Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 07:41 AM GMT

PDB ID	:	3BLX
Title	:	Yeast Isocitrate Dehydrogenase (Apo Form)
Authors	:	Taylor, A.B.; Hu, G.; Hart, P.J.; McAlister-Henn, L.
Deposited on	:	2007-12-11
Resolution	:	2.70 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

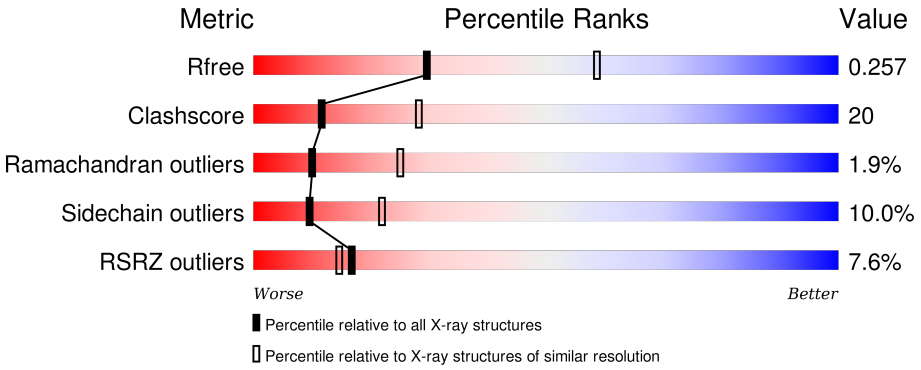
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.70 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	2103 (2.70-2.70)
Clashscore	102246	2422 (2.70-2.70)
Ramachandran outliers	100387	2382 (2.70-2.70)
Sidechain outliers	100360	2382 (2.70-2.70)
RSRZ outliers	91569	2107 (2.70-2.70)

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	349	4% 65% 27%
1	C	349	% 66% 27%
1	E	349	% 68% 25%
1	G	349	% 65% 26%
1	I	349	4% 64% 26% 5% 5%

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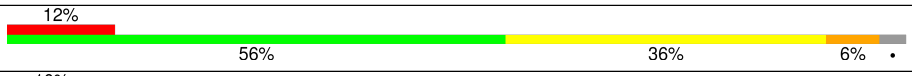
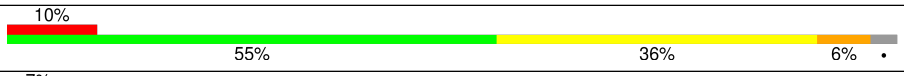
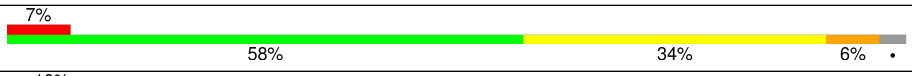
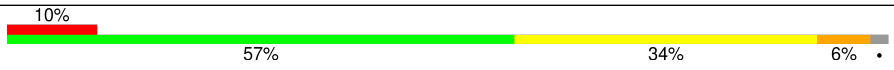
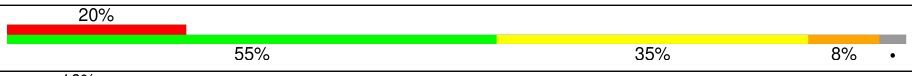
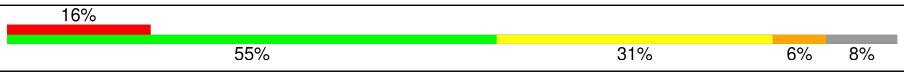
Mol	Chain	Length	Quality of chain
1	K	349	
1	M	349	
1	O	349	
2	B	354	
2	D	354	
2	F	354	
2	H	354	
2	J	354	
2	L	354	
2	N	354	
2	P	354	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 41336 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 Isocitrate dehydrogenase [NAD] subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	0	0
			2575	1626	451	491	7			
1	C	338	Total	C	N	O	S	0	0	0
			2605	1645	458	495	7			
1	E	341	Total	C	N	O	S	0	0	0
			2626	1659	461	499	7			
1	G	334	Total	C	N	O	S	0	0	0
			2567	1620	450	490	7			
1	I	333	Total	C	N	O	S	0	0	0
			2562	1617	448	490	7			
1	K	338	Total	C	N	O	S	0	0	0
			2605	1645	458	495	7			
1	M	337	Total	C	N	O	S	0	0	0
			2590	1638	453	492	7			
1	O	332	Total	C	N	O	S	0	0	0
			2546	1605	447	487	7			

- Molecule 2 is a protein called Isocitrate dehydrogenase [NAD] subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	346	Total	C	N	O	S	0	0	0
			2608	1646	447	509	6			
2	D	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	F	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	H	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	J	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	L	346	Total	C	N	O	S	0	0	0
			2608	1646	447	509	6			

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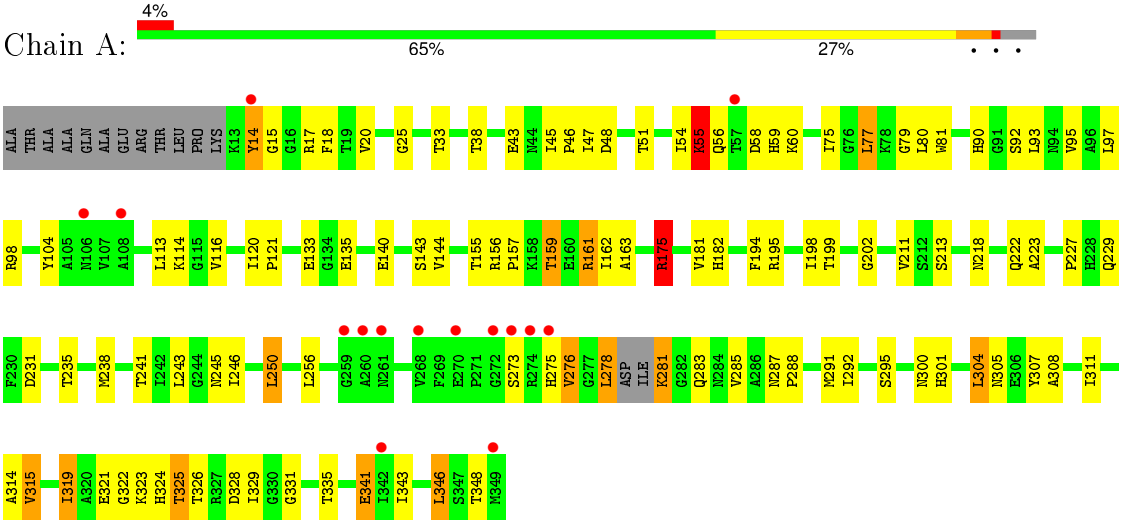
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	N	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	P	326	Total	C	N	O	S	0	0	0
			2454	1549	418	481	6			

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.

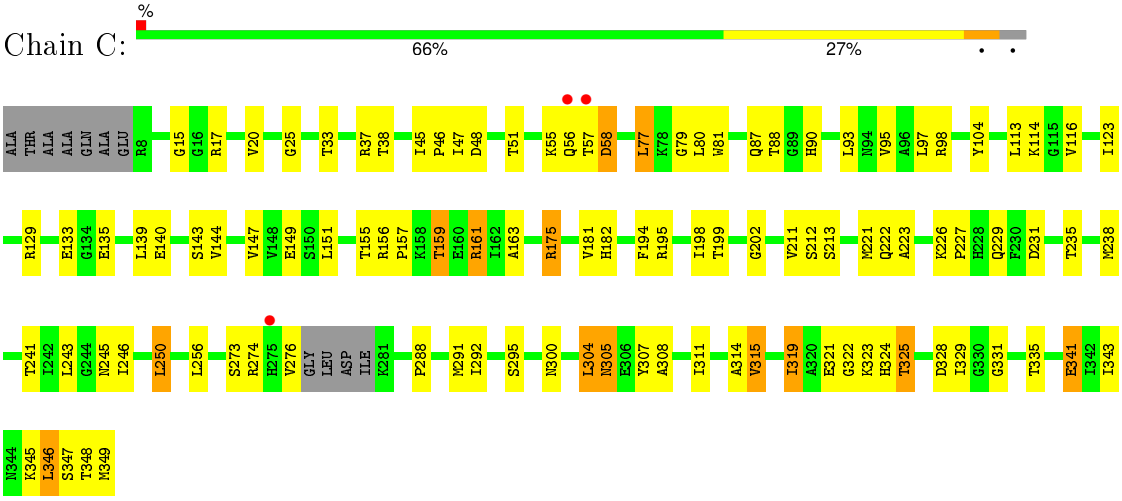
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

Chain A:



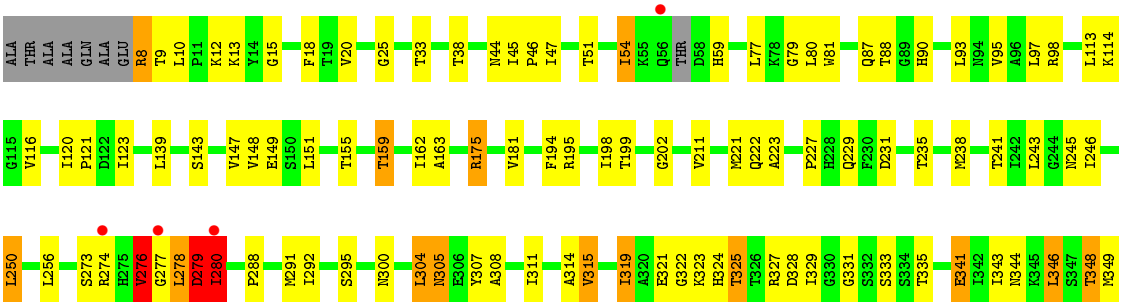
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

Chain C:



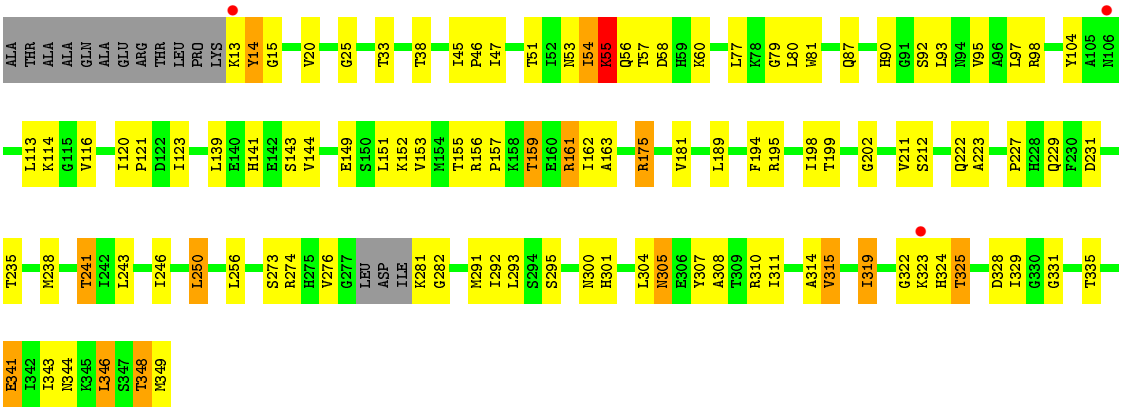
- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

Chain E:



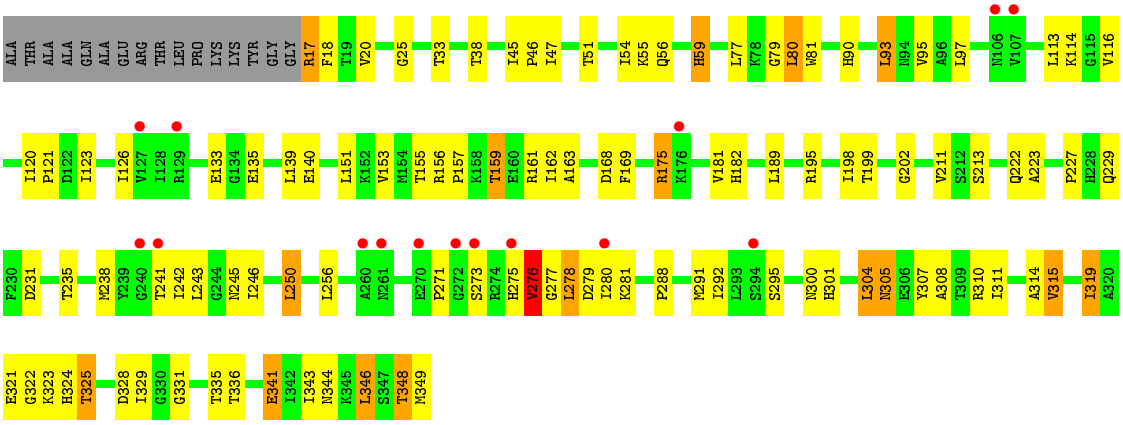
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

Chain G:



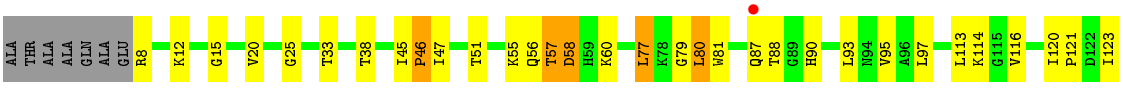
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

