



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:47 AM UTC

PDB ID : 1TAB / pdb_00001tab
Title : STRUCTURE OF THE TRYPSIN-BINDING DOMAIN OF BOWMAN-BIRK TYPE PROTEASE INHIBITOR AND ITS INTERACTION WITH TRYPSIN
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Deposited on : 1990-10-15
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 ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtrriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

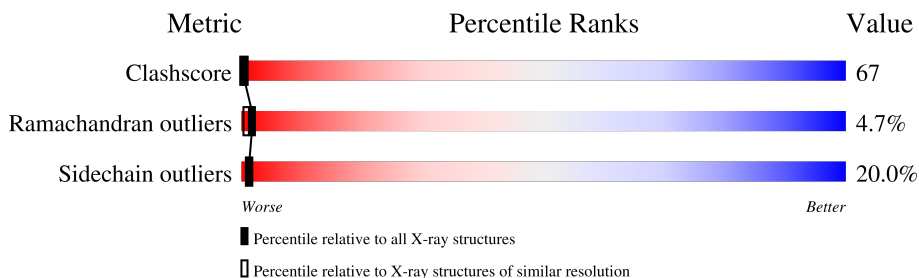
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (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 $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	E	223	 21% 41% 31% 8%
2	I	82	 • 12% 16% 15% 56%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 2044 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 TRYPSIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	E	223	1629	1012	279	324	14	0	0	0

- Molecule 2 is a protein called BOWMAN-BIRK TYPE PROTEINASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	I	36	275	162	48	56	9	0	0	0

- Molecule 3 is water.

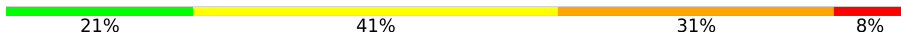
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	136	Total	O	0	0
			136	136		
3	I	4	Total	O	0	0
			4	4		

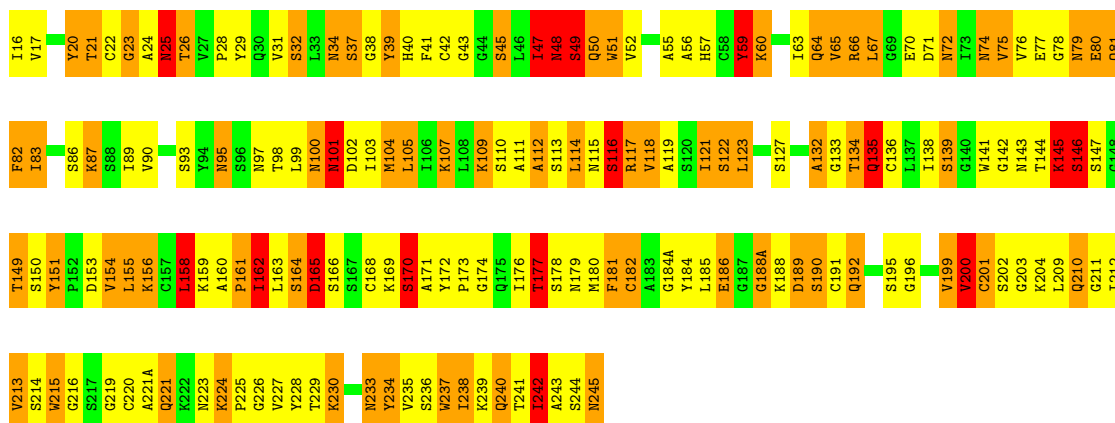
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

- Molecule 1: TRYPSIN

Chain E: 



- Molecule 2: BOWMAN-BIRK TYPE PROTEINASE INHIBITOR

Chain I: 



4 Data and refinement statistics

Xtrriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	55.42Å 55.42Å 181.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.200 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	2044	wwPDB-VP
Average B, all atoms (Å ²)	12.0	wwPDB-VP

5 Model quality i

5.1 Standard geometry i

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	E	1.77	17/1660 (1.0%)	3.02	206/2250 (9.2%)
2	I	2.07	8/279 (2.9%)	4.93	63/371 (17.0%)
All	All	1.82	25/1939 (1.3%)	3.36	269/2621 (10.3%)

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	66	ASP	N-CA	-10.39	1.32	1.46
2	I	72	CYS	N-CA	-10.28	1.32	1.46
2	I	67	PHE	N-CA	-7.66	1.36	1.46
2	I	71	PRO	CA-CB	7.28	1.66	1.53
1	E	200	VAL	N-CA	6.49	1.54	1.46
1	E	158	LEU	N-CA	6.36	1.53	1.46
1	E	149	THR	CA-CB	6.18	1.61	1.53
1	E	111	ALA	CA-CB	-6.11	1.43	1.53
1	E	89	ILE	CA-CB	5.96	1.61	1.53
1	E	26	THR	N-CA	5.91	1.53	1.46
2	I	37	ILE	N-CA	5.78	1.53	1.46
1	E	104	MET	C-N	-5.74	1.25	1.33
1	E	241	THR	C-N	-5.69	1.26	1.33
1	E	60	LYS	C-O	-5.58	1.17	1.23
1	E	43	GLY	N-CA	5.55	1.50	1.44
1	E	172	TYR	N-CA	-5.54	1.40	1.46
1	E	149	THR	C-O	5.40	1.30	1.24
1	E	97	ASN	C-O	5.32	1.30	1.24
1	E	66	ARG	N-CA	5.31	1.52	1.46
2	I	23	SER	C-N	-5.17	1.25	1.33
2	I	65	ASN	C-N	-5.16	1.26	1.33
1	E	60	LYS	CA-C	5.16	1.58	1.52
2	I	66	ASP	CA-CB	5.10	1.62	1.53
1	E	40	HIS	CD2-NE2	-5.08	1.32	1.37
1	E	105	LEU	N-CA	5.01	1.52	1.46

