



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:09 am GMT

PDB ID : 2LBP
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : recalc28949

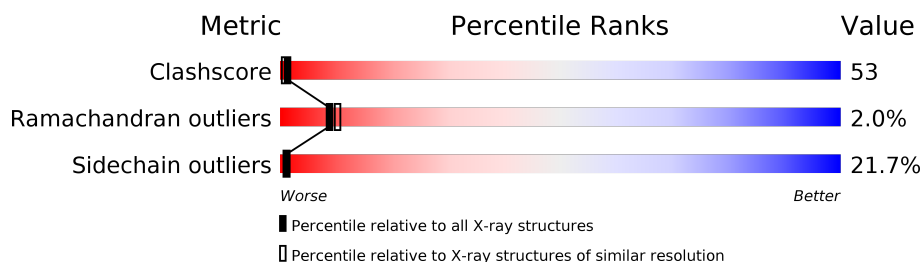
1 Overall quality at a glance

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	112137	3674 (2.40-2.40)
Ramachandran outliers	110173	3616 (2.40-2.40)
Sidechain outliers	110143	3617 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	346	

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.

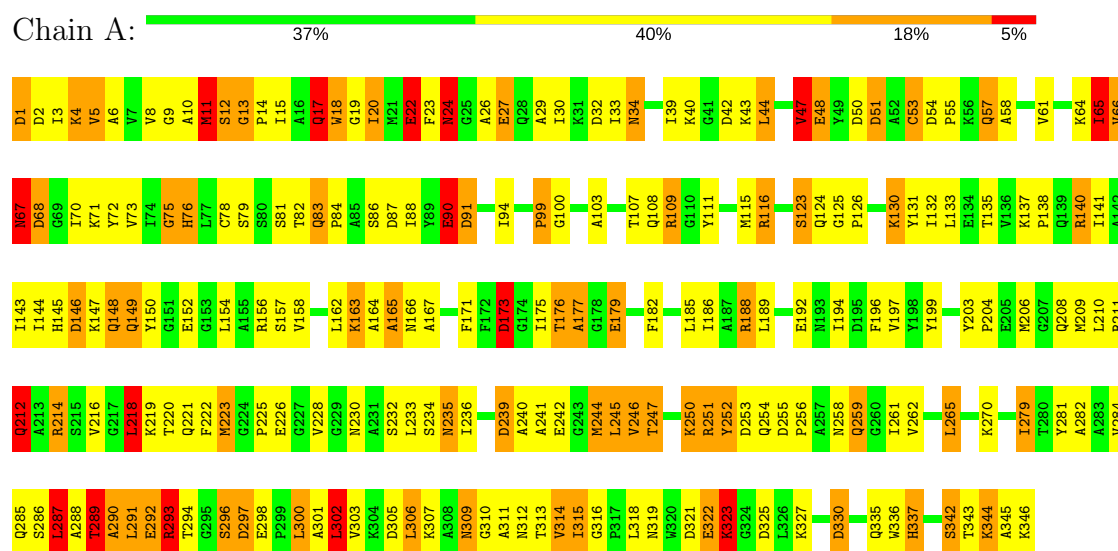
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	91	Total	O	0	0
			91	91		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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	1.10	11/2648 (0.4%)	2.18	114/3581 (3.2%)

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 (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	22	GLU	CB-CG	-7.55	1.37	1.52
1	A	13	GLY	N-CA	7.50	1.57	1.46
1	A	27	GLU	CG-CD	-7.14	1.41	1.51
1	A	310	GLY	N-CA	6.54	1.55	1.46
1	A	292	GLU	CD-OE1	-6.22	1.18	1.25
1	A	90	GLU	CD-OE1	-6.01	1.19	1.25
1	A	22	GLU	CG-CD	-5.77	1.43	1.51
1	A	342	SER	CA-CB	5.47	1.61	1.52
1	A	12	SER	C-O	5.21	1.33	1.23
1	A	48	GLU	CD-OE1	-5.15	1.20	1.25
1	A	291	LEU	N-CA	-5.12	1.36	1.46

