Full wwPDB X-ray Structure Validation Report ⓘ

Oct 26, 2023 – 07:43 AM EDT

PDB ID	:	3H4J
Title	:	crystal structure of pombe AMPK KDAID fragment
Authors	:	Chen, L.; Jiao, Z.-H.; Zheng, L.-S.; Zhang, Y.-Y.; Xie, S.-T.; Wang, Z.-X.; Wu, J.-W.
Deposited on	:	2009-04-20
Resolution	:	2.80 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:

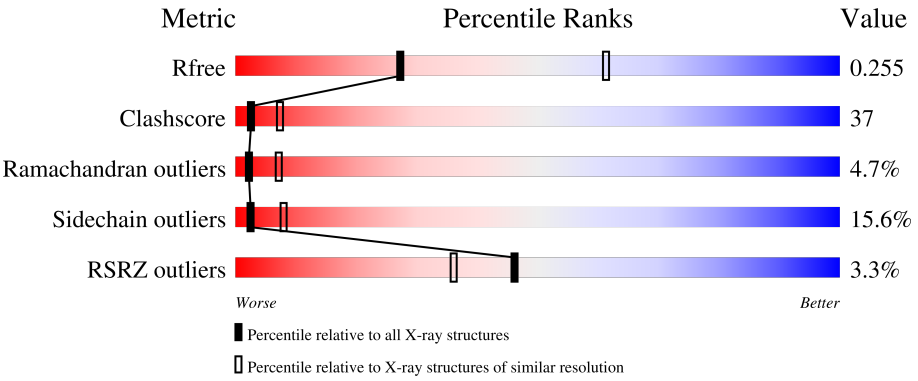
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.80 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}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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 <=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	336	5% 30% 48% 15% • 6%
1	B	336	% 48% 40% 9% ••

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 5364 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 SNF1-like protein kinase ssp2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	330	Total	C	N	O	S	0	0	0
			2686	1716	464	490	16			
1	A	316	Total	C	N	O	S	0	0	0
			2574	1645	442	472	15			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	24	MET	-	expression tag	UNP O74536
B	352	LEU	-	expression tag	UNP O74536
B	353	GLU	-	expression tag	UNP O74536
B	354	HIS	-	expression tag	UNP O74536
B	355	HIS	-	expression tag	UNP O74536
B	356	HIS	-	expression tag	UNP O74536
B	357	HIS	-	expression tag	UNP O74536
B	358	HIS	-	expression tag	UNP O74536
B	359	HIS	-	expression tag	UNP O74536
A	24	MET	-	expression tag	UNP O74536
A	352	LEU	-	expression tag	UNP O74536
A	353	GLU	-	expression tag	UNP O74536
A	354	HIS	-	expression tag	UNP O74536
A	355	HIS	-	expression tag	UNP O74536
A	356	HIS	-	expression tag	UNP O74536
A	357	HIS	-	expression tag	UNP O74536
A	358	HIS	-	expression tag	UNP O74536
A	359	HIS	-	expression tag	UNP O74536

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	81	Total	O	0	0
			81	81		

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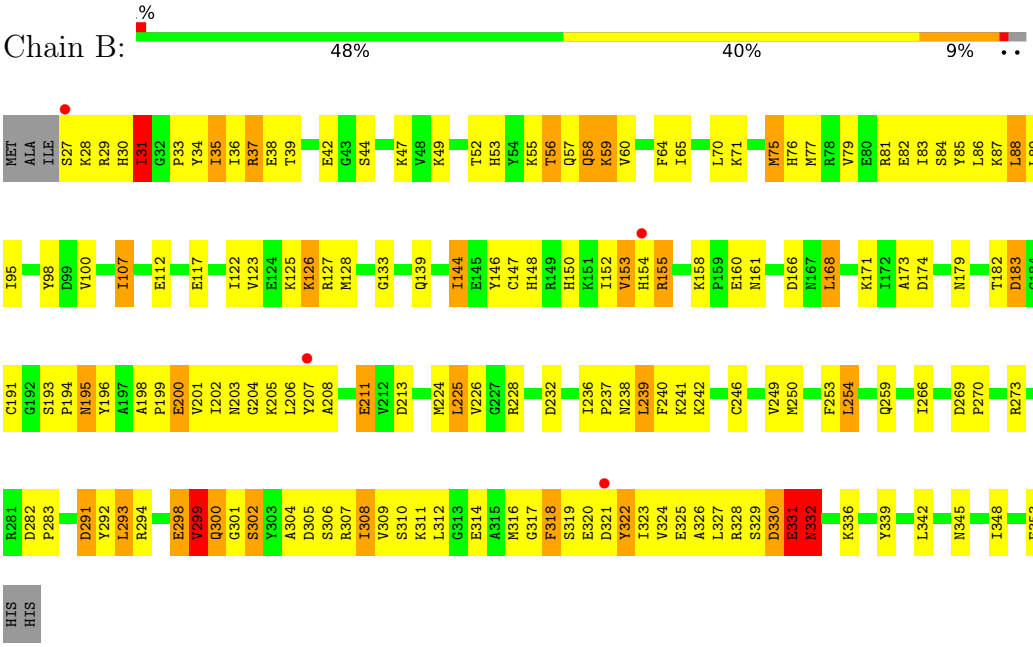
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	23	Total	O	0	0
			23	23		

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry 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.