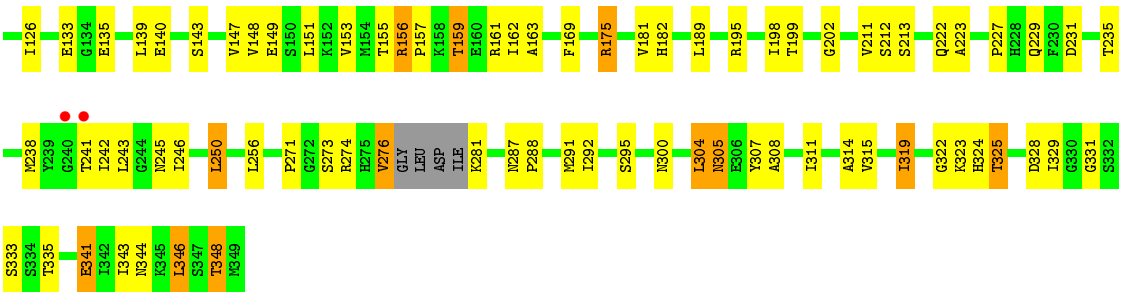
Chain I:



• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

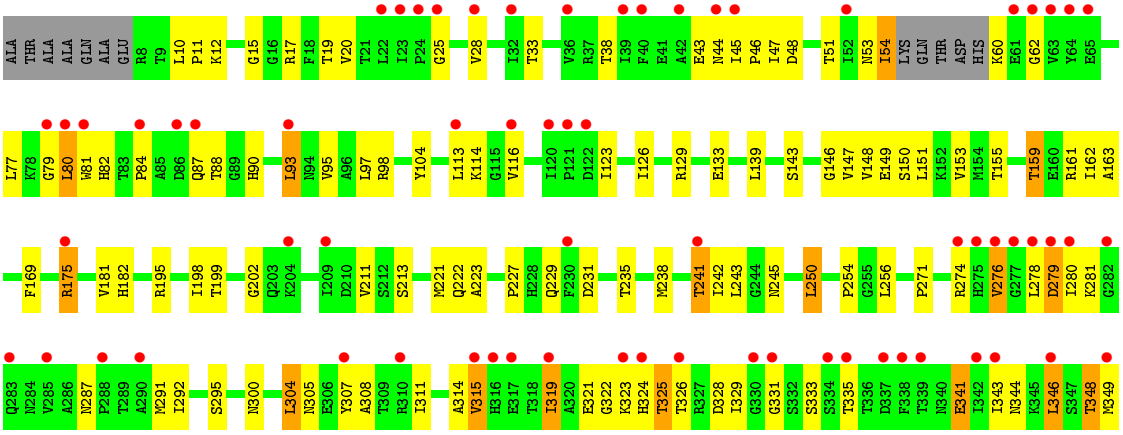
Chain K:





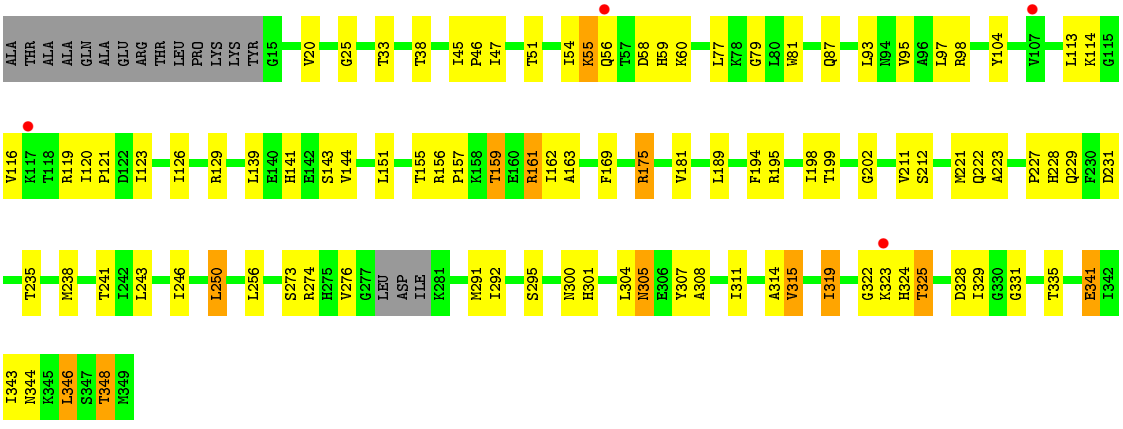
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

Chain M:



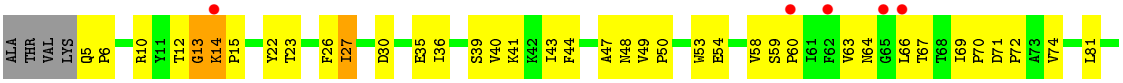
• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

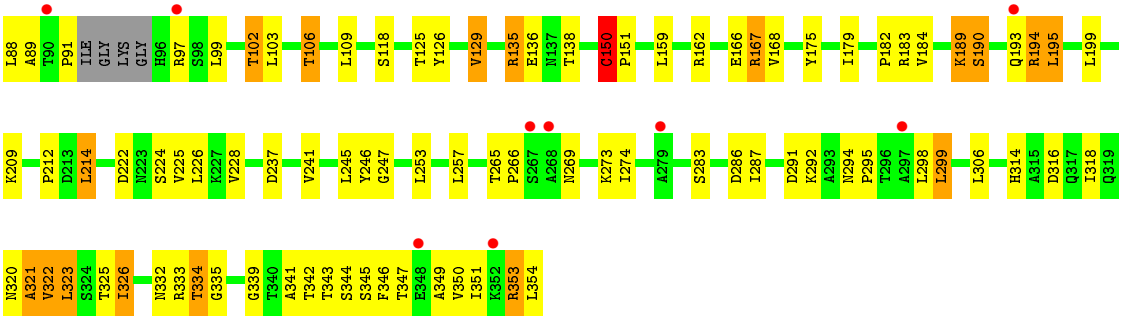
Chain O:



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

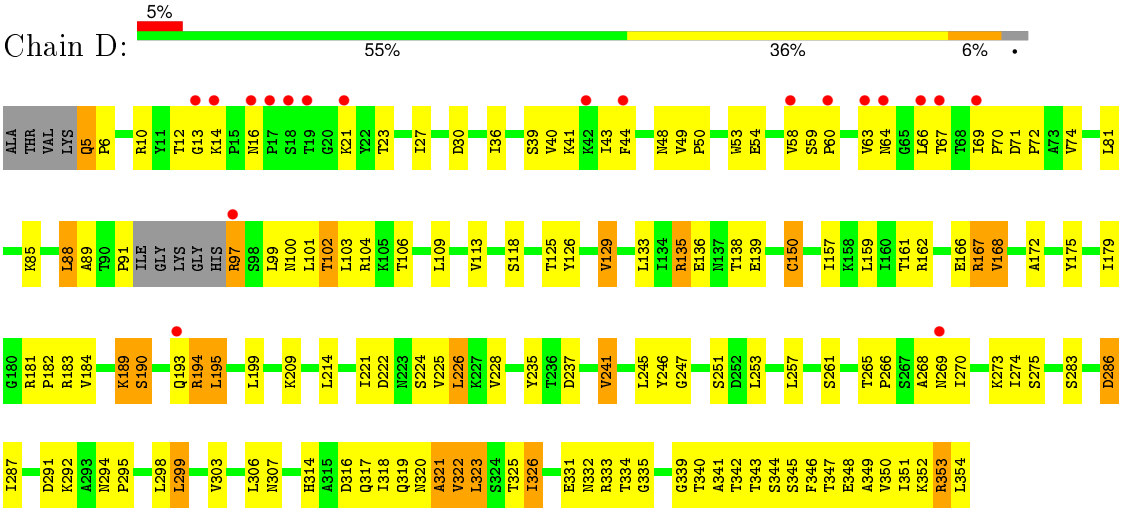
Chain B:





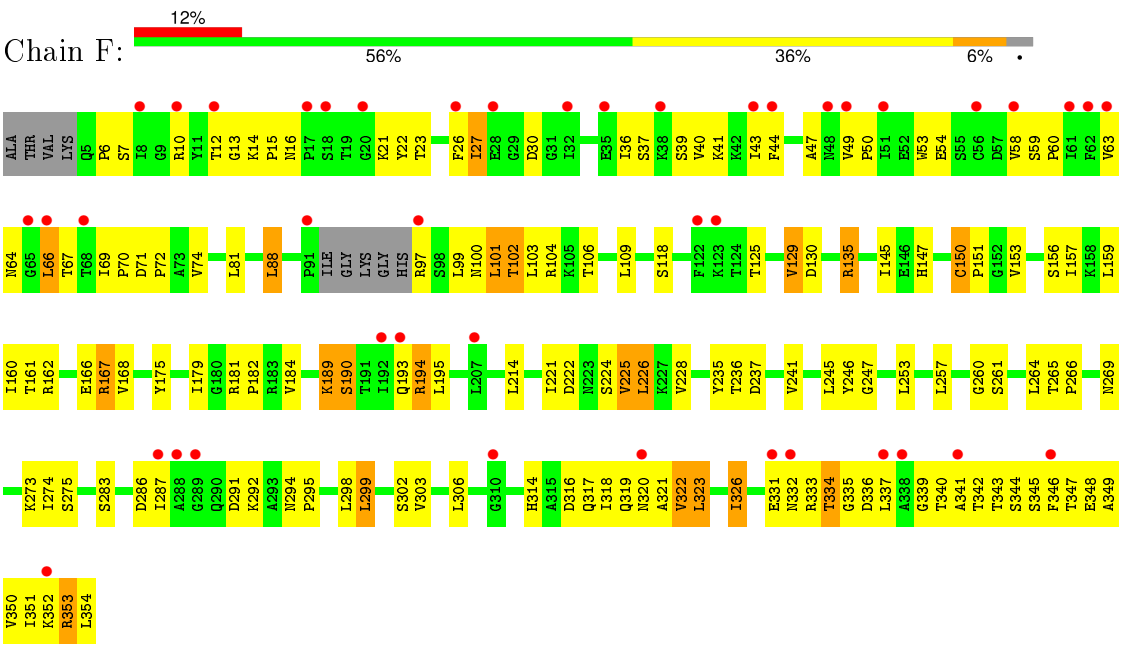
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

Chain D:



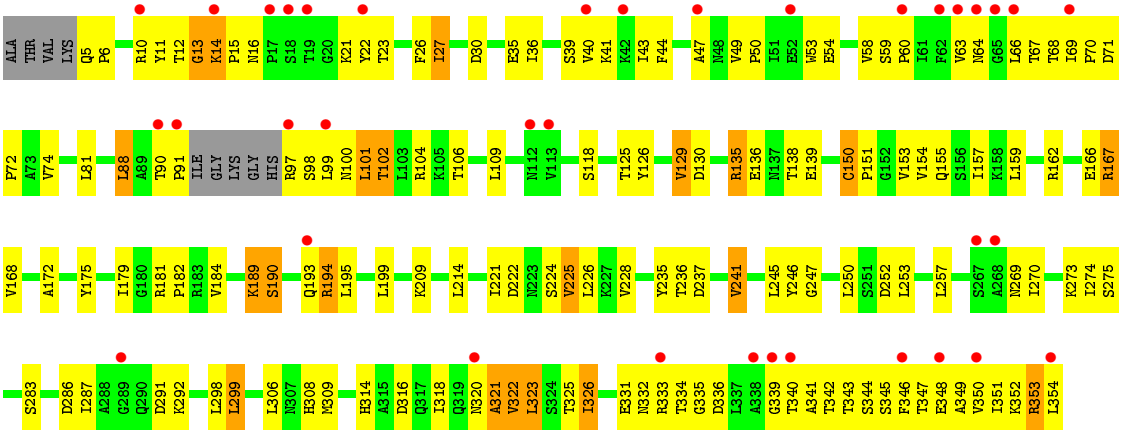
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

Chain F:



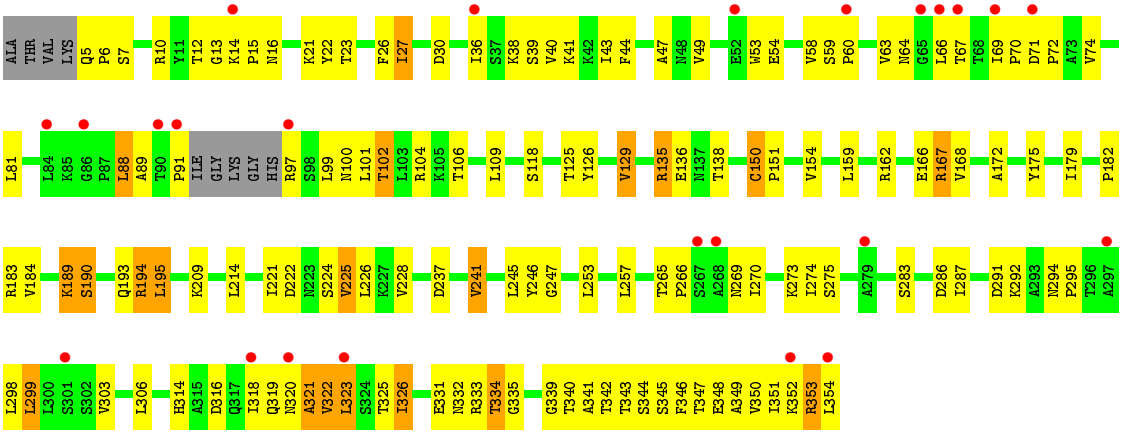
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