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	307	LYS	CA-CB-CG	20.04	157.49	113.40
1	A	22	GLU	CB-CG-CD	17.15	160.49	114.20
1	A	22	GLU	CA-CB-CG	16.65	150.04	113.40
1	A	27	GLU	CB-CG-CD	15.06	154.85	114.20
1	A	156	ARG	NE-CZ-NH1	14.23	127.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	156	ARG	NE-CZ-NH2	-13.41	113.59	120.30
1	A	51	ASP	CB-CG-OD2	-13.28	106.35	118.30
1	A	116	ARG	CD-NE-CZ	12.93	141.70	123.60
1	A	34	ASN	CB-CA-C	12.85	136.10	110.40
1	A	47	VAL	CB-CA-C	12.23	134.63	111.40
1	A	75	GLY	C-N-CA	11.65	150.82	121.70
1	A	330	ASP	CA-CB-CG	11.34	138.35	113.40
1	A	116	ARG	NE-CZ-NH1	10.90	125.75	120.30
1	A	188	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	A	27	GLU	CG-CD-OE1	10.32	138.95	118.30
1	A	290	ALA	C-N-CA	10.03	146.78	121.70
1	A	239	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	A	188	ARG	NE-CZ-NH2	-9.61	115.50	120.30
1	A	290	ALA	CB-CA-C	9.54	124.40	110.10
1	A	51	ASP	CB-CG-OD1	9.32	126.69	118.30
1	A	27	GLU	OE1-CD-OE2	-8.94	112.58	123.30
1	A	235	ASN	CA-CB-CG	8.90	132.98	113.40
1	A	5	VAL	CB-CA-C	-8.89	94.50	111.40
1	A	12	SER	CA-C-N	8.62	133.43	116.20
1	A	24	ASN	N-CA-CB	-8.33	95.60	110.60
1	A	223	MET	N-CA-CB	8.27	125.49	110.60
1	A	292	GLU	CG-CD-OE1	8.23	134.77	118.30
1	A	211	ARG	NE-CZ-NH1	-8.13	116.23	120.30
1	A	293	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	108	GLN	CA-CB-CG	7.87	130.72	113.40
1	A	246	VAL	CA-CB-CG2	7.75	122.52	110.90
1	A	2	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	A	34	ASN	CA-CB-CG	7.62	130.16	113.40
1	A	289	THR	CA-CB-CG2	7.58	123.01	112.40
1	A	226	GLU	CA-CB-CG	7.54	129.99	113.40
1	A	50	ASP	CB-CG-OD2	7.52	125.07	118.30
1	A	252	TYR	CB-CG-CD2	-7.41	116.55	121.00
1	A	109	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	A	48	GLU	CG-CD-OE1	7.34	132.99	118.30
1	A	90	GLU	C-N-CA	7.24	139.80	121.70
1	A	297	ASP	CB-CA-C	7.21	124.81	110.40
1	A	146	ASP	CB-CG-OD2	-7.14	111.88	118.30
1	A	327	LYS	CA-CB-CG	7.07	128.96	113.40
1	A	4	LYS	C-N-CA	6.98	139.15	121.70
1	A	211	ARG	CD-NE-CZ	-6.94	113.88	123.60
1	A	246	VAL	CB-CA-C	-6.67	98.72	111.40
1	A	287	LEU	CA-C-O	6.66	134.08	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ASP	CB-CG-OD1	6.63	124.27	118.30
1	A	91	ASP	N-CA-CB	-6.62	98.69	110.60
1	A	11	MET	CA-CB-CG	6.60	124.53	113.30
1	A	289	THR	C-N-CA	-6.53	105.36	121.70
1	A	327	LYS	N-CA-CB	6.53	122.36	110.60
1	A	292	GLU	CG-CD-OE2	-6.49	105.32	118.30
1	A	173	ASP	CB-CG-OD1	6.46	124.11	118.30
1	A	47	VAL	CA-CB-CG1	6.45	120.58	110.90