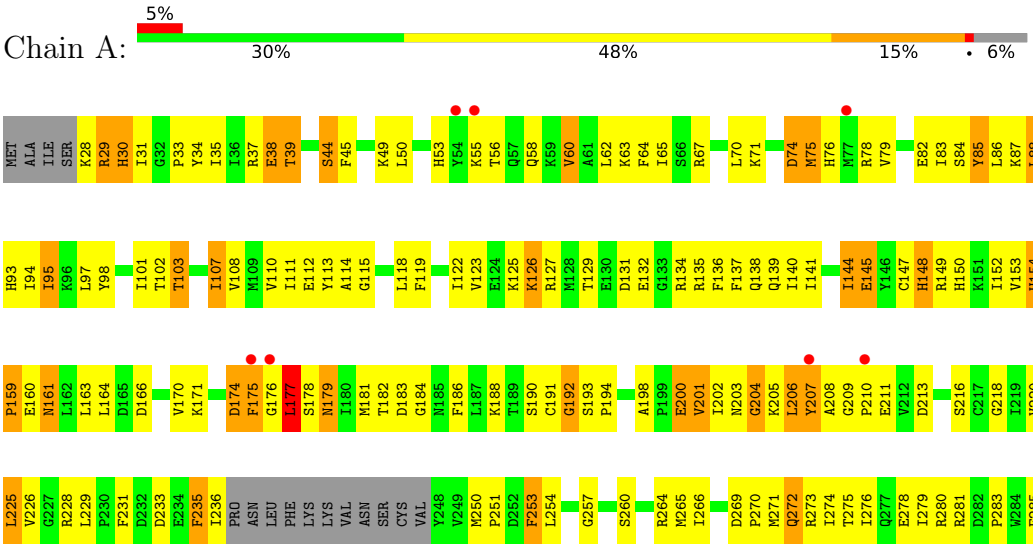
• Molecule 1: SNF1-like protein kinase ssp2

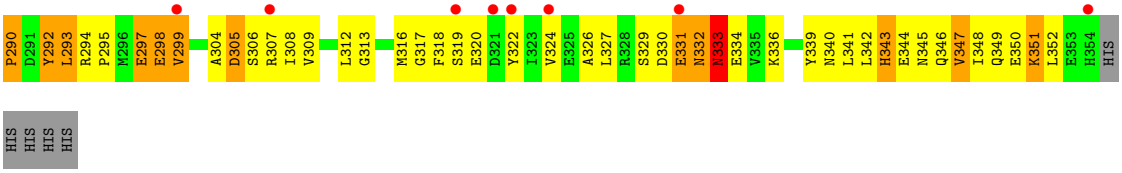
Chain B:



• Molecule 1: SNF1-like protein kinase ssp2

Chain A:




P290
D291
Y292
L293
R294
P295
M296
E297
E298
V299
A304
D305
S306
R307
I308
V309
L312
G313
M316
G317
F318
S319
E320
D321
Y322
I323
V324
E325
A326
L327
R328
S329
D330
E331
M332
N333
E334
V335
K336
Y339
N340
L341
L342
H343
E344
N345
Q346
V347
I348
Q349
E350
K351
L352
E353
H354
HIS

HIS
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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α, β, γ	128.96Å 128.96Å 106.87Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	39.26 – 2.80 39.26 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.9 (39.26-2.80) 99.8 (39.26-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 2.69Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.218 , 0.257 0.217 , 0.255	Depositor DCC
R_{free} test set	1399 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	71.1	Xtriage
Anisotropy	0.413	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 68.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.038 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	5364	wwPDB-VP
Average B, all atoms (Å^2)	102.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.72% 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, 0.333 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	0.45	0/2627	0.83	8/3545 (0.2%)
1	B	0.51	0/2744	0.85	7/3705 (0.2%)
All	All	0.48	0/5371	0.84	15/7250 (0.2%)

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	1

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	299	VAL	CB-CA-C	-8.47	95.30	111.40
1	A	75	MET	N-CA-C	-7.86	89.77	111.00
1	B	299	VAL	CB-CA-C	-7.36	97.43	111.40
1	A	154	HIS	N-CA-C	-6.99	92.12	111.00
1	B	331	GLU	N-CA-C	6.82	129.41	111.00
1	B	205	LYS	N-CA-C	-6.34	93.89	111.00
1	A	183	ASP	CB-CG-OD2	6.33	124.00	118.30
1	B	299	VAL	N-CA-C	-6.27	94.08	111.00
1	A	177	LEU	CA-CB-CG	6.10	129.34	115.30
1	B	126	LYS	N-CA-C	-6.04	94.68	111.00
1	B	298	GLU	N-CA-C	5.67	126.32	111.00
1	B	332	ASN	N-CA-C	5.57	126.03	111.00
1	A	155	ARG	N-CA-C	5.45	125.71	111.00
1	A	182	THR	CB-CA-C	-5.26	97.39	111.60
1	A	192	GLY	N-CA-C	-5.19	100.13	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	235	PHE	Peptide