Chain H:



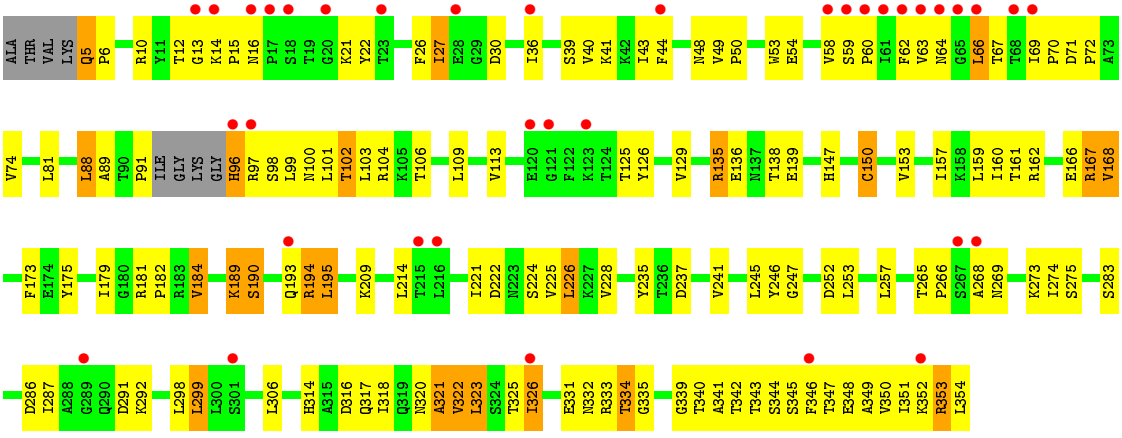
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

Chain J:



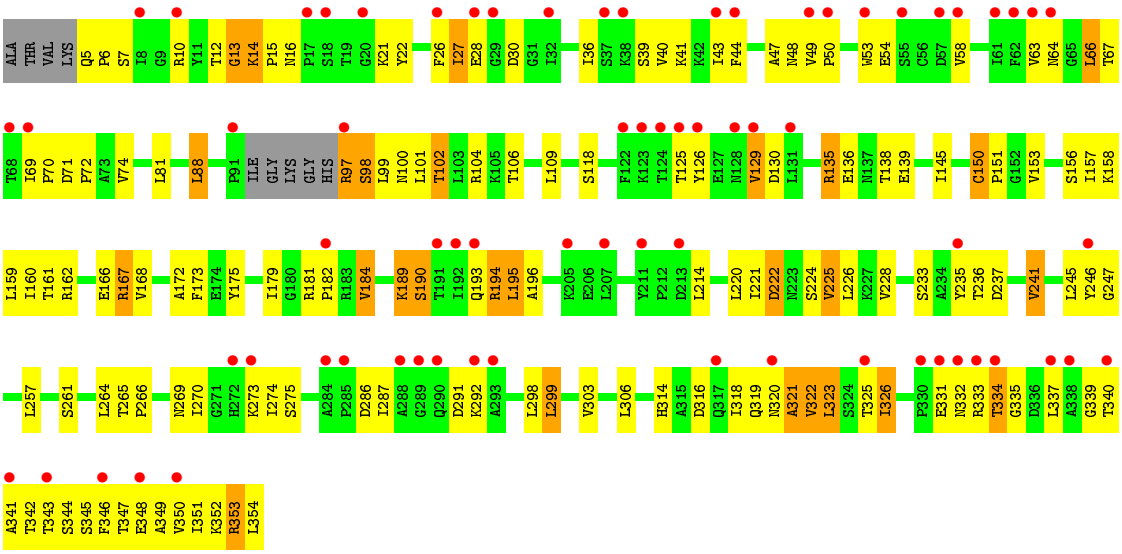
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

Chain L:



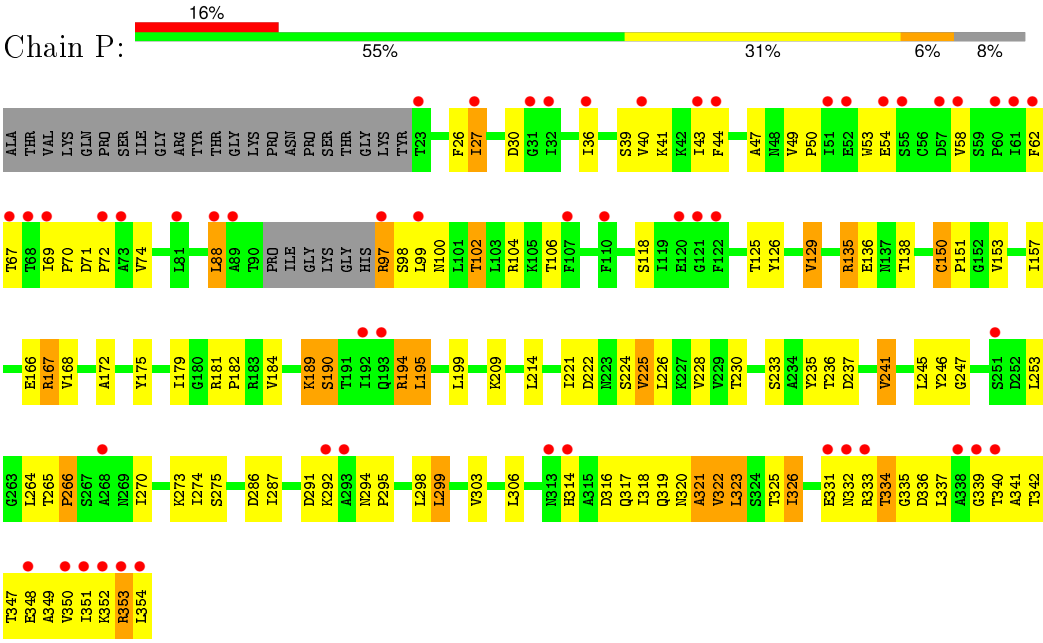
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

Chain N:



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	112.44Å 115.21Å 159.25Å 111.03° 96.08° 107.13°	Depositor
Resolution (Å)	35.74 – 2.70 35.74 – 2.70	Depositor EDS
% Data completeness (in resolution range)	96.5 (35.74-2.70) 82.4 (35.74-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	2.01 (at 2.68Å)	Xtriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.239 , 0.264 0.227 , 0.257	Depositor DCC
R_{free} test set	9226 reflections (5.03%)	DCC
Wilson B-factor (Å^2)	71.3	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 41.0	EDS
Estimated twinning fraction	0.005 for k,h,-h-k-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 183471 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	41336	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% 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	0.60	0/2619	0.71	2/3538 (0.1%)
1	C	0.60	0/2650	0.67	0/3580
1	E	0.56	0/2671	0.69	0/3608
1	G	0.56	0/2611	0.67	0/3527
1	I	0.58	0/2606	0.68	0/3524
1	K	0.57	0/2650	0.67	0/3580
1	M	0.64	0/2634	0.69	0/3559
1	O	0.54	0/2589	0.66	0/3498
2	B	0.51	1/2654 (0.0%)	0.62	0/3610
2	D	0.48	0/2643	0.62	1/3595 (0.0%)
2	F	0.47	0/2643	0.60	0/3595
2	H	0.46	0/2643	0.59	0/3595
2	J	0.43	0/2643	0.56	0/3595
2	L	0.46	1/2654 (0.0%)	0.60	0/3610
2	N	0.50	0/2643	0.59	0/3595
2	P	0.46	0/2493	0.59	0/3390
All	All	0.53	2/42046 (0.0%)	0.64	3/56999 (0.0%)

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	M	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	150	CYS	CB-SG	5.76	1.92	1.82
2	B	150	CYS	CB-SG	5.60	1.91	1.82

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	175	ARG	NE-CZ-NH1	5.99	123.30	120.30
2	D	150	CYS	CA-CB-SG	5.47	123.84	114.00
1	A	278	LEU	CA-CB-CG	5.40	127.72	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	M	53	ASN	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	2575	0	2608	87	0
1	C	2605	0	2645	85	0
1	E	2626	0	2667	94	0
1	G	2567	0	2597	89	0
1	I	2562	0	2596	90	0
1	K	2605	0	2645	82	0
1	M	2590	0	2635	116	0
1	O	2546	0	2575	82	0
2	B	2608	0	2648	124	0
2	D	2598	0	2641	138	0
2	F	2598	0	2641	151	0
2	H	2598	0	2641	148	0
2	J	2598	0	2641	132	0
2	L	2608	0	2648	138	0
2	N	2598	0	2641	169	0
2	P	2454	0	2498	124	0
All	All	41336	0	41967	1692	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 20.