1	A	90	GLU	CG-CD-OE2	-6.40	105.51	118.30
1	A	177	ALA	CB-CA-C	6.26	119.48	110.10
1	A	214	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	A	291	LEU	N-CA-C	6.12	127.52	111.00
1	A	173	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	A	301	ALA	C-N-CA	6.08	136.89	121.70
1	A	163	LYS	N-CA-CB	6.08	121.53	110.60
1	A	293	ARG	C-N-CA	6.05	136.84	121.70
1	A	12	SER	O-C-N	-6.04	112.93	123.20
1	A	176	THR	CA-CB-CG2	6.03	120.83	112.40
1	A	116	ARG	CA-CB-CG	6.02	126.65	113.40
1	A	5	VAL	N-CA-CB	5.97	124.64	111.50
1	A	146	ASP	C-N-CA	5.92	136.49	121.70
1	A	78	CYS	O-C-N	5.90	132.14	122.70
1	A	342	SER	N-CA-CB	-5.90	101.66	110.50
1	A	226	GLU	N-CA-CB	5.84	121.12	110.60
1	A	307	LYS	N-CA-CB	5.83	121.10	110.60
1	A	251	ARG	NE-CZ-NH2	5.81	123.21	120.30
1	A	50	ASP	O-C-N	5.75	131.91	122.70
1	A	12	SER	C-N-CA	-5.75	110.22	122.30
1	A	212	GLN	CA-CB-CG	5.75	126.04	113.40
1	A	291	LEU	CA-CB-CG	-5.70	102.19	115.30
1	A	253	ASP	CB-CG-OD1	5.69	123.42	118.30
1	A	252	TYR	CB-CG-CD1	5.67	124.40	121.00
1	A	51	ASP	CB-CA-C	-5.61	99.17	110.40
1	A	297	ASP	C-N-CA	5.61	135.73	121.70
1	A	330	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	323	LYS	CA-CB-CG	5.59	125.69	113.40
1	A	265	LEU	CB-CA-C	5.57	120.78	110.20
1	A	307	LYS	CB-CG-CD	5.57	126.07	111.60
1	A	235	ASN	CB-CA-C	5.56	121.53	110.40
1	A	291	LEU	CA-C-O	-5.56	108.42	120.10
1	A	298	GLU	OE1-CD-OE2	5.54	129.95	123.30
1	A	17	GLN	N-CA-CB	5.52	120.54	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	44	LEU	O-C-N	5.44	131.40	122.70
1	A	311	ALA	O-C-N	5.40	131.34	122.70
1	A	68	ASP	CB-CA-C	5.40	121.20	110.40
1	A	23	PHE	N-CA-CB	5.34	120.21	110.60
1	A	290	ALA	O-C-N	-5.32	114.18	122.70
1	A	293	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	A	211	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	A	154	LEU	CA-CB-CG	5.24	127.35	115.30
1	A	18	TRP	CB-CA-C	5.22	120.85	110.40
1	A	218	LEU	CB-CA-C	5.22	120.11	110.20
1	A	50	ASP	C-N-CA	5.21	134.74	121.70
1	A	311	ALA	N-CA-CB	5.21	117.40	110.10
1	A	309	ASN	C-N-CA	-5.20	111.38	122.30
1	A	302	LEU	CB-CG-CD2	-5.19	102.18	111.00
1	A	65	ILE	CB-CA-C	5.19	121.97	111.60
1	A	291	LEU	N-CA-CB	5.18	120.77	110.40
1	A	290	ALA	N-CA-C	-5.18	97.02	111.00
1	A	188	ARG	CD-NE-CZ	5.17	130.84	123.60
1	A	244	MET	CG-SD-CE	5.14	108.42	100.20
1	A	253	ASP	CA-CB-CG	5.13	124.70	113.40
1	A	259	GLN	N-CA-CB	5.11	119.79	110.60
1	A	337	HIS	CA-CB-CG	-5.10	104.92	113.60
1	A	5	VAL	O-C-N	5.09	130.84	122.70
1	A	68	ASP	N-CA-CB	-5.08	101.45	110.60
1	A	2	ASP	CA-C-O	-5.06	109.47	120.10

