Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 04:33 PM GMT

PDB ID	:	4FE4
Title	:	Crystal structure of apo E. coli XylR
Authors	:	Schumacher, M.A.; Ni, L.
Deposited on	:	2012-05-29
Resolution	:	3.45 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:

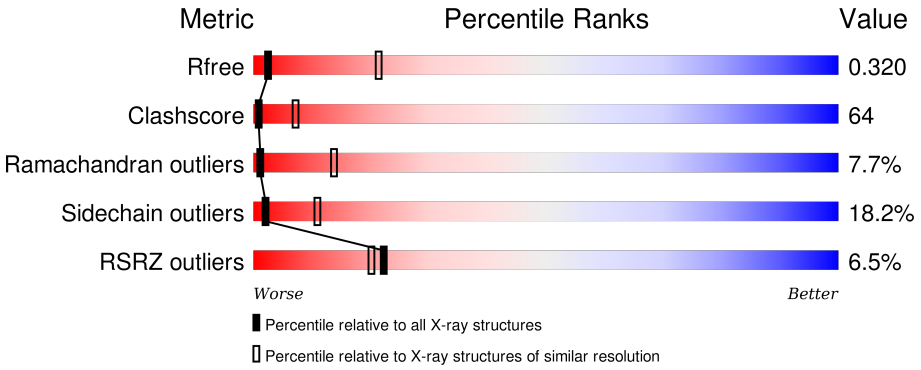
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.45 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}	91344	1000 (3.56-3.36)
Clashscore	102246	1090 (3.56-3.36)
Ramachandran outliers	100387	1057 (3.56-3.36)
Sidechain outliers	100360	1058 (3.56-3.36)
RSRZ outliers	91569	1005 (3.56-3.36)

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	392	6% 22% 57% 16%
1	B	392	3% 26% 55% 15%
1	C	392	10% 25% 56% 14%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9189 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 Xylose operon regulatory protein.

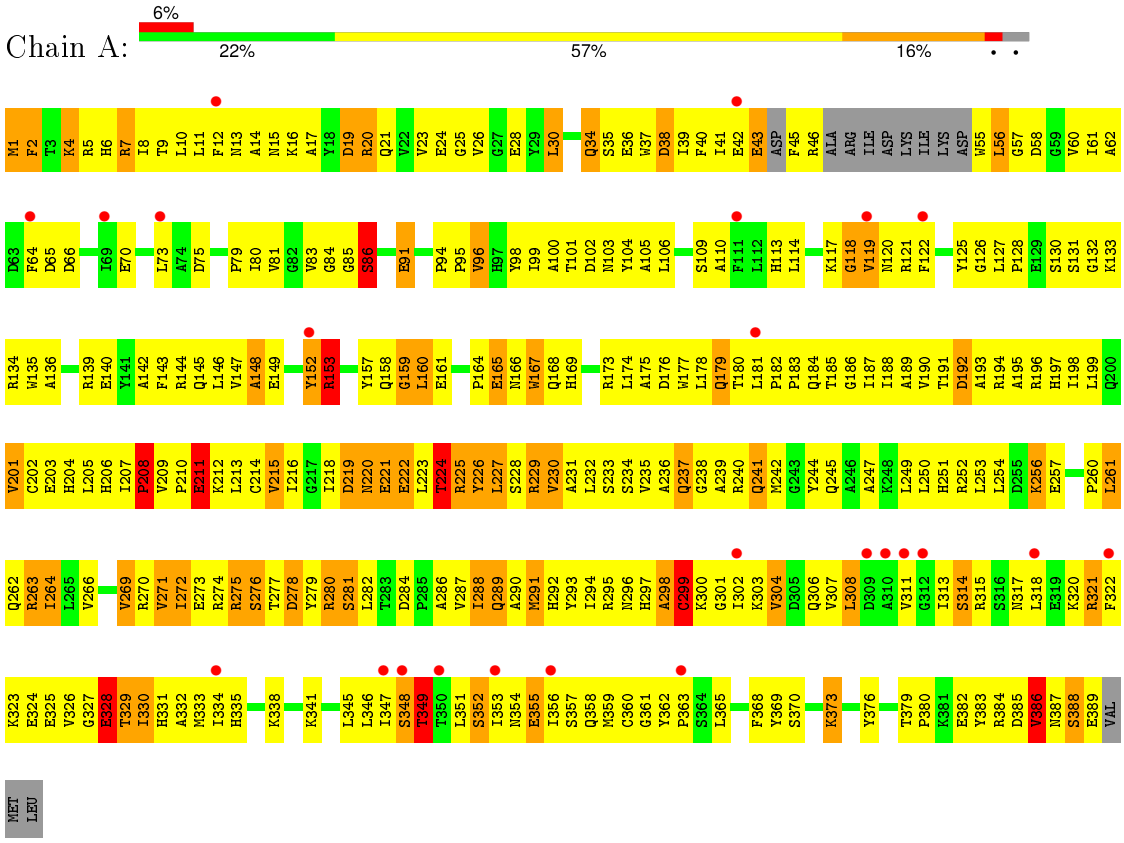
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			3063	1946	538	569	10			
1	B	380	Total	C	N	O	S	0	0	0
			3063	1946	538	569	10			
1	C	380	Total	C	N	O	S	0	0	0
			3063	1946	538	569	10			

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.

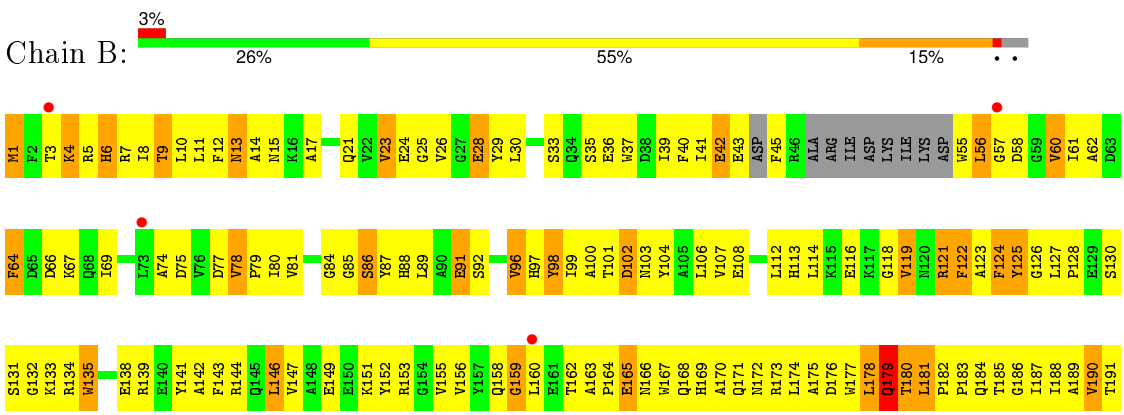
- Molecule 1: Xylose operon regulatory protein

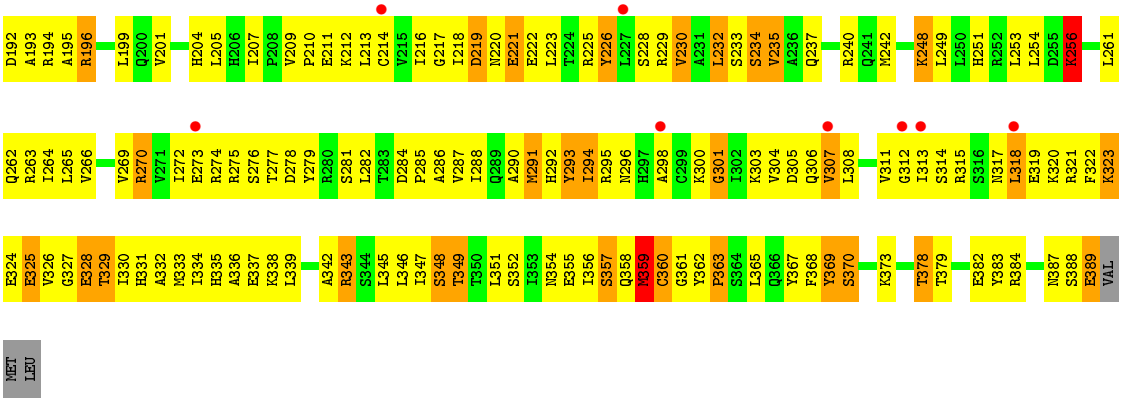
Chain A:



- Molecule 1: Xylose operon regulatory protein

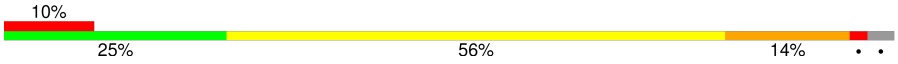
Chain B:

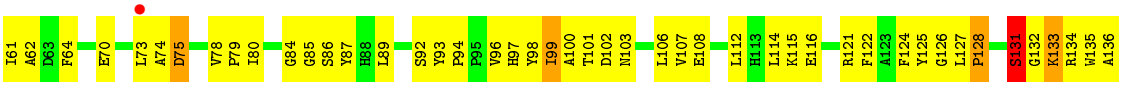


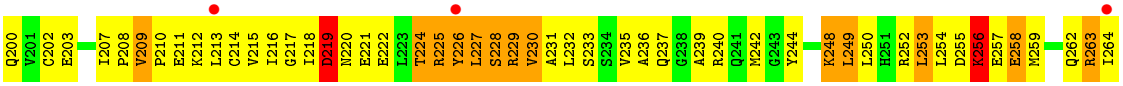


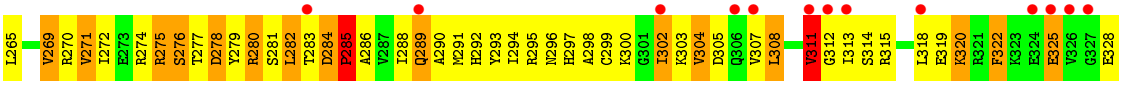
- Molecule 1: Xylose operon regulatory protein

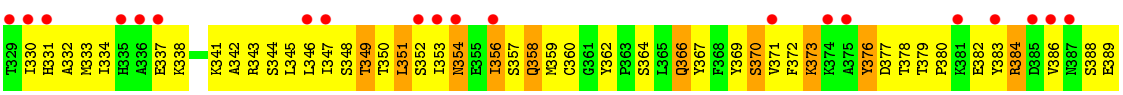
Chain C:











4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α, β, γ	124.50Å 124.50Å 189.80Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	107.80 – 3.45 107.82 – 3.45	Depositor EDS
% Data completeness (in resolution range)	96.3 (107.80-3.45) 96.3 (107.82-3.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.71 (at 3.49Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.289 , 0.318 0.290 , 0.320	Depositor DCC
R_{free} test set	1222 reflections (5.52%)	DCC
Wilson B-factor (Å^2)	97.2	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 80.1	EDS
Estimated twinning fraction	0.109 for -h,-k,l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.40$, $< L^2 > = 0.23$	Xtriage
Outliers	3 of 22149 reflections (0.014%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	9189	wwPDB-VP
Average B, all atoms (Å^2)	115.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.71% 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	0.55	1/3129 (0.0%)	0.79	2/4238 (0.0%)
1	B	0.58	0/3129	0.76	1/4238 (0.0%)
1	C	0.62	2/3129 (0.1%)	0.80	2/4238 (0.0%)
All	All	0.58	3/9387 (0.0%)	0.78	5/12714 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	140	GLU	CG-CD	-6.95	1.41	1.51
1	C	311	VAL	CB-CG1	-5.92	1.40	1.52
1	A	386	VAL	CB-CG2	-5.58	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	235	VAL	CB-CA-C	-7.39	97.36	111.40
1	A	325	GLU	N-CA-C	6.39	128.25	111.00
1	C	99	ILE	N-CA-C	-5.61	95.85	111.00
1	A	324	GLU	N-CA-C	5.35	125.44	111.00
1	C	219	ASP	CB-CG-OD2	-5.32	113.51	118.30

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	3063	0	3028	426	0
1	B	3063	0	3028	346	0
1	C	3063	0	3028	424	1
All	All	9189	0	9084	1169	1

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 64.

