Full wwPDB X-ray Structure Validation Report (i)

Nov 14, 2022 – 03:52 PM EST

PDB ID	:	4TLN
Title	:	BINDING OF HYDROXAMIC ACID INHIBITORS TO CRYSTALLINE THERMOLYSIN SUGGESTS A PENTACOORDINATE ZINC INTERMEDIATE 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

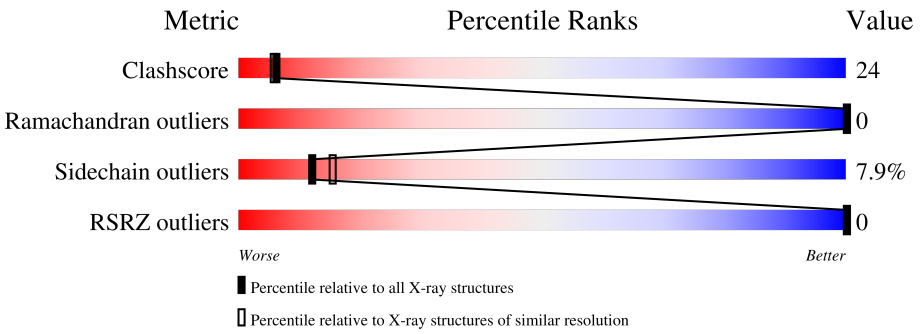
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (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 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 <=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	24% 52% 22% •

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	LNO	A	322	-	X	-	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 2597 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
			Total	C	N	O	S			
1	A	316	2432	1528	408	494	2	0	0	0

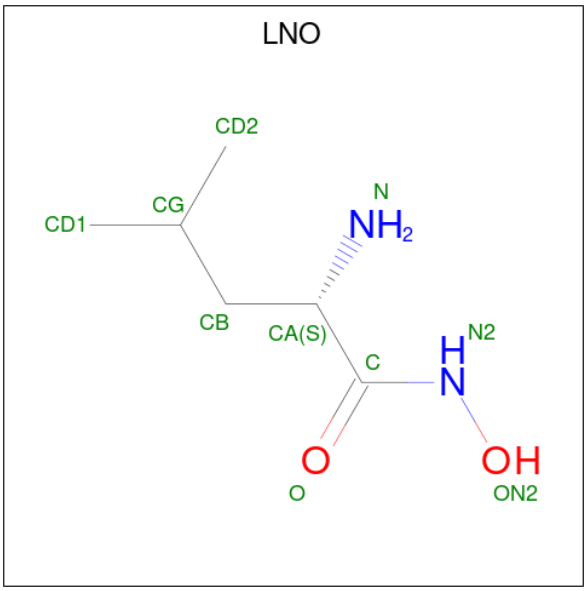
- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

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

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

- Molecule 4 is L-LEUCYL-HYDROXYLAMINE (three-letter code: LNO) (formula: $C_6H_{14}N_2O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
4	A	1	10	6	2	2	0	0

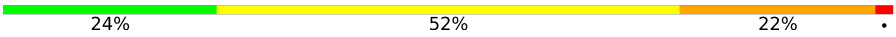
- Molecule 5 is water.

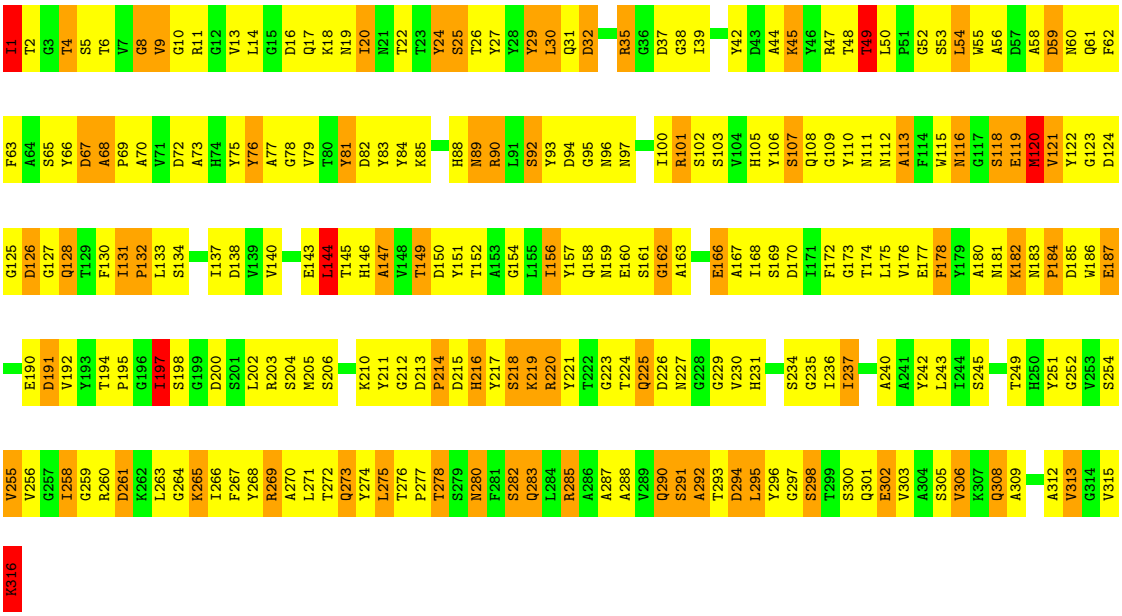
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	150	150	150	0	0

3 Residue-property plots (i)

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: THERMOLYSIN

Chain A: 



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α, β, γ	94.20Å 94.20Å 131.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	10.00 – 2.30 26.63 – 2.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-2.30) 76.2 (26.63-2.31)	Depositor EDS
R_{merge}	0.03	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	114125.00 (at 2.31Å)	Xtriage
Refinement program	TNT, PROLSQ	Depositor
R, R_{free}	0.169 , (Not available) 0.156 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	18.7	Xtriage
Anisotropy	0.054	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 68.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	2597	wwPDB-VP
Average B, all atoms (Å^2)	11.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	2.26	81/2491 (3.3%)	3.20	317/3391 (9.3%)

