



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:06 AM UTC

PDB ID : 2LIV / pdb_00002liv
Title : PERIPLASMIC BINDING PROTEIN STRUCTURE AND FUNCTION. RE-
FINED X-RAY STRUCTURES OF THE LEUCINE/ISOLEUCINE/VALIN
E-BINDING PROTEIN AND ITS COMPLEX WITH LEUCINE
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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

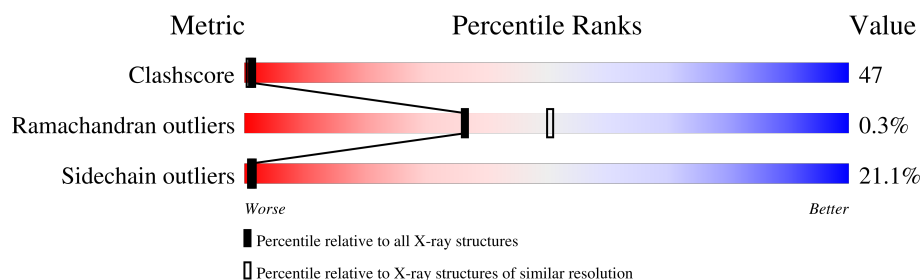
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

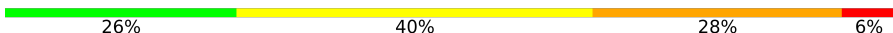
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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	344	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 2710 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2589	1633	439	510	7			

- Molecule 2 is water.

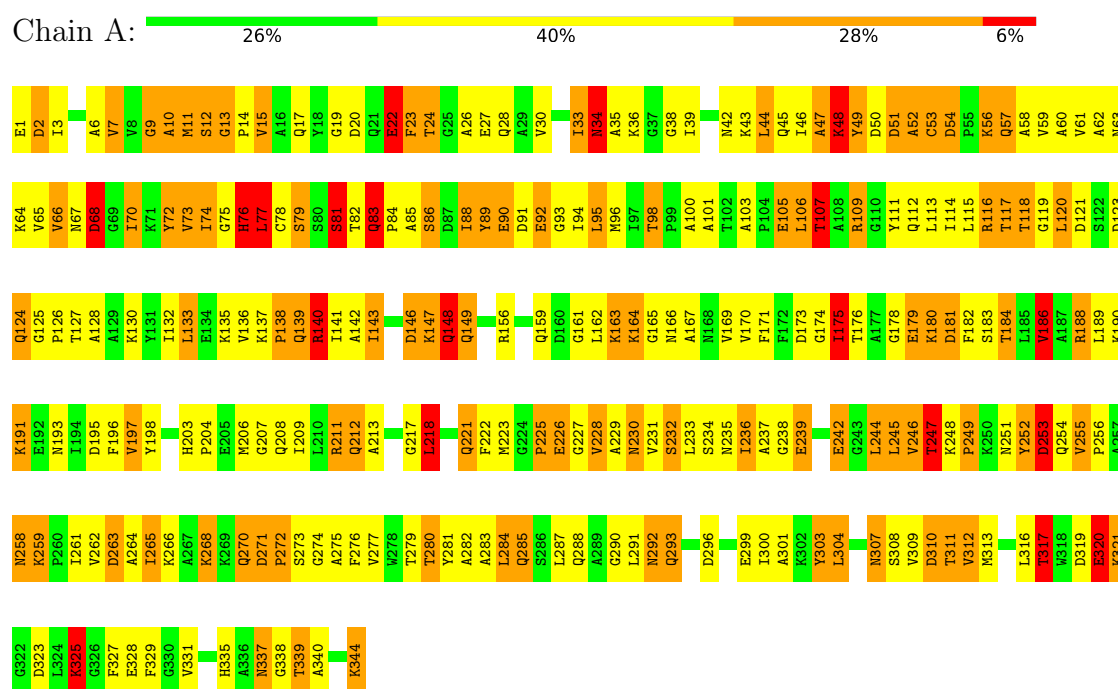
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	121	Total	O	0	0
			121	121		

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



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	39.88Å 70.99Å 115.63Å 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}	0.179 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	2710	wwPDB-VP
Average B, all atoms (Å ²)	11.0	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	1.43	10/2636 (0.4%)	2.85	271/3570 (7.6%)

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	2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	2	ASP	N-CA	-6.08	1.38	1.46
1	A	76	HIS	N-CA	-6.01	1.38	1.46
1	A	164	LYS	N-CA	5.96	1.54	1.46
1	A	252	TYR	C-N	-5.64	1.26	1.33
1	A	165	GLY	N-CA	5.61	1.53	1.45
1	A	22	GLU	CA-CB	-5.47	1.44	1.53
1	A	1	GLU	C-N	-5.30	1.25	1.33
1	A	292	ASN	C-N	-5.27	1.26	1.33
1	A	164	LYS	C-N	-5.25	1.25	1.33
1	A	118	THR	CA-C	5.24	1.59	1.52