All (1692) 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)
2:N:97:ARG:NH1	2:N:102:THR:HG23	1.63	1.12
1:E:54:ILE:H	1:E:54:ILE:HD12	1.19	1.06
1:O:181:VAL:HB	1:O:235:THR:HG22	1.37	1.04
1:E:181:VAL:HB	1:E:235:THR:HG22	1.38	1.04
1:A:181:VAL:HB	1:A:235:THR:HG22	1.38	1.03
1:C:181:VAL:HB	1:C:235:THR:HG22	1.40	1.02
2:B:318:ILE:O	2:B:322:VAL:HG21	1.61	1.01
1:I:18:PHE:CZ	1:M:44:ASN:ND2	2.29	1.00
1:K:181:VAL:HB	1:K:235:THR:HG22	1.40	1.00
1:M:54:ILE:HA	1:M:62:GLY:HA3	1.43	1.00
1:I:181:VAL:HB	1:I:235:THR:HG22	1.42	0.99
1:G:181:VAL:HB	1:G:235:THR:HG22	1.43	0.99
1:M:147:VAL:HG22	2:N:161:THR:HG22	1.41	0.99
2:F:287:ILE:HD11	2:F:292:LYS:HD2	1.44	0.98
1:I:18:PHE:HZ	1:M:44:ASN:HD21	1.03	0.98
1:K:175:ARG:HH11	1:K:175:ARG:HG3	1.27	0.98
1:G:54:ILE:HD12	1:G:54:ILE:H	1.29	0.96
1:E:175:ARG:HG3	1:E:175:ARG:HH11	1.29	0.96
1:O:175:ARG:HH11	1:O:175:ARG:HG3	1.29	0.96
2:N:97:ARG:HH12	2:N:102:THR:HG23	1.28	0.96
2:P:135:ARG:HD3	2:P:247:GLY:HA3	1.48	0.96
1:M:175:ARG:HG3	1:M:175:ARG:HH11	1.29	0.95
1:G:175:ARG:HG3	1:G:175:ARG:HH11	1.31	0.95
2:N:287:ILE:HD11	2:N:292:LYS:HD2	1.46	0.95
2:H:194:ARG:HG3	2:H:194:ARG:HH21	1.30	0.95
1:E:280:ILE:HG22	1:E:327:ARG:HE	1.31	0.95
2:H:287:ILE:HD11	2:H:292:LYS:HD2	1.48	0.94
2:F:318:ILE:O	2:F:322:VAL:HG21	1.66	0.94
2:P:287:ILE:HD11	2:P:292:LYS:HD2	1.47	0.94
1:M:181:VAL:HB	1:M:235:THR:HG22	1.47	0.94
2:J:318:ILE:O	2:J:322:VAL:HG21	1.68	0.94
2:L:189:LYS:HD2	2:L:190:SER:H	1.32	0.94
2:B:189:LYS:HD2	2:B:190:SER:H	1.29	0.94
2:N:135:ARG:HD3	2:N:247:GLY:HA3	1.48	0.94
2:N:194:ARG:HG3	2:N:194:ARG:HH21	1.33	0.93
2:D:189:LYS:HD2	2:D:190:SER:H	1.33	0.93
2:L:135:ARG:HD3	2:L:247:GLY:HA3	1.50	0.93
1:M:148:VAL:HB	2:N:160:ILE:HG22	1.47	0.93
2:F:159:LEU:HD21	1:G:144:VAL:HG12	1.49	0.93
2:N:97:ARG:HD2	2:N:101:LEU:HD12	1.50	0.92
2:F:189:LYS:HD2	2:F:190:SER:H	1.32	0.92
1:C:175:ARG:HG3	1:C:175:ARG:HH11	1.33	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:47:ALA:HB2	2:H:354:LEU:HD11	1.50	0.92
1:I:175:ARG:HG3	1:I:175:ARG:HH11	1.35	0.92
2:J:135:ARG:HD3	2:J:247:GLY:HA3	1.51	0.92
2:N:318:ILE:O	2:N:322:VAL:HG21	1.70	0.91
2:F:135:ARG:HD3	2:F:247:GLY:HA3	1.51	0.91
2:J:189:LYS:HD2	2:J:190:SER:H	1.31	0.91
1:I:17:ARG:HH21	1:I:46:PRO:HA	1.34	0.91
2:D:194:ARG:HG3	2:D:194:ARG:HH21	1.35	0.91
2:P:194:ARG:HG3	2:P:194:ARG:HH21	1.36	0.91
2:H:194:ARG:CG	2:H:194:ARG:HH21	1.84	0.91
2:D:135:ARG:HD3	2:D:247:GLY:HA3	1.51	0.90
2:D:318:ILE:O	2:D:322:VAL:HG21	1.71	0.90
1:M:151:LEU:HD23	2:N:157:ILE:HG12	1.53	0.90
2:P:318:ILE:O	2:P:322:VAL:HG21	1.69	0.90
2:P:189:LYS:HD2	2:P:190:SER:H	1.34	0.90
2:N:189:LYS:HD2	2:N:190:SER:H	1.34	0.90
2:H:189:LYS:HD2	2:H:190:SER:H	1.35	0.90
2:H:135:ARG:HD3	2:H:247:GLY:HA3	1.54	0.90
1:E:143:SER:HB3	2:H:159:LEU:HD22	1.53	0.89
2:N:194:ARG:HH21	2:N:194:ARG:CG	1.84	0.89
2:J:287:ILE:HD11	2:J:292:LYS:HD2	1.52	0.89
2:J:194:ARG:HH21	2:J:194:ARG:HG3	1.36	0.89
2:F:194:ARG:HG3	2:F:194:ARG:HH21	1.37	0.88
2:B:135:ARG:HD3	2:B:247:GLY:HA3	1.53	0.88
2:L:194:ARG:HH21	2:L:194:ARG:HG3	1.37	0.88
2:B:194:ARG:HG3	2:B:194:ARG:HH21	1.34	0.88
2:P:194:ARG:CG	2:P:194:ARG:HH21	1.86	0.88
1:I:275:HIS:ND1	1:I:278:LEU:HD12	1.88	0.88
1:A:275:HIS:ND1	1:A:278:LEU:HD12	1.87	0.88
2:D:194:ARG:HH21	2:D:194:ARG:CG	1.87	0.88
2:D:287:ILE:HD11	2:D:292:LYS:HD2	1.56	0.87
2:B:159:LEU:HD22	1:C:143:SER:HB3	1.54	0.87
1:K:175:ARG:HH11	1:K:175:ARG:CG	1.87	0.87
2:F:194:ARG:CG	2:F:194:ARG:HH21	1.87	0.87
1:A:301:HIS:HE1	1:E:15:GLY:O	1.57	0.87
1:A:175:ARG:HG3	1:A:175:ARG:HH11	1.40	0.87
2:H:318:ILE:O	2:H:322:VAL:HG21	1.74	0.86
2:B:322:VAL:O	2:B:326:ILE:HG23	1.75	0.86
2:J:194:ARG:CG	2:J:194:ARG:HH21	1.88	0.86
2:F:159:LEU:CD2	1:G:144:VAL:HG12	2.06	0.86
1:E:151:LEU:HD23	2:F:157:ILE:HG12	1.56	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:287:ILE:HD11	2:L:292:LYS:HD2	1.59	0.85
2:B:194:ARG:CG	2:B:194:ARG:HH21	1.89	0.84
1:A:325:THR:HG22	1:A:331:GLY:HA3	1.60	0.84
2:B:343:THR:O	2:B:347:THR:HG23	1.78	0.84
2:P:318:ILE:HA	2:P:322:VAL:HG11	1.60	0.84
2:J:47:ALA:HB2	2:J:354:LEU:HD11	1.59	0.83
2:P:47:ALA:HB2	2:P:354:LEU:HD11	1.60	0.83
1:A:18:PHE:HZ	1:E:44:ASN:ND2	1.75	0.83
1:I:175:ARG:HH11	1:I:175:ARG:CG	1.90	0.83
1:E:175:ARG:CG	1:E:175:ARG:HH11	1.91	0.83
1:O:175:ARG:HH11	1:O:175:ARG:CG	1.92	0.83
1:G:175:ARG:CG	1:G:175:ARG:HH11	1.91	0.83
2:H:343:THR:O	2:H:347:THR:HG23	1.78	0.83
2:L:194:ARG:HH21	2:L:194:ARG:CG	1.91	0.83
2:N:318:ILE:HA	2:N:322:VAL:HG11	1.60	0.83
2:B:287:ILE:HD11	2:B:292:LYS:HD2	1.61	0.83
2:J:343:THR:O	2:J:347:THR:HG23	1.80	0.82
2:F:323:LEU:HD23	2:F:323:LEU:H	1.44	0.82
2:J:67:THR:HG21	2:J:97:ARG:N	1.95	0.82
2:B:102:THR:O	2:B:106:THR:HG23	1.79	0.82
2:L:318:ILE:HA	2:L:322:VAL:HG11	1.61	0.82
2:F:318:ILE:HA	2:F:322:VAL:HG11	1.61	0.82
1:C:175:ARG:CG	1:C:175:ARG:HH11	1.93	0.81
1:M:175:ARG:CG	1:M:175:ARG:HH11	1.93	0.81
2:L:318:ILE:O	2:L:322:VAL:HG21	1.79	0.81
2:F:343:THR:O	2:F:347:THR:HG23	1.81	0.81
2:P:343:THR:O	2:P:347:THR:HG23	1.81	0.81
2:D:322:VAL:O	2:D:326:ILE:HG23	1.81	0.80
2:N:343:THR:O	2:N:347:THR:HG23	1.80	0.80
1:E:280:ILE:CG2	1:E:327:ARG:HE	1.95	0.80
2:F:322:VAL:HB	2:F:323:LEU:HD23	1.63	0.80
2:F:322:VAL:O	2:F:326:ILE:HG23	1.81	0.80
2:D:318:ILE:HA	2:D:322:VAL:HG11	1.64	0.80
2:D:343:THR:O	2:D:347:THR:HG23	1.81	0.80
2:J:318:ILE:HA	2:J:322:VAL:HG11	1.63	0.80
1:M:82:HIS:HB3	1:M:279:ASP:HB3	1.63	0.80
1:A:38:THR:HG22	1:A:343:ILE:HD11	1.63	0.80
1:A:300:ASN:HA	1:A:305:ASN:HB3	1.64	0.80
2:J:159:LEU:HD22	1:K:143:SER:HB3	1.64	0.80
2:J:322:VAL:O	2:J:326:ILE:HG23	1.82	0.79
2:P:66:LEU:HD21	2:P:97:ARG:HH21	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ILE:HG22	1:E:327:ARG:NE	1.98	0.78
2:L:343:THR:O	2:L:347:THR:HG23	1.81	0.78
2:N:97:ARG:HH12	2:N:102:THR:CG2	1.96	0.78
1:M:151:LEU:CD2	2:N:157:ILE:HG12	2.14	0.78
2:L:97:ARG:HG2	2:L:98:SER:H	1.48	0.78
2:N:159:LEU:HD21	1:O:144:VAL:HG12	1.65	0.78
2:H:318:ILE:HA	2:H:322:VAL:HG11	1.63	0.78
1:M:38:THR:HG22	1:M:343:ILE:HD11	1.64	0.78
1:M:88:THR:HB	2:N:189:LYS:HE3	1.64	0.78
1:M:54:ILE:HD13	1:M:81:TRP:HZ2	1.50	0.77
2:N:314:HIS:O	2:N:318:ILE:HG13	1.84	0.77
1:E:151:LEU:CD2	2:F:157:ILE:HG12	2.14	0.77
2:L:322:VAL:O	2:L:326:ILE:HG23	1.84	0.77
2:H:322:VAL:O	2:H:326:ILE:HG23	1.85	0.77
2:P:97:ARG:HG3	2:P:98:SER:H	1.49	0.77
1:K:15:GLY:O	1:O:301:HIS:HE1	1.68	0.77
1:E:325:THR:HG23	1:E:329:ILE:HG13	1.66	0.77
2:B:212:PRO:HG2	1:O:228:HIS:CD2	2.20	0.76
2:F:159:LEU:HD21	1:G:144:VAL:CG1	2.16	0.76
2:J:5:GLN:HG3	2:J:6:PRO:HD2	1.65	0.76
1:O:315:VAL:O	1:O:319:ILE:HG23	1.85	0.76
2:N:323:LEU:HD23	2:N:323:LEU:H	1.49	0.76
1:A:175:ARG:CG	1:A:175:ARG:HH11	1.98	0.76
1:O:38:THR:HG22	1:O:343:ILE:HD11	1.67	0.76
1:G:151:LEU:HD23	2:H:157:ILE:HG12	1.66	0.76
2:N:322:VAL:O	2:N:326:ILE:HG23	1.84	0.75
2:H:97:ARG:NH2	2:H:102:THR:HG23	2.00	0.75
2:B:318:ILE:HA	2:B:322:VAL:HG11	1.66	0.75
1:G:38:THR:HG22	1:G:343:ILE:HD11	1.66	0.75
1:I:315:VAL:O	1:I:319:ILE:HG23	1.86	0.75
1:E:38:THR:HG22	1:E:343:ILE:HD11	1.69	0.75
1:I:310:ARG:HA	1:I:349:MET:HE1	1.69	0.74
1:I:17:ARG:NH2	1:I:46:PRO:HA	2.01	0.74
1:C:17:ARG:NH1	1:C:48:ASP:OD1	2.21	0.73
2:H:323:LEU:H	2:H:323:LEU:HD23	1.52	0.73
1:M:325:THR:HG23	1:M:329:ILE:HG13	1.71	0.73
1:M:17:ARG:NH1	1:M:48:ASP:OD1	2.20	0.73
1:C:211:VAL:O	2:J:38:LYS:HE3	1.87	0.73
