



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:29 PM UTC

PDB ID : 2LBP / pdb_00002lbp
Title : STRUCTURE OF THE L-LEUCINE-BINDING PROTEIN REFINED AT 2.4
ANGSTROMS RESOLUTION AND COMPARISON WITH THE LEU(SLA
SH)ILE(SLASH)VAL-BINDING PROTEIN STRUCTURE
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Deposited on : 1989-04-10
Resolution : 2.40 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **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

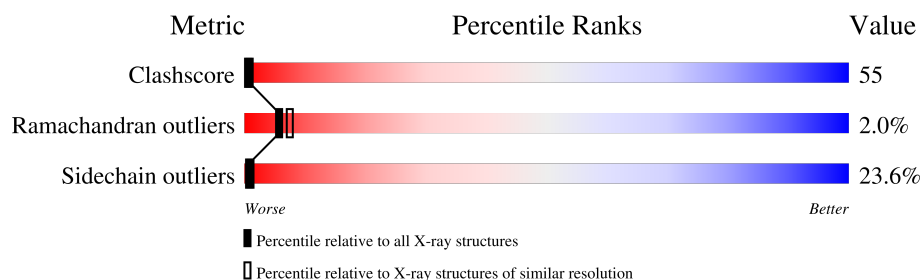
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	A	346	27% 40% 27% 6%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2691 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 LEUCINE-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	346	2600	1636	442	511	11	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	344	LYS	ALA	conflict	UNP P04816

- Molecule 2 is water.

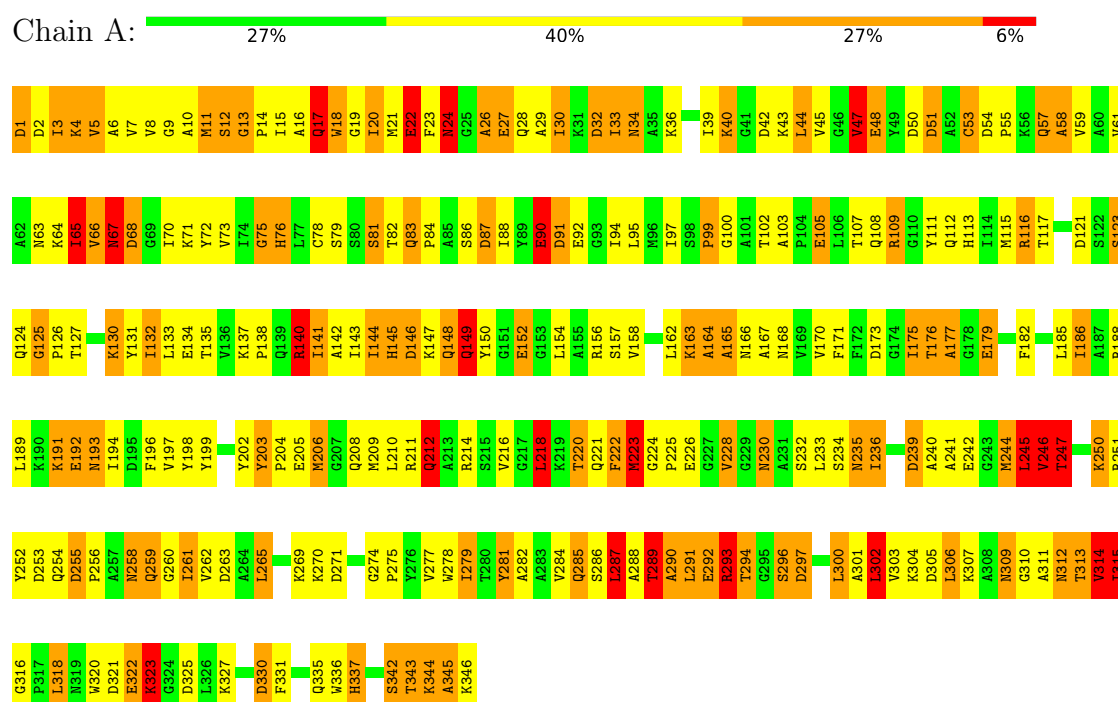
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		

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: LEUCINE-BINDING PROTEIN



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	68.80Å 69.34Å 74.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	10.00 – 2.40	Depositor
% Data completeness (in resolution range)	(Not available) (10.00-2.40)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	PROLSQ	Depositor
R, R_{free}	0.213 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2691	wwPDB-VP
Average B, all atoms (Å ²)	9.0	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	A	1.40	16/2648 (0.6%)	2.89	257/3581 (7.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	5

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	13	GLY	N-CA	9.19	1.57	1.44
1	A	291	LEU	N-CA	-7.82	1.36	1.46
1	A	12	SER	C-O	7.36	1.33	1.24
1	A	310	GLY	N-CA	7.23	1.55	1.45
1	A	23	PHE	C-N	-6.78	1.25	1.33
1	A	68	ASP	N-CA	6.30	1.52	1.46
1	A	290	ALA	N-CA	5.97	1.53	1.46
1	A	289	THR	C-O	5.75	1.31	1.24
1	A	141	ILE	CA-CB	5.72	1.61	1.54
1	A	51	ASP	CA-CB	5.67	1.62	1.53
1	A	313	THR	CA-CB	5.55	1.63	1.54
1	A	47	VAL	N-CA	5.46	1.53	1.46
1	A	90	GLU	C-N	-5.20	1.26	1.33
1	A	307	LYS	CA-CB	-5.16	1.44	1.53
1	A	309	ASN	C-O	5.13	1.31	1.23
1	A	245	LEU	N-CA	5.01	1.52	1.46