All (271) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1	GLU	CA-C-N	25.66	164.30	122.73
1	A	1	GLU	C-N-CA	25.66	164.30	122.73
1	A	75	GLY	CA-C-N	21.45	162.51	121.54
1	A	75	GLY	C-N-CA	21.45	162.51	121.54
1	A	22	GLU	CA-CB-CG	13.51	141.13	114.10
1	A	253	ASP	CA-CB-CG	13.05	125.66	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	12	SER	N-CA-C	12.63	129.43	112.13
1	A	34	ASN	CB-CA-C	12.58	135.09	109.55
1	A	164	LYS	N-CA-C	-12.55	91.08	109.15
1	A	116	ARG	CD-NE-CZ	12.21	141.50	124.40
1	A	67	ASN	CA-CB-CG	11.64	124.24	112.60
1	A	195	ASP	CA-CB-CG	11.26	123.86	112.60
1	A	181	ASP	CA-C-O	-11.04	109.06	120.54
1	A	34	ASN	OD1-CG-ND2	10.74	133.34	122.60
1	A	47	ALA	CA-C-N	10.71	136.08	120.87
1	A	47	ALA	C-N-CA	10.71	136.08	120.87
1	A	238	GLY	CA-C-N	10.17	134.31	120.38
1	A	238	GLY	C-N-CA	10.17	134.31	120.38
1	A	2	ASP	CA-CB-CG	9.87	122.47	112.60
1	A	164	LYS	CA-C-O	-9.39	109.44	120.62
1	A	163	LYS	N-CA-CB	9.38	124.40	110.33
1	A	293	GLN	CB-CG-CD	-9.35	96.70	112.60
1	A	320	GLU	CB-CG-CD	9.29	128.39	112.60
1	A	252	TYR	CA-C-N	9.23	134.67	120.82
1	A	252	TYR	C-N-CA	9.23	134.67	120.82
1	A	159	GLN	O-C-N	9.15	131.82	122.12
1	A	173	ASP	CA-CB-CG	9.15	121.75	112.60
1	A	180	LYS	CA-CB-CG	9.10	132.30	114.10
1	A	190	LYS	CA-C-N	8.99	132.51	120.65
1	A	190	LYS	C-N-CA	8.99	132.51	120.65
1	A	94	ILE	O-C-N	8.94	132.72	123.07
1	A	94	ILE	CA-C-O	-8.87	110.76	120.43
1	A	76	HIS	N-CA-CB	8.84	125.44	110.49
1	A	77	LEU	N-CA-C	8.81	120.57	110.97
1	A	86	SER	CA-CB-OG	8.79	128.68	111.10
1	A	74	ILE	N-CA-CB	8.73	122.67	111.67
1	A	116	ARG	NE-CZ-NH1	8.69	130.19	121.50
1	A	156	ARG	NE-CZ-NH2	8.63	126.97	119.20
1	A	107	THR	CA-CB-OG1	-8.61	96.68	109.60
1	A	156	ARG	NE-CZ-NH1	-8.50	113.00	121.50
1	A	236	ILE	N-CA-C	8.49	119.11	111.81
1	A	68	ASP	CA-CB-CG	8.48	121.08	112.60
1	A	179	GLU	N-CA-CB	8.44	122.37	109.97
1	A	139	GLN	OE1-CD-NE2	-8.38	114.22	122.60
1	A	181	ASP	CA-CB-CG	-8.33	104.27	112.60
1	A	132	ILE	CA-C-N	8.28	131.58	120.65
1	A	132	ILE	C-N-CA	8.28	131.58	120.65
1	A	340	ALA	CA-C-N	8.27	135.80	122.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	ALA	C-N-CA	8.27	135.80	122.81
1	A	231	VAL	CA-C-N	8.21	131.28	120.28
1	A	231	VAL	C-N-CA	8.21	131.28	120.28
1	A	253	ASP	N-CA-CB	-8.20	96.41	109.78
1	A	156	ARG	CD-NE-CZ	-8.15	112.98	124.40
1	A	159	GLN	CA-C-O	-8.11	111.95	120.55
1	A	146	ASP	CA-CB-CG	8.08	120.68	112.60
1	A	148	GLN	N-CA-C	-8.06	98.58	110.52
1	A	143	ILE	CA-C-O	-7.98	111.90	120.36
1	A	81	SER	CA-C-N	7.90	131.19	120.44
1	A	81	SER	C-N-CA	7.90	131.19	120.44
1	A	11	MET	CA-C-N	7.89	134.40	122.56
1	A	11	MET	C-N-CA	7.89	134.40	122.56
1	A	12	SER	CB-CA-C	-7.84	98.44	110.83
1	A	310	ASP	CA-CB-CG	-7.84	104.76	112.60
1	A	179	GLU	CA-CB-CG	7.83	129.76	114.10
1	A	319	ASP	CA-CB-CG	7.83	120.43	112.60
1	A	312	VAL	CA-C-N	7.81	135.43	122.54
1	A	312	VAL	C-N-CA	7.81	135.43	122.54
1	A	52	ALA	CA-C-N	7.68	133.65	122.36
1	A	52	ALA	C-N-CA	7.68	133.65	122.36
1	A	252	TYR	CA-C-O	7.66	128.80	119.38
1	A	180	LYS	N-CA-C	-7.63	104.46	114.31
1	A	68	ASP	CA-C-O	7.50	128.25	119.32
1	A	218	LEU	CB-CA-C	7.50	122.07	109.84
1	A	98	THR	CA-CB-OG1	-7.45	98.42	109.60
1	A	263	ASP	CA-C-N	7.45	131.26	120.38
1	A	263	ASP	C-N-CA	7.45	131.26	120.38
1	A	156	ARG	CB-CA-C	7.42	123.47	110.85
1	A	166	ASN	CA-CB-CG	7.41	120.01	112.60
1	A	133	LEU	O-C-N	7.35	129.67	122.03
1	A	271	ASP	CA-CB-CG	7.35	119.95	112.60
1	A	9	GLY	CA-C-N	7.32	134.19	123.13
1	A	9	GLY	C-N-CA	7.32	134.19	123.13
1	A	275	ALA	CA-C-O	-7.31	112.68	120.42
1	A	53	CYS	O-C-N	7.29	130.91	122.67
1	A	147	LYS	N-CA-CB	7.29	123.14	112.28
1	A	139	GLN	CA-CB-CG	7.12	128.35	114.10
1	A	148	GLN	OE1-CD-NE2	7.12	129.72	122.60
1	A	235	ASN	CA-CB-CG	7.03	119.63	112.60
1	A	7	VAL	CB-CA-C	6.91	120.98	111.31
