Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 12:46 AM GMT

PDB ID	:	2BLS
Title	:	AMPC BETA-LACTAMASE FROM ESCHERICHIA COLI
Authors	:	Usher, K.C.; Wery, J.-P.; Blaszczak, L.C.; Remington, S.J.
Deposited on	:	1998-06-03
Resolution	:	2.00 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

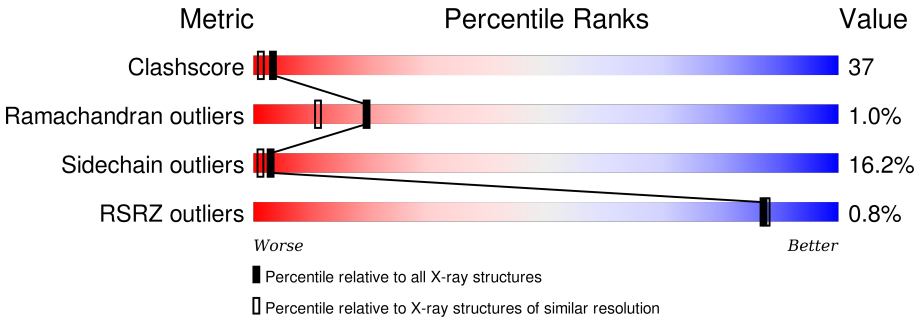
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 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 <=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	358	% 39% 44% 14%
1	B	358	% 38% 46% 14%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5662 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 AMPC BETA-LACTAMASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	4	0	0
			2790	1799	474	511	6			
1	B	357	Total	C	N	O	S	4	0	0
			2790	1799	474	511	6			

- Molecule 2 is water.

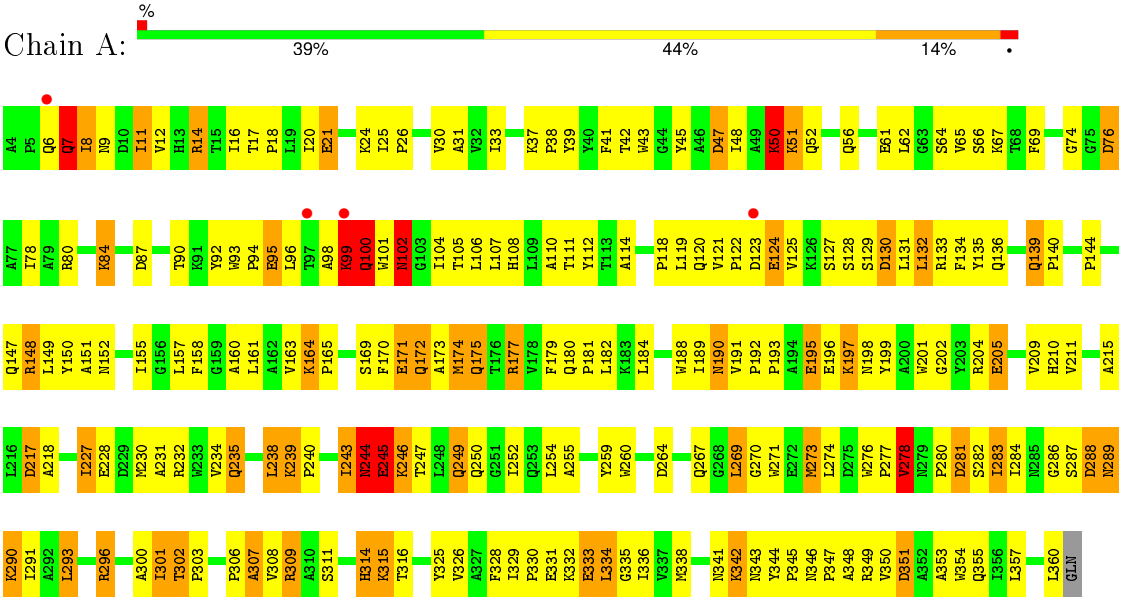
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	40	Total	O	0	0
			40	40		
2	B	42	Total	O	0	0
			42	42		

3 Residue-property plots (i)

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.

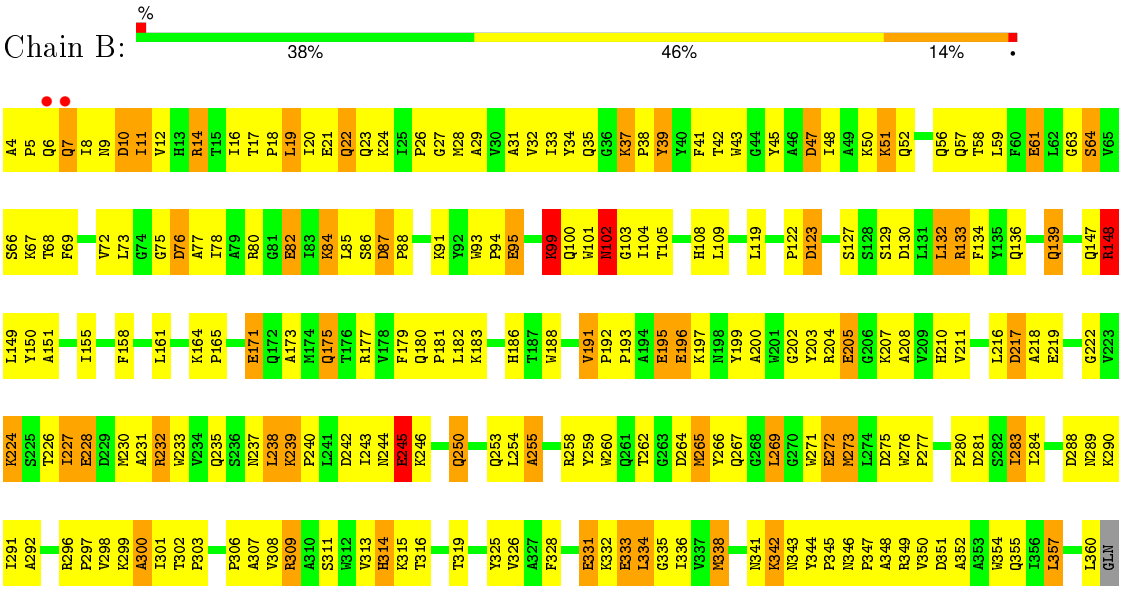
- Molecule 1: AMPC BETA-LACTAMASE

Chain A:



- Molecule 1: AMPC BETA-LACTAMASE

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	117.73Å 77.35Å 97.59Å 90.00° 116.45° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 62.36 – 1.90	Depositor EDS
% Data completeness (in resolution range)	77.4 (25.00-2.00) 69.4 (62.36-1.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.05 (at 1.90Å)	Xtriage
Refinement program	TNT V. 5-F	Depositor
R, R_{free}	0.216 , (Not available) 0.209 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.292	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 101.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 43486 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5662	wwPDB-VP
Average B, all atoms (Å^2)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.34% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	1.18	10/2870 (0.3%)	1.53	33/3921 (0.8%)
1	B	1.17	16/2870 (0.6%)	1.53	34/3921 (0.9%)
All	All	1.18	26/5740 (0.5%)	1.53	67/7842 (0.9%)

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	195	GLU	CD-OE2	8.61	1.35	1.25
1	A	21	GLU	CD-OE1	8.22	1.34	1.25
1	A	171	GLU	CD-OE2	7.88	1.34	1.25
1	B	61	GLU	CD-OE2	7.44	1.33	1.25
1	B	272	GLU	CD-OE2	-7.33	1.17	1.25
1	A	196	GLU	CD-OE2	7.12	1.33	1.25
1	B	195	GLU	CD-OE2	7.11	1.33	1.25
1	A	333	GLU	CD-OE2	7.01	1.33	1.25
1	B	219	GLU	CD-OE2	6.85	1.33	1.25
1	B	171	GLU	CD-OE2	6.48	1.32	1.25
1	A	205	GLU	CD-OE1	6.43	1.32	1.25
1	A	95	GLU	CD-OE2	6.31	1.32	1.25
1	B	196	GLU	CD-OE2	6.21	1.32	1.25
1	A	245	GLU	CD-OE2	6.15	1.32	1.25
1	B	21	GLU	CD-OE1	5.97	1.32	1.25
1	B	331	GLU	CD-OE1	5.96	1.32	1.25
1	A	331	GLU	CD-OE1	5.95	1.32	1.25
1	B	205	GLU	CD-OE1	5.83	1.32	1.25
1	B	245	GLU	CD-OE2	5.79	1.32	1.25
1	B	82	GLU	CD-OE2	5.74	1.31	1.25
1	B	82	GLU	CD-OE1	-5.60	1.19	1.25
1	B	228	GLU	CD-OE2	5.44	1.31	1.25
1	B	195	GLU	CD-OE1	-5.38	1.19	1.25
1	B	333	GLU	CD-OE1	5.30	1.31	1.25
1	A	50	LYS	CD-CE	5.26	1.64	1.51
1	B	87	ASP	CG-OD1	5.18	1.37	1.25

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	99	LYS	CB-CA-C	-9.40	91.60	110.40
1	A	123	ASP	CB-CG-OD2	-8.61	110.56	118.30
1	B	82	GLU	N-CA-CB	-8.53	95.25	110.60
1	B	123	ASP	CB-CG-OD2	-8.53	110.63	118.30
1	B	76	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	A	76	ASP	CB-CG-OD1	7.59	125.13	118.30
1	A	147	GLN	N-CA-CB	-7.38	97.32	110.60
1	B	281	ASP	CB-CG-OD1	-7.22	111.80	118.30
1	B	10	ASP	CB-CG-OD1	-7.20	111.82	118.30
1	A	148	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	A	130	ASP	CB-CG-OD2	6.92	124.53	118.30
1	B	232	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	296	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	B	132	LEU	CB-CG-CD2	6.85	122.64	111.00
1	B	264	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	B	264	ASP	CB-CG-OD1	6.77	124.39	118.30
1	A	288	ASP	CB-CG-OD1	6.76	124.38	118.30
1	B	123	ASP	CB-CG-OD1	6.72	124.34	118.30
1	B	338	MET	CG-SD-CE	-6.68	89.52	100.20
1	A	123	ASP	CB-CG-OD1	6.63	124.27	118.30
1	B	217	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	A	111	THR	CA-CB-CG2	-6.57	103.21	112.40
1	B	272	GLU	N-CA-CB	6.56	122.41	110.60
1	A	130	ASP	CB-CG-OD1	-6.46	112.48	118.30
1	A	174	MET	CG-SD-CE	-6.45	89.87	100.20
1	A	351	ASP	CB-CG-OD1	-6.43	112.52	118.30
1	A	177	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	275	ASP	CB-CG-OD1	-6.28	112.65	118.30
1	A	47	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	A	278	VAL	CB-CA-C	-6.26	99.51	111.40
1	A	296	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	296	ARG	NE-CZ-NH1	6.25	123.43	120.30
1	B	351	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	B	242	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	B	255	ALA	CB-CA-C	6.20	119.39	110.10
1	A	281	ASP	CB-CG-OD1	-6.19	112.73	118.30
1	B	58	THR	CA-CB-CG2	-6.01	103.98	112.40
1	A	14	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	B	133	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	A	43	TRP	CB-CA-C	-5.88	98.64	110.40
1	B	281	ASP	CB-CG-OD2	5.88	123.59	118.30
1	B	275	ASP	CB-CG-OD2	5.85	123.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	300	ALA	CB-CA-C	5.82	118.83	110.10
1	A	217	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	144	PRO	N-CA-CB	5.80	110.26	103.30
1	A	76	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	351	ASP	CB-CG-OD2	5.79	123.51	118.30
1	A	50	LYS	CD-CE-NZ	5.77	124.97	111.70
1	A	47	ASP	CB-CG-OD1	5.76	123.48	118.30
1	B	39	TYR	CB-CG-CD2	-5.74	117.56	121.00
1	A	302	THR	N-CA-CB	-5.71	99.44	110.30
1	A	264	ASP	CB-CG-OD2	-5.68	113.19	118.30
1	B	296	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	B	99	LYS	CB-CA-C	-5.52	99.35	110.40
1	A	122	PRO	N-CA-CB	5.50	109.90	103.30
1	B	258	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	A	14	ARG	CB-CA-C	-5.34	99.73	110.40
1	B	242	ASP	CB-CG-OD2	5.33	123.10	118.30
1	A	244	ASN	CA-CB-CG	-5.33	101.66	113.40
1	A	132	LEU	CB-CG-CD2	5.33	120.05	111.00
1	A	351	ASP	CB-CG-OD2	5.25	123.03	118.30
1	B	47	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	100	GLN	CG-CD-OE1	-5.16	111.28	121.60
1	B	47	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	B	341	ASN	N-CA-CB	5.14	119.86	110.60
1	B	148	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	B	331	GLU	CB-CA-C	5.10	120.60	110.40

There are no chirality outliers.

There are no planarity outliers.

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	2790	0	2770	216	0
1	B	2790	0	2770	202	0
2	A	40	0	0	1	0
2	B	42	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5662	0	5540	412	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 37.