All (257) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	GLU	CB-CG-CD	28.17	160.49	112.60
1	A	330	ASP	CA-CB-CG	25.75	138.35	112.60
1	A	27	GLU	CB-CG-CD	24.85	154.85	112.60
1	A	307	LYS	CA-CB-CG	21.70	157.49	114.10
1	A	235	ASN	CA-CB-CG	20.38	132.98	112.60
1	A	22	GLU	CA-CB-CG	17.97	150.04	114.10
1	A	34	ASN	CA-CB-CG	17.56	130.16	112.60
1	A	47	VAL	CB-CA-C	17.26	134.63	110.98
1	A	75	GLY	CA-C-N	15.33	150.82	121.54
1	A	75	GLY	C-N-CA	15.33	150.82	121.54
1	A	34	ASN	CB-CA-C	13.24	136.10	110.67
1	A	290	ALA	CA-C-N	13.21	146.78	121.54
1	A	290	ALA	C-N-CA	13.21	146.78	121.54
1	A	287	LEU	CA-C-O	12.80	134.08	120.90
1	A	116	ARG	CD-NE-CZ	12.36	141.70	124.40
1	A	253	ASP	CA-CB-CG	12.10	124.70	112.60
1	A	290	ALA	CB-CA-C	11.87	124.40	109.80
1	A	301	ALA	CA-C-N	11.69	136.89	120.29
1	A	301	ALA	C-N-CA	11.69	136.89	120.29
1	A	4	LYS	CA-C-N	11.62	139.15	122.99
1	A	4	LYS	C-N-CA	11.62	139.15	122.99
1	A	5	VAL	CB-CA-C	-10.84	94.50	110.33
1	A	34	ASN	OD1-CG-ND2	-10.64	111.96	122.60
1	A	51	ASP	CA-CB-CG	-10.01	102.59	112.60
1	A	239	ASP	CA-CB-CG	-10.00	102.60	112.60
1	A	289	THR	CA-C-N	-9.60	105.36	121.97
1	A	289	THR	C-N-CA	-9.60	105.36	121.97
1	A	121	ASP	CA-CB-CG	9.59	122.19	112.60
1	A	90	GLU	CA-C-N	9.56	139.80	121.54
1	A	90	GLU	C-N-CA	9.56	139.80	121.54
1	A	236	ILE	N-CA-C	9.36	119.48	111.90
1	A	290	ALA	N-CA-C	-9.21	97.02	110.64
1	A	297	ASP	CB-CA-C	9.02	124.81	109.65
1	A	5	VAL	N-CA-CB	8.99	124.64	111.52
1	A	27	GLU	CG-CD-OE1	8.93	138.95	118.40
1	A	337	HIS	CA-CB-CG	-8.88	104.92	113.80
1	A	342	SER	N-CA-C	8.84	122.93	108.26
1	A	32	ASP	CA-CB-CG	8.83	121.43	112.60
1	A	24	ASN	N-CA-CB	-8.70	95.60	109.78
1	A	22	GLU	CA-C-O	-8.58	111.86	120.70
1	A	23	PHE	CA-C-N	8.55	133.64	120.82
1	A	23	PHE	C-N-CA	8.55	133.64	120.82
1	A	291	LEU	CA-C-O	-8.46	108.42	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	223	MET	N-CA-CB	8.43	125.49	111.08
1	A	108	GLN	CA-CB-CG	8.31	130.72	114.10
1	A	331	PHE	CA-CB-CG	8.28	122.08	113.80
1	A	226	GLU	CA-C-O	-8.22	110.99	120.20
1	A	168	ASN	CA-CB-CG	8.15	120.75	112.60
1	A	78	CYS	O-C-N	8.12	132.14	122.96
1	A	271	ASP	CA-CB-CG	7.99	120.58	112.60
1	A	293	ARG	CA-C-N	7.95	136.84	122.06
1	A	293	ARG	C-N-CA	7.95	136.84	122.06
1	A	226	GLU	CA-CB-CG	7.94	129.99	114.10
1	A	291	LEU	N-CA-C	7.85	127.52	110.80
1	A	113	HIS	CA-CB-CG	7.83	121.63	113.80
1	A	152	GLU	CA-C-N	7.77	128.56	119.94
1	A	152	GLU	C-N-CA	7.77	128.56	119.94
1	A	236	ILE	CB-CA-C	-7.76	103.86	111.30
1	A	226	GLU	CB-CG-CD	7.75	125.78	112.60
1	A	163	LYS	N-CA-CB	7.71	121.53	110.13
1	A	50	ASP	O-C-N	7.62	131.91	123.22
1	A	17	GLN	N-CA-C	-7.61	103.99	113.20
1	A	313	THR	N-CA-C	7.55	120.88	109.41
1	A	211	ARG	CD-NE-CZ	-7.51	113.88	124.40
1	A	203	TYR	O-C-N	7.49	127.66	120.55
1	A	246	VAL	CB-CA-C	-7.48	98.72	110.69
1	A	24	ASN	OD1-CG-ND2	7.46	130.06	122.60
1	A	327	LYS	CA-CB-CG	7.43	128.96	114.10
1	A	12	SER	CA-C-N	-7.42	110.22	121.87
1	A	12	SER	C-N-CA	-7.42	110.22	121.87
1	A	149	GLN	CA-C-O	-7.39	113.24	121.00
1	A	289	THR	CA-CB-CG2	7.36	123.01	110.50
1	A	297	ASP	N-CA-C	-7.36	104.16	113.43
1	A	65	ILE	CB-CA-C	7.32	121.97	111.65
1	A	146	ASP	CA-C-N	7.29	136.49	124.31
1	A	146	ASP	C-N-CA	7.29	136.49	124.31
1	A	12	SER	O-C-N	-7.26	112.93	122.59
1	A	211	ARG	CA-C-N	7.26	130.60	120.29
1	A	211	ARG	C-N-CA	7.26	130.60	120.29
1	A	331	PHE	O-C-N	-7.26	114.81	122.94
1	A	87	ASP	O-C-N	7.25	129.92	122.09
1	A	44	LEU	O-C-N	7.20	131.40	123.27
1	A	58	ALA	CA-C-N	7.19	131.84	120.47
1	A	58	ALA	C-N-CA	7.19	131.84	120.47
1	A	327	LYS	N-CA-CB	7.19	122.36	110.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	ILE	CA-C-N	-7.13	109.47	120.31