2:F:69:ILE:HD12	2:F:70:PRO:HD2	1.69	0.73
1:C:15:GLY:O	1:G:301:HIS:HE1	1.71	0.73
2:H:97:ARG:HG2	2:H:98:SER:H	1.54	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:47:ALA:HB2	2:N:354:LEU:HD21	1.71	0.73
2:F:97:ARG:NH2	2:F:102:THR:HG23	2.04	0.72
1:I:325:THR:HG23	1:I:329:ILE:HG13	1.71	0.72
2:B:36:ILE:HG22	2:B:298:LEU:HD23	1.70	0.72
1:M:315:VAL:O	1:M:319:ILE:HG23	1.89	0.72
1:C:38:THR:HG22	1:C:343:ILE:HD11	1.71	0.72
2:L:323:LEU:HD23	2:L:323:LEU:H	1.54	0.72
2:L:342:THR:CG2	2:L:345:SER:H	2.02	0.72
2:H:273:LYS:HG3	2:H:274:ILE:HD12	1.71	0.72
1:M:79:GLY:HA2	1:M:291:MET:HE1	1.69	0.72
2:P:323:LEU:HD23	2:P:323:LEU:H	1.54	0.72
2:N:322:VAL:HB	2:N:323:LEU:HD23	1.72	0.72
2:P:322:VAL:O	2:P:326:ILE:HG23	1.89	0.71
2:L:342:THR:HG22	2:L:345:SER:H	1.53	0.71
2:F:349:ALA:O	2:F:353:ARG:HD3	1.91	0.71
2:N:159:LEU:CD2	1:O:144:VAL:HG12	2.20	0.71
1:C:325:THR:HG23	1:C:329:ILE:HG13	1.71	0.71
2:B:342:THR:CG2	2:B:345:SER:H	2.04	0.71
1:G:281:LYS:HG2	1:G:282:GLY:H	1.55	0.71
1:I:38:THR:HG22	1:I:343:ILE:HD11	1.72	0.71
1:G:315:VAL:O	1:G:319:ILE:HG23	1.91	0.71
2:H:314:HIS:O	2:H:318:ILE:HG13	1.90	0.71
1:M:113:LEU:HD13	1:M:256:LEU:HD22	1.71	0.71
2:D:89:ALA:O	2:D:91:PRO:HD3	1.91	0.70
2:F:287:ILE:HD11	2:F:292:LYS:CD	2.21	0.70
1:K:315:VAL:O	1:K:319:ILE:HG23	1.91	0.70
2:J:323:LEU:HD23	2:J:323:LEU:H	1.55	0.70
2:P:314:HIS:O	2:P:318:ILE:HG13	1.90	0.70
1:A:181:VAL:HB	1:A:235:THR:CG2	2.19	0.70
2:D:342:THR:CG2	2:D:345:SER:H	2.05	0.70
2:D:342:THR:HG22	2:D:345:SER:H	1.55	0.70
2:P:194:ARG:CB	2:P:194:ARG:HH21	2.05	0.70
1:O:325:THR:HG23	1:O:329:ILE:HG13	1.72	0.70
2:D:323:LEU:HD23	2:D:323:LEU:H	1.56	0.70
2:B:323:LEU:H	2:B:323:LEU:HD23	1.55	0.70
1:M:147:VAL:HG22	2:N:161:THR:CG2	2.21	0.70
2:F:189:LYS:HD2	2:F:190:SER:N	2.05	0.70
2:D:322:VAL:HB	2:D:323:LEU:HD23	1.74	0.70
2:J:342:THR:CG2	2:J:345:SER:H	2.05	0.69
1:O:55:LYS:HD3	1:O:59:HIS:CD2	2.27	0.69
1:M:90:HIS:CB	2:N:193:GLN:HG3	2.22	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:194:ARG:HG3	2:F:194:ARG:NH2	2.07	0.69
1:K:38:THR:HG22	1:K:343:ILE:HD11	1.75	0.69
1:A:325:THR:HG23	1:A:329:ILE:HG13	1.74	0.69
2:J:102:THR:O	2:J:106:THR:HG23	1.92	0.69
1:A:79:GLY:HA2	1:A:291:MET:HE1	1.73	0.69
2:B:322:VAL:HG23	2:B:323:LEU:N	2.07	0.69
2:N:287:ILE:HD11	2:N:292:LYS:CD	2.21	0.69
1:K:325:THR:HG23	1:K:329:ILE:HG13	1.74	0.69
2:F:314:HIS:O	2:F:318:ILE:HG13	1.93	0.69
1:O:325:THR:HG22	1:O:331:GLY:HA3	1.75	0.69
2:P:189:LYS:HD2	2:P:190:SER:N	2.08	0.69
1:G:56:GLN:C	1:G:58:ASP:H	1.94	0.69
2:B:189:LYS:HD2	2:B:190:SER:N	2.06	0.68
2:L:66:LEU:CD2	2:L:97:ARG:HH21	2.06	0.68
2:F:273:LYS:HG3	2:F:274:ILE:HD12	1.75	0.68
2:P:194:ARG:HG3	2:P:194:ARG:NH2	2.05	0.68
2:P:102:THR:O	2:P:106:THR:HG23	1.93	0.68
2:J:342:THR:HG22	2:J:345:SER:H	1.58	0.68
2:H:342:THR:CG2	2:H:345:SER:H	2.05	0.68
2:H:102:THR:O	2:H:106:THR:HG23	1.93	0.68
1:E:147:VAL:HG22	2:F:161:THR:HG22	1.74	0.68
2:N:194:ARG:CB	2:N:194:ARG:HH21	2.06	0.68
2:F:97:ARG:HH11	2:F:101:LEU:HD12	1.59	0.68
1:G:325:THR:HG23	1:G:329:ILE:HG13	1.73	0.68
2:B:89:ALA:O	2:B:91:PRO:HD3	1.92	0.68
2:H:189:LYS:HD2	2:H:190:SER:N	2.09	0.68
2:L:36:ILE:HG22	2:L:298:LEU:HD23	1.76	0.68
1:A:113:LEU:HD13	1:A:256:LEU:HD22	1.76	0.68
2:D:97:ARG:HH21	2:D:102:THR:HG23	1.58	0.68
2:P:342:THR:CG2	2:P:345:SER:H	2.07	0.68
2:J:314:HIS:O	2:J:318:ILE:HG13	1.94	0.68
2:L:314:HIS:O	2:L:318:ILE:HG13	1.93	0.68
2:J:194:ARG:HG3	2:J:194:ARG:NH2	2.08	0.68
2:L:273:LYS:HG3	2:L:274:ILE:HD12	1.76	0.68
2:N:349:ALA:O	2:N:353:ARG:HD3	1.93	0.67
2:P:273:LYS:HG3	2:P:274:ILE:HD12	1.76	0.67
2:F:194:ARG:CB	2:F:194:ARG:HH21	2.06	0.67
1:M:90:HIS:HB3	2:N:193:GLN:HG3	1.76	0.67
1:G:175:ARG:HG3	1:G:175:ARG:NH1	2.09	0.67
2:D:273:LYS:HG3	2:D:274:ILE:HD12	1.75	0.67
2:L:189:LYS:HD2	2:L:190:SER:N	2.05	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:36:ILE:HG22	2:F:298:LEU:HD23	1.77	0.67
2:L:333:ARG:HB2	2:L:339:GLY:HA3	1.77	0.67
2:H:97:ARG:NH2	2:H:102:THR:CG2	2.57	0.67
1:E:90:HIS:CB	2:F:193:GLN:HG3	2.25	0.67
2:D:349:ALA:O	2:D:353:ARG:HD3	1.94	0.67
2:D:314:HIS:O	2:D:318:ILE:HG13	1.95	0.66
1:A:58:ASP:HA	1:A:92:SER:HB2	1.77	0.66
1:A:315:VAL:O	1:A:319:ILE:HG23	1.95	0.66
1:G:151:LEU:CD2	2:H:157:ILE:HG12	2.26	0.66
1:G:281:LYS:CG	1:G:282:GLY:H	2.08	0.66
2:H:342:THR:HG22	2:H:345:SER:H	1.60	0.66
2:P:342:THR:HG22	2:P:345:SER:H	1.58	0.66
2:F:342:THR:CG2	2:F:345:SER:H	2.09	0.66
2:H:194:ARG:HG3	2:H:194:ARG:NH2	2.03	0.66
1:I:140:GLU:OE2	2:J:194:ARG:HA	1.95	0.66
1:O:300:ASN:HA	1:O:305:ASN:HB3	1.77	0.66
2:P:318:ILE:C	2:P:322:VAL:HG21	2.15	0.66
1:A:163:ALA:HB2	1:A:198:ILE:HD13	1.76	0.66
2:N:273:LYS:HG3	2:N:274:ILE:HD12	1.76	0.66
2:B:314:HIS:O	2:B:318:ILE:HG13	1.95	0.66
1:A:300:ASN:OD1	1:A:305:ASN:HB2	1.96	0.66
1:M:149:GLU:HG3	2:N:159:LEU:CD1	2.25	0.66
2:H:69:ILE:HD12	2:H:70:PRO:HD2	1.77	0.66
2:P:273:LYS:HE3	2:P:274:ILE:HD11	1.78	0.66
1:G:300:ASN:HA	1:G:305:ASN:HB3	1.78	0.66
2:J:273:LYS:HG3	2:J:274:ILE:HD12	1.76	0.66
2:P:97:ARG:CG	2:P:98:SER:H	2.07	0.66
1:C:315:VAL:O	1:C:319:ILE:HG23	1.96	0.66
2:D:194:ARG:HH21	2:D:194:ARG:CB	2.09	0.66
2:F:97:ARG:NH1	2:F:101:LEU:HD12	2.11	0.66
2:D:102:THR:O	2:D:106:THR:HG23	1.96	0.65
2:P:287:ILE:HD11	2:P:292:LYS:CD	2.24	0.65
2:N:189:LYS:HD2	2:N:190:SER:N	2.07	0.65
2:L:349:ALA:O	2:L:353:ARG:HD3	1.96	0.65
2:N:69:ILE:HD12	2:N:70:PRO:HD2	1.78	0.65
2:D:291:ASP:O	2:D:343:THR:HG22	1.95	0.65
1:O:151:LEU:HD23	2:P:157:ILE:HG12	1.78	0.65
1:I:245:ASN:OD1	1:I:276:VAL:HG21	1.97	0.65
2:F:326:ILE:HD11	2:F:346:PHE:CE1	2.32	0.65
2:J:189:LYS:HD2	2:J:190:SER:N	2.06	0.65
1:A:301:HIS:CE1	1:E:15:GLY:O	2.45	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:325:THR:HG22	1:G:331:GLY:HA3	1.78	0.65
2:P:69:ILE:HD12	2:P:70:PRO:HD2	1.79	0.65
1:C:325:THR:HG22	1:C:331:GLY:HA3	1.79	0.65
2:H:333:ARG:HB2	2:H:339:GLY:HA3	1.77	0.65
2:P:347:THR:O	2:P:351:ILE:HG13	1.97	0.65
2:B:322:VAL:HB	2:B:323:LEU:HD23	1.79	0.65
2:N:326:ILE:HG21	2:N:350:VAL:HA	1.79	0.65
2:N:342:THR:CG2	2:N:345:SER:H	2.10	0.65
2:D:286:ASP:OD2	2:J:287:ILE:HG12	1.98	0.64
1:A:305:ASN:HA	1:A:308:ALA:HB3	1.79	0.64
2:L:273:LYS:HE3	2:L:274:ILE:HD11	1.78	0.64
2:P:326:ILE:HG21	2:P:350:VAL:HA	1.80	0.64
1:A:325:THR:HG22	1:A:331:GLY:CA	2.25	0.64
2:H:273:LYS:HE3	2:H:274:ILE:HD11	1.78	0.64
2:F:342:THR:HG22	2:F:345:SER:H	1.63	0.64
1:C:300:ASN:HA	1:C:305:ASN:HB3	1.77	0.64
1:E:315:VAL:O	1:E:319:ILE:HG23	1.97	0.64
2:F:322:VAL:C	2:F:326:ILE:HG23	2.18	0.64
2:J:322:VAL:HB	2:J:323:LEU:HD23	1.78	0.64
2:J:194:ARG:CB	2:J:194:ARG:HH21	2.11	0.64
2:N:342:THR:HG22	2:N:345:SER:H	1.61	0.64
1:I:300:ASN:HA	1:I:305:ASN:HB3	1.78	0.64
2:D:333:ARG:HB2	2:D:339:GLY:HA3	1.78	0.64
1:M:223:ALA:O	1:M:227:PRO:HG3	1.98	0.64
2:H:322:VAL:HB	2:H:323:LEU:HD23	1.80	0.64
2:J:349:ALA:O	2:J:353:ARG:HD3	1.97	0.64
2:J:36:ILE:HG22	2:J:298:LEU:HD23	1.78	0.64
2:B:347:THR:O	2:B:351:ILE:HG13	1.98	0.64
2:H:349:ALA:O	2:H:353:ARG:HD3	1.98	0.64
2:L:102:THR:O	2:L:106:THR:HG23	1.98	0.64
1:O:175:ARG:NH1	1:O:175:ARG:HG3	2.08	0.64
2:B:5:GLN:NE2	2:B:6:PRO:HD2	2.12	0.64
1:K:175:ARG:HG3	1:K:175:ARG:NH1	2.05	0.64
1:K:175:ARG:CG	1:K:175:ARG:NH1	2.55	0.64
2:H:326:ILE:HG21	2:H:350:VAL:HA	1.80	0.64
1:E:181:VAL:HB	1:E:235:THR:CG2	2.22	0.63
2:H:194:ARG:CB	2:H:194:ARG:HH21	2.10	0.63