All (1169) 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:320:LYS:O	1:B:323:LYS:HE2	1.42	1.18
1:A:280:ARG:HG2	1:A:282:LEU:HD12	1.28	1.12
1:A:282:LEU:HD21	1:A:326:VAL:HG21	1.12	1.11
1:A:280:ARG:HG2	1:A:282:LEU:CD1	1.81	1.09
1:B:320:LYS:O	1:B:323:LYS:CE	2.01	1.07
1:A:272:ILE:H	1:A:272:ILE:HD12	1.15	1.06
1:A:382:GLU:O	1:A:386:VAL:HG23	1.58	1.03
1:B:98:TYR:HD2	1:B:100:ALA:HB2	1.24	1.01
1:A:223:LEU:HD12	1:C:24:GLU:HG3	1.41	1.01
1:A:308:LEU:HA	1:A:318:LEU:HG	1.43	1.00
1:C:79:PRO:HB3	1:C:253:LEU:HD22	1.42	1.00
1:A:210:PRO:HD2	1:A:295:ARG:NH1	1.78	0.99
1:A:282:LEU:CD2	1:A:326:VAL:HG21	1.93	0.98
1:B:225:ARG:NH2	1:B:389:GLU:O	1.94	0.98
1:C:190:VAL:HG23	1:C:191:THR:HG23	1.45	0.98
1:A:207:ILE:HG23	1:A:212:LYS:HD2	1.43	0.98
1:C:298:ALA:HA	1:C:302:ILE:HD11	1.39	0.98
1:B:79:PRO:HB3	1:B:253:LEU:HD23	1.46	0.97
1:A:4:LYS:HZ3	1:A:4:LYS:HA	1.28	0.96
1:C:11:LEU:HB3	1:C:43:GLU:OE1	1.65	0.96
1:A:269:VAL:HG12	1:A:270:ARG:HG3	1.49	0.94
1:B:354:ASN:HA	1:B:365:LEU:HD13	1.47	0.94
1:A:210:PRO:HD2	1:A:295:ARG:HH12	1.31	0.94
1:B:98:TYR:CD2	1:B:100:ALA:HB2	2.02	0.94
1:A:382:GLU:O	1:A:386:VAL:CG2	2.14	0.93
1:A:282:LEU:HD21	1:A:326:VAL:CG2	1.99	0.93
1:A:280:ARG:CG	1:A:282:LEU:CD1	2.47	0.93
1:A:346:LEU:HD23	1:A:384:ARG:HH11	1.34	0.92
1:A:280:ARG:CG	1:A:282:LEU:HD11	2.00	0.91
1:C:275:ARG:HG2	1:C:295:ARG:HH11	1.34	0.91
1:A:280:ARG:HG3	1:A:282:LEU:HD11	1.53	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:LYS:HA	1:A:4:LYS:NZ	1.84	0.91
1:B:37:TRP:HZ2	1:B:251:HIS:HB2	1.33	0.90
1:C:225:ARG:HE	1:C:274:ARG:NH2	1.69	0.90
1:B:242:MET:HA	1:B:266:VAL:HG21	1.53	0.90
1:C:160:LEU:H	1:C:194:ARG:HH12	1.17	0.89
1:A:274:ARG:HG3	1:A:274:ARG:HH11	1.34	0.89
1:C:311:VAL:HB	1:C:318:LEU:HD11	1.56	0.88
1:A:303:LYS:O	1:A:307:VAL:HG23	1.72	0.88
1:C:60:VAL:HB	1:C:80:ILE:HD13	1.53	0.88
1:A:10:LEU:HD22	1:A:61:ILE:HB	1.54	0.88
1:A:60:VAL:HB	1:A:80:ILE:HG22	1.55	0.88
1:C:224:THR:HA	1:C:227:LEU:HD12	1.54	0.88
1:C:283:THR:O	1:C:285:PRO:HD3	1.74	0.87
1:C:286:ALA:O	1:C:311:VAL:HG11	1.73	0.87
1:C:192:ASP:HB2	1:C:219:ASP:HB2	1.56	0.87
1:C:161:GLU:HB3	1:C:164:PRO:HB3	1.56	0.86
1:B:323:LYS:N	1:B:323:LYS:HD3	1.90	0.86
1:A:160:LEU:HD22	1:A:164:PRO:HB3	1.55	0.86
1:C:269:VAL:HG23	1:C:270:ARG:H	1.40	0.86
1:C:150:GLU:HG3	1:C:151:LYS:H	1.38	0.86
1:A:73:LEU:HD21	1:A:80:ILE:HG21	1.56	0.85
1:C:286:ALA:O	1:C:311:VAL:CG1	2.25	0.85
1:B:345:LEU:HA	1:B:349:THR:HG23	1.56	0.85
1:A:328:GLU:HG3	1:A:332:ALA:HB1	1.58	0.84
1:A:354:ASN:ND2	1:A:365:LEU:HD13	1.93	0.84
1:A:351:LEU:H	1:A:384:ARG:NH2	1.75	0.84
1:C:290:ALA:O	1:C:294:ILE:HG13	1.78	0.83
1:C:239:ALA:HA	1:C:242:MET:HG3	1.60	0.83
1:C:225:ARG:HE	1:C:274:ARG:HH22	1.27	0.83
1:A:230:VAL:HG12	1:A:275:ARG:HD2	1.59	0.83
1:C:235:VAL:HA	1:C:271:VAL:HG13	1.61	0.82
1:B:17:ALA:O	1:B:21:GLN:HG3	1.79	0.82
1:B:275:ARG:NH2	1:B:295:ARG:HD2	1.94	0.82
1:A:79:PRO:HG3	1:A:253:LEU:HD22	1.61	0.82
1:A:386:VAL:HG12	1:A:387:ASN:OD1	1.79	0.82
1:A:275:ARG:HH11	1:A:275:ARG:HG3	1.43	0.81
1:A:347:ILE:HG23	1:A:389:GLU:H	1.45	0.81
1:B:128:PRO:HB2	1:B:130:SER:HB3	1.62	0.81
1:A:346:LEU:HD23	1:A:384:ARG:NH1	1.96	0.81
1:B:96:VAL:HG22	1:B:97:HIS:H	1.46	0.81
1:B:304:VAL:O	1:B:307:VAL:HG23	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:ILE:HG23	1:A:317:ASN:HD22	1.44	0.80
1:C:218:ILE:HG22	1:C:218:ILE:O	1.80	0.80
1:A:167:TRP:CZ3	1:A:168:GLN:HB2	2.16	0.80
1:B:275:ARG:HH21	1:B:295:ARG:HD2	1.44	0.80
1:B:311:VAL:HG21	1:B:318:LEU:HD11	1.63	0.80
1:B:56:LEU:HG	1:B:57:GLY:H	1.44	0.80
1:B:308:LEU:HD23	1:B:318:LEU:HD13	1.64	0.79
1:C:308:LEU:O	1:C:318:LEU:CD1	2.31	0.79
1:A:196:ARG:NH2	1:A:225:ARG:HA	1.97	0.79
1:C:125:TYR:HE2	1:C:194:ARG:HB3	1.47	0.79
1:B:307:VAL:O	1:B:311:VAL:HG23	1.82	0.79
1:C:308:LEU:O	1:C:318:LEU:HD13	1.83	0.79
1:A:8:ILE:HD12	1:A:37:TRP:CE3	2.17	0.78
1:C:151:LYS:HB3	1:C:152:TYR:HD1	1.48	0.78
1:C:192:ASP:HB2	1:C:219:ASP:CB	2.13	0.78
1:B:166:ASN:HB2	1:B:169:HIS:HB3	1.66	0.78
1:C:73:LEU:HD13	1:C:80:ILE:HD12	1.66	0.78
1:B:186:GLY:HA2	1:B:214:CYS:HB2	1.66	0.78
1:A:160:LEU:HD13	1:A:164:PRO:HG3	1.64	0.77
1:C:107:VAL:HG22	1:C:139:ARG:HG2	1.65	0.77
1:A:282:LEU:CD2	1:A:326:VAL:CG2	2.60	0.77
1:A:313:ILE:HB	1:A:318:LEU:HD23	1.66	0.77
1:A:373:LYS:HA	1:A:376:TYR:O	1.84	0.77
1:B:262:GLN:C	1:B:263:ARG:HD2	2.04	0.77
1:B:42:GLU:O	1:B:43:GLU:HB2	1.82	0.77
1:A:215:VAL:HG23	1:A:276:SER:HB2	1.67	0.77
1:B:191:THR:HG22	1:B:193:ALA:H	1.49	0.77
1:B:124:PHE:CZ	1:B:190:VAL:HG13	2.20	0.77
1:A:229:ARG:HH12	1:A:296:ASN:HB3	1.48	0.77
1:B:210:PRO:HD2	1:B:295:ARG:HH12	1.49	0.77
1:B:311:VAL:CG2	1:B:318:LEU:HD11	2.15	0.77
1:C:14:ALA:O	1:C:20:ARG:HD2	1.84	0.77
1:C:79:PRO:CB	1:C:253:LEU:HD22	2.15	0.77
1:A:179:GLN:HE22	1:A:207:ILE:HD11	1.50	0.76
1:B:133:LYS:HD2	1:B:133:LYS:H	1.50	0.76
1:C:297:HIS:HB3	1:C:300:LYS:HD2	1.66	0.76
1:C:380:PRO:O	1:C:384:ARG:HB2	1.86	0.76
1:A:359:MET:SD	1:C:32:ALA:HB1	2.25	0.76
1:C:112:LEU:O	1:C:116:GLU:HG3	1.84	0.76
1:B:37:TRP:CZ2	1:B:251:HIS:HB2	2.21	0.76
1:B:303:LYS:H	1:B:306:GLN:HB2	1.51	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LEU:HA	1:C:194:ARG:HH21	1.51	0.76
1:C:290:ALA:HA	1:C:311:VAL:HG22	1.66	0.76
1:C:25:GLY:HA2	1:C:28:GLU:HG3	1.68	0.76
1:B:10:LEU:HD23	1:B:61:ILE:HB	1.66	0.75
1:C:79:PRO:HB3	1:C:253:LEU:CD2	2.17	0.75
1:A:354:ASN:HD21	1:A:365:LEU:HD13	1.47	0.75
1:B:8:ILE:HD13	1:B:37:TRP:HB3	1.68	0.75
1:C:5:ARG:HA	1:C:36:GLU:O	1.85	0.75
1:C:160:LEU:N	1:C:194:ARG:HH12	1.85	0.75
1:B:345:LEU:HA	1:B:349:THR:CG2	2.16	0.75
1:C:151:LYS:HB3	1:C:152:TYR:CD1	2.22	0.74
1:B:192:ASP:OD1	1:B:219:ASP:N	2.20	0.74
1:C:289:GLN:HB3	1:C:311:VAL:HA	1.66	0.74
1:B:292:HIS:CE1	1:B:296:ASN:HD21	2.06	0.74
1:B:272:ILE:HG21	1:B:274:ARG:HE	1.51	0.74
1:B:314:SER:O	1:B:318:LEU:HB2	1.87	0.74
1:C:89:LEU:O	1:C:92:SER:HB2	1.88	0.73
1:A:313:ILE:HG22	1:A:317:ASN:HB3	1.71	0.73
1:B:17:ALA:HB2	1:B:221:GLU:HA	1.70	0.73
1:B:294:ILE:HG22	1:B:298:ALA:HB2	1.70	0.73
1:C:378:THR:HG1	1:C:383:TYR:HD1	1.36	0.73
1:A:189:ALA:HB3	1:A:195:ALA:HB2	1.69	0.73
1:B:23:VAL:HG21	1:B:41:ILE:HD11	1.68	0.73
1:A:223:LEU:HD12	1:C:24:GLU:CG	2.18	0.73
1:B:308:LEU:CD2	1:B:318:LEU:HD13	2.18	0.73
1:C:208:PRO:HB3	1:C:211:GLU:HB2	1.70	0.73
1:B:249:LEU:O	1:B:249:LEU:HD23	1.88	0.73
1:A:41:ILE:HG22	1:A:41:ILE:O	1.88	0.73
1:B:367:TYR:O	1:B:370:SER:HB3	1.89	0.73
1:A:275:ARG:NH1	1:A:275:ARG:HG3	2.04	0.73
1:A:277:THR:O	1:A:279:TYR:N	2.21	0.73
1:A:216:ILE:HD12	1:A:233:SER:O	1.89	0.72
1:B:343:ARG:HG2	1:B:383:TYR:CE2	2.24	0.72
1:B:343:ARG:HH11	1:B:383:TYR:HE2	1.35	0.72
1:C:131:SER:O	1:C:133:LYS:N	2.21	0.72
1:B:114:LEU:O	1:B:119:VAL:HB	1.89	0.72
1:B:262:GLN:O	1:B:263:ARG:HD2	1.90	0.72
1:A:230:VAL:CG1	1:A:275:ARG:HD2	2.18	0.72
1:A:227:LEU:HB3	1:C:27:GLY:CA	2.19	0.72
1:A:101:THR:HB	1:A:242:MET:CE	2.19	0.72
1:C:328:GLU:HB2	1:C:332:ALA:HB3	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:PRO:HD2	1:B:367:TYR:CD2	2.24	0.72
1:A:179:GLN:NE2	1:A:207:ILE:HD11	2.04	0.72
1:C:292:HIS:O	1:C:296:ASN:HB2	1.89	0.71
1:A:46:ARG:NH1	1:A:46:ARG:HB2	2.04	0.71
1:B:67:LYS:HE2	1:B:134:ARG:NH1	2.05	0.71
1:B:11:LEU:HB2	1:B:62:ALA:CB	2.20	0.71
1:A:11:LEU:HB2	1:A:62:ALA:HB2	1.72	0.71
1:C:155:VAL:HG11	1:C:177:TRP:HE1	1.56	0.71
1:A:175:ALA:HA	1:A:178:LEU:HD13	1.72	0.71
1:C:56:LEU:HD21	1:C:60:VAL:HG21	1.72	0.71
1:A:34:GLN:NE2	1:C:229:ARG:HD2	2.06	0.71
1:C:160:LEU:H	1:C:194:ARG:NH1	1.88	0.71
1:A:212:LYS:HG2	1:A:213:LEU:HG	1.72	0.71
1:B:188:ILE:HA	1:B:216:ILE:HG22	1.73	0.71
1:B:89:LEU:HB3	1:B:91:GLU:OE1	1.91	0.71
1:A:199:LEU:HD21	1:A:215:VAL:HG21	1.71	0.70
1:A:6:HIS:O	1:A:8:ILE:HG13	1.91	0.70
1:A:133:LYS:H	1:A:133:LYS:HD2	1.55	0.70
1:C:108:GLU:O	1:C:112:LEU:HD12	1.92	0.70
1:A:20:ARG:O	1:A:24:GLU:HG3	1.91	0.70
1:A:272:ILE:H	1:A:272:ILE:CD1	1.93	0.70
1:C:131:SER:C	1:C:133:LYS:H	1.95	0.70
1:A:60:VAL:HG12	1:A:61:ILE:H	1.56	0.70
1:C:362:TYR:HD1	1:C:367:TYR:HD2	1.39	0.70
1:A:133:LYS:HD2	1:A:133:LYS:N	2.06	0.69
1:C:364:SER:HB2	1:C:366:GLN:HG3	1.74	0.69
1:B:317:ASN:HB3	1:B:321:ARG:HD2	1.74	0.69
1:A:11:LEU:HB2	1:A:62:ALA:CB	2.22	0.69
1:B:284:ASP:HB3	1:B:325:GLU:OE1	1.92	0.69
1:C:196:ARG:HG3	1:C:224:THR:HG21	1.74	0.69
1:B:335:HIS:HA	1:B:338:LYS:HE2	1.74	0.69
1:A:15:ASN:CG	1:A:16:LYS:H	1.94	0.69
1:A:160:LEU:H	1:A:194:ARG:HH22	1.39	0.69
1:A:225:ARG:HH21	1:A:274:ARG:CZ	2.05	0.69
1:B:7:ARG:HD3	1:B:57:GLY:HA2	1.75	0.69
1:A:240:ARG:HD3	1:C:350:THR:HG21	1.73	0.69
1:B:183:PRO:HG3	1:B:212:LYS:HE2	1.74	0.69
1:A:225:ARG:HE	1:A:274:ARG:NH1	1.91	0.69
1:A:34:GLN:HE21	1:C:229:ARG:HD2	1.58	0.69
1:A:25:GLY:O	1:A:28:GLU:HB3	1.91	0.69
1:C:299:CYS:HA	1:C:338:LYS:CG	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:342:ALA:HB2	1:C:360:CYS:SG	2.33	0.69
1:A:328:GLU:HB3	1:A:333:MET:HG2	1.75	0.68
1:B:123:ALA:HB2	1:B:181:LEU:HD21	1.73	0.68
1:C:21:GLN:HB3	1:C:239:ALA:HB3	1.74	0.68
1:C:311:VAL:CB	1:C:318:LEU:HD11	2.23	0.68
1:B:133:LYS:HD2	1:B:133:LYS:N	2.08	0.68
1:A:121:ARG:HG2	1:A:152:TYR:CD1	2.29	0.68
1:A:13:ASN:O	1:A:19:ASP:HB3	1.92	0.68
1:A:42:GLU:O	1:A:43:GLU:HB2	1.93	0.68
1:A:95:PRO:O	1:A:96:VAL:HB	1.92	0.68
1:B:369:TYR:CZ	1:B:373:LYS:HD2	2.28	0.67
1:A:348:SER:O	1:A:349:THR:HG23	1.94	0.67
1:C:197:HIS:HA	1:C:200:GLN:NE2	2.10	0.67
1:C:197:HIS:N	1:C:200:GLN:HE21	1.92	0.67
1:C:70:GLU:OE2	1:C:94:PRO:HB3	1.94	0.67
1:B:343:ARG:HB3	1:B:343:ARG:CZ	2.24	0.67
1:C:161:GLU:HB3	1:C:164:PRO:CB	2.24	0.67
1:B:210:PRO:HD2	1:B:295:ARG:NH1	2.10	0.67
1:C:313:ILE:HG22	1:C:314:SER:H	1.60	0.67
1:A:61:ILE:HD13	1:A:81:VAL:HB	1.77	0.67
1:A:167:TRP:CE3	1:A:168:GLN:HB2	2.29	0.67
1:B:5:ARG:HA	1:B:36:GLU:O	1.95	0.67
1:A:26:VAL:HG13	1:A:247:ALA:HB2	1.76	0.67
1:C:299:CYS:HA	1:C:338:LYS:HG3	1.76	0.67
1:B:30:LEU:HD23	1:B:30:LEU:O	1.94	0.67
1:B:218:ILE:HA	1:B:235:VAL:HG23	1.76	0.66
1:A:253:LEU:O	1:A:253:LEU:HD23	1.94	0.66
1:B:56:LEU:CD2	1:B:78:VAL:HG21	2.24	0.66
1:A:185:THR:HG22	1:A:186:GLY:N	2.11	0.66
1:C:293:TYR:HE2	1:C:302:ILE:HG13	1.59	0.66
1:A:43:GLU:HG2	1:A:45:PHE:O	1.96	0.66
1:C:33:SER:O	1:C:34:GLN:HB2	1.95	0.66
1:B:135:TRP:HE3	1:B:139:ARG:NH2	1.94	0.66
1:A:304:VAL:HG12	1:A:308:LEU:HD21	1.78	0.66
1:B:345:LEU:HB3	1:B:356:ILE:HD12	1.77	0.66
1:A:160:LEU:HD23	1:A:161:GLU:H	1.61	0.65
1:B:43:GLU:HG2	1:B:45:PHE:O	1.96	0.65
