



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:22 AM UTC

PDB ID : 5HV6 / pdb_00005hv6
Title : The ATP binding domain of rifampin phosphotransferase from *Listeria monocytogenes*
Authors : Zhang, P.; Qi, X.
Deposited on : 2016-01-28
Resolution : 3.00 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) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

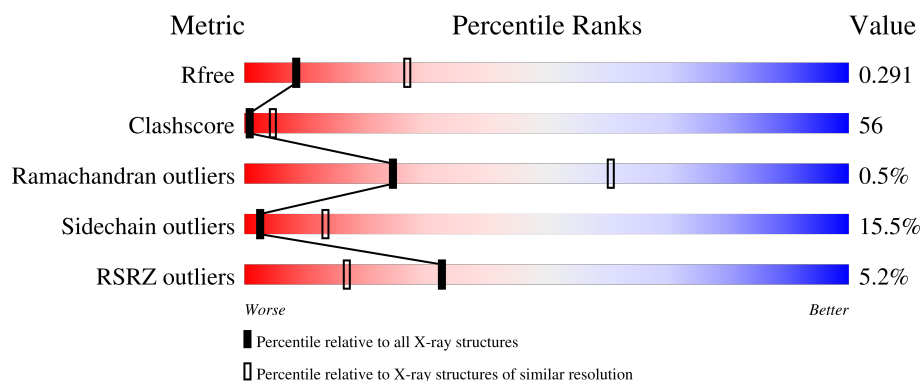
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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.

Mol	Chain	Length	Quality of chain
1	A	327	5% 45% 35% 12% 6%
1	B	327	5% 39% 35% 12% 11%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4678 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 Phosphoenolpyruvate synthase.

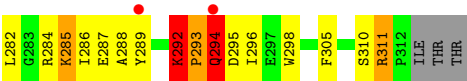
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	308	Total	C	N	O	S	0	0	0
			2400	1518	410	462	10			
1	B	291	Total	C	N	O	S	0	0	0
			2277	1442	391	434	10			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP A0A0S2YLC8
A	-10	ARG	-	expression tag	UNP A0A0S2YLC8
A	-9	GLY	-	expression tag	UNP A0A0S2YLC8
A	-8	SER	-	expression tag	UNP A0A0S2YLC8
A	-7	HIS	-	expression tag	UNP A0A0S2YLC8
A	-6	HIS	-	expression tag	UNP A0A0S2YLC8
A	-5	HIS	-	expression tag	UNP A0A0S2YLC8
A	-4	HIS	-	expression tag	UNP A0A0S2YLC8
A	-3	HIS	-	expression tag	UNP A0A0S2YLC8
A	-2	HIS	-	expression tag	UNP A0A0S2YLC8
A	-1	GLY	-	expression tag	UNP A0A0S2YLC8
A	0	SER	-	expression tag	UNP A0A0S2YLC8
B	-11	MET	-	expression tag	UNP A0A0S2YLC8
B	-10	ARG	-	expression tag	UNP A0A0S2YLC8
B	-9	GLY	-	expression tag	UNP A0A0S2YLC8
B	-8	SER	-	expression tag	UNP A0A0S2YLC8
B	-7	HIS	-	expression tag	UNP A0A0S2YLC8
B	-6	HIS	-	expression tag	UNP A0A0S2YLC8
B	-5	HIS	-	expression tag	UNP A0A0S2YLC8
B	-4	HIS	-	expression tag	UNP A0A0S2YLC8
B	-3	HIS	-	expression tag	UNP A0A0S2YLC8
B	-2	HIS	-	expression tag	UNP A0A0S2YLC8
B	-1	GLY	-	expression tag	UNP A0A0S2YLC8
B	0	SER	-	expression tag	UNP A0A0S2YLC8

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	O	0	0
			1	1		



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	85.01Å 86.18Å 100.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.27 – 3.00 29.27 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.9 (29.27-3.00) 84.6 (29.27-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.24 (at 3.00Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.241 , 0.295 0.245 , 0.291	Depositor DCC
R_{free} test set	1326 reflections (8.71%)	wwPDB-VP
Wilson B-factor (Å ²)	48.2	Xtriage
Anisotropy	0.060	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4678	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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	1.32	12/2438 (0.5%)	1.59	52/3295 (1.6%)
1	B	1.27	8/2310 (0.3%)	1.73	37/3116 (1.2%)
All	All	1.30	20/4748 (0.4%)	1.66	89/6411 (1.4%)

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	3
1	B	0	5
All	All	0	8

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	182	ILE	C-O	-11.18	1.11	1.24
1	A	181	VAL	C-O	-8.72	1.14	1.24
1	A	5	VAL	C-O	-6.86	1.17	1.24
1	A	7	LYS	CA-C	-6.63	1.44	1.52
1	A	183	GLN	C-O	-6.41	1.15	1.23
1	B	12	ARG	C-N	6.12	1.41	1.33
1	A	136	THR	CA-C	-6.04	1.45	1.52
1	A	30	SER	CA-C	-5.91	1.44	1.52
1	A	185	MET	CA-C	-5.77	1.45	1.52
1	A	135	ASP	C-O	-5.70	1.16	1.23
1	B	103	THR	CA-C	-5.56	1.45	1.52
1	A	7	LYS	C-O	-5.54	1.17	1.23
1	B	292	LYS	C-N	5.53	1.40	1.33
1	A	6	LEU	C-O	-5.33	1.17	1.23
1	B	137	TYR	C-O	-5.23	1.17	1.24
1	B	149	HIS	CA-C	-5.21	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	293	PRO	N-CD	5.19	1.55	1.47
1	B	25	ASN	CA-C	-5.18	1.46	1.52
1	A	93	PRO	N-CD	5.16	1.54	1.47
1	B	38	PRO	N-CD	5.05	1.54	1.47