All (412) 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:26:PRO:HB3	1:A:48:ILE:HD11	1.37	1.04
1:A:244:ASN:ND2	1:A:244:ASN:H	1.54	1.01
1:B:8:ILE:HA	1:B:11:ILE:HD11	1.46	0.95
1:A:67:LYS:HD3	1:A:155:ILE:HG21	1.49	0.92
1:B:67:LYS:HD3	1:B:155:ILE:HG21	1.51	0.91
1:B:8:ILE:HD12	1:B:41:PHE:HZ	1.38	0.88
1:A:98:ALA:HB3	1:A:101:TRP:HD1	1.39	0.87
1:A:334:LEU:HD12	1:A:335:GLY:N	1.88	0.87
1:A:260:TRP:CZ3	1:A:300:ALA:HB2	2.13	0.84
1:A:338:MET:HE1	1:A:353:ALA:HB2	1.60	0.84
1:B:17:THR:HB	1:B:18:PRO:HD3	1.61	0.83
1:B:11:ILE:H	1:B:11:ILE:HD13	1.43	0.82
1:A:119:LEU:HA	1:A:151:ALA:HA	1.62	0.82
1:A:316:THR:HG22	1:A:325:TYR:HD1	1.45	0.82
1:B:316:THR:HG22	1:B:325:TYR:CD1	2.15	0.81
1:A:232:ARG:HA	1:A:235:GLN:NE2	1.96	0.80
1:B:260:TRP:CZ3	1:B:300:ALA:HB2	2.16	0.80
1:B:334:LEU:HD13	1:B:357:LEU:HG	1.64	0.79
1:A:56:GLN:CB	1:A:227:ILE:HD11	2.12	0.79
1:A:244:ASN:ND2	1:A:244:ASN:N	2.29	0.78
1:B:316:THR:HG22	1:B:325:TYR:HD1	1.47	0.78
1:B:164:LYS:HB2	1:B:165:PRO:HD3	1.65	0.78
1:A:344:TYR:CZ	1:A:349:ARG:HG2	2.18	0.78
1:A:357:LEU:O	1:A:360:LEU:HD12	1.84	0.78
1:A:316:THR:HG22	1:A:325:TYR:CD1	2.18	0.77
1:B:56:GLN:HA	1:B:227:ILE:HD11	1.66	0.77
1:A:17:THR:O	1:A:21:GLU:HG2	1.84	0.77
1:A:118:PRO:O	1:A:151:ALA:HB1	1.85	0.76
1:B:77:ALA:O	1:B:82:GLU:HB2	1.85	0.76
1:B:101:TRP:HA	1:B:104:ILE:HD12	1.67	0.76
1:A:107:LEU:HD22	1:B:303:PRO:HD3	1.67	0.76
1:A:255:ALA:HA	1:A:269:LEU:HB2	1.66	0.76
1:B:10:ASP:HB3	1:B:14:ARG:HH21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:171:GLU:HG2	1:B:175:GLN:HE22	1.50	0.76
1:B:67:LYS:HE2	1:B:150:TYR:OH	1.86	0.74
1:B:334:LEU:CD1	1:B:357:LEU:HG	2.17	0.74
1:B:8:ILE:HD12	1:B:41:PHE:CZ	2.23	0.73
1:B:259:TYR:CE2	1:B:269:LEU:HD13	2.23	0.73
1:A:7:GLN:O	1:A:11:ILE:HG23	1.88	0.73
1:B:80:ARG:HB3	1:B:82:GLU:HG3	1.71	0.73
1:A:130:ASP:HA	1:A:133:ARG:HH11	1.53	0.73
1:B:8:ILE:O	1:B:12:VAL:HG23	1.89	0.72
1:A:56:GLN:HA	1:A:227:ILE:HD11	1.70	0.72
1:A:336:ILE:HD13	1:A:338:MET:CE	2.20	0.72
1:B:47:ASP:OD2	1:B:50:LYS:HD2	1.90	0.72
1:A:260:TRP:HZ3	1:A:300:ALA:HB2	1.55	0.72
1:B:357:LEU:O	1:B:360:LEU:HD12	1.90	0.71
1:B:344:TYR:CZ	1:B:349:ARG:HG2	2.25	0.71
1:A:98:ALA:HB3	1:A:101:TRP:CD1	2.24	0.71
1:B:161:LEU:HA	1:B:164:LYS:HG2	1.71	0.71
1:B:181:PRO:HB3	1:B:245:GLU:OE2	1.90	0.70
1:B:26:PRO:HB3	1:B:48:ILE:HD11	1.74	0.70
1:A:7:GLN:O	1:A:11:ILE:HD13	1.92	0.70
1:B:11:ILE:HD13	1:B:11:ILE:N	2.03	0.69
1:B:336:ILE:HD13	1:B:338:MET:CE	2.22	0.69
1:A:56:GLN:CA	1:A:227:ILE:HD11	2.22	0.69
1:A:47:ASP:OD2	1:A:50:LYS:HD2	1.92	0.69
1:A:7:GLN:HG3	1:A:7:GLN:O	1.91	0.68
1:A:67:LYS:HE2	1:A:150:TYR:OH	1.94	0.68
1:B:56:GLN:CB	1:B:227:ILE:HD11	2.23	0.68
1:B:173:ALA:O	1:B:177:ARG:HB2	1.93	0.68
1:B:232:ARG:HA	1:B:235:GLN:HE21	1.59	0.67
1:B:95:GLU:OE1	1:B:95:GLU:N	2.28	0.67
1:B:80:ARG:HD2	1:B:177:ARG:NH2	2.10	0.66
1:A:280:PRO:O	1:A:284:ILE:HG13	1.95	0.66
1:B:29:ALA:HB1	1:B:227:ILE:HG12	1.77	0.66
1:A:8:ILE:O	1:A:12:VAL:HG23	1.95	0.66
1:B:4:ALA:HB3	1:B:9:ASN:HD21	1.59	0.66
1:B:192:PRO:HG2	1:B:195:GLU:HG3	1.77	0.66
1:A:8:ILE:HA	1:A:11:ILE:HD13	1.78	0.66
1:A:66:SER:O	1:A:69:PHE:HB2	1.94	0.66
1:A:336:ILE:HD13	1:A:338:MET:HE3	1.77	0.66
1:A:238:LEU:HD13	1:A:328:PHE:CD2	2.31	0.66
1:B:8:ILE:CA	1:B:11:ILE:HD11	2.24	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:O	1:A:20:ILE:HG13	1.95	0.65
1:A:197:LYS:HD3	1:A:198:ASN:OD1	1.96	0.65
1:B:238:LEU:HD11	1:B:328:PHE:HB2	1.77	0.65
1:B:37:LYS:HG3	1:B:38:PRO:N	2.11	0.65
1:A:8:ILE:HA	1:A:11:ILE:CD1	2.26	0.65
1:A:105:THR:H	1:A:108:HIS:CD2	2.15	0.65
1:A:173:ALA:O	1:A:177:ARG:HB2	1.96	0.65