1	A	33	ILE	C-N-CA	-7.13	109.47	120.31
1	A	246	VAL	CA-CB-CG2	7.13	122.52	110.40
1	A	292	GLU	CG-CD-OE1	7.12	134.77	118.40
1	A	5	VAL	O-C-N	7.07	130.84	123.20
1	A	50	ASP	CA-C-N	7.06	134.74	122.09
1	A	50	ASP	C-N-CA	7.06	134.74	122.09
1	A	2	ASP	CA-C-O	-7.04	109.47	120.81
1	A	277	VAL	O-C-N	7.04	128.81	121.91
1	A	290	ALA	O-C-N	-7.02	114.18	122.89
1	A	91	ASP	N-CA-CB	-6.98	98.69	110.49
1	A	307	LYS	N-CA-CB	6.98	121.10	110.28
1	A	34	ASN	CA-C-N	6.96	130.31	120.28
1	A	34	ASN	C-N-CA	6.96	130.31	120.28
1	A	311	ALA	N-CA-C	-6.96	98.58	109.72
1	A	289	THR	CB-CA-C	6.95	124.26	110.42
1	A	226	GLU	N-CA-CB	6.95	121.12	110.14
1	A	235	ASN	OD1-CG-ND2	-6.94	115.66	122.60
1	A	152	GLU	CA-C-O	6.93	127.77	120.42
1	A	206	MET	CA-C-N	6.91	127.64	119.98
1	A	206	MET	C-N-CA	6.91	127.64	119.98
1	A	78	CYS	CA-C-O	-6.90	113.53	121.47
1	A	23	PHE	N-CA-CB	6.89	120.21	109.94
1	A	7	VAL	CB-CA-C	6.87	119.93	110.99
1	A	235	ASN	N-CA-C	-6.75	104.91	113.01
1	A	313	THR	CA-C-O	6.68	129.33	121.58
1	A	18	TRP	CB-CA-C	6.63	120.85	109.24
1	A	141	ILE	N-CA-CB	-6.63	103.11	111.46
1	A	134	GLU	CB-CG-CD	6.60	123.82	112.60
1	A	157	SER	CA-C-N	6.59	129.77	120.42
1	A	157	SER	C-N-CA	6.59	129.77	120.42
1	A	193	ASN	N-CA-CB	-6.59	101.95	111.70
1	A	141	ILE	N-CA-C	6.57	117.32	107.80
1	A	345	ALA	N-CA-C	6.56	120.59	110.42
1	A	145	HIS	CA-CB-CG	-6.51	107.29	113.80
1	A	285	GLN	CB-CG-CD	6.47	123.60	112.60
1	A	170	VAL	N-CA-C	6.45	116.56	110.30
1	A	271	ASP	CB-CA-C	6.44	118.66	109.38
1	A	309	ASN	CA-CB-CG	-6.43	106.17	112.60
1	A	125	GLY	CA-C-N	6.42	126.34	119.28
1	A	125	GLY	C-N-CA	6.42	126.34	119.28
1	A	307	LYS	CB-CG-CD	6.42	126.07	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ASP	CB-CA-C	-6.41	102.98	111.82
1	A	260	GLY	CA-C-N	6.37	129.46	120.42
1	A	260	GLY	C-N-CA	6.37	129.46	120.42
1	A	343	THR	CA-C-O	-6.37	113.60	120.92
1	A	48	GLU	CG-CD-OE1	6.34	132.99	118.40
1	A	116	ARG	CA-CB-CG	6.27	126.65	114.10
1	A	311	ALA	O-C-N	6.27	131.34	123.19
1	A	17	GLN	N-CA-CB	6.25	120.54	110.42
1	A	175	ILE	CA-C-O	-6.25	114.38	121.75
1	A	112	GLN	OE1-CD-NE2	6.23	128.83	122.60
1	A	156	ARG	NE-CZ-NH2	-6.23	113.59	119.20
1	A	198	TYR	N-CA-C	-6.22	99.06	109.07
1	A	259	GLN	N-CA-CB	6.21	119.79	110.22
1	A	318	LEU	CA-C-O	6.18	127.26	120.71
1	A	277	VAL	N-CA-CB	6.13	117.73	110.55
1	A	218	LEU	CB-CA-C	6.12	120.11	109.65
1	A	92	GLU	N-CA-C	6.10	120.34	113.02
1	A	68	ASP	CB-CA-C	6.09	121.20	110.35
1	A	291	LEU	N-CA-CB	6.08	120.77	110.49
1	A	176	THR	CA-CB-CG2	6.08	120.83	110.50
1	A	177	ALA	N-CA-C	-6.04	101.47	110.23
1	A	63	ASN	N-CA-C	-6.02	104.28	111.69
1	A	287	LEU	N-CA-C	-6.01	104.36	111.03
1	A	222	PHE	CA-C-N	6.00	132.23	122.81
1	A	222	PHE	C-N-CA	6.00	132.23	122.81
1	A	47	VAL	CA-CB-CG1	5.99	120.58	110.40
1	A	278	TRP	N-CA-C	5.99	117.60	111.14
1	A	22	GLU	N-CA-CB	5.98	118.74	110.07
1	A	212	GLN	CA-CB-CG	5.97	126.04	114.10
1	A	312	ASN	N-CA-C	-5.97	98.79	108.52
1	A	261	ILE	CA-C-N	5.97	128.08	120.56
1	A	261	ILE	C-N-CA	5.97	128.08	120.56
1	A	154	LEU	CA-C-O	-5.96	113.11	119.97
1	A	315	ILE	N-CA-CB	-5.95	103.40	112.15
1	A	24	ASN	CB-CG-ND2	-5.95	107.48	116.40
1	A	265	LEU	CB-CA-C	5.94	120.78	110.79
1	A	230	ASN	OD1-CG-ND2	-5.93	116.67	122.60
1	A	263	ASP	CA-CB-CG	5.92	118.52	112.60
1	A	156	ARG	NE-CZ-NH1	5.92	127.42	121.50
1	A	28	GLN	OE1-CD-NE2	-5.89	116.71	122.60
1	A	102	THR	N-CA-C	5.88	120.47	112.88
1	A	239	ASP	N-CA-C	5.88	117.77	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	177	ALA	CB-CA-C	5.88	119.48	109.72
1	A	23	PHE	CA-CB-CG	-5.85	107.95	113.80