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	253	GLU	CA-C-N	26.80	151.32	122.38
1	B	253	GLU	C-N-CA	26.80	151.32	122.38
1	B	253	GLU	CB-CA-C	-24.98	79.07	109.80
1	A	53	ALA	N-CA-C	-20.14	82.95	110.35
1	A	233	GLU	CB-CA-C	-19.38	71.85	110.42
1	A	33	GLU	N-CA-C	18.72	136.55	111.28
1	B	56	ASN	CB-CA-C	-17.60	76.66	110.10
1	A	264	SER	N-CA-C	-17.53	91.21	113.12
1	B	107	VAL	N-CA-C	16.50	126.04	110.53
1	A	73	MET	N-CA-C	13.92	134.33	111.37
1	B	158	PHE	CA-C-N	13.76	141.39	121.02
1	B	158	PHE	C-N-CA	13.76	141.39	121.02
1	B	159	THR	O-C-N	-13.51	105.05	123.01
1	A	54	GLU	N-CA-CB	12.30	131.28	110.49
1	B	252	LYS	CA-C-N	11.93	142.61	121.97
1	B	252	LYS	C-N-CA	11.93	142.61	121.97
1	B	253	GLU	O-C-N	-11.83	108.22	122.89
1	B	56	ASN	N-CA-C	10.59	140.65	111.00
1	B	56	ASN	CA-C-N	10.36	151.47	122.15
1	B	56	ASN	C-N-CA	10.36	151.47	122.15
1	B	15	SER	CB-CA-C	-9.88	91.34	110.10
1	A	69	LYS	CB-CA-C	9.29	130.18	111.78
1	A	73	MET	CB-CA-C	-8.97	95.84	110.74
1	A	136	THR	N-CA-C	-8.92	95.41	109.50
1	A	53	ALA	CB-CA-C	-8.85	93.78	109.62
1	A	31	ASN	N-CA-C	8.77	120.84	111.28
1	B	168	GLN	N-CA-C	8.77	123.54	113.02
1	A	33	GLU	CB-CA-C	-8.72	99.37	112.11
1	A	57	GLU	N-CA-C	-8.53	101.94	111.07
1	B	25	ASN	N-CA-C	-8.31	102.18	111.07
1	A	120	ALA	N-CA-C	8.30	122.21	110.50
1	A	36	HIS	N-CA-C	-8.05	99.68	110.55
1	A	234	ASN	N-CA-C	8.05	125.23	113.40
1	B	33	GLU	N-CA-C	-7.74	96.50	108.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	58	PHE	N-CA-C	7.57	119.17	111.07
1	B	215	LEU	N-CA-C	7.46	121.57	110.52
1	B	55	ASN	N-CA-C	-7.45	99.25	110.28
1	B	169	ASN	N-CA-C	7.43	124.45	114.12
1	A	204	ARG	CA-C-N	-7.08	109.57	122.38
1	A	204	ARG	C-N-CA	-7.08	109.57	122.38
1	A	65	LEU	N-CA-C	6.89	118.44	111.07
1	A	69	LYS	N-CA-C	-6.89	98.17	107.88
1	B	12	ARG	CA-C-N	-6.78	113.31	120.03
1	B	12	ARG	C-N-CA	-6.78	113.31	120.03
1	B	252	LYS	N-CA-C	6.74	118.42	111.14
1	A	233	GLU	CA-C-N	-6.71	113.60	123.93
1	A	233	GLU	C-N-CA	-6.71	113.60	123.93
1	A	19	VAL	N-CA-C	6.63	118.47	112.17
1	A	177	GLN	N-CA-C	-6.60	99.29	109.52
1	B	103	THR	CB-CA-C	-6.60	99.84	110.79
1	A	67	SER	N-CA-C	-6.57	104.27	113.20
1	A	7	LYS	N-CA-C	-6.45	99.79	110.17
1	B	140	ILE	CB-CA-C	-6.42	102.95	110.91
1	B	224	VAL	N-CA-C	-6.30	99.40	108.53
1	A	312	PRO	CA-N-CD	-6.28	103.21	112.00
1	A	283	GLY	N-CA-C	-6.25	106.60	114.16
1	A	203	ASN	CA-C-N	6.16	131.91	121.14
1	A	203	ASN	C-N-CA	6.16	131.91	121.14
1	A	233	GLU	N-CA-C	6.11	123.81	110.80
1	B	294	GLN	N-CA-C	6.11	119.45	110.59
1	A	110	TYR	N-CA-C	-5.99	106.62	112.97
1	B	218	ALA	N-CA-C	-5.91	100.51	109.85
1	B	292	LYS	CA-C-N	-5.85	113.52	120.13
1	B	292	LYS	C-N-CA	-5.85	113.52	120.13
1	A	184	GLN	CA-C-N	-5.66	114.21	122.65
1	A	184	GLN	C-N-CA	-5.66	114.21	122.65
1	A	181	VAL	CB-CA-C	-5.64	103.17	110.84
1	B	285	LYS	N-CA-C	-5.64	105.13	111.28
1	A	120	ALA	CA-C-N	5.61	128.26	120.29
1	A	120	ALA	C-N-CA	5.61	128.26	120.29
1	B	35	VAL	N-CA-C	-5.61	99.47	107.77
1	A	185	MET	CA-C-N	-5.59	114.57	122.34
1	A	185	MET	C-N-CA	-5.59	114.57	122.34
1	A	51	THR	N-CA-C	5.58	117.16	111.14
1	A	92	ILE	CA-C-N	-5.50	114.03	119.92
1	A	92	ILE	C-N-CA	-5.50	114.03	119.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	74	ASP	N-CA-C	-5.50	106.53	113.18
1	B	25	ASN	CB-CA-C	-5.43	102.36	110.88
1	A	204	ARG	N-CA-C	5.33	119.51	112.89
1	A	238	ASN	CB-CA-C	5.29	118.24	109.72
1	A	107	VAL	N-CA-C	5.24	119.74	112.35
1	A	234	ASN	N-CA-CB	5.13	122.08	113.10
1	A	37	VAL	CA-C-N	-5.13	114.29	119.83
1	A	37	VAL	C-N-CA	-5.13	114.29	119.83
1	B	165	TYR	N-CA-C	-5.11	105.71	111.28
1	B	122	ALA	N-CA-C	-5.11	101.14	108.60
1	A	11	ILE	N-CA-C	5.09	116.96	109.63
1	B	12	ARG	N-CA-C	-5.07	103.66	108.22
1	A	93	PRO	CA-N-CD	-5.01	104.99	112.00

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	204	ARG	Mainchain
1	A	205	LYS	Mainchain
1	A	33	GLU	Peptide
1	B	159	THR	Mainchain
1	B	216	GLY	Peptide
1	B	252	LYS	Peptide
1	B	253	GLU	Peptide
1	B	56	ASN	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	2400	0	2423	198	0
1	B	2277	0	2302	338	0
2	A	1	0	0	0	0
All	All	4678	0	4725	525	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 56.