1:A:338:MET:HE1	1:A:353:ALA:CB	2.26	0.65
1:A:37:LYS:HG2	1:A:39:TYR:CZ	2.32	0.65
1:B:183:LYS:O	1:B:232:ARG:NH1	2.30	0.65
1:A:217:ASP:OD1	1:A:218:ALA:N	2.29	0.64
1:B:10:ASP:CB	1:B:14:ARG:HH21	2.10	0.64
1:A:276:TRP:CZ3	1:A:278:VAL:HG22	2.32	0.64
1:A:8:ILE:HD11	1:A:41:PHE:CE1	2.32	0.64
1:A:148:ARG:NH1	1:A:267:GLN:OE1	2.29	0.64
1:A:130:ASP:HA	1:A:133:ARG:NH1	2.12	0.64
1:A:50:LYS:O	1:A:52:GLN:NE2	2.28	0.64
1:B:288:ASP:OD2	1:B:290:LYS:HD2	1.98	0.63
1:A:74:GLY:O	1:A:78:ILE:HG13	1.97	0.63
1:B:308:VAL:HG22	1:B:311:SER:OG	1.98	0.63
1:B:228:GLU:O	1:B:231:ALA:HB3	1.98	0.63
1:B:232:ARG:HA	1:B:235:GLN:NE2	2.14	0.62
1:B:129:SER:OG	1:B:133:ARG:NH1	2.32	0.62
1:B:11:ILE:HG12	1:B:12:VAL:N	2.14	0.62
1:B:355:GLN:HA	1:B:355:GLN:NE2	2.14	0.62
1:B:240:PRO:HA	1:B:243:ILE:CD1	2.30	0.62
1:B:203:TYR:HA	1:B:207:LYS:O	2.00	0.61
1:B:68:THR:HG21	1:B:271:TRP:CZ3	2.35	0.61
1:A:11:ILE:HG12	1:A:12:VAL:N	2.15	0.61
1:A:243:ILE:HD11	1:A:249:GLN:HA	1.81	0.61
1:B:171:GLU:HG2	1:B:175:GLN:NE2	2.16	0.61
1:A:351:ASP:OD1	1:A:355:GLN:NE2	2.34	0.61
1:B:72:VAL:HG21	1:B:233:TRP:CH2	2.36	0.61
1:A:303:PRO:CG	1:B:85:LEU:HB2	2.30	0.61
1:B:260:TRP:HZ3	1:B:300:ALA:HB2	1.66	0.61
1:A:276:TRP:CE3	1:A:278:VAL:HG22	2.35	0.60
1:B:127:SER:OG	1:B:130:ASP:N	2.28	0.60
1:B:344:TYR:CE1	1:B:349:ARG:HG2	2.36	0.60
1:A:308:VAL:HG22	1:A:311:SER:OG	2.02	0.60
1:B:148:ARG:HB2	1:B:298:VAL:CG1	2.32	0.60
1:B:193:PRO:O	1:B:196:GLU:HB2	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:ARG:HA	1:A:235:GLN:HE21	1.67	0.60
1:B:127:SER:OG	1:B:129:SER:HB3	2.01	0.60
1:B:240:PRO:O	1:B:243:ILE:HD12	2.01	0.60
1:B:56:GLN:CA	1:B:227:ILE:HD11	2.30	0.59
1:A:217:ASP:O	1:A:218:ALA:C	2.40	0.59
1:A:93:TRP:CE3	1:A:96:LEU:HD13	2.38	0.59
1:A:99:LYS:NZ	1:A:99:LYS:HB3	2.06	0.58
1:A:99:LYS:O	1:A:102:ASN:HB2	2.03	0.58
1:A:345:PRO:O	1:A:348:ALA:HB3	2.03	0.58
1:B:5:PRO:O	1:B:8:ILE:HG13	2.03	0.58
1:B:59:LEU:HD21	1:B:186:HIS:O	2.03	0.58
1:A:100:GLN:NE2	1:A:136:GLN:O	2.36	0.58
1:A:243:ILE:HD11	1:A:249:GLN:CA	2.33	0.58
1:A:56:GLN:HB3	1:A:228:GLU:HG3	1.85	0.57
1:A:338:MET:HE1	1:A:353:ALA:CA	2.34	0.57
1:A:8:ILE:HD11	1:A:41:PHE:CZ	2.40	0.57
1:B:200:ALA:O	1:B:210:HIS:NE2	2.30	0.57
1:B:271:TRP:HB3	1:B:273:MET:HE2	1.87	0.56
1:B:336:ILE:HD13	1:B:338:MET:HE3	1.86	0.56
1:A:33:ILE:HD12	1:A:33:ILE:N	2.20	0.56
1:A:188:TRP:CZ3	1:A:192:PRO:HG3	2.40	0.56
1:B:148:ARG:NH1	1:B:267:GLN:OE1	2.37	0.56
1:A:303:PRO:HD2	1:B:86:SER:N	2.20	0.56
1:B:16:ILE:O	1:B:20:ILE:HG13	2.05	0.56
1:A:120:GLN:OE1	1:A:152:ASN:ND2	2.29	0.56
1:A:238:LEU:HD12	1:A:330:PRO:HA	1.88	0.56
1:A:228:GLU:O	1:A:231:ALA:HB3	2.06	0.56
1:B:33:ILE:N	1:B:33:ILE:HD12	2.21	0.56
1:B:105:THR:H	1:B:108:HIS:CD2	2.24	0.56
1:B:37:LYS:HG2	1:B:39:TYR:CZ	2.41	0.55
1:B:28:MET:CE	1:B:338:MET:HB3	2.37	0.55
1:A:336:ILE:HD13	1:A:338:MET:HE2	1.88	0.55
1:A:62:LEU:HB3	1:A:65:VAL:HB	1.87	0.55
1:A:104:ILE:HA	1:A:108:HIS:HD2	1.72	0.55
1:B:240:PRO:HA	1:B:243:ILE:HD11	1.89	0.54
1:A:56:GLN:HB3	1:A:228:GLU:CG	2.38	0.54
1:A:139:GLN:CA	1:A:139:GLN:HE21	2.20	0.54
1:B:119:LEU:HA	1:B:151:ALA:HA	1.89	0.54
1:A:56:GLN:HB3	1:A:227:ILE:HD11	1.87	0.54
1:B:66:SER:O	1:B:69:PHE:HB2	2.08	0.54
1:B:10:ASP:CG	1:B:14:ARG:HH21	2.11	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:TRP:HB3	1:A:273:MET:HE3	1.90	0.54
1:A:234:VAL:HG12	1:A:238:LEU:HD22	1.89	0.54
1:A:119:LEU:HA	1:A:151:ALA:CA	2.37	0.53
1:A:56:GLN:CG	1:A:227:ILE:HD11	2.38	0.53
1:B:271:TRP:O	1:B:273:MET:HE3	2.08	0.53
1:A:164:LYS:HB2	1:A:165:PRO:HD3	1.90	0.53
1:B:276:TRP:CD2	1:B:277:PRO:HA	2.43	0.53