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	Mainchain,Peptide

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	2562	274	0
2	A	91	0	0	7	0
All	All	2691	0	2562	274	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 53.

All (274) 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:NE2	1:A:17:GLN:H	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
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:29:ALA:HB1	1:A:284:VAL:CG1	1.86	1.04
1:A:289:THR:O	1:A:290:ALA:C	1.98	1.00
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:HG	1:A:291:LEU:O	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:210:LEU:HD11	1:A:244:MET:HE2	1.58	0.84
1:A:208:GLN:O	1:A:212:GLN:HB2	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:A:107:THR:HG22	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: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
1:A:209:MET:HE1	1:A:222:PHE:HE1	1.48	0.76
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:143:ILE:C	1:A:144:ILE:HG13	2.05	0.75
1:A:88:ILE:O	1:A:91:ASP:HB3	1.87	0.75
1:A:291:LEU:CG	1:A:291:LEU:O	2.35	0.75
1:A:144:ILE:HD11	1:A:171:PHE:CE2	2.22	0.75
1:A:17:GLN:NE2	1:A:17:GLN:N	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:HD21	1:A:302:LEU:HG	1.68	0.73
1:A:291:LEU:CD1	1:A:305:ASP:HB3	2.15	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: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:OE1	1:A:149:GLN:N	2.22	0.71
1:A:218:LEU:HG	1:A:220:THR:OG1	1.91	0.71
1:A:103:ALA:O	1:A:116:ARG:NH2	2.17	0.71
1:A:17:GLN:OE1	1:A:18:TRP:CZ3	2.43	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:209:MET:CE	1:A:222:PHE:CE1	2.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD11	1:A:288:ALA:HB1	1.74	0.69
1:A:209:MET:HE1	1:A:222:PHE:CE1	2.28	0.68
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: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:291:LEU:HG	1:A:294:THR:HB	1.76	0.67
1:A:282:ALA:CB	1:A:313:THR:HG21	2.25	0.67
1:A:29:ALA:O	1:A:33:ILE:HG13	1.94	0.67
1:A:107:THR:CG2	1:A:323:LYS:O	2.43	0.67
1:A:1:ASP:N	2:A:525:HOH:O	2.28	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
1:A:186:ILE:HD12	1:A:212:GLN:HG2	1.78	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:210:LEU:CD1	1:A:244:MET:HE2	2.27	0.63
1:A:51:ASP:C	1:A:53:CYS:H	2.00	0.63
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:66:VAL:C	1:A:68:ASP:H	1.98	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:291:LEU:HD13	1:A:302:LEU:C	2.19	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: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:233:LEU:HD21	1:A:244:MET:HE3	1.82	0.60
1:A:291:LEU:HD23	1:A:291:LEU:C	2.21	0.60
1:A:107:THR:HG21	1:A:323:LYS:CG	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:TYR:CD2	1:A:111:TYR:N	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:337:HIS:HE1	1:A:343:THR:OG1	1.84	0.59