5.2 Too-close contacts (i)

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	2574	0	2584	241	0
1	B	2686	0	2697	167	0
2	A	23	0	0	7	0
2	B	81	0	0	11	0
All	All	5364	0	5281	388	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 (388) 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:71:LYS:HG2	2:B:408:HOH:O	1.18	1.25
1:A:235:PHE:O	1:A:236:ILE:HG23	1.53	1.07
1:A:235:PHE:C	1:A:236:ILE:HG23	1.70	1.05
1:A:126:LYS:HG2	1:A:127:ARG:H	1.23	1.04
1:A:147:CYS:HA	1:A:152:ILE:HD11	1.38	1.03
1:B:56:THR:HG22	1:B:58:GLN:H	1.26	0.96
1:B:89:LEU:O	1:B:90:ARG:HD2	1.67	0.95
1:A:126:LYS:CG	1:A:127:ARG:H	1.78	0.94
1:A:91:HIS:HD2	1:A:93:HIS:H	0.94	0.93
1:A:91:HIS:CD2	1:A:93:HIS:H	1.86	0.93
1:A:70:LEU:HD12	1:A:107:ILE:HD11	1.52	0.91
1:A:327:LEU:HA	1:A:336:LYS:HE3	1.51	0.90
1:B:311:LYS:NZ	2:B:372:HOH:O	2.04	0.90
1:A:235:PHE:O	1:A:236:ILE:HG12	1.74	0.87
1:A:144:ILE:HG13	1:A:148:HIS:NE2	1.91	0.85
1:A:316:MET:HB3	1:A:318:PHE:HE1	1.41	0.84
1:B:57:GLN:NE2	2:B:373:HOH:O	2.10	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:83:ILE:HD13	1:B:100:VAL:HG21	1.60	0.81
1:A:28:LYS:HG2	1:A:29:ARG:H	1.46	0.81
1:B:144:ILE:HD12	1:B:213:ASP:HB3	1.63	0.80
1:B:55:LYS:HD2	2:B:414:HOH:O	1.81	0.79
1:A:28:LYS:HE2	1:A:29:ARG:NH2	1.98	0.79
1:A:251:PRO:HD2	1:A:254:LEU:HD12	1.64	0.78
1:A:318:PHE:HD2	1:A:322:TYR:HE2	1.32	0.78
1:B:201:VAL:HG22	1:A:206:LEU:HB3	1.63	0.78
1:A:235:PHE:O	1:A:236:ILE:CG2	2.30	0.78
1:B:158:LYS:H	1:B:161:ASN:HD22	1.32	0.77
1:A:31:ILE:HD11	1:A:62:LEU:HD13	1.66	0.77
1:B:320:GLU:O	1:B:324:VAL:HG23	1.85	0.77
1:A:297:GLU:HG2	1:A:298:GLU:H	1.49	0.76
1:A:292:TYR:HA	1:A:351:LYS:HE2	1.67	0.76
1:A:144:ILE:HG23	1:A:148:HIS:CE1	2.21	0.76
1:B:203:ASN:CG	1:A:203:ASN:HB3	2.05	0.75
1:B:316:MET:HG2	1:B:318:PHE:CE2	2.22	0.75
1:B:84:SER:HA	1:B:87:LYS:HG3	1.68	0.74
1:B:250:MET:HE1	1:B:259:GLN:HA	1.69	0.74
1:A:126:LYS:HG2	1:A:127:ARG:N	2.01	0.74
1:B:90:ARG:HH11	1:B:90:ARG:HG2	1.52	0.74
1:A:91:HIS:HD2	1:A:93:HIS:N	1.79	0.74
1:A:91:HIS:HB3	1:A:94:ILE:HG12	1.71	0.72
1:B:154:HIS:CD2	1:B:174:ASP:HB2	2.24	0.72
1:B:35:ILE:HD11	1:B:37:ARG:CZ	2.19	0.71
1:A:29:ARG:HD3	2:A:372:HOH:O	1.88	0.71
1:B:128:MET:HE1	1:B:224:MET:HB3	1.73	0.71
1:B:250:MET:HE3	1:B:254:LEU:HD23	1.71	0.71
1:A:319:SER:OG	1:A:322:TYR:HB3	1.89	0.70
1:A:28:LYS:HE2	1:A:29:ARG:HH21	1.56	0.70
1:B:90:ARG:NH2	1:B:98:TYR:HA	2.06	0.70
1:B:70:LEU:HD13	1:B:76:HIS:HD2	1.56	0.70
1:B:292:TYR:CE1	1:B:293:LEU:HD13	2.26	0.70
1:A:126:LYS:CG	1:A:127:ARG:N	2.51	0.70
1:B:75:MET:CE	1:B:75:MET:HA	2.21	0.70
1:A:91:HIS:HB3	1:A:94:ILE:CG1	2.22	0.70
1:A:70:LEU:HD22	1:A:76:HIS:HB2	1.72	0.69
1:A:235:PHE:C	1:A:236:ILE:CG2	2.45	0.69
1:B:330:ASP:O	1:B:331:GLU:HB2	1.91	0.69
1:A:29:ARG:NH1	1:A:29:ARG:HB2	2.06	0.69
1:A:144:ILE:HG21	1:A:276:ILE:HD12	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:59:LYS:NZ	1:B:59:LYS:H	1.91	0.69
1:A:316:MET:HB3	1:A:318:PHE:CE1	2.26	0.68
1:B:250:MET:HE2	1:B:259:GLN:HG2	1.76	0.67
1:A:297:GLU:HG2	1:A:298:GLU:N	2.08	0.67
1:A:190:SER:O	1:A:193:SER:HB3	1.95	0.67
1:B:195:ASN:OD1	1:B:195:ASN:N	2.28	0.67
1:A:145:GLU:HG3	1:A:280:ARG:HH11	1.60	0.67
1:A:194:PRO:O	1:A:202:ILE:HD13	1.95	0.66
1:A:67:ARG:O	1:A:71:LYS:HG3	1.95	0.66
1:B:325:GLU:HG2	1:B:328:ARG:HH12	1.61	0.66
1:B:155:ARG:NH1	2:B:405:HOH:O	2.29	0.66
1:A:153:VAL:HG12	1:A:153:VAL:O	1.94	0.66
1:B:202:ILE:HD12	1:B:202:ILE:O	1.96	0.65
1:B:31:ILE:HG23	1:B:36:ILE:HD11	1.79	0.65
