C-O	5.56	1.33	1.23
1	A	93	TYR	N-CA	5.55	1.57	1.46
1	A	203	ARG	CZ-NH2	5.55	1.40	1.33
1	A	162	GLY	C-O	5.51	1.32	1.23
1	A	44	ALA	CA-CB	-5.49	1.41	1.52
1	A	4	THR	C-O	5.47	1.33	1.23
1	A	115	TRP	NE1-CE2	5.46	1.44	1.37
1	A	306	VAL	C-O	5.46	1.33	1.23
1	A	265	LYS	CD-CE	5.46	1.65	1.51
1	A	168	ILE	C-O	5.40	1.33	1.23
1	A	39	ILE	C-N	-5.40	1.21	1.34
1	A	182	LYS	CE-NZ	5.39	1.62	1.49
1	A	217	TYR	C-O	5.39	1.33	1.23
1	A	132	PRO	N-CD	5.34	1.55	1.47
1	A	278	THR	C-N	-5.33	1.21	1.34
1	A	295	LEU	N-CA	-5.33	1.35	1.46
1	A	290	GLN	C-O	5.30	1.33	1.23
1	A	302	GLU	CD-OE1	-5.28	1.19	1.25
1	A	101	ARG	CZ-NH1	5.28	1.40	1.33
1	A	105	HIS	C-N	-5.27	1.22	1.34
1	A	47	ARG	NE-CZ	-5.26	1.26	1.33
1	A	76	TYR	C-N	-5.25	1.22	1.34
1	A	11	ARG	C-N	-5.23	1.23	1.33
1	A	3	GLY	C-O	5.23	1.32	1.23
1	A	55	TRP	CD2-CE2	-5.20	1.35	1.41
1	A	24	TYR	C-O	5.15	1.33	1.23
1	A	78	GLY	CA-C	5.14	1.60	1.51
1	A	39	ILE	CA-CB	5.11	1.66	1.54
1	A	58	ALA	CA-CB	5.08	1.63	1.52
1	A	10	GLY	N-CA	5.07	1.53	1.46
1	A	55	TRP	NE1-CE2	5.06	1.44	1.37
1	A	265	LYS	N-CA	5.05	1.56	1.46
1	A	177	GLU	CG-CD	-5.02	1.44	1.51
1	A	149	THR	C-O	5.02	1.32	1.23
1	A	45	LYS	CE-NZ	5.00	1.61	1.49
1	A	126	ASP	C-N	-5.00	1.24	1.33
1	A	265	LYS	CE-NZ	5.00	1.61	1.49
1	A	148	VAL	C-O	5.00	1.32	1.23