1:A:1:ASP:CA	1:A:42:ASP:OD1	2.38	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: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:294:THR:CG2	1:A:296:SER:H	2.17	0.57
1:A:66:VAL:O	1:A:68:ASP:N	2.34	0.57
1:A:344:LYS:HD2	1:A:344:LYS:C	2.25	0.57
1:A:313:THR:CG2	1:A:314:VAL:N	2.68	0.57
1:A:51:ASP:C	1:A:53:CYS:N	2.57	0.57
1:A:315:ILE:CG2	1:A:318:LEU:HD21	2.34	0.57
1:A:250:LYS:CE	2:A:574:HOH:O	2.52	0.57
1:A:8:VAL:CG1	1:A:76:HIS:CE1	2.84	0.57
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:51:ASP:HB3	1:A:53:CYS:H	1.69	0.56
1:A:107:THR:CG2	1:A:323:LYS:CB	2.83	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:322:GLU:CD	1:A:322:GLU:H	2.10	0.54
1:A:68:ASP:O	1:A:68:ASP:OD1	2.25	0.54
1:A:17:GLN:OE1	1:A:18:TRP:CH2	2.60	0.54
1:A:346:LYS:HG3	1:A:346:LYS:OXT	2.06	0.54
1:A:64:LYS:O	1:A:68:ASP:HB3	2.07	0.54
1:A:148:GLN:N	1:A:148:GLN:NE2	2.56	0.54
1:A:285:GLN:OE1	1:A:314:VAL:HB	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:66:VAL:HG22	1:A:94:ILE:CD1	2.36	0.54
1:A:107:THR:CG2	1:A:323:LYS:CG	2.85	0.54
1:A:39:ILE:CD1	1:A:44:LEU:HG	2.38	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:192:GLU:HA	1:A:192:GLU:OE2	2.09	0.53
1:A:144:ILE:HD11	1:A:171:PHE:HE2	1.71	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:197:VAL:HG23	1:A:220:THR:HG21	1.91	0.53
1:A:67:ASN:O	1:A:67:ASN:CG	2.47	0.53
1:A:90:GLU:OE1	1:A:111:TYR:HA	2.09	0.52
1:A:233:LEU:HD21	1:A:244:MET:HE1	1.91	0.52
1:A:306:LEU:O	1:A:309:ASN:O	2.27	0.52
1:A:246:VAL:HG21	1:A:336:TRP:CE3	2.44	0.52
1:A:203:TYR:CD1	1:A:204:PRO:HD3	2.43	0.52
1:A:209:MET:HE2	1:A:222:PHE:CE1	2.44	0.52
1:A:287:LEU:HG	1:A:288:ALA:N	2.21	0.52
1:A:86:SER:OG	1:A:109:ARG:NH2	2.35	0.52
1:A:149:GLN:CD	1:A:149:GLN:N	2.59	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: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: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:115:MET:HE1	1:A:303:VAL:HA	1.92	0.50
1:A:189:LEU:HD22	1:A:194:ILE:CG2	2.39	0.50
1:A:246:VAL:HG12	1:A:247:THR:N	2.27	0.50
1:A:131:TYR:OH	1:A:346:LYS:OXT	2.23	0.50
1:A:67:ASN:O	1:A:67:ASN:OD1	2.30	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: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:66:VAL:C	1:A:68:ASP:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:LYS:C	1:A:148:GLN:NE2	2.67	0.48
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:252:TYR:O	1:A:258:ASN:ND2	2.41	0.48
1:A:64:LYS:O	1:A:64:LYS:CG	2.61	0.48
1:A:163:LYS:O	1:A:165:ALA:N	2.46	0.48
1:A:44:LEU:HD11	1:A:288:ALA:CB	2.44	0.47
1:A:132:ILE:CG1	1:A:223:MET:HE3	2.45	0.47
1:A:164:ALA:O	1:A:165:ALA:HB2	2.15	0.47
1:A:147:LYS:C	1:A:148:GLN:HE21	2.17	0.47
1:A:158:VAL:O	1:A:162:LEU:HG	2.15	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:HG3	1:A:130:LYS:O	2.15	0.46
1:A:145:HIS:CE1	1:A:152:GLU:HG3	2.51	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:148:GLN:N	1:A:148:GLN:HE21	2.13	0.46
1:A:57:GLN:NE2	2:A:508:HOH:O	2.48	0.46
1:A:282:ALA:HB2	1:A:313:THR:CG2	2.46	0.46