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	101	ARG	CG-CD	12.14	1.82	1.51
1	A	119	GLU	CD-OE1	-12.14	1.12	1.25
1	A	166	GLU	CD-OE1	-11.57	1.12	1.25
1	A	25	SER	CB-OG	11.37	1.57	1.42
1	A	53	SER	CA-CB	10.91	1.69	1.52
1	A	35	ARG	C-N	-9.64	1.15	1.33
1	A	8	GLY	N-CA	9.34	1.60	1.46
1	A	265	LYS	CE-NZ	8.15	1.69	1.49
1	A	260	ARG	C-N	-7.91	1.15	1.34
1	A	11	ARG	NE-CZ	7.78	1.43	1.33
1	A	160	GLU	CD-OE2	-7.68	1.17	1.25
1	A	186	TRP	CG-CD2	7.39	1.56	1.43
1	A	316	LYS	C-OXT	7.32	1.37	1.23
1	A	101	ARG	NE-CZ	-7.21	1.23	1.33
1	A	235	GLY	C-O	7.20	1.35	1.23
1	A	108	GLN	C-O	7.13	1.36	1.23
1	A	278	THR	CB-OG1	7.11	1.57	1.43
1	A	256	VAL	N-CA	7.10	1.60	1.46
1	A	119	GLU	CB-CG	-7.07	1.38	1.52
1	A	101	ARG	CZ-NH2	7.06	1.42	1.33
1	A	5	SER	CB-OG	7.02	1.51	1.42
1	A	95	GLY	C-O	7.00	1.34	1.23
1	A	143	GLU	CD-OE1	-6.99	1.18	1.25
1	A	102	SER	CA-CB	6.95	1.63	1.52
1	A	190	GLU	CD-OE1	-6.93	1.18	1.25
1	A	173	GLY	CA-C	-6.91	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	118	SER	CB-OG	-6.90	1.33	1.42
1	A	92	SER	CB-OG	6.88	1.51	1.42
1	A	267	PHE	C-O	6.77	1.36	1.23
1	A	218	SER	CB-OG	-6.75	1.33	1.42
1	A	194	THR	CB-OG1	6.71	1.56	1.43
1	A	162	GLY	C-O	6.69	1.34	1.23
1	A	52	GLY	C-O	6.60	1.34	1.23
1	A	265	LYS	CA-CB	-6.55	1.39	1.53
1	A	252	GLY	C-O	6.33	1.33	1.23
1	A	77	ALA	C-O	-6.26	1.11	1.23
1	A	182	LYS	CE-NZ	6.17	1.64	1.49
1	A	20	ILE	C-O	6.17	1.35	1.23
1	A	213	ASP	CG-OD2	6.14	1.39	1.25
1	A	4	THR	C-O	6.13	1.35	1.23
1	A	123	GLY	CA-C	6.12	1.61	1.51
1	A	10	GLY	C-O	6.01	1.33	1.23
1	A	234	SER	CB-OG	-5.84	1.34	1.42
1	A	166	GLU	CD-OE2	5.82	1.32	1.25
1	A	187	GLU	CD-OE2	5.78	1.32	1.25
1	A	174	THR	C-O	5.75	1.34	1.23
1	A	163	ALA	C-N	-5.71	1.21	1.34
1	A	144	LEU	C-O	5.71	1.34	1.23
1	A	302	GLU	CD-OE2	-5.66	1.19	1.25
1	A	47	ARG	NE-CZ	-5.66	1.25	1.33
1	A	116	ASN	CG-ND2	-5.64	1.18	1.32
1	A	308	GLN	CD-NE2	5.63	1.47	1.32
1	A	288	ALA	C-O	5.62	1.34	1.23
1	A	47	ARG	C-N	-5.62	1.21	1.34
1	A	282	SER	CA-CB	-5.62	1.44	1.52
1	A	107	SER	CA-CB	-5.58	1.44	1.52
1	A	298	SER	CB-OG	-5.51	1.35	1.42
1	A	183	ASN	N-CA	5.48	1.57	1.46
1	A	285	ARG	C-N	5.45	1.46	1.34
1	A	10	GLY	C-N	-5.42	1.21	1.34
1	A	295	LEU	N-CA	-5.41	1.35	1.46
1	A	190	GLU	CG-CD	5.39	1.60	1.51
1	A	115	TRP	NE1-CE2	5.36	1.44	1.37
1	A	259	GLY	C-O	-5.36	1.15	1.23
1	A	11	ARG	CZ-NH2	5.34	1.40	1.33
1	A	216	HIS	CG-ND1	-5.32	1.27	1.38
1	A	78	GLY	CA-C	5.30	1.60	1.51
1	A	265	LYS	CB-CG	-5.28	1.38	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	ASN	CG-OD1	5.27	1.35	1.24
1	A	105	HIS	CB-CG	-5.23	1.40	1.50
1	A	132	PRO	N-CD	5.23	1.55	1.47
1	A	297	GLY	C-N	-5.21	1.22	1.34
1	A	221	TYR	CB-CG	-5.21	1.43	1.51
1	A	305	SER	CA-CB	-5.16	1.45	1.52
1	A	255	VAL	CB-CG1	-5.16	1.42	1.52
1	A	223	GLY	CA-C	5.12	1.60	1.51
1	A	44	ALA	C-O	5.10	1.33	1.23
1	A	101	ARG	CZ-NH1	5.08	1.39	1.33
1	A	4	THR	N-CA	5.04	1.56	1.46
1	A	245	SER	CB-OG	5.02	1.48	1.42
1	A	118	SER	CA-CB	-5.01	1.45	1.52