1:C:362:TYR:HD1	1:C:367:TYR:CD2	2.13	0.65
1:C:56:LEU:CD2	1:C:60:VAL:HG21	2.26	0.65
1:A:254:LEU:C	1:A:256:LYS:H	2.00	0.65
1:C:378:THR:HG22	1:C:382:GLU:OE1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:PHE:O	1:C:154:GLY:HA2	1.97	0.65
1:C:127:LEU:HA	1:C:194:ARG:NH2	2.11	0.65
1:B:363:PRO:HD2	1:B:367:TYR:CE2	2.32	0.65
1:A:227:LEU:HB3	1:C:27:GLY:HA3	1.79	0.65
1:A:7:ARG:HH12	1:A:57:GLY:HA2	1.60	0.65
1:A:286:ALA:HA	1:A:311:VAL:HG11	1.79	0.65
1:C:125:TYR:CE2	1:C:194:ARG:HB3	2.31	0.65
1:C:384:ARG:O	1:C:388:SER:HB2	1.96	0.65
1:A:303:LYS:O	1:A:307:VAL:CG2	2.43	0.65
1:A:175:ALA:HB1	1:A:205:LEU:HD21	1.79	0.65
1:B:124:PHE:HZ	1:B:190:VAL:HG13	1.60	0.65
1:C:366:GLN:O	1:C:369:TYR:HB3	1.97	0.65
1:B:162:THR:HG23	1:B:163:ALA:N	2.11	0.65
1:A:101:THR:HB	1:A:242:MET:HE1	1.79	0.65
1:A:106:LEU:O	1:A:109:SER:HB3	1.97	0.65
1:B:195:ALA:HB3	1:B:232:LEU:HD11	1.79	0.65
1:A:272:ILE:HG21	1:A:274:ARG:HH21	1.62	0.64
1:C:272:ILE:HG21	1:C:274:ARG:CZ	2.27	0.64
1:C:12:PHE:HD2	1:C:23:VAL:HG22	1.61	0.64
1:A:160:LEU:HD22	1:A:164:PRO:CB	2.28	0.64
1:A:199:LEU:CD2	1:A:215:VAL:HG21	2.26	0.64
1:C:93:TYR:OH	1:C:265:LEU:HD21	1.96	0.64
1:A:121:ARG:HG2	1:A:152:TYR:HD1	1.61	0.64
1:B:108:GLU:HG2	1:B:112:LEU:HD12	1.79	0.64
1:A:272:ILE:HD12	1:A:272:ILE:N	2.01	0.64
1:C:225:ARG:NE	1:C:274:ARG:NH2	2.44	0.64
1:B:143:PHE:CE2	1:B:147:VAL:HG11	2.32	0.64
1:C:185:THR:HB	1:C:213:LEU:HD22	1.79	0.64
1:A:99:ILE:HD12	1:A:264:ILE:HG12	1.77	0.64
1:C:184:GLN:NE2	1:C:211:GLU:O	2.31	0.64
1:C:299:CYS:HB3	1:C:341:LYS:HB2	1.79	0.64
1:B:354:ASN:O	1:B:357:SER:HB3	1.98	0.64
1:B:311:VAL:HG21	1:B:318:LEU:HD21	1.79	0.64
1:B:355:GLU:O	1:B:359:MET:HB3	1.97	0.64
1:C:17:ALA:HB2	1:C:221:GLU:OE1	1.98	0.64
1:B:133:LYS:HB3	1:B:135:TRP:CD1	2.33	0.64
1:C:155:VAL:CG1	1:C:177:TRP:HE1	2.10	0.64
1:C:220:ASN:ND2	1:C:225:ARG:HH22	1.96	0.63
1:A:86:SER:HB3	1:A:102:ASP:HA	1.80	0.63
1:C:131:SER:HB2	1:C:133:LYS:HD2	1.80	0.63
1:B:345:LEU:CA	1:B:349:THR:HG23	2.27	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:386:VAL:HG12	1:A:387:ASN:N	2.13	0.63
1:C:302:ILE:H	1:C:302:ILE:HD13	1.63	0.63
1:B:230:VAL:HG12	1:B:275:ARG:HD3	1.81	0.63
1:B:143:PHE:CZ	1:B:147:VAL:HG21	2.34	0.63
1:C:262:GLN:O	1:C:263:ARG:HD2	1.97	0.63
1:B:84:GLY:O	1:B:101:THR:HG22	1.99	0.63
1:A:298:ALA:HB3	1:A:341:LYS:HD2	1.81	0.63
1:A:302:ILE:HG13	1:A:334:ILE:CD1	2.29	0.63
1:A:346:LEU:HA	1:A:384:ARG:NH1	2.14	0.63
1:B:292:HIS:O	1:B:295:ARG:N	2.32	0.63
1:A:43:GLU:HA	1:A:45:PHE:O	1.99	0.63
1:A:169:HIS:NE2	1:A:173:ARG:HD2	2.13	0.63
1:C:308:LEU:HD13	1:C:315:ARG:HB2	1.81	0.62
1:C:328:GLU:HB2	1:C:332:ALA:CB	2.28	0.62
1:C:174:LEU:HD11	1:C:178:LEU:HD11	1.81	0.62
1:A:279:TYR:CE2	1:A:281:SER:HA	2.33	0.62
1:B:347:ILE:O	1:B:389:GLU:N	2.31	0.62
1:C:286:ALA:HA	1:C:311:VAL:CG1	2.29	0.62
1:C:296:ASN:HB3	1:C:297:HIS:ND1	2.15	0.62
1:B:151:LYS:HB3	1:B:152:TYR:CE1	2.34	0.62
1:B:225:ARG:HH12	1:B:389:GLU:C	2.03	0.62
1:C:13:ASN:O	1:C:19:ASP:HB2	1.99	0.62
1:B:292:HIS:HA	1:B:295:ARG:HG3	1.82	0.62
1:A:232:LEU:HD23	1:A:233:SER:O	2.00	0.62
1:C:302:ILE:HD13	1:C:302:ILE:N	2.14	0.62
1:A:240:ARG:HD3	1:C:350:THR:CB	2.29	0.62
1:C:4:LYS:NZ	1:C:4:LYS:HA	2.15	0.62
1:A:292:HIS:CD2	1:A:296:ASN:HD21	2.18	0.61
1:C:290:ALA:CA	1:C:311:VAL:HG22	2.30	0.61
1:A:121:ARG:HH11	1:A:121:ARG:HG3	1.65	0.61
1:B:347:ILE:HG13	1:B:387:ASN:O	1.99	0.61
1:A:10:LEU:CD2	1:A:61:ILE:HB	2.29	0.61
1:B:308:LEU:HA	1:B:318:LEU:CD1	2.30	0.61
1:B:131:SER:O	1:B:133:LYS:N	2.33	0.61
1:B:135:TRP:HE3	1:B:139:ARG:CZ	2.13	0.61
1:A:15:ASN:CG	1:A:16:LYS:N	2.54	0.61
1:A:382:GLU:O	1:A:386:VAL:HG21	2.00	0.61
1:C:342:ALA:HB1	1:C:356:ILE:HG22	1.81	0.61
1:C:39:ILE:HD12	1:C:39:ILE:H	1.65	0.61
1:B:211:GLU:OE2	1:B:211:GLU:HA	1.99	0.61
1:B:207:ILE:O	1:B:209:VAL:HG23	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:269:VAL:HG12	1:A:270:ARG:N	2.14	0.61
1:A:64:PHE:CD2	1:A:70:GLU:HB2	2.34	0.61
1:B:333:MET:O	1:B:337:GLU:N	2.33	0.61
1:B:96:VAL:HG22	1:B:97:HIS:N	2.13	0.61
1:B:43:GLU:HA	1:B:45:PHE:N	2.16	0.61
1:A:286:ALA:HB3	1:A:321:ARG:HG2	1.82	0.61
1:B:313:ILE:HG13	1:B:321:ARG:HH12	1.66	0.61
1:B:144:ARG:HH11	1:B:144:ARG:HG3	1.65	0.61
1:B:220:ASN:HD21	1:B:272:ILE:HG13	1.66	0.61
1:C:185:THR:HB	1:C:213:LEU:CD2	2.31	0.61
1:A:160:LEU:CD2	1:A:161:GLU:H	2.14	0.61
1:C:87:TYR:HD2	1:C:92:SER:HB3	1.66	0.60
1:C:150:GLU:CG	1:C:151:LYS:H	2.12	0.60
1:C:388:SER:O	1:C:389:GLU:HB3	2.00	0.60
1:C:345:LEU:HD23	1:C:349:THR:HG21	1.83	0.60
1:C:42:GLU:HA	1:C:45:PHE:HZ	1.64	0.60
1:B:294:ILE:O	1:B:298:ALA:CB	2.49	0.60
1:B:56:LEU:HG	1:B:57:GLY:N	2.15	0.60
1:A:227:LEU:HB3	1:C:27:GLY:HA2	1.83	0.60
1:B:175:ALA:CB	1:B:205:LEU:HD21	2.31	0.60
1:A:144:ARG:O	1:A:147:VAL:HG12	2.02	0.60
1:A:274:ARG:HG3	1:A:274:ARG:NH1	2.12	0.60
1:C:342:ALA:O	1:C:356:ILE:HG21	2.01	0.60
1:C:298:ALA:N	1:C:341:LYS:NZ	2.50	0.60
1:A:328:GLU:HG2	1:A:333:MET:SD	2.41	0.60
1:B:358:GLN:HG3	1:B:359:MET:H	1.66	0.60
1:B:1:MET:HA	1:B:1:MET:CE	2.31	0.60
1:C:135:TRP:HB2	1:C:139:ARG:HH21	1.66	0.60
1:C:235:VAL:O	1:C:235:VAL:HG12	2.00	0.60
1:C:311:VAL:CG2	1:C:318:LEU:HD11	2.32	0.60
1:B:223:LEU:H	1:B:223:LEU:HD23	1.67	0.60
1:A:7:ARG:HB3	1:A:7:ARG:CZ	2.32	0.60
1:A:229:ARG:NH1	1:A:296:ASN:HB3	2.16	0.60
1:C:197:HIS:CA	1:C:200:GLN:HE21	2.15	0.60
1:C:319:GLU:O	1:C:322:PHE:HB2	2.02	0.60
1:C:304:VAL:O	1:C:304:VAL:HG12	2.02	0.60
1:A:158:GLN:O	1:A:159:GLY:O	2.19	0.60
1:B:328:GLU:OE1	1:B:328:GLU:HA	2.01	0.60
1:A:315:ARG:HH11	1:A:315:ARG:HG3	1.65	0.59
1:A:238:GLY:O	1:A:242:MET:HB2	2.02	0.59
1:A:269:VAL:CG1	1:A:270:ARG:HG3	2.28	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:97:HIS:NE2	1:B:261:LEU:HA	2.17	0.59
1:A:353:ILE:HD11	1:A:384:ARG:HD3	1.85	0.59
1:C:97:HIS:CD2	1:C:262:GLN:H	2.20	0.59
1:B:336:ALA:O	1:B:339:LEU:HB2	2.02	0.59
1:B:311:VAL:HG12	1:B:312:GLY:N	2.17	0.59
1:A:222:GLU:OE2	1:C:20:ARG:NH2	2.33	0.59
1:B:11:LEU:HB2	1:B:62:ALA:HB2	1.84	0.59
1:B:85:GLY:O	1:B:87:TYR:HD1	1.85	0.59
1:A:298:ALA:O	1:A:338:LYS:HE2	2.02	0.59
1:A:212:LYS:O	1:A:213:LEU:HD23	2.02	0.59
1:C:174:LEU:HD11	1:C:178:LEU:CD1	2.32	0.59
1:A:351:LEU:H	1:A:384:ARG:HH22	1.46	0.59
1:A:240:ARG:HD3	1:C:350:THR:CG2	2.32	0.59
1:C:98:TYR:CD2	1:C:100:ALA:HB2	2.38	0.59
1:A:121:ARG:HD3	1:A:182:PRO:HB2	1.84	0.59
1:A:303:LYS:HG2	1:A:306:GLN:NE2	2.18	0.59
1:C:299:CYS:HB3	1:C:341:LYS:HD3	1.83	0.59
1:B:133:LYS:CG	1:B:135:TRP:HE1	2.16	0.59
1:A:262:GLN:O	1:A:263:ARG:HG3	2.03	0.59
1:B:162:THR:HG23	1:B:163:ALA:H	1.67	0.59
1:A:302:ILE:H	1:A:334:ILE:HD11	1.68	0.59
1:A:188:ILE:HG12	1:A:216:ILE:HG23	1.84	0.59
1:A:190:VAL:HG23	1:A:191:THR:N	2.17	0.59
1:B:86:SER:HB3	1:B:265:LEU:HD22	1.85	0.59
1:A:34:GLN:HG3	1:C:300:LYS:HZ2	1.67	0.59
1:B:275:ARG:O	1:B:277:THR:N	2.35	0.59
1:B:126:GLY:HA2	1:B:190:VAL:HG22	1.85	0.59
1:C:376:TYR:O	1:C:378:THR:N	2.35	0.59
1:A:224:THR:O	1:A:226:TYR:N	2.36	0.58
1:A:240:ARG:HG2	1:C:350:THR:HG21	1.85	0.58
1:A:300:LYS:HE2	1:C:2:PHE:HZ	1.68	0.58
1:B:221:GLU:HG2	1:B:223:LEU:HD21	1.86	0.58
1:C:10:LEU:CD2	1:C:61:ILE:HD12	2.32	0.58
1:A:355:GLU:HA	1:A:358:GLN:OE1	2.03	0.58
1:C:313:ILE:HB	1:C:318:LEU:HB2	1.83	0.58
1:C:231:ALA:HB1	1:C:274:ARG:HG2	1.85	0.58
1:B:185:THR:HB	1:B:213:LEU:HD22	1.85	0.58
1:B:30:LEU:HD12	1:B:39:ILE:HD13	1.84	0.58
1:B:88:HIS:HB2	1:B:138:GLU:OE1	2.03	0.58
1:A:226:TYR:HB3	1:A:227:LEU:HD23	1.86	0.58
1:B:55:TRP:O	1:B:56:LEU:O	2.22	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:GLY:O	1:A:266:VAL:HG11	2.03	0.58
1:C:286:ALA:O	1:C:311:VAL:HG13	2.01	0.58
1:A:4:LYS:CA	1:A:4:LYS:NZ	2.63	0.58
1:B:119:VAL:HG12	1:B:122:PHE:CE2	2.38	0.58
1:B:124:PHE:CD2	1:B:124:PHE:C	2.78	0.58
1:C:220:ASN:HB2	1:C:236:ALA:HA	1.85	0.58
1:B:290:ALA:O	1:B:294:ILE:HG12	2.04	0.57
1:C:64:PHE:HB2	1:C:98:TYR:HE1	1.68	0.57
1:B:86:SER:OG	1:B:103:ASN:N	2.36	0.57
1:B:17:ALA:CB	1:B:221:GLU:HA	2.34	0.57
1:B:113:HIS:HE1	1:B:273:GLU:OE1	1.87	0.57
1:C:135:TRP:CE3	1:C:136:ALA:N	2.72	0.57
1:B:308:LEU:HD13	1:B:315:ARG:HB2	1.84	0.57
1:A:135:TRP:O	1:A:139:ARG:HG3	2.02	0.57
1:C:191:THR:O	1:C:195:ALA:HB2	2.04	0.57
1:C:11:LEU:CB	1:C:43:GLU:OE1	2.45	0.57
1:B:155:VAL:HG11	1:B:177:TRP:HE1	1.68	0.57
1:C:224:THR:O	1:C:225:ARG:C	2.43	0.57
1:C:73:LEU:HD13	1:C:80:ILE:CD1	2.34	0.57
1:A:140:GLU:O	1:A:144:ARG:HG2	2.03	0.57
1:A:249:LEU:C	1:A:249:LEU:HD23	2.25	0.57
1:A:34:GLN:HE21	1:C:229:ARG:CD	2.17	0.57
1:C:293:TYR:CE1	1:C:297:HIS:HB2	2.40	0.57
1:C:197:HIS:HA	1:C:200:GLN:HE21	1.69	0.57
1:B:292:HIS:O	1:B:294:ILE:N	2.38	0.57
1:A:126:GLY:HA2	1:A:190:VAL:HG13	1.86	0.57
1:C:220:ASN:OD1	1:C:272:ILE:HD12	2.03	0.57
1:B:24:GLU:HB3	1:B:240:ARG:NH2	2.20	0.57
1:B:251:HIS:O	1:B:254:LEU:HB2	2.04	0.57
1:C:96:VAL:HG22	1:C:97:HIS:H	1.68	0.57
1:A:12:PHE:HD2	1:A:23:VAL:HG23	1.70	0.57
1:A:330:ILE:HG22	1:A:331:HIS:N	2.19	0.57
1:C:8:ILE:HG13	1:C:37:TRP:CE3	2.40	0.57
1:A:244:TYR:HD1	1:A:245:GLN:HE21	1.53	0.57
1:A:286:ALA:O	1:A:290:ALA:HB2	2.04	0.57
1:B:107:VAL:HG12	1:B:146:LEU:HD11	1.86	0.57
1:B:264:ILE:HD12	1:B:265:LEU:N	2.20	0.57
1:A:356:ILE:O	1:A:360:CYS:HB2	2.05	0.57
1:A:261:LEU:HB3	1:A:263:ARG:HH21	1.70	0.57
1:C:263:ARG:HG2	1:C:263:ARG:HH11	1.70	0.57
1:A:110:ALA:O	1:A:113:HIS:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:PRO:CG	1:A:253:LEU:HD22	2.32	0.56
1:C:328:GLU:HG3	1:C:332:ALA:O	2.05	0.56
1:A:46:ARG:HH11	1:A:46:ARG:HB2	1.69	0.56
1:B:174:LEU:HG	1:B:178:LEU:HD13	1.87	0.56
1:C:85:GLY:HA2	1:C:101:THR:HG22	1.87	0.56
1:A:289:GLN:HB3	1:A:311:VAL:HG13	1.87	0.56
1:C:308:LEU:HB2	1:C:314:SER:O	2.05	0.56
1:B:124:PHE:C	1:B:124:PHE:HD2	2.09	0.56
1:A:43:GLU:C	1:A:45:PHE:N	2.58	0.56
1:C:85:GLY:HA2	1:C:101:THR:CG2	2.35	0.56
1:C:256:LYS:HE3	1:C:256:LYS:N	2.20	0.56
1:B:343:ARG:NH1	1:B:383:TYR:OH	2.38	0.56
1:C:126:GLY:O	1:C:158:GLN:HA	2.05	0.56
1:C:252:ARG:NH2	1:C:259:MET:CE	2.68	0.56
1:C:87:TYR:CD2	1:C:92:SER:HB3	2.40	0.56
1:A:221:GLU:O	1:A:225:ARG:HG2	2.04	0.56
1:C:232:LEU:HD22	1:C:233:SER:N	2.20	0.56
1:B:311:VAL:CB	1:B:318:LEU:HD11	2.36	0.56
1:B:151:LYS:HG2	1:B:151:LYS:O	2.05	0.56
1:C:103:ASN:O	1:C:107:VAL:HG23	2.05	0.56
1:C:152:TYR:N	1:C:152:TYR:CD1	2.73	0.56
1:C:259:MET:HG2	1:C:262:GLN:NE2	2.20	0.56
1:A:291:MET:O	1:A:292:HIS:C	2.42	0.56
1:B:269:VAL:HG12	1:B:270:ARG:HD3	1.87	0.56