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	65	ASN	CA-CB-CG	37.13	149.73	112.60
2	I	65	ASN	CA-C-N	24.18	167.72	121.54
2	I	65	ASN	C-N-CA	24.18	167.72	121.54
2	I	71	PRO	CA-C-N	23.41	166.25	121.54
2	I	71	PRO	C-N-CA	23.41	166.25	121.54
1	E	97	ASN	CA-CB-CG	18.97	131.57	112.60
1	E	245	ASN	CA-CB-CG	18.83	131.43	112.60
1	E	101	ASN	OD1-CG-ND2	-15.04	107.56	122.60
2	I	66	ASP	CA-C-N	14.90	149.99	121.54
2	I	66	ASP	C-N-CA	14.90	149.99	121.54
1	E	181	PHE	CA-CB-CG	14.81	128.61	113.80
1	E	101	ASN	CA-CB-CG	14.02	126.62	112.60
1	E	171	ALA	CA-C-N	13.33	139.56	123.16
1	E	171	ALA	C-N-CA	13.33	139.56	123.16
2	I	66	ASP	CA-C-O	13.19	139.37	120.51
2	I	36	ASP	CA-CB-CG	12.17	124.77	112.60
1	E	25	ASN	CA-CB-CG	11.78	124.38	112.60
2	I	69	TYR	CA-C-O	11.58	133.31	120.80
2	I	65	ASN	OD1-CG-ND2	-11.41	111.19	122.60
1	E	26	THR	N-CA-C	-11.04	99.92	113.50
1	E	199	VAL	N-CA-CB	10.91	125.35	112.15
1	E	101	ASN	CB-CG-OD1	10.82	142.43	120.80
1	E	233	ASN	OD1-CG-ND2	-10.54	112.06	122.60
1	E	105	LEU	CB-CA-C	10.29	128.53	109.71
2	I	66	ASP	N-CA-C	10.19	132.51	110.80
2	I	22	CYS	N-CA-CB	10.18	129.63	110.90
2	I	33	ARG	CA-C-O	-9.99	109.18	120.66
2	I	69	TYR	N-CA-C	9.77	124.95	110.30
1	E	115	ASN	N-CA-C	9.74	121.51	108.07
2	I	67	PHE	CA-CB-CG	-9.65	104.15	113.80
1	E	34	ASN	CA-CB-CG	9.53	122.12	112.60
1	E	66	ARG	NE-CZ-NH1	9.33	130.83	121.50
1	E	100	ASN	CA-C-N	9.26	135.21	122.34
1	E	100	ASN	C-N-CA	9.26	135.21	122.34
2	I	19	CYS	N-CA-CB	9.16	125.97	110.49
1	E	153	ASP	N-CA-C	-8.97	102.47	113.50
1	E	105	LEU	N-CA-CB	-8.92	95.69	110.68
1	E	233	ASN	CA-CB-CG	8.92	121.52	112.60
2	I	18	CYS	CA-C-N	8.77	138.29	121.54
2	I	18	CYS	C-N-CA	8.77	138.29	121.54
1	E	111	ALA	N-CA-CB	8.71	125.20	110.49
1	E	142	GLY	CA-C-N	8.70	134.27	121.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	142	GLY	C-N-CA	8.70	134.27	121.31
2	I	71	PRO	N-CA-C	8.65	134.59	112.10
1	E	37	SER	N-CA-C	-8.62	98.97	111.30
1	E	59	TYR	CA-C-N	8.60	136.51	121.80
1	E	59	TYR	C-N-CA	8.60	136.51	121.80
2	I	67	PHE	N-CA-CB	8.37	124.64	110.49
1	E	116	SER	O-C-N	8.37	131.03	122.08
1	E	97	ASN	CA-C-N	-8.34	109.59	122.60
1	E	97	ASN	C-N-CA	-8.34	109.59	122.60
2	I	31	LYS	CB-CA-C	8.32	123.45	110.14
1	E	230	LYS	CA-C-O	-8.21	112.47	122.41
1	E	72	ASN	CA-C-O	-8.21	111.32	120.60
1	E	210	GLN	OE1-CD-NE2	-8.20	114.40	122.60
1	E	26	THR	CB-CA-C	8.12	124.06	109.29
1	E	103	ILE	CA-C-N	8.08	135.62	122.29
1	E	103	ILE	C-N-CA	8.08	135.62	122.29
2	I	65	ASN	O-C-N	-8.03	110.14	123.00
1	E	185	LEU	N-CA-C	-7.97	102.82	112.54
2	I	67	PHE	CA-C-N	7.92	136.66	121.54
2	I	67	PHE	C-N-CA	7.92	136.66	121.54
1	E	95	ASN	CA-CB-CG	7.87	120.47	112.60
1	E	86	SER	CA-C-O	7.80	127.31	118.97
1	E	97	ASN	N-CA-CB	7.74	122.22	110.30
1	E	146	SER	CA-CB-OG	7.73	126.56	111.10
1	E	214	SER	CA-C-O	7.63	125.10	119.68
1	E	170	SER	CA-CB-OG	-7.61	95.88	111.10
2	I	20	ASP	CA-C-O	7.61	131.39	120.51
1	E	150	SER	CA-C-N	7.60	138.12	121.63
1	E	150	SER	C-N-CA	7.60	138.12	121.63
2	I	72	CYS	CA-C-N	7.57	135.33	121.70
2	I	72	CYS	C-N-CA	7.57	135.33	121.70
1	E	200	VAL	CB-CA-C	7.52	122.67	111.31
2	I	16	LYS	CA-C-N	7.44	129.14	119.84
2	I	16	LYS	C-N-CA	7.44	129.14	119.84
1	E	171	ALA	N-CA-C	7.43	119.38	111.28
1	E	240	GLN	CA-C-N	7.41	130.08	120.44
1	E	240	GLN	C-N-CA	7.41	130.08	120.44
2	I	68	CYS	CB-CA-C	7.29	124.93	110.42
1	E	188(A)	GLY	N-CA-C	-7.21	104.88	114.25
1	E	109	LYS	CA-C-N	7.18	135.25	121.54
1	E	109	LYS	C-N-CA	7.18	135.25	121.54
2	I	72	CYS	N-CA-CB	7.18	122.62	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	225	PRO	CA-C-N	7.14	127.60	120.31
1	E	225	PRO	C-N-CA	7.14	127.60	120.31
1	E	122	SER	O-C-N	7.12	131.42	123.16
1	E	242	ILE	N-CA-C	-7.12	103.36	110.62