All (317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	47	ARG	NE-CZ-NH1	24.51	132.56	120.30
1	A	47	ARG	CD-NE-CZ	22.79	155.50	123.60
1	A	101	ARG	CD-NE-CZ	22.76	155.47	123.60
1	A	260	ARG	NE-CZ-NH2	-18.95	110.82	120.30
1	A	90	ARG	NE-CZ-NH1	17.86	129.23	120.30
1	A	182	LYS	CG-CD-CE	17.07	163.09	111.90
1	A	101	ARG	NE-CZ-NH1	16.16	128.38	120.30
1	A	27	TYR	CB-CG-CD2	-16.09	111.35	121.00
1	A	168	ILE	CB-CG1-CD1	16.07	158.89	113.90
1	A	211	TYR	CB-CG-CD2	-15.36	111.79	121.00
1	A	11	ARG	NE-CZ-NH2	-15.26	112.67	120.30
1	A	67	ASP	CB-CG-OD1	15.25	132.03	118.30
1	A	120	MET	CG-SD-CE	14.27	123.03	100.20
1	A	101	ARG	CA-CB-CG	12.63	141.19	113.40
1	A	37	ASP	CB-CG-OD2	12.56	129.60	118.30
1	A	27	TYR	CZ-CE2-CD2	-12.38	108.66	119.80
1	A	101	ARG	NE-CZ-NH2	-12.08	114.26	120.30
1	A	90	ARG	NE-CZ-NH2	-12.00	114.30	120.30
1	A	138	ASP	CB-CG-OD1	11.75	128.87	118.30
1	A	308	GLN	CG-CD-OE1	11.69	144.97	121.60
1	A	296	TYR	CB-CG-CD1	11.57	127.94	121.00
1	A	11	ARG	CD-NE-CZ	-11.53	107.46	123.60
1	A	47	ARG	NE-CZ-NH2	-11.50	114.55	120.30
1	A	35	ARG	NE-CZ-NH1	11.43	126.02	120.30
1	A	101	ARG	CG-CD-NE	-11.16	88.36	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	264	GLY	CA-C-O	11.13	140.63	120.60
1	A	143	GLU	CG-CD-OE1	11.12	140.53	118.30
1	A	220	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	A	101	ARG	CB-CA-C	10.53	131.46	110.40
1	A	35	ARG	NE-CZ-NH2	-10.44	115.08	120.30
1	A	221	TYR	CB-CG-CD1	-10.38	114.77	121.00
1	A	126	ASP	CB-CG-OD1	-10.28	109.05	118.30
1	A	200	ASP	CB-CG-OD1	10.24	127.52	118.30
1	A	24	TYR	CG-CD1-CE1	10.24	129.49	121.30
1	A	261	ASP	CB-CG-OD2	-10.13	109.18	118.30
1	A	151	TYR	CB-CG-CD1	10.12	127.08	121.00
1	A	29	TYR	CB-CG-CD2	10.02	127.02	121.00
1	A	59	ASP	CB-CG-OD2	10.00	127.30	118.30
1	A	296	TYR	CB-CG-CD2	-9.91	115.06	121.00
1	A	288	ALA	CB-CA-C	9.89	124.94	110.10
1	A	27	TYR	CB-CG-CD1	9.85	126.91	121.00
1	A	157	TYR	CB-CG-CD2	9.78	126.87	121.00
1	A	113	ALA	C-N-CA	9.76	146.10	121.70
1	A	82	ASP	CB-CG-OD1	9.74	127.07	118.30
1	A	211	TYR	CB-CG-CD1	9.62	126.77	121.00
1	A	29	TYR	CB-CG-CD1	-9.51	115.30	121.00
1	A	121	VAL	CA-CB-CG2	-9.33	96.91	110.90
1	A	37	ASP	C-N-CA	9.29	141.82	122.30
1	A	198	SER	CB-CA-C	9.21	127.59	110.10
1	A	24	TYR	CB-CG-CD2	9.20	126.52	121.00
1	A	225	GLN	CB-CA-C	9.10	128.61	110.40
1	A	227	ASN	O-C-N	9.08	138.64	123.20
1	A	282	SER	CB-CA-C	9.06	127.31	110.10
1	A	274	TYR	CZ-CE2-CD2	-9.05	111.65	119.80
1	A	166	GLU	OE1-CD-OE2	-8.84	112.69	123.30
1	A	130	PHE	CB-CG-CD1	8.55	126.79	120.80
1	A	198	SER	N-CA-CB	-8.49	97.77	110.50
1	A	297	GLY	C-N-CA	8.47	142.87	121.70
1	A	108	GLN	CG-CD-OE1	-8.45	104.70	121.60
1	A	119	GLU	N-CA-CB	-8.39	95.49	110.60
1	A	138	ASP	OD1-CG-OD2	-8.39	107.36	123.30
1	A	220	ARG	NH1-CZ-NH2	8.39	128.62	119.40
1	A	78	GLY	CA-C-O	-8.20	105.84	120.60
1	A	66	TYR	C-N-CA	8.16	142.11	121.70
1	A	269	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	A	11	ARG	NH1-CZ-NH2	8.14	128.36	119.40
1	A	191	ASP	CB-CG-OD1	8.10	125.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	274	TYR	CG-CD2-CE2	8.10	127.78	121.30
1	A	301	GLN	CG-CD-OE1	8.01	137.61	121.60
1	A	190	GLU	OE1-CD-OE2	7.90	132.78	123.30
1	A	203	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	312	ALA	C-N-CA	7.86	141.34	121.70
1	A	103	SER	O-C-N	7.83	135.24	122.70
1	A	223	GLY	C-N-CA	7.82	141.26	121.70
1	A	9	VAL	CB-CA-C	-7.76	96.65	111.40