1:C:147:VAL:HG21	1:C:154:GLY:H	1.70	0.56
1:C:79:PRO:HB3	1:C:253:LEU:HD13	1.86	0.55
1:A:127:LEU:CD1	1:A:194:ARG:NE	2.69	0.55
1:B:81:VAL:HG21	1:B:249:LEU:HD22	1.88	0.55
1:B:11:LEU:HB2	1:B:62:ALA:HB1	1.88	0.55
1:B:211:GLU:OE1	1:B:295:ARG:NH2	2.38	0.55
1:A:7:ARG:HA	1:A:38:ASP:HB3	1.88	0.55
1:B:358:GLN:O	1:B:359:MET:C	2.45	0.55
1:C:79:PRO:CG	1:C:253:LEU:HD22	2.36	0.55
1:B:320:LYS:O	1:B:323:LYS:CD	2.54	0.55
1:C:345:LEU:HA	1:C:349:THR:HG21	1.87	0.55
1:C:286:ALA:HA	1:C:311:VAL:HG12	1.89	0.55
1:C:12:PHE:O	1:C:43:GLU:HB3	2.07	0.55
1:B:221:GLU:HG2	1:B:223:LEU:CD2	2.36	0.55
1:B:135:TRP:CE3	1:B:139:ARG:NH2	2.74	0.55
1:A:146:LEU:HD12	1:A:147:VAL:N	2.21	0.55
1:C:282:LEU:HD22	1:C:325:GLU:HG3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135:TRP:CE3	1:A:136:ALA:N	2.74	0.55
1:A:280:ARG:HB3	1:A:280:ARG:CZ	2.36	0.55
1:A:272:ILE:HG21	1:A:274:ARG:NH2	2.21	0.55
1:A:274:ARG:HH11	1:A:274:ARG:CG	2.10	0.55
1:A:347:ILE:CG2	1:A:389:GLU:H	2.18	0.55
1:C:18:TYR:O	1:C:21:GLN:HB2	2.07	0.55
1:C:382:GLU:HG2	1:C:382:GLU:O	2.05	0.55
1:B:108:GLU:HG2	1:B:112:LEU:CD1	2.36	0.55
1:B:13:ASN:O	1:B:15:ASN:N	2.39	0.55
1:A:286:ALA:HA	1:A:311:VAL:CG1	2.36	0.54
1:A:313:ILE:CG2	1:A:317:ASN:HB3	2.37	0.54
1:B:320:LYS:O	1:B:323:LYS:NZ	2.39	0.54
1:A:235:VAL:HA	1:A:271:VAL:HG13	1.89	0.54
1:A:60:VAL:O	1:A:61:ILE:HG12	2.07	0.54
1:C:345:LEU:HA	1:C:349:THR:CG2	2.37	0.54
1:C:232:LEU:HD22	1:C:233:SER:H	1.73	0.54
1:A:160:LEU:N	1:A:194:ARG:HH22	2.04	0.54
1:C:150:GLU:HG3	1:C:151:LYS:N	2.17	0.54
1:A:329:THR:N	1:A:332:ALA:HB3	2.22	0.54
1:C:174:LEU:CD1	1:C:178:LEU:CD1	2.85	0.54
1:A:126:GLY:HA2	1:A:190:VAL:CG1	2.37	0.54
1:C:151:LYS:HD2	1:C:152:TYR:CE1	2.43	0.54
1:C:372:PHE:O	1:C:372:PHE:HD2	1.90	0.54
1:C:162:THR:HG23	1:C:163:ALA:N	2.23	0.54
1:B:351:LEU:H	1:B:384:ARG:NH2	2.05	0.54
1:B:313:ILE:HG13	1:B:321:ARG:NH1	2.22	0.54
1:A:347:ILE:HD11	1:A:383:TYR:CZ	2.43	0.54
1:A:388:SER:O	1:A:389:GLU:HB2	2.07	0.54
1:A:178:LEU:HD23	1:A:202:CYS:SG	2.48	0.54
1:B:6:HIS:ND1	1:B:6:HIS:N	2.56	0.54
1:B:275:ARG:HH21	1:B:295:ARG:HH11	1.56	0.54
1:A:240:ARG:CD	1:C:350:THR:HG21	2.37	0.54
1:A:165:GLU:HG2	1:A:166:ASN:H	1.72	0.54
1:A:314:SER:O	1:A:318:LEU:HB2	2.06	0.54
1:C:139:ARG:HD3	1:C:218:ILE:HD12	1.89	0.54
1:C:127:LEU:CD2	1:C:190:VAL:HG21	2.38	0.54
1:B:275:ARG:C	1:B:277:THR:H	2.11	0.54
1:B:23:VAL:CG1	1:B:24:GLU:N	2.70	0.54
1:A:100:ALA:O	1:A:266:VAL:HG23	2.08	0.54
1:C:24:GLU:HB3	1:C:240:ARG:NH1	2.22	0.54
1:B:85:GLY:O	1:B:87:TYR:CD1	2.61	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:87:TYR:HE2	1:C:134:ARG:HE	1.55	0.54
1:A:30:LEU:CD2	1:A:39:ILE:HD11	2.38	0.54
1:B:159:GLY:HA3	1:B:194:ARG:NH2	2.22	0.54
1:A:99:ILE:HD12	1:A:264:ILE:CG1	2.38	0.54
1:A:188:ILE:HG12	1:A:216:ILE:CG2	2.38	0.54
1:C:42:GLU:O	1:C:43:GLU:HB2	2.07	0.54
1:C:11:LEU:HD12	1:C:62:ALA:HB2	1.90	0.54
1:B:356:ILE:O	1:B:360:CYS:HB2	2.08	0.54
1:A:30:LEU:HD21	1:A:39:ILE:HD11	1.90	0.54
1:C:345:LEU:HD22	1:C:351:LEU:HD12	1.88	0.54
1:A:104:TYR:HA	1:A:142:ALA:HB1	1.89	0.54
1:C:218:ILE:HA	1:C:235:VAL:HB	1.90	0.53
1:C:192:ASP:H	1:C:219:ASP:HB2	1.73	0.53
1:A:159:GLY:HA3	1:A:194:ARG:HH21	1.73	0.53
1:A:328:GLU:HG3	1:A:332:ALA:CB	2.35	0.53
1:B:97:HIS:CE1	1:B:262:GLN:H	2.26	0.53
1:B:9:THR:O	1:B:60:VAL:HG12	2.08	0.53
1:A:24:GLU:OE1	1:A:240:ARG:NH2	2.33	0.53
1:B:149:GLU:O	1:B:149:GLU:HG2	2.06	0.53
1:A:311:VAL:CG2	1:A:318:LEU:HD21	2.39	0.53
1:C:128:PRO:HG2	1:C:160:LEU:O	2.08	0.53
1:B:182:PRO:O	1:B:213:LEU:HD21	2.09	0.53
1:A:195:ALA:HB3	1:A:232:LEU:HD11	1.90	0.53
1:A:326:VAL:HG12	1:A:326:VAL:O	2.09	0.53
1:A:178:LEU:HD22	1:A:201:VAL:HG12	1.90	0.53
1:A:227:LEU:HD23	1:A:227:LEU:H	1.72	0.53
1:C:131:SER:C	1:C:133:LYS:N	2.61	0.53
1:C:218:ILE:O	1:C:218:ILE:CG2	2.53	0.53
1:A:353:ILE:CD1	1:A:384:ARG:HD3	2.39	0.53
1:B:272:ILE:CG2	1:B:274:ARG:HE	2.18	0.53
1:A:1:MET:HG2	1:A:2:PHE:N	2.24	0.53
1:B:319:GLU:O	1:B:323:LYS:HD2	2.08	0.53
1:A:225:ARG:HE	1:A:274:ARG:HH12	1.55	0.53
1:C:220:ASN:C	1:C:225:ARG:HH12	2.12	0.53
1:B:233:SER:HA	1:B:274:ARG:HG2	1.89	0.53
1:C:275:ARG:HG2	1:C:295:ARG:NH1	2.13	0.53
1:A:169:HIS:CE1	1:A:173:ARG:HD2	2.44	0.53
1:A:225:ARG:NH2	1:A:274:ARG:CZ	2.72	0.53
1:C:220:ASN:HD21	1:C:225:ARG:HH22	1.56	0.53
1:A:73:LEU:CD2	1:A:80:ILE:HD13	2.38	0.53
1:C:161:GLU:HG2	1:C:164:PRO:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:269:VAL:HG23	1:C:270:ARG:N	2.18	0.53
1:A:190:VAL:O	1:A:218:ILE:HD13	2.09	0.53
1:A:235:VAL:HG12	1:A:236:ALA:H	1.74	0.53
1:C:11:LEU:HA	1:C:42:GLU:O	2.09	0.53
1:C:196:ARG:C	1:C:200:GLN:HE21	2.13	0.52
1:A:61:ILE:HD11	1:A:250:LEU:HD22	1.92	0.52
1:B:126:GLY:HA2	1:B:190:VAL:CG2	2.39	0.52
1:C:26:VAL:C	1:C:28:GLU:H	2.12	0.52
1:B:175:ALA:HB2	1:B:205:LEU:HD21	1.90	0.52
1:C:174:LEU:O	1:C:178:LEU:HB2	2.08	0.52
1:C:142:ALA:O	1:C:146:LEU:HG	2.09	0.52
1:A:177:TRP:NE1	1:A:181:LEU:HD21	2.25	0.52
1:A:128:PRO:C	1:A:130:SER:H	2.12	0.52
1:C:99:ILE:HD13	1:C:264:ILE:CG2	2.40	0.52
1:C:275:ARG:HH22	1:C:296:ASN:HD21	1.57	0.52
1:B:187:ILE:O	1:B:216:ILE:HG22	2.09	0.52
1:A:98:TYR:O	1:A:263:ARG:HA	2.09	0.52
1:B:369:TYR:O	1:B:373:LYS:HG3	2.10	0.52
1:B:135:TRP:CE3	1:B:139:ARG:CZ	2.92	0.52
1:C:353:ILE:HD11	1:C:384:ARG:HG3	1.91	0.52
1:A:299:CYS:HA	1:A:338:LYS:HG3	1.91	0.52
1:C:159:GLY:HA3	1:C:194:ARG:NH1	2.25	0.52
1:C:42:GLU:HA	1:C:45:PHE:CZ	2.44	0.52
1:B:205:LEU:HD12	1:B:205:LEU:N	2.25	0.52
1:A:192:ASP:OD2	1:A:232:LEU:HD22	2.10	0.52
1:A:345:LEU:HA	1:A:349:THR:OG1	2.10	0.52
1:A:61:ILE:CD1	1:A:81:VAL:HB	2.40	0.52
1:C:369:TYR:HE1	1:C:379:THR:HG22	1.75	0.52
1:A:7:ARG:HA	1:A:38:ASP:CB	2.40	0.52
1:A:83:VAL:HA	1:A:99:ILE:O	2.09	0.52
1:C:280:ARG:O	1:C:282:LEU:HG	2.10	0.52
1:A:91:GLU:HG2	1:A:91:GLU:O	2.10	0.52
1:C:89:LEU:HB2	1:C:92:SER:OG	2.10	0.52
1:C:376:TYR:C	1:C:378:THR:H	2.14	0.52
1:C:291:MET:HG2	1:C:291:MET:O	2.10	0.52
1:A:182:PRO:O	1:A:185:THR:OG1	2.27	0.52
1:A:102:ASP:OD2	1:A:105:ALA:HB2	2.10	0.52
1:A:308:LEU:HD22	1:A:315:ARG:HA	1.91	0.51
1:A:299:CYS:HB2	1:A:360:CYS:HA	1.92	0.51
1:A:254:LEU:C	1:A:256:LYS:N	2.63	0.51
1:A:174:LEU:HD12	1:A:178:LEU:HD13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:ILE:HG21	1:C:215:VAL:HG13	1.93	0.51
1:B:311:VAL:HB	1:B:318:LEU:HD11	1.93	0.51
1:A:241:GLN:O	1:A:245:GLN:HG2	2.10	0.51
1:B:66:ASP:OD2	1:B:69:ILE:HD13	2.09	0.51
1:A:347:ILE:HG23	1:A:387:ASN:O	2.10	0.51
1:A:174:LEU:HD12	1:A:178:LEU:CD1	2.39	0.51
1:C:296:ASN:HB3	1:C:297:HIS:CE1	2.46	0.51
1:A:240:ARG:CG	1:C:350:THR:HG21	2.40	0.51
1:C:256:LYS:HE3	1:C:256:LYS:H	1.74	0.51
1:A:210:PRO:CD	1:A:295:ARG:HH12	2.14	0.51
1:C:298:ALA:HA	1:C:302:ILE:CD1	2.27	0.51
1:B:135:TRP:H	1:B:135:TRP:HD1	1.59	0.51
1:C:86:SER:HB3	1:C:102:ASP:HA	1.91	0.51
1:A:157:TYR:CZ	1:A:174:LEU:HA	2.46	0.51
1:A:347:ILE:HG23	1:A:388:SER:HA	1.93	0.51
1:B:126:GLY:O	1:B:127:LEU:HD12	2.10	0.51
1:B:384:ARG:O	1:B:388:SER:HB2	2.11	0.51
1:B:119:VAL:HG23	1:B:279:TYR:CD2	2.46	0.51
1:B:67:LYS:HE2	1:B:134:ARG:HH12	1.76	0.51
1:A:311:VAL:HG21	1:A:318:LEU:HD21	1.93	0.50
1:B:6:HIS:CD2	1:B:254:LEU:HD13	2.47	0.50
1:C:199:LEU:HD22	1:C:230:VAL:HG21	1.92	0.50
1:B:294:ILE:HG22	1:B:298:ALA:CB	2.39	0.50
1:A:13:ASN:O	1:A:19:ASP:CB	2.59	0.50
1:A:193:ALA:O	1:A:196:ARG:HB2	2.11	0.50
1:A:110:ALA:HB2	1:A:235:VAL:CG2	2.41	0.50
1:B:351:LEU:H	1:B:384:ARG:HH22	1.59	0.50
1:B:191:THR:HG22	1:B:193:ALA:N	2.22	0.50
1:C:378:THR:OG1	1:C:383:TYR:HD1	1.93	0.50
1:C:345:LEU:HD13	1:C:356:ILE:HD12	1.93	0.50
1:C:86:SER:C	1:C:87:TYR:CD1	2.84	0.50
1:B:124:PHE:CE2	1:B:190:VAL:HG13	2.45	0.50
1:B:183:PRO:O	1:B:184:GLN:HG2	2.11	0.50
1:C:84:GLY:HA3	1:C:98:TYR:OH	2.12	0.50
1:A:282:LEU:HD23	1:A:326:VAL:CG2	2.40	0.50
1:B:101:THR:HA	1:B:242:MET:HE2	1.93	0.50
1:A:290:ALA:O	1:A:294:ILE:HG13	2.12	0.50
1:C:347:ILE:HD12	1:C:347:ILE:H	1.77	0.50
1:C:357:SER:O	1:C:362:TYR:N	2.44	0.50
1:A:174:LEU:C	1:A:174:LEU:HD12	2.32	0.50
1:C:298:ALA:H	1:C:341:LYS:NZ	2.08	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:LYS:HG3	1:B:135:TRP:HE1	1.76	0.50
1:B:10:LEU:CD2	1:B:61:ILE:HB	2.39	0.50
1:C:97:HIS:HB3	1:C:262:GLN:HB2	1.94	0.50
1:B:358:GLN:O	1:B:361:GLY:N	2.44	0.50
1:B:347:ILE:HA	1:B:388:SER:HA	1.93	0.50
1:C:133:LYS:HD2	1:C:133:LYS:H	1.77	0.50
1:A:304:VAL:O	1:A:308:LEU:HG	2.12	0.50
1:A:313:ILE:CG2	1:A:317:ASN:HD22	2.18	0.50
1:C:192:ASP:OD1	1:C:217:GLY:HA3	2.11	0.50
1:B:112:LEU:O	1:B:116:GLU:HB2	2.12	0.50
1:C:4:LYS:C	1:C:4:LYS:HD3	2.32	0.50
1:A:104:TYR:CD1	1:A:142:ALA:HA	2.47	0.50
1:B:99:ILE:HG21	1:B:242:MET:O	2.11	0.49
1:A:346:LEU:CD2	1:A:384:ARG:HH11	2.14	0.49
1:C:70:GLU:OE2	1:C:94:PRO:CB	2.60	0.49
1:B:162:THR:CG2	1:B:163:ALA:H	2.25	0.49
1:C:358:GLN:HE22	1:C:359:MET:CE	2.24	0.49
1:A:229:ARG:NH2	1:A:296:ASN:OD1	2.45	0.49
1:B:86:SER:CB	1:B:265:LEU:HD22	2.42	0.49
1:B:86:SER:HB3	1:B:102:ASP:HA	1.93	0.49
1:C:189:ALA:O	1:C:191:THR:N	2.45	0.49
1:B:313:ILE:HG21	1:B:317:ASN:HB2	1.94	0.49
1:C:98:TYR:CE2	1:C:100:ALA:HB2	2.47	0.49
1:C:74:ALA:O	1:C:75:ASP:HB3	2.12	0.49
1:C:347:ILE:HD12	1:C:347:ILE:N	2.28	0.49
1:C:39:ILE:CD1	1:C:39:ILE:H	2.23	0.49
1:A:143:PHE:O	1:A:146:LEU:HG	2.12	0.49
1:C:330:ILE:O	1:C:334:ILE:HG12	2.13	0.49
1:A:218:ILE:N	1:A:218:ILE:HD12	2.28	0.49
1:A:225:ARG:HG3	1:A:225:ARG:HH11	1.77	0.49
1:A:275:ARG:O	1:A:277:THR:N	2.45	0.49
1:B:158:GLN:O	1:B:159:GLY:O	2.31	0.49
1:B:155:VAL:HG12	1:B:156:VAL:N	2.28	0.49
1:A:185:THR:HG22	1:A:186:GLY:H	1.78	0.49
1:A:104:TYR:HD1	1:A:142:ALA:HA	1.77	0.49
1:B:308:LEU:HA	1:B:318:LEU:HD13	1.94	0.49
1:A:261:LEU:HD22	1:A:263:ARG:NH2	2.28	0.49
1:A:184:GLN:HG2	1:A:279:TYR:OH	2.13	0.49
1:B:183:PRO:O	1:B:184:GLN:CG	2.61	0.49
1:B:342:ALA:O	1:B:346:LEU:HG	2.13	0.49
1:A:292:HIS:O	1:A:295:ARG:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:347:ILE:HD11	1:B:383:TYR:CE2	2.48	0.49
1:C:294:ILE:HA	1:C:298:ALA:HB2	1.95	0.49
1:C:114:LEU:HB2	1:C:122:PHE:CE2	2.47	0.49
1:A:7:ARG:CZ	1:A:7:ARG:CB	2.91	0.49
1:C:6:HIS:HB2	1:C:8:ILE:HD11	1.95	0.49
1:B:264:ILE:HD12	1:B:265:LEU:H	1.77	0.49
1:A:4:LYS:N	1:A:36:GLU:HG3	2.28	0.49
1:C:188:ILE:HA	1:C:216:ILE:CG2	2.42	0.49
1:C:147:VAL:HG13	1:C:148:ALA:N	2.28	0.49
1:C:122:PHE:O	1:C:154:GLY:CA	2.61	0.49
1:A:102:ASP:O	1:A:103:ASN:C	2.51	0.49
1:C:169:HIS:O	1:C:172:ASN:HB2	2.11	0.49