1	E	20	TYR	CA-C-O	-7.10	113.66	121.33
1	E	64	GLN	OE1-CD-NE2	-7.09	115.51	122.60
1	E	49	SER	N-CA-C	7.07	121.73	113.18
1	E	199	VAL	CA-C-O	-7.07	111.51	120.69
1	E	100	ASN	CB-CA-C	7.06	121.72	109.65
1	E	100	ASN	CB-CG-ND2	7.05	126.98	116.40
1	E	151	TYR	N-CA-CB	-7.05	96.19	109.37
1	E	199	VAL	CA-CB-CG2	7.04	122.37	110.40
1	E	82	PHE	CA-C-O	-7.02	113.24	120.54
1	E	64	GLN	CB-CG-CD	7.01	124.51	112.60
1	E	177	THR	CA-C-O	-7.00	113.00	121.89
1	E	97	ASN	OD1-CG-ND2	-6.99	115.61	122.60
1	E	240	GLN	CG-CD-OE1	6.98	134.77	120.80
1	E	63	ILE	CA-C-O	-6.96	112.77	120.84
2	I	69	TYR	CA-C-N	6.94	138.74	121.80
2	I	69	TYR	C-N-CA	6.94	138.74	121.80
2	I	13	GLU	CA-C-N	6.92	134.75	121.54
2	I	13	GLU	C-N-CA	6.92	134.75	121.54
1	E	23	GLY	CA-C-O	-6.91	115.58	121.66
1	E	111	ALA	N-CA-C	-6.90	96.10	110.80
1	E	230	LYS	N-CA-CB	6.90	120.51	110.58
1	E	86	SER	O-C-N	-6.84	114.20	122.48
1	E	132	ALA	CA-C-O	-6.83	113.63	121.15
1	E	34	ASN	OD1-CG-ND2	-6.81	115.79	122.60
1	E	81	GLN	CA-CB-CG	6.81	127.72	114.10
1	E	230	LYS	CG-CD-CE	6.80	126.93	111.30
1	E	213	VAL	O-C-N	6.78	131.04	122.57
2	I	31	LYS	N-CA-C	-6.78	97.23	108.34
2	I	23	SER	CA-C-O	-6.78	113.87	120.92
1	E	190	SER	N-CA-C	-6.77	101.80	110.53
1	E	86	SER	CA-C-N	6.76	133.84	121.94
1	E	86	SER	C-N-CA	6.76	133.84	121.94
1	E	25	ASN	OD1-CG-ND2	-6.73	115.87	122.60
1	E	240	GLN	O-C-N	6.67	128.94	122.07
2	I	30	PRO	CB-CA-C	-6.66	100.57	111.56
1	E	60	LYS	CA-CB-CG	6.66	127.42	114.10
1	E	230	LYS	CB-CA-C	-6.61	101.26	111.83
2	I	68	CYS	O-C-N	-6.58	113.84	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	47	ILE	CA-C-N	6.56	133.87	122.32
1	E	47	ILE	C-N-CA	6.56	133.87	122.32
1	E	67	LEU	CA-C-N	6.54	132.57	120.87
1	E	67	LEU	C-N-CA	6.54	132.57	120.87
1	E	173	PRO	CB-CA-C	-6.54	103.55	111.46
1	E	66	ARG	NH1-CZ-NH2	-6.53	110.81	119.30
1	E	196	GLY	N-CA-C	-6.50	107.34	115.08
2	I	38	ARG	CD-NE-CZ	6.50	133.50	124.40
1	E	20	TYR	O-C-N	6.48	130.63	123.25
1	E	51	TRP	CA-C-N	6.48	131.94	122.94
1	E	51	TRP	C-N-CA	6.48	131.94	122.94
1	E	102	ASP	CA-C-O	-6.46	114.57	122.64
1	E	95	ASN	N-CA-CB	-6.45	99.56	110.46
1	E	160	ALA	O-C-N	6.45	126.36	121.85
1	E	240	GLN	CB-CG-CD	6.44	123.55	112.60
1	E	230	LYS	O-C-N	6.44	130.88	122.38
1	E	47	ILE	CB-CA-C	6.42	120.46	110.95
1	E	60	LYS	N-CA-CB	6.42	121.35	111.46
1	E	81	GLN	N-CA-CB	6.42	120.92	110.90
1	E	156	LYS	CB-CA-C	6.40	120.23	109.48
1	E	65	VAL	CB-CA-C	6.38	119.95	111.21
2	I	21	GLN	N-CA-CB	6.36	121.25	110.49
1	E	165	ASP	CA-CB-CG	6.33	118.93	112.60
1	E	135	GLN	CB-CG-CD	-6.32	101.86	112.60
1	E	234	TYR	O-C-N	6.29	129.62	122.20
1	E	161	PRO	CA-C-N	6.28	130.22	122.37
1	E	161	PRO	C-N-CA	6.28	130.22	122.37
2	I	21	GLN	O-C-N	6.27	130.93	122.59
1	E	165	ASP	N-CA-C	-6.27	104.89	112.54
1	E	47	ILE	CB-CG1-CD1	6.26	126.95	113.80
1	E	21	THR	CA-CB-OG1	-6.25	100.22	109.60
1	E	72	ASN	O-C-N	6.21	130.89	122.82
2	I	18	CYS	CA-C-O	6.18	129.35	120.51
2	I	38	ARG	NE-CZ-NH1	6.16	127.66	121.50
1	E	168	CYS	CA-C-O	6.16	127.05	119.97
1	E	86	SER	N-CA-C	-6.08	106.19	113.97
1	E	79	ASN	O-C-N	6.06	129.57	122.24
1	E	112	ALA	O-C-N	6.04	129.73	122.85
1	E	114	LEU	N-CA-C	6.02	118.01	108.67
2	I	72	CYS	N-CA-C	6.00	123.57	110.80
1	E	190	SER	CA-CB-OG	5.97	123.05	111.10
1	E	230	LYS	CA-CB-CG	5.97	126.04	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	242	ILE	CB-CA-C	5.94	120.16	112.14
1	E	189	ASP	N-CA-C	5.91	117.24	107.73
1	E	87	LYS	CB-CG-CD	5.90	124.86	111.30
1	E	170	SER	CA-C-N	5.87	128.15	120.28
1	E	170	SER	C-N-CA	5.87	128.15	120.28
2	I	38	ARG	CA-CB-CG	5.86	125.82	114.10
1	E	186	GLU	CB-CG-CD	-5.85	102.65	112.60
1	E	216	GLY	N-CA-C	-5.85	102.20	110.75
1	E	39	TYR	CA-C-O	-5.85	114.46	120.89
1	E	171	ALA	CB-CA-C	-5.84	101.10	110.79
2	I	20	ASP	N-CA-CB	5.82	120.33	110.49
