



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:54 AM GMT

PDB ID : 2LIV
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
<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
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

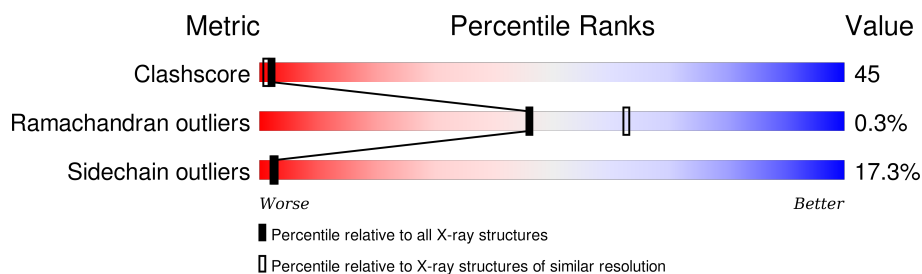
1 Overall quality at a glance

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	102246	3407 (2.40-2.40)
Ramachandran outliers	100387	3351 (2.40-2.40)
Sidechain outliers	100360	3352 (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	344	 38% 41% 19%

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.

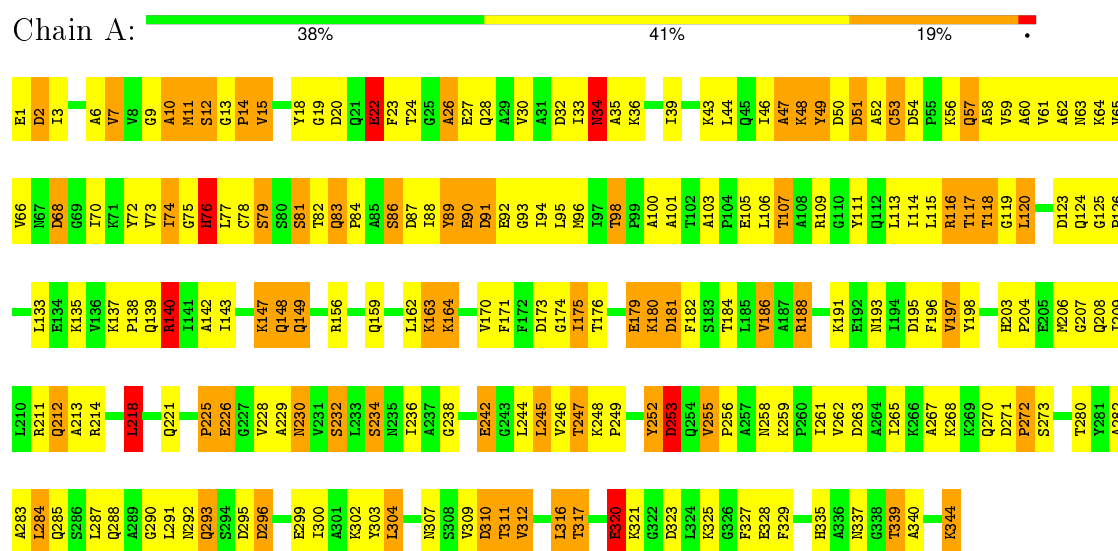
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	121	Total	O	0	0
			121	121		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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



4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section will therefore be 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	1.11	2/2636 (0.1%)	2.19	114/3570 (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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	12	SER	CA-CB	5.89	1.61	1.52
1	A	234	SER	CB-OG	5.02	1.48	1.42