1	A	95	LEU	CB-CA-C	5.84	119.41	109.53
1	A	224	GLY	O-C-N	5.83	127.60	121.77
1	A	146	ASP	N-CA-C	5.80	119.91	112.26
1	A	168	ASN	OD1-CG-ND2	-5.80	116.80	122.60
1	A	323	LYS	CA-CB-CG	5.80	125.69	114.10
1	A	275	PRO	CB-CA-C	5.77	121.22	112.21
1	A	193	ASN	CA-CB-CG	5.76	118.36	112.60
1	A	239	ASP	O-C-N	5.76	128.72	122.15
1	A	51	ASP	CB-CA-C	-5.75	99.17	109.24
1	A	105	GLU	CB-CG-CD	5.75	122.37	112.60
1	A	258	ASN	OD1-CG-ND2	5.74	128.34	122.60
1	A	294	THR	CB-CA-C	-5.72	98.74	109.72
1	A	297	ASP	CA-C-N	5.71	135.73	121.80
1	A	297	ASP	C-N-CA	5.71	135.73	121.80
1	A	50	ASP	CB-CA-C	-5.70	100.95	110.19
1	A	312	ASN	OD1-CG-ND2	5.70	128.30	122.60
1	A	292	GLU	CG-CD-OE2	-5.68	105.32	118.40
1	A	144	ILE	CB-CA-C	5.68	119.78	110.69
1	A	144	ILE	N-CA-CB	-5.67	101.44	111.93
1	A	327	LYS	N-CA-C	-5.65	100.97	109.95
1	A	345	ALA	CA-C-O	5.64	128.54	121.66
1	A	281	TYR	O-C-N	5.64	128.58	122.15
1	A	205	GLU	CB-CG-CD	5.63	122.18	112.60
1	A	90	GLU	CG-CD-OE2	-5.61	105.51	118.40
1	A	302	LEU	N-CA-CB	-5.59	101.88	110.16
1	A	342	SER	N-CA-CB	-5.59	101.66	110.77
1	A	247	THR	CB-CA-C	5.58	119.33	110.19
1	A	235	ASN	CB-CA-C	5.57	121.53	110.17
1	A	164	ALA	N-CA-C	-5.56	98.95	110.80
1	A	13	GLY	CA-C-N	5.54	125.24	119.64
1	A	13	GLY	C-N-CA	5.54	125.24	119.64
1	A	95	LEU	CA-C-N	5.53	130.58	122.39
1	A	95	LEU	C-N-CA	5.53	130.58	122.39
1	A	140	ARG	CD-NE-CZ	-5.53	116.65	124.40
1	A	48	GLU	CB-CG-CD	5.53	122.00	112.60
1	A	228	VAL	CA-C-O	5.52	124.50	119.20
1	A	132	ILE	CB-CA-C	-5.51	104.70	112.14
1	A	292	GLU	CB-CG-CD	-5.50	103.24	112.60
1	A	314	VAL	CA-C-N	5.49	130.08	122.28
1	A	314	VAL	C-N-CA	5.49	130.08	122.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	117	THR	N-CA-CB	5.49	118.98	110.80
1	A	127	THR	CA-CB-OG1	-5.46	101.40	109.60
1	A	313	THR	CA-CB-OG1	-5.45	101.42	109.60
1	A	65	ILE	CB-CG1-CD1	-5.45	102.35	113.80
1	A	30	ILE	CB-CA-C	5.41	118.89	111.97
1	A	320	TRP	O-C-N	5.39	130.19	123.19
1	A	81	SER	N-CA-C	-5.35	106.88	113.41
1	A	289	THR	N-CA-C	-5.33	99.45	110.80
1	A	304	LYS	CA-C-N	5.33	127.85	120.29
1	A	304	LYS	C-N-CA	5.33	127.85	120.29
1	A	26	ALA	CA-C-N	5.32	127.72	120.54
1	A	26	ALA	C-N-CA	5.32	127.72	120.54
1	A	68	ASP	N-CA-CB	-5.31	101.45	111.43
1	A	109	ARG	CB-CA-C	5.30	117.55	109.34
1	A	323	LYS	N-CA-CB	5.27	118.39	110.53
1	A	211	ARG	NE-CZ-NH1	-5.27	116.23	121.50
1	A	65	ILE	CA-CB-CG2	5.26	119.44	110.50
1	A	191	LYS	N-CA-C	5.26	117.69	111.33
1	A	202	TYR	O-C-N	5.25	130.26	122.97
1	A	87	ASP	N-CA-C	-5.25	105.47	111.14
1	A	51	ASP	CB-CG-OD2	-5.24	106.35	118.40
1	A	11	MET	CA-CB-CG	5.21	124.53	114.10
1	A	320	TRP	CA-C-O	-5.20	115.24	121.11
1	A	142	ALA	CA-C-O	-5.18	115.22	120.71
1	A	30	ILE	CA-CB-CG2	5.18	119.30	110.50
1	A	68	ASP	CA-C-O	5.16	124.40	119.08
1	A	97	ILE	N-CA-CB	5.16	118.40	112.15
1	A	198	TYR	N-CA-CB	5.13	118.62	110.57
1	A	175	ILE	O-C-N	5.12	128.45	122.97
1	A	309	ASN	CA-C-N	-5.12	111.38	121.41
1	A	309	ASN	C-N-CA	-5.12	111.38	121.41
1	A	3	ILE	N-CA-CB	-5.11	105.14	110.82
1	A	36	LYS	CA-C-O	-5.10	113.26	119.43
1	A	186	ILE	O-C-N	5.10	126.82	121.87
1	A	259	GLN	CA-CB-CG	-5.08	103.93	114.10
1	A	247	THR	O-C-N	-5.08	117.28	123.27
1	A	255	ASP	N-CA-C	-5.06	103.39	109.72
1	A	228	VAL	O-C-N	-5.06	117.27	122.23
1	A	34	ASN	N-CA-C	-5.04	105.97	111.82
1	A	192	GLU	N-CA-C	-5.04	107.19	113.19
1	A	67	ASN	OD1-CG-ND2	5.03	127.63	122.60
1	A	230	ASN	CA-C-N	5.03	127.95	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	230	ASN	C-N-CA	5.03	127.95	120.31
1	A	112	GLN	CA-CB-CG	-5.02	104.06	114.10
1	A	152	GLU	CB-CG-CD	5.02	121.13	112.60
1	A	186	ILE	CA-C-O	-5.01	115.74	120.95