1	A	285	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	A	265	LYS	CD-CE-NZ	-7.75	93.88	111.70
1	A	298	SER	N-CA-CB	-7.74	98.89	110.50
1	A	56	ALA	CA-C-O	7.72	136.32	120.10
1	A	215	ASP	CB-CG-OD2	-7.72	111.35	118.30
1	A	315	VAL	O-C-N	7.70	135.02	122.70
1	A	226	ASP	CB-CG-OD1	7.69	125.22	118.30
1	A	42	TYR	CZ-CE2-CD2	-7.68	112.88	119.80
1	A	263	LEU	O-C-N	-7.63	110.23	123.20
1	A	261	ASP	N-CA-CB	-7.59	96.94	110.60
1	A	160	GLU	OE1-CD-OE2	-7.56	114.22	123.30
1	A	61	GLN	O-C-N	7.55	134.78	122.70
1	A	81	TYR	CG-CD1-CE1	7.53	127.33	121.30
1	A	76	TYR	CZ-CE2-CD2	-7.53	113.03	119.80
1	A	151	TYR	CB-CG-CD2	-7.52	116.49	121.00
1	A	18	LYS	O-C-N	7.47	134.66	122.70
1	A	178	PHE	CB-CG-CD2	7.46	126.03	120.80
1	A	130	PHE	CB-CA-C	-7.45	95.50	110.40
1	A	270	ALA	O-C-N	-7.44	110.80	122.70
1	A	220	ARG	NE-CZ-NH1	-7.38	116.61	120.30
1	A	251	TYR	CB-CG-CD2	7.38	125.43	121.00
1	A	83	TYR	CB-CG-CD1	7.37	125.42	121.00
1	A	197	ILE	CA-C-O	7.36	135.56	120.10
1	A	147	ALA	CB-CA-C	7.36	121.14	110.10
1	A	38	GLY	CA-C-O	-7.34	107.38	120.60
1	A	49	THR	O-C-N	7.32	134.41	122.70
1	A	308	GLN	CG-CD-NE2	-7.29	99.19	116.70
1	A	309	ALA	CB-CA-C	7.25	120.98	110.10
1	A	53	SER	CB-CA-C	-7.24	96.35	110.10
1	A	143	GLU	CG-CD-OE2	-7.24	103.83	118.30
1	A	101	ARG	CB-CG-CD	7.21	130.35	111.60
1	A	84	TYR	CB-CG-CD2	7.18	125.31	121.00
1	A	218	SER	C-N-CA	7.18	139.64	121.70
1	A	221	TYR	CD1-CE1-CZ	-7.16	113.36	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	39	ILE	CB-CG1-CD1	7.14	133.90	113.90
1	A	5	SER	N-CA-CB	7.14	121.21	110.50
1	A	56	ALA	O-C-N	-7.13	111.29	122.70
1	A	122	TYR	CB-CG-CD1	-7.09	116.75	121.00
1	A	220	ARG	O-C-N	-7.08	111.38	122.70
1	A	101	ARG	C-N-CA	7.06	139.35	121.70
1	A	147	ALA	N-CA-CB	-7.02	100.27	110.10
1	A	32	ASP	CB-CG-OD1	7.02	124.61	118.30
1	A	204	SER	CA-C-N	7.00	132.59	117.20
1	A	265	LYS	O-C-N	-6.99	111.51	122.70
1	A	261	ASP	OD1-CG-OD2	6.98	136.57	123.30
1	A	156	ILE	CA-CB-CG2	6.98	124.86	110.90
1	A	16	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	A	169	SER	O-C-N	-6.96	111.56	122.70
1	A	283	GLN	CA-CB-CG	-6.96	98.08	113.40
1	A	162	GLY	O-C-N	-6.94	111.59	122.70
1	A	47	ARG	NH1-CZ-NH2	-6.93	111.78	119.40
1	A	260	ARG	C-N-CA	6.90	138.96	121.70
1	A	282	SER	N-CA-CB	-6.90	100.14	110.50
1	A	42	TYR	CG-CD1-CE1	-6.89	115.79	121.30
1	A	101	ARG	N-CA-CB	-6.89	98.20	110.60
1	A	180	ALA	CB-CA-C	6.87	120.40	110.10
1	A	96	ASN	O-C-N	6.84	133.65	122.70
1	A	83	TYR	CD1-CE1-CZ	-6.83	113.65	119.80
1	A	270	ALA	CA-C-O	6.83	134.44	120.10
1	A	8	GLY	O-C-N	-6.82	111.79	122.70
1	A	184	PRO	O-C-N	6.81	133.60	122.70
1	A	264	GLY	O-C-N	-6.81	111.80	122.70
1	A	94	ASP	CB-CG-OD2	6.78	124.40	118.30
1	A	278	THR	CA-CB-CG2	-6.78	102.91	112.40
1	A	38	GLY	O-C-N	6.78	133.54	122.70
1	A	254	SER	CA-CB-OG	6.75	129.44	111.20
1	A	146	HIS	CG-ND1-CE1	6.65	117.51	108.20
1	A	133	LEU	CA-C-N	6.65	131.82	117.20
1	A	296	TYR	C-N-CA	6.64	136.25	122.30
1	A	274	TYR	CB-CG-CD2	6.61	124.97	121.00
1	A	75	TYR	CE1-CZ-CE2	6.58	130.33	119.80
1	A	211	TYR	CA-CB-CG	-6.58	100.91	113.40
1	A	39	ILE	C-N-CA	6.57	138.13	121.70
1	A	45	LYS	CB-CA-C	-6.56	97.28	110.40
1	A	45	LYS	O-C-N	6.54	133.17	122.70
1	A	75	TYR	CZ-CE2-CD2	-6.52	113.94	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	SER	CA-C-O	-6.50	106.44	120.10
1	A	127	GLY	O-C-N	6.49	133.09	122.70
1	A	260	ARG	NH1-CZ-NH2	6.48	126.53	119.40
1	A	66	TYR	CG-CD2-CE2	6.47	126.48	121.30
1	A	70	ALA	O-C-N	-6.45	112.38	122.70
1	A	224	THR	C-N-CA	-6.44	105.60	121.70