All (332) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	47	ARG	NE-CZ-NH1	24.91	132.75	120.30
1	A	211	TYR	CB-CG-CD2	-24.86	106.09	121.00
1	A	47	ARG	CD-NE-CZ	22.68	155.35	123.60
1	A	101	ARG	CD-NE-CZ	22.42	154.99	123.60
1	A	260	ARG	NE-CZ-NH2	-18.65	110.97	120.30
1	A	90	ARG	NE-CZ-NH1	17.34	128.97	120.30
1	A	101	ARG	NE-CZ-NH1	16.75	128.67	120.30
1	A	211	TYR	CB-CG-CD1	16.61	130.97	121.00
1	A	67	ASP	CB-CG-OD1	15.73	132.46	118.30
1	A	11	ARG	NE-CZ-NH2	-14.71	112.95	120.30
1	A	138	ASP	CB-CG-OD1	14.28	131.15	118.30
1	A	29	TYR	CB-CG-CD2	14.21	129.53	121.00
1	A	143	GLU	CG-CD-OE1	13.98	146.26	118.30
1	A	200	ASP	CB-CG-OD1	13.56	130.50	118.30
1	A	27	TYR	CB-CG-CD1	13.39	129.03	121.00
1	A	27	TYR	CB-CG-CD2	-13.38	112.97	121.00
1	A	101	ARG	NE-CZ-NH2	-13.16	113.72	120.30
1	A	227	ASN	O-C-N	13.10	145.47	123.20
1	A	261	ASP	CB-CG-OD1	-13.00	106.60	118.30
1	A	182	LYS	CG-CD-CE	12.71	150.05	111.90
1	A	101	ARG	CA-CB-CG	12.59	141.09	113.40
1	A	130	PHE	CB-CG-CD1	12.46	129.52	120.80
1	A	90	ARG	NE-CZ-NH2	-12.28	114.16	120.30
1	A	29	TYR	CB-CG-CD1	-12.04	113.78	121.00
1	A	120	MET	CG-SD-CE	12.00	119.39	100.20
1	A	226	ASP	CB-CG-OD1	11.99	129.09	118.30
1	A	27	TYR	CZ-CE2-CD2	-11.58	109.38	119.80
1	A	35	ARG	NE-CZ-NH1	11.53	126.06	120.30
1	A	297	GLY	C-N-CA	11.45	150.33	121.70
1	A	11	ARG	CD-NE-CZ	-11.31	107.77	123.60
1	A	101	ARG	CG-CD-NE	-11.24	88.19	111.80
1	A	47	ARG	NE-CZ-NH2	-11.12	114.74	120.30
1	A	200	ASP	CB-CG-OD2	-11.08	108.33	118.30
1	A	101	ARG	CB-CA-C	10.67	131.74	110.40
1	A	178	PHE	CB-CG-CD2	10.64	128.25	120.80
1	A	264	GLY	CA-C-O	10.63	139.73	120.60
1	A	265	LYS	CA-CB-CG	10.55	136.60	113.40
1	A	220	ARG	NE-CZ-NH2	-10.51	115.04	120.30
1	A	315	VAL	O-C-N	10.48	139.48	122.70
1	A	198	SER	N-CA-CB	-10.45	94.83	110.50
1	A	16	ASP	CB-CG-OD2	-10.38	108.96	118.30
1	A	119	GLU	OE1-CD-OE2	10.35	135.72	123.30
1	A	39	ILE	CB-CG1-CD1	10.30	142.74	113.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	ALA	C-N-CA	10.02	146.75	121.70
1	A	282	SER	CB-CA-C	9.97	129.05	110.10
1	A	151	TYR	CB-CG-CD1	9.86	126.91	121.00
1	A	308	GLN	CG-CD-OE1	9.72	141.03	121.60
1	A	261	ASP	OD1-CG-OD2	9.58	141.50	123.30
1	A	212	GLY	CA-C-O	-9.50	103.50	120.60
1	A	126	ASP	CB-CG-OD1	-9.30	109.93	118.30
1	A	143	GLU	CG-CD-OE2	-9.18	99.93	118.30
1	A	35	ARG	NE-CZ-NH2	-9.11	115.75	120.30
1	A	66	TYR	C-N-CA	9.04	144.29	121.70
1	A	122	TYR	CG-CD2-CE2	9.00	128.50	121.30
1	A	27	TYR	CG-CD2-CE2	8.98	128.49	121.30
1	A	251	TYR	CB-CG-CD1	-8.97	115.62	121.00
1	A	130	PHE	CB-CG-CD2	-8.96	114.53	120.80
1	A	198	SER	CB-CA-C	8.91	127.03	110.10
1	A	251	TYR	CB-CG-CD2	8.76	126.26	121.00
1	A	32	ASP	CB-CG-OD1	8.68	126.11	118.30
1	A	151	TYR	CB-CG-CD2	-8.65	115.81	121.00
1	A	273	GLN	CA-CB-CG	8.64	132.41	113.40
1	A	261	ASP	N-CA-CB	-8.60	95.11	110.60
1	A	298	SER	N-CA-CB	-8.57	97.64	110.50
1	A	138	ASP	OD1-CG-OD2	-8.54	107.06	123.30
1	A	101	ARG	C-N-CA	8.51	142.99	121.70
1	A	203	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	A	162	GLY	O-C-N	-8.45	109.19	122.70
1	A	191	ASP	CB-CG-OD1	8.44	125.89	118.30
1	A	94	ASP	CB-CG-OD2	8.36	125.83	118.30
1	A	150	ASP	CB-CG-OD2	8.36	125.82	118.30
1	A	309	ALA	CB-CA-C	8.35	122.62	110.10
1	A	166	GLU	OE1-CD-OE2	-8.34	113.30	123.30
1	A	147	ALA	CB-CA-C	8.26	122.48	110.10
1	A	177	GLU	OE1-CD-OE2	-8.17	113.49	123.30
1	A	269	ARG	NE-CZ-NH2	-8.17	116.22	120.30
1	A	103	SER	O-C-N	8.17	135.77	122.70
1	A	78	GLY	CA-C-O	-8.15	105.94	120.60
1	A	274	TYR	CG-CD2-CE2	8.12	127.80	121.30
1	A	220	ARG	NH1-CZ-NH2	8.03	128.24	119.40
1	A	11	ARG	NH1-CZ-NH2	8.01	128.21	119.40