1:A:286:GLY:O	1:A:291:ILE:HG23	2.08	0.53
1:A:311:SER:O	1:A:330:PRO:HD2	2.08	0.53
1:A:150:TYR:OH	1:A:315:LYS:NZ	2.42	0.53
1:A:230:MET:O	1:A:234:VAL:HG23	2.07	0.53
1:B:148:ARG:HB2	1:B:298:VAL:HG11	1.91	0.53
1:A:139:GLN:H	1:A:139:GLN:NE2	2.06	0.53
1:A:51:LYS:N	1:A:51:LYS:HD3	2.24	0.53
1:A:346:ASN:HB2	1:A:347:PRO:HD3	1.89	0.53
1:A:201:TRP:O	1:A:341:ASN:HB2	2.07	0.53
1:A:314:HIS:HB2	1:A:326:VAL:O	2.09	0.53
1:B:8:ILE:CD1	1:B:41:PHE:HZ	2.18	0.53
1:B:227:ILE:HG13	2:B:385:HOH:O	2.09	0.53
1:B:336:ILE:HD13	1:B:338:MET:HE2	1.90	0.52
1:B:80:ARG:CB	1:B:82:GLU:HG3	2.39	0.52
1:A:92:TYR:CE1	1:A:106:LEU:HD11	2.44	0.52
1:A:114:ALA:HB3	2:A:380:HOH:O	2.09	0.52
1:A:6:GLN:O	1:A:8:ILE:N	2.43	0.52
1:A:101:TRP:CZ2	1:A:135:TYR:HB3	2.45	0.52
1:A:303:PRO:HG2	1:B:85:LEU:HB2	1.91	0.52
1:B:147:GLN:NE2	1:B:297:PRO:HA	2.24	0.52
1:B:265:MET:HG2	1:B:266:TYR:N	2.25	0.51
1:A:20:ILE:HG23	1:A:25:ILE:HB	1.92	0.51
1:A:355:GLN:OE1	1:A:355:GLN:HA	2.11	0.51
1:B:222:GLY:O	1:B:224:LYS:HE3	2.10	0.51
1:A:127:SER:OG	1:A:129:SER:HB3	2.10	0.51
1:B:336:ILE:CD1	1:B:338:MET:HE2	2.40	0.51
1:A:110:ALA:O	1:A:155:ILE:HD12	2.10	0.51
1:A:67:LYS:NZ	1:A:152:ASN:OD1	2.43	0.51
1:A:182:LEU:HB2	1:A:184:LEU:HG	1.93	0.51
1:B:238:LEU:CD1	1:B:328:PHE:CD2	2.94	0.51
1:A:332:LYS:O	1:A:333:GLU:HB2	2.11	0.51
1:A:6:GLN:O	1:A:9:ASN:N	2.43	0.51
1:B:199:TYR:CZ	1:B:210:HIS:CD2	2.99	0.51
1:B:19:LEU:HD12	1:B:19:LEU:O	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:HIS:N	1:B:314:HIS:CD2	2.79	0.51
1:A:280:PRO:HG3	1:A:354:TRP:CZ2	2.46	0.51
1:B:280:PRO:HG3	1:B:354:TRP:CZ2	2.45	0.51
1:A:118:PRO:HG2	1:A:134:PHE:HZ	1.76	0.51
1:B:164:LYS:HB2	1:B:165:PRO:CD	2.37	0.51
1:B:59:LEU:HB2	1:B:199:TYR:HA	1.93	0.51
1:B:16:ILE:HG21	1:B:43:TRP:CH2	2.46	0.51
1:A:112:TYR:CE2	1:A:148:ARG:NH1	2.79	0.50
1:A:288:ASP:OD1	1:A:290:LYS:HD3	2.09	0.50
1:B:32:VAL:C	1:B:33:ILE:HD12	2.32	0.50
1:B:61:GLU:CD	1:B:211:VAL:H	2.14	0.50
1:A:56:GLN:HG2	1:A:227:ILE:HD11	1.94	0.50
1:A:139:GLN:CA	1:A:139:GLN:NE2	2.74	0.50
1:A:80:ARG:HH21	1:A:177:ARG:HG2	1.77	0.50
1:B:188:TRP:CD2	1:B:192:PRO:HD3	2.47	0.49
1:B:105:THR:H	1:B:108:HIS:HD2	1.59	0.49
1:B:6:GLN:C	1:B:8:ILE:H	2.16	0.49
1:B:8:ILE:HA	1:B:11:ILE:CD1	2.32	0.49
1:A:243:ILE:CD1	1:A:249:GLN:HA	2.42	0.49
1:A:98:ALA:HB1	1:A:100:GLN:NE2	2.28	0.49
1:B:47:ASP:O	1:B:52:GLN:N	2.35	0.49
1:A:334:LEU:HD12	1:A:334:LEU:C	2.32	0.49
1:B:26:PRO:HG2	1:B:203:TYR:CD2	2.47	0.49
1:A:344:TYR:CE2	1:A:349:ARG:HG2	2.48	0.49
1:A:45:TYR:N	1:A:45:TYR:CD1	2.80	0.49
1:B:12:VAL:HG21	1:B:41:PHE:CZ	2.47	0.49
1:B:164:LYS:CB	1:B:165:PRO:HD3	2.39	0.49
1:A:17:THR:N	1:A:18:PRO:CD	2.76	0.49
1:A:99:LYS:HZ1	1:A:99:LYS:HB3	1.78	0.49
1:B:202:GLY:O	1:B:208:ALA:HA	2.13	0.49
1:B:23:GLN:O	1:B:24:LYS:HB2	2.12	0.49
1:B:17:THR:HB	1:B:18:PRO:CD	2.39	0.49
1:B:4:ALA:CB	1:B:9:ASN:HD21	2.25	0.49
1:A:124:GLU:N	1:A:124:GLU:OE1	2.46	0.49
1:A:202:GLY:O	1:A:209:VAL:N	2.37	0.48
1:A:160:ALA:O	1:A:163:VAL:HG22	2.14	0.48
1:A:192:PRO:HG2	1:A:195:GLU:HG3	1.95	0.48
1:B:265:MET:HE3	1:B:272:GLU:HB3	1.95	0.48
1:A:169:SER:OG	1:A:172:GLN:HB2	2.13	0.48
1:B:23:GLN:NE2	1:B:23:GLN:HA	2.28	0.48
1:A:124:GLU:H	1:A:124:GLU:CD	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:94:PRO:HG2	1:A:95:GLU:OE1	2.13	0.48
1:B:217:ASP:OD1	1:B:218:ALA:N	2.47	0.48
1:B:18:PRO:O	1:B:22:GLN:HB2	2.14	0.48
1:A:174:MET:HG3	1:A:179:PHE:CZ	2.48	0.48
1:A:180:GLN:O	1:A:181:PRO:C	2.47	0.48
1:B:32:VAL:HG22	1:B:336:ILE:HG13	1.94	0.48
1:B:188:TRP:CZ2	1:B:192:PRO:HG3	2.48	0.48
1:A:234:VAL:HG12	1:A:238:LEU:CD2	2.44	0.48