1:B:276:ILE:HD13	1:B:277:GLN:N	2.12	0.65
1:A:144:ILE:CG2	1:A:145:GLU:N	2.60	0.65
1:B:49:LYS:HD2	1:B:64:PHE:CE1	2.32	0.65
1:A:70:LEU:HD22	1:A:76:HIS:CB	2.27	0.65
1:B:238:ASN:HB3	1:A:186:PHE:CE1	2.32	0.64
1:A:275:THR:O	1:A:279:ILE:HG13	1.97	0.64
1:A:135:ARG:O	1:A:138:GLN:HG2	1.98	0.64
1:B:306:SER:HA	1:B:309:VAL:HB	1.79	0.64
1:A:49:LYS:HD2	1:A:64:PHE:CE1	2.33	0.64
1:B:44:SER:HB2	1:A:229:LEU:O	1.98	0.64
1:A:266:ILE:HG22	1:A:266:ILE:O	1.98	0.64
1:B:56:THR:O	1:B:57:GLN:HB2	1.98	0.63
1:A:144:ILE:HG23	1:A:148:HIS:HE1	1.64	0.63
1:A:222:TYR:C	1:A:222:TYR:CD2	2.72	0.63
1:B:194:PRO:HB2	1:A:231:PHE:CD1	2.33	0.63
1:A:235:PHE:O	1:A:236:ILE:CG1	2.47	0.63
1:A:37:ARG:O	1:A:38:GLU:HB2	1.97	0.63
1:A:158:LYS:HB2	1:A:159:PRO:HD2	1.79	0.63
1:A:331:GLU:O	1:A:333:ASN:N	2.32	0.63
1:A:155:ARG:O	1:A:157:LEU:N	2.31	0.63
1:B:75:MET:HA	1:B:75:MET:HE2	1.81	0.62
1:B:89:LEU:C	1:B:90:ARG:HD2	2.19	0.62
1:B:298:GLU:C	1:B:299:VAL:O	2.36	0.62
1:A:344:GLU:HA	1:A:347:VAL:CG1	2.29	0.62
1:A:53:HIS:CG	1:A:56:THR:HG22	2.35	0.61
1:A:125:LYS:NZ	2:A:380:HOH:O	2.31	0.61
1:A:93:HIS:CE1	1:A:139:GLN:HE21	2.18	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:306:SER:HA	1:A:309:VAL:HB	1.81	0.61
1:A:176:GLY:C	1:A:177:LEU:HD22	2.20	0.61
1:A:29:ARG:HB2	1:A:29:ARG:CZ	2.31	0.61
1:A:31:ILE:HD12	1:A:108:VAL:HG11	1.81	0.61
1:A:208:ALA:HB3	1:A:211:GLU:OE1	2.01	0.60
1:B:59:LYS:H	1:B:59:LYS:HZ2	1.49	0.60
1:B:198:ALA:HB1	1:B:200:GLU:OE2	2.01	0.60
1:B:200:GLU:HG2	1:A:270:PRO:HG3	1.83	0.60
1:B:250:MET:CE	1:B:254:LEU:HD23	2.31	0.60
1:B:107:ILE:HG13	1:B:107:ILE:O	2.02	0.60
1:A:94:ILE:HD12	1:A:94:ILE:O	2.02	0.60
1:A:326:ALA:O	1:A:333:ASN:OD1	2.20	0.60
1:A:318:PHE:CD2	1:A:322:TYR:HE2	2.19	0.60
1:A:119:PHE:O	1:A:123:VAL:HG23	2.02	0.59
1:A:155:ARG:HH22	1:A:209:GLY:C	2.06	0.59
1:A:289:LEU:HD21	1:A:293:LEU:HB3	1.84	0.59
1:A:159:PRO:O	1:A:161:ASN:N	2.36	0.59
1:B:203:ASN:ND2	1:A:203:ASN:HB3	2.18	0.59
1:B:128:MET:CE	1:B:224:MET:HB3	2.33	0.58
1:B:193:SER:OG	1:A:233:ASP:OD1	2.20	0.58
1:B:330:ASP:O	1:B:331:GLU:CB	2.51	0.58
1:B:200:GLU:HG2	1:A:270:PRO:CG	2.33	0.58
1:A:320:GLU:O	1:A:324:VAL:HG23	2.03	0.58
1:B:236:ILE:HG22	1:B:239:LEU:HB2	1.84	0.58
1:A:140:ILE:HG13	1:A:170:VAL:HG11	1.85	0.58
1:A:274:ILE:HG13	1:A:278:GLU:HB3	1.86	0.58
1:A:144:ILE:HG22	1:A:145:GLU:N	2.19	0.58
1:A:177:LEU:O	1:A:178:SER:CB	2.51	0.57
1:B:319:SER:OG	1:B:322:TYR:HB3	2.03	0.57
1:A:91:HIS:CD2	1:A:92:PRO:HD2	2.39	0.57
1:B:189:THR:HG22	1:A:159:PRO:HG2	1.85	0.57
1:B:305:ASP:OD2	1:B:307:ARG:N	2.38	0.57
1:A:308:ILE:HD11	1:A:339:TYR:CE1	2.40	0.57
1:B:93:HIS:NE2	1:B:139:GLN:HG2	2.20	0.57
1:B:150:HIS:HB2	1:B:152:ILE:CD1	2.35	0.57
1:A:201:VAL:HG12	1:A:202:ILE:HG23	1.87	0.57
1:B:146:TYR:OH	1:B:345:ASN:ND2	2.36	0.57
1:B:202:ILE:O	1:B:204:GLY:N	2.36	0.56
1:B:308:ILE:HD11	1:B:339:TYR:CD1	2.39	0.56
1:B:65:ILE:HB	1:B:107:ILE:HG13	1.88	0.56
1:A:177:LEU:N	1:A:177:LEU:CD2	2.68	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:HIS:HE1	2:A:368:HOH:O	1.88	0.56
1:A:137:PHE:CG	1:A:221:LEU:HD13	2.41	0.56
1:A:251:PRO:HD2	1:A:254:LEU:CD1	2.33	0.56
1:B:56:THR:CG2	1:B:58:GLN:HB2	2.36	0.55
1:A:344:GLU:O	1:A:348:ILE:HG12	2.06	0.55
1:A:122:ILE:HD13	1:A:224:MET:HA	1.87	0.55
1:A:177:LEU:O	1:A:178:SER:HB2	2.06	0.55
1:A:225:LEU:HB3	1:A:254:LEU:HD21	1.88	0.55
1:A:157:LEU:HD12	1:A:157:LEU:H	1.72	0.55
1:B:90:ARG:HH11	1:B:90:ARG:CG	2.19	0.55
1:B:152:ILE:HG22	1:B:154:HIS:H	1.72	0.55
1:B:183:ASP:HB3	1:B:185:ASN:H	1.72	0.55