1	A	143	GLU	OE1-CD-OE2	-7.92	113.80	123.30
1	A	274	TYR	CZ-CE2-CD2	-7.88	112.71	119.80
1	A	219	LYS	CB-CG-CD	7.87	132.06	111.60
1	A	119	GLU	CG-CD-OE2	-7.86	102.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	46	TYR	CB-CG-CD2	7.85	125.71	121.00
1	A	53	SER	CA-C-O	-7.83	103.66	120.10
1	A	168	ILE	CB-CG1-CD1	7.83	135.82	113.90
1	A	270	ALA	CA-C-O	7.82	136.53	120.10
1	A	234	SER	O-C-N	-7.81	109.92	123.20
1	A	239	LYS	CB-CG-CD	7.81	131.91	111.60
1	A	38	GLY	CA-C-O	-7.80	106.55	120.60
1	A	18	LYS	O-C-N	7.79	135.16	122.70
1	A	84	TYR	CB-CG-CD2	7.76	125.66	121.00
1	A	270	ALA	O-C-N	-7.74	110.32	122.70
1	A	290	GLN	CA-CB-CG	-7.69	96.47	113.40
1	A	308	GLN	CG-CD-NE2	-7.64	98.36	116.70
1	A	119	GLU	N-CA-CB	-7.64	96.86	110.60
1	A	14	LEU	CB-CG-CD1	7.55	123.84	111.00
1	A	46	TYR	CB-CG-CD1	-7.51	116.50	121.00
1	A	53	SER	CB-CA-C	-7.47	95.91	110.10
1	A	264	GLY	O-C-N	-7.45	110.79	122.70
1	A	9	VAL	CB-CA-C	-7.44	97.26	111.40
1	A	45	LYS	CB-CA-C	-7.39	95.62	110.40
1	A	2	THR	CA-C-N	7.38	130.96	116.20
1	A	167	ALA	CB-CA-C	7.38	121.17	110.10
1	A	56	ALA	CA-C-O	7.31	135.46	120.10
1	A	268	TYR	CB-CG-CD1	7.30	125.38	121.00
1	A	282	SER	N-CA-CB	-7.28	99.58	110.50
1	A	231	HIS	N-CA-CB	7.26	123.67	110.60
1	A	259	GLY	O-C-N	-7.25	111.11	122.70
1	A	211	TYR	CA-CB-CG	-7.24	99.65	113.40
1	A	101	ARG	CB-CG-CD	7.20	130.33	111.60
1	A	47	ARG	NH1-CZ-NH2	-7.19	111.49	119.40
1	A	261	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	A	217	TYR	CG-CD2-CE2	-7.18	115.56	121.30
1	A	122	TYR	CZ-CE2-CD2	-7.17	113.34	119.80
1	A	220	ARG	NE-CZ-NH1	-7.16	116.72	120.30
1	A	167	ALA	O-C-N	-7.14	111.27	122.70
1	A	225	GLN	CB-CA-C	7.13	124.67	110.40
1	A	26	THR	CA-CB-CG2	7.12	122.38	112.40
1	A	85	LYS	O-C-N	-7.10	111.34	122.70
1	A	285	ARG	NE-CZ-NH1	6.98	123.79	120.30
1	A	72	ASP	CB-CG-OD2	6.97	124.58	118.30
1	A	296	TYR	CB-CG-CD1	6.94	125.16	121.00
1	A	224	THR	CA-CB-CG2	6.92	122.09	112.40
1	A	85	LYS	CA-C-O	6.92	134.63	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	9	VAL	CA-CB-CG1	6.91	121.27	110.90
1	A	197	ILE	CA-C-O	6.90	134.58	120.10
1	A	163	ALA	C-N-CA	6.85	138.82	121.70
1	A	315	VAL	CA-C-N	-6.83	102.17	117.20
1	A	158	GLN	N-CA-CB	6.82	122.87	110.60
1	A	48	THR	O-C-N	-6.82	111.80	122.70
1	A	77	ALA	N-CA-CB	6.82	119.64	110.10
1	A	258	ILE	O-C-N	-6.81	111.63	123.20
1	A	140	VAL	O-C-N	-6.80	111.82	122.70
1	A	184	PRO	O-C-N	6.80	133.58	122.70
1	A	56	ALA	O-C-N	-6.78	111.86	122.70
1	A	113	ALA	CA-C-N	6.73	132.00	117.20
1	A	45	LYS	CB-CG-CD	6.71	129.05	111.60
1	A	312	ALA	C-N-CA	6.68	138.41	121.70
1	A	61	GLN	O-C-N	6.65	133.34	122.70
1	A	85	LYS	CA-CB-CG	-6.65	98.77	113.40
1	A	224	THR	N-CA-C	6.65	128.96	111.00
1	A	256	VAL	CG1-CB-CG2	-6.64	100.27	110.90
1	A	101	ARG	N-CA-CB	-6.64	98.65	110.60
1	A	66	TYR	CG-CD2-CE2	6.63	126.61	121.30
1	A	124	ASP	CB-CG-OD1	-6.63	112.34	118.30
1	A	42	TYR	CZ-CE2-CD2	-6.61	113.86	119.80
1	A	45	LYS	O-C-N	6.60	133.26	122.70
1	A	88	HIS	CA-CB-CG	-6.59	102.39	113.60
1	A	186	TRP	CA-C-N	-6.57	102.75	117.20
1	A	267	PHE	CB-CG-CD1	6.53	125.37	120.80
1	A	129	THR	O-C-N	-6.51	112.28	122.70
1	A	115	TRP	CA-C-N	6.50	131.50	117.20
1	A	293	THR	O-C-N	6.49	133.09	122.70
1	A	130	PHE	CB-CA-C	-6.46	97.49	110.40
1	A	49	THR	CA-CB-OG1	-6.43	95.49	109.00
1	A	186	TRP	CD1-CG-CD2	-6.43	101.16	106.30
1	A	263	LEU	O-C-N	-6.42	112.28	123.20
1	A	156	ILE	CA-CB-CG2	6.42	123.73	110.90
1	A	157	TYR	CZ-CE2-CD2	-6.40	114.04	119.80
1	A	211	TYR	CB-CA-C	-6.39	97.62	110.40
1	A	57	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	54	LEU	O-C-N	6.37	132.89	122.70