1:B:238:LEU:HA	1:B:238:LEU:HD12	1.47	0.48
1:B:240:PRO:HA	1:B:243:ILE:HD12	1.96	0.48
1:A:288:ASP:O	1:A:291:ILE:HG22	2.14	0.48
1:B:72:VAL:HG21	1:B:233:TRP:HH2	1.79	0.48
1:B:276:TRP:HA	1:B:277:PRO:C	2.34	0.48
1:B:289:ASN:HA	1:B:292:ALA:HB3	1.96	0.48
1:B:306:PRO:O	1:B:307:ALA:C	2.53	0.48
1:A:182:LEU:O	1:A:232:ARG:HD3	2.14	0.47
1:A:287:SER:HB2	1:A:346:ASN:HB3	1.96	0.47
1:A:287:SER:HB3	1:A:350:VAL:HG21	1.96	0.47
1:A:306:PRO:O	1:A:307:ALA:C	2.52	0.47
1:B:175:GLN:HB2	1:B:175:GLN:HE21	1.28	0.47
1:A:8:ILE:CD1	1:A:41:PHE:CE1	2.98	0.47
1:B:34:TYR:O	1:B:35:GLN:C	2.50	0.47
1:B:33:ILE:N	1:B:33:ILE:CD1	2.77	0.47
1:A:121:VAL:HG11	1:A:215:ALA:HB3	1.96	0.47
1:A:342:LYS:HG2	1:A:343:ASN:N	2.30	0.47
1:A:302:THR:O	1:B:86:SER:HA	2.15	0.47
1:A:130:ASP:CA	1:A:133:ARG:NH1	2.77	0.47
1:A:246:LYS:HG2	1:A:247:THR:N	2.29	0.47
1:A:80:ARG:CD	1:A:177:ARG:NH2	2.79	0.46
1:A:181:PRO:HB3	1:A:245:GLU:OE2	2.16	0.46
1:B:12:VAL:HG21	1:B:41:PHE:CE1	2.50	0.46
1:A:100:GLN:HG3	1:A:100:GLN:H	1.23	0.46
1:A:271:TRP:HB3	1:A:273:MET:CE	2.45	0.46
1:A:188:TRP:CE3	1:A:192:PRO:HG3	2.50	0.46
1:A:47:ASP:CG	1:A:50:LYS:HD2	2.36	0.46
1:B:182:LEU:O	1:B:183:LYS:HB2	2.15	0.46
1:A:309:ARG:O	1:A:330:PRO:HG2	2.16	0.46
1:B:273:MET:HG3	1:B:313:VAL:HG13	1.97	0.46
1:A:274:LEU:HD22	1:A:283:ILE:CG2	2.45	0.46
1:A:67:LYS:O	1:A:270:GLY:HA3	2.15	0.46
1:B:31:ALA:HA	1:B:39:TYR:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:99:LYS:O	1:B:102:ASN:HB2	2.16	0.46
1:B:6:GLN:O	1:B:8:ILE:N	2.49	0.46
1:A:139:GLN:N	1:A:139:GLN:NE2	2.64	0.46
1:A:171:GLU:HG3	1:A:189:ILE:HB	1.98	0.46
1:B:61:GLU:OE2	1:B:199:TYR:OH	2.28	0.45
1:A:289:ASN:CG	1:A:293:LEU:HD22	2.36	0.45
1:A:289:ASN:OD1	1:A:293:LEU:HD22	2.17	0.45
1:B:226:THR:O	1:B:230:MET:HG2	2.17	0.45
1:B:149:LEU:O	1:B:150:TYR:C	2.54	0.45
1:B:19:LEU:HD12	1:B:19:LEU:C	2.37	0.45
1:A:139:GLN:CB	1:A:140:PRO:HD2	2.43	0.45
1:B:109:LEU:HB3	1:B:158:PHE:HB2	1.98	0.45
1:B:27:GLY:HA3	1:B:45:TYR:O	2.16	0.45
1:A:112:TYR:HB3	1:A:149:LEU:O	2.16	0.45
1:A:188:TRP:HB3	1:A:190:ASN:O	2.17	0.45
1:B:346:ASN:N	1:B:347:PRO:CD	2.80	0.45
1:A:315:LYS:HG3	1:A:316:THR:N	2.32	0.45
1:B:80:ARG:CD	1:B:177:ARG:NH2	2.79	0.45
1:A:37:LYS:HG2	1:A:39:TYR:CE2	2.52	0.45
1:A:280:PRO:HA	1:A:283:ILE:HD11	1.99	0.45
1:B:191:VAL:HG23	1:B:195:GLU:HB2	1.99	0.45
1:A:346:ASN:N	1:A:347:PRO:CD	2.79	0.45
1:A:238:LEU:CD1	1:A:328:PHE:CD2	2.99	0.45
1:A:276:TRP:CD2	1:A:277:PRO:HA	2.52	0.45
1:A:119:LEU:O	1:A:152:ASN:HB2	2.17	0.45
1:A:179:PHE:CD1	1:A:179:PHE:N	2.82	0.45
1:A:157:LEU:O	1:A:158:PHE:C	2.54	0.45
1:B:23:GLN:NE2	1:B:23:GLN:CA	2.81	0.45
1:B:237:ASN:HB3	1:B:328:PHE:CZ	2.52	0.44
1:A:33:ILE:HA	1:A:37:LYS:O	2.17	0.44
1:A:139:GLN:HB3	1:A:140:PRO:HD2	1.99	0.44
1:B:280:PRO:O	1:B:284:ILE:HD12	2.17	0.44
1:B:332:LYS:O	1:B:333:GLU:C	2.53	0.44
1:A:243:ILE:HD11	1:A:249:GLN:N	2.32	0.44
1:A:125:VAL:HG12	1:A:125:VAL:O	2.16	0.44
1:B:227:ILE:H	1:B:227:ILE:HG13	1.59	0.44
1:B:50:LYS:O	1:B:51:LYS:HB2	2.18	0.44
1:A:276:TRP:CZ3	1:A:278:VAL:CG2	2.99	0.44
1:A:271:TRP:CB	1:A:273:MET:CE	2.95	0.44
1:A:199:TYR:CZ	1:A:210:HIS:CD2	3.06	0.44
1:B:259:TYR:CE2	1:B:269:LEU:CD1	2.97	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:336:ILE:HB	1:A:357:LEU:HD11	2.00	0.44
1:B:26:PRO:CB	1:B:48:ILE:HD11	2.45	0.44
1:B:179:PHE:N	1:B:179:PHE:CD1	2.85	0.44
1:B:175:GLN:O	1:B:180:GLN:HB2	2.18	0.43
1:A:273:MET:C	1:A:274:LEU:HD12	2.38	0.43
1:A:99:LYS:HB3	1:A:99:LYS:HE3	1.66	0.43
1:A:245:GLU:N	1:A:245:GLU:OE1	2.51	0.43
1:A:240:PRO:HB3	1:A:252:ILE:HG21	1.99	0.43
1:A:334:LEU:HD12	1:A:335:GLY:H	1.75	0.43