1:B:308:ILE:HD12	1:B:342:LEU:HB2	1.88	0.55
1:A:83:ILE:HD12	1:A:84:SER:N	2.22	0.55
1:B:191:CYS:HB2	1:A:192:GLY:O	2.06	0.54
1:B:325:GLU:HG2	1:B:328:ARG:NH1	2.22	0.54
1:A:88:LEU:O	1:A:341:LEU:HD21	2.08	0.54
1:B:70:LEU:HD13	1:B:76:HIS:CD2	2.40	0.54
1:A:131:ASP:O	1:A:134:ARG:HG2	2.08	0.54
1:A:50:LEU:HD11	1:A:113:TYR:CE1	2.42	0.54
1:A:157:LEU:O	1:A:157:LEU:HD22	2.07	0.54
1:B:305:ASP:OD2	1:B:307:ARG:HB2	2.06	0.54
1:A:28:LYS:NZ	2:A:368:HOH:O	2.40	0.54
1:A:326:ALA:HB1	1:A:333:ASN:OD1	2.08	0.53
1:A:55:LYS:HD2	1:A:55:LYS:O	2.08	0.53
1:A:147:CYS:HA	1:A:152:ILE:CD1	2.26	0.53
1:B:35:ILE:HD11	1:B:37:ARG:NH2	2.23	0.53
1:A:70:LEU:CD2	1:A:76:HIS:HB2	2.39	0.53
1:A:198:ALA:HB1	1:A:200:GLU:OE1	2.08	0.53
1:A:297:GLU:O	1:A:298:GLU:HB2	2.09	0.53
1:B:127:ARG:HD2	1:B:253:PHE:CE1	2.43	0.53
1:A:63:LYS:HZ2	1:A:177:LEU:HA	1.73	0.53
1:A:74:ASP:C	1:A:76:HIS:H	2.12	0.53
1:A:251:PRO:HB2	1:A:253:PHE:CE2	2.43	0.53
1:B:144:ILE:CD1	1:B:213:ASP:HB3	2.38	0.53
1:B:152:ILE:HG22	1:B:153:VAL:N	2.24	0.53
1:A:33:PRO:HB3	1:A:53:HIS:CE1	2.44	0.53
1:B:37:ARG:O	1:B:38:GLU:HB3	2.08	0.52
1:A:313:GLY:HA2	1:A:317:GLY:O	2.09	0.52
1:A:327:LEU:HD23	1:A:327:LEU:C	2.29	0.52
1:A:136:PHE:HA	1:A:139:GLN:OE1	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:HIS:HB2	1:A:152:ILE:HG23	1.90	0.52
1:A:264:ARG:O	1:A:274:ILE:HG22	2.08	0.52
1:B:56:THR:HG22	1:B:58:GLN:N	2.10	0.52
1:A:137:PHE:CD1	1:A:221:LEU:HD13	2.45	0.52
1:A:144:ILE:CG1	1:A:148:HIS:NE2	2.69	0.52
1:A:28:LYS:HG2	1:A:29:ARG:N	2.21	0.51
1:A:78:ARG:O	1:A:82:GLU:HB2	2.10	0.51
1:B:291:ASP:HB2	1:B:294:ARG:NH1	2.25	0.51
1:B:150:HIS:HB2	1:B:152:ILE:HD11	1.93	0.51
1:B:353:GLU:C	1:B:355:HIS:H	2.13	0.51
1:A:141:ILE:HG21	1:A:285:PHE:CE1	2.46	0.51
1:A:201:VAL:CG1	1:A:202:ILE:HG23	2.41	0.51
1:B:83:ILE:HD12	1:B:84:SER:N	2.26	0.51
1:B:203:ASN:ND2	1:A:203:ASN:O	2.44	0.51
2:B:406:HOH:O	1:A:228:ARG:CD	2.58	0.51
1:A:346:GLN:O	1:A:349:GLN:HB3	2.11	0.51
1:B:29:ARG:O	1:B:36:ILE:HG12	2.11	0.50
1:A:91:HIS:HB3	1:A:94:ILE:HG13	1.93	0.50
1:A:129:THR:OG1	1:A:132:GLU:HG2	2.11	0.50
1:B:270:PRO:HG3	1:A:200:GLU:CD	2.31	0.50
1:A:84:SER:C	1:A:86:LEU:H	2.13	0.50
1:A:145:GLU:HG3	1:A:280:ARG:NH1	2.24	0.50
1:B:56:THR:HG22	1:B:58:GLN:HB2	1.92	0.50
1:B:158:LYS:H	1:B:161:ASN:ND2	2.06	0.50
1:B:226:VAL:HG12	1:B:228:ARG:HG2	1.93	0.50
1:B:305:ASP:HB3	1:B:339:TYR:OH	2.11	0.50
1:A:305:ASP:C	1:A:307:ARG:H	2.15	0.50
1:A:67:ARG:HH11	1:A:102:THR:CG2	2.25	0.50
1:B:31:ILE:CG2	1:B:36:ILE:HD11	2.41	0.50
1:B:182:THR:HG23	1:B:183:ASP:N	2.26	0.50
1:A:31:ILE:HD12	1:A:108:VAL:HG21	1.94	0.50
1:B:79:VAL:HG22	1:A:235:PHE:CD1	2.47	0.49
1:A:218:GLY:C	1:A:266:ILE:HD11	2.33	0.49
1:A:345:ASN:N	1:A:345:ASN:HD22	2.10	0.49
1:A:287:VAL:HG12	1:A:288:ASN:OD1	2.12	0.49
1:B:325:GLU:HA	1:B:328:ARG:NH1	2.27	0.49
1:A:286:ASN:HD22	1:A:289:LEU:HD12	1.77	0.49
1:B:211:GLU:O	1:B:273:ARG:NH1	2.40	0.49
1:A:114:ALA:HB1	1:A:164:LEU:C	2.33	0.49
1:A:341:LEU:HD23	1:A:342:LEU:N	2.27	0.49
1:A:344:GLU:O	1:A:347:VAL:HG13	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:ILE:CG1	1:A:170:VAL:HG11	2.42	0.49
1:A:177:LEU:HD22	1:A:177:LEU:N	2.28	0.49
1:B:305:ASP:OD2	1:B:305:ASP:C	2.51	0.49
1:B:308:ILE:HD11	1:B:339:TYR:CG	2.48	0.49
1:A:34:TYR:N	1:A:34:TYR:CD1	2.81	0.49
1:B:27:SER:N	2:B:418:HOH:O	2.46	0.48
1:A:235:PHE:O	1:A:236:ILE:CB	2.60	0.48
1:A:264:ARG:NH2	2:A:373:HOH:O	2.41	0.48
1:B:200:GLU:CG	1:A:270:PRO:HG3	2.43	0.48
1:A:98:TYR:HB2	1:A:110:VAL:HG12	1.94	0.48