1	E	177	THR	O-C-N	5.82	129.59	122.84
1	E	95	ASN	OD1-CG-ND2	5.82	128.42	122.60
1	E	81	GLN	OE1-CD-NE2	-5.80	116.80	122.60
1	E	75	VAL	N-CA-CB	5.80	120.97	111.58
2	I	71	PRO	CA-C-O	5.79	134.10	120.20
1	E	190	SER	CB-CA-C	5.75	122.31	110.40
1	E	67	LEU	CB-CA-C	5.73	119.85	109.37
2	I	26	LYS	O-C-N	5.72	130.19	122.59
1	E	199	VAL	N-CA-C	-5.70	97.65	106.72
2	I	71	PRO	N-CA-CB	-5.68	96.36	102.60
1	E	38	GLY	N-CA-C	-5.67	107.22	114.37
1	E	226	GLY	CA-C-N	-5.67	115.79	122.93
1	E	226	GLY	C-N-CA	-5.67	115.79	122.93
2	I	73	LYS	N-CA-CB	5.66	120.11	110.50
1	E	132	ALA	O-C-N	5.64	129.85	122.97
1	E	213	VAL	N-CA-CB	5.63	120.53	111.23
1	E	158	LEU	CA-CB-CG	5.63	136.01	116.30
1	E	50	GLN	OE1-CD-NE2	5.62	128.22	122.60
1	E	80	GLU	CB-CG-CD	5.62	122.16	112.60
1	E	51	TRP	N-CA-C	5.62	118.56	109.40
2	I	66	ASP	O-C-N	-5.62	115.11	122.59
1	E	100	ASN	CA-C-O	5.62	127.45	121.16
1	E	240	GLN	CG-CD-NE2	-5.59	108.02	116.40
2	I	66	ASP	CA-CB-CG	5.58	118.19	112.60
1	E	174	GLY	O-C-N	5.58	129.38	122.41
1	E	115	ASN	CA-C-N	5.55	128.50	120.79
1	E	115	ASN	C-N-CA	5.55	128.50	120.79
1	E	118	VAL	O-C-N	5.54	129.42	122.66
1	E	37	SER	CA-C-N	-5.53	115.61	123.08
1	E	37	SER	C-N-CA	-5.53	115.61	123.08
1	E	186	GLU	N-CA-C	5.52	119.19	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	25	THR	N-CA-CB	5.51	119.01	110.46
2	I	36	ASP	CA-C-O	-5.51	112.62	120.51
1	E	134	THR	CA-CB-CG2	5.51	119.86	110.50
2	I	32	CYS	O-C-N	5.50	130.39	123.23
2	I	72	CYS	CA-CB-SG	-5.50	101.74	114.40
1	E	190	SER	CA-C-O	-5.50	115.62	121.94
2	I	71	PRO	O-C-N	-5.48	110.69	121.10
1	E	170	SER	N-CA-CB	-5.47	102.12	110.33
1	E	95	ASN	CB-CG-ND2	-5.47	108.20	116.40
2	I	13	GLU	CB-CG-CD	5.46	121.89	112.60
1	E	60	LYS	CB-CA-C	-5.40	100.58	111.17
1	E	240	GLN	OE1-CD-NE2	-5.40	117.20	122.60
1	E	204	LYS	CA-C-O	-5.39	114.46	120.66
1	E	102	ASP	O-C-N	5.38	129.61	122.56
1	E	215	TRP	CA-C-N	5.37	129.07	120.97
1	E	215	TRP	C-N-CA	5.37	129.07	120.97
1	E	186	GLU	CG-CD-OE2	-5.35	106.09	118.40
2	I	18	CYS	CB-CA-C	5.34	121.05	110.42
1	E	238	ILE	CA-C-N	5.33	127.73	120.54
1	E	238	ILE	C-N-CA	5.33	127.73	120.54
1	E	178	SER	CA-C-N	5.33	131.01	122.86
1	E	178	SER	C-N-CA	5.33	131.01	122.86
1	E	237	TRP	N-CA-CB	5.31	117.71	110.01
1	E	60	LYS	CA-C-N	5.30	130.03	122.72
1	E	60	LYS	C-N-CA	5.30	130.03	122.72
1	E	40	HIS	CA-CB-CG	5.29	119.09	113.80
2	I	13	GLU	CA-C-O	5.28	128.07	120.51
1	E	171	ALA	CA-C-O	5.28	126.14	120.55
1	E	43	GLY	CA-C-O	-5.27	114.83	122.52
1	E	184	TYR	CA-C-O	5.23	126.12	120.32
1	E	212	ILE	N-CA-CB	5.22	118.92	111.82
1	E	162	ILE	O-C-N	5.20	129.28	122.94
1	E	107	LYS	CB-CG-CD	5.19	123.25	111.30
1	E	116	SER	CB-CA-C	-5.19	102.67	110.92
1	E	127	SER	CB-CA-C	5.19	121.00	109.94
1	E	139	SER	N-CA-CB	-5.18	102.87	111.57
1	E	87	LYS	N-CA-C	5.16	117.58	108.75
1	E	112	ALA	CA-C-N	-5.16	116.14	122.84
1	E	112	ALA	C-N-CA	-5.16	116.14	122.84
1	E	23	GLY	O-C-N	5.15	127.69	122.65
1	E	111	ALA	O-C-N	5.13	129.41	122.59
1	E	237	TRP	CA-C-N	5.13	127.11	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	237	TRP	C-N-CA	5.13	127.11	120.70
1	E	26	THR	CA-C-N	5.12	131.60	122.13
1	E	26	THR	C-N-CA	5.12	131.60	122.13
1	E	115	ASN	CA-C-O	5.12	128.28	121.47
1	E	182	CYS	N-CA-CB	5.12	118.97	110.52
1	E	113	SER	CA-C-N	5.10	129.58	121.99
1	E	113	SER	C-N-CA	5.10	129.58	121.99
2	I	31	LYS	O-C-N	5.09	129.23	123.27
1	E	76	VAL	CB-CA-C	5.07	116.88	111.35
1	E	146	SER	N-CA-CB	5.06	118.14	110.14
1	E	42	CYS	O-C-N	5.06	128.83	123.42
1	E	145	LYS	CA-CB-CG	5.05	124.21	114.10
1	E	154	VAL	CA-CB-CG2	5.05	118.98	110.40
1	E	47	ILE	O-C-N	5.04	127.17	122.23
1	E	48	ASN	CA-CB-CG	5.03	117.63	112.60
1	E	32	SER	O-C-N	5.01	129.21	123.29
1	E	143	ASN	CA-C-O	-5.01	115.66	121.07