1:A:243:ILE:HG23	1:A:243:ILE:HD13	1.57	0.43
1:A:191:VAL:HA	1:A:192:PRO:HD3	1.54	0.43
1:B:265:MET:CE	1:B:272:GLU:HB3	2.48	0.43
1:B:253:GLN:HG3	1:B:253:GLN:H	1.62	0.43
1:A:259:TYR:C	1:A:301:ILE:HG13	2.38	0.43
1:A:8:ILE:HD11	1:A:41:PHE:HE1	1.78	0.43
1:B:342:LYS:HG2	1:B:343:ASN:N	2.33	0.43
1:B:109:LEU:HD23	1:B:109:LEU:HA	1.70	0.43
1:A:8:ILE:HA	1:A:11:ILE:HD11	2.00	0.43
1:A:84:LYS:HB2	1:A:84:LYS:HE3	1.41	0.43
1:A:329:ILE:O	1:A:330:PRO:C	2.56	0.43
1:B:271:TRP:HB3	1:B:273:MET:CE	2.48	0.43
1:A:192:PRO:HA	1:A:193:PRO:HD3	1.88	0.43
1:A:287:SER:OG	1:A:347:PRO:HA	2.18	0.43
1:B:84:LYS:HB2	1:B:84:LYS:HE3	1.55	0.43
1:B:239:LYS:HA	1:B:240:PRO:HD2	1.86	0.43
1:A:99:LYS:CB	1:A:99:LYS:NZ	2.78	0.43
1:B:164:LYS:CB	1:B:165:PRO:CD	2.96	0.43
1:A:6:GLN:O	1:A:7:GLN:C	2.55	0.43
1:B:99:LYS:HB3	1:B:99:LYS:HE3	1.14	0.43
1:A:56:GLN:HG2	1:A:227:ILE:CD1	2.48	0.42
1:B:216:LEU:HA	1:B:216:LEU:HD23	1.79	0.42
1:A:334:LEU:HD11	1:A:357:LEU:HG	2.02	0.42
1:B:16:ILE:O	1:B:19:LEU:HB3	2.20	0.42
1:A:336:ILE:CD1	1:A:338:MET:HE2	2.47	0.42
1:B:328:PHE:HA	1:B:335:GLY:HA2	2.01	0.42
1:A:76:ASP:O	1:A:80:ARG:N	2.47	0.42
1:B:61:GLU:HA	1:B:224:LYS:HG3	2.02	0.42
1:A:179:PHE:O	1:A:180:GLN:C	2.57	0.42
1:B:139:GLN:HE21	1:B:139:GLN:CA	2.23	0.42
1:B:255:ALA:HA	1:B:269:LEU:HB2	2.00	0.42
1:B:283:ILE:HG13	1:B:350:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ILE:CD1	1:A:41:PHE:CZ	3.02	0.42
1:B:271:TRP:CB	1:B:273:MET:CE	2.97	0.42
1:B:276:TRP:CG	1:B:277:PRO:HA	2.55	0.42
1:B:75:GLY:HA2	1:B:78:ILE:HD12	2.01	0.42
1:B:161:LEU:CD1	1:B:161:LEU:N	2.82	0.42
1:A:271:TRP:C	1:A:273:MET:HE1	2.40	0.42
1:B:47:ASP:CG	1:B:50:LYS:HD2	2.40	0.42
1:B:122:PRO:HD2	1:B:134:PHE:CE1	2.55	0.42
1:B:4:ALA:O	1:B:9:ASN:ND2	2.52	0.42
1:A:37:LYS:HG3	1:A:38:PRO:N	2.35	0.42
1:A:243:ILE:HG21	1:A:243:ILE:HD12	1.58	0.42
1:B:345:PRO:O	1:B:348:ALA:HB3	2.20	0.42
1:B:127:SER:HG	1:B:129:SER:HB3	1.85	0.41
1:A:239:LYS:HE3	1:A:239:LYS:HB2	1.50	0.41
1:A:119:LEU:HA	1:A:151:ALA:CB	2.50	0.41
1:A:227:ILE:HD12	1:A:228:GLU:N	2.35	0.41
1:A:169:SER:O	1:A:170:PHE:C	2.58	0.41
1:B:8:ILE:CA	1:B:11:ILE:CD1	2.96	0.41
1:A:301:ILE:O	1:A:303:PRO:C	2.58	0.41
1:B:302:THR:HA	1:B:303:PRO:HA	1.82	0.41
1:B:283:ILE:HD12	1:B:283:ILE:HG21	1.78	0.41
1:B:100:GLN:NE2	1:B:136:GLN:O	2.52	0.41
1:A:281:ASP:O	1:A:282:SER:C	2.58	0.41
1:B:63:GLY:CA	1:B:319:THR:HG23	2.50	0.41
1:B:139:GLN:HE21	1:B:139:GLN:HA	1.84	0.41
1:A:260:TRP:N	1:A:301:ILE:HG13	2.36	0.41
1:B:66:SER:O	1:B:69:PHE:N	2.50	0.41
1:A:30:VAL:CG1	1:A:31:ALA:N	2.83	0.41
1:B:10:ASP:HB3	1:B:14:ARG:NH2	2.27	0.41
1:B:314:HIS:HB2	1:B:326:VAL:O	2.21	0.41
1:A:175:GLN:HG2	1:A:180:GLN:HE21	1.85	0.41
1:A:80:ARG:HD2	1:A:177:ARG:NH2	2.36	0.41
1:B:102:ASN:HB3	1:B:103:GLY:H	1.43	0.41
1:A:246:LYS:NZ	1:B:309:ARG:HD3	2.35	0.41
1:A:128:SER:O	1:A:131:LEU:HB3	2.21	0.41
1:A:329:ILE:HA	1:A:330:PRO:HD2	1.64	0.41
1:B:289:ASN:HA	1:B:289:ASN:HD22	1.47	0.41
1:B:291:ILE:HG21	1:B:291:ILE:HD13	1.75	0.41
1:B:250:GLN:O	1:B:254:LEU:HG	2.20	0.41
1:B:87:ASP:HB3	1:B:88:PRO:HD2	2.03	0.40
1:B:93:TRP:N	1:B:94:PRO:HD3	2.35	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:THR:HG22	1:A:96:LEU:HB3	2.04	0.40
1:B:265:MET:HE3	1:B:272:GLU:OE1	2.21	0.40
1:A:61:GLU:CD	1:A:211:VAL:H	2.23	0.40
1:B:85:LEU:HD23	1:B:85:LEU:HA	1.84	0.40
1:A:93:TRP:O	1:A:96:LEU:HB2	2.20	0.40
1:A:87:ASP:OD2	1:A:92:TYR:OH	2.30	0.40
1:B:5:PRO:HD2	1:B:8:ILE:HG12	2.01	0.40
1:B:182:LEU:O	1:B:232:ARG:HD2	2.22	0.40
1:B:352:ALA:O	1:B:355:GLN:HB2	2.21	0.40
1:B:73:LEU:O	1:B:76:ASP:HB3	2.22	0.40