1:A:30:HIS:CE1	2:A:368:HOH:O	2.66	0.48
1:A:350:GLU:C	1:A:352:LEU:H	2.16	0.48
1:A:138:GLN:HA	1:A:141:ILE:HG22	1.94	0.48
1:A:87:LYS:HG2	1:A:97:LEU:HD23	1.96	0.47
1:A:221:LEU:HA	1:A:224:MET:HE2	1.96	0.47
2:B:406:HOH:O	1:A:228:ARG:HD3	2.13	0.47
1:A:95:ILE:CD1	1:A:171:LYS:HB3	2.43	0.47
1:A:344:GLU:HA	1:A:347:VAL:HG12	1.93	0.47
1:B:30:HIS:O	1:B:31:ILE:HG22	2.13	0.47
1:B:327:LEU:HD23	1:B:336:LYS:HG2	1.96	0.47
1:B:83:ILE:CD1	1:B:100:VAL:HG21	2.40	0.47
1:B:308:ILE:HG12	1:B:339:TYR:CE1	2.49	0.47
1:B:317:GLY:O	1:B:318:PHE:O	2.32	0.47
1:A:50:LEU:HD12	1:A:50:LEU:HA	1.62	0.47
1:B:28:LYS:O	1:B:29:ARG:CB	2.62	0.47
1:B:203:ASN:HD22	1:B:203:ASN:H	1.61	0.47
1:A:134:ARG:HG3	1:A:135:ARG:N	2.29	0.47
1:A:204:GLY:O	1:A:207:TYR:CZ	2.67	0.47
1:A:218:GLY:HA3	1:A:266:ILE:HD12	1.96	0.47
1:A:159:PRO:C	1:A:161:ASN:H	2.18	0.47
1:B:95:ILE:HG13	1:B:173:ALA:HB2	1.96	0.47
1:A:327:LEU:HB2	2:A:374:HOH:O	2.14	0.47
1:A:144:ILE:HG22	1:A:145:GLU:H	1.79	0.47
1:A:343:HIS:O	1:A:347:VAL:HG12	2.15	0.46
1:B:236:ILE:CG2	1:B:239:LEU:HB2	2.45	0.46
1:A:144:ILE:HD11	1:A:213:ASP:OD2	2.16	0.46
1:A:222:TYR:C	1:A:222:TYR:HD2	2.18	0.46
1:A:44:SER:OG	1:A:45:PHE:N	2.48	0.46
1:B:250:MET:CE	1:B:259:GLN:HG2	2.43	0.46
1:A:76:HIS:HB2	1:A:79:VAL:HB	1.97	0.46
1:B:77:MET:O	1:B:81:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:179:ASN:HB3	1:B:183:ASP:HB2	1.98	0.46
1:B:42:GLU:OE2	1:B:47:LYS:HG2	2.15	0.46
1:B:84:SER:HA	1:B:87:LYS:CG	2.42	0.46
1:B:147:CYS:O	1:B:150:HIS:N	2.41	0.46
1:B:291:ASP:HA	1:B:294:ARG:HG3	1.97	0.46
1:A:269:ASP:OD2	1:A:272:GLN:HB2	2.15	0.46
1:B:52:THR:HA	1:B:58:GLN:O	2.17	0.46
1:B:266:ILE:HG22	1:B:266:ILE:O	2.16	0.45
1:B:298:GLU:O	1:B:299:VAL:O	2.34	0.45
1:B:95:ILE:HG23	1:B:112:GLU:HB3	1.97	0.45
1:B:189:THR:HG23	1:B:196:TYR:HD1	1.81	0.45
1:A:210:PRO:HB3	1:A:276:ILE:HG12	1.99	0.45
1:A:70:LEU:HD21	1:A:79:VAL:HG11	1.98	0.45
1:A:74:ASP:HA	1:A:76:HIS:ND1	2.31	0.45
1:A:111:ILE:HG22	1:A:112:GLU:O	2.17	0.45
1:A:292:TYR:CD1	1:A:293:LEU:HD13	2.51	0.45
1:B:33:PRO:HD2	1:B:34:TYR:CD1	2.51	0.45
1:A:288:ASN:O	1:A:290:PRO:HD3	2.16	0.45
1:A:304:ALA:O	1:A:305:ASP:C	2.55	0.45
1:A:174:ASP:HB3	1:A:175:PHE:H	1.54	0.45
1:B:86:LEU:HD23	1:B:86:LEU:HA	1.74	0.45
1:B:28:LYS:O	1:B:28:LYS:HG2	2.17	0.45
1:A:38:GLU:HB3	1:A:50:LEU:HB3	1.99	0.45
1:B:88:LEU:N	1:B:88:LEU:HD23	2.33	0.44
1:B:312:LEU:HD11	1:B:339:TYR:HA	1.99	0.44
1:A:286:ASN:O	1:A:289:LEU:HB2	2.18	0.44
1:A:58:GLN:HE21	1:A:58:GLN:HB3	1.69	0.44
1:A:67:ARG:NH1	1:A:102:THR:HG22	2.33	0.44
1:A:95:ILE:HD12	1:A:171:LYS:HB3	1.99	0.44
1:A:101:ILE:O	1:A:108:VAL:HG22	2.17	0.44
1:B:47:LYS:O	1:B:64:PHE:HB2	2.17	0.44
1:B:31:ILE:O	1:B:31:ILE:CG1	2.66	0.44
1:B:182:THR:HG23	1:B:183:ASP:H	1.82	0.44
1:B:225:LEU:HB3	1:B:254:LEU:HD11	2.00	0.44
1:A:144:ILE:O	1:A:147:CYS:N	2.51	0.44
1:B:33:PRO:HB2	1:B:53:HIS:CD2	2.53	0.44
1:B:206:LEU:HD12	1:B:206:LEU:C	2.38	0.44
1:B:270:PRO:HG3	1:A:200:GLU:CG	2.48	0.44
1:A:200:GLU:H	1:A:200:GLU:HG3	1.07	0.44
1:A:331:GLU:O	1:A:332:ASN:C	2.55	0.44
1:B:89:LEU:HD11	1:B:152:ILE:HG12	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:67:ARG:NH1	1:A:103:THR:O	2.51	0.43
1:A:137:PHE:CZ	1:A:141:ILE:HD13	2.53	0.43
1:B:246:CYS:HB2	2:B:3:HOH:O	2.18	0.43
1:B:320:GLU:C	1:B:324:VAL:HG23	2.38	0.43
1:A:84:SER:C	1:A:86:LEU:N	2.72	0.43
1:B:299:VAL:HB	1:B:300:GLN:H	1.00	0.43
1:B:236:ILE:HA	1:B:237:PRO:HD3	1.85	0.43
1:A:86:LEU:HD23	1:A:89:LEU:HD12	2.01	0.43