1	A	113	ALA	CA-C-O	-6.35	106.76	120.10
1	A	126	ASP	CB-CG-OD2	6.34	124.00	118.30
1	A	260	ARG	NH1-CZ-NH2	6.31	126.34	119.40
1	A	85	LYS	N-CA-CB	-6.25	99.36	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	TYR	O-C-N	6.24	133.81	123.20
1	A	108	GLN	CG-CD-OE1	-6.19	109.23	121.60
1	A	89	ASN	CB-CG-OD1	-6.18	109.23	121.60
1	A	157	TYR	CB-CG-CD2	6.18	124.71	121.00
1	A	90	ARG	CG-CD-NE	-6.15	98.88	111.80
1	A	82	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	212	GLY	O-C-N	6.10	132.46	122.70
1	A	201	SER	CA-CB-OG	-6.09	94.77	111.20
1	A	288	ALA	O-C-N	-6.09	112.96	122.70
1	A	65	SER	CB-CA-C	6.08	121.64	110.10
1	A	265	LYS	CD-CE-NZ	-6.08	97.73	111.70
1	A	296	TYR	C-N-CA	6.08	135.06	122.30
1	A	242	TYR	C-N-CA	6.06	136.86	121.70
1	A	47	ARG	C-N-CA	6.06	136.84	121.70
1	A	169	SER	O-C-N	-6.04	113.03	122.70
1	A	287	ALA	CB-CA-C	-6.04	101.05	110.10
1	A	217	TYR	CB-CG-CD1	-6.02	117.39	121.00
1	A	310	PHE	CG-CD1-CE1	-6.02	114.18	120.80
1	A	93	TYR	N-CA-CB	-6.00	99.80	110.60
1	A	275	LEU	CB-CA-C	6.00	121.59	110.20
1	A	1	ILE	CA-CB-CG1	-5.99	99.62	111.00
1	A	14	LEU	CA-C-N	5.97	128.15	116.20
1	A	288	ALA	C-N-CA	5.97	136.63	121.70
1	A	41	THR	CA-C-N	-5.97	104.07	117.20
1	A	233	ASN	O-C-N	5.96	132.24	122.70
1	A	170	ASP	N-CA-CB	5.96	121.32	110.60
1	A	33	ASN	N-CA-CB	-5.95	99.89	110.60
1	A	9	VAL	CA-C-N	5.94	128.09	116.20
1	A	278	THR	CA-CB-CG2	-5.94	104.08	112.40
1	A	300	SER	CA-C-O	5.94	132.57	120.10
1	A	81	TYR	CG-CD1-CE1	5.93	126.04	121.30
1	A	178	PHE	CE1-CZ-CE2	-5.92	109.35	120.00
1	A	243	LEU	O-C-N	-5.92	113.24	122.70
1	A	288	ALA	N-CA-CB	-5.91	101.83	110.10
1	A	186	TRP	O-C-N	5.90	132.14	122.70
1	A	186	TRP	CB-CG-CD1	5.90	134.67	127.00
1	A	166	GLU	CA-C-O	-5.90	107.72	120.10
1	A	53	SER	CA-C-N	5.89	130.17	117.20
1	A	291	SER	CB-CA-C	-5.89	98.90	110.10
1	A	24	TYR	CD1-CE1-CZ	-5.89	114.50	119.80
1	A	185	ASP	CB-CG-OD1	-5.89	113.00	118.30
1	A	221	TYR	CB-CG-CD1	-5.89	117.47	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	283	GLN	CA-CB-CG	-5.88	100.45	113.40
1	A	157	TYR	CG-CD2-CE2	5.88	126.00	121.30
1	A	257	GLY	CA-C-O	-5.87	110.04	120.60
1	A	227	ASN	CA-C-O	-5.85	107.81	120.10
1	A	251	TYR	CZ-CE2-CD2	-5.85	114.53	119.80
1	A	215	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	84	TYR	CZ-CE2-CD2	5.83	125.05	119.80
1	A	178	PHE	CZ-CE2-CD2	5.82	127.08	120.10
1	A	135	GLY	CA-C-O	5.80	131.04	120.60
1	A	186	TRP	CZ3-CH2-CZ2	-5.78	114.67	121.60
1	A	211	TYR	O-C-N	5.77	133.01	123.20
1	A	8	GLY	O-C-N	-5.76	113.48	122.70
1	A	288	ALA	CB-CA-C	5.76	118.74	110.10
1	A	103	SER	CA-C-O	-5.74	108.04	120.10
1	A	223	GLY	C-N-CA	5.74	136.05	121.70
1	A	29	TYR	CZ-CE2-CD2	5.73	124.95	119.80
1	A	108	GLN	O-C-N	5.72	132.92	123.20
1	A	4	THR	CA-CB-CG2	5.71	120.40	112.40
1	A	183	ASN	CB-CG-OD1	-5.68	110.25	121.60
1	A	81	TYR	CB-CG-CD1	5.67	124.41	121.00
1	A	260	ARG	C-N-CA	5.67	135.86	121.70
1	A	38	GLY	N-CA-C	5.66	127.25	113.10
1	A	83	TYR	CD1-CE1-CZ	-5.66	114.71	119.80
1	A	242	TYR	CA-C-N	5.65	129.62	117.20
1	A	21	ASN	CB-CG-OD1	5.64	132.88	121.60
1	A	155	LEU	CB-CG-CD1	5.63	120.58	111.00
1	A	70	ALA	O-C-N	-5.62	113.71	122.70
1	A	5	SER	N-CA-CB	5.62	118.93	110.50
1	A	46	TYR	CD1-CE1-CZ	-5.61	114.75	119.80
1	A	149	THR	CA-CB-CG2	5.57	120.20	112.40
1	A	21	ASN	CA-CB-CG	-5.57	101.16	113.40
1	A	311	ASP	O-C-N	-5.56	113.81	122.70
1	A	92	SER	C-N-CA	-5.55	107.83	121.70
1	A	275	LEU	O-C-N	5.54	131.56	122.70
1	A	106	TYR	CZ-CE2-CD2	5.53	124.77	119.80
1	A	207	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	254	SER	CA-CB-OG	5.52	126.09	111.20
1	A	133	LEU	CA-C-N	5.51	129.33	117.20