1	A	211	ARG	CA-C-O	6.91	128.67	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	ASN	CA-CB-CG	-6.90	105.70	112.60
1	A	67	ASN	OD1-CG-ND2	-6.90	115.70	122.60
1	A	75	GLY	CA-C-O	6.89	132.56	120.57
1	A	251	ASN	CA-C-O	-6.86	113.63	121.66
1	A	148	GLN	CB-CG-CD	-6.84	100.97	112.60
1	A	277	VAL	CA-C-O	-6.83	113.61	120.85
1	A	156	ARG	CA-CB-CG	6.81	127.72	114.10
1	A	149	GLN	CA-CB-CG	-6.80	100.51	114.10
1	A	186	VAL	CA-C-O	-6.74	113.94	120.95
1	A	118	THR	CB-CA-C	-6.72	96.04	109.35
1	A	147	LYS	CA-CB-CG	6.72	127.54	114.10
1	A	277	VAL	N-CA-C	-6.67	103.98	110.72
1	A	227	GLY	CA-C-N	6.65	130.99	121.55
1	A	227	GLY	C-N-CA	6.65	130.99	121.55
1	A	127	THR	N-CA-CB	6.64	119.61	109.91
1	A	141	ILE	N-CA-C	6.59	117.79	108.36
1	A	107	THR	N-CA-CB	-6.56	100.71	110.61
1	A	165	GLY	CA-C-N	6.56	131.43	122.19
1	A	165	GLY	C-N-CA	6.56	131.43	122.19
1	A	48	LYS	N-CA-C	6.54	119.96	110.28
1	A	90	GLU	N-CA-CB	6.52	119.81	110.16
1	A	56	LYS	CA-C-O	6.41	127.82	120.00
1	A	239	GLU	O-C-N	6.40	128.91	122.12
1	A	109	ARG	N-CA-C	6.40	121.17	113.23
1	A	149	GLN	CB-CA-C	6.40	120.87	110.95
1	A	148	GLN	N-CA-CB	6.34	120.61	110.46
1	A	337	ASN	CA-CB-CG	-6.33	106.27	112.60
1	A	13	GLY	CA-C-N	6.32	127.73	119.84
1	A	13	GLY	C-N-CA	6.32	127.73	119.84
1	A	181	ASP	O-C-N	6.30	130.55	123.05
1	A	111	TYR	CB-CA-C	6.27	122.54	109.68
1	A	124	GLN	OE1-CD-NE2	-6.27	116.33	122.60
1	A	301	ALA	CA-C-N	6.26	129.14	120.63
1	A	301	ALA	C-N-CA	6.26	129.14	120.63
1	A	88	ILE	CA-C-O	-6.25	114.78	121.27
1	A	159	GLN	N-CA-CB	6.24	119.30	110.12
1	A	111	TYR	O-C-N	-6.24	115.68	122.79
1	A	117	THR	N-CA-CB	6.19	120.52	111.54
1	A	89	TYR	N-CA-CB	6.19	119.32	110.16
1	A	198	TYR	N-CA-CB	6.14	120.19	110.55
1	A	293	GLN	N-CA-CB	-6.13	100.03	110.33
1	A	49	TYR	O-C-N	6.13	130.68	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	188	ARG	NE-CZ-NH2	-6.12	113.69	119.20
1	A	281	TYR	CA-C-N	6.12	129.09	120.28
1	A	281	TYR	C-N-CA	6.12	129.09	120.28
1	A	280	THR	N-CA-CB	6.10	119.15	110.13
1	A	161	GLY	N-CA-C	-6.08	107.99	114.67
1	A	66	VAL	O-C-N	6.05	128.17	121.94
1	A	226	GLU	CA-C-O	-6.05	113.43	120.20
1	A	141	ILE	N-CA-CB	-6.04	103.74	110.99
1	A	175	ILE	O-C-N	6.04	129.75	123.05
1	A	222	PHE	CA-CB-CG	6.02	119.82	113.80
1	A	233	LEU	CA-C-N	-6.02	110.61	121.14
1	A	233	LEU	C-N-CA	-6.02	110.61	121.14
1	A	276	PHE	CA-CB-CG	-6.01	107.79	113.80
1	A	120	LEU	CA-C-O	-6.00	114.44	121.46
1	A	130	LYS	CA-C-N	5.99	128.23	120.44
1	A	130	LYS	C-N-CA	5.99	128.23	120.44
1	A	166	ASN	OD1-CG-ND2	-5.95	116.65	122.60
1	A	11	MET	N-CA-C	-5.89	104.75	112.41
1	A	279	THR	CA-C-O	-5.89	113.20	119.97
1	A	50	ASP	CA-C-N	5.87	134.49	121.80
1	A	50	ASP	C-N-CA	5.87	134.49	121.80
1	A	53	CYS	CA-C-O	-5.85	114.44	121.40
1	A	180	LYS	CB-CG-CD	5.84	124.73	111.30
1	A	73	VAL	O-C-N	5.82	129.29	123.18
1	A	321	LYS	N-CA-C	-5.81	106.35	113.50
1	A	217	GLY	CA-C-O	5.80	126.98	119.44
1	A	325	LYS	CA-C-O	-5.79	114.45	121.28
1	A	328	GLU	N-CA-C	5.79	118.90	109.06
1	A	264	ALA	N-CA-C	5.76	119.13	111.75
1	A	242	GLU	CG-CD-OE2	-5.76	105.15	118.40
1	A	107	THR	CA-CB-CG2	5.76	120.28	110.50
1	A	253	ASP	CA-C-O	5.73	127.34	120.92
1	A	17	GLN	OE1-CD-NE2	5.72	128.32	122.60
1	A	184	THR	CA-C-O	5.71	126.48	120.42
1	A	277	VAL	O-C-N	5.70	127.70	121.83
1	A	112	GLN	O-C-N	5.69	128.87	122.27
1	A	189	LEU	N-CA-C	-5.69	105.16	111.36
1	A	274	GLY	CA-C-N	5.69	128.37	120.29
1	A	274	GLY	C-N-CA	5.69	128.37	120.29
1	A	63	ASN	N-CA-CB	-5.68	101.56	110.30
1	A	53	CYS	N-CA-CB	5.67	121.33	112.25
1	A	124	GLN	CA-C-N	5.63	130.72	121.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	GLN	C-N-CA	5.63	130.72	121.87
1	A	268	LYS	O-C-N	5.63	129.27	122.35
1	A	118	THR	CA-C-N	5.61	128.98	121.01
1	A	118	THR	C-N-CA	5.61	128.98	121.01
1	A	340	ALA	N-CA-CB	-5.61	101.08	111.13
1	A	265	ILE	CA-C-N	5.58	130.04	120.72