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	140	ARG	Sidechain
1	A	214	ARG	Sidechain
1	A	293	ARG	Sidechain
1	A	75	GLY	Peptide,Mainchain

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	2600	0	2567	286	0
2	A	91	0	0	7	0
All	All	2691	0	2567	286	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 55.

All (286) 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:291:LEU:HD22	1:A:302:LEU:CG	1.53	1.36
1:A:291:LEU:CD2	1:A:302:LEU:HG	1.53	1.35
1:A:17:GLN:HE21	1:A:17:GLN:N	1.28	1.31
1:A:291:LEU:CD1	1:A:302:LEU:HA	1.61	1.29
1:A:17:GLN:H	1:A:17:GLN:NE2	1.31	1.27
1:A:65:ILE:HD11	1:A:73:VAL:HG22	1.21	1.11
1:A:291:LEU:HD13	1:A:302:LEU:CA	1.79	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:ASP:HA	1:A:42:ASP:OD1	1.49	1.10
1:A:291:LEU:HD12	1:A:305:ASP:HB3	1.27	1.10
1:A:65:ILE:HD11	1:A:73:VAL:CG2	1.84	1.07
1:A:29:ALA:CB	1:A:284:VAL:HG11	1.83	1.07
1:A:313:THR:HG22	1:A:315:ILE:H	1.16	1.06
1:A:289:THR:O	1:A:290:ALA:C	1.98	1.05
1:A:29:ALA:HB1	1:A:284:VAL:CG1	1.86	1.04
1:A:206:MET:HG2	1:A:228:VAL:HG11	1.43	1.00
1:A:32:ASP:OD1	1:A:281:TYR:OH	1.82	0.97
1:A:20:ILE:O	1:A:24:ASN:HB2	1.64	0.96
1:A:291:LEU:O	1:A:291:LEU:HG	1.63	0.96
1:A:8:VAL:HG11	1:A:76:HIS:CE1	2.02	0.94
1:A:230:ASN:HD22	1:A:232:SER:H	1.15	0.94
1:A:206:MET:HG2	1:A:228:VAL:CG1	1.98	0.93
1:A:291:LEU:HD13	1:A:302:LEU:HA	0.94	0.93
1:A:281:TYR:O	1:A:284:VAL:HG12	1.70	0.91
1:A:291:LEU:HD22	1:A:302:LEU:CD2	2.01	0.90
1:A:223:MET:HG2	1:A:245:LEU:HB3	1.54	0.89
1:A:107:THR:HG23	1:A:323:LYS:O	1.73	0.89
1:A:26:ALA:O	1:A:29:ALA:HB3	1.72	0.88
1:A:230:ASN:ND2	1:A:232:SER:H	1.70	0.88
1:A:99:PRO:O	1:A:279:ILE:HD11	1.75	0.87
1:A:289:THR:O	1:A:291:LEU:N	2.09	0.85
1:A:209:MET:HE2	1:A:222:PHE:CE1	2.12	0.85
1:A:208:GLN:O	1:A:212:GLN:HB2	1.77	0.84
1:A:291:LEU:HD22	1:A:302:LEU:HG	0.85	0.84
1:A:3:ILE:HB	1:A:44:LEU:HD23	1.59	0.84
1:A:107:THR:HG22	1:A:107:THR:O	1.77	0.83
1:A:291:LEU:HD12	1:A:305:ASP:CB	2.09	0.83
1:A:344:LYS:HD2	1:A:345:ALA:N	1.94	0.82
1:A:124:GLN:HB3	1:A:247:THR:HG21	1.60	0.81
1:A:27:GLU:OE2	1:A:48:GLU:OE2	2.00	0.80
1:A:143:ILE:C	1:A:144:ILE:HG13	2.05	0.80
1:A:29:ALA:HB1	1:A:284:VAL:HG11	0.90	0.78
1:A:40:LYS:HE2	2:A:505:HOH:O	1.83	0.78
1:A:321:ASP:OD1	1:A:323:LYS:HE3	1.83	0.78
1:A:209:MET:CE	1:A:222:PHE:HE1	1.95	0.78
1:A:65:ILE:CD1	1:A:73:VAL:HG22	2.11	0.78
1:A:203:TYR:CG	1:A:204:PRO:HD3	2.20	0.77
1:A:282:ALA:HB1	1:A:313:THR:HG21	1.67	0.76
1:A:186:ILE:HD12	1:A:212:GLN:CG	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD11	1:A:244:MET:CE	2.15	0.76
1:A:291:LEU:O	1:A:294:THR:HB	1.86	0.75
1:A:88:ILE:O	1:A:91:ASP:HB3	1.87	0.75
1:A:291:LEU:O	1:A:291:LEU:CG	2.35	0.75
1:A:144:ILE:HD11	1:A:171:PHE:CE2	2.22	0.75
1:A:17:GLN:N	1:A:17:GLN:NE2	2.07	0.75
1:A:107:THR:HG22	1:A:323:LYS:HB2	1.68	0.74
1:A:189:LEU:HD22	1:A:194:ILE:HG21	1.68	0.74
1:A:291:LEU:CD1	1:A:305:ASP:HB3	2.15	0.73
1:A:291:LEU:HD21	1:A:302:LEU:HG	1.68	0.73
1:A:107:THR:CG2	1:A:323:LYS:HB2	2.18	0.73
1:A:186:ILE:HD11	1:A:212:GLN:HB3	1.70	0.72
1:A:284:VAL:HG13	1:A:285:GLN:N	2.03	0.72
1:A:286:SER:O	1:A:290:ALA:O	2.08	0.72
1:A:66:VAL:HG22	1:A:94:ILE:HD12	1.72	0.72
1:A:210:LEU:HD11	1:A:244:MET:HE2	1.72	0.71
1:A:233:LEU:HD21	1:A:244:MET:CE	2.19	0.71
1:A:58:ALA:HB2	1:A:81:SER:HB2	1.72	0.71
1:A:149:GLN:N	1:A:149:GLN:OE1	2.22	0.71
1:A:218:LEU:HG	1:A:220:THR:OG1	1.91	0.71
1:A:17:GLN:OE1	1:A:18:TRP:CZ3	2.43	0.71
1:A:103:ALA:O	1:A:116:ARG:NH2	2.17	0.71
1:A:57:GLN:O	1:A:61:VAL:HG23	1.91	0.71
1:A:313:THR:HG22	1:A:315:ILE:N	2.00	0.70
1:A:44:LEU:HD11	1:A:288:ALA:HB1	1.74	0.69
1:A:223:MET:HG2	1:A:245:LEU:CB	2.22	0.68
1:A:131:TYR:CE2	1:A:346:LYS:OXT	2.47	0.68
1:A:66:VAL:C	1:A:68:ASP:H	1.98	0.68
1:A:107:THR:CG2	1:A:323:LYS:HG3	2.24	0.68
1:A:17:GLN:HE21	1:A:17:GLN:H	0.69	0.68
1:A:51:ASP:C	1:A:53:CYS:H	2.00	0.67
1:A:291:LEU:HG	1:A:294:THR:HB	1.76	0.67
1:A:29:ALA:O	1:A:33:ILE:HG13	1.94	0.67
1:A:282:ALA:CB	1:A:313:THR:HG21	2.25	0.67
1:A:107:THR:CG2	1:A:323:LYS:O	2.43	0.67
1:A:291:LEU:HD13	1:A:302:LEU:C	2.19	0.67
1:A:1:ASP:N	2:A:525:HOH:O	2.28	0.66
1:A:233:LEU:HD21	1:A:244:MET:HE1	1.77	0.66
1:A:99:PRO:O	1:A:279:ILE:CD1	2.43	0.66
1:A:87:ASP:O	1:A:91:ASP:HB2	1.96	0.66
1:A:1:ASP:N	1:A:1:ASP:OD2	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:ILE:HD12	1:A:212:GLN:HG2	1.78	0.65