1:A:140:ARG:HG2	1:A:140:ARG:NH1	2.30	0.45
1:A:186:ILE:CD1	1:A:212:GLN:HB3	2.44	0.45
1:A:291:LEU:C	1:A:293:ARG:N	2.69	0.45
1:A:11:MET:HE1	1:A:48:GLU:HB3	1.98	0.45
1:A:186:ILE:CD1	1:A:212:GLN:CB	2.94	0.45
1:A:291:LEU:HD23	1:A:292:GLU:N	2.32	0.45
1:A:3:ILE:N	1:A:43:LYS:O	2.50	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:199:TYR:O	1:A:225:PRO:HD3	2.16	0.44
1:A:54:ASP:HA	1:A:55:PRO:HD3	1.79	0.44
1:A:125:GLY:N	1:A:126:PRO:CD	2.81	0.44
1:A:65:ILE:HD11	1:A:73:VAL:HG21	1.88	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:83:GLN:CB	1:A:84:PRO:HD3	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:291:LEU:CD2	1:A:291:LEU:O	2.65	0.44
1:A:144:ILE:HA	1:A:173:ASP:O	2.18	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:HD12	1:A:185:LEU:O	2.18	0.43
1:A:64:LYS:O	1:A:68:ASP:CB	2.65	0.43
1:A:210:LEU:HD13	1:A:241:ALA:HA	1.99	0.43
1:A:291:LEU:CD2	1:A:291:LEU:C	2.80	0.43
1:A:132:ILE:HG13	1:A:223:MET:HE3	2.01	0.43
1:A:270:LYS:HE2	2:A:511:HOH:O	2.19	0.43
1:A:322:GLU:N	1:A:322:GLU:CD	2.71	0.43
1:A:306:LEU:HA	1:A:306:LEU:HD12	1.94	0.43
1:A:47:VAL:HG13	1:A:70:ILE:HD13	2.01	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:148:GLN:CA	1:A:148:GLN:HE21	2.33	0.42
1:A:206:MET:HG3	1:A:244:MET:HE2	2.01	0.42
1:A:51:ASP:O	1:A:53:CYS:N	2.53	0.42
1:A:65:ILE:CD1	1:A:73:VAL:CG2	2.76	0.42
1:A:176:THR:HB	1:A:179:GLU:HG3	2.02	0.41
1:A:131:TYR:CZ	1:A:346:LYS:OXT	2.73	0.41
1:A:163:LYS:HD3	1:A:163:LYS:O	2.20	0.41
1:A:47:VAL:CG1	1:A:70:ILE:HD11	2.49	0.41
1:A:233:LEU:CD2	1:A:244:MET:HE1	2.49	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:300:LEU:HA	1:A:303:VAL:HG12	2.01	0.41
1:A:107:THR:O	1:A:107:THR:CG2	2.50	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:176:THR:HB	1:A:179:GLU:CG	2.51	0.41
1:A:284:VAL:CG1	1:A:285:GLN:H	2.33	0.41
1:A:192:GLU:HB3	1:A:194:ILE:CD1	2.50	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%)	9	10

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%)	209 (78%)	58 (22%)	1	1

All (58) 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	47	VAL
1	A	53	CYS
1	A	57	GLN
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	123	SER
1	A	130	LYS
1	A	135	THR
1	A	148	GLN
1	A	149	GLN
1	A	157	SER
1	A	173	ASP
1	A	175	ILE
1	A	179	GLU
1	A	212	GLN
1	A	216	VAL
1	A	218	LEU
1	A	219	LYS
1	A	221	GLN
1	A	234	SER
1	A	235	ASN
1	A	239	ASP
1	A	245	LEU
1	A	247	THR
1	A	250	LYS
1	A	259	GLN
1	A	279	ILE
1	A	287	LEU
1	A	289	THR
1	A	296	SER
1	A	300	LEU

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Mol	Chain	Res	Type
1	A	302	LEU
1	A	306	LEU
1	A	312	ASN
1	A	314	VAL
1	A	315	ILE
1	A	319	ASN
1	A	322	GLU
1	A	323	LYS
1	A	330	ASP
1	A	335	GLN
1	A	342	SER
1	A	344	LYS

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

Mol	Chain	Res	Type
1	A	17	GLN
1	A	148	GLN
1	A	208	GLN
1	A	230	ASN
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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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.