1:A:91:HIS:HA	1:A:92:PRO:HD3	1.85	0.43
1:A:294:ARG:HA	1:A:295:PRO:HD3	1.89	0.43
1:B:27:SER:OG	1:B:28:LYS:N	2.51	0.43
1:B:200:GLU:HG2	1:A:270:PRO:HG2	2.00	0.43
1:A:184:GLY:O	1:A:188:LYS:HG3	2.18	0.43
1:B:85:TYR:C	1:B:85:TYR:CD2	2.91	0.43
1:B:125:LYS:O	1:B:126:LYS:HB2	2.18	0.43
1:B:282:ASP:HA	1:B:283:PRO:HD3	1.93	0.43
1:B:302:SER:OG	1:B:304:ALA:HB3	2.18	0.43
1:A:39:THR:O	1:A:39:THR:CG2	2.66	0.43
1:A:45:PHE:CD1	1:A:176:GLY:O	2.72	0.43
1:A:308:ILE:O	1:A:312:LEU:HG	2.18	0.43
1:A:49:LYS:HD2	1:A:64:PHE:CZ	2.53	0.43
1:A:163:LEU:HD23	1:A:163:LEU:N	2.34	0.42
1:A:305:ASP:O	1:A:306:SER:OG	2.34	0.42
1:A:102:THR:HG23	1:A:107:ILE:HG23	2.02	0.42
1:A:125:LYS:O	1:A:126:LYS:HB3	2.19	0.42
1:A:289:LEU:HD21	1:A:293:LEU:CB	2.49	0.42
1:A:318:PHE:HB3	1:A:322:TYR:CD2	2.54	0.42
1:B:240:PHE:N	2:B:402:HOH:O	2.49	0.42
1:B:280:ARG:NH2	1:B:293:LEU:O	2.44	0.42
1:A:38:GLU:HB3	1:A:50:LEU:CB	2.49	0.42
1:B:59:LYS:H	1:B:59:LYS:HZ3	1.65	0.42
1:A:155:ARG:O	1:A:157:LEU:HD12	2.20	0.42
1:A:216:SER:O	1:A:220:VAL:HG23	2.19	0.42
1:A:318:PHE:HD2	1:A:322:TYR:CE2	2.23	0.42
1:A:63:LYS:HB2	1:A:63:LYS:HE3	1.92	0.42
1:B:318:PHE:N	1:B:318:PHE:CD1	2.85	0.42
1:A:45:PHE:HB3	1:A:65:ILE:HG12	2.02	0.42
1:A:269:ASP:HA	1:A:270:PRO:HD3	1.68	0.42
1:B:147:CYS:O	1:B:148:HIS:C	2.57	0.42
1:B:168:LEU:HD12	1:B:168:LEU:HA	1.80	0.42
1:A:98:TYR:HB2	1:A:110:VAL:CG1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:H	1:A:152:ILE:HG12	1.73	0.42
1:B:71:LYS:CG	2:B:408:HOH:O	2.05	0.42
1:B:269:ASP:OD2	1:B:269:ASP:C	2.58	0.42
1:B:276:ILE:HD13	1:B:276:ILE:C	2.40	0.42
1:A:235:PHE:CA	1:A:236:ILE:HG23	2.46	0.42
1:A:211:GLU:O	1:A:273:ARG:NH1	2.52	0.41
1:B:122:ILE:O	1:B:126:LYS:O	2.37	0.41
1:A:31:ILE:CD1	1:A:62:LEU:HD13	2.44	0.41
1:A:155:ARG:C	1:A:155:ARG:HD3	2.32	0.41
1:A:297:GLU:CG	1:A:298:GLU:H	2.26	0.41
1:B:302:SER:C	1:B:304:ALA:H	2.23	0.41
1:A:260:SER:HG	1:A:264:ARG:HH12	1.65	0.41
1:B:56:THR:O	1:B:57:GLN:CB	2.67	0.41
1:A:67:ARG:NH1	1:A:102:THR:CG2	2.84	0.41
1:A:156:ASP:HB3	1:A:158:LYS:HE2	2.02	0.41
1:B:133:GLY:HA3	1:B:225:LEU:CD1	2.51	0.41
1:B:320:GLU:O	1:B:323:ILE:HB	2.21	0.41
1:A:265:MET:O	1:A:273:ARG:HD3	2.20	0.41
1:B:70:LEU:HA	1:B:70:LEU:HD23	1.79	0.41
1:B:207:TYR:CD2	1:A:201:VAL:HG21	2.56	0.41
1:A:155:ARG:HD3	1:A:155:ARG:HA	1.74	0.41
1:B:31:ILE:O	1:B:31:ILE:HG13	2.20	0.41
1:B:95:ILE:HG12	1:B:171:LYS:HB3	2.03	0.41
1:B:322:TYR:C	1:B:322:TYR:CD1	2.94	0.41
1:B:353:GLU:C	1:B:355:HIS:N	2.75	0.41
1:A:226:VAL:HG22	1:A:251:PRO:HG2	2.03	0.41
1:B:198:ALA:HA	1:B:199:PRO:HD3	1.99	0.41
1:A:83:ILE:H	1:A:83:ILE:HG13	1.73	0.41
1:A:101:ILE:HB	1:A:108:VAL:HG22	2.03	0.41
1:B:237:PRO:O	1:A:44:SER:O	2.39	0.40
1:A:34:TYR:CD2	1:A:60:VAL:HG11	2.56	0.40
1:A:179:ASN:HD21	1:A:181:MET:HB3	1.86	0.40
1:A:208:ALA:CB	1:A:211:GLU:OE1	2.67	0.40
1:B:195:ASN:HD22	1:A:229:LEU:HD22	1.85	0.40
1:B:202:ILE:C	1:B:204:GLY:N	2.75	0.40
1:B:206:LEU:C	1:B:208:ALA:H	2.24	0.40
1:B:241:LYS:HB3	1:B:242:LYS:H	1.67	0.40
1:A:76:HIS:C	1:A:78:ARG:H	2.24	0.40
1:A:85:TYR:O	1:A:85:TYR:CD2	2.74	0.40
1:A:257:GLY:O	1:A:260:SER:HB3	2.21	0.40
1:A:327:LEU:HG	1:A:336:LYS:CE	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:340:ASN:HD22	1:A:340:ASN:H	1.68	0.40
1:A:102:THR:HG23	1:A:107:ILE:CG2	2.52	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	312/336 (93%)	243 (78%)	50 (16%)	19 (6%)	1 4
1	B	328/336 (98%)	277 (84%)	40 (12%)	11 (3%)	3 13
All	All	640/672 (95%)	520 (81%)	90 (14%)	30 (5%)	2 7