1	A	1	ILE	O-C-N	-5.51	113.88	122.70
1	A	211	TYR	CA-C-O	-5.51	108.53	120.10
1	A	2	THR	O-C-N	-5.51	113.84	123.20
1	A	299	THR	CA-CB-CG2	-5.49	104.71	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187	GLU	CG-CD-OE1	5.47	129.24	118.30
1	A	180	ALA	CB-CA-C	5.47	118.30	110.10
1	A	188	ILE	CA-CB-CG1	-5.47	100.61	111.00
1	A	217	TYR	CD1-CE1-CZ	-5.47	114.88	119.80
1	A	44	ALA	C-N-CA	5.47	135.36	121.70
1	A	30	LEU	C-N-CA	5.46	135.35	121.70
1	A	18	LYS	CG-CD-CE	5.46	128.27	111.90
1	A	73	ALA	N-CA-CB	-5.45	102.47	110.10
1	A	76	TYR	CZ-CE2-CD2	-5.44	114.90	119.80
1	A	224	THR	CA-CB-OG1	-5.44	97.58	109.00
1	A	274	TYR	N-CA-CB	-5.43	100.83	110.60
1	A	96	ASN	O-C-N	5.43	131.38	122.70
1	A	236	ILE	CA-CB-CG2	-5.42	100.06	110.90
1	A	156	ILE	CB-CG1-CD1	-5.41	98.75	113.90
1	A	265	LYS	O-C-N	-5.40	114.06	122.70
1	A	122	TYR	C-N-CA	-5.39	110.99	122.30
1	A	274	TYR	CB-CG-CD2	5.37	124.22	121.00
1	A	191	ASP	OD1-CG-OD2	-5.37	113.10	123.30
1	A	260	ARG	CA-CB-CG	5.37	125.21	113.40
1	A	14	LEU	CB-CG-CD2	-5.36	101.89	111.00
1	A	268	TYR	O-C-N	-5.36	114.13	122.70
1	A	45	LYS	N-CA-CB	5.35	120.23	110.60
1	A	116	ASN	CA-C-N	5.35	126.89	116.20
1	A	148	VAL	CA-C-N	5.34	128.96	117.20
1	A	133	LEU	CA-CB-CG	-5.34	103.02	115.30
1	A	315	VAL	CA-CB-CG1	5.33	118.90	110.90
1	A	236	ILE	CB-CG1-CD1	5.33	128.82	113.90
1	A	25	SER	CA-CB-OG	-5.32	96.83	111.20
1	A	224	THR	C-N-CA	-5.32	108.40	121.70
1	A	168	ILE	CA-CB-CG1	-5.32	100.90	111.00
1	A	76	TYR	CA-C-O	-5.31	108.95	120.10
1	A	286	ALA	CA-C-O	5.31	131.25	120.10
1	A	41	THR	O-C-N	5.30	131.18	122.70
1	A	183	ASN	N-CA-CB	-5.30	101.06	110.60
1	A	259	GLY	CA-C-O	5.29	130.13	120.60
1	A	316	LYS	N-CA-CB	-5.29	101.07	110.60
1	A	128	GLN	CA-CB-CG	-5.29	101.77	113.40
1	A	310	PHE	CZ-CE2-CD2	-5.27	113.78	120.10
1	A	255	VAL	CG1-CB-CG2	5.26	119.31	110.90
1	A	79	VAL	CG1-CB-CG2	5.25	119.31	110.90
1	A	218	SER	CB-CA-C	-5.25	100.12	110.10
1	A	301	GLN	CG-CD-OE1	5.25	132.09	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	106	TYR	CB-CG-CD2	5.25	124.15	121.00
1	A	47	ARG	CG-CD-NE	-5.24	100.79	111.80
1	A	42	TYR	CG-CD1-CE1	-5.23	117.11	121.30
1	A	187	GLU	OE1-CD-OE2	-5.23	117.03	123.30
1	A	186	TRP	CH2-CZ2-CE2	5.21	122.61	117.40
1	A	198	SER	CA-CB-OG	5.21	125.26	111.20
1	A	301	GLN	OE1-CD-NE2	-5.19	109.96	121.90
1	A	15	GLY	CA-C-O	5.19	129.93	120.60
1	A	121	VAL	N-CA-CB	-5.19	100.09	111.50
1	A	8	GLY	CA-C-N	5.18	128.60	117.20
1	A	106	TYR	N-CA-CB	-5.18	101.27	110.60
1	A	260	ARG	CA-C-N	5.18	128.60	117.20
1	A	192	VAL	CA-CB-CG2	5.17	118.65	110.90
1	A	202	LEU	CB-CA-C	5.17	120.02	110.20
1	A	115	TRP	CA-C-O	-5.16	109.26	120.10
1	A	265	LYS	CB-CG-CD	-5.16	98.19	111.60
1	A	73	ALA	CA-C-O	5.14	130.90	120.10
1	A	145	THR	CA-CB-CG2	-5.13	105.21	112.40
1	A	148	VAL	CA-C-O	-5.12	109.34	120.10
1	A	83	TYR	CG-CD1-CE1	5.11	125.39	121.30
1	A	174	THR	CA-C-N	5.08	128.38	117.20
1	A	23	THR	CA-C-N	-5.08	106.03	117.20
1	A	229	GLY	C-N-CA	5.08	134.39	121.70
1	A	209	ALA	C-N-CA	5.07	134.38	121.70
1	A	197	ILE	O-C-N	-5.07	114.60	122.70
1	A	184	PRO	CA-C-O	-5.06	108.05	120.20
1	A	7	VAL	CA-C-O	-5.06	109.47	120.10
1	A	94	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	A	102	SER	CB-CA-C	-5.06	100.49	110.10
1	A	96	ASN	OD1-CG-ND2	5.05	133.53	121.90
1	A	67	ASP	OD1-CG-OD2	-5.05	113.70	123.30
1	A	239	LYS	CG-CD-CE	5.05	127.04	111.90
1	A	157	TYR	CA-C-N	5.04	128.29	117.20
1	A	296	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	A	68	ALA	CB-CA-C	5.03	117.64	110.10
1	A	251	TYR	CG-CD2-CE2	5.03	125.32	121.30
1	A	303	VAL	CA-CB-CG1	5.03	118.44	110.90