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	E	1629	0	1588	184	4
2	I	275	0	247	70	0
3	E	136	0	0	32	4
3	I	4	0	0	0	0
All	All	2044	0	1835	250	5

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 67.

All (250) 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)
2:I:13:GLU:HG3	2:I:14:SER:H	1.08	1.17
1:E:87:LYS:HE3	3:E:332:HOH:O	1.48	1.14
2:I:12:SER:HA	2:I:16:LYS:HD3	1.31	1.10
2:I:28:MET:HE2	2:I:29:PRO:HA	1.17	1.10
1:E:149:THR:HG23	1:E:151:TYR:CE2	1.89	1.07
2:I:17:PRO:O	2:I:20:ASP:HB2	1.57	1.05
1:E:135:GLN:HE21	1:E:159:LYS:HB3	1.17	1.04
2:I:17:PRO:O	2:I:18:CYS:C	2.04	1.01
2:I:36:ASP:O	2:I:37:ILE:HB	1.24	0.99
1:E:121:ILE:HD12	1:E:122:SER:H	1.25	0.98
1:E:149:THR:HG23	1:E:151:TYR:HE2	1.26	0.98
1:E:87:LYS:NZ	1:E:245:ASN:OD1	1.96	0.97
2:I:13:GLU:CG	2:I:14:SER:H	1.56	0.97
1:E:220:CYS:N	3:E:303:HOH:O	1.94	0.95
2:I:13:GLU:CG	2:I:14:SER:N	2.26	0.95
2:I:28:MET:CE	2:I:29:PRO:HA	1.95	0.94
2:I:33:ARG:HH11	2:I:33:ARG:HG3	1.31	0.94
2:I:72:CYS:SG	2:I:73:LYS:N	2.36	0.94
1:E:48:ASN:HD22	1:E:49:SER:N	1.65	0.93
3:E:256:HOH:O	2:I:26:LYS:HE3	1.69	0.93
2:I:36:ASP:O	2:I:37:ILE:CB	2.15	0.93
1:E:164:SER:HB3	1:E:166:SER:OG	1.69	0.93
2:I:13:GLU:HG3	2:I:14:SER:N	1.83	0.92
2:I:17:PRO:O	2:I:18:CYS:O	1.90	0.89
1:E:25:ASN:CG	1:E:117:ARG:HB3	1.96	0.89
1:E:55:ALA:O	1:E:104:MET:HE2	1.73	0.88
1:E:55:ALA:O	1:E:104:MET:CE	2.22	0.88
1:E:135:GLN:NE2	1:E:159:LYS:HB3	1.87	0.88
2:I:21:GLN:O	2:I:34:CYS:HA	1.75	0.86
1:E:224:LYS:N	1:E:224:LYS:HD2	1.91	0.85
2:I:12:SER:HA	2:I:16:LYS:CD	2.07	0.85
1:E:192:GLN:HG3	3:E:247:HOH:O	1.78	0.84
2:I:67:PHE:C	2:I:68:CYS:SG	2.60	0.83
1:E:25:ASN:HA	3:E:260:HOH:O	1.78	0.83
2:I:67:PHE:O	2:I:68:CYS:SG	2.37	0.82
1:E:25:ASN:ND2	1:E:117:ARG:HA	1.94	0.82
1:E:31:VAL:CG1	1:E:65:VAL:HG13	2.09	0.81
1:E:238:ILE:HG23	1:E:242:ILE:CD1	2.10	0.81
2:I:28:MET:HE2	2:I:29:PRO:CA	2.08	0.81
2:I:28:MET:HE2	2:I:28:MET:HA	1.62	0.81
1:E:223:ASN:C	1:E:224:LYS:HD2	2.06	0.81
2:I:19:CYS:HA	2:I:36:ASP:OD1	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:18:CYS:O	2:I:69:TYR:HE2	1.64	0.80
1:E:80:GLU:HB3	1:E:82:PHE:CE2	2.17	0.80
1:E:25:ASN:CB	1:E:117:ARG:HB3	2.12	0.80
2:I:21:GLN:HA	2:I:21:GLN:OE1	1.73	0.79
1:E:119:ALA:HB2	3:E:372:HOH:O	1.83	0.79
1:E:146:SER:OG	3:E:305:HOH:O	2.02	0.78
1:E:67:LEU:O	1:E:80:GLU:HA	1.83	0.78
1:E:105:LEU:HD11	1:E:242:ILE:HD11	1.67	0.77
1:E:121:ILE:HD12	1:E:122:SER:N	1.98	0.76
1:E:121:ILE:HG21	1:E:209:LEU:HD22	1.67	0.76
1:E:31:VAL:HG22	1:E:67:LEU:HD23	1.67	0.75
1:E:83:ILE:HG21	1:E:110:SER:HB2	1.69	0.74
1:E:79:ASN:O	3:E:333:HOH:O	2.05	0.74
1:E:93:SER:HB2	1:E:101:ASN:HD21	1.53	0.73
2:I:37:ILE:O	2:I:38:ARG:HG2	1.89	0.72
2:I:15:SER:O	2:I:16:LYS:O	2.08	0.72
1:E:176:ILE:O	3:E:355:HOH:O	2.08	0.71
1:E:64:GLN:HE22	1:E:66:ARG:HH21	1.39	0.71
1:E:64:GLN:NE2	1:E:66:ARG:HH21	1.89	0.71
1:E:186:GLU:HG3	3:E:276:HOH:O	1.89	0.71
1:E:146:SER:HB3	1:E:220:CYS:O	1.90	0.71
1:E:17:VAL:HG11	3:E:305:HOH:O	1.89	0.70
2:I:17:PRO:O	2:I:20:ASP:CB	2.37	0.70
1:E:93:SER:HB2	1:E:101:ASN:ND2	2.06	0.70
1:E:188(A):GLY:H	1:E:221(A):ALA:HB1	1.57	0.70
1:E:132:ALA:HA	1:E:162:ILE:HG22	1.72	0.70
1:E:72:ASN:O	3:E:381:HOH:O	2.10	0.69
1:E:135:GLN:HG3	3:E:367:HOH:O	1.92	0.69
1:E:25:ASN:HB3	3:E:348:HOH:O	1.92	0.69
2:I:21:GLN:HB3	2:I:35:SER:OG	1.93	0.69
1:E:25:ASN:CG	1:E:25:ASN:O	2.33	0.68
2:I:67:PHE:CD1	2:I:68:CYS:N	2.62	0.68
1:E:186:GLU:HB2	3:E:276:HOH:O	1.94	0.68
1:E:117:ARG:HD3	3:E:348:HOH:O	1.94	0.68
1:E:238:ILE:CG2	1:E:242:ILE:CD1	2.72	0.68
1:E:166:SER:O	1:E:170:SER:OG	2.12	0.67
1:E:138:ILE:HG12	1:E:199:VAL:HG22	1.76	0.67
1:E:99:LEU:HD12	1:E:215:TRP:CD1	2.30	0.67