All (525) 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:B:220:VAL:HG21	1:B:223:LEU:CB	1.23	1.66
1:B:110:TYR:CE1	1:B:143:LYS:HB2	1.15	1.65
1:B:110:TYR:CD1	1:B:143:LYS:CB	1.82	1.62
1:A:263:LYS:CA	1:A:266:GLN:HG3	1.16	1.61
1:B:13:PRO:HB3	1:B:14:HIS:CE1	1.09	1.61
1:B:65:LEU:HD21	1:B:79:ILE:CG2	1.29	1.61
1:B:13:PRO:HB2	1:B:14:HIS:CG	1.36	1.60
1:A:263:LYS:HA	1:A:266:GLN:CG	1.24	1.59
1:B:220:VAL:HG11	1:B:223:LEU:CD1	1.30	1.55
1:A:6:LEU:CB	1:A:11:ILE:HD11	1.35	1.54
1:B:13:PRO:CB	1:B:14:HIS:ND1	1.73	1.52
1:B:110:TYR:CD1	1:B:143:LYS:HB3	1.40	1.52
1:B:196:THR:HG21	1:B:287:GLU:CD	1.34	1.52
1:A:6:LEU:HB3	1:A:11:ILE:CD1	1.39	1.47
1:B:249:TYR:CD2	1:B:259:ARG:HD2	1.48	1.46
1:B:13:PRO:CB	1:B:14:HIS:CE1	2.00	1.44
1:B:220:VAL:CG2	1:B:223:LEU:HB2	1.48	1.43
1:B:110:TYR:CE1	1:B:143:LYS:CB	1.90	1.41
1:B:48:TYR:CE1	1:B:52:LEU:HD12	1.56	1.40
1:B:286:ILE:CG2	1:B:294:GLN:OE1	1.67	1.39
1:B:65:LEU:CD2	1:B:79:ILE:HG21	1.54	1.36
1:B:55:ASN:CA	1:B:56:ASN:HB2	1.01	1.36
1:B:13:PRO:HB3	1:B:14:HIS:ND1	1.33	1.33
1:B:13:PRO:CB	1:B:14:HIS:CG	2.06	1.33
1:B:65:LEU:CD2	1:B:79:ILE:CG2	2.06	1.31
1:B:16:GLU:O	1:B:121:THR:CG2	1.77	1.30
1:B:220:VAL:CG1	1:B:223:LEU:CD1	2.08	1.30
1:B:55:ASN:HA	1:B:56:ASN:CB	1.17	1.29
1:B:196:THR:CG2	1:B:287:GLU:CD	2.05	1.27
1:B:22:LYS:HB2	1:B:119:SER:OG	1.16	1.27
1:B:157:LEU:O	1:B:166:ARG:NH1	1.65	1.27
1:A:68:LEU:O	1:A:69:LYS:HG3	1.34	1.24
1:B:286:ILE:HG21	1:B:294:GLN:OE1	1.18	1.22
1:B:220:VAL:HG11	1:B:223:LEU:CG	1.70	1.21
1:A:174:ARG:NH2	1:B:217:GLU:OE1	1.74	1.19
1:B:159:THR:HG22	1:B:162:ALA:N	1.57	1.19
1:B:16:GLU:O	1:B:121:THR:HG21	1.03	1.18
1:B:13:PRO:HB2	1:B:14:HIS:CD2	1.78	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:HG21	1:B:223:LEU:CG	1.73	1.17
1:B:249:TYR:CE2	1:B:259:ARG:HD2	1.79	1.16
1:A:68:LEU:CD1	1:A:167:ILE:HD11	1.74	1.16
1:A:6:LEU:HD22	1:A:11:ILE:CD1	1.77	1.15
1:B:249:TYR:CD2	1:B:259:ARG:CD	2.30	1.15
1:B:220:VAL:CG1	1:B:223:LEU:HD12	1.75	1.15
1:B:16:GLU:N	1:B:24:MET:HE1	1.62	1.14
1:A:6:LEU:CD2	1:A:11:ILE:HD13	1.78	1.13
1:A:68:LEU:HD12	1:A:167:ILE:HD11	1.15	1.13
1:A:294:GLN:OE1	1:A:311:ARG:O	1.67	1.12
1:A:263:LYS:O	1:A:263:LYS:HG2	1.49	1.11
1:B:14:HIS:HA	1:B:15:SER:HB2	1.19	1.11
1:B:16:GLU:CA	1:B:24:MET:HE1	1.81	1.10
1:A:200:ILE:HD12	1:A:201:THR:H	1.14	1.09
1:B:65:LEU:HD23	1:B:79:ILE:HG21	1.26	1.08
1:B:220:VAL:HG11	1:B:223:LEU:HD11	1.20	1.08
1:B:48:TYR:HE1	1:B:52:LEU:CD1	1.66	1.08
1:B:107:VAL:HB	1:B:184:GLN:NE2	1.68	1.07
1:A:198:ASP:OD1	1:A:200:ILE:CD1	2.01	1.07
1:B:196:THR:HG21	1:B:287:GLU:OE2	1.52	1.07
1:B:220:VAL:CG2	1:B:223:LEU:CB	2.18	1.06
1:B:159:THR:CG2	1:B:162:ALA:H	1.66	1.06
1:A:44:THR:HG22	1:A:46:GLU:H	1.20	1.06
1:B:56:ASN:N	1:B:59:THR:OG1	1.87	1.05
1:B:16:GLU:HG2	1:B:24:MET:HE3	1.38	1.05
1:A:65:LEU:O	1:A:68:LEU:HB3	1.54	1.05
1:B:104:LEU:HD23	1:B:110:TYR:CE2	1.91	1.05
1:A:68:LEU:CD1	1:A:167:ILE:CD1	2.34	1.04
1:B:65:LEU:HD21	1:B:79:ILE:HG23	1.10	1.04
1:A:15:SER:O	1:A:19:VAL:HG22	1.58	1.03
1:A:198:ASP:OD1	1:A:200:ILE:HD11	1.55	1.03
1:B:55:ASN:CB	1:B:56:ASN:HB2	1.89	1.03
1:B:110:TYR:HD1	1:B:143:LYS:CA	1.72	1.03
1:A:175:LYS:HA	1:B:220:VAL:CG1	1.89	1.03
1:B:65:LEU:CD1	1:B:83:ILE:HD11	1.88	1.02
1:A:6:LEU:CB	1:A:11:ILE:CD1	2.13	1.02
1:A:313:ILE:HG22	1:A:314:THR:HA	1.41	1.02
1:A:200:ILE:HD12	1:A:201:THR:N	1.74	1.02
1:B:32:ILE:HD11	1:B:289:TYR:CE1	1.94	1.01
1:A:6:LEU:HD13	1:A:11:ILE:HD12	1.43	1.00
1:B:15:SER:C	1:B:24:MET:HE1	1.87	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:TYR:HD1	1:B:143:LYS:CB	1.42	0.99
1:B:249:TYR:HD2	1:B:259:ARG:CD	1.69	0.99
1:A:263:LYS:HA	1:A:266:GLN:CB	1.92	0.99
1:B:22:LYS:CB	1:B:119:SER:OG	2.11	0.98
1:A:175:LYS:HA	1:B:220:VAL:HG12	1.46	0.98
1:B:32:ILE:HD11	1:B:289:TYR:CZ	1.99	0.97
1:B:83:ILE:HG21	1:B:158:PHE:CD2	1.99	0.97
1:B:48:TYR:HE1	1:B:52:LEU:HD12	0.88	0.97
1:B:159:THR:HG22	1:B:162:ALA:H	0.82	0.97
1:B:22:LYS:O	1:B:26:LEU:HB2	1.64	0.97
1:B:16:GLU:HA	1:B:24:MET:HE1	1.44	0.96
1:B:58:PHE:CZ	1:B:62:LEU:HD11	2.01	0.96
1:A:52:LEU:HD13	1:A:87:ILE:HD13	1.43	0.96
1:B:13:PRO:CA	1:B:14:HIS:ND1	2.29	0.95
1:A:32:ILE:HD12	1:A:35:VAL:HG11	1.49	0.95
1:B:22:LYS:HD2	1:B:118:SER:O	1.66	0.95
1:B:110:TYR:CD1	1:B:143:LYS:CA	2.49	0.95
1:A:204:ARG:HG3	1:A:204:ARG:HH11	1.29	0.94
1:B:220:VAL:CB	1:B:223:LEU:HG	1.98	0.94
1:A:6:LEU:CG	1:A:11:ILE:CD1	2.45	0.94
1:B:14:HIS:HA	1:B:15:SER:CB	1.98	0.94
1:A:11:ILE:HG22	1:A:15:SER:OG	1.66	0.93
1:B:81:GLU:O	1:B:85:THR:OG1	1.85	0.93
1:B:13:PRO:HB3	1:B:14:HIS:NE2	1.83	0.93
1:A:6:LEU:CD2	1:A:11:ILE:CD1	2.42	0.92
1:B:196:THR:CG2	1:B:287:GLU:OE1	2.15	0.92