There are no chirality outliers.

There are no planarity outliers.

## 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	2432	0	2249	113	1
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	23	0	15	3	0
5	A	146	0	0	34	10
All	All	2606	0	2264	113	10

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 24.

All (113) 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:A:101:ARG:CG	1:A:101:ARG:CD	1.82	1.51
1:A:92:SER:CB	5:A:451:HOH:O	1.88	1.19
1:A:92:SER:OG	5:A:451:HOH:O	1.65	1.15
1:A:118:SER:N	5:A:442:HOH:O	1.78	1.13
1:A:308:GLN:HG2	5:A:388:HOH:O	1.52	1.09
1:A:92:SER:HA	5:A:451:HOH:O	1.52	1.08
1:A:228:GLY:C	5:A:382:HOH:O	1.94	1.04
1:A:218:SER:HB3	5:A:435:HOH:O	1.54	1.03
1:A:101:ARG:CG	1:A:101:ARG:NE	2.29	0.96
1:A:119:GLU:OE1	5:A:447:HOH:O	1.85	0.94
1:A:219:LYS:HE2	5:A:391:HOH:O	1.72	0.89
1:A:228:GLY:CA	5:A:382:HOH:O	2.26	0.82
1:A:219:LYS:CE	5:A:391:HOH:O	2.26	0.81
1:A:278:THR:HG22	1:A:278:THR:O	1.82	0.80
1:A:216:HIS:ND1	5:A:435:HOH:O	2.17	0.78
1:A:116:ASN:OD1	5:A:442:HOH:O	2.02	0.77
1:A:111:ASN:O	1:A:112:ASN:HB2	1.83	0.77
1:A:137:ILE:HG22	1:A:182:LYS:NZ	2.00	0.76
1:A:269:ARG:NH1	1:A:294:ASP:OD2	2.18	0.76
1:A:228:GLY:HA2	5:A:382:HOH:O	1.85	0.73
1:A:197:ILE:N	1:A:197:ILE:HD13	2.05	0.71
1:A:273:GLN:CG	5:A:372:HOH:O	2.38	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HG22	1:A:182:LYS:HZ3	1.54	0.70
1:A:131:ILE:HB	1:A:132:PRO:CD	2.21	0.70
1:A:280:ASN:ND2	1:A:283:GLN:H	1.90	0.69
1:A:216:HIS:CE1	5:A:435:HOH:O	2.46	0.68
1:A:273:GLN:HG3	5:A:372:HOH:O	1.94	0.67
1:A:1:ILE:N	1:A:31:GLN:HE22	1.92	0.67
1:A:128:GLN:O	1:A:195:PRO:HD2	1.96	0.66
1:A:150:ASP:HA	5:A:379:HOH:O	1.94	0.66
1:A:191:ASP:HB2	5:A:350:HOH:O	1.94	0.65
1:A:278:THR:O	1:A:278:THR:CG2	2.45	0.65
1:A:280:ASN:C	1:A:280:ASN:HD22	2.00	0.65
1:A:217:TYR:O	1:A:220:ARG:HB2	1.97	0.64
1:A:273:GLN:HB3	5:A:372:HOH:O	1.96	0.64
1:A:144:LEU:O	1:A:147:ALA:HB3	1.96	0.64
1:A:187:GLU:OE1	5:A:411:HOH:O	2.15	0.63
1:A:120:MET:SD	1:A:144:LEU:HD23	2.38	0.62
1:A:229:GLY:N	5:A:382:HOH:O	2.26	0.62
1:A:30:LEU:HB2	1:A:55:TRP:HB3	1.81	0.62
1:A:101:ARG:HG3	1:A:101:ARG:NE	2.12	0.61
1:A:131:ILE:HG23	1:A:195:PRO:HG3	1.82	0.61
1:A:152:THR:HG21	1:A:272:THR:HG22	1.84	0.60
1:A:126:ASP:OD2	1:A:128:GLN:N	2.31	0.58
1:A:172:PHE:O	1:A:176:VAL:HG23	2.04	0.58
1:A:33:ASN:ND2	5:A:459:HOH:O	2.37	0.57
1:A:273:GLN:CB	5:A:372:HOH:O	2.53	0.56
1:A:188:ILE:HG22	4:A:322:BAN:H15	1.89	0.55
1:A:276:THR:HB	1:A:277:PRO:CD	2.37	0.55
1:A:282:SER:HA	1:A:316:LYS:HD2	1.88	0.54
1:A:240:ALA:O	1:A:244:ILE:HG13	2.08	0.53
1:A:120:MET:C	1:A:121:VAL:HG23	2.28	0.52
1:A:308:GLN:CG	5:A:388:HOH:O	2.31	0.52