1	A	265	ILE	C-N-CA	5.58	130.04	120.72
1	A	44	LEU	O-C-N	5.58	129.63	123.16
1	A	338	GLY	CA-C-O	5.58	125.93	119.13
1	A	85	ALA	CA-C-N	5.57	128.06	120.54
1	A	85	ALA	C-N-CA	5.57	128.06	120.54
1	A	22	GLU	N-CA-CB	5.56	118.14	110.07
1	A	118	THR	CA-C-O	-5.55	114.27	120.66
1	A	33	ILE	CA-C-N	-5.55	111.89	121.66
1	A	33	ILE	C-N-CA	-5.55	111.89	121.66
1	A	254	GLN	N-CA-C	5.54	120.15	113.17
1	A	38	GLY	CA-C-O	-5.54	115.42	122.01
1	A	12	SER	CA-CB-OG	-5.53	100.04	111.10
1	A	317	THR	CA-C-O	-5.53	113.96	120.60
1	A	66	VAL	N-CA-C	5.53	115.66	110.30
1	A	121	ASP	CA-CB-CG	-5.53	107.07	112.60
1	A	270	GLN	N-CA-C	-5.50	101.15	109.85
1	A	143	ILE	O-C-N	5.50	129.14	123.20
1	A	94	ILE	N-CA-C	-5.48	100.17	108.17
1	A	136	VAL	CA-C-O	-5.48	114.84	120.71
1	A	253	ASP	CB-CA-C	-5.46	101.67	110.74
1	A	317	THR	N-CA-CB	-5.46	101.35	111.13
1	A	10	ALA	O-C-N	5.46	131.26	122.96
1	A	237	ALA	O-C-N	5.46	128.78	122.17
1	A	218	LEU	N-CA-CB	-5.46	101.49	109.95
1	A	264	ALA	CA-C-O	-5.45	114.10	120.20
1	A	23	PHE	CA-CB-CG	-5.43	108.37	113.80
1	A	52	ALA	N-CA-CB	-5.43	105.67	113.65
1	A	128	ALA	CA-C-N	5.42	127.86	120.54
1	A	128	ALA	C-N-CA	5.42	127.86	120.54
1	A	169	VAL	CA-C-O	-5.41	117.92	122.63
1	A	266	LYS	CA-C-N	5.41	129.88	120.68
1	A	266	LYS	C-N-CA	5.41	129.88	120.68
1	A	138	PRO	CA-C-O	-5.41	114.52	122.31
1	A	167	ALA	CA-C-N	5.40	130.26	122.16
1	A	167	ALA	C-N-CA	5.40	130.26	122.16
1	A	51	ASP	O-C-N	5.40	129.59	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	CA-C-O	-5.39	115.06	121.16
1	A	149	GLN	N-CA-CB	-5.37	102.19	109.98
1	A	303	TYR	CA-C-N	5.37	127.74	120.44
1	A	303	TYR	C-N-CA	5.37	127.74	120.44
1	A	118	THR	OG1-CB-CG2	5.36	120.02	109.30
1	A	238	GLY	CA-C-O	5.34	128.88	121.40
1	A	45	GLN	CA-C-N	5.33	128.31	120.91
1	A	45	GLN	C-N-CA	5.33	128.31	120.91
1	A	183	SER	CB-CA-C	-5.33	101.62	110.68
1	A	285	GLN	OE1-CD-NE2	5.32	127.92	122.60
1	A	328	GLU	CB-CA-C	-5.32	98.59	109.38
1	A	120	LEU	O-C-N	5.30	130.22	123.11
1	A	47	ALA	CB-CA-C	5.30	118.76	111.23
1	A	258	ASN	CA-C-O	5.29	125.69	119.28
1	A	274	GLY	O-C-N	-5.29	115.82	122.70
1	A	181	ASP	CB-CA-C	-5.27	102.35	110.78
1	A	293	GLN	CA-CB-CG	-5.27	103.57	114.10
1	A	7	VAL	CA-C-O	-5.24	114.66	120.74
1	A	221	GLN	CB-CG-CD	5.24	121.51	112.60
1	A	319	ASP	N-CA-C	-5.22	102.27	110.36
1	A	106	LEU	CA-C-O	5.21	125.98	120.10
1	A	139	GLN	CB-CG-CD	5.20	121.44	112.60
1	A	320	GLU	CA-C-O	5.19	125.75	119.11
1	A	249	PRO	CB-CA-C	5.19	118.03	111.39
1	A	72	TYR	CA-C-N	-5.19	116.76	123.19
1	A	72	TYR	C-N-CA	-5.19	116.76	123.19
1	A	274	GLY	CA-C-O	5.17	129.57	120.57
1	A	307	ASN	OD1-CG-ND2	5.17	127.77	122.60
1	A	140	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	A	184	THR	N-CA-CB	-5.15	102.54	110.16
1	A	117	THR	CA-C-N	5.15	131.07	122.73
1	A	117	THR	C-N-CA	5.15	131.07	122.73
1	A	81	SER	CB-CA-C	-5.13	101.30	110.70
1	A	308	SER	CA-C-N	-5.11	116.44	123.14
1	A	308	SER	C-N-CA	-5.11	116.44	123.14
1	A	111	TYR	N-CA-C	-5.10	103.80	110.53
1	A	191	LYS	N-CA-C	5.09	116.52	110.97
1	A	83	GLN	CA-C-N	5.09	124.53	119.24
1	A	83	GLN	C-N-CA	5.09	124.53	119.24
1	A	52	ALA	CA-C-O	5.09	125.93	119.16
1	A	42	ASN	OD1-CG-ND2	5.08	127.68	122.60
1	A	54	ASP	CA-C-N	5.08	124.74	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	54	ASP	C-N-CA	5.08	124.74	119.56
1	A	247	THR	OG1-CB-CG2	5.08	119.45	109.30
1	A	92	GLU	N-CA-C	5.07	119.02	111.87
1	A	197	VAL	N-CA-CB	5.06	120.20	111.39
1	A	178	GLY	N-CA-C	-5.06	107.56	114.64
1	A	237	ALA	CA-C-O	-5.05	115.15	120.55
1	A	140	ARG	CD-NE-CZ	5.05	131.47	124.40
1	A	275	ALA	N-CA-C	5.04	116.86	111.36
1	A	20	ASP	O-C-N	5.04	127.89	122.15
1	A	331	VAL	O-C-N	5.03	128.46	123.18
1	A	24	THR	N-CA-CB	5.02	118.07	110.28
1	A	156	ARG	CA-C-N	5.02	127.42	120.29
1	A	156	ARG	C-N-CA	5.02	127.42	120.29