There are no symmetry-related clashes.

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	355/358 (99%)	328 (92%)	23 (6%)	4 (1%)	17 9
1	B	355/358 (99%)	326 (92%)	26 (7%)	3 (1%)	24 15
All	All	710/716 (99%)	654 (92%)	49 (7%)	7 (1%)	19 11

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	102	ASN
1	B	102	ASN
1	A	7	GLN
1	B	64	SER
1	A	175	GLN
1	A	307	ALA
1	B	7	GLN

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	291/292 (100%)	243 (84%)	48 (16%)	3 1
1	B	291/292 (100%)	245 (84%)	46 (16%)	3 1
All	All	582/584 (100%)	488 (84%)	94 (16%)	3 1

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	8	ILE
1	A	11	ILE
1	A	14	ARG
1	A	24	LYS
1	A	42	THR
1	A	50	LYS
1	A	51	LYS
1	A	64	SER
1	A	84	LYS
1	A	99	LYS
1	A	100	GLN
1	A	102	ASN
1	A	124	GLU
1	A	132	LEU
1	A	139	GLN
1	A	161	LEU
1	A	164	LYS
1	A	172	GLN
1	A	190	ASN
1	A	197	LYS
1	A	204	ARG
1	A	205	GLU
1	A	227	ILE
1	A	235	GLN
1	A	238	LEU
1	A	239	LYS

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Mol	Chain	Res	Type
1	A	243	ILE
1	A	244	ASN
1	A	245	GLU
1	A	246	LYS
1	A	249	GLN
1	A	250	GLN
1	A	254	LEU
1	A	269	LEU
1	A	273	MET
1	A	278	VAL
1	A	283	ILE
1	A	289	ASN
1	A	290	LYS
1	A	293	LEU
1	A	296	ARG
1	A	301	ILE
1	A	309	ARG
1	A	314	HIS
1	A	315	LYS
1	A	334	LEU
1	A	342	LYS
1	B	7	GLN
1	B	11	ILE
1	B	14	ARG
1	B	19	LEU
1	B	22	GLN
1	B	37	LYS
1	B	42	THR
1	B	51	LYS
1	B	57	GLN
1	B	64	SER
1	B	84	LYS
1	B	91	LYS
1	B	95	GLU
1	B	99	LYS
1	B	102	ASN
1	B	123	ASP
1	B	132	LEU
1	B	139	GLN
1	B	148	ARG
1	B	175	GLN
1	B	191	VAL

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Mol	Chain	Res	Type
1	B	197	LYS
1	B	204	ARG
1	B	205	GLU
1	B	224	LYS
1	B	227	ILE
1	B	238	LEU
1	B	239	LYS
1	B	244	ASN
1	B	245	GLU
1	B	246	LYS
1	B	250	GLN
1	B	262	THR
1	B	265	MET
1	B	269	LEU
1	B	273	MET
1	B	283	ILE
1	B	299	LYS
1	B	301	ILE
1	B	309	ARG
1	B	314	HIS
1	B	315	LYS
1	B	331	GLU
1	B	334	LEU
1	B	342	LYS
1	B	357	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	9	ASN
1	A	56	GLN
1	A	102	ASN
1	A	108	HIS
1	A	139	GLN
1	A	147	GLN
1	A	235	GLN
1	A	244	ASN
1	A	253	GLN
1	A	289	ASN
1	B	9	ASN
1	B	23	GLN
1	B	56	GLN

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Mol	Chain	Res	Type
1	B	102	ASN
1	B	108	HIS
1	B	137	ASN
1	B	139	GLN
1	B	147	GLN
1	B	175	GLN
1	B	235	GLN
1	B	250	GLN
1	B	285	ASN
1	B	289	ASN
1	B	355	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	357/358 (99%)	-0.00	4 (1%)	82	83	19, 34, 63, 97	1 (0%)
1	B	357/358 (99%)	0.04	2 (0%)	90	90	21, 34, 63, 97	1 (0%)
All	All	714/716 (99%)	0.02	6 (0%)	87	88	19, 34, 63, 97	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	6	GLN	5.8
1	A	6	GLN	3.5
1	A	123	ASP	2.8
1	A	97	THR	2.7
1	A	99	LYS	2.5
1	B	7	GLN	2.4

6.2 Non-standard residues in protein, DNA, RNA chains

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

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.