1:A:291:LEU:HD23	1:A:291:LEU:C	2.21	0.65
1:A:17:GLN:HE21	1:A:17:GLN:CA	1.87	0.65
1:A:76:HIS:HB2	1:A:82:THR:OG1	1.95	0.65
1:A:143:ILE:HD11	1:A:162:LEU:HD12	1.79	0.64
1:A:284:VAL:CG1	1:A:285:GLN:N	2.60	0.64
1:A:242:GLU:OE1	1:A:337:HIS:HD2	1.82	0.63
1:A:288:ALA:O	1:A:289:THR:HG22	1.99	0.63
1:A:289:THR:OG1	1:A:293:ARG:NH2	2.32	0.62
1:A:90:GLU:HG3	1:A:111:TYR:HB3	1.80	0.62
1:A:107:THR:HG21	1:A:323:LYS:HG3	1.82	0.62
1:A:344:LYS:HD2	1:A:344:LYS:C	2.25	0.62
1:A:10:ALA:O	1:A:19:GLY:HA3	2.00	0.62
1:A:258:ASN:O	1:A:262:VAL:HG23	1.99	0.62
1:A:131:TYR:HE2	1:A:346:LYS:OXT	1.83	0.62
1:A:51:ASP:C	1:A:53:CYS:N	2.57	0.61
1:A:15:ILE:HG22	1:A:15:ILE:O	1.99	0.61
1:A:47:VAL:HG11	1:A:70:ILE:HD11	1.82	0.61
1:A:111:TYR:HD2	1:A:111:TYR:N	1.99	0.61
1:A:291:LEU:CD1	1:A:302:LEU:CA	2.56	0.61
1:A:232:SER:O	1:A:236:ILE:HD12	2.00	0.61
1:A:6:ALA:CB	1:A:65:ILE:HD12	2.31	0.61
1:A:223:MET:CG	1:A:245:LEU:HB3	2.31	0.61
1:A:107:THR:HG21	1:A:323:LYS:CG	2.31	0.60
1:A:111:TYR:N	1:A:111:TYR:CD2	2.68	0.60
1:A:313:THR:CG2	1:A:315:ILE:HG22	2.31	0.60
1:A:294:THR:HG23	1:A:296:SER:H	1.67	0.60
1:A:313:THR:HG22	1:A:314:VAL:N	2.17	0.60
1:A:143:ILE:O	1:A:144:ILE:HG13	2.02	0.59
1:A:1:ASP:CA	1:A:42:ASP:OD1	2.38	0.59
1:A:337:HIS:HE1	1:A:343:THR:OG1	1.84	0.59
1:A:99:PRO:O	1:A:279:ILE:CG1	2.51	0.59
1:A:9:GLY:HA3	1:A:22:GLU:OE1	2.03	0.58
1:A:209:MET:CE	1:A:222:PHE:CE1	2.75	0.58
1:A:21:MET:HE2	1:A:274:GLY:HA3	1.85	0.58
1:A:282:ALA:CB	1:A:313:THR:CG2	2.80	0.58
1:A:163:LYS:O	1:A:166:ASN:N	2.37	0.58
1:A:186:ILE:CD1	1:A:212:GLN:CG	2.81	0.58
1:A:288:ALA:O	1:A:289:THR:HB	2.04	0.58
1:A:149:GLN:N	1:A:149:GLN:CD	2.59	0.58
1:A:66:VAL:O	1:A:68:ASP:N	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ASN:O	1:A:67:ASN:CG	2.47	0.57
1:A:294:THR:CG2	1:A:296:SER:H	2.17	0.57
1:A:322:GLU:CD	1:A:322:GLU:H	2.10	0.57
1:A:315:ILE:CG2	1:A:318:LEU:HD21	2.34	0.57
1:A:8:VAL:CG1	1:A:76:HIS:CE1	2.84	0.57
1:A:250:LYS:CE	2:A:574:HOH:O	2.52	0.57
1:A:51:ASP:HB3	1:A:53:CYS:H	1.69	0.56
1:A:210:LEU:CD1	1:A:244:MET:CE	2.83	0.56
1:A:291:LEU:O	1:A:294:THR:CB	2.52	0.56
1:A:107:THR:CG2	1:A:323:LYS:CB	2.83	0.56
1:A:313:THR:CG2	1:A:314:VAL:N	2.68	0.56
1:A:230:ASN:HD22	1:A:232:SER:N	1.94	0.56
1:A:250:LYS:HE2	2:A:574:HOH:O	2.05	0.56
1:A:313:THR:HB	1:A:315:ILE:HG22	1.88	0.55
1:A:90:GLU:HG3	1:A:111:TYR:CB	2.36	0.55
1:A:186:ILE:HD12	1:A:212:GLN:HG3	1.85	0.55
1:A:285:GLN:O	1:A:289:THR:HG22	2.07	0.55
1:A:294:THR:HG23	1:A:294:THR:O	2.06	0.55
1:A:315:ILE:O	1:A:315:ILE:HG23	2.07	0.55
1:A:288:ALA:O	1:A:289:THR:CB	2.55	0.55
1:A:68:ASP:OD1	1:A:68:ASP:O	2.25	0.54
1:A:17:GLN:OE1	1:A:18:TRP:CH2	2.60	0.54
1:A:346:LYS:OXT	1:A:346:LYS:HG3	2.06	0.54
1:A:64:LYS:O	1:A:68:ASP:HB3	2.07	0.54
1:A:66:VAL:HG22	1:A:94:ILE:CD1	2.36	0.54
1:A:148:GLN:NE2	1:A:148:GLN:N	2.56	0.54
1:A:285:GLN:OE1	1:A:314:VAL:HB	2.08	0.54
1:A:39:ILE:CD1	1:A:44:LEU:HG	2.38	0.54
1:A:107:THR:CG2	1:A:323:LYS:CG	2.85	0.54
1:A:233:LEU:CD2	1:A:244:MET:HE1	2.37	0.54
1:A:313:THR:HB	1:A:316:GLY:O	2.07	0.54
1:A:124:GLN:HB3	1:A:247:THR:CG2	2.33	0.53
1:A:291:LEU:HD11	1:A:302:LEU:HA	1.74	0.53
1:A:76:HIS:H	1:A:76:HIS:CD2	2.25	0.53
1:A:192:GLU:OE2	1:A:192:GLU:HA	2.09	0.53
1:A:144:ILE:HD11	1:A:171:PHE:HE2	1.71	0.53
1:A:147:LYS:C	1:A:148:GLN:NE2	2.67	0.53
1:A:176:THR:O	1:A:179:GLU:HG3	2.08	0.53
1:A:321:ASP:OD1	1:A:323:LYS:CE	2.56	0.53
1:A:132:ILE:CG1	1:A:223:MET:HE3	2.38	0.53
1:A:197:VAL:HG23	1:A:220:THR:HG21	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:C	1:A:68:ASP:N	2.66	0.53
1:A:90:GLU:OE1	1:A:111:TYR:HA	2.09	0.52
1:A:246:VAL:HG21	1:A:336:TRP:CE3	2.44	0.52
1:A:306:LEU:O	1:A:309:ASN:O	2.27	0.52
1:A:203:TYR:CD1	1:A:204:PRO:HD3	2.43	0.52
1:A:86:SER:OG	1:A:109:ARG:NH2	2.35	0.52
1:A:147:LYS:C	1:A:148:GLN:HE21	2.17	0.52
1:A:287:LEU:HG	1:A:288:ALA:N	2.21	0.52
1:A:192:GLU:HB3	1:A:194:ILE:HD11	1.91	0.52
1:A:289:THR:HA	1:A:293:ARG:HG3	1.90	0.52
1:A:210:LEU:HD11	1:A:244:MET:HE3	1.92	0.51
1:A:107:THR:HG22	1:A:323:LYS:HG3	1.92	0.51
1:A:286:SER:O	1:A:306:LEU:HD21	2.10	0.51
1:A:132:ILE:HG13	1:A:223:MET:HE3	1.93	0.51
1:A:206:MET:HG3	1:A:244:MET:HE2	1.92	0.51
1:A:313:THR:HG21	1:A:315:ILE:CG2	2.40	0.51
1:A:261:ILE:HG22	1:A:265:LEU:HD12	1.93	0.51