1:B:220:VAL:HG11	1:B:223:LEU:HG	1.51	0.92
1:B:65:LEU:HD11	1:B:83:ILE:CD1	1.99	0.92
1:B:13:PRO:CB	1:B:14:HIS:CD2	2.45	0.91
1:B:196:THR:CG2	1:B:287:GLU:OE2	2.13	0.91
1:B:22:LYS:HB2	1:B:119:SER:HG	1.29	0.91
1:B:65:LEU:HD12	1:B:83:ILE:HD11	1.52	0.91
1:A:252:LYS:HB2	1:A:252:LYS:NZ	1.86	0.90
1:A:68:LEU:O	1:A:69:LYS:CG	2.18	0.90
1:A:6:LEU:HD22	1:A:11:ILE:HD13	0.91	0.90
1:B:65:LEU:CD1	1:B:83:ILE:CD1	2.50	0.90
1:A:86:LEU:O	1:A:90:THR:OG1	1.90	0.90
1:A:263:LYS:N	1:A:266:GLN:HG3	1.87	0.90
1:B:159:THR:HB	1:B:162:ALA:HB3	1.53	0.90
1:B:159:THR:CG2	1:B:162:ALA:N	2.31	0.89
1:B:8:PHE:O	1:B:11:ILE:HG22	1.73	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:ILE:HG22	1:B:294:GLN:OE1	1.72	0.89
1:A:16:GLU:OE2	1:A:123:GLU:HB3	1.71	0.89
1:B:48:TYR:CE2	1:B:177:GLN:HA	2.08	0.88
1:B:58:PHE:CE1	1:B:62:LEU:HD11	2.09	0.88
1:B:220:VAL:CG1	1:B:223:LEU:HG	2.02	0.88
1:B:107:VAL:CG2	1:B:108:GLY:HA2	2.03	0.88
1:A:55:ASN:OD1	1:A:56:ASN:N	2.06	0.87
1:B:159:THR:HB	1:B:162:ALA:CB	2.04	0.87
1:B:220:VAL:CG2	1:B:223:LEU:CG	2.49	0.86
1:B:233:GLU:N	1:B:284:ARG:HH22	1.73	0.86
1:A:272:THR:H	1:A:275:GLN:HE21	1.21	0.86
1:B:23:GLY:O	1:B:27:GLY:N	2.08	0.86
1:B:197:ALA:HB2	1:B:204:ARG:HA	1.56	0.85
1:B:294:GLN:HG2	1:B:296:ILE:HG13	1.58	0.85
1:B:55:ASN:HA	1:B:56:ASN:CG	2.00	0.85
1:A:81:GLU:O	1:A:85:THR:HG23	1.77	0.85
1:B:197:ALA:CB	1:B:204:ARG:HA	2.07	0.85
1:B:220:VAL:HG13	1:B:223:LEU:HD12	1.56	0.85
1:B:107:VAL:HG22	1:B:108:GLY:HA2	1.59	0.84
1:B:233:GLU:H	1:B:284:ARG:HH22	1.24	0.84
1:A:18:LEU:O	1:A:45:THR:HG23	1.76	0.84
1:A:201:THR:O	1:A:202:SER:OG	1.95	0.84
1:A:168:GLN:HE22	1:B:160:GLU:CD	1.86	0.84
1:B:104:LEU:O	1:B:107:VAL:HG22	1.77	0.84
1:B:101:ASP:OD1	1:B:110:TYR:OH	1.96	0.83
1:A:52:LEU:HD13	1:A:87:ILE:CD1	2.07	0.83
1:B:249:TYR:HD2	1:B:259:ARG:HD2	1.18	0.83
1:A:68:LEU:HD11	1:A:167:ILE:CD1	2.08	0.83
1:A:119:SER:HB2	1:A:181:VAL:HG23	1.59	0.83
1:A:11:ILE:CG2	1:A:15:SER:OG	2.27	0.82
1:B:13:PRO:CB	1:B:14:HIS:NE2	2.40	0.82
1:A:101:ASP:O	1:A:105:LEU:HG	1.79	0.82
1:B:16:GLU:HA	1:B:24:MET:CE	2.10	0.81
1:A:79:ILE:O	1:A:83:ILE:HD12	1.81	0.81
1:B:110:TYR:HE1	1:B:143:LYS:CB	1.58	0.81
1:A:263:LYS:CB	1:A:266:GLN:HG3	2.09	0.81
1:B:294:GLN:HG2	1:B:296:ILE:CG1	2.11	0.81
1:A:165:TYR:OH	1:B:161:ARG:HD2	1.81	0.81
1:A:200:ILE:CD1	1:A:201:THR:N	2.45	0.80
1:B:77:ARG:H	1:B:77:ARG:HD2	1.45	0.80
1:A:68:LEU:HG	1:A:167:ILE:HD13	1.64	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:HG22	1:A:314:THR:CA	2.12	0.79
1:B:65:LEU:HD11	1:B:83:ILE:HD11	1.56	0.79
1:B:294:GLN:HG3	1:B:295:ASP:H	1.48	0.79
1:B:33:GLU:HA	1:B:35:VAL:H	1.47	0.79
1:B:107:VAL:HB	1:B:184:GLN:HE21	1.45	0.78
1:B:16:GLU:CA	1:B:24:MET:CE	2.61	0.78
1:B:110:TYR:CD1	1:B:143:LYS:HB2	1.69	0.78
1:B:32:ILE:HG22	1:B:35:VAL:CG1	2.14	0.78
1:A:169:ASN:OD1	1:B:159:THR:HG23	1.83	0.78
1:A:79:ILE:HD12	1:A:79:ILE:H	1.46	0.77
1:B:32:ILE:O	1:B:33:GLU:HG3	1.84	0.77
1:A:6:LEU:CD1	1:A:11:ILE:HD12	2.15	0.77
1:A:55:ASN:O	1:A:59:THR:OG1	2.03	0.77
1:A:135:ASP:OD2	1:A:156:SER:OG	1.99	0.77
1:B:251:LEU:CB	1:B:253:GLU:O	2.33	0.77
1:B:251:LEU:HB3	1:B:253:GLU:O	1.85	0.76
1:B:65:LEU:O	1:B:66:SER:OG	2.03	0.76
1:A:200:ILE:HD13	1:A:201:THR:HB	1.66	0.76
1:B:32:ILE:CD1	1:B:289:TYR:CZ	2.68	0.75
1:B:119:SER:O	1:B:178:LEU:HD12	1.87	0.75
1:A:6:LEU:HD13	1:A:11:ILE:CD1	2.16	0.75
1:B:249:TYR:HD2	1:B:259:ARG:CG	1.99	0.75
1:B:15:SER:HB3	1:B:24:MET:SD	2.27	0.74
1:B:141:ILE:HD12	1:B:141:ILE:O	1.86	0.74
1:B:287:GLU:HG3	1:B:292:LYS:O	1.88	0.74
1:A:100:MET:HE1	1:A:146:LEU:HD11	1.70	0.74
1:A:232:ARG:O	1:A:233:GLU:HB2	1.86	0.73
1:B:55:ASN:CA	1:B:56:ASN:CB	1.95	0.73
1:B:146:LEU:HD12	1:B:146:LEU:O	1.87	0.73
1:B:55:ASN:CB	1:B:56:ASN:CB	2.60	0.72
1:B:104:LEU:HD11	1:B:114:PHE:CZ	2.24	0.72
1:B:233:GLU:H	1:B:284:ARG:NH2	1.87	0.72
1:B:48:TYR:CE1	1:B:52:LEU:CD1	2.49	0.72
1:B:196:THR:HG21	1:B:287:GLU:CG	2.19	0.72
1:B:48:TYR:CD1	1:B:52:LEU:HD12	2.22	0.72
1:B:220:VAL:HG21	1:B:223:LEU:HB2	0.73	0.72
1:B:65:LEU:HD11	1:B:83:ILE:HD12	1.72	0.72
1:A:252:LYS:HB2	1:A:252:LYS:HZ1	1.54	0.72
1:B:11:ILE:C	1:B:12:ARG:HG3	2.15	0.72
1:B:15:SER:O	1:B:24:MET:SD	2.47	0.72
1:A:204:ARG:HG3	1:A:204:ARG:NH1	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:CB	1:B:223:LEU:CG	2.67	0.72
1:B:15:SER:C	1:B:24:MET:CE	2.63	0.71
1:B:14:HIS:CA	1:B:15:SER:HB2	2.10	0.71
1:B:11:ILE:HD11	1:B:19:VAL:HG21	1.73	0.71
1:B:15:SER:O	1:B:24:MET:HE1	1.89	0.71
1:A:68:LEU:C	1:A:68:LEU:HD23	2.15	0.70
1:A:110:TYR:HB3	1:A:142:GLY:HA2	1.73	0.70
1:B:107:VAL:CB	1:B:184:GLN:NE2	2.52	0.70