1	A	121	VAL	CG1-CB-CG2	6.44	121.20	110.90
1	A	44	ALA	C-N-CA	6.43	137.76	121.70
1	A	110	TYR	CD1-CE1-CZ	-6.40	114.04	119.80
1	A	143	GLU	OE1-CD-OE2	-6.38	115.64	123.30
1	A	65	SER	CB-CA-C	6.35	122.16	110.10
1	A	265	LYS	N-CA-CB	-6.32	99.22	110.60
1	A	67	ASP	OD1-CG-OD2	-6.32	111.30	123.30
1	A	200	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	A	251	TYR	CB-CG-CD1	-6.31	117.21	121.00
1	A	18	LYS	CG-CD-CE	6.31	130.83	111.90
1	A	268	TYR	CG-CD1-CE1	-6.31	116.25	121.30
1	A	122	TYR	CG-CD1-CE1	-6.30	116.26	121.30
1	A	75	TYR	CD1-CE1-CZ	-6.27	114.16	119.80
1	A	174	THR	OG1-CB-CG2	6.26	124.39	110.00
1	A	300	SER	C-N-CA	6.24	137.29	121.70
1	A	290	GLN	CA-CB-CG	-6.22	99.72	113.40
1	A	70	ALA	CA-C-O	6.21	133.13	120.10
1	A	9	VAL	CA-C-N	6.17	128.55	116.20
1	A	106	TYR	N-CA-CB	-6.13	99.56	110.60
1	A	130	PHE	O-C-N	6.12	132.49	122.70
1	A	219	LYS	CB-CG-CD	6.09	127.43	111.60
1	A	90	ARG	CG-CD-NE	-6.08	99.03	111.80
1	A	93	TYR	CB-CG-CD1	6.08	124.65	121.00
1	A	49	THR	CA-CB-OG1	-6.07	96.24	109.00
1	A	315	VAL	CA-C-N	-6.06	103.86	117.20
1	A	82	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	A	260	ARG	CA-C-N	6.04	130.50	117.20
1	A	187	GLU	CG-CD-OE1	6.04	130.37	118.30
1	A	237	ILE	CA-CB-CG1	-6.03	99.54	111.00
1	A	53	SER	CA-C-N	6.02	130.45	117.20
1	A	231	HIS	N-CA-CB	6.02	121.43	110.60
1	A	138	ASP	CB-CG-OD2	6.01	123.71	118.30
1	A	140	VAL	O-C-N	-6.00	113.10	122.70
1	A	302	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	A	115	TRP	CD2-CE3-CZ3	5.99	126.58	118.80
1	A	183	ASN	N-CA-CB	-5.96	99.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	205	MET	N-CA-CB	5.92	121.26	110.60
1	A	224	THR	N-CA-C	5.92	126.97	111.00
1	A	145	THR	O-C-N	-5.92	113.24	122.70
1	A	288	ALA	N-CA-CB	-5.91	101.82	110.10
1	A	197	ILE	O-C-N	-5.90	113.26	122.70
1	A	27	TYR	CG-CD2-CE2	5.89	126.01	121.30
1	A	27	TYR	CE1-CZ-CE2	5.87	129.19	119.80
1	A	66	TYR	CZ-CE2-CD2	-5.86	114.52	119.80
1	A	170	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	126	ASP	N-CA-CB	5.84	121.11	110.60
1	A	291	SER	O-C-N	5.83	132.02	122.70
1	A	229	GLY	N-CA-C	5.80	127.61	113.10
1	A	265	LYS	CA-CB-CG	5.80	126.16	113.40
1	A	273	GLN	CA-CB-CG	5.80	126.16	113.40
1	A	128	GLN	CA-CB-CG	-5.79	100.65	113.40
1	A	53	SER	CA-C-O	-5.78	107.96	120.10
1	A	76	TYR	CE1-CZ-CE2	5.78	129.05	119.80
1	A	211	TYR	CB-CA-C	-5.76	98.88	110.40
1	A	88	HIS	CA-CB-CG	-5.76	103.81	113.60
1	A	96	ASN	CB-CA-C	-5.75	98.89	110.40
1	A	292	ALA	N-CA-CB	5.75	118.15	110.10
1	A	258	ILE	O-C-N	-5.75	113.43	123.20
1	A	126	ASP	CA-C-O	-5.73	108.06	120.10
1	A	61	GLN	CA-CB-CG	-5.73	100.80	113.40
1	A	296	TYR	CA-C-N	5.73	127.65	116.20
1	A	14	LEU	CB-CG-CD1	5.71	120.70	111.00
1	A	182	LYS	CB-CA-C	5.66	121.72	110.40
1	A	85	LYS	CA-CB-CG	-5.66	100.96	113.40
1	A	236	ILE	C-N-CA	5.65	135.83	121.70
1	A	177	GLU	O-C-N	-5.64	113.68	122.70
1	A	212	GLY	CA-C-O	-5.63	110.46	120.60
1	A	234	SER	O-C-N	-5.61	113.66	123.20
1	A	159	ASN	CB-CG-OD1	5.61	132.81	121.60
1	A	223	GLY	O-C-N	5.59	131.64	122.70
1	A	81	TYR	CB-CG-CD1	5.58	124.35	121.00
1	A	166	GLU	CG-CD-OE1	5.57	129.44	118.30
1	A	58	ALA	CA-C-N	5.56	129.44	117.20
1	A	302	GLU	CG-CD-OE1	5.56	129.42	118.30
1	A	53	SER	CA-CB-OG	-5.56	96.19	111.20
1	A	75	TYR	N-CA-CB	-5.56	100.60	110.60
1	A	220	ARG	CA-C-N	5.55	129.42	117.20
1	A	242	TYR	CA-C-N	5.55	129.40	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	166	GLU	CB-CG-CD	-5.54	99.25	114.20
1	A	240	ALA	N-CA-CB	5.54	117.85	110.10