1:A:313:THR:HG21	1:A:315:ILE:HG22	1.92	0.50
1:A:189:LEU:HD22	1:A:194:ILE:CG2	2.39	0.50
1:A:210:LEU:CD1	1:A:244:MET:HE2	2.40	0.50
1:A:210:LEU:CD1	1:A:244:MET:HE3	2.41	0.50
1:A:67:ASN:O	1:A:67:ASN:OD1	2.30	0.50
1:A:131:TYR:OH	1:A:346:LYS:OXT	2.23	0.50
1:A:246:VAL:HG12	1:A:247:THR:N	2.27	0.50
1:A:146:ASP:HB2	1:A:177:ALA:HB2	1.94	0.50
1:A:144:ILE:O	1:A:199:TYR:HA	2.12	0.50
1:A:164:ALA:O	1:A:165:ALA:CB	2.60	0.49
1:A:138:PRO:HG2	1:A:141:ILE:HD11	1.94	0.49
1:A:24:ASN:OD1	1:A:270:LYS:HD3	2.13	0.49
1:A:291:LEU:C	1:A:293:ARG:N	2.69	0.49
1:A:206:MET:HG2	1:A:228:VAL:HG13	1.91	0.49
1:A:132:ILE:HG13	1:A:223:MET:CE	2.43	0.49
1:A:24:ASN:OD1	2:A:511:HOH:O	2.20	0.48
1:A:291:LEU:HD13	1:A:302:LEU:O	2.13	0.48
1:A:64:LYS:O	1:A:64:LYS:CG	2.61	0.48
1:A:115:MET:HE2	1:A:303:VAL:HG23	1.95	0.48
1:A:252:TYR:O	1:A:258:ASN:ND2	2.41	0.48
1:A:291:LEU:CD2	1:A:291:LEU:C	2.80	0.48
1:A:163:LYS:O	1:A:165:ALA:N	2.46	0.48
1:A:322:GLU:CD	1:A:322:GLU:N	2.71	0.47
1:A:44:LEU:HD11	1:A:288:ALA:CB	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:GLN:CD	1:A:149:GLN:H	2.18	0.47
1:A:164:ALA:O	1:A:165:ALA:HB2	2.15	0.47
1:A:158:VAL:O	1:A:162:LEU:HG	2.15	0.47
1:A:233:LEU:HD21	1:A:244:MET:HE3	1.96	0.47
1:A:282:ALA:HB1	1:A:313:THR:CG2	2.40	0.47
1:A:288:ALA:O	1:A:289:THR:CG2	2.63	0.47
1:A:163:LYS:HD3	1:A:166:ASN:HA	1.98	0.46
1:A:130:LYS:O	1:A:130:LYS:HG3	2.15	0.46
1:A:145:HIS:CE1	1:A:152:GLU:HG3	2.51	0.46
1:A:209:MET:HE1	1:A:222:PHE:HE1	1.77	0.46
1:A:255:ASP:OD2	1:A:256:PRO:HD2	2.16	0.46
1:A:12:SER:O	1:A:13:GLY:O	2.32	0.46
1:A:57:GLN:NE2	2:A:508:HOH:O	2.48	0.46
1:A:148:GLN:N	1:A:148:GLN:HE21	2.13	0.46
1:A:282:ALA:HB2	1:A:313:THR:CG2	2.46	0.46
1:A:140:ARG:NH1	1:A:140:ARG:HG2	2.30	0.45
1:A:186:ILE:CD1	1:A:212:GLN:HB3	2.44	0.45
1:A:3:ILE:N	1:A:43:LYS:O	2.50	0.45
1:A:186:ILE:CD1	1:A:212:GLN:CB	2.94	0.45
1:A:115:MET:HE2	1:A:303:VAL:HA	1.99	0.45
1:A:230:ASN:ND2	1:A:232:SER:HB2	2.32	0.45
1:A:186:ILE:HD11	1:A:212:GLN:CB	2.42	0.44
1:A:251:ARG:HD3	1:A:254:GLN:OE1	2.17	0.44
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.79	0.44
1:A:199:TYR:O	1:A:225:PRO:HD3	2.16	0.44
1:A:65:ILE:HD11	1:A:73:VAL:HG21	1.88	0.44
1:A:125:GLY:N	1:A:126:PRO:CD	2.81	0.44
1:A:83:GLN:CB	1:A:84:PRO:HD3	2.48	0.44
1:A:132:ILE:HG12	1:A:196:PHE:CZ	2.53	0.44
1:A:321:ASP:OD1	1:A:325:ASP:HB2	2.18	0.44
1:A:13:GLY:HA3	1:A:14:PRO:HD3	1.79	0.44
1:A:15:ILE:O	1:A:15:ILE:CG2	2.65	0.44
1:A:124:GLN:OE1	1:A:247:THR:CG2	2.66	0.44
1:A:291:LEU:CD2	1:A:291:LEU:O	2.65	0.44
1:A:1:ASP:HA	1:A:42:ASP:CG	2.34	0.44
1:A:291:LEU:HD23	1:A:292:GLU:N	2.32	0.44
1:A:144:ILE:HA	1:A:173:ASP:O	2.18	0.43
1:A:64:LYS:O	1:A:68:ASP:CB	2.65	0.43
1:A:123:SER:O	1:A:126:PRO:HD2	2.17	0.43
1:A:133:LEU:HD21	1:A:167:ALA:HB2	2.00	0.43
1:A:185:LEU:O	1:A:185:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HD13	1:A:241:ALA:HA	1.99	0.43
1:A:186:ILE:CD1	1:A:212:GLN:C	2.91	0.43
1:A:206:MET:CG	1:A:244:MET:HE2	2.48	0.43
1:A:270:LYS:HE2	2:A:511:HOH:O	2.19	0.43
1:A:47:VAL:HG13	1:A:70:ILE:HD13	2.01	0.43
1:A:306:LEU:HD12	1:A:306:LEU:HA	1.94	0.43
1:A:203:TYR:CD2	1:A:204:PRO:HD3	2.53	0.42
1:A:225:PRO:HA	1:A:247:THR:HG22	2.01	0.42
1:A:191:LYS:C	1:A:193:ASN:H	2.26	0.42
1:A:16:ALA:C	1:A:18:TRP:H	2.26	0.42
1:A:123:SER:C	1:A:126:PRO:HD2	2.44	0.42
1:A:51:ASP:O	1:A:53:CYS:N	2.53	0.42
1:A:148:GLN:HE21	1:A:148:GLN:CA	2.33	0.42
1:A:65:ILE:CD1	1:A:73:VAL:CG2	2.76	0.42
1:A:12:SER:O	1:A:13:GLY:C	2.59	0.41
1:A:131:TYR:CZ	1:A:346:LYS:OXT	2.73	0.41
1:A:176:THR:HB	1:A:179:GLU:HG3	2.02	0.41
1:A:47:VAL:CG1	1:A:70:ILE:HD11	2.49	0.41
1:A:163:LYS:O	1:A:163:LYS:HD3	2.20	0.41
1:A:210:LEU:O	1:A:240:ALA:HB1	2.21	0.41
1:A:182:PHE:HE2	1:A:208:GLN:HB2	1.86	0.41
1:A:186:ILE:HD13	1:A:212:GLN:C	2.46	0.41
1:A:300:LEU:HA	1:A:303:VAL:HG12	2.01	0.41
1:A:15:ILE:HA	1:A:18:TRP:CE3	2.56	0.41
1:A:15:ILE:HA	1:A:18:TRP:HE3	1.86	0.41
1:A:107:THR:O	1:A:107:THR:CG2	2.50	0.41
1:A:176:THR:HB	1:A:179:GLU:CG	2.51	0.41
1:A:192:GLU:HB3	1:A:194:ILE:CD1	2.50	0.41
1:A:284:VAL:CG1	1:A:285:GLN:H	2.33	0.41
1:A:115:MET:CE	1:A:303:VAL:HA	2.50	0.40
1:A:137:LYS:N	1:A:138:PRO:CD	2.84	0.40
1:A:188:ARG:O	1:A:188:ARG:HG2	2.22	0.40
1:A:72:TYR:OH	1:A:297:ASP:O	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	344/346 (99%)	327 (95%)	10 (3%)	7 (2%)	6 7