1:A:280:ARG:CG	1:A:282:LEU:HD12	2.16	0.49
1:A:274:ARG:CG	1:A:274:ARG:NH1	2.71	0.49
1:B:85:GLY:C	1:B:100:ALA:HB1	2.33	0.49
1:A:207:ILE:O	1:A:207:ILE:HG22	2.13	0.49
1:C:225:ARG:NE	1:C:274:ARG:HH22	2.04	0.49
1:A:260:PRO:O	1:A:261:LEU:C	2.49	0.49
1:C:345:LEU:HB3	1:C:356:ILE:HD12	1.94	0.49
1:B:368:PHE:C	1:B:368:PHE:CD2	2.86	0.49
1:C:308:LEU:HD13	1:C:315:ARG:HA	1.95	0.48
1:C:60:VAL:HB	1:C:80:ILE:CD1	2.36	0.48
1:B:193:ALA:O	1:B:196:ARG:HB2	2.13	0.48
1:A:45:PHE:C	1:A:46:ARG:HG3	2.33	0.48
1:A:12:PHE:CD2	1:A:23:VAL:HG23	2.48	0.48
1:C:4:LYS:HA	1:C:4:LYS:HZ3	1.76	0.48
1:C:121:ARG:HD2	1:C:182:PRO:HG2	1.95	0.48
1:A:216:ILE:CD1	1:A:234:SER:HA	2.43	0.48
1:C:299:CYS:H	1:C:341:LYS:NZ	2.11	0.48
1:C:152:TYR:HD1	1:C:152:TYR:N	2.10	0.48
1:C:252:ARG:NH2	1:C:259:MET:HE1	2.27	0.48
1:A:157:TYR:CE2	1:A:174:LEU:HA	2.48	0.48
1:C:26:VAL:C	1:C:28:GLU:N	2.67	0.48
1:B:121:ARG:NH1	1:B:184:GLN:HG3	2.28	0.48
1:A:218:ILE:HG22	1:A:219:ASP:N	2.27	0.48
1:C:11:LEU:HB3	1:C:43:GLU:CD	2.32	0.48
1:B:294:ILE:O	1:B:298:ALA:HB2	2.13	0.48
1:C:135:TRP:CZ3	1:C:136:ALA:HB2	2.49	0.48
1:B:160:LEU:HD12	1:B:170:ALA:HA	1.95	0.48
1:C:106:LEU:HD13	1:C:218:ILE:HG21	1.95	0.48
1:B:277:THR:C	1:B:279:TYR:H	2.17	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:MET:HG3	1:A:266:VAL:HG21	1.95	0.48
1:A:379:THR:HB	1:A:380:PRO:HD2	1.95	0.48
1:B:226:TYR:HD2	1:B:348:SER:HG	1.58	0.48
1:B:323:LYS:HD3	1:B:323:LYS:H	1.72	0.48
1:B:118:GLY:O	1:B:119:VAL:C	2.52	0.48
1:B:220:ASN:ND2	1:B:272:ILE:HG13	2.29	0.48
1:A:79:PRO:HG2	1:A:254:LEU:HD23	1.96	0.48
1:A:204:HIS:C	1:A:206:HIS:H	2.17	0.48
1:C:343:ARG:HG2	1:C:343:ARG:O	2.14	0.48
1:B:282:LEU:HD21	1:B:326:VAL:HG22	1.94	0.48
1:A:303:LYS:CG	1:A:306:GLN:HE21	2.27	0.48
1:A:127:LEU:HD11	1:A:194:ARG:NE	2.29	0.48
1:A:227:LEU:HD23	1:A:227:LEU:N	2.28	0.48
1:C:94:PRO:O	1:C:263:ARG:NH2	2.31	0.48
1:A:70:GLU:O	1:A:70:GLU:HG2	2.14	0.48
1:C:250:LEU:O	1:C:254:LEU:HG	2.13	0.48
1:C:161:GLU:O	1:C:164:PRO:HD3	2.13	0.48
1:B:223:LEU:H	1:B:223:LEU:CD2	2.27	0.48
1:B:284:ASP:OD1	1:B:286:ALA:N	2.37	0.48
1:B:177:TRP:CZ2	1:B:181:LEU:HD11	2.49	0.48
1:B:138:GLU:O	1:B:141:TYR:N	2.46	0.48
1:A:284:ASP:O	1:A:288:ILE:HG13	2.14	0.48
1:B:343:ARG:NH1	1:B:383:TYR:CE2	2.74	0.48
1:B:175:ALA:HB1	1:B:205:LEU:HD21	1.95	0.48
1:A:299:CYS:HB3	1:A:341:LYS:HD3	1.95	0.47
1:C:214:CYS:SG	1:C:279:TYR:HB2	2.54	0.47
1:C:286:ALA:C	1:C:311:VAL:HG11	2.35	0.47
1:A:7:ARG:NH1	1:A:7:ARG:HB2	2.28	0.47
1:B:9:THR:HA	1:B:40:PHE:O	2.14	0.47
1:C:252:ARG:NH2	1:C:259:MET:HE2	2.28	0.47
1:A:56:LEU:HG	1:A:57:GLY:N	2.29	0.47
1:B:162:THR:CG2	1:B:163:ALA:N	2.75	0.47
1:A:302:ILE:HG13	1:A:334:ILE:HG13	1.97	0.47
1:C:17:ALA:HB2	1:C:221:GLU:CD	2.35	0.47
1:A:261:LEU:HB3	1:A:263:ARG:HE	1.78	0.47
1:A:261:LEU:HD22	1:A:263:ARG:HH21	1.80	0.47
1:A:294:ILE:O	1:A:298:ALA:HB2	2.15	0.47
1:C:133:LYS:HB3	1:C:135:TRP:CZ2	2.50	0.47
1:C:199:LEU:HG	1:C:215:VAL:HG21	1.95	0.47
1:B:321:ARG:O	1:B:324:GLU:HB3	2.14	0.47
1:A:370:SER:O	1:A:373:LYS:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:SER:OG	1:B:355:GLU:HB3	2.14	0.47
1:A:17:ALA:O	1:A:21:GLN:HG3	2.13	0.47
1:C:308:LEU:HD13	1:C:315:ARG:CA	2.44	0.47
1:A:253:LEU:O	1:A:253:LEU:CD2	2.63	0.47
1:A:331:HIS:HA	1:A:334:ILE:HG22	1.96	0.47
1:C:253:LEU:C	1:C:255:ASP:H	2.18	0.47
1:C:299:CYS:HB3	1:C:341:LYS:CB	2.44	0.47
1:B:251:HIS:O	1:B:254:LEU:N	2.47	0.47
1:B:292:HIS:O	1:B:293:TYR:C	2.53	0.47
1:C:351:LEU:CD2	1:C:352:SER:H	2.28	0.47
1:B:178:LEU:C	1:B:180:THR:H	2.18	0.47
1:C:168:GLN:O	1:C:171:GLN:HB3	2.15	0.47
1:A:326:VAL:CG1	1:A:326:VAL:O	2.62	0.47
1:B:242:MET:HE2	1:B:266:VAL:HB	1.96	0.47
1:B:343:ARG:HB3	1:B:343:ARG:NH1	2.30	0.47
1:C:192:ASP:OD1	1:C:232:LEU:HD11	2.15	0.47
1:A:161:GLU:O	1:A:164:PRO:HD3	2.15	0.47
1:B:134:ARG:HH11	1:B:134:ARG:HG3	1.80	0.47
1:B:355:GLU:OE1	1:B:359:MET:HB2	2.14	0.47
1:A:5:ARG:NH2	1:C:203:GLU:HB3	2.30	0.47
1:A:286:ALA:CA	1:A:311:VAL:HG11	2.44	0.47
1:A:174:LEU:O	1:A:177:TRP:HB3	2.15	0.47
1:A:179:GLN:HE22	1:A:205:LEU:HD23	1.80	0.47
1:C:233:SER:N	1:C:276:SER:OG	2.47	0.47
1:C:29:TYR:HD1	1:C:244:TYR:CE2	2.33	0.47
1:A:313:ILE:HG23	1:A:317:ASN:ND2	2.23	0.47
1:C:103:ASN:O	1:C:106:LEU:HB2	2.15	0.47
1:C:174:LEU:CD1	1:C:178:LEU:HD12	2.44	0.47
1:C:10:LEU:HD21	1:C:61:ILE:HD12	1.97	0.47
1:B:343:ARG:NH1	1:B:383:TYR:HE2	2.09	0.47
1:C:124:PHE:CZ	1:C:190:VAL:HG12	2.49	0.47
1:A:60:VAL:HG12	1:A:61:ILE:N	2.26	0.47
1:B:9:THR:OG1	1:B:60:VAL:HG13	2.15	0.47
1:A:223:LEU:CD1	1:C:24:GLU:HG3	2.27	0.46
1:A:12:PHE:HZ	1:A:83:VAL:HG21	1.80	0.46
1:A:235:VAL:HG12	1:A:236:ALA:N	2.30	0.46
1:C:127:LEU:HB3	1:C:131:SER:OG	2.16	0.46
1:C:299:CYS:HA	1:C:338:LYS:HG2	1.96	0.46
1:C:20:ARG:HB3	1:C:20:ARG:NH1	2.31	0.46
1:B:329:THR:C	1:B:331:HIS:H	2.18	0.46
1:B:3:THR:HG23	1:B:3:THR:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:TYR:HE1	1:C:145:GLN:NE2	2.13	0.46
1:A:190:VAL:HG23	1:A:191:THR:HG23	1.97	0.46
1:C:291:MET:HA	1:C:294:ILE:HD12	1.97	0.46
1:C:11:LEU:O	1:C:12:PHE:CD1	2.68	0.46
1:C:283:THR:O	1:C:285:PRO:CD	2.56	0.46
1:B:223:LEU:HD23	1:B:223:LEU:N	2.29	0.46
1:A:313:ILE:CB	1:A:318:LEU:HD23	2.42	0.46
1:C:86:SER:N	1:C:103:ASN:ND2	2.63	0.46
1:C:102:ASP:HB2	1:C:265:LEU:HB3	1.96	0.46
1:A:159:GLY:HA3	1:A:194:ARG:NH2	2.29	0.46
1:B:332:ALA:O	1:B:336:ALA:HB3	2.15	0.46
1:A:209:VAL:HG13	1:A:213:LEU:O	2.16	0.46
1:C:298:ALA:HB3	1:C:341:LYS:HZ2	1.80	0.46
1:C:221:GLU:O	1:C:225:ARG:HG2	2.15	0.46
1:A:98:TYR:CE2	1:A:100:ALA:HB2	2.50	0.46
1:B:378:THR:HB	1:B:379:THR:H	1.45	0.46
1:C:311:VAL:HG21	1:C:318:LEU:HD11	1.97	0.46
1:C:150:GLU:CG	1:C:151:LYS:N	2.78	0.46
1:B:274:ARG:HG3	1:B:274:ARG:HH11	1.81	0.46
1:C:209:VAL:HA	1:C:210:PRO:HA	1.75	0.46
1:A:192:ASP:O	1:A:196:ARG:HG2	2.15	0.46
1:A:341:LYS:O	1:A:345:LEU:HG	2.16	0.46
1:C:21:GLN:HB3	1:C:239:ALA:CB	2.44	0.46
1:B:61:ILE:HD13	1:B:81:VAL:O	2.15	0.46
1:C:333:MET:O	1:C:337:GLU:HB2	2.16	0.46
1:B:168:GLN:NE2	1:B:172:ASN:OD1	2.44	0.46
1:B:26:VAL:O	1:B:29:TYR:N	2.49	0.46
1:C:318:LEU:C	1:C:318:LEU:HD23	2.35	0.46
1:A:240:ARG:HD3	1:C:350:THR:HB	1.97	0.46
1:B:121:ARG:NH1	1:B:121:ARG:HG3	2.31	0.46
1:B:201:VAL:HG13	1:B:205:LEU:HD13	1.96	0.46
1:B:13:ASN:C	1:B:15:ASN:H	2.19	0.46
1:B:300:LYS:O	1:B:301:GLY:O	2.33	0.46
1:A:357:SER:O	1:A:362:TYR:HB2	2.16	0.46
1:C:128:PRO:HA	1:C:158:GLN:HB3	1.96	0.46
1:C:125:TYR:OH	1:C:194:ARG:NH1	2.49	0.46
1:C:9:THR:OG1	1:C:60:VAL:HG22	2.15	0.46
1:A:7:ARG:NH1	1:A:7:ARG:CB	2.79	0.46
1:C:39:ILE:N	1:C:39:ILE:HD12	2.30	0.46
1:A:34:GLN:NE2	1:C:229:ARG:CD	2.75	0.46
1:B:303:LYS:H	1:B:306:GLN:CB	2.25	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:VAL:HG22	1:C:97:HIS:N	2.30	0.46
1:C:13:ASN:HB3	1:C:15:ASN:OD1	2.16	0.45
1:A:114:LEU:HD13	1:A:186:GLY:HA3	1.97	0.45
1:A:330:ILE:CG2	1:A:331:HIS:N	2.79	0.45
1:A:244:TYR:C	1:A:244:TYR:CD1	2.89	0.45
1:A:216:ILE:HD12	1:A:233:SER:C	2.36	0.45
1:B:189:ALA:HB1	1:B:194:ARG:HB2	1.97	0.45
1:C:376:TYR:C	1:C:378:THR:N	2.69	0.45
1:A:239:ALA:HA	1:A:242:MET:HE3	1.97	0.45
1:A:45:PHE:O	1:A:46:ARG:HG3	2.16	0.45
1:C:208:PRO:HB2	1:C:212:LYS:HB2	1.97	0.45
1:A:34:GLN:CG	1:C:300:LYS:HZ2	2.29	0.45
1:C:114:LEU:C	1:C:116:GLU:H	2.20	0.45
1:B:178:LEU:HA	1:B:181:LEU:HD12	1.98	0.45
1:B:165:GLU:N	1:B:165:GLU:OE1	2.46	0.45
1:C:184:GLN:HE21	1:C:279:TYR:HE1	1.58	0.45
1:C:12:PHE:HB3	1:C:19:ASP:HB3	1.98	0.45
1:C:161:GLU:HB3	1:C:164:PRO:CA	2.46	0.45
1:B:56:LEU:HD23	1:B:78:VAL:HG21	1.98	0.45
1:B:127:LEU:HD13	1:B:190:VAL:HG21	1.97	0.45
1:A:65:ASP:OD2	1:A:84:GLY:HA2	2.16	0.45
1:A:6:HIS:CE1	1:A:254:LEU:HD13	2.51	0.45
1:C:263:ARG:HG2	1:C:263:ARG:NH1	2.30	0.45
1:A:64:PHE:CE2	1:A:70:GLU:HA	2.51	0.45
1:A:70:GLU:CD	1:A:94:PRO:HB3	2.37	0.45
1:A:297:HIS:O	1:A:300:LYS:HB2	2.17	0.45
1:A:207:ILE:HG23	1:A:212:LYS:CD	2.31	0.45
1:C:18:TYR:O	1:C:19:ASP:C	2.53	0.45
1:B:345:LEU:CB	1:B:356:ILE:HD12	2.44	0.45
1:B:64:PHE:CE2	1:B:96:VAL:HG11	2.51	0.45
1:B:60:VAL:HG23	1:B:80:ILE:HG12	1.98	0.45
1:C:97:HIS:HD2	1:C:262:GLN:HG2	1.82	0.45
1:A:128:PRO:C	1:A:130:SER:N	2.70	0.45
1:C:344:SER:C	1:C:346:LEU:H	2.19	0.45
1:B:184:GLN:O	1:B:184:GLN:HG3	2.17	0.45
1:A:282:LEU:HD23	1:A:326:VAL:HG23	1.97	0.45
1:A:190:VAL:CG2	1:A:191:THR:N	2.78	0.45
1:A:386:VAL:CG1	1:A:387:ASN:OD1	2.60	0.45
1:A:345:LEU:HB3	1:A:356:ILE:HD12	1.98	0.45
1:A:352:SER:O	1:A:356:ILE:HG12	2.17	0.45
1:C:107:VAL:CG2	1:C:139:ARG:HG2	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:216:ILE:HG13	1:C:233:SER:O	2.16	0.45
1:A:251:HIS:HA	1:A:254:LEU:HD12	1.98	0.45
1:C:258:GLU:OE1	1:C:258:GLU:HA	2.17	0.45
1:A:184:GLN:N	1:A:212:LYS:O	2.44	0.45
1:B:284:ASP:HA	1:B:285:PRO:HD3	1.81	0.45
1:A:383:TYR:O	1:A:386:VAL:HB	2.17	0.45
1:C:79:PRO:HB3	1:C:253:LEU:CD1	2.46	0.45
1:A:178:LEU:HD22	1:A:201:VAL:CG1	2.47	0.45
1:B:305:ASP:C	1:B:307:VAL:N	2.69	0.45
1:B:12:PHE:CE1	1:B:62:ALA:C	2.91	0.45
1:A:121:ARG:NH1	1:A:121:ARG:HG3	2.30	0.45
1:C:64:PHE:CB	1:C:98:TYR:HE1	2.28	0.45
1:A:232:LEU:C	1:A:232:LEU:HD23	2.37	0.44
1:A:347:ILE:HD11	1:A:383:TYR:OH	2.17	0.44
1:A:4:LYS:CA	1:A:4:LYS:HZ2	2.30	0.44
1:B:165:GLU:CD	1:B:165:GLU:H	2.21	0.44
1:C:275:ARG:O	1:C:277:THR:N	2.50	0.44
1:C:279:TYR:OH	1:C:281:SER:HA	2.18	0.44
1:B:127:LEU:HB3	1:B:131:SER:OG	2.17	0.44
1:A:41:ILE:CG2	1:A:41:ILE:O	2.61	0.44
1:A:43:GLU:HG2	1:A:46:ARG:HG3	1.98	0.44
1:B:160:LEU:CD1	1:B:170:ALA:HA	2.47	0.44
1:C:43:GLU:O	1:C:45:PHE:N	2.50	0.44
1:B:291:MET:HE3	1:B:295:ARG:NH2	2.32	0.44
1:B:311:VAL:HG11	1:B:318:LEU:HG	1.98	0.44
1:B:135:TRP:HB2	1:B:139:ARG:HE	1.82	0.44
1:C:369:TYR:HE1	1:C:379:THR:CG2	2.30	0.44
1:A:185:THR:CG2	1:A:186:GLY:N	2.78	0.44
1:C:181:LEU:HA	1:C:182:PRO:HD3	1.83	0.44
1:C:115:LYS:O	1:C:115:LYS:HG3	2.18	0.44
1:A:286:ALA:C	1:A:311:VAL:HG11	2.38	0.44
1:A:157:TYR:OH	1:A:174:LEU:HA	2.17	0.44
1:B:67:LYS:HG3	1:B:134:ARG:NH2	2.32	0.44
1:B:4:LYS:HE2	1:B:4:LYS:HA	2.00	0.44
1:A:303:LYS:HG2	1:A:306:GLN:HE21	1.81	0.44
1:C:235:VAL:HA	1:C:271:VAL:CG1	2.42	0.44
1:B:354:ASN:HA	1:B:365:LEU:CD1	2.34	0.44
1:A:152:TYR:O	1:A:153:ARG:O	2.35	0.44
1:C:386:VAL:O	1:C:386:VAL:HG12	2.18	0.44
1:A:287:VAL:HG22	1:A:322:PHE:HA	1.99	0.44
1:C:305:ASP:C	1:C:307:VAL:H	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:ALA:HB2	1:A:272:ILE:HD11	1.99	0.44
1:A:211:GLU:OE1	1:A:295:ARG:NH1	2.51	0.44