1	A	265	LYS	CB-CG-CD	-5.53	97.22	111.60
1	A	161	SER	O-C-N	-5.50	113.84	123.20
1	A	133	LEU	CA-CB-CG	-5.49	102.68	115.30
1	A	192	VAL	CA-CB-CG2	5.49	119.13	110.90
1	A	1	ILE	CA-CB-CG1	-5.47	100.60	111.00
1	A	106	TYR	CZ-CE2-CD2	5.47	124.72	119.80
1	A	24	TYR	CD1-CG-CD2	-5.46	111.89	117.90
1	A	108	GLN	O-C-N	5.45	132.46	123.20
1	A	261	ASP	CA-CB-CG	-5.45	101.42	113.40
1	A	89	ASN	CB-CG-OD1	-5.44	110.72	121.60
1	A	260	ARG	CA-CB-CG	5.44	125.37	113.40
1	A	287	ALA	CB-CA-C	-5.44	101.94	110.10
1	A	115	TRP	CA-C-N	5.43	129.15	117.20
1	A	25	SER	CA-CB-OG	-5.43	96.54	111.20
1	A	126	ASP	CB-CG-OD2	5.42	123.18	118.30
1	A	294	ASP	C-N-CA	5.42	135.26	121.70
1	A	167	ALA	O-C-N	-5.40	114.06	122.70
1	A	156	ILE	CB-CG1-CD1	-5.40	98.79	113.90
1	A	79	VAL	CG1-CB-CG2	5.39	119.53	110.90
1	A	8	GLY	CA-C-N	5.38	129.04	117.20
1	A	116	ASN	CA-C-O	-5.38	108.81	120.10
1	A	27	TYR	CG-CD1-CE1	-5.37	117.01	121.30
1	A	242	TYR	C-N-CA	5.34	135.06	121.70
1	A	157	TYR	CB-CG-CD1	-5.34	117.79	121.00
1	A	105	HIS	O-C-N	5.34	131.24	122.70
1	A	180	ALA	N-CA-CB	-5.34	102.63	110.10
1	A	38	GLY	N-CA-C	5.33	126.43	113.10
1	A	30	LEU	C-N-CA	5.33	135.01	121.70
1	A	2	THR	O-C-N	-5.32	114.16	123.20
1	A	191	ASP	OD1-CG-OD2	-5.32	113.20	123.30
1	A	2	THR	CA-C-N	5.32	126.83	116.20
1	A	83	TYR	CG-CD1-CE1	5.32	125.55	121.30
1	A	149	THR	CA-CB-CG2	5.32	119.84	112.40
1	A	9	VAL	CA-C-O	-5.31	108.94	120.10
1	A	29	TYR	CZ-CE2-CD2	5.31	124.58	119.80
1	A	221	TYR	CB-CG-CD2	5.29	124.17	121.00
1	A	124	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	45	LYS	N-CA-CB	5.27	120.08	110.60
1	A	59	ASP	OD1-CG-OD2	-5.26	113.30	123.30
1	A	130	PHE	CB-CG-CD2	-5.26	117.12	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	240	ALA	CB-CA-C	-5.26	102.22	110.10
1	A	301	GLN	OE1-CD-NE2	-5.25	109.82	121.90
1	A	131	ILE	N-CA-CB	5.25	122.88	110.80
1	A	315	VAL	CA-CB-CG2	-5.24	103.04	110.90
1	A	170	ASP	CB-CG-OD1	5.24	123.02	118.30
1	A	268	TYR	O-C-N	-5.24	114.32	122.70
1	A	204	SER	CA-C-O	-5.23	109.11	120.10
1	A	210	LYS	CD-CE-NZ	-5.23	99.68	111.70
1	A	54	LEU	CB-CG-CD1	-5.22	102.12	111.00
1	A	81	TYR	CD1-CE1-CZ	-5.22	115.10	119.80
1	A	47	ARG	CG-CD-NE	-5.22	100.84	111.80
1	A	49	THR	CA-C-O	-5.22	109.15	120.10
1	A	25	SER	C-N-CA	5.21	134.72	121.70
1	A	183	ASN	CB-CG-OD1	-5.20	111.19	121.60
1	A	206	SER	C-N-CA	5.20	134.69	121.70
1	A	17	GLN	CG-CD-OE1	5.19	131.98	121.60
1	A	14	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	A	275	LEU	CB-CA-C	5.18	120.04	110.20
1	A	263	LEU	CA-C-N	5.18	126.56	116.20
1	A	106	TYR	CG-CD2-CE2	-5.17	117.16	121.30
1	A	68	ALA	CB-CA-C	5.17	117.86	110.10
1	A	83	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	48	THR	O-C-N	-5.17	114.43	122.70
1	A	288	ALA	C-N-CA	5.14	134.55	121.70
1	A	22	THR	CA-CB-CG2	5.14	119.59	112.40
1	A	211	TYR	CZ-CE2-CD2	-5.13	115.18	119.80
1	A	181	ASN	CA-C-N	-5.13	105.92	117.20
1	A	306	VAL	CA-C-O	5.12	130.85	120.10
1	A	73	ALA	CA-C-O	5.12	130.85	120.10
1	A	85	LYS	N-CA-CB	-5.12	101.39	110.60
1	A	115	TRP	CE3-CZ3-CH2	-5.11	115.58	121.20
1	A	265	LYS	CA-C-N	5.09	128.40	117.20
1	A	119	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	A	178	PHE	CZ-CE2-CD2	5.05	126.16	120.10
1	A	166	GLU	CA-C-O	-5.05	109.50	120.10
1	A	313	VAL	CB-CA-C	5.04	120.98	111.40
1	A	305	SER	CA-C-N	5.04	128.28	117.20
1	A	63	PHE	CD1-CG-CD2	-5.02	111.78	118.30
1	A	255	VAL	CA-CB-CG1	5.00	118.41	110.90
1	A	214	PRO	N-CD-CG	-5.00	95.70	103.20