2:N:318:ILE:C	2:N:322:VAL:HG21	2.19	0.63
2:D:273:LYS:HE3	2:D:274:ILE:HD11	1.81	0.63
2:B:224:SER:O	2:B:228:VAL:HG23	1.98	0.63
1:M:222:GLN:HG3	1:M:229:GLN:OE1	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:347:THR:O	2:L:351:ILE:HG13	1.98	0.63
2:F:318:ILE:C	2:F:322:VAL:HG21	2.17	0.63
2:F:159:LEU:HD22	1:G:143:SER:HB3	1.80	0.63
2:B:342:THR:HG22	2:B:345:SER:H	1.61	0.63
2:J:273:LYS:HE3	2:J:274:ILE:HD11	1.80	0.63
1:C:113:LEU:HD13	1:C:256:LEU:HD22	1.79	0.63
1:E:222:GLN:HG3	1:E:229:GLN:OE1	1.98	0.63
1:I:175:ARG:NH1	1:I:231:ASP:OD1	2.32	0.63
1:M:143:SER:HB3	2:P:159:LEU:HD22	1.81	0.63
1:C:345:LYS:O	1:C:349:MET:HG3	1.99	0.63
1:M:300:ASN:HA	1:M:305:ASN:HB3	1.80	0.63
2:F:347:THR:O	2:F:351:ILE:HG13	1.98	0.63
2:B:291:ASP:O	2:B:343:THR:HG22	1.98	0.63
2:B:322:VAL:C	2:B:326:ILE:HG23	2.18	0.63
1:K:113:LEU:HD13	1:K:256:LEU:HD22	1.79	0.63
1:I:135:GLU:OE2	2:J:189:LYS:HE2	1.99	0.63
2:P:326:ILE:HD11	2:P:346:PHE:CE1	2.34	0.63
2:L:322:VAL:HB	2:L:323:LEU:HD23	1.79	0.63
1:I:305:ASN:HA	1:I:308:ALA:HB3	1.81	0.63
1:O:123:ILE:HD13	1:O:250:LEU:HB3	1.81	0.63
1:C:246:ILE:HD11	2:D:253:LEU:HD12	1.81	0.63
2:F:245:LEU:HD23	2:F:246:TYR:CE1	2.34	0.63
2:P:322:VAL:HB	2:P:323:LEU:HD23	1.81	0.62
2:J:69:ILE:HD12	2:J:70:PRO:HD2	1.79	0.62
1:E:325:THR:HG22	1:E:331:GLY:HA3	1.81	0.62
2:J:322:VAL:HG23	2:J:323:LEU:N	2.13	0.62
2:D:36:ILE:HG22	2:D:298:LEU:HD23	1.80	0.62
2:B:349:ALA:O	2:B:353:ARG:HD3	1.99	0.62
2:N:194:ARG:HG3	2:N:194:ARG:NH2	2.03	0.62
2:J:333:ARG:HB2	2:J:339:GLY:HA3	1.81	0.62
2:L:351:ILE:HA	2:L:354:LEU:HB2	1.80	0.62
1:G:113:LEU:HD13	1:G:256:LEU:HD22	1.82	0.62
1:K:300:ASN:HA	1:K:305:ASN:HB3	1.81	0.62
1:K:175:ARG:NH1	1:K:231:ASP:OD1	2.32	0.62
1:I:181:VAL:HB	1:I:235:THR:CG2	2.23	0.62
2:B:194:ARG:HG3	2:B:194:ARG:NH2	2.08	0.62
2:H:318:ILE:C	2:H:322:VAL:HG21	2.19	0.62
2:L:326:ILE:HG21	2:L:350:VAL:HA	1.82	0.62
2:B:318:ILE:C	2:B:322:VAL:HG21	2.19	0.62
1:G:175:ARG:NH1	1:G:231:ASP:OD1	2.33	0.62
2:J:318:ILE:C	2:J:322:VAL:HG21	2.18	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:305:ASN:HA	1:G:308:ALA:HB3	1.81	0.62
1:C:222:GLN:HG3	1:C:229:GLN:OE1	1.99	0.62
1:E:54:ILE:H	1:E:54:ILE:CD1	1.88	0.62
2:F:326:ILE:HG21	2:F:350:VAL:HA	1.81	0.62
1:M:311:ILE:O	1:M:315:VAL:HG13	1.99	0.62
2:D:69:ILE:HD12	2:D:70:PRO:HD2	1.81	0.62
1:M:10:LEU:CD2	1:M:11:PRO:HD2	2.30	0.62
2:H:97:ARG:HH11	2:H:101:LEU:HD12	1.64	0.62
2:N:36:ILE:HG22	2:N:298:LEU:HD23	1.81	0.62
2:L:194:ARG:HG3	2:L:194:ARG:NH2	2.10	0.61
1:K:222:GLN:HG3	1:K:229:GLN:OE1	1.99	0.61
2:J:326:ILE:HG21	2:J:350:VAL:HA	1.80	0.61
1:C:175:ARG:HG3	1:C:175:ARG:NH1	2.10	0.61
2:N:159:LEU:HD21	1:O:144:VAL:CG1	2.28	0.61
2:B:326:ILE:HG21	2:B:350:VAL:HA	1.81	0.61
1:M:305:ASN:HA	1:M:308:ALA:HB3	1.82	0.61
1:C:90:HIS:CB	2:D:193:GLN:HG3	2.31	0.61
1:E:300:ASN:HA	1:E:305:ASN:HB3	1.81	0.61
2:L:97:ARG:CG	2:L:98:SER:H	2.13	0.61
2:J:347:THR:O	2:J:351:ILE:HG13	1.99	0.61
2:P:66:LEU:CD2	2:P:97:ARG:HH21	2.14	0.61
2:N:273:LYS:HE3	2:N:274:ILE:HD11	1.82	0.61
2:P:349:ALA:O	2:P:353:ARG:HD3	2.00	0.61
1:A:18:PHE:CZ	1:E:44:ASN:ND2	2.64	0.61
1:K:245:ASN:OD1	1:K:276:VAL:HG21	2.00	0.61
1:K:151:LEU:HD23	2:L:157:ILE:HG12	1.83	0.61
1:I:275:HIS:ND1	1:I:278:LEU:CD1	2.61	0.61
1:G:222:GLN:HG3	1:G:229:GLN:OE1	2.00	0.61
1:M:146:GLY:O	2:N:161:THR:HA	2.01	0.61
2:D:189:LYS:HD2	2:D:190:SER:N	2.10	0.61
2:D:322:VAL:C	2:D:326:ILE:HG23	2.21	0.61
2:J:291:ASP:O	2:J:343:THR:HG22	2.01	0.61
2:N:333:ARG:HB2	2:N:339:GLY:HA3	1.83	0.61
1:O:181:VAL:HB	1:O:235:THR:CG2	2.23	0.61
2:J:287:ILE:HD11	2:J:292:LYS:CD	2.30	0.61
2:H:97:ARG:NH1	2:H:101:LEU:CD1	2.63	0.61
1:A:155:THR:O	1:A:159:THR:CG2	2.48	0.61
1:K:55:LYS:HB3	1:K:57:THR:HG22	1.81	0.61
2:P:333:ARG:HB2	2:P:339:GLY:HA3	1.81	0.61
1:O:175:ARG:NH1	1:O:231:ASP:OD1	2.35	0.60
2:D:318:ILE:C	2:D:322:VAL:HG21	2.21	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:97:ARG:HH21	2:J:102:THR:HG23	1.66	0.60
1:I:325:THR:HG22	1:I:331:GLY:HA3	1.82	0.60
1:I:113:LEU:HD13	1:I:256:LEU:HD22	1.82	0.60
1:I:222:GLN:HG3	1:I:229:GLN:OE1	2.01	0.60
2:J:97:ARG:HH21	2:J:102:THR:CG2	2.14	0.60
2:B:97:ARG:NH2	2:B:102:THR:HG23	2.16	0.60
2:D:194:ARG:HG3	2:D:194:ARG:NH2	2.07	0.60
2:D:326:ILE:HG21	2:D:350:VAL:HA	1.82	0.60
2:H:6:PRO:O	2:H:10:ARG:HG2	2.01	0.60
1:O:222:GLN:HG3	1:O:229:GLN:OE1	2.01	0.60
1:I:300:ASN:OD1	1:I:305:ASN:HB2	2.02	0.60
2:B:69:ILE:HD12	2:B:70:PRO:HD2	1.83	0.60
1:C:163:ALA:HB2	1:C:198:ILE:HD13	1.84	0.60
2:J:322:VAL:C	2:J:326:ILE:HG23	2.22	0.60
2:L:291:ASP:O	2:L:343:THR:HG22	2.02	0.60
1:M:305:ASN:HA	1:M:308:ALA:CB	2.32	0.60
2:L:322:VAL:HG23	2:L:323:LEU:N	2.16	0.60
2:L:322:VAL:C	2:L:326:ILE:HG23	2.22	0.60
2:F:273:LYS:HE3	2:F:274:ILE:HD11	1.84	0.60
1:C:305:ASN:HA	1:C:308:ALA:HB3	1.83	0.60
2:N:118:SER:OG	2:N:129:VAL:HG13	2.02	0.60
1:G:55:LYS:HB3	1:G:56:GLN:NE2	2.15	0.60
1:M:155:THR:O	1:M:159:THR:CG2	2.50	0.60
1:C:175:ARG:NH1	1:C:231:ASP:OD1	2.35	0.59
2:D:322:VAL:HG23	2:D:323:LEU:N	2.16	0.59
1:C:300:ASN:OD1	1:C:305:ASN:HB2	2.02	0.59
1:A:305:ASN:HA	1:A:308:ALA:CB	2.31	0.59
2:P:97:ARG:CZ	2:P:102:THR:HG23	2.32	0.59
1:A:144:VAL:HG12	2:D:159:LEU:HD21	1.83	0.59
2:B:175:TYR:O	2:B:179:ILE:HG12	2.02	0.59
2:B:40:VAL:HG22	2:B:299:LEU:HD13	1.84	0.59
1:A:18:PHE:HZ	1:E:44:ASN:HD22	1.51	0.59
2:L:318:ILE:C	2:L:322:VAL:HG21	2.23	0.59
2:N:291:ASP:O	2:N:343:THR:HG22	2.02	0.59
2:F:97:ARG:NH1	2:F:101:LEU:CD1	2.66	0.59
1:G:155:THR:O	1:G:159:THR:HG22	2.02	0.59
2:H:39:SER:O	2:H:43:ILE:HG13	2.03	0.59
1:I:163:ALA:HB2	1:I:198:ILE:HD13	1.84	0.59
2:B:194:ARG:CB	2:B:194:ARG:HH21	2.15	0.59
1:E:175:ARG:NH1	1:E:231:ASP:OD1	2.36	0.59
1:M:123:ILE:HD13	1:M:250:LEU:HB3	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:6:PRO:O	2:F:10:ARG:HG2	2.03	0.59
2:H:36:ILE:HG22	2:H:298:LEU:HD23	1.85	0.59
1:O:292:ILE:O	1:O:295:SER:HB3	2.03	0.59
2:H:347:THR:O	2:H:351:ILE:HG13	2.02	0.59
1:G:79:GLY:HA2	1:G:291:MET:HE1	1.83	0.59
2:P:97:ARG:HG3	2:P:98:SER:N	2.17	0.59
1:K:79:GLY:HA2	1:K:291:MET:HE1	1.85	0.59
2:P:36:ILE:HG22	2:P:298:LEU:HD23	1.85	0.59
2:F:333:ARG:HB2	2:F:339:GLY:HA3	1.84	0.59
1:K:181:VAL:HB	1:K:235:THR:CG2	2.25	0.58
2:F:322:VAL:HG23	2:F:323:LEU:N	2.16	0.58
2:D:326:ILE:HD11	2:D:346:PHE:CE1	2.38	0.58
2:F:102:THR:O	2:F:106:THR:HG23	2.03	0.58
1:M:221:MET:SD	2:N:261:SER:HA	2.42	0.58
2:N:347:THR:O	2:N:351:ILE:HG13	2.02	0.58
2:N:97:ARG:HG3	2:N:98:SER:N	2.16	0.58
1:C:181:VAL:HB	1:C:235:THR:CG2	2.24	0.58
1:C:305:ASN:HA	1:C:308:ALA:CB	2.32	0.58
1:K:223:ALA:O	1:K:227:PRO:HG3	2.03	0.58
1:E:223:ALA:O	1:E:227:PRO:HG3	2.03	0.58
2:N:322:VAL:C	2:N:326:ILE:HG23	2.23	0.58
1:I:140:GLU:HB3	2:J:195:LEU:CD2	2.34	0.58
1:A:175:ARG:NH1	1:A:231:ASP:OD1	2.37	0.58
2:H:326:ILE:HD11	2:H:346:PHE:CE1	2.38	0.58
1:E:305:ASN:HA	1:E:308:ALA:HB3	1.84	0.58
1:I:155:THR:O	1:I:159:THR:HG23	2.03	0.58
1:E:245:ASN:OD1	1:E:276:VAL:HG21	2.03	0.58
2:L:89:ALA:O	2:L:91:PRO:HD3	2.04	0.58
1:M:151:LEU:HA	2:N:156:SER:O	2.02	0.58
2:P:318:ILE:CA	2:P:322:VAL:HG11	2.34	0.58
1:M:149:GLU:HG3	2:N:159:LEU:HD12	1.86	0.58
1:K:305:ASN:HA	1:K:308:ALA:CB	2.34	0.58
1:A:323:LYS:O	1:A:324:HIS:HB2	2.03	0.58
2:L:194:ARG:HH21	2:L:194:ARG:CB	2.16	0.58
2:H:322:VAL:C	2:H:326:ILE:HG23	2.24	0.58
2:J:97:ARG:NH2	2:J:102:THR:HG23	2.18	0.58