1:B:15:SER:CB	1:B:24:MET:SD	2.80	0.70
1:B:16:GLU:CG	1:B:24:MET:HE3	2.20	0.70
1:A:16:GLU:HB2	1:A:24:MET:HG3	1.74	0.70
1:B:110:TYR:HD1	1:B:143:LYS:N	1.89	0.70
1:B:79:ILE:O	1:B:82:THR:OG1	2.10	0.69
1:A:263:LYS:CA	1:A:266:GLN:CG	2.11	0.69
1:B:32:ILE:HG22	1:B:35:VAL:HG12	1.74	0.69
1:B:159:THR:O	1:B:163:ILE:HG13	1.93	0.69
1:B:13:PRO:HA	1:B:14:HIS:ND1	2.06	0.69
1:A:168:GLN:NE2	1:B:160:GLU:CD	2.51	0.69
1:B:220:VAL:HB	1:B:223:LEU:HG	1.74	0.68
1:B:44:THR:HG22	1:B:46:GLU:H	1.59	0.68
1:B:104:LEU:CD2	1:B:110:TYR:CE2	2.74	0.68
1:A:68:LEU:HD11	1:A:167:ILE:HG12	1.74	0.68
1:B:122:ALA:O	1:B:123:GLU:HB2	1.93	0.68
1:B:164:ILE:O	1:B:168:GLN:HG2	1.93	0.68
1:A:6:LEU:CD1	1:A:11:ILE:CD1	2.71	0.68
1:A:135:ASP:HB3	1:A:137:TYR:HE1	1.59	0.68
1:A:198:ASP:OD1	1:A:200:ILE:HD12	1.91	0.68
1:B:14:HIS:CA	1:B:15:SER:CB	2.72	0.67
1:A:119:SER:HB3	1:A:179:ALA:O	1.94	0.67
1:B:104:LEU:HD23	1:B:110:TYR:CD2	2.29	0.67
1:A:120:ALA:HB2	1:A:133:GLN:HB3	1.77	0.67
1:B:16:GLU:N	1:B:24:MET:CE	2.50	0.67
1:B:286:ILE:CG2	1:B:294:GLN:CD	2.66	0.66
1:B:282:LEU:O	1:B:286:ILE:HD13	1.96	0.66
1:A:157:LEU:HD11	1:A:178:LEU:HB2	1.77	0.66
1:A:34:GLY:HA2	1:A:35:VAL:HB	1.78	0.65
1:A:123:GLU:N	1:A:123:GLU:OE2	2.28	0.65
1:A:68:LEU:HD11	1:A:167:ILE:CG1	2.26	0.65
1:B:58:PHE:O	1:B:62:LEU:HD12	1.96	0.65
1:A:200:ILE:CD1	1:A:201:THR:HB	2.26	0.65
1:A:263:LYS:HB2	1:A:266:GLN:CD	2.22	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:CG1	1:B:223:LEU:HD11	1.99	0.64
1:A:313:ILE:HA	1:A:314:THR:C	2.23	0.64
1:A:15:SER:HB3	1:A:19:VAL:CG2	2.27	0.64
1:A:198:ASP:CG	1:A:200:ILE:HD11	2.22	0.64
1:A:38:PRO:HB2	1:A:183:GLN:HG2	1.80	0.64
1:A:194:LEU:HD22	1:A:296:ILE:HD12	1.78	0.64
1:B:48:TYR:HE2	1:B:177:GLN:HA	1.58	0.64
1:A:15:SER:HB3	1:A:19:VAL:HG22	1.80	0.63
1:A:168:GLN:HG3	1:B:84:ARG:NH2	2.13	0.63
1:B:15:SER:O	1:B:24:MET:CE	2.45	0.63
1:B:110:TYR:HD1	1:B:143:LYS:HB3	1.05	0.63
1:B:167:ILE:O	1:B:170:GLN:CD	2.42	0.63
1:B:16:GLU:HG2	1:B:24:MET:CE	2.23	0.62
1:B:107:VAL:HG23	1:B:108:GLY:HA2	1.80	0.62
1:B:16:GLU:O	1:B:121:THR:HG22	1.93	0.62
1:B:107:VAL:CB	1:B:184:GLN:HE21	2.11	0.62
1:B:203:ASN:O	1:B:204:ARG:HB2	2.00	0.62
1:A:52:LEU:C	1:A:53:ALA:O	2.28	0.62
1:B:215:LEU:N	1:B:215:LEU:HD12	2.15	0.62
1:A:34:GLY:HA3	1:A:36:HIS:CD2	2.35	0.61
1:A:92:ILE:HD12	1:A:147:LEU:HD23	1.81	0.61
1:B:77:ARG:HG2	1:B:77:ARG:HH11	1.63	0.61
1:B:146:LEU:O	1:B:150:ILE:HG13	2.00	0.61
1:B:220:VAL:CG2	1:B:223:LEU:HG	2.25	0.61
1:B:251:LEU:HB2	1:B:253:GLU:O	2.00	0.61
1:B:27:GLY:O	1:B:30:SER:N	2.33	0.61
1:B:157:LEU:C	1:B:166:ARG:HH12	1.98	0.61
1:B:233:GLU:O	1:B:234:ASN:HB2	2.00	0.61
1:A:135:ASP:HB3	1:A:137:TYR:CE1	2.35	0.61
1:B:19:VAL:HG12	1:B:42:CYS:SG	2.41	0.61
1:B:136:THR:CG2	1:B:217:GLU:HG2	2.31	0.61
1:A:15:SER:O	1:A:19:VAL:CG2	2.43	0.60
1:A:68:LEU:CG	1:A:167:ILE:HD13	2.30	0.60
1:A:272:THR:HG23	1:A:275:GLN:NE2	2.17	0.60
1:B:48:TYR:CD2	1:B:177:GLN:HA	2.35	0.60
1:A:265:GLN:HA	1:A:268:LYS:HB2	1.84	0.60
1:B:65:LEU:HD21	1:B:79:ILE:HG22	1.63	0.60
1:A:165:TYR:OH	1:B:161:ARG:CD	2.47	0.59
1:B:286:ILE:HG22	1:B:294:GLN:CD	2.27	0.59
1:B:11:ILE:O	1:B:12:ARG:HG3	2.02	0.59
1:A:74:ASP:OD1	1:A:77:ARG:NH2	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:ASP:OD1	1:A:110:TYR:OH	2.18	0.59
1:A:314:THR:HG22	1:A:314:THR:O	2.01	0.59
1:A:2:LYS:O	1:A:2:LYS:HD3	2.03	0.59
1:B:58:PHE:CE2	1:B:62:LEU:CD1	2.86	0.58
1:B:194:LEU:CD2	1:B:207:LEU:HD11	2.33	0.58
1:B:294:GLN:HG3	1:B:295:ASP:N	2.16	0.58
1:B:153:CYS:O	1:B:156:SER:HB3	2.04	0.58
1:B:65:LEU:HD12	1:B:83:ILE:CD1	2.23	0.58
1:B:169:ASN:N	1:B:170:GLN:HA	2.19	0.58
1:B:194:LEU:HD21	1:B:207:LEU:HD11	1.86	0.58
1:B:11:ILE:CG2	1:B:27:GLY:HA3	2.34	0.57
1:A:7:LYS:O	1:A:11:ILE:HG12	2.04	0.57
1:B:22:LYS:CB	1:B:119:SER:HG	2.06	0.57
1:A:15:SER:C	1:A:19:VAL:HG22	2.28	0.57
1:A:201:THR:C	1:A:202:SER:HG	1.98	0.57
1:A:52:LEU:CD1	1:A:87:ILE:CD1	2.80	0.57
1:B:58:PHE:CE2	1:B:62:LEU:HD11	2.38	0.57
1:B:210:ASP:OD2	1:B:219:LEU:HD11	2.04	0.57
1:A:2:LYS:CA	1:A:46:GLU:OE1	2.53	0.57
1:B:171:PHE:CD1	1:B:171:PHE:N	2.73	0.57
1:A:265:GLN:HG3	1:A:268:LYS:HD3	1.86	0.56
1:B:20:GLY:HA2	1:B:121:THR:HG23	1.85	0.56
1:A:34:GLY:HA2	1:A:35:VAL:C	2.30	0.56
1:A:262:GLU:O	1:A:263:LYS:HB3	2.05	0.56
1:B:196:THR:HG22	1:B:287:GLU:CD	2.21	0.56
1:B:220:VAL:CG2	1:B:223:LEU:HD12	2.34	0.56
1:B:15:SER:HB2	1:B:24:MET:SD	2.46	0.55
1:B:169:ASN:HB3	1:B:171:PHE:HE1	1.71	0.55
1:B:49:LYS:O	1:B:53:ALA:HB3	2.07	0.55
1:B:51:THR:HG23	1:B:93:PRO:HD3	1.87	0.55
1:A:32:ILE:HD12	1:A:35:VAL:CG1	2.32	0.55
1:A:68:LEU:CG	1:A:167:ILE:CD1	2.84	0.55
1:B:65:LEU:CD2	1:B:79:ILE:HG23	2.01	0.54