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	299	VAL
1	B	318	PHE
1	B	331	GLU
1	A	159	PRO
1	A	160	GLU
1	A	332	ASN
1	A	333	ASN
1	B	300	GLN
1	B	301	GLY
1	B	314	GLU
1	B	329	SER
1	B	332	ASN
1	A	38	GLU
1	A	44	SER
1	A	74	ASP
1	A	253	PHE

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Mol	Chain	Res	Type
1	B	302	SER
1	B	326	ALA
1	A	297	GLU
1	A	305	ASP
1	A	292	TYR
1	A	126	LYS
1	A	156	ASP
1	A	204	GLY
1	A	351	LYS
1	A	290	PRO
1	A	298	GLU
1	B	31	ILE
1	A	115	GLY
1	A	283	PRO

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	284/303 (94%)	235 (83%)	49 (17%)	2 6
1	B	298/303 (98%)	256 (86%)	42 (14%)	3 10
All	All	582/606 (96%)	491 (84%)	91 (16%)	2 8

All (91) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	31	ILE
1	B	35	ILE
1	B	37	ARG
1	B	39	THR
1	B	56	THR
1	B	58	GLN
1	B	59	LYS
1	B	60	VAL
1	B	75	MET

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Mol	Chain	Res	Type
1	B	82	GLU
1	B	88	LEU
1	B	90	ARG
1	B	107	ILE
1	B	117	GLU
1	B	123	VAL
1	B	144	ILE
1	B	153	VAL
1	B	155	ARG
1	B	160	GLU
1	B	166	ASP
1	B	168	LEU
1	B	183	ASP
1	B	195	ASN
1	B	200	GLU
1	B	211	GLU
1	B	225	LEU
1	B	232	ASP
1	B	239	LEU
1	B	249	VAL
1	B	254	LEU
1	B	276	ILE
1	B	291	ASP
1	B	293	LEU
1	B	299	VAL
1	B	308	ILE
1	B	310	SER
1	B	321	ASP
1	B	322	TYR
1	B	330	ASP
1	B	332	ASN
1	B	348	ILE
1	B	356	HIS
1	A	29	ARG
1	A	30	HIS
1	A	35	ILE
1	A	39	THR
1	A	60	VAL
1	A	75	MET
1	A	85	TYR
1	A	88	LEU
1	A	90	ARG

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Mol	Chain	Res	Type
1	A	95	ILE
1	A	103	THR
1	A	107	ILE
1	A	118	LEU
1	A	144	ILE
1	A	145	GLU
1	A	148	HIS
1	A	149	ARG
1	A	154	HIS
1	A	155	ARG
1	A	157	LEU
1	A	158	LYS
1	A	161	ASN
1	A	166	ASP
1	A	174	ASP
1	A	175	PHE
1	A	177	LEU
1	A	179	ASN
1	A	191	CYS
1	A	200	GLU
1	A	201	VAL
1	A	205	LYS
1	A	206	LEU
1	A	207	TYR
1	A	222	TYR
1	A	225	LEU
1	A	250	MET
1	A	271	MET
1	A	272	GLN
1	A	281	ARG
1	A	289	LEU
1	A	293	LEU
1	A	299	VAL
1	A	329	SER
1	A	330	ASP
1	A	331	GLU
1	A	333	ASN
1	A	334	GLU
1	A	343	HIS
1	A	347	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	30	HIS
1	B	58	GLN
1	B	76	HIS
1	B	161	ASN
1	B	203	ASN
1	B	340	ASN
1	B	345	ASN
1	B	355	HIS
1	A	58	GLN
1	A	91	HIS
1	A	93	HIS
1	A	138	GLN
1	A	161	ASN
1	A	179	ASN
1	A	185	ASN
1	A	203	ASN
1	A	277	GLN
1	A	286	ASN
1	A	340	ASN
1	A	345	ASN
1	A	346	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 monosaccharides in this entry.

5.6 Ligand geometry

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, 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	316/336 (94%)	0.20	17 (5%) 25 17	54, 109, 201, 271	0
1	B	330/336 (98%)	-0.15	4 (1%) 79 73	41, 70, 165, 232	0
All	All	646/672 (96%)	0.02	21 (3%) 46 36	41, 90, 189, 271	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	155	ARG	6.6
1	A	207	TYR	5.6
1	A	77	MET	5.4
1	A	299	VAL	5.0
1	A	354	HIS	3.8
1	A	55	LYS	3.3
1	A	307	ARG	3.1
1	A	321	ASP	2.9
1	A	319	SER	2.9
1	A	322	TYR	2.9
1	A	175	PHE	2.8
1	A	324	VAL	2.8
1	A	331	GLU	2.6
1	A	176	GLY	2.4
1	A	156	ASP	2.4
1	A	54	TYR	2.2
1	B	207	TYR	2.2
1	B	154	HIS	2.2
1	A	210	PRO	2.1
1	B	27	SER	2.0
1	B	321	ASP	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 monosaccharides 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.