1:E:215:TRP:CZ3	2:I:23:SER:OG	2.48	0.66
1:E:31:VAL:HG13	1:E:65:VAL:HG13	1.75	0.66
1:E:165:ASP:O	1:E:169:LYS:HB2	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:238:ILE:HG23	1:E:242:ILE:HD12	1.78	0.66
2:I:67:PHE:CZ	2:I:68:CYS:O	2.49	0.66
1:E:165:ASP:OD2	1:E:169:LYS:HD2	1.97	0.65
1:E:87:LYS:HZ1	1:E:245:ASN:HB3	1.62	0.65
1:E:17:VAL:HG22	1:E:144:THR:C	2.22	0.64
1:E:195:SER:OG	2:I:26:LYS:C	2.40	0.64
2:I:19:CYS:CA	2:I:36:ASP:OD1	2.46	0.63
2:I:37:ILE:O	2:I:38:ARG:CG	2.46	0.63
1:E:48:ASN:ND2	1:E:50:GLN:H	1.97	0.62
1:E:25:ASN:ND2	1:E:25:ASN:O	2.33	0.62
2:I:18:CYS:O	2:I:69:TYR:CE2	2.50	0.62
1:E:51:TRP:CZ2	1:E:107:LYS:HD2	2.35	0.62
2:I:17:PRO:O	2:I:20:ASP:N	2.32	0.61
1:E:48:ASN:HD22	1:E:48:ASN:C	2.08	0.61
1:E:243:ALA:HB2	3:E:266:HOH:O	2.00	0.61
2:I:67:PHE:CG	2:I:68:CYS:N	2.50	0.61
1:E:64:GLN:HE21	1:E:66:ARG:HE	1.48	0.60
1:E:238:ILE:O	1:E:242:ILE:HD12	2.01	0.60
1:E:25:ASN:HB2	1:E:117:ARG:HB3	1.83	0.60
2:I:13:GLU:HG3	2:I:14:SER:CB	2.32	0.60
1:E:39:TYR:CE2	1:E:41:PHE:HB3	2.37	0.60
1:E:163:LEU:HD12	1:E:182:CYS:CB	2.31	0.60
1:E:17:VAL:O	1:E:188:LYS:HA	2.02	0.60
1:E:99:LEU:CD1	1:E:215:TRP:CD1	2.85	0.59
1:E:31:VAL:HG22	1:E:67:LEU:CD2	2.32	0.59
1:E:138:ILE:CG1	1:E:199:VAL:HG22	2.33	0.59
1:E:87:LYS:NZ	1:E:245:ASN:HB3	2.17	0.59
1:E:192:GLN:CG	3:E:247:HOH:O	2.45	0.59
1:E:20:TYR:HA	3:E:254:HOH:O	2.01	0.58
1:E:24:ALA:O	1:E:26:THR:HG23	2.03	0.58
1:E:56:ALA:HB1	1:E:90:VAL:HG13	1.84	0.58
1:E:238:ILE:CG2	1:E:242:ILE:HD12	2.31	0.58
1:E:31:VAL:HG11	1:E:65:VAL:HG13	1.84	0.58
2:I:22:CYS:SG	2:I:22:CYS:O	2.62	0.57
1:E:101:ASN:HA	1:E:234:TYR:OH	2.05	0.57
1:E:163:LEU:HD12	1:E:182:CYS:HB2	1.86	0.57
1:E:145:LYS:HB2	1:E:147:SER:O	2.05	0.56
1:E:95:ASN:O	1:E:99:LEU:N	2.38	0.56
1:E:186:GLU:CB	3:E:276:HOH:O	2.53	0.56
1:E:70:GLU:HB2	3:E:261:HOH:O	2.06	0.56
1:E:25:ASN:N	3:E:316:HOH:O	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:80:GLU:HB3	1:E:82:PHE:HE2	1.66	0.55
1:E:235:VAL:O	1:E:239:LYS:HG3	2.06	0.55
1:E:99:LEU:HD12	1:E:215:TRP:CG	2.41	0.55
1:E:136:CYS:HB3	1:E:200:VAL:O	2.07	0.55
1:E:79:ASN:CG	1:E:117:ARG:HD2	2.31	0.55
1:E:158:LEU:HD21	1:E:188:LYS:HB3	1.86	0.55
1:E:221:GLN:O	1:E:224:LYS:HB2	2.07	0.55
2:I:33:ARG:HG3	2:I:33:ARG:NH1	2.08	0.55
1:E:191:CYS:O	2:I:26:LYS:HB3	2.07	0.55
1:E:135:GLN:HE22	1:E:159:LYS:HD3	1.73	0.54
2:I:28:MET:CE	2:I:28:MET:HA	2.37	0.54
1:E:59:TYR:C	1:E:59:TYR:CD2	2.85	0.54
2:I:16:LYS:O	2:I:20:ASP:HB2	2.08	0.54
2:I:19:CYS:N	2:I:36:ASP:OD1	2.40	0.54
1:E:47:ILE:HG22	1:E:121:ILE:HG22	1.91	0.53
2:I:21:GLN:O	2:I:34:CYS:CA	2.53	0.53
1:E:32:SER:HB3	1:E:66:ARG:HB2	1.91	0.53
1:E:135:GLN:HE22	1:E:159:LYS:CD	2.22	0.53
1:E:64:GLN:HE22	1:E:66:ARG:NH2	2.05	0.53
1:E:149:THR:HG23	1:E:151:TYR:CD2	2.41	0.53
1:E:162:ILE:HD13	1:E:181:PHE:CE1	2.45	0.52
1:E:164:SER:CB	1:E:166:SER:OG	2.51	0.52
1:E:100:ASN:ND2	1:E:179:ASN:HB2	2.23	0.52
1:E:47:ILE:HG22	1:E:121:ILE:CG2	2.40	0.52
1:E:28:PRO:HB2	1:E:119:ALA:H	1.75	0.52
1:E:162:ILE:CD1	1:E:181:PHE:CE1	2.93	0.52
1:E:186:GLU:CG	3:E:276:HOH:O	2.53	0.51
1:E:29:TYR:HB3	1:E:119:ALA:O	2.11	0.51
1:E:21:THR:OG1	1:E:156:LYS:HE2	2.10	0.51
1:E:78:GLY:N	1:E:80:GLU:OE1	2.32	0.51
1:E:23:GLY:O	1:E:26:THR:HG23	2.10	0.51
1:E:240:GLN:NE2	3:E:298:HOH:O	2.43	0.51
1:E:149:THR:CG2	1:E:151:TYR:CE2	2.81	0.51
1:E:188(A):GLY:N	1:E:221(A):ALA:HB1	2.25	0.51
2:I:19:CYS:H	2:I:36:ASP:CG	2.19	0.51
1:E:163:LEU:HD12	1:E:182:CYS:HB3	1.93	0.50
1:E:134:THR:O	1:E:161:PRO:HA	2.12	0.50
1:E:165:ASP:OD1	1:E:169:LYS:HE3	2.11	0.50
1:E:98:THR:C	1:E:100:ASN:H	2.21	0.49
1:E:28:PRO:HB3	1:E:117:ARG:O	2.12	0.49