1:A:2:LYS:HD3	1:A:2:LYS:C	2.31	0.54
1:B:15:SER:C	1:B:24:MET:SD	2.89	0.54
1:B:58:PHE:CZ	1:B:62:LEU:CD1	2.85	0.54
1:A:18:LEU:HG	1:A:44:THR:HG23	1.89	0.54
1:A:109:GLY:C	1:A:111:GLU:H	2.14	0.54
1:B:20:GLY:HA2	1:B:121:THR:CG2	2.38	0.54
1:B:119:SER:O	1:B:178:LEU:CD1	2.54	0.54
1:B:15:SER:O	1:B:19:VAL:CG2	2.56	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:220:VAL:CG2	1:B:223:LEU:N	2.70	0.54
1:A:204:ARG:NH1	1:A:204:ARG:CG	2.68	0.54
1:A:6:LEU:CB	1:A:11:ILE:HD12	2.30	0.54
1:B:32:ILE:CG2	1:B:35:VAL:CG1	2.85	0.54
1:B:196:THR:HG22	1:B:287:GLU:OE2	2.01	0.54
1:B:294:GLN:HG2	1:B:296:ILE:HG12	1.88	0.54
1:B:159:THR:HB	1:B:162:ALA:HB2	1.85	0.54
1:B:101:ASP:O	1:B:105:LEU:HD13	2.07	0.53
1:B:220:VAL:HG21	1:B:223:LEU:CD1	2.35	0.53
1:B:233:GLU:CA	1:B:284:ARG:HH22	2.20	0.53
1:B:272:THR:O	1:B:276:ILE:HG13	2.08	0.53
1:B:4:TYR:OH	1:B:50:ARG:HG3	2.08	0.53
1:B:136:THR:HG22	1:B:217:GLU:HG2	1.88	0.53
1:B:171:PHE:N	1:B:171:PHE:HD1	2.07	0.53
1:A:35:VAL:HG12	1:A:35:VAL:O	2.07	0.53
1:B:220:VAL:CG2	1:B:223:LEU:CD1	2.86	0.53
1:B:104:LEU:HD23	1:B:110:TYR:HE2	1.63	0.53
1:B:107:VAL:HG23	1:B:108:GLY:CA	2.38	0.53
1:A:66:SER:C	1:A:68:LEU:H	2.17	0.53
1:B:197:ALA:HB1	1:B:204:ARG:HA	1.90	0.53
1:B:293:PRO:O	1:B:293:PRO:HG2	2.08	0.52
1:B:233:GLU:OE1	1:B:233:GLU:HA	2.10	0.52
1:A:174:ARG:O	1:B:220:VAL:CG1	2.44	0.52
1:B:107:VAL:CG2	1:B:108:GLY:CA	2.85	0.52
1:A:239:LYS:NZ	1:A:273:ASP:OD1	2.30	0.52
1:B:251:LEU:HD21	1:B:257:GLU:HB3	1.92	0.52
1:A:68:LEU:HG	1:A:167:ILE:CD1	2.37	0.52
1:B:136:THR:O	1:B:217:GLU:OE2	2.28	0.52
1:B:194:LEU:HD23	1:B:195:PHE:N	2.25	0.52
1:B:59:THR:O	1:B:63:GLN:HB2	2.10	0.52
1:B:104:LEU:CD2	1:B:110:TYR:CD2	2.93	0.52
1:B:159:THR:HG22	1:B:161:ARG:N	2.24	0.52
1:B:220:VAL:HG21	1:B:223:LEU:CA	2.24	0.52
1:B:151:SER:O	1:B:152:MET:C	2.53	0.51
1:A:263:LYS:O	1:A:263:LYS:CG	2.33	0.51
1:B:13:PRO:HA	1:B:15:SER:HB2	1.91	0.51
1:B:295:ASP:HB3	1:B:311:ARG:O	2.10	0.51
1:A:172:ASP:OD1	1:A:175:LYS:HD2	2.10	0.51
1:A:263:LYS:CB	1:A:266:GLN:CG	2.81	0.51
1:B:26:LEU:HD11	1:B:183:GLN:HE21	1.75	0.51
1:A:313:ILE:HG22	1:A:314:THR:C	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ALA:HB3	1:B:184:GLN:OE1	2.10	0.51
1:B:77:ARG:HG2	1:B:77:ARG:NH1	2.26	0.51
1:B:193:ILE:HG22	1:B:194:LEU:N	2.26	0.51
1:A:68:LEU:CD1	1:A:167:ILE:HD13	2.31	0.51
1:B:49:LYS:O	1:B:53:ALA:CB	2.58	0.51
1:B:78:GLU:O	1:B:81:GLU:HB3	2.11	0.51
1:B:292:LYS:HG2	1:B:293:PRO:HD2	1.93	0.50
1:A:300:LEU:HD13	1:A:305:PHE:CZ	2.46	0.50
1:B:107:VAL:O	1:B:184:GLN:NE2	2.44	0.50
1:A:51:THR:HG22	1:A:52:LEU:HD23	1.93	0.50
1:A:112:MET:HB2	1:A:184:GLN:NE2	2.26	0.50
1:A:252:LYS:HB2	1:A:252:LYS:HZ2	1.72	0.50
1:B:2:LYS:CB	1:B:46:GLU:HG3	2.42	0.50
1:B:163:ILE:O	1:B:166:ARG:HB3	2.11	0.50
1:B:196:THR:HG23	1:B:287:GLU:OE1	2.06	0.50
1:B:31:ASN:O	1:B:32:ILE:HD12	2.11	0.50
1:A:2:LYS:C	1:A:2:LYS:CD	2.85	0.49
1:B:32:ILE:CD1	1:B:289:TYR:CE2	2.95	0.49
1:A:191:SER:HB3	1:A:216:GLY:HA2	1.93	0.49
1:A:313:ILE:CA	1:A:314:THR:C	2.85	0.49
1:B:286:ILE:N	1:B:286:ILE:CD1	2.75	0.49
1:A:34:GLY:CA	1:A:35:VAL:C	2.85	0.49
1:A:263:LYS:CB	1:A:266:GLN:CD	2.86	0.49
1:A:2:LYS:HA	1:A:46:GLU:OE1	2.12	0.49
1:B:32:ILE:HG22	1:B:33:GLU:N	2.27	0.49
1:A:148:GLN:O	1:A:152:MET:HG3	2.13	0.49
1:B:13:PRO:CA	1:B:14:HIS:CG	2.86	0.49
1:A:2:LYS:HB3	1:A:3:PRO:HD3	1.94	0.49
1:B:36:HIS:C	1:B:37:VAL:HG23	2.38	0.49
1:A:165:TYR:OH	1:B:161:ARG:NH1	2.46	0.49
1:A:52:LEU:CD1	1:A:87:ILE:HD13	2.29	0.48
1:A:253:GLU:HG2	1:A:254:GLY:N	2.27	0.48
1:A:2:LYS:C	1:A:46:GLU:OE1	2.55	0.48
1:A:196:THR:HG22	1:A:207:LEU:HD12	1.94	0.48
1:B:220:VAL:HG23	1:B:223:LEU:N	2.27	0.48
1:A:198:ASP:HB3	1:A:201:THR:HG22	1.95	0.48
1:B:122:ALA:HB3	1:B:123:GLU:OE1	2.12	0.48
1:A:312:PRO:HD2	1:A:312:PRO:O	2.14	0.48
1:B:172:ASP:OD1	1:B:173:HIS:N	2.47	0.48
1:B:58:PHE:CD2	1:B:62:LEU:HD13	2.49	0.48
1:B:286:ILE:N	1:B:286:ILE:HD12	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:ARG:HG2	1:A:160:GLU:OE1	2.14	0.48
1:B:150:ILE:O	1:B:153:CYS:HB2	2.13	0.48
1:B:294:GLN:CD	1:B:310:SER:OG	2.57	0.48
1:B:173:HIS:O	1:B:176:VAL:HG12	2.14	0.48
1:A:281:LYS:O	1:A:285:LYS:N	2.41	0.48
1:B:285:LYS:O	1:B:288:ALA:HB3	2.14	0.47
1:A:35:VAL:H	1:A:282:LEU:HD11	1.79	0.47
1:A:68:LEU:HG	1:A:69:LYS:N	2.30	0.47
1:B:107:VAL:C	1:B:184:GLN:NE2	2.72	0.47
1:B:193:ILE:HG22	1:B:194:LEU:H	1.80	0.47
1:A:66:SER:C	1:A:68:LEU:N	2.73	0.47
1:A:272:THR:O	1:A:275:GLN:N	2.48	0.47
1:B:2:LYS:HB3	1:B:46:GLU:HG3	1.97	0.47
1:A:76:ILE:O	1:A:80:SER:HB3	2.15	0.47
1:B:15:SER:O	1:B:19:VAL:HG22	2.15	0.47
1:B:192:GLY:HA3	1:B:210:ASP:O	2.15	0.47