1:A:207:ASP:OD1	5:A:361:HOH:O	2.18	0.52
1:A:137:ILE:H	1:A:182:LYS:HZ2	1.56	0.52
1:A:131:ILE:HB	1:A:132:PRO:HD2	1.93	0.51
1:A:100:ILE:HD11	5:A:451:HOH:O	2.10	0.51
1:A:271:LEU:HA	1:A:275:LEU:HD12	1.93	0.51
1:A:214:PRO:HB3	1:A:219:LYS:HB3	1.92	0.50
1:A:32:ASP:OD1	1:A:35:ARG:NH1	2.42	0.50
1:A:4:THR:HG22	1:A:24:TYR:HB3	1.93	0.50
1:A:35:ARG:HD2	1:A:39:ILE:HD12	1.92	0.50
1:A:285:ARG:HD3	1:A:316:LYS:HD3	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:SER:CB	5:A:435:HOH:O	2.30	0.49
1:A:111:ASN:O	1:A:112:ASN:CB	2.56	0.49
1:A:298:SER:CB	5:A:424:HOH:O	2.61	0.48
1:A:1:ILE:N	1:A:31:GLN:NE2	2.61	0.48
1:A:137:ILE:HG22	1:A:182:LYS:HZ2	1.78	0.47
1:A:131:ILE:HG21	1:A:131:ILE:HD13	1.47	0.47
1:A:133:LEU:HD12	1:A:133:LEU:H	1.79	0.47
1:A:178:PHE:CD1	1:A:184:PRO:HB2	2.49	0.47
1:A:298:SER:HB3	5:A:424:HOH:O	2.14	0.47
1:A:249:THR:HA	1:A:253:VAL:O	2.14	0.46
1:A:178:PHE:CE1	1:A:184:PRO:HB2	2.51	0.46
1:A:258:ILE:HG21	1:A:302:GLU:HA	1.97	0.46
1:A:300:SER:HB2	1:A:302:GLU:OE1	2.15	0.45
1:A:68:ALA:HB3	1:A:69:PRO:HD3	1.98	0.45
1:A:185:ASP:OD2	1:A:187:GLU:HB2	2.17	0.44
1:A:109:GLY:HA2	1:A:125:GLY:O	2.18	0.44
1:A:139:VAL:HG22	4:A:322:BAN:CZ2	2.48	0.44
1:A:92:SER:HB2	1:A:97:ASN:HA	1.99	0.43
1:A:285:ARG:CD	1:A:316:LYS:HD3	2.48	0.43
1:A:167:ALA:CB	1:A:237:ILE:HB	2.49	0.43
1:A:116:ASN:C	5:A:442:HOH:O	2.57	0.43
1:A:21:ASN:HA	1:A:21:ASN:HD22	1.49	0.43
1:A:96:ASN:O	1:A:97:ASN:HB2	2.17	0.43
1:A:32:ASP:O	1:A:38:GLY:HA2	2.19	0.43
1:A:269:ARG:HG3	1:A:273:GLN:HG2	2.00	0.43
1:A:99:ALA:CB	1:A:101:ARG:NH1	2.82	0.42
1:A:221:TYR:CD2	5:A:382:HOH:O	2.71	0.42
1:A:197:ILE:N	1:A:197:ILE:CD1	2.75	0.42
1:A:166:GLU:HG3	1:A:230:VAL:HG12	2.00	0.42
1:A:30:LEU:HA	1:A:30:LEU:HD23	1.74	0.42
1:A:221:TYR:CE2	5:A:382:HOH:O	2.57	0.42
1:A:76:TYR:OH	1:A:182:LYS:HE3	2.20	0.42
1:A:1:ILE:H2	1:A:31:GLN:HE22	1.67	0.42
1:A:130:PHE:HZ	1:A:202:LEU:HD22	1.83	0.42
1:A:154:GLY:HA2	5:A:379:HOH:O	2.19	0.42
1:A:285:ARG:HD3	1:A:316:LYS:NZ	2.35	0.42
1:A:280:ASN:C	1:A:280:ASN:ND2	2.69	0.42
1:A:202:LEU:HD12	1:A:202:LEU:HA	1.78	0.42
1:A:285:ARG:HD3	1:A:316:LYS:HZ3	1.85	0.41
1:A:217:TYR:N	1:A:313:VAL:O	2.44	0.41
1:A:25:SER:O	1:A:27:TYR:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:255:VAL:HG11	1:A:309:ALA:HB2	2.03	0.41
1:A:293:THR:HA	1:A:303:VAL:HG21	2.02	0.41
1:A:255:VAL:HG22	1:A:308:GLN:HB3	2.03	0.41
1:A:237:ILE:HD13	1:A:237:ILE:HA	1.71	0.41
1:A:128:GLN:O	1:A:194:THR:HA	2.21	0.41
1:A:226:ASP:OD1	4:A:322:BAN:H29	2.21	0.41
1:A:156:ILE:HD13	1:A:156:ILE:HG21	1.91	0.41
1:A:167:ALA:HB1	1:A:237:ILE:HB	2.03	0.40
1:A:144:LEU:HD22	1:A:144:LEU:HA	1.66	0.40