1:E:64:GLN:NE2	1:E:66:ARG:NH2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:114:LEU:HA	1:E:118:VAL:O	2.13	0.49
2:I:21:GLN:HB3	2:I:35:SER:CB	2.41	0.49
2:I:13:GLU:HG2	2:I:14:SER:N	2.24	0.49
1:E:95:ASN:ND2	3:E:287:HOH:O	2.45	0.49
1:E:221(A):ALA:HA	3:E:302:HOH:O	2.13	0.48
2:I:37:ILE:C	2:I:38:ARG:CG	2.86	0.48
1:E:211:GLY:HA2	1:E:229:THR:O	2.14	0.48
1:E:81:GLN:OE1	1:E:112:ALA:HB1	2.14	0.48
1:E:45:SER:O	1:E:52:VAL:HA	2.14	0.48
1:E:80:GLU:CB	1:E:82:PHE:CE2	2.95	0.48
1:E:144:THR:OG1	1:E:145:LYS:HD3	2.14	0.48
1:E:223:ASN:O	1:E:224:LYS:HD2	2.13	0.47
2:I:18:CYS:HB3	2:I:71:PRO:HG2	1.96	0.47
1:E:64:GLN:NE2	1:E:66:ARG:HE	2.12	0.47
2:I:67:PHE:CE1	2:I:68:CYS:O	2.67	0.47
1:E:48:ASN:ND2	1:E:48:ASN:C	2.73	0.47
2:I:16:LYS:H	2:I:16:LYS:HG2	1.49	0.47
1:E:177:THR:HG23	1:E:180:MET:HE3	1.96	0.47
1:E:25:ASN:HB2	1:E:117:ARG:CB	2.44	0.47
1:E:100:ASN:ND2	1:E:177:THR:OG1	2.48	0.47
2:I:72:CYS:SG	2:I:73:LYS:C	2.98	0.46
1:E:56:ALA:HB1	1:E:90:VAL:CG1	2.45	0.46
1:E:83:ILE:CG2	1:E:110:SER:HB2	2.41	0.46
1:E:141:TRP:CD2	1:E:155:LEU:HD23	2.51	0.46
2:I:13:GLU:HG3	2:I:14:SER:CA	2.45	0.46
1:E:82:PHE:C	1:E:83:ILE:HG12	2.40	0.46
1:E:82:PHE:N	1:E:82:PHE:CD2	2.81	0.46
1:E:123:LEU:HD12	1:E:123:LEU:HA	1.82	0.46
1:E:163:LEU:HD21	1:E:184(A):GLY:O	2.15	0.46
1:E:22:CYS:HB3	1:E:26:THR:OG1	2.16	0.46
2:I:67:PHE:HZ	2:I:70:GLU:HB2	1.81	0.46
1:E:25:ASN:CB	3:E:348:HOH:O	2.58	0.45
1:E:99:LEU:CD1	1:E:215:TRP:CG	2.99	0.45
2:I:16:LYS:HB3	2:I:17:PRO:HD2	1.99	0.45
1:E:230:LYS:NZ	3:E:366:HOH:O	2.48	0.45
1:E:48:ASN:HD21	1:E:50:GLN:H	1.64	0.45
1:E:219:GLY:CA	3:E:303:HOH:O	2.65	0.45
1:E:133:GLY:N	1:E:162:ILE:O	2.40	0.45
1:E:87:LYS:HB3	1:E:107:LYS:HB3	1.99	0.45
1:E:203:GLY:N	3:E:338:HOH:O	2.50	0.45
1:E:236:SER:O	1:E:240:GLN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:27:SER:OG	2:I:30:PRO:HA	2.17	0.44
1:E:213:VAL:HA	1:E:228:TYR:CD1	2.52	0.44
1:E:71:ASP:HB3	1:E:77:GLU:OE1	2.18	0.44
2:I:13:GLU:C	2:I:15:SER:H	2.26	0.44
1:E:24:ALA:O	1:E:25:ASN:C	2.61	0.44
1:E:179:ASN:OD1	1:E:233:ASN:ND2	2.43	0.44
1:E:16:ILE:HD11	1:E:138:ILE:HG22	1.99	0.44
1:E:72:ASN:H	1:E:77:GLU:CD	2.24	0.44
2:I:29:PRO:HB2	2:I:65:ASN:N	2.33	0.44
1:E:16:ILE:CD1	1:E:138:ILE:HG22	2.48	0.44
1:E:189:ASP:OD2	1:E:190:SER:N	2.51	0.44
2:I:13:GLU:HG3	2:I:14:SER:HB3	2.00	0.44
2:I:21:GLN:O	2:I:34:CYS:SG	2.76	0.44
1:E:145:LYS:C	1:E:147:SER:N	2.73	0.43
2:I:70:GLU:HA	2:I:71:PRO:HA	1.95	0.43
1:E:87:LYS:NZ	1:E:245:ASN:CG	2.74	0.43
1:E:34:ASN:HB2	3:E:269:HOH:O	2.18	0.43
2:I:73:LYS:HA	2:I:73:LYS:HD3	1.70	0.43
1:E:98:THR:C	1:E:100:ASN:N	2.75	0.43
2:I:17:PRO:O	2:I:20:ASP:CA	2.66	0.43
2:I:28:MET:CE	2:I:30:PRO:HD3	2.49	0.43
1:E:221:GLN:HB3	1:E:224:LYS:CB	2.49	0.43
1:E:238:ILE:O	1:E:242:ILE:HB	2.19	0.42
1:E:83:ILE:HD11	3:E:304:HOH:O	2.20	0.42
1:E:224:LYS:N	1:E:224:LYS:CD	2.70	0.42
1:E:138:ILE:O	1:E:139:SER:HB3	2.19	0.42
2:I:16:LYS:O	2:I:20:ASP:CB	2.66	0.42
1:E:41:PHE:CE2	1:E:60:LYS:HD2	2.54	0.42
1:E:17:VAL:HG12	1:E:188(A):GLY:O	2.20	0.42
1:E:116:SER:OG	1:E:117:ARG:N	2.52	0.42
2:I:28:MET:HE2	2:I:30:PRO:HD3	2.00	0.42
1:E:48:ASN:HD22	1:E:49:SER:H	1.61	0.41
1:E:105:LEU:HD22	1:E:237:TRP:CZ3	2.54	0.41
1:E:121:ILE:CG2	1:E:209:LEU:HD22	2.46	0.41
1:E:188:LYS:O	1:E:189:ASP:HB2	2.20	0.41
1:E:135:GLN:NE2	1:E:159:LYS:HD3	2.33	0.41
1:E:16:ILE:HG21	1:E:158:LEU:HB2	2.03	0.41
1:E:29:TYR:O	1:E:31:VAL:HG23	2.21	0.41
2:I:65:ASN:OD1	2:I:66:ASP:OD2	2.39	0.41
1:E:201:CYS:SG	1:E:210:GLN:HG3	2.61	0.40
1:E:37:SER:OG	1:E:60:LYS:HE2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:135:GLN:NE2	1:E:159:LYS:CD	2.83	0.40
2:I:29:PRO:HA	2:I:30:PRO:HD3	1.96	0.40
1:E:57:HIS:CD2	2:I:27:SER:HB3	2.56	0.40