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	ARG	NE-CZ-NH1	19.78	130.19	120.30
1	A	1	GLU	C-N-CA	17.04	164.30	121.70
1	A	75	GLY	C-N-CA	16.32	162.51	121.70
1	A	156	ARG	NE-CZ-NH1	-14.60	113.00	120.30
1	A	156	ARG	NE-CZ-NH2	13.34	126.97	120.30
1	A	188	ARG	NE-CZ-NH2	-13.22	113.69	120.30
1	A	116	ARG	CD-NE-CZ	12.78	141.50	123.60
1	A	140	ARG	NE-CZ-NH1	12.71	126.66	120.30
1	A	22	GLU	CA-CB-CG	12.60	141.13	113.40
1	A	34	ASN	CB-CA-C	12.34	135.09	110.40
1	A	111	TYR	CB-CG-CD2	11.97	128.18	121.00
1	A	87	ASP	CB-CG-OD2	-10.46	108.89	118.30
1	A	195	ASP	CB-CG-OD2	9.81	127.13	118.30
1	A	111	TYR	CB-CG-CD1	-8.90	115.66	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	214	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	116	ARG	NE-CZ-NH2	-8.77	115.92	120.30
1	A	180	LYS	CA-CB-CG	8.59	132.30	113.40
1	A	295	ASP	CB-CG-OD2	-8.55	110.60	118.30
1	A	76	HIS	N-CA-CB	8.24	125.44	110.60
1	A	188	ARG	NE-CZ-NH1	8.18	124.39	120.30
1	A	253	ASP	N-CA-CB	-7.88	96.41	110.60
1	A	91	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	A	214	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	A	75	GLY	CA-C-N	-7.76	100.13	117.20
1	A	163	LYS	N-CA-CB	7.67	124.40	110.60
1	A	156	ARG	CD-NE-CZ	-7.58	112.98	123.60
1	A	18	TYR	CB-CG-CD2	-7.49	116.51	121.00
1	A	226	GLU	OE1-CD-OE2	7.47	132.27	123.30
1	A	179	GLU	CA-CB-CG	7.43	129.76	113.40
1	A	164	LYS	N-CA-C	-7.38	91.08	111.00
1	A	310	ASP	CB-CG-OD2	-7.29	111.74	118.30
1	A	51	ASP	CB-CG-OD1	7.19	124.77	118.30
1	A	91	ASP	CB-CG-OD1	7.13	124.72	118.30
1	A	51	ASP	CB-CG-OD2	-7.00	112.00	118.30
1	A	147	LYS	N-CA-CB	6.97	123.14	110.60
1	A	49	TYR	CB-CG-CD1	-6.84	116.90	121.00
1	A	12	SER	N-CA-C	6.83	129.43	111.00
1	A	139	GLN	CA-CB-CG	6.79	128.35	113.40
1	A	2	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	A	75	GLY	CA-C-O	6.64	132.56	120.60
1	A	2	ASP	CB-CG-OD2	6.62	124.26	118.30
1	A	316	LEU	CA-CB-CG	6.59	130.47	115.30
1	A	242	GLU	CG-CD-OE2	-6.58	105.15	118.30
1	A	179	GLU	N-CA-CB	6.54	122.37	110.60
1	A	156	ARG	CB-CA-C	6.54	123.47	110.40
1	A	156	ARG	CA-CB-CG	6.51	127.72	113.40
1	A	296	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	86	SER	CA-CB-OG	6.47	128.68	111.20
1	A	340	ALA	N-CA-CB	-6.44	101.08	110.10
1	A	147	LYS	CA-CB-CG	6.43	127.54	113.40
1	A	173	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	253	ASP	CB-CG-OD1	6.33	124.00	118.30
1	A	94	ILE	O-C-N	6.26	132.72	122.70
1	A	218	LEU	CB-CA-C	6.25	122.07	110.20
1	A	120	LEU	CA-CB-CG	6.24	129.66	115.30