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	109	ARG	Sidechain
1	A	140	ARG	Sidechain

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2589	0	2566	243	2
2	A	121	0	0	44	3
All	All	2710	0	2566	243	3

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 47.

All (243) 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:47:ALA:HB1	2:A:413:HOH:O	1.23	1.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:ILE:HG12	2:A:412:HOH:O	1.31	1.26
1:A:317:THR:HG22	1:A:325:LYS:HB2	1.22	1.20
1:A:249:PRO:HB3	2:A:514:HOH:O	1.45	1.14
1:A:107:THR:HG21	1:A:323:ASP:OD2	1.45	1.13
1:A:293:GLN:NE2	1:A:303:TYR:CD2	2.18	1.11
1:A:39:ILE:HG23	1:A:292:ASN:ND2	1.69	1.08
1:A:107:THR:HG21	1:A:323:ASP:CG	1.76	1.08
1:A:107:THR:CG2	1:A:321:LYS:HG2	1.87	1.03
1:A:23:PHE:CD2	1:A:48:LYS:HD2	1.93	1.03
1:A:107:THR:HG23	1:A:321:LYS:CG	1.88	1.03
1:A:106:LEU:HB3	1:A:116:ARG:NH2	1.77	0.99
1:A:317:THR:HG22	1:A:325:LYS:CB	1.93	0.98
1:A:107:THR:HG23	1:A:321:LYS:HG2	0.98	0.98
1:A:83:GLN:O	1:A:86:SER:HB3	1.63	0.98
1:A:107:THR:O	1:A:321:LYS:HG3	1.68	0.93
1:A:39:ILE:HG23	1:A:292:ASN:HD22	1.29	0.90
1:A:120:LEU:O	1:A:123:ASP:HB2	1.72	0.90
1:A:230:ASN:ND2	1:A:232:SER:HB2	1.86	0.89
1:A:229:ALA:CB	2:A:420:HOH:O	2.20	0.89
1:A:14:PRO:HD2	1:A:15:VAL:HG22	1.54	0.88
1:A:193:ASN:OD1	1:A:193:ASN:O	1.92	0.88
1:A:253:ASP:OD2	1:A:273:SER:HA	1.73	0.88
1:A:229:ALA:HB2	2:A:420:HOH:O	1.73	0.87
1:A:107:THR:CG2	1:A:323:ASP:OD2	2.22	0.87
1:A:76:HIS:HE2	1:A:89:TYR:HH	0.86	0.86
1:A:225:PRO:HA	1:A:247:THR:HG22	1.58	0.85
1:A:230:ASN:ND2	1:A:232:SER:H	1.74	0.84
1:A:23:PHE:HD2	1:A:48:LYS:HD2	1.37	0.83
1:A:23:PHE:CE2	1:A:48:LYS:HG3	2.14	0.82
1:A:14:PRO:HD2	1:A:15:VAL:H	1.44	0.82
1:A:39:ILE:CD1	2:A:410:HOH:O	2.28	0.81
1:A:81:SER:HB2	2:A:417:HOH:O	1.79	0.81
1:A:34:ASN:HB2	1:A:43:LYS:HD2	1.61	0.81
1:A:317:THR:CG2	1:A:325:LYS:HD2	2.10	0.81
1:A:23:PHE:CE2	1:A:48:LYS:HD2	2.18	0.79
1:A:64:LYS:O	1:A:68:ASP:HB2	1.84	0.77
1:A:242:GLU:OE1	1:A:335:HIS:HD2	1.66	0.77
1:A:23:PHE:HE2	1:A:48:LYS:HG3	1.46	0.77
1:A:174:GLY:O	1:A:175:ILE:HD12	1.84	0.77
1:A:19:GLY:O	1:A:23:PHE:HD1	1.66	0.77
1:A:35:ALA:HB2	2:A:408:HOH:O	1.85	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:LEU:HB3	1:A:116:ARG:HH22	1.50	0.76
1:A:337:ASN:OD1	1:A:339:THR:HB	1.85	0.76
1:A:96:MET:HE2	1:A:114:ILE:HG23	1.68	0.76
1:A:61:VAL:O	1:A:65:VAL:HG23	1.87	0.75
1:A:23:PHE:CE2	1:A:48:LYS:CG	2.70	0.74
1:A:263:ASP:OD1	2:A:421:HOH:O	2.02	0.74
1:A:107:THR:O	1:A:321:LYS:CG	2.36	0.74
1:A:24:THR:HG23	1:A:270:GLN:NE2	2.02	0.73
1:A:39:ILE:HD12	2:A:410:HOH:O	1.87	0.73
1:A:282:ALA:HA	1:A:311:THR:HG22	1.70	0.73
1:A:12:SER:OG	1:A:13:GLY:N	2.20	0.73
1:A:47:ALA:CB	2:A:413:HOH:O	2.02	0.73
1:A:24:THR:HG23	1:A:270:GLN:HE21	1.51	0.73
1:A:290:GLY:O	1:A:293:GLN:HB2	1.89	0.73
1:A:230:ASN:HD22	1:A:232:SER:H	1.36	0.73
1:A:81:SER:CB	2:A:417:HOH:O	2.37	0.72
1:A:14:PRO:CD	1:A:15:VAL:H	2.00	0.72
1:A:119:GLY:HA3	1:A:327:PHE:CE1	2.25	0.72
1:A:206:MET:HE3	1:A:244:LEU:CD1	2.20	0.71
1:A:3:ILE:HB	1:A:44:LEU:HD23	1.71	0.71
1:A:307:ASN:ND2	2:A:425:HOH:O	2.19	0.71
1:A:106:LEU:CD2	1:A:116:ARG:HH21	2.04	0.70
1:A:106:LEU:HD23	1:A:116:ARG:HH21	1.54	0.70
1:A:23:PHE:CD2	1:A:48:LYS:CD	2.72	0.70
1:A:59:VAL:HG13	1:A:88:ILE:CD1	2.20	0.70
1:A:33:ILE:CD1	2:A:411:HOH:O	2.37	0.70
1:A:261:ILE:O	1:A:265:ILE:HG13	1.92	0.70
1:A:76:HIS:O	1:A:98:THR:HG23	1.92	0.70
1:A:163:LYS:O	1:A:163:LYS:HG3	1.91	0.69
1:A:230:ASN:HD22	1:A:232:SER:HB2	1.56	0.69
1:A:206:MET:HE3	1:A:244:LEU:HD11	1.74	0.69
1:A:107:THR:HG21	1:A:323:ASP:OD1	1.91	0.69
1:A:252:TYR:O	1:A:258:ASN:ND2	2.19	0.69