1:B:32:ILE:CG2	1:B:33:GLU:N	2.78	0.47
1:A:100:MET:HE2	1:A:100:MET:HB3	1.60	0.47
1:B:110:TYR:HE1	1:B:143:LYS:HB2	0.69	0.47
1:B:230:THR:O	1:B:237:THR:HB	2.16	0.46
1:B:58:PHE:CE2	1:B:62:LEU:HD13	2.49	0.46
1:B:83:ILE:CD1	1:B:158:PHE:HD2	2.29	0.46
1:B:176:VAL:HG22	1:B:177:GLN:N	2.29	0.46
1:B:169:ASN:H	1:B:170:GLN:HA	1.80	0.46
1:B:178:LEU:HD12	1:B:179:ALA:H	1.81	0.46
1:B:185:MET:HE2	1:B:185:MET:HB3	1.88	0.46
1:B:45:THR:O	1:B:48:TYR:HB3	2.15	0.46
1:A:68:LEU:C	1:A:69:LYS:HG3	2.28	0.46
1:A:263:LYS:HA	1:A:266:GLN:HB2	1.90	0.46
1:B:194:LEU:HD12	1:B:279:LEU:HG	1.98	0.46
1:A:11:ILE:CG2	1:A:15:SER:CB	2.93	0.45
1:A:32:ILE:H	1:A:32:ILE:HG13	1.64	0.45
1:B:22:LYS:O	1:B:26:LEU:CB	2.51	0.45
1:B:32:ILE:HD13	1:B:289:TYR:CE2	2.52	0.45
1:A:289:TYR:C	1:A:289:TYR:CD2	2.94	0.45
1:B:83:ILE:HD13	1:B:158:PHE:CD2	2.51	0.45
1:B:294:GLN:CG	1:B:295:ASP:N	2.79	0.45
1:B:79:ILE:HD12	1:B:79:ILE:HA	1.66	0.45
1:A:93:PRO:HD2	1:A:96:ILE:CD1	2.47	0.45
1:A:119:SER:CB	1:A:181:VAL:HG23	2.39	0.45
1:A:232:ARG:O	1:A:233:GLU:CB	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:THR:HG22	1:A:179:ALA:HB2	1.98	0.44
1:A:112:MET:HE3	1:A:184:GLN:NE2	2.32	0.44
1:B:137:TYR:N	1:B:137:TYR:CD2	2.85	0.44
1:A:15:SER:HB3	1:A:19:VAL:HG21	1.98	0.44
1:A:191:SER:OG	1:A:214:GLY:O	2.22	0.44
1:B:279:LEU:HB2	1:B:305:PHE:CE1	2.51	0.44
1:A:11:ILE:HG22	1:A:15:SER:CB	2.45	0.44
1:A:273:ASP:HA	1:A:276:ILE:HD12	1.98	0.44
1:B:114:PHE:O	1:B:140:ILE:HG12	2.17	0.44
1:A:77:ARG:HG2	1:A:160:GLU:CD	2.42	0.44
1:A:104:LEU:HD12	1:A:104:LEU:HA	1.72	0.44
1:A:123:GLU:C	1:A:123:GLU:CD	2.85	0.44
1:A:166:ARG:HG2	1:A:171:PHE:HB2	2.00	0.44
1:B:44:THR:HG22	1:B:45:THR:N	2.32	0.44
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.76	0.43
1:A:68:LEU:CG	1:A:69:LYS:N	2.80	0.43
1:B:110:TYR:HD2	1:B:110:TYR:N	2.16	0.43
1:A:34:GLY:HA2	1:A:35:VAL:CB	2.42	0.43
1:A:204:ARG:O	1:A:284:ARG:NH2	2.51	0.43
1:B:58:PHE:CD1	1:B:62:LEU:HD11	2.52	0.43
1:B:58:PHE:CD2	1:B:62:LEU:CD1	3.00	0.43
1:B:110:TYR:CD1	1:B:143:LYS:HA	2.47	0.43
1:A:160:GLU:O	1:A:164:ILE:HG12	2.19	0.43
1:A:107:VAL:HG23	1:A:108:GLY:HA2	2.00	0.43
1:B:151:SER:O	1:B:154:TRP:N	2.52	0.43
1:A:292:LYS:HA	1:A:292:LYS:HD3	1.84	0.43
1:B:19:VAL:CG1	1:B:42:CYS:SG	3.07	0.43
1:B:33:GLU:HA	1:B:35:VAL:N	2.24	0.43
1:B:284:ARG:O	1:B:285:LYS:C	2.62	0.43
1:A:112:MET:HB2	1:A:184:GLN:HE21	1.84	0.43
1:B:82:THR:HA	1:B:85:THR:OG1	2.19	0.43
1:B:110:TYR:CE1	1:B:143:LYS:CD	3.02	0.43
1:A:199:PRO:HD2	1:A:200:ILE:H	1.84	0.42
1:B:110:TYR:CD2	1:B:110:TYR:N	2.86	0.42
1:A:51:THR:C	1:A:52:LEU:HD23	2.44	0.42
1:B:193:ILE:O	1:B:298:TRP:NE1	2.46	0.42
1:B:249:TYR:CD2	1:B:259:ARG:NE	2.84	0.42
1:A:119:SER:CB	1:A:179:ALA:O	2.65	0.42
1:B:36:HIS:O	1:B:37:VAL:HG23	2.20	0.42
1:B:24:MET:O	1:B:25:ASN:C	2.59	0.42
1:B:168:GLN:HE21	1:B:168:GLN:HB3	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:TYR:O	1:A:44:THR:N	2.40	0.42
1:A:129:SER:OG	1:A:130:PHE:N	2.49	0.42
1:B:31:ASN:O	1:B:32:ILE:HG13	2.20	0.41
1:B:295:ASP:HB3	1:B:311:ARG:HG3	2.02	0.41
1:B:14:HIS:CE1	1:B:24:MET:HG2	2.55	0.41
1:B:79:ILE:HA	1:B:82:THR:OG1	2.19	0.41
1:A:93:PRO:HD2	1:A:96:ILE:HD12	2.02	0.41
1:B:2:LYS:HB2	1:B:46:GLU:HG3	2.03	0.41
1:B:220:VAL:HG13	1:B:223:LEU:CD1	2.21	0.41
1:A:198:ASP:OD1	1:A:200:ILE:CG1	2.66	0.41
1:B:157:LEU:HB2	1:B:158:PHE:HD1	1.85	0.41
1:B:168:GLN:HG2	1:B:168:GLN:H	1.73	0.41
1:B:203:ASN:O	1:B:204:ARG:CB	2.68	0.41
1:A:198:ASP:CG	1:A:200:ILE:CD1	2.87	0.41
1:A:197:ALA:O	1:A:198:ASP:C	2.63	0.41
1:B:31:ASN:O	1:B:32:ILE:CG1	2.69	0.41
1:B:109:GLY:C	1:B:111:GLU:H	2.27	0.41
1:B:210:ASP:HA	1:B:227:ASP:O	2.21	0.41
1:B:233:GLU:N	1:B:284:ARG:NH2	2.51	0.41
1:A:67:SER:O	1:A:67:SER:OG	2.39	0.41
1:B:11:ILE:HG21	1:B:27:GLY:HA3	2.02	0.41
1:B:13:PRO:HB2	1:B:14:HIS:CB	2.28	0.41
1:B:101:ASP:O	1:B:105:LEU:CD1	2.69	0.41
1:A:93:PRO:HB2	1:A:96:ILE:HG13	2.02	0.41
1:A:272:THR:HG23	1:A:275:GLN:HE21	1.85	0.41
1:B:284:ARG:O	1:B:287:GLU:N	2.54	0.40
1:B:37:VAL:HG13	1:B:38:PRO:HD2	2.03	0.40
1:A:123:GLU:OE2	1:A:123:GLU:CA	2.70	0.40
1:A:313:ILE:H	1:A:313:ILE:HG13	1.79	0.40
1:B:83:ILE:HD12	1:B:158:PHE:HD2	1.86	0.40
1:A:198:ASP:CG	1:A:201:THR:HG22	2.46	0.40
1:B:36:HIS:O	1:B:37:VAL:CG2	2.69	0.40
1:B:92:ILE:HA	1:B:93:PRO:HD3	1.85	0.40
1:B:141:ILE:H	1:B:141:ILE:HG13	1.69	0.40
1:A:187:SER:HA	1:A:188:PRO:HD3	1.77	0.40
1:A:196:THR:HG22	1:A:207:LEU:CD1	2.50	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	304/327 (93%)	277 (91%)	26 (9%)	1 (0%)	36	70
1	B	281/327 (86%)	259 (92%)	20 (7%)	2 (1%)	18	53
All	All	585/654 (89%)	536 (92%)	46 (8%)	3 (0%)	24	60