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	HIS
1	A	165	ALA
1	A	289	THR
1	A	67	ASN
1	A	150	TYR
1	A	100	GLY
1	A	66	VAL

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	267/267 (100%)	204 (76%)	63 (24%)	1 1

All (63) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	ASP
1	A	4	LYS
1	A	5	VAL
1	A	11	MET

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Mol	Chain	Res	Type
1	A	17	GLN
1	A	20	ILE
1	A	22	GLU
1	A	24	ASN
1	A	30	ILE
1	A	34	ASN
1	A	40	LYS
1	A	45	VAL
1	A	47	VAL
1	A	53	CYS
1	A	57	GLN
1	A	59	VAL
1	A	65	ILE
1	A	67	ASN
1	A	71	LYS
1	A	79	SER
1	A	83	GLN
1	A	90	GLU
1	A	99	PRO
1	A	105	GLU
1	A	123	SER
1	A	130	LYS
1	A	135	THR
1	A	148	GLN
1	A	149	GLN
1	A	175	ILE
1	A	179	GLU
1	A	212	GLN
1	A	216	VAL
1	A	218	LEU
1	A	220	THR
1	A	221	GLN
1	A	223	MET
1	A	234	SER
1	A	235	ASN
1	A	239	ASP
1	A	244	MET
1	A	245	LEU
1	A	246	VAL
1	A	247	THR
1	A	250	LYS
1	A	259	GLN

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Mol	Chain	Res	Type
1	A	269	LYS
1	A	279	ILE
1	A	287	LEU
1	A	289	THR
1	A	296	SER
1	A	300	LEU
1	A	302	LEU
1	A	306	LEU
1	A	312	ASN
1	A	314	VAL
1	A	315	ILE
1	A	322	GLU
1	A	323	LYS
1	A	330	ASP
1	A	335	GLN
1	A	342	SER
1	A	344	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	17	GLN
1	A	28	GLN
1	A	63	ASN
1	A	148	GLN
1	A	168	ASN
1	A	208	GLN
1	A	230	ASN
1	A	254	GLN
1	A	319	ASN
1	A	337	HIS

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.