1:A:337:ASN:ND2	2:A:430:HOH:O	2.18	0.68
1:A:296:ASP:HB3	1:A:299:GLU:HB2	1.74	0.68
1:A:62:ALA:O	1:A:66:VAL:HG23	1.94	0.68
1:A:248:LYS:HB2	1:A:249:PRO:HD2	1.75	0.68
1:A:285:GLN:OE1	1:A:311:THR:HG22	1.94	0.68
1:A:36:LYS:HE3	2:A:437:HOH:O	1.92	0.68
1:A:23:PHE:O	1:A:27:GLU:HG3	1.95	0.67
1:A:133:LEU:O	2:A:504:HOH:O	2.11	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ALA:HA	1:A:311:THR:CG2	2.25	0.66
1:A:282:ALA:HB1	1:A:311:THR:HG21	1.79	0.64
1:A:163:LYS:HE2	2:A:474:HOH:O	1.97	0.64
1:A:293:GLN:NE2	1:A:303:TYR:HD2	1.92	0.64
1:A:285:GLN:HB2	1:A:311:THR:HG23	1.80	0.63
1:A:317:THR:HG21	1:A:325:LYS:HD2	1.79	0.63
1:A:23:PHE:CE2	1:A:48:LYS:CD	2.82	0.63
1:A:236:ILE:CD1	2:A:429:HOH:O	2.47	0.63
1:A:182:PHE:CE2	1:A:208:GLN:HB3	2.34	0.62
1:A:105:GLU:CD	1:A:105:GLU:H	2.08	0.61
1:A:300:ILE:HD13	2:A:424:HOH:O	2.00	0.61
1:A:124:GLN:HB3	1:A:247:THR:HG21	1.82	0.61
1:A:6:ALA:HB2	1:A:70:ILE:HG21	1.81	0.60
1:A:119:GLY:HA3	1:A:327:PHE:CD1	2.36	0.60
1:A:26:ALA:HB2	1:A:280:THR:HG21	1.82	0.60
1:A:317:THR:CG2	1:A:325:LYS:CB	2.76	0.60
1:A:143:ILE:HD11	1:A:162:LEU:HD12	1.83	0.60
1:A:10:ALA:O	1:A:19:GLY:HA3	2.01	0.60
1:A:33:ILE:HD12	2:A:411:HOH:O	1.97	0.60
1:A:236:ILE:HD11	2:A:429:HOH:O	2.02	0.59
1:A:287:LEU:CD1	2:A:424:HOH:O	2.50	0.59
1:A:14:PRO:HD2	1:A:15:VAL:N	2.17	0.59
1:A:84:PRO:HG3	2:A:418:HOH:O	2.02	0.59
1:A:163:LYS:HB2	2:A:474:HOH:O	2.03	0.58
1:A:242:GLU:OE1	1:A:335:HIS:CD2	2.53	0.58
1:A:182:PHE:HE2	1:A:208:GLN:CB	2.16	0.58
1:A:171:PHE:CZ	1:A:188:ARG:HD3	2.39	0.58
1:A:39:ILE:HG23	1:A:292:ASN:HD21	1.65	0.58
1:A:59:VAL:HG13	1:A:88:ILE:HD11	1.85	0.57
1:A:163:LYS:O	1:A:163:LYS:CG	2.52	0.57
1:A:303:TYR:CD1	1:A:303:TYR:C	2.83	0.57
1:A:182:PHE:HE2	1:A:208:GLN:HB3	1.70	0.56
1:A:103:ALA:O	1:A:116:ARG:NH2	2.38	0.56
1:A:19:GLY:O	1:A:23:PHE:CD1	2.53	0.56
1:A:213:ALA:O	1:A:218:LEU:HB2	2.05	0.56
1:A:335:HIS:ND1	1:A:339:THR:HG22	2.21	0.56
1:A:230:ASN:HD22	1:A:232:SER:N	2.03	0.56
1:A:255:VAL:HG12	1:A:256:PRO:HD2	1.86	0.56
1:A:253:ASP:O	1:A:262:VAL:HG21	2.05	0.56
1:A:106:LEU:HD23	1:A:116:ARG:NH2	2.19	0.56
1:A:107:THR:O	1:A:321:LYS:CD	2.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PHE:HE2	1:A:48:LYS:CG	2.15	0.55
1:A:77:LEU:CB	2:A:415:HOH:O	2.54	0.55
1:A:124:GLN:OE1	1:A:247:THR:CG2	2.55	0.55
1:A:51:ASP:C	1:A:53:CYS:H	2.14	0.55
1:A:7:VAL:HG22	1:A:74:ILE:HB	1.89	0.54
1:A:34:ASN:C	1:A:34:ASN:HD22	2.15	0.54
1:A:225:PRO:O	1:A:228:VAL:HB	2.07	0.54
1:A:76:HIS:HB2	1:A:82:THR:OG1	2.08	0.54
1:A:98:THR:HG22	1:A:100:ALA:H	1.73	0.54
1:A:252:TYR:CE2	1:A:313:MET:HE3	2.43	0.54
1:A:221:GLN:OE1	1:A:245:LEU:HD22	2.07	0.54
1:A:6:ALA:HA	1:A:47:ALA:O	2.07	0.54
1:A:137:LYS:N	1:A:138:PRO:HD3	2.23	0.54
1:A:33:ILE:HD13	2:A:411:HOH:O	2.04	0.53
1:A:206:MET:HE3	1:A:244:LEU:HD13	1.90	0.53
1:A:77:LEU:HB2	2:A:415:HOH:O	2.08	0.53
1:A:14:PRO:CD	1:A:15:VAL:N	2.69	0.53
1:A:58:ALA:HB1	1:A:81:SER:O	2.09	0.53
1:A:79:SER:HB3	1:A:103:ALA:HB2	1.91	0.53
1:A:26:ALA:HA	1:A:284:LEU:HD13	1.91	0.53
1:A:36:LYS:CE	2:A:437:HOH:O	2.54	0.52
1:A:28:GLN:OE1	1:A:268:LYS:NZ	2.41	0.52
1:A:226:GLU:C	1:A:228:VAL:H	2.18	0.52
1:A:72:TYR:CD2	2:A:424:HOH:O	2.54	0.52
1:A:193:ASN:O	1:A:193:ASN:CG	2.51	0.52
1:A:248:LYS:HD3	2:A:420:HOH:O	2.09	0.52
1:A:182:PHE:O	1:A:186:VAL:HG13	2.10	0.52
1:A:282:ALA:CB	1:A:311:THR:HG21	2.40	0.51
1:A:226:GLU:HG3	2:A:405:HOH:O	2.10	0.51
1:A:120:LEU:HD13	2:A:433:HOH:O	2.11	0.51
1:A:9:GLY:HA3	1:A:23:PHE:HE1	1.77	0.50
1:A:293:GLN:NE2	1:A:303:TYR:CE2	2.76	0.50
1:A:23:PHE:HD2	1:A:48:LYS:CD	2.18	0.49
1:A:76:HIS:CB	1:A:82:THR:OG1	2.60	0.49
1:A:30:VAL:HG11	1:A:46:ILE:CD1	2.43	0.49