There are no chirality outliers.

There are no planarity outliers.

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	2432	0	2249	112	2
2	A	4	0	0	0	0
3	A	1	0	0	0	0
4	A	10	0	13	4	0
5	A	150	0	0	34	10
All	All	2597	0	2262	115	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 (115) 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:265:LYS:CE	1:A:265:LYS:NZ	1.69	1.56
1:A:101:ARG:CD	1:A:101:ARG:CG	1.82	1.54
4:A:322:LNO:N	4:A:322:LNO:HD13	1.45	1.18
1:A:308:GLN:HG2	5:A:388:HOH:O	1.44	1.15
1:A:218:SER:HB3	5:A:435:HOH:O	1.43	1.14
1:A:118:SER:N	5:A:442:HOH:O	1.78	1.11
1:A:216:HIS:ND1	5:A:435:HOH:O	1.88	1.04
4:A:322:LNO:N	4:A:322:LNO:CD1	2.15	1.02
1:A:116:ASN:OD1	5:A:442:HOH:O	1.78	1.01
1:A:92:SER:HA	5:A:451:HOH:O	1.61	0.99
1:A:101:ARG:CG	1:A:101:ARG:NE	2.29	0.96
4:A:322:LNO:HD13	4:A:322:LNO:HN1	1.04	0.95
1:A:137:ILE:HG22	1:A:182:LYS:NZ	1.83	0.94
1:A:280:ASN:HD22	1:A:280:ASN:C	1.72	0.91
1:A:219:LYS:HE2	5:A:391:HOH:O	1.71	0.90
1:A:219:LYS:CE	5:A:391:HOH:O	2.22	0.85
1:A:100:ILE:HD11	5:A:451:HOH:O	1.79	0.83
1:A:265:LYS:NZ	1:A:265:LYS:CD	2.40	0.83
1:A:137:ILE:HG22	1:A:182:LYS:HZ3	1.43	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:OE1	5:A:447:HOH:O	1.97	0.81
1:A:273:GLN:CG	5:A:372:HOH:O	2.29	0.81
1:A:216:HIS:CE1	5:A:435:HOH:O	2.31	0.81
1:A:278:THR:HG22	1:A:278:THR:O	1.79	0.80
1:A:269:ARG:NH1	1:A:294:ASP:OD2	2.18	0.77
1:A:111:ASN:O	1:A:112:ASN:HB2	1.86	0.75
1:A:92:SER:OG	5:A:451:HOH:O	2.04	0.74
1:A:191:ASP:HB2	5:A:350:HOH:O	1.90	0.71
1:A:92:SER:CB	5:A:451:HOH:O	2.37	0.71
1:A:1:ILE:HD13	1:A:29:TYR:CE2	2.26	0.71
1:A:280:ASN:ND2	1:A:283:GLN:H	1.89	0.70
1:A:137:ILE:HG22	1:A:182:LYS:HZ2	1.57	0.68
1:A:144:LEU:O	1:A:147:ALA:HB3	1.93	0.68
1:A:116:ASN:C	5:A:442:HOH:O	2.32	0.68
1:A:126:ASP:OD2	1:A:128:GLN:N	2.25	0.67
1:A:273:GLN:HB3	5:A:372:HOH:O	1.94	0.67
1:A:131:ILE:HB	1:A:132:PRO:CD	2.24	0.67
1:A:280:ASN:C	1:A:280:ASN:ND2	2.47	0.67
1:A:172:PHE:O	1:A:176:VAL:HG23	1.96	0.66
1:A:162:GLY:O	1:A:230:VAL:HG13	1.94	0.66
1:A:101:ARG:NE	1:A:101:ARG:HG3	2.12	0.65
1:A:273:GLN:CB	5:A:372:HOH:O	2.45	0.65
1:A:278:THR:O	1:A:278:THR:CG2	2.46	0.64
1:A:30:LEU:HB2	1:A:55:TRP:HB3	1.81	0.62
1:A:120:MET:SD	1:A:144:LEU:HD23	2.40	0.62
1:A:152:THR:HG21	1:A:272:THR:HG22	1.82	0.62
1:A:150:ASP:HA	5:A:379:HOH:O	2.00	0.61
1:A:187:GLU:OE1	5:A:411:HOH:O	2.16	0.61
1:A:197:ILE:HD13	1:A:197:ILE:N	2.16	0.61
1:A:154:GLY:HA2	5:A:379:HOH:O	2.01	0.60
1:A:137:ILE:H	1:A:182:LYS:HZ2	1.49	0.60
1:A:131:ILE:HG23	1:A:195:PRO:HG3	1.84	0.59
1:A:217:TYR:O	1:A:220:ARG:HB2	2.02	0.59
1:A:50:LEU:HD12	5:A:336:HOH:O	2.04	0.58
1:A:178:PHE:CE1	1:A:184:PRO:HB2	2.39	0.58
1:A:308:GLN:CG	5:A:388:HOH:O	2.22	0.58
1:A:120:MET:C	1:A:121:VAL:HG23	2.21	0.57
1:A:218:SER:N	5:A:435:HOH:O	2.30	0.57
1:A:68:ALA:HB3	1:A:69:PRO:HD3	1.86	0.57
1:A:273:GLN:HG3	5:A:372:HOH:O	1.99	0.56
1:A:280:ASN:HD21	1:A:283:GLN:H	1.52	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:GLN:O	1:A:195:PRO:HD2	2.09	0.53
1:A:131:ILE:HB	1:A:132:PRO:HD2	1.90	0.53
1:A:166:GLU:HG3	1:A:230:VAL:HG12	1.91	0.52
1:A:273:GLN:CD	5:A:372:HOH:O	2.49	0.51
1:A:1:ILE:N	1:A:31:GLN:HE22	2.10	0.50
1:A:137:ILE:H	1:A:182:LYS:NZ	2.08	0.50
1:A:4:THR:HG22	1:A:24:TYR:HB3	1.93	0.49
1:A:265:LYS:HE2	5:A:446:HOH:O	2.13	0.49
1:A:285:ARG:HD3	1:A:316:LYS:HD3	1.94	0.49
1:A:298:SER:HB2	5:A:424:HOH:O	2.12	0.49
1:A:282:SER:HA	1:A:316:LYS:HD2	1.94	0.48
1:A:276:THR:HB	1:A:277:PRO:CD	2.43	0.48
1:A:13:VAL:CG1	1:A:131:ILE:HD12	2.43	0.48
1:A:149:THR:O	1:A:154:GLY:N	2.41	0.48
1:A:178:PHE:CD1	1:A:184:PRO:HB2	2.49	0.48
1:A:218:SER:CB	5:A:435:HOH:O	2.26	0.48
1:A:49:THR:O	1:A:49:THR:HG22	2.15	0.47
1:A:156:ILE:HD13	1:A:156:ILE:HG21	1.70	0.47
1:A:290:GLN:O	1:A:290:GLN:HG3	2.11	0.47
1:A:291:SER:O	1:A:295:LEU:HD12	2.13	0.47
1:A:62:PHE:HA	1:A:67:ASP:OD2	2.14	0.47
1:A:113:ALA:O	4:A:322:LNO:HB1	2.14	0.47
1:A:271:LEU:HA	1:A:275:LEU:HD12	1.97	0.47
1:A:76:TYR:OH	1:A:182:LYS:HE3	2.15	0.46
1:A:81:TYR:HD1	5:A:451:HOH:O	1.97	0.46
1:A:293:THR:HA	1:A:303:VAL:HG21	1.97	0.46
1:A:249:THR:HG22	5:A:454:HOH:O	2.16	0.46
1:A:32:ASP:OD1	1:A:35:ARG:NH1	2.48	0.45
1:A:92:SER:HB2	1:A:97:ASN:HA	1.99	0.45
1:A:116:ASN:CG	5:A:442:HOH:O	2.43	0.45
1:A:137:ILE:HG22	1:A:137:ILE:H	1.37	0.45
1:A:1:ILE:HD13	1:A:29:TYR:CZ	2.52	0.44
1:A:45:LYS:NZ	5:A:412:HOH:O	2.45	0.44
1:A:258:ILE:HG21	1:A:302:GLU:HA	1.99	0.44
1:A:302:GLU:O	1:A:306:VAL:HG23	2.17	0.44
1:A:166:GLU:CG	1:A:230:VAL:HG12	2.47	0.44
1:A:237:ILE:HG23	1:A:237:ILE:HD12	1.80	0.43
1:A:280:ASN:ND2	1:A:282:SER:H	2.17	0.43
1:A:265:LYS:HE3	1:A:265:LYS:HB2	1.83	0.43
1:A:269:ARG:HD2	1:A:295:LEU:HD11	2.01	0.43
1:A:197:ILE:N	1:A:197:ILE:CD1	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:GLY:HA2	1:A:125:GLY:O	2.20	0.42
1:A:202:LEU:HA	1:A:202:LEU:HD12	1.61	0.42
1:A:214:PRO:HB3	1:A:219:LYS:HB3	2.00	0.42
1:A:162:GLY:C	1:A:230:VAL:HG13	2.40	0.42
1:A:72:ASP:HB3	1:A:134:SER:O	2.19	0.42
1:A:131:ILE:HD13	1:A:131:ILE:HG21	1.90	0.41
1:A:266:ILE:HG12	1:A:292:ALA:HA	2.01	0.41
1:A:30:LEU:HD23	1:A:30:LEU:HA	1.78	0.41
1:A:59:ASP:O	1:A:60:ASN:CB	2.68	0.41
1:A:255:VAL:HG22	1:A:308:GLN:HB3	2.02	0.41
1:A:285:ARG:CD	1:A:316:LYS:HD3	2.50	0.41
1:A:158:GLN:OE1	5:A:375:HOH:O	2.21	0.41
1:A:8:GLY:O	1:A:19:ASN:HA	2.20	0.41
1:A:90:ARG:NH1	1:A:90:ARG:HG3	2.36	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]	0.93	1.27
5:A:369:HOH:O	5:A:407:HOH:O[5_564]	1.42	0.78
5:A:333:HOH:O	5:A:337:HOH:O[10_664]	1.74	0.46
5:A:332:HOH:O	5:A:336:HOH:O[10_664]	1.75	0.45
5:A:418:HOH:O	5:A:418:HOH:O[12_565]	1.75	0.45
5:A:485:HOH:O	5:A:485:HOH:O[7_555]	1.80	0.40
5:A:379:HOH:O	5:A:396:HOH:O[10_664]	2.01	0.19
1:A:6:THR:CB	5:A:473:HOH:O[12_565]	2.03	0.17
1:A:116:ASN:O	5:A:336:HOH:O[10_664]	2.11	0.09
5:A:372:HOH:O	5:A:463:HOH:O[5_564]	2.14	0.06