1	A	12	SER	CB-CA-C	-6.14	98.44	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TYR	CB-CA-C	6.07	122.54	110.40
1	A	252	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	140	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	164	LYS	CA-C-N	5.99	128.18	116.20
1	A	12	SER	N-CA-CB	-5.99	101.52	110.50
1	A	53	CYS	N-CA-CB	5.96	121.33	110.60
1	A	310	ASP	OD1-CG-OD2	5.96	134.62	123.30
1	A	328	GLU	CB-CA-C	-5.91	98.59	110.40
1	A	293	GLN	N-CA-CB	-5.87	100.03	110.60
1	A	107	THR	CA-CB-OG1	-5.87	96.68	109.00
1	A	149	GLN	CA-CB-CG	-5.86	100.51	113.40
1	A	173	ASP	CB-CG-OD2	-5.85	113.03	118.30
1	A	47	ALA	CB-CA-C	5.77	118.76	110.10
1	A	118	THR	CB-CA-C	-5.76	96.04	111.60
1	A	47	ALA	C-N-CA	5.75	136.08	121.70
1	A	293	GLN	CB-CG-CD	-5.73	96.70	111.60
1	A	195	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	A	159	GLN	O-C-N	5.70	131.82	122.70
1	A	89	TYR	CB-CG-CD2	5.65	124.39	121.00
1	A	340	ALA	C-N-CA	5.64	135.80	121.70
1	A	107	THR	CA-CB-CG2	5.63	120.28	112.40
1	A	32	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	140	ARG	CD-NE-CZ	5.62	131.47	123.60
1	A	20	ASP	CB-CG-OD1	5.59	123.33	118.30
1	A	253	ASP	CA-CB-CG	5.57	125.66	113.40
1	A	310	ASP	CB-CG-OD1	-5.56	113.29	118.30
1	A	148	GLN	N-CA-CB	5.56	120.61	110.60
1	A	312	VAL	C-N-CA	5.49	135.43	121.70
1	A	90	GLU	CG-CD-OE1	5.39	129.07	118.30
1	A	117	THR	N-CA-CB	5.38	120.52	110.30
1	A	10	ALA	O-C-N	5.35	131.26	122.70
1	A	198	TYR	N-CA-CB	5.33	120.19	110.60
1	A	312	VAL	N-CA-CB	-5.29	99.86	111.50
1	A	181	ASP	CA-C-O	-5.26	109.06	120.10
1	A	320	GLU	CB-CG-CD	5.25	128.39	114.20
1	A	149	GLN	CB-CA-C	5.24	120.87	110.40
1	A	197	VAL	CA-CB-CG2	5.24	118.75	110.90
1	A	320	GLU	CG-CD-OE1	5.22	128.74	118.30
1	A	267	ALA	CB-CA-C	-5.21	102.28	110.10
1	A	252	TYR	C-N-CA	5.19	134.67	121.70
1	A	74	ILE	N-CA-CB	5.16	122.67	110.80
1	A	179	GLU	CG-CD-OE1	5.16	128.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	TYR	CB-CG-CD2	-5.14	117.91	121.00
1	A	295	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	53	CYS	O-C-N	5.13	130.91	122.70
1	A	90	GLU	N-CA-CB	5.12	119.81	110.60
1	A	50	ASP	C-N-CA	5.12	134.49	121.70
1	A	11	MET	C-N-CA	5.08	134.40	121.70
1	A	164	LYS	CA-C-O	-5.08	109.44	120.10
1	A	180	LYS	CB-CG-CD	5.05	124.73	111.60
1	A	107	THR	N-CA-CB	-5.05	100.71	110.30
1	A	116	ARG	NH1-CZ-NH2	-5.05	113.85	119.40
1	A	238	GLY	C-N-CA	5.04	134.31	121.70
1	A	7	VAL	CB-CA-C	5.04	120.98	111.40
1	A	26	ALA	CB-CA-C	5.04	117.66	110.10
1	A	98	THR	CA-CB-OG1	-5.04	98.42	109.00
1	A	63	ASN	N-CA-CB	-5.02	101.56	110.60
1	A	295	ASP	CB-CA-C	-5.01	100.37	110.40