1:A:3:ILE:HD13	1:A:291:LEU:HD13	1.94	0.49
1:A:9:GLY:HA3	1:A:23:PHE:CE1	2.48	0.49
1:A:30:VAL:HG23	1:A:284:LEU:HD22	1.94	0.49
1:A:47:ALA:CA	2:A:413:HOH:O	2.52	0.49
1:A:282:ALA:CA	1:A:311:THR:CG2	2.90	0.49
1:A:72:TYR:HD2	2:A:424:HOH:O	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:CB	1:A:46:ILE:HD11	2.43	0.48
1:A:223:MET:HE2	1:A:245:LEU:HB3	1.94	0.48
1:A:28:GLN:HG2	1:A:265:ILE:HG12	1.95	0.48
1:A:179:GLU:OE2	1:A:181:ASP:O	2.31	0.48
1:A:191:LYS:C	1:A:193:ASN:H	2.22	0.48
1:A:93:GLY:HA2	1:A:113:LEU:CD1	2.43	0.48
1:A:182:PHE:CE2	1:A:208:GLN:CB	2.95	0.48
1:A:284:LEU:HD23	2:A:411:HOH:O	2.14	0.48
1:A:320:GLU:CD	1:A:320:GLU:H	2.20	0.48
1:A:65:VAL:HG11	1:A:73:VAL:CG2	2.45	0.47
1:A:225:PRO:HA	1:A:247:THR:CG2	2.37	0.47
1:A:91:ASP:C	1:A:92:GLU:HG2	2.39	0.47
1:A:206:MET:CE	1:A:244:LEU:HD11	2.43	0.47
1:A:54:ASP:HB3	1:A:57:GLN:HB2	1.96	0.47
1:A:209:ILE:O	1:A:213:ALA:HB2	2.15	0.47
1:A:76:HIS:O	1:A:98:THR:CG2	2.63	0.47
1:A:271:ASP:HA	1:A:272:PRO:HD2	1.80	0.47
1:A:196:PHE:HA	1:A:221:GLN:O	2.15	0.46
1:A:115:LEU:HD22	1:A:304:LEU:HD23	1.96	0.46
1:A:125:GLY:N	1:A:126:PRO:CD	2.78	0.46
1:A:335:HIS:N	1:A:339:THR:O	2.47	0.46
1:A:13:GLY:HA3	1:A:14:PRO:HD3	1.66	0.46
1:A:282:ALA:CA	1:A:311:THR:HG21	2.45	0.46
1:A:203:HIS:N	1:A:204:PRO:CD	2.79	0.46
1:A:140:ARG:HB3	1:A:170:VAL:HG21	1.98	0.46
1:A:255:VAL:CG1	1:A:256:PRO:HD2	2.46	0.45
1:A:262:VAL:O	1:A:263:ASP:C	2.58	0.45
1:A:113:LEU:C	1:A:114:ILE:HD13	2.41	0.45
1:A:142:ALA:HB3	1:A:197:VAL:HG22	1.98	0.45
1:A:27:GLU:CD	2:A:409:HOH:O	2.60	0.45
1:A:171:PHE:CE1	1:A:188:ARG:HD3	2.52	0.45
1:A:256:PRO:O	1:A:259:LYS:HB2	2.17	0.45
1:A:133:LEU:HA	1:A:133:LEU:HD23	1.55	0.44
1:A:103:ALA:HB1	1:A:105:GLU:OE1	2.17	0.44
1:A:117:THR:HG21	1:A:283:ALA:HA	1.98	0.44
1:A:26:ALA:HB2	1:A:280:THR:CG2	2.48	0.44
1:A:83:GLN:N	1:A:84:PRO:HD2	2.32	0.44
1:A:138:PRO:HB3	1:A:196:PHE:HB2	2.00	0.44
1:A:49:TYR:HE1	1:A:64:LYS:HG2	1.82	0.43
1:A:123:ASP:HB2	1:A:329:PHE:HE2	1.82	0.43
1:A:249:PRO:CB	2:A:514:HOH:O	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HG	2:A:410:HOH:O	2.18	0.43
1:A:51:ASP:O	1:A:52:ALA:HB3	2.16	0.43
1:A:335:HIS:HB2	1:A:339:THR:O	2.19	0.43
1:A:30:VAL:HG21	1:A:46:ILE:HG13	2.01	0.43
1:A:114:ILE:HD13	1:A:114:ILE:N	2.32	0.43
1:A:44:LEU:CD1	2:A:411:HOH:O	2.67	0.43
1:A:146:ASP:C	1:A:148:GLN:N	2.75	0.43
1:A:46:ILE:HG21	2:A:412:HOH:O	2.18	0.43
1:A:344:LYS:OXT	1:A:344:LYS:HG3	2.18	0.43
1:A:163:LYS:HE2	1:A:163:LYS:HB2	1.79	0.43
1:A:207:GLY:O	1:A:211:ARG:HG3	2.19	0.42
1:A:30:VAL:HB	1:A:46:ILE:HD11	2.01	0.42
1:A:106:LEU:HB3	1:A:116:ARG:HH21	1.73	0.42
1:A:226:GLU:C	1:A:228:VAL:N	2.75	0.42
1:A:30:VAL:HG11	1:A:46:ILE:HD12	2.02	0.42
1:A:96:MET:HE3	1:A:98:THR:OG1	2.20	0.42
1:A:98:THR:HG22	1:A:101:ALA:H	1.85	0.42
1:A:107:THR:CG2	1:A:321:LYS:CG	2.70	0.42
1:A:164:LYS:HB3	1:A:164:LYS:HE3	1.54	0.42
1:A:255:VAL:O	1:A:256:PRO:C	2.62	0.42
1:A:209:ILE:O	1:A:213:ALA:CB	2.68	0.41
1:A:107:THR:HG22	1:A:321:LYS:HD2	2.02	0.41
1:A:175:ILE:HD12	1:A:175:ILE:HA	1.68	0.41
1:A:203:HIS:N	1:A:204:PRO:HD3	2.34	0.41
1:A:95:LEU:CD2	2:A:424:HOH:O	2.68	0.41
1:A:213:ALA:O	1:A:218:LEU:CB	2.67	0.41
1:A:309:VAL:O	1:A:316:LEU:N	2.44	0.41
1:A:123:ASP:CB	1:A:329:PHE:HE2	2.33	0.41
1:A:57:GLN:O	1:A:60:ALA:HB3	2.20	0.41
1:A:246:VAL:HG11	2:A:420:HOH:O	2.20	0.41
1:A:22:GLU:HB3	1:A:280:THR:OG1	2.21	0.40
1:A:30:VAL:HG11	1:A:46:ILE:HD11	2.04	0.40
1:A:30:VAL:HG21	1:A:46:ILE:HD11	2.03	0.40
1:A:58:ALA:CB	1:A:81:SER:O	2.69	0.40
1:A:208:GLN:O	1:A:212:GLN:HB2	2.21	0.40
1:A:22:GLU:OE1	1:A:77:LEU:HD13	2.21	0.40
1:A:78:CYS:HB2	2:A:417:HOH:O	2.22	0.40