All (5) 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)
1:E:170:SER:CB	3:E:295:HOH:O[3_645]	0.55	1.65
1:E:170:SER:CA	3:E:295:HOH:O[3_645]	1.78	0.42
1:E:170:SER:OG	3:E:295:HOH:O[3_645]	1.96	0.24
3:E:297:HOH:O	3:E:300:HOH:O[6_555]	2.12	0.08
1:E:74:ASN:ND2	1:E:90:VAL:CG2[6_455]	2.18	0.02

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	E	221/223 (99%)	202 (91%)	19 (9%)	0	100	100
2	I	32/82 (39%)	13 (41%)	7 (22%)	12 (38%)	0	0
All	All	253/305 (83%)	215 (85%)	26 (10%)	12 (5%)	2	1

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	I	16	LYS
2	I	17	PRO
2	I	18	CYS
2	I	37	ILE
2	I	66	ASP
2	I	67	PHE

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Mol	Chain	Res	Type
2	I	68	CYS
2	I	70	GLU
2	I	71	PRO
2	I	72	CYS
2	I	21	GLN
2	I	36	ASP

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	E	184/184 (100%)	149 (81%)	35 (19%)	1	1
2	I	36/78 (46%)	27 (75%)	9 (25%)	0	0
All	All	220/262 (84%)	176 (80%)	44 (20%)	1	1

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	25	ASN
1	E	45	SER
1	E	47	ILE
1	E	48	ASN
1	E	49	SER
1	E	59	TYR
1	E	74	ASN
1	E	75	VAL
1	E	83	ILE
1	E	101	ASN
1	E	109	LYS
1	E	116	SER
1	E	117	ARG
1	E	121	ILE
1	E	123	LEU
1	E	135	GLN
1	E	145	LYS

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Mol	Chain	Res	Type
1	E	146	SER
1	E	154	VAL
1	E	155	LEU
1	E	158	LEU
1	E	162	ILE
1	E	164	SER
1	E	165	ASP
1	E	170	SER
1	E	177	THR
1	E	192	GLN
1	E	200	VAL
1	E	201	CYS
1	E	202	SER
1	E	221	GLN
1	E	224	LYS
1	E	227	VAL
1	E	242	ILE
1	E	244	SER
2	I	16	LYS
2	I	21	GLN
2	I	28	MET
2	I	33	ARG
2	I	37	ILE
2	I	66	ASP
2	I	71	PRO
2	I	72	CYS
2	I	73	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	30	GLN
1	E	48	ASN
1	E	50	GLN
1	E	64	GLN
1	E	100	ASN
1	E	135	GLN
1	E	192	GLN
1	E	240	GLN
2	I	65	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.