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	94	SER
1	A	312	PRO
1	B	188	PRO

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	262/278 (94%)	222 (85%)	40 (15%)	3	14
1	B	247/278 (89%)	208 (84%)	39 (16%)	2	13
All	All	509/556 (92%)	430 (84%)	79 (16%)	2	13

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LYS
1	A	7	LYS
1	A	9	GLN

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Mol	Chain	Res	Type
1	A	10	GLU
1	A	11	ILE
1	A	30	SER
1	A	32	ILE
1	A	33	GLU
1	A	38	PRO
1	A	44	THR
1	A	45	THR
1	A	50	ARG
1	A	54	GLU
1	A	59	THR
1	A	62	LEU
1	A	65	LEU
1	A	68	LEU
1	A	71	SER
1	A	79	ILE
1	A	90	THR
1	A	93	PRO
1	A	94	SER
1	A	96	ILE
1	A	112	MET
1	A	123	GLU
1	A	141	ILE
1	A	178	LEU
1	A	183	GLN
1	A	200	ILE
1	A	201	THR
1	A	224	VAL
1	A	235	THR
1	A	245	LYS
1	A	250	SER
1	A	252	LYS
1	A	256	THR
1	A	263	LYS
1	A	289	TYR
1	A	292	LYS
1	A	313	ILE
1	B	10	GLU
1	B	24	MET
1	B	26	LEU
1	B	30	SER
1	B	32	ILE

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Mol	Chain	Res	Type
1	B	35	VAL
1	B	50	ARG
1	B	59	THR
1	B	62	LEU
1	B	79	ILE
1	B	82	THR
1	B	85	THR
1	B	88	GLN
1	B	89	HIS
1	B	103	THR
1	B	105	LEU
1	B	107	VAL
1	B	112	MET
1	B	119	SER
1	B	141	ILE
1	B	143	LYS
1	B	159	THR
1	B	161	ARG
1	B	164	ILE
1	B	167	ILE
1	B	168	GLN
1	B	170	GLN
1	B	171	PHE
1	B	174	ARG
1	B	220	VAL
1	B	224	VAL
1	B	233	GLU
1	B	237	THR
1	B	265	GLN
1	B	268	LYS
1	B	271	LEU
1	B	292	LYS
1	B	294	GLN
1	B	311	ARG

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	36	HIS
1	A	168	GLN
1	A	170	GLN
1	A	183	GLN

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Mol	Chain	Res	Type
1	A	184	GLN
1	A	234	ASN
1	A	275	GLN
1	B	36	HIS
1	B	56	ASN
1	B	139	ASN
1	B	168	GLN
1	B	184	GLN

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	308/327 (94%)	0.17	16 (5%) 33 17	8, 31, 80, 110	0
1	B	291/327 (88%)	0.39	15 (5%) 33 17	9, 48, 92, 113	0
All	All	599/654 (91%)	0.28	31 (5%) 33 17	8, 40, 89, 113	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	ALA	5.4
1	A	15	SER	4.6
1	B	294	GLN	4.3
1	A	129	SER	4.2
1	A	11	ILE	3.9
1	A	31	ASN	3.6
1	A	10	GLU	3.6
1	B	289	TYR	3.5
1	B	14	HIS	3.3
1	A	263	LYS	3.1
1	B	233	GLU	3.0
1	A	33	GLU	2.9
1	A	14	HIS	2.8
1	B	174	ARG	2.8
1	A	130	PHE	2.7
1	B	122	ALA	2.6
1	A	9	GLN	2.5
1	B	234	ASN	2.5
1	B	203	ASN	2.4
1	B	123	GLU	2.3
1	B	223	LEU	2.3
1	A	72	ASP	2.3
1	A	179	ALA	2.2
1	A	161	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	205	LYS	2.2
1	A	67	SER	2.2
1	A	34	GLY	2.1
1	B	172	ASP	2.1
1	B	16	GLU	2.1
1	B	9	GLN	2.0
1	B	254	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.