All (10) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:372:HOH:O	5:A:409:HOH:O[5_564]	1.17	1.03
5:A:369:HOH:O	5:A:407:HOH:O[5_564]	1.19	1.01
5:A:332:HOH:O	5:A:336:HOH:O[10_664]	1.34	0.86
5:A:485:HOH:O	5:A:485:HOH:O[7_555]	1.54	0.66
5:A:436:HOH:O	5:A:447:HOH:O[10_664]	1.78	0.42
5:A:372:HOH:O	5:A:463:HOH:O[5_564]	1.92	0.28
5:A:418:HOH:O	5:A:418:HOH:O[12_565]	1.95	0.25
5:A:379:HOH:O	5:A:396:HOH:O[10_664]	2.00	0.20
5:A:333:HOH:O	5:A:337:HOH:O[10_664]	2.10	0.10
1:A:6:THR:CB	5:A:473:HOH:O[12_565]	2.12	0.08

## 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	314/316 (99%)	297 (95%)	17 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	252/252 (100%)	226 (90%)	26 (10%)	9 10

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ILE
1	A	9	VAL
1	A	20	ILE
1	A	25	SER
1	A	26	THR
1	A	49	THR
1	A	54	LEU
1	A	89	ASN
1	A	107	SER
1	A	120	MET
1	A	132	PRO
1	A	144	LEU
1	A	175	LEU
1	A	185	ASP
1	A	197	ILE
1	A	208	PRO
1	A	219	LYS
1	A	224	THR
1	A	225	GLN
1	A	239	LYS
1	A	243	LEU
1	A	261	ASP
1	A	273	GLN
1	A	280	ASN
1	A	313	VAL
1	A	316	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	31	GLN
1	A	33	ASN
1	A	97	ASN
1	A	280	ASN
1	A	308	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 5 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
4	BAN	A	322	3	22,23,34	4.42	14 (63%)	23,29,45	4.46	16 (69%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BAN	A	322	3	-	1/25/26/35	0/1/1/2

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	322	BAN	CB2-CA2	-9.74	1.34	1.54
4	A	322	BAN	CA2-C2	-9.23	1.41	1.52
4	A	322	BAN	CB3-CA3	-6.23	1.35	1.52
4	A	322	BAN	CA2-C1	-3.29	1.48	1.52
4	A	322	BAN	CE2-CD2	-2.88	1.33	1.38
4	A	322	BAN	CE1-CD1	-2.48	1.33	1.38
4	A	322	BAN	O4-C4	2.42	1.35	1.19
4	A	322	BAN	C3-N4	2.59	1.39	1.33
4	A	322	BAN	O3-C3	3.08	1.29	1.23
4	A	322	BAN	C2-N3	3.15	1.41	1.34
4	A	322	BAN	OH1-N1	3.36	1.45	1.39
4	A	322	BAN	CA4-C4	5.17	1.68	1.49
4	A	322	BAN	CA3-N3	6.79	1.59	1.46
4	A	322	BAN	O1-C1	7.93	1.38	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	322	BAN	OH1-N1-C1	-11.53	103.55	119.86
4	A	322	BAN	O4-C4-CA4	-9.62	90.56	125.23
4	A	322	BAN	C4-CA4-N4	-5.29	95.13	112.93
4	A	322	BAN	O3-C3-CA3	-5.23	107.92	120.45
4	A	322	BAN	O2-C2-CA2	-4.07	117.45	122.23
4	A	322	BAN	CB2-CG2-CD1	-3.46	113.66	120.90
4	A	322	BAN	C3-CA3-N3	-3.00	104.17	111.67
4	A	322	BAN	CA3-N3-C2	-2.64	115.21	121.27
4	A	322	BAN	CA4-N4-C3	-2.29	115.98	123.00
4	A	322	BAN	O3-C3-N4	2.23	127.55	123.08
4	A	322	BAN	CD2-CG2-CD1	2.68	122.42	118.13
4	A	322	BAN	CB3-CA3-N3	2.97	115.92	110.31
4	A	322	BAN	CA3-C3-N4	3.69	124.48	116.43
4	A	322	BAN	O2-C2-N3	4.13	131.02	122.93
4	A	322	BAN	CG2-CB2-CA2	5.29	126.16	113.89
4	A	322	BAN	CB3-CA3-C3	6.30	122.64	110.19

There are no chirality outliers.

All (1) torsion outliers are listed below:



Mol	Chain	Res	Type	Atoms
4	A	322	BAN	CB2-CA2-C1-N1

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	322	BAN	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	210/316 (66%)	-0.64	3 (1%) 78 83	2, 9, 19, 27	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	20	ILE	2.5
1	A	22	THR	2.4
1	A	128	GLN	2.2

### 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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	BAN	A	322	23/33	0.93	0.15	2.05	21,23,31,33	0
2	CA	A	318	1/1	0.98	0.05	-0.95	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CA	A	320	1/1	0.99	0.06	-1.42	13,13,13,13	0
3	ZN	A	321	1/1	0.99	0.06	-1.70	16,16,16,16	0
2	CA	A	317	1/1	1.00	0.04	-3.69	9,9,9,9	0
2	CA	A	319	1/1	0.99	0.03	-4.22	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.