1:K:305:ASN:HA	1:K:308:ALA:HB3	1.85	0.58
2:B:273:LYS:HE3	2:B:274:ILE:HD11	1.86	0.58
2:D:287:ILE:HD11	2:D:292:LYS:CD	2.33	0.58
1:G:305:ASN:HA	1:G:308:ALA:CB	2.33	0.58
1:I:155:THR:O	1:I:159:THR:CG2	2.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:292:ILE:O	1:K:295:SER:HB3	2.03	0.58
1:O:305:ASN:HA	1:O:308:ALA:HB3	1.86	0.58
2:B:182:PRO:HD2	2:B:237:ASP:O	2.03	0.58
1:E:79:GLY:HA2	1:E:291:MET:HE1	1.85	0.58
1:K:151:LEU:CD2	2:L:157:ILE:HG12	2.34	0.58
1:E:175:ARG:HG3	1:E:175:ARG:NH1	2.09	0.57
2:H:97:ARG:CG	2:H:98:SER:H	2.15	0.57
1:G:55:LYS:HD2	1:G:55:LYS:N	2.18	0.57
1:G:300:ASN:OD1	1:G:305:ASN:HB2	2.02	0.57
1:M:175:ARG:NH1	1:M:231:ASP:OD1	2.37	0.57
2:J:326:ILE:HD11	2:J:346:PHE:CE1	2.38	0.57
2:D:318:ILE:CA	2:D:322:VAL:HG11	2.33	0.57
1:A:275:HIS:CE1	1:A:278:LEU:HD12	2.40	0.57
1:I:90:HIS:CB	2:J:193:GLN:HG3	2.35	0.57
2:L:175:TYR:O	2:L:179:ILE:HG12	2.04	0.57
2:F:287:ILE:HG13	2:F:292:LYS:HB2	1.87	0.57
2:B:273:LYS:HG3	2:B:274:ILE:HD12	1.85	0.57
2:F:39:SER:O	2:F:43:ILE:HG13	2.04	0.57
1:G:155:THR:O	1:G:159:THR:CG2	2.52	0.57
1:E:113:LEU:HD13	1:E:256:LEU:HD22	1.87	0.57
2:D:88:LEU:HD13	2:D:99:LEU:HD23	1.87	0.57
1:M:116:VAL:HG23	1:M:319:ILE:CD1	2.35	0.57
1:A:324:HIS:CG	1:A:341:GLU:HG3	2.40	0.57
2:D:6:PRO:O	2:D:10:ARG:HG2	2.03	0.57
1:M:199:THR:HA	1:M:211:VAL:HG11	1.86	0.57
1:I:54:ILE:HG23	1:I:59:HIS:HB3	1.86	0.57
1:C:151:LEU:HD23	2:D:157:ILE:HG12	1.87	0.57
1:E:54:ILE:N	1:E:54:ILE:HD12	2.04	0.57
2:N:326:ILE:HD11	2:N:346:PHE:CE1	2.39	0.57
1:I:278:LEU:HD22	1:I:280:ILE:HG12	1.85	0.57
2:L:351:ILE:HG23	2:L:354:LEU:HD23	1.86	0.57
1:I:310:ARG:HG2	1:I:349:MET:CE	2.35	0.57
1:C:79:GLY:HA2	1:C:291:MET:CE	2.35	0.57
2:F:44:PHE:CD2	2:F:49:VAL:HG21	2.39	0.57
1:I:292:ILE:O	1:I:295:SER:HB3	2.05	0.57
2:H:287:ILE:HD11	2:H:292:LYS:CD	2.28	0.57
2:B:67:THR:OG1	2:B:97:ARG:HB3	2.04	0.57
1:I:54:ILE:HG22	1:I:56:GLN:O	2.04	0.57
1:O:113:LEU:HD13	1:O:256:LEU:HD22	1.86	0.57
1:E:314:ALA:HB2	1:E:346:LEU:HD13	1.86	0.57
2:N:12:THR:HB	2:N:81:LEU:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:163:ALA:HB2	1:K:198:ILE:HD13	1.86	0.57
2:B:333:ARG:HB2	2:B:339:GLY:HA3	1.86	0.57
1:O:163:ALA:HB2	1:O:198:ILE:HD13	1.87	0.57
1:C:195:ARG:O	1:C:199:THR:HG23	2.05	0.56
1:I:199:THR:HA	1:I:211:VAL:HG11	1.86	0.56
2:B:47:ALA:HB2	2:B:354:LEU:HD21	1.87	0.56
2:J:6:PRO:O	2:J:10:ARG:HG2	2.05	0.56
2:L:69:ILE:HD12	2:L:70:PRO:HD2	1.86	0.56
2:B:6:PRO:O	2:B:10:ARG:HG2	2.05	0.56
1:O:79:GLY:HA2	1:O:291:MET:HE1	1.87	0.56
1:E:163:ALA:HB2	1:E:198:ILE:HD13	1.86	0.56
1:E:123:ILE:HD13	1:E:250:LEU:HB3	1.86	0.56
1:E:139:LEU:HD23	1:E:151:LEU:HD12	1.87	0.56
2:N:39:SER:O	2:N:43:ILE:HG13	2.05	0.56
2:D:347:THR:O	2:D:351:ILE:HG13	2.05	0.56
1:E:90:HIS:HB3	2:F:193:GLN:HG3	1.86	0.56
1:A:311:ILE:O	1:A:315:VAL:HG13	2.05	0.56
1:I:189:LEU:HB3	2:J:154:VAL:HG11	1.87	0.56
2:D:245:LEU:HD23	2:D:246:TYR:CE1	2.39	0.56
1:O:25:GLY:HA2	1:O:81:TRP:CZ2	2.39	0.56
2:F:318:ILE:CA	2:F:322:VAL:HG11	2.34	0.56
2:N:322:VAL:HG23	2:N:323:LEU:N	2.20	0.56
2:P:39:SER:O	2:P:43:ILE:HG13	2.06	0.56
1:K:325:THR:HG22	1:K:331:GLY:HA3	1.87	0.56
1:I:280:ILE:HD12	1:I:280:ILE:O	2.05	0.56
1:G:20:VAL:HG13	1:G:47:ILE:HG23	1.88	0.56
1:A:222:GLN:HG3	1:A:229:GLN:OE1	2.06	0.56
2:B:97:ARG:NH2	2:B:102:THR:CG2	2.69	0.56
1:M:325:THR:CG2	1:M:329:ILE:HG13	2.35	0.56
2:N:63:VAL:O	2:N:64:ASN:HB2	2.06	0.56
1:G:123:ILE:HD13	1:G:250:LEU:HB3	1.86	0.56
2:H:318:ILE:CA	2:H:322:VAL:HG11	2.34	0.56
2:B:40:VAL:HG22	2:B:299:LEU:CD1	2.36	0.56
1:E:199:THR:HA	1:E:211:VAL:HG11	1.86	0.56
1:C:155:THR:O	1:C:159:THR:CG2	2.54	0.56
1:A:223:ALA:O	1:A:227:PRO:HG3	2.05	0.56
2:F:291:ASP:O	2:F:343:THR:HG22	2.06	0.56
2:N:274:ILE:HG22	2:N:275:SER:N	2.20	0.56
2:J:318:ILE:CA	2:J:322:VAL:HG11	2.35	0.56
1:I:310:ARG:HG2	1:I:349:MET:HE2	1.88	0.56
1:M:300:ASN:OD1	1:M:305:ASN:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:10:LEU:HD22	1:M:11:PRO:HD2	1.88	0.56
1:E:292:ILE:O	1:E:295:SER:HB3	2.06	0.56
2:H:12:THR:HB	2:H:81:LEU:CD1	2.36	0.56
2:L:318:ILE:CA	2:L:322:VAL:HG11	2.33	0.56
1:E:79:GLY:HA2	1:E:291:MET:CE	2.36	0.56
2:F:47:ALA:HB2	2:F:354:LEU:HD11	1.87	0.56
2:B:47:ALA:HB2	2:B:354:LEU:HD11	1.88	0.55
1:E:175:ARG:CG	1:E:175:ARG:NH1	2.59	0.55
2:J:47:ALA:CA	2:J:354:LEU:HD21	2.35	0.55
1:M:84:PRO:HB3	2:N:220:LEU:HD11	1.87	0.55
1:M:235:THR:HG21	1:M:243:LEU:HD12	1.89	0.55
2:L:135:ARG:CD	2:L:247:GLY:HA3	2.32	0.55
2:P:47:ALA:CB	2:P:354:LEU:HD11	2.36	0.55
1:E:305:ASN:HA	1:E:308:ALA:CB	2.37	0.55
1:E:246:ILE:HD11	2:F:253:LEU:HD12	1.88	0.55
1:C:276:VAL:O	2:D:226:LEU:HD12	2.06	0.55
2:H:291:ASP:O	2:H:343:THR:HG22	2.07	0.55
1:M:195:ARG:O	1:M:199:THR:HG23	2.07	0.55
2:P:63:VAL:O	2:P:64:ASN:HB2	2.05	0.55
2:D:166:GLU:O	2:D:167:ARG:HB2	2.05	0.55
2:P:322:VAL:HG23	2:P:323:LEU:N	2.21	0.55
1:K:281:LYS:HD2	1:K:281:LYS:O	2.06	0.55
1:G:116:VAL:HG23	1:G:319:ILE:CD1	2.37	0.55
1:A:79:GLY:HA2	1:A:291:MET:CE	2.36	0.55
1:G:58:ASP:HA	1:G:92:SER:HB2	1.88	0.55
1:C:79:GLY:HA2	1:C:291:MET:HE1	1.87	0.55
1:K:246:ILE:HD11	2:L:253:LEU:HD12	1.89	0.55
2:L:6:PRO:O	2:L:10:ARG:HG2	2.06	0.55
1:C:223:ALA:O	1:C:227:PRO:HG3	2.07	0.55
2:N:5:GLN:HG3	2:N:6:PRO:HD2	1.89	0.55
1:A:246:ILE:HD11	2:B:253:LEU:HD12	1.88	0.55
1:O:54:ILE:CG2	1:O:59:HIS:HB3	2.37	0.55
1:K:79:GLY:HA2	1:K:291:MET:CE	2.37	0.55
2:N:6:PRO:O	2:N:10:ARG:HG2	2.07	0.55
1:O:199:THR:HA	1:O:211:VAL:HG11	1.88	0.55
2:L:332:ASN:HA	2:L:341:ALA:HB2	1.89	0.55
1:E:149:GLU:HG3	2:F:159:LEU:HD12	1.89	0.55
1:I:305:ASN:HA	1:I:308:ALA:CB	2.37	0.55
1:M:155:THR:HG22	2:N:153:VAL:HG13	1.88	0.55
1:M:292:ILE:O	1:M:295:SER:HB3	2.07	0.55
2:N:287:ILE:HG13	2:N:292:LYS:HB2	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:181:VAL:HB	1:M:235:THR:CG2	2.29	0.55
2:N:318:ILE:CA	2:N:322:VAL:HG11	2.33	0.55
1:E:143:SER:HB3	2:H:159:LEU:CD2	2.32	0.55
1:G:199:THR:HA	1:G:211:VAL:HG11	1.88	0.55
1:I:55:LYS:N	1:I:55:LYS:HD3	2.20	0.55
1:O:235:THR:HG21	1:O:243:LEU:HD12	1.88	0.54
2:B:318:ILE:CA	2:B:322:VAL:HG11	2.37	0.54
2:F:97:ARG:NH2	2:F:102:THR:CG2	2.70	0.54
1:M:113:LEU:CD1	1:M:256:LEU:HD22	2.37	0.54
1:K:276:VAL:O	2:L:226:LEU:HD12	2.07	0.54
2:F:175:TYR:O	2:F:179:ILE:HG12	2.06	0.54
1:G:25:GLY:HA2	1:G:81:TRP:CZ2	2.43	0.54
1:M:139:LEU:HD23	1:M:151:LEU:HD12	1.87	0.54
2:P:322:VAL:C	2:P:326:ILE:HG23	2.28	0.54
1:I:277:GLY:O	1:I:279:ASP:N	2.40	0.54
2:H:67:THR:OG1	2:H:97:ARG:HB3	2.07	0.54
1:O:305:ASN:HA	1:O:308:ALA:CB	2.38	0.54
2:P:126:TYR:HB2	2:P:257:LEU:O	2.08	0.54
2:N:332:ASN:HA	2:N:341:ALA:HB2	1.89	0.54
1:A:90:HIS:CB	2:B:193:GLN:HG3	2.37	0.54
2:H:97:ARG:NH1	2:H:101:LEU:HD12	2.22	0.54
2:H:224:SER:O	2:H:228:VAL:HG23	2.07	0.54
2:P:97:ARG:CG	2:P:98:SER:N	2.71	0.54
2:J:245:LEU:HD23	2:J:246:TYR:CE1	2.43	0.54
1:I:175:ARG:HG3	1:I:175:ARG:NH1	2.11	0.54
1:O:116:VAL:HG23	1:O:319:ILE:CD1	2.37	0.54
2:L:342:THR:HG23	2:L:344:SER:H	1.73	0.54
1:E:300:ASN:OD1	1:E:305:ASN:HB2	2.07	0.54
2:D:224:SER:O	2:D:228:VAL:HG23	2.07	0.54
1:A:288:PRO:O	1:A:292:ILE:HG13	2.08	0.54
1:C:292:ILE:O	1:C:295:SER:HB3	2.08	0.54
2:N:102:THR:O	2:N:106:THR:HG23	2.07	0.54
2:H:322:VAL:HG23	2:H:323:LEU:N	2.20	0.54
1:O:195:ARG:O	1:O:199:THR:HG23	2.08	0.54
1:I:223:ALA:O	1:I:227:PRO:HG3	2.07	0.54
2:N:157:ILE:CD1	1:O:151:LEU:HD11	2.38	0.54
2:F:97:ARG:HH22	2:F:102:THR:HG23	1.73	0.54