All (3) 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:A:335:HIS:CE1	2:A:429:HOH:O[4_444]	1.80	0.40
1:A:335:HIS:NE2	2:A:429:HOH:O[4_444]	2.00	0.20
2:A:425:HOH:O	2:A:431:HOH:O[3_454]	2.08	0.12

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	342/344 (99%)	328 (96%)	13 (4%)	1 (0%)	36 50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	76	HIS

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	266/266 (100%)	210 (79%)	56 (21%)	1 1

All (56) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	11	MET
1	A	15	VAL

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Mol	Chain	Res	Type
1	A	22	GLU
1	A	34	ASN
1	A	48	LYS
1	A	56	LYS
1	A	57	GLN
1	A	68	ASP
1	A	70	ILE
1	A	77	LEU
1	A	79	SER
1	A	81	SER
1	A	83	GLN
1	A	90	GLU
1	A	95	LEU
1	A	105	GLU
1	A	107	THR
1	A	118	THR
1	A	135	LYS
1	A	139	GLN
1	A	147	LYS
1	A	148	GLN
1	A	149	GLN
1	A	175	ILE
1	A	176	THR
1	A	180	LYS
1	A	184	THR
1	A	186	VAL
1	A	212	GLN
1	A	218	LEU
1	A	225	PRO
1	A	228	VAL
1	A	230	ASN
1	A	232	SER
1	A	234	SER
1	A	239	GLU
1	A	244	LEU
1	A	245	LEU
1	A	246	VAL
1	A	247	THR
1	A	253	ASP
1	A	255	VAL
1	A	259	LYS
1	A	272	PRO

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Mol	Chain	Res	Type
1	A	284	LEU
1	A	288	GLN
1	A	304	LEU
1	A	310	ASP
1	A	311	THR
1	A	312	VAL
1	A	317	THR
1	A	320	GLU
1	A	325	LYS
1	A	339	THR
1	A	344	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	63	ASN
1	A	112	GLN
1	A	149	GLN
1	A	159	GLN
1	A	168	ASN
1	A	208	GLN
1	A	230	ASN
1	A	251	ASN
1	A	270	GLN
1	A	292	ASN
1	A	335	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

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.