1:A:175:ALA:O	1:A:178:LEU:N	2.50	0.44
1:B:25:GLY:HA2	1:B:240:ARG:HG3	1.99	0.44
1:A:278:ASP:OD1	1:A:280:ARG:NH2	2.50	0.44
1:B:242:MET:CE	1:B:266:VAL:HB	2.47	0.44
1:A:34:GLN:HE21	1:A:34:GLN:HB3	1.54	0.44
1:C:291:MET:HA	1:C:294:ILE:HB	1.98	0.44
1:A:61:ILE:CD1	1:A:250:LEU:HD22	2.47	0.44
1:C:20:ARG:CB	1:C:20:ARG:NH1	2.80	0.44
1:B:134:ARG:HG3	1:B:134:ARG:NH1	2.33	0.44
1:C:64:PHE:CE2	1:C:70:GLU:HG2	2.53	0.44
1:B:327:GLY:O	1:B:328:GLU:CD	2.56	0.44
1:C:107:VAL:HG22	1:C:139:ARG:CG	2.42	0.44
1:C:127:LEU:HD13	1:C:194:ARG:NE	2.33	0.44
1:C:208:PRO:HG3	1:C:289:GLN:OE1	2.18	0.44
1:C:192:ASP:HB2	1:C:219:ASP:HB3	1.94	0.44
1:A:160:LEU:HD13	1:A:164:PRO:CG	2.42	0.44
1:A:328:GLU:C	1:A:332:ALA:HB3	2.38	0.44
1:A:8:ILE:O	1:A:39:ILE:HA	2.17	0.44
1:B:191:THR:HB	1:B:194:ARG:HG2	2.00	0.44
1:B:133:LYS:HB3	1:B:135:TRP:NE1	2.33	0.44
1:B:142:ALA:O	1:B:143:PHE:C	2.54	0.44
1:A:220:ASN:O	1:A:221:GLU:C	2.56	0.44
1:A:308:LEU:HB3	1:A:313:ILE:O	2.18	0.44
1:C:372:PHE:CD2	1:C:372:PHE:O	2.70	0.44
1:C:179:GLN:OE1	1:C:207:ILE:HD11	2.18	0.44
1:A:113:HIS:HE1	1:A:273:GLU:OE1	2.00	0.43
1:C:159:GLY:HA3	1:C:194:ARG:HH12	1.83	0.43
1:A:127:LEU:HD11	1:A:194:ARG:CZ	2.48	0.43
1:A:300:LYS:HE2	1:C:2:PHE:CZ	2.50	0.43
1:A:180:THR:O	1:A:180:THR:HG22	2.18	0.43
1:A:232:LEU:HA	1:A:276:SER:HB3	1.99	0.43
1:A:313:ILE:HG21	1:A:317:ASN:O	2.18	0.43
1:C:222:GLU:OE1	1:C:225:ARG:HG3	2.18	0.43
1:B:345:LEU:C	1:B:349:THR:HG23	2.37	0.43
1:B:313:ILE:HG22	1:B:314:SER:N	2.33	0.43
1:B:179:GLN:NE2	1:B:207:ILE:HD11	2.32	0.43
1:A:249:LEU:HD23	1:A:249:LEU:O	2.18	0.43
1:B:228:SER:OG	1:B:229:ARG:N	2.51	0.43
1:C:293:TYR:CE2	1:C:302:ILE:HG13	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:372:PHE:CD1	1:C:380:PRO:HG3	2.53	0.43
1:C:249:LEU:HD23	1:C:249:LEU:HA	1.88	0.43
1:B:66:ASP:O	1:B:69:ILE:HB	2.18	0.43
1:B:217:GLY:O	1:B:234:SER:HA	2.18	0.43
1:A:293:TYR:O	1:A:294:ILE:C	2.56	0.43
1:B:343:ARG:CB	1:B:343:ARG:CZ	2.96	0.43
1:C:208:PRO:HA	1:C:292:HIS:CE1	2.53	0.43
1:C:295:ARG:HG2	1:C:295:ARG:O	2.18	0.43
1:B:254:LEU:HD23	1:B:254:LEU:HA	1.89	0.43
1:C:112:LEU:HB3	1:C:116:GLU:OE2	2.17	0.43
1:A:147:VAL:HG13	1:A:148:ALA:N	2.33	0.43
1:A:291:MET:C	1:A:293:TYR:N	2.72	0.43
1:A:313:ILE:O	1:A:318:LEU:HB2	2.17	0.43
1:C:308:LEU:HD13	1:C:315:ARG:CB	2.46	0.43
1:B:125:TYR:HE1	1:B:159:GLY:CA	2.30	0.43
1:C:147:VAL:HG21	1:C:154:GLY:N	2.33	0.43
1:B:33:SER:C	1:B:35:SER:N	2.72	0.43
1:C:293:TYR:CZ	1:C:297:HIS:HB2	2.53	0.43
1:C:229:ARG:NH2	1:C:296:ASN:OD1	2.52	0.43
1:C:226:TYR:O	1:C:228:SER:N	2.52	0.43
1:B:56:LEU:HD11	1:B:60:VAL:HG11	2.00	0.43
1:A:370:SER:HA	1:A:373:LYS:NZ	2.33	0.43
1:B:121:ARG:HH12	1:B:184:GLN:HG3	1.83	0.43
1:C:98:TYR:N	1:C:262:GLN:O	2.47	0.43
1:C:228:SER:O	1:C:230:VAL:N	2.52	0.43
1:B:345:LEU:HD12	1:B:356:ILE:HG23	2.00	0.43
1:A:7:ARG:HB2	1:A:7:ARG:HH11	1.84	0.43
1:A:379:THR:HB	1:A:380:PRO:CD	2.48	0.43
1:C:305:ASP:O	1:C:305:ASP:OD1	2.36	0.43
1:A:231:ALA:O	1:A:276:SER:HB3	2.18	0.43
1:C:299:CYS:H	1:C:341:LYS:HZ2	1.67	0.43
1:A:79:PRO:CB	1:A:253:LEU:HD22	2.49	0.43
1:C:328:GLU:OE2	1:C:333:MET:HG2	2.19	0.43
1:C:159:GLY:CA	1:C:194:ARG:HH22	2.31	0.43
1:A:175:ALA:O	1:A:176:ASP:C	2.58	0.43
1:C:288:ILE:HG22	1:C:289:GLN:N	2.33	0.43
1:C:304:VAL:O	1:C:315:ARG:NH2	2.52	0.43
1:A:14:ALA:HB3	1:C:15:ASN:O	2.19	0.43
1:B:317:ASN:HB3	1:B:321:ARG:CD	2.45	0.43
1:C:370:SER:C	1:C:372:PHE:H	2.21	0.43
1:B:1:MET:HA	1:B:1:MET:HE3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:133:LYS:HE3	1:C:133:LYS:N	2.34	0.43
1:B:60:VAL:HG23	1:B:80:ILE:HG23	2.01	0.43
1:C:20:ARG:CZ	1:C:20:ARG:HB3	2.48	0.43
1:A:20:ARG:HE	1:A:20:ARG:HB3	1.63	0.43
1:A:166:ASN:HB2	1:A:169:HIS:HB2	2.00	0.43
1:C:278:ASP:CA	1:C:280:ARG:NH2	2.82	0.43
1:C:303:LYS:C	1:C:305:ASP:H	2.23	0.43
1:A:233:SER:OG	1:A:273:GLU:HA	2.19	0.42
1:C:225:ARG:NH2	1:C:272:ILE:HD12	2.34	0.42
1:C:114:LEU:HB2	1:C:122:PHE:HE2	1.84	0.42
1:C:248:LYS:O	1:C:252:ARG:HG3	2.19	0.42
1:A:12:PHE:HD2	1:A:23:VAL:CG2	2.31	0.42
1:B:199:LEU:HD23	1:B:199:LEU:HA	1.84	0.42
1:A:218:ILE:O	1:A:220:ASN:N	2.52	0.42
1:A:219:ASP:C	1:A:221:GLU:H	2.23	0.42
1:A:79:PRO:HB3	1:A:253:LEU:HD13	2.00	0.42
1:B:56:LEU:HD21	1:B:60:VAL:HG22	2.00	0.42
1:C:14:ALA:O	1:C:20:ARG:CD	2.63	0.42
1:A:101:THR:HG21	1:A:237:GLN:OE1	2.18	0.42
1:B:378:THR:HG22	1:B:382:GLU:OE1	2.20	0.42
1:C:305:ASP:C	1:C:307:VAL:N	2.71	0.42
1:B:272:ILE:CG2	1:B:274:ARG:NE	2.82	0.42
1:C:25:GLY:O	1:C:28:GLU:HB2	2.19	0.42
1:B:185:THR:HB	1:B:213:LEU:CD2	2.47	0.42
1:C:144:ARG:HG3	1:C:144:ARG:HH11	1.85	0.42
1:B:143:PHE:CZ	1:B:147:VAL:HG11	2.54	0.42
1:C:346:LEU:HB2	1:C:347:ILE:HD12	2.01	0.42
1:C:159:GLY:HA3	1:C:194:ARG:CZ	2.50	0.42
1:C:354:ASN:HD22	1:C:354:ASN:HA	1.61	0.42
1:A:220:ASN:HB2	1:A:235:VAL:O	2.19	0.42
1:A:365:LEU:O	1:A:368:PHE:HB3	2.18	0.42
1:A:233:SER:HA	1:A:274:ARG:CG	2.50	0.42
1:B:99:ILE:HD13	1:B:264:ILE:CG2	2.50	0.42
1:C:18:TYR:O	1:C:21:GLN:N	2.53	0.42
1:B:274:ARG:HG3	1:B:274:ARG:NH1	2.35	0.42
1:C:360:CYS:HB3	1:C:362:TYR:CE2	2.55	0.42
1:A:173:ARG:HE	1:A:173:ARG:HA	1.85	0.42
1:C:140:GLU:O	1:C:143:PHE:HB3	2.20	0.42
1:C:86:SER:H	1:C:103:ASN:ND2	2.18	0.42
1:A:351:LEU:N	1:A:384:ARG:HH22	2.15	0.42
1:B:327:GLY:O	1:B:328:GLU:OE2	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:THR:HB	1:B:242:MET:HE1	2.01	0.42
1:B:28:GLU:OE1	1:B:240:ARG:HD3	2.20	0.42
1:A:182:PRO:HA	1:A:183:PRO:HD3	1.91	0.42
1:B:104:TYR:HE2	1:B:108:GLU:OE1	2.02	0.42
1:A:189:ALA:CB	1:A:195:ALA:HB2	2.46	0.42
1:A:347:ILE:HA	1:A:388:SER:HA	2.01	0.42
1:A:304:VAL:O	1:A:307:VAL:HB	2.20	0.42
1:B:216:ILE:HD12	1:B:233:SER:HB2	2.02	0.42
1:C:373:LYS:HA	1:C:376:TYR:O	2.20	0.42
1:C:373:LYS:HE2	1:C:373:LYS:HB2	1.83	0.41
1:B:284:ASP:CB	1:B:325:GLU:OE1	2.65	0.41
1:A:302:ILE:O	1:A:334:ILE:HD12	2.20	0.41
1:C:7:ARG:CB	1:C:7:ARG:HH11	2.33	0.41
1:C:11:LEU:HB2	1:C:62:ALA:CB	2.51	0.41
1:B:89:LEU:HB2	1:B:92:SER:HB2	2.01	0.41
1:B:121:ARG:CG	1:B:121:ARG:HH11	2.33	0.41
1:B:155:VAL:HG12	1:B:156:VAL:H	1.85	0.41
1:A:102:ASP:HB3	1:A:105:ALA:HB3	2.02	0.41
1:A:234:SER:OG	1:A:235:VAL:N	2.54	0.41
1:C:291:MET:HA	1:C:294:ILE:CG1	2.51	0.41
1:B:305:ASP:C	1:B:307:VAL:H	2.23	0.41
1:B:55:TRP:C	1:B:56:LEU:O	2.59	0.41
1:B:192:ASP:OD1	1:B:218:ILE:N	2.53	0.41
1:B:124:PHE:CD1	1:B:143:PHE:HB2	2.55	0.41
1:A:84:GLY:O	1:A:100:ALA:HB1	2.20	0.41
1:C:259:MET:HG2	1:C:262:GLN:HE21	1.85	0.41
1:C:144:ARG:HG3	1:C:144:ARG:NH1	2.34	0.41
1:C:184:GLN:HA	1:C:212:LYS:O	2.19	0.41
1:A:203:GLU:HB3	1:C:5:ARG:NH1	2.34	0.41
1:A:122:PHE:N	1:A:122:PHE:CD1	2.88	0.41
1:C:2:PHE:O	1:C:2:PHE:HD1	2.02	0.41
1:A:118:GLY:O	1:A:119:VAL:O	2.39	0.41
1:B:84:GLY:HA3	1:B:98:TYR:OH	2.20	0.41
1:A:174:LEU:HD12	1:A:175:ALA:N	2.35	0.41
1:A:187:ILE:HD11	1:A:213:LEU:HD13	2.01	0.41
1:C:164:PRO:HG2	1:C:167:TRP:HA	2.02	0.41
1:B:311:VAL:CG1	1:B:312:GLY:N	2.82	0.41
1:B:218:ILE:HG13	1:B:235:VAL:CG2	2.51	0.41
1:A:121:ARG:O	1:A:185:THR:HG23	2.21	0.41
1:C:46:ARG:NH1	1:C:46:ARG:HG2	2.35	0.41
1:A:347:ILE:HG23	1:A:389:GLU:N	2.22	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:C	1:B:256:LYS:H	2.23	0.41
1:C:222:GLU:HA	1:C:222:GLU:OE1	2.21	0.41
1:A:373:LYS:HE2	1:A:373:LYS:HB2	1.96	0.41
1:C:346:LEU:HD13	1:C:384:ARG:HG2	2.01	0.41
1:C:351:LEU:HD22	1:C:352:SER:H	1.85	0.41
1:B:178:LEU:O	1:B:181:LEU:HB2	2.21	0.41
1:B:204:HIS:CD2	1:B:205:LEU:HD12	2.55	0.41
1:B:205:LEU:CD1	1:B:205:LEU:N	2.83	0.41
1:B:287:VAL:O	1:B:288:ILE:C	2.59	0.41
1:A:198:ILE:HG21	1:A:215:VAL:CG1	2.51	0.41
1:A:211:GLU:HG2	1:A:292:HIS:HB2	2.01	0.41
1:C:127:LEU:HD22	1:C:190:VAL:HG21	2.02	0.41
1:C:86:SER:C	1:C:87:TYR:HD1	2.23	0.41
1:C:311:VAL:HB	1:C:318:LEU:CD1	2.38	0.41
1:B:313:ILE:HG22	1:B:314:SER:O	2.21	0.41
1:B:308:LEU:HD22	1:B:315:ARG:HA	2.02	0.41
1:C:22:VAL:O	1:C:25:GLY:N	2.54	0.41
1:C:249:LEU:HD11	1:C:262:GLN:HG3	2.02	0.41
1:C:284:ASP:HB3	1:C:325:GLU:OE2	2.20	0.41
1:C:159:GLY:HA3	1:C:194:ARG:NH2	2.35	0.41
1:C:275:ARG:HH22	1:C:296:ASN:ND2	2.17	0.41
1:C:23:VAL:HG11	1:C:41:ILE:HD13	2.02	0.41
1:C:233:SER:CB	1:C:276:SER:OG	2.68	0.41
1:B:188:ILE:HG12	1:B:216:ILE:HG21	2.03	0.41
1:B:106:LEU:HB3	1:B:218:ILE:HD11	2.02	0.41
1:B:191:THR:HG22	1:B:192:ASP:N	2.35	0.41
1:C:356:ILE:N	1:C:356:ILE:HD13	2.36	0.41
1:B:174:LEU:O	1:B:175:ALA:C	2.58	0.41
1:C:84:GLY:O	1:C:100:ALA:HA	2.21	0.41
1:C:185:THR:HG22	1:C:186:GLY:N	2.36	0.41
1:B:152:TYR:N	1:B:152:TYR:CD1	2.89	0.41
1:C:4:LYS:HZ2	1:C:4:LYS:HA	1.86	0.41
1:A:244:TYR:HD1	1:A:245:GLN:NE2	2.16	0.41
1:B:164:PRO:HB2	1:B:170:ALA:HB2	2.01	0.41
1:A:206:HIS:O	1:A:208:PRO:HD3	2.21	0.41
1:C:141:TYR:CD1	1:C:141:TYR:C	2.95	0.41
1:B:216:ILE:CD1	1:B:277:THR:HG21	2.51	0.41
1:C:278:ASP:O	1:C:280:ARG:CZ	2.69	0.41
1:C:75:ASP:O	1:C:75:ASP:CG	2.59	0.41
1:B:29:TYR:CE1	1:B:248:LYS:HA	2.55	0.41
1:C:308:LEU:CD1	1:C:315:ARG:HB2	2.49	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:VAL:O	1:C:231:ALA:C	2.59	0.40
1:B:292:HIS:C	1:B:294:ILE:N	2.75	0.40
1:B:308:LEU:HD13	1:B:315:ARG:CB	2.51	0.40
1:B:369:TYR:CE2	1:B:373:LYS:HD2	2.56	0.40
1:A:99:ILE:HG23	1:A:264:ILE:HG13	2.02	0.40
1:B:331:HIS:C	1:B:333:MET:N	2.73	0.40
1:C:58:ASP:O	1:C:78:VAL:HB	2.21	0.40
1:A:157:TYR:CE1	1:A:177:TRP:HB2	2.56	0.40
1:A:114:LEU:HB2	1:A:122:PHE:HE2	1.86	0.40
1:A:216:ILE:HD11	1:A:234:SER:HA	2.03	0.40
1:B:41:ILE:O	1:B:41:ILE:HG22	2.21	0.40
1:A:65:ASP:OD1	1:A:85:GLY:N	2.52	0.40
1:B:144:ARG:HG3	1:B:144:ARG:NH1	2.31	0.40
1:A:131:SER:O	1:A:132:GLY:C	2.59	0.40
1:C:272:ILE:HB	1:C:274:ARG:NH1	2.37	0.40
1:B:291:MET:CE	1:B:295:ARG:NH2	2.84	0.40
1:A:24:GLU:HB3	1:A:240:ARG:HH12	1.86	0.40
1:A:185:THR:O	1:A:214:CYS:HB2	2.22	0.40
1:C:209:VAL:HG12	1:C:213:LEU:O	2.22	0.40
1:A:147:VAL:C	1:A:149:GLU:H	2.24	0.40
1:A:297:HIS:NE2	1:C:1:MET:SD	2.94	0.40
1:C:180:THR:HG22	1:C:180:THR:O	2.22	0.40
1:A:125:TYR:CD2	1:A:198:ILE:HD11	2.57	0.40
1:A:188:ILE:HA	1:A:216:ILE:HG23	2.02	0.40
1:A:352:SER:OG	1:A:355:GLU:HB3	2.20	0.40
1:B:222:GLU:O	1:B:225:ARG:HB2	2.21	0.40
1:C:86:SER:O	1:C:87:TYR:CD1	2.75	0.40
1:B:216:ILE:HD13	1:B:277:THR:HG21	2.03	0.40
1:B:135:TRP:O	1:B:139:ARG:HD2	2.21	0.40
1:B:181:LEU:HA	1:B:182:PRO:HD3	1.92	0.40
1:B:74:ALA:C	1:B:75:ASP:OD1	2.59	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:320:LYS:NZ	1:C:320:LYS:NZ[6_554]	1.76	0.44