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	314/316 (99%)	299 (95%)	15 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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%)	232 (92%)	20 (8%)	12	15

All (20) 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	144	LEU
1	A	175	LEU
1	A	185	ASP
1	A	197	ILE
1	A	225	GLN
1	A	243	LEU
1	A	261	ASP
1	A	280	ASN
1	A	313	VAL
1	A	316	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) 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

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 monosaccharides 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	LNO	A	322	3	9,9,9	1.59	3 (33%)	10,11,11	3.16	6 (60%)

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	LNO	A	322	3	-	4/10/10/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	322	LNO	CB-CA	2.88	1.61	1.53
4	A	322	LNO	C-N2	-2.77	1.29	1.33
4	A	322	LNO	O-C	2.27	1.27	1.23

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	322	LNO	CB-CA-N	-5.83	97.35	110.32
4	A	322	LNO	CB-CA-C	-5.05	99.91	110.85
4	A	322	LNO	O-C-CA	3.57	127.74	120.18
4	A	322	LNO	CA-C-N2	-2.80	111.37	115.87
4	A	322	LNO	CD1-CG-CB	-2.53	101.80	111.11
4	A	322	LNO	C-CA-N	2.13	117.62	109.40

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	322	LNO	N-CA-CB-CG
4	A	322	LNO	C-CA-CB-CG
4	A	322	LNO	O-C-CA-CB
4	A	322	LNO	N2-C-CA-CB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	322	LNO	4	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

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Mol	Chain	Number of breaks

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	35:ARG	C	36:GLY	N	1.15
1	A	260:ARG	C	261:ASP	N	1.15

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	316/316 (100%)	-0.75	0	100	100	2, 9, 20, 29	0

There are no RSRZ outliers to report.

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 monosaccharides 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. The B-factors column lists the minimum, median, 95th 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	B-factors(Å^2)	Q<0.9
4	LNO	A	322	10/10	0.88	0.18	23,27,29,29	0
2	CA	A	319	1/1	0.99	0.04	11,11,11,11	0
2	CA	A	320	1/1	0.99	0.04	14,14,14,14	0
3	ZN	A	321	1/1	0.99	0.05	14,14,14,14	0
2	CA	A	318	1/1	0.99	0.05	13,13,13,13	0
2	CA	A	317	1/1	1.00	0.04	8,8,8,8	0

6.5 Other polymers (i)

There are no such residues in this entry.