1:K:300:ASN:OD1	1:K:305:ASN:HB2	2.07	0.54
2:D:63:VAL:O	2:D:64:ASN:HB2	2.08	0.54
2:H:175:TYR:O	2:H:179:ILE:HG12	2.07	0.54
1:E:88:THR:HB	2:F:189:LYS:HE3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:155:THR:O	1:M:159:THR:HG23	2.08	0.54
2:L:5:GLN:HA	2:L:5:GLN:HE21	1.73	0.54
1:G:235:THR:HG21	1:G:243:LEU:HD12	1.90	0.54
2:D:291:ASP:C	2:D:343:THR:HG22	2.28	0.54
1:O:300:ASN:OD1	1:O:305:ASN:HB2	2.06	0.54
1:I:25:GLY:HA2	1:I:81:TRP:CZ2	2.42	0.54
2:N:41:LYS:HG2	2:N:53:TRP:NE1	2.23	0.54
2:L:194:ARG:CG	2:L:194:ARG:NH2	2.61	0.54
1:A:18:PHE:HZ	1:E:44:ASN:HD21	1.53	0.54
1:G:163:ALA:HB2	1:G:198:ILE:HD13	1.89	0.54
1:I:314:ALA:HB2	1:I:346:LEU:HD13	1.88	0.54
2:F:63:VAL:O	2:F:64:ASN:HB2	2.08	0.54
2:B:326:ILE:HD11	2:B:346:PHE:CE1	2.44	0.53
2:F:41:LYS:HG2	2:F:53:TRP:NE1	2.22	0.53
1:I:325:THR:CG2	1:I:329:ILE:HG13	2.37	0.53
2:N:221:ILE:O	2:N:225:VAL:HG13	2.08	0.53
2:H:150:CYS:HB2	2:H:151:PRO:CD	2.38	0.53
1:G:181:VAL:HB	1:G:235:THR:CG2	2.27	0.53
1:M:148:VAL:HB	2:N:160:ILE:CG2	2.31	0.53
2:N:44:PHE:CD2	2:N:49:VAL:HG21	2.44	0.53
1:I:140:GLU:HB3	2:J:195:LEU:HD21	1.91	0.53
2:F:274:ILE:HG22	2:F:275:SER:N	2.24	0.53
1:G:79:GLY:HA2	1:G:291:MET:CE	2.37	0.53
2:F:348:GLU:O	2:F:352:LYS:HG2	2.09	0.53
2:P:291:ASP:O	2:P:343:THR:HG22	2.08	0.53
1:E:325:THR:CG2	1:E:329:ILE:HG13	2.36	0.53
1:E:116:VAL:HG23	1:E:319:ILE:CD1	2.38	0.53
1:E:148:VAL:HB	2:F:160:ILE:HG22	1.90	0.53
2:L:326:ILE:O	2:L:326:ILE:HD12	2.08	0.53
2:L:66:LEU:HD21	2:L:97:ARG:HH21	1.74	0.53
1:G:325:THR:CG2	1:G:329:ILE:HG13	2.39	0.53
1:K:199:THR:HA	1:K:211:VAL:HG11	1.89	0.53
2:P:88:LEU:HD13	2:P:99:LEU:HD23	1.89	0.53
2:F:118:SER:OG	2:F:129:VAL:HG13	2.08	0.53
1:I:116:VAL:HG23	1:I:319:ILE:CD1	2.39	0.53
2:D:342:THR:HG23	2:D:344:SER:H	1.74	0.53
1:A:245:ASN:OD1	1:A:276:VAL:HG21	2.09	0.53
2:P:44:PHE:CD2	2:P:49:VAL:HG21	2.44	0.53
1:M:79:GLY:HA2	1:M:291:MET:CE	2.38	0.53
1:E:195:ARG:O	1:E:199:THR:HG23	2.09	0.53
1:K:45:ILE:HG23	1:K:46:PRO:HD2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:314:ALA:HB2	1:C:346:LEU:HD13	1.90	0.53
1:K:25:GLY:HA2	1:K:81:TRP:CZ2	2.43	0.53
1:M:25:GLY:HA2	1:M:81:TRP:CZ2	2.44	0.53
1:K:325:THR:CG2	1:K:329:ILE:HG13	2.39	0.53
2:H:332:ASN:HA	2:H:341:ALA:HB2	1.90	0.53
1:K:123:ILE:HD13	1:K:250:LEU:HB3	1.91	0.53
2:P:332:ASN:HA	2:P:341:ALA:HB2	1.91	0.53
2:B:12:THR:HB	2:B:81:LEU:CD1	2.39	0.53
2:P:334:THR:HG22	2:P:335:GLY:H	1.72	0.53
2:L:326:ILE:HD11	2:L:346:PHE:CE1	2.44	0.52
2:D:39:SER:O	2:D:43:ILE:HG13	2.09	0.52
1:C:323:LYS:O	1:C:324:HIS:HB2	2.09	0.52
1:I:175:ARG:NH1	1:I:175:ARG:CG	2.59	0.52
1:O:79:GLY:HA2	1:O:291:MET:CE	2.39	0.52
2:H:88:LEU:HD13	2:H:99:LEU:HD23	1.91	0.52
1:E:25:GLY:HA2	1:E:81:TRP:CZ2	2.44	0.52
1:M:54:ILE:HD12	1:M:54:ILE:H	1.74	0.52
2:D:5:GLN:HE21	2:D:5:GLN:HA	1.72	0.52
1:I:20:VAL:HG13	1:I:47:ILE:HG23	1.90	0.52
1:A:199:THR:HA	1:A:211:VAL:HG11	1.90	0.52
1:O:56:GLN:C	1:O:58:ASP:H	2.12	0.52
1:C:55:LYS:HB3	1:C:57:THR:HG22	1.90	0.52
1:G:54:ILE:N	1:G:54:ILE:CD1	2.72	0.52
2:H:12:THR:HB	2:H:81:LEU:HD12	1.92	0.52
2:F:12:THR:HB	2:F:81:LEU:CD1	2.40	0.52
1:M:314:ALA:HB2	1:M:346:LEU:HD13	1.89	0.52
2:H:334:THR:HG22	2:H:335:GLY:H	1.73	0.52
2:J:224:SER:O	2:J:228:VAL:HG23	2.09	0.52
2:L:63:VAL:O	2:L:64:ASN:HB2	2.09	0.52
2:H:245:LEU:HD23	2:H:246:TYR:CE1	2.44	0.52
1:C:245:ASN:OD1	1:C:276:VAL:HG21	2.09	0.52
2:H:126:TYR:HB2	2:H:257:LEU:O	2.10	0.52
2:H:97:ARG:CG	2:H:98:SER:N	2.70	0.52
2:N:270:ILE:HD12	2:N:270:ILE:N	2.25	0.52
2:B:245:LEU:HD23	2:B:246:TYR:CE1	2.44	0.52
1:K:15:GLY:O	1:O:301:HIS:CE1	2.56	0.52
2:B:342:THR:HG22	2:B:345:SER:HB3	1.90	0.52
1:I:195:ARG:O	1:I:199:THR:HG23	2.10	0.52
1:O:314:ALA:HB2	1:O:346:LEU:HD13	1.92	0.52
2:D:12:THR:HB	2:D:81:LEU:CD1	2.40	0.52
1:C:199:THR:HA	1:C:211:VAL:HG11	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:311:ILE:O	1:C:315:VAL:HG13	2.10	0.52
1:I:79:GLY:HA2	1:I:291:MET:HE1	1.92	0.52
2:P:135:ARG:CD	2:P:247:GLY:HA3	2.29	0.52
1:M:148:VAL:N	2:N:160:ILE:O	2.34	0.52
2:N:326:ILE:HG12	2:N:350:VAL:CG2	2.40	0.52
2:N:157:ILE:HD11	1:O:151:LEU:CD1	2.40	0.52
2:B:342:THR:HG23	2:B:344:SER:H	1.74	0.52
1:A:155:THR:O	1:A:159:THR:HG22	2.09	0.52
1:G:314:ALA:HB2	1:G:346:LEU:HD13	1.92	0.52
1:E:235:THR:HG21	1:E:243:LEU:HD12	1.90	0.52
1:M:163:ALA:HB2	1:M:198:ILE:HD13	1.91	0.52
1:C:347:SER:HA	1:G:14:TYR:CE1	2.45	0.52
2:J:175:TYR:O	2:J:179:ILE:HG12	2.10	0.52
1:G:38:THR:HG22	1:G:343:ILE:CD1	2.40	0.51
1:M:325:THR:HG22	1:M:331:GLY:HA3	1.92	0.51
1:O:155:THR:O	1:O:159:THR:CG2	2.57	0.51
1:C:235:THR:HG21	1:C:243:LEU:HD12	1.92	0.51
1:M:175:ARG:HG3	1:M:175:ARG:NH1	2.09	0.51
1:M:88:THR:CB	2:N:189:LYS:HE3	2.34	0.51
1:A:275:HIS:ND1	1:A:278:LEU:CD1	2.66	0.51
2:H:97:ARG:CZ	2:H:102:THR:HG23	2.40	0.51
2:F:70:PRO:O	2:F:74:VAL:HG23	2.11	0.51
1:M:202:GLY:HA3	1:M:211:VAL:HG21	1.91	0.51
2:J:12:THR:HB	2:J:81:LEU:CD1	2.39	0.51
2:N:69:ILE:HG22	2:N:106:THR:HG21	1.93	0.51
2:B:159:LEU:CD2	1:C:143:SER:HB3	2.35	0.51
1:A:175:ARG:HG3	1:A:175:ARG:NH1	2.15	0.51
2:F:12:THR:HB	2:F:81:LEU:HD12	1.91	0.51
2:D:332:ASN:HA	2:D:341:ALA:HB2	1.92	0.51
2:B:291:ASP:C	2:B:343:THR:HG22	2.31	0.51
1:E:149:GLU:HG3	2:F:159:LEU:CD1	2.40	0.51
2:J:135:ARG:CD	2:J:247:GLY:HA3	2.34	0.51
2:H:67:THR:HG21	2:H:97:ARG:N	2.25	0.51
2:P:273:LYS:HE3	2:P:274:ILE:CD1	2.40	0.51
1:E:311:ILE:O	1:E:315:VAL:HG13	2.10	0.51
1:I:123:ILE:HD13	1:I:250:LEU:HB3	1.92	0.51
2:P:166:GLU:O	2:P:167:ARG:HB2	2.10	0.51
1:K:235:THR:HG21	1:K:243:LEU:HD12	1.93	0.51
2:N:145:ILE:HD12	1:O:141:HIS:ND1	2.26	0.51
2:P:224:SER:O	2:P:228:VAL:HG23	2.10	0.51
1:M:20:VAL:HG13	1:M:47:ILE:HG23	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:GLU:OE2	2:D:189:LYS:HE2	2.10	0.51
2:J:342:THR:HG23	2:J:344:SER:H	1.75	0.51
1:C:324:HIS:CG	1:C:341:GLU:HG3	2.46	0.51
2:L:348:GLU:O	2:L:352:LYS:HG2	2.10	0.51
1:A:314:ALA:HB2	1:A:346:LEU:HD13	1.93	0.51
2:J:47:ALA:HA	2:J:354:LEU:HD21	1.91	0.51
1:C:325:THR:CG2	1:C:329:ILE:HG13	2.38	0.51
1:A:143:SER:HB3	2:D:159:LEU:HD22	1.93	0.51
1:K:311:ILE:O	1:K:315:VAL:HG13	2.10	0.51
2:D:70:PRO:O	2:D:74:VAL:HG23	2.11	0.51
2:N:334:THR:HG22	2:N:335:GLY:H	1.76	0.51
1:M:45:ILE:HG12	1:M:307:TYR:CD2	2.45	0.51
2:D:334:THR:HG22	2:D:335:GLY:H	1.75	0.51
2:B:41:LYS:HG2	2:B:53:TRP:NE1	2.26	0.51
1:E:54:ILE:HD13	1:E:81:TRP:CZ2	2.46	0.51
2:P:97:ARG:NH2	2:P:102:THR:HG23	2.26	0.51
1:I:311:ILE:O	1:I:315:VAL:HG13	2.11	0.51
2:P:342:THR:HG23	2:P:344:SER:H	1.75	0.51
2:P:44:PHE:O	2:P:49:VAL:HG22	2.11	0.51
2:D:71:ASP:N	2:D:72:PRO:CD	2.74	0.51
1:G:292:ILE:O	1:G:295:SER:HB3	2.11	0.51
2:F:303:VAL:HG21	2:F:319:GLN:HB2	1.93	0.51
2:P:41:LYS:HG2	2:P:53:TRP:NE1	2.26	0.51
2:P:274:ILE:HG22	2:P:275:SER:N	2.26	0.50
1:E:45:ILE:HG12	1:E:307:TYR:CD2	2.47	0.50
2:B:332:ASN:HA	2:B:341:ALA:HB2	1.92	0.50
2:H:15:PRO:HG3	2:H:22:TYR:CZ	2.46	0.50
1:K:323:LYS:O	1:K:324:HIS:HB2	2.11	0.50
2:J:5:GLN:HG3	2:J:6:PRO:CD	2.38	0.50
2:B:183:ARG:HD2	2:B:237:ASP:OD2	2.12	0.50
1:I:79:GLY:HA2	1:I:291:MET:CE	2.41	0.50
2:N:58:VAL:HG12	2:N:69:ILE:HD11	1.92	0.50
2:F:166:GLU:HG2	2:F:166:GLU:O	2.11	0.50
1:M:175:ARG:CG	1:M:175:ARG:NH1	2.61	0.50
2:F:135:ARG:HD3	2:F:247:GLY:CA	2.34	0.50
2:F:135:ARG:CD	2:F:247:GLY:HA3	2.34	0.50
2:L:287:ILE:HD11	2:L:292:LYS:CD	2.34	0.50
1:M:116:VAL:HG23	1:M:319:ILE:HD13	1.93	0.50