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	374/392 (95%)	272 (73%)	64 (17%)	38 (10%)	1 9
1	B	374/392 (95%)	277 (74%)	74 (20%)	23 (6%)	2 19
1	C	374/392 (95%)	292 (78%)	57 (15%)	25 (7%)	1 18
All	All	1122/1176 (95%)	841 (75%)	195 (17%)	86 (8%)	1 14

All (86) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	VAL
1	A	119	VAL
1	A	153	ARG
1	A	159	GLY
1	A	225	ARG
1	A	269	VAL
1	A	278	ASP
1	A	386	VAL
1	B	56	LEU
1	B	132	GLY
1	B	276	SER
1	C	56	LEU
1	C	227	LEU
1	A	2	PHE
1	A	7	ARG
1	A	56	LEU
1	A	219	ASP
1	A	237	GLN
1	A	276	SER
1	A	298	ALA
1	A	299	CYS
1	A	327	GLY
1	A	328	GLU
1	B	14	ALA

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Mol	Chain	Res	Type
1	B	96	VAL
1	B	119	VAL
1	B	159	GLY
1	B	293	TYR
1	B	301	GLY
1	B	363	PRO
1	C	132	GLY
1	C	159	GLY
1	C	167	TRP
1	C	229	ARG
1	C	256	LYS
1	C	269	VAL
1	C	276	SER
1	C	325	GLU
1	C	370	SER
1	C	377	ASP
1	A	118	GLY
1	A	220	ASN
1	A	281	SER
1	A	288	ILE
1	A	329	THR
1	B	86	SER
1	B	237	GLN
1	B	357	SER
1	C	190	VAL
1	C	225	ARG
1	C	226	TYR
1	A	86	SER
1	A	148	ALA
1	A	211	GLU
1	A	224	THR
1	A	301	GLY
1	A	308	LEU
1	A	361	GLY
1	B	78	VAL
1	B	102	ASP
1	C	131	SER
1	C	160	LEU
1	C	304	VAL
1	C	311	VAL
1	C	312	GLY
1	C	371	VAL