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	2565	234	2
2	A	121	0	0	43	3
All	All	2710	0	2565	234	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 45.

All (234) 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
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	1.03
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:253:ASP:OD2	1:A:273:SER:HA	1.73	0.88
1:A:193:ASN:O	1:A:193:ASN:OD1	1.92	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:242:GLU:OE1	1:A:335:HIS:HD2	1.66	0.77
1:A:64:LYS:O	1:A:68:ASP:HB2	1.84	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:106:LEU:HB3	1:A:116:ARG:HH22	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ALA:HB2	2:A:408:HOH:O	1.85	0.76
1:A:337:ASN:OD1	1:A:339:THR:HB	1.85	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:290:GLY:O	1:A:293:GLN:HB2	1.89	0.73
1:A:24:THR:HG23	1:A:270:GLN:HE21	1.51	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: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:230:ASN:HD22	1:A:232:SER:HB2	1.56	0.69
1:A:163:LYS:HG3	1:A:163:LYS:O	1.91	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:GLN:NE2	1:A:303:TYR:HD2	1.92	0.64
1:A:317:THR:HG21	1:A:325:LYS:HD2	1.79	0.63
1:A:285:GLN:HB2	1:A:311:THR:HG23	1.80	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: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:84:PRO:HG3	2:A:418:HOH:O	2.02	0.59
1:A:14:PRO:HD2	1:A:15:VAL:N	2.17	0.59
1:A:242:GLU:OE1	1:A:335:HIS:CD2	2.53	0.58
1:A:163:LYS:HB2	2:A:474:HOH:O	2.03	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: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:107:THR:O	1:A:321:LYS:CD	2.54	0.56
1:A:106:LEU:HD23	1:A:116:ARG:NH2	2.19	0.56
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:105:GLU:H	1:A:105:GLU:CD	2.08	0.55
1:A:124:GLN:OE1	1:A:247:THR:CG2	2.55	0.55
1:A:7:VAL:HG22	1:A:74:ILE:HB	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:77:LEU:HB2	2:A:415:HOH:O	2.08	0.53
1:A:79:SER:HB3	1:A:103:ALA:HB2	1.91	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:26:ALA:HA	1:A:284:LEU:HD13	1.91	0.53
1:A:303:TYR:CD1	1:A:303:TYR:C	2.83	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:248:LYS:HD3	2:A:420:HOH:O	2.09	0.52
1:A:72:TYR:CD2	2:A:424:HOH:O	2.54	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:34:ASN:HD22	1:A:34:ASN:C	2.15	0.50
1:A:23:PHE:HD2	1:A:48:LYS:CD	2.18	0.49
1:A:51:ASP:C	1:A:53:CYS:H	2.14	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:47:ALA:CA	2:A:413:HOH:O	2.52	0.49
1:A:30:VAL:HG23	1:A:284:LEU:HD22	1.94	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
1:A:30:VAL:CB	1:A:46:ILE:HD11	2.43	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:284:LEU:HD23	2:A:411:HOH:O	2.14	0.48
1:A:182:PHE:CE2	1:A:208:GLN:CB	2.95	0.48
1:A:93:GLY:HA2	1:A:113:LEU:CD1	2.43	0.48
1:A:226:GLU:C	1:A:228:VAL:H	2.18	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:206:MET:CE	1:A:244:LEU:HD11	2.43	0.47
1:A:209:ILE:O	1:A:213:ALA:HB2	2.15	0.47
1:A:54:ASP:HB3	1:A:57:GLN:HB2	1.96	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:96:MET:CE	1:A:114:ILE:HG23	2.46	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:142:ALA:HB3	1:A:197:VAL:HG22	1.98	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:HD23	1:A:133:LEU:HA	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:249:PRO:CB	2:A:514:HOH:O	2.27	0.43
1:A:123:ASP:HB2	1:A:329:PHE:HE2	1.82	0.43
1:A:49:TYR:HE1	1:A:64:LYS:HG2	1.82	0.43
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:320:GLU:H	1:A:320:GLU:CD	2.20	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:191:LYS:C	1:A:193:ASN:H	2.22	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: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:HB2	1:A:163:LYS:HE2	1.79	0.43
1:A:207:GLY:O	1:A:211:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASP:C	1:A:92:GLU:HG2	2.39	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:30:VAL:HG11	1:A:46:ILE:HD12	2.02	0.42
1:A:107:THR:CG2	1:A:321:LYS:CG	2.70	0.42
1:A:98:THR:HG22	1:A:101:ALA:H	1.85	0.42
1:A:164:LYS:HE3	1:A:164:LYS:HB3	1.54	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:HA	1:A:175:ILE:HD12	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:96:MET:HE1	1:A:114:ILE:HG23	2.01	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:246:VAL:HG11	2:A:420:HOH:O	2.20	0.41
1:A:262:VAL:O	1:A:263:ASP:C	2.58	0.41
1:A:57:GLN:O	1:A:60:ALA:HB3	2.20	0.41
1:A:113:LEU:C	1:A:114:ILE:HD13	2.41	0.41
1:A:206:MET:HE1	1:A:244:LEU:CD1	2.51	0.40
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%)	46 63

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%)	220 (83%)	46 (17%)	2 2

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	ASP
1	A	11	MET
1	A	14	PRO
1	A	15	VAL
1	A	22	GLU
1	A	34	ASN
1	A	48	LYS
1	A	56	LYS
1	A	57	GLN
1	A	68	ASP

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Mol	Chain	Res	Type
1	A	79	SER
1	A	81	SER
1	A	83	GLN
1	A	90	GLU
1	A	118	THR
1	A	135	LYS
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	230	ASN
1	A	232	SER
1	A	234	SER
1	A	245	LEU
1	A	247	THR
1	A	253	ASP
1	A	255	VAL
1	A	272	PRO
1	A	284	LEU
1	A	288	GLN
1	A	302	LYS
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	339	THR
1	A	344	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	ASN
1	A	63	ASN

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Mol	Chain	Res	Type
1	A	112	GLN
1	A	149	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 [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 [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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates [i](#)

EDS was not executed - this section will therefore be empty.

6.4 Ligands [i](#)

EDS was not executed - this section will therefore be empty.

6.5 Other polymers [i](#)

EDS was not executed - this section will therefore be empty.