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Mol	Chain	Res	Type
1	A	228	SER
1	A	261	LEU
1	A	314	SER
1	A	349	THR
1	A	388	SER
1	B	256	LYS
1	B	278	ASP
1	B	359	MET
1	B	370	SER
1	C	285	PRO
1	A	208	PRO
1	B	179	GLN
1	B	322	PHE
1	C	128	PRO
1	C	278	ASP
1	A	363	PRO
1	B	334	ILE
1	B	362	TYR
1	C	284	ASP
1	A	271	VAL

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	326/338 (96%)	260 (80%)	66 (20%)	1 7
1	B	326/338 (96%)	267 (82%)	59 (18%)	2 11
1	C	326/338 (96%)	273 (84%)	53 (16%)	3 16
All	All	978/1014 (96%)	800 (82%)	178 (18%)	2 11

All (178) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	4	LYS

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Mol	Chain	Res	Type
1	A	9	THR
1	A	19	ASP
1	A	20	ARG
1	A	30	LEU
1	A	34	GLN
1	A	35	SER
1	A	38	ASP
1	A	40	PHE
1	A	43	GLU
1	A	55	TRP
1	A	58	ASP
1	A	66	ASP
1	A	75	ASP
1	A	86	SER
1	A	91	GLU
1	A	117	LYS
1	A	120	ASN
1	A	134	ARG
1	A	145	GLN
1	A	152	TYR
1	A	153	ARG
1	A	160	LEU
1	A	165	GLU
1	A	167	TRP
1	A	179	GLN
1	A	192	ASP
1	A	197	HIS
1	A	201	VAL
1	A	208	PRO
1	A	211	GLU
1	A	215	VAL
1	A	221	GLU
1	A	222	GLU
1	A	224	THR
1	A	226	TYR
1	A	227	LEU
1	A	229	ARG
1	A	230	VAL
1	A	241	GLN
1	A	252	ARG
1	A	256	LYS
1	A	257	GLU

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Mol	Chain	Res	Type
1	A	263	ARG
1	A	264	ILE
1	A	272	ILE
1	A	275	ARG
1	A	280	ARG
1	A	289	GLN
1	A	291	MET
1	A	299	CYS
1	A	304	VAL
1	A	320	LYS
1	A	321	ARG
1	A	323	LYS
1	A	328	GLU
1	A	330	ILE
1	A	335	HIS
1	A	348	SER
1	A	349	THR
1	A	352	SER
1	A	355	GLU
1	A	369	TYR
1	A	373	LYS
1	A	385	ASP
1	B	1	MET
1	B	4	LYS
1	B	6	HIS
1	B	9	THR
1	B	13	ASN
1	B	23	VAL
1	B	28	GLU
1	B	42	GLU
1	B	58	ASP
1	B	60	VAL
1	B	64	PHE
1	B	77	ASP
1	B	91	GLU
1	B	98	TYR
1	B	121	ARG
1	B	122	PHE
1	B	124	PHE
1	B	125	TYR
1	B	135	TRP
1	B	146	LEU

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Mol	Chain	Res	Type
1	B	153	ARG
1	B	165	GLU
1	B	167	TRP
1	B	171	GLN
1	B	173	ARG
1	B	176	ASP
1	B	178	LEU
1	B	179	GLN
1	B	180	THR
1	B	181	LEU
1	B	190	VAL
1	B	196	ARG
1	B	219	ASP
1	B	221	GLU
1	B	226	TYR
1	B	230	VAL
1	B	232	LEU
1	B	234	SER
1	B	248	LYS
1	B	256	LYS
1	B	270	ARG
1	B	281	SER
1	B	291	MET
1	B	294	ILE
1	B	307	VAL
1	B	318	LEU
1	B	323	LYS
1	B	325	GLU
1	B	328	GLU
1	B	329	THR
1	B	330	ILE
1	B	343	ARG
1	B	348	SER
1	B	349	THR
1	B	359	MET
1	B	360	CYS
1	B	369	TYR
1	B	378	THR
1	B	389	GLU
1	C	4	LYS
1	C	19	ASP
1	C	30	LEU

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Mol	Chain	Res	Type
1	C	38	ASP
1	C	39	ILE
1	C	75	ASP
1	C	131	SER
1	C	133	LYS
1	C	141	TYR
1	C	144	ARG
1	C	152	TYR
1	C	160	LEU
1	C	165	GLU
1	C	166	ASN
1	C	167	TRP
1	C	172	ASN
1	C	174	LEU
1	C	192	ASP
1	C	202	CYS
1	C	209	VAL
1	C	219	ASP
1	C	224	THR
1	C	228	SER
1	C	230	VAL
1	C	237	GLN
1	C	248	LYS
1	C	249	LEU
1	C	253	LEU
1	C	256	LYS
1	C	257	GLU
1	C	258	GLU
1	C	263	ARG
1	C	271	VAL
1	C	275	ARG
1	C	280	ARG
1	C	282	LEU
1	C	285	PRO
1	C	289	GLN
1	C	302	ILE
1	C	308	LEU
1	C	320	LYS
1	C	322	PHE
1	C	331	HIS
1	C	348	SER
1	C	349	THR

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Mol	Chain	Res	Type
1	C	351	LEU
1	C	354	ASN
1	C	356	ILE
1	C	358	GLN
1	C	366	GLN
1	C	373	LYS
1	C	376	TYR
1	C	384	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	113	HIS
1	A	179	GLN
1	A	245	GLN
1	A	289	GLN
1	A	292	HIS
1	A	306	GLN
1	A	317	ASN
1	A	354	ASN
1	B	13	ASN
1	B	15	ASN
1	B	88	HIS
1	B	97	HIS
1	B	113	HIS
1	B	168	GLN
1	B	171	GLN
1	B	172	ASN
1	B	179	GLN
1	B	184	GLN
1	B	200	GLN
1	B	204	HIS
1	B	245	GLN
1	B	292	HIS
1	B	297	HIS
1	B	331	HIS
1	C	21	GLN
1	C	97	HIS
1	C	113	HIS
1	C	145	GLN
1	C	172	ASN

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Mol	Chain	Res	Type
1	C	200	GLN
1	C	241	GLN
1	C	251	HIS
1	C	262	GLN
1	C	292	HIS
1	C	317	ASN
1	C	354	ASN
1	C	358	GLN
1	C	366	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 carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

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	380/392 (96%)	0.36	24 (6%)	23	21	70, 120, 159, 178	0
1	B	380/392 (96%)	0.36	12 (3%)	51	45	56, 102, 140, 162	0
1	C	380/392 (96%)	0.57	38 (10%)	9	10	69, 114, 166, 178	0
All	All	1140/1176 (96%)	0.43	74 (6%)	22	20	56, 112, 160, 178	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	353	ILE	9.1
1	A	347	ILE	6.1
1	A	311	VAL	5.7
1	C	347	ILE	5.7
1	C	318	LEU	5.2
1	C	330	ILE	4.7
1	A	73	LEU	4.5
1	C	327	GLY	4.5
1	C	386	VAL	4.3
1	C	325	GLU	4.2
1	C	311	VAL	4.2
1	B	312	GLY	4.0
1	C	337	GLU	3.9
1	C	289	GLN	3.8
1	A	356	ILE	3.8
1	A	348	SER	3.8
1	A	42	GLU	3.6
1	B	73	LEU	3.6
1	C	335	HIS	3.6
1	A	309	ASP	3.4
1	C	346	LEU	3.4
1	C	374	LYS	3.3
1	C	354	ASN	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	329	THR	3.2
1	C	375	ALA	3.2
1	A	69	ILE	3.2
1	B	313	ILE	3.1
1	B	160	LEU	3.1
1	C	383	TYR	3.1
1	C	371	VAL	3.1
1	A	350	THR	2.9
1	A	310	ALA	2.8
1	C	387	ASN	2.8
1	A	318	LEU	2.7
1	C	306	GLN	2.7
1	B	318	LEU	2.7
1	C	226	TYR	2.6
1	C	213	LEU	2.6
1	A	302	ILE	2.6
1	C	352	SER	2.6
1	A	334	ILE	2.5
1	C	73	LEU	2.5
1	C	312	GLY	2.5
1	B	273	GLU	2.5
1	A	111	PHE	2.5
1	C	307	VAL	2.5
1	C	381	LYS	2.5
1	B	298	ALA	2.4
1	C	302	ILE	2.4
1	C	336	ALA	2.4
1	B	3	THR	2.4
1	C	356	ILE	2.4
1	C	283	THR	2.4
1	A	122	PHE	2.4
1	A	152	TYR	2.3
1	A	312	GLY	2.3
1	C	264	ILE	2.3
1	C	41	ILE	2.3
1	C	313	ILE	2.2
1	A	119	VAL	2.2
1	B	227	LEU	2.2
1	A	12	PHE	2.2
1	B	57	GLY	2.2
1	C	326	VAL	2.1
1	C	331	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	363	PRO	2.1
1	C	324	GLU	2.1
1	A	64	PHE	2.1
1	A	353	ILE	2.1
1	C	385	ASP	2.1
1	B	307	VAL	2.1
1	B	214	CYS	2.0
1	A	322	PHE	2.0
1	A	181	LEU	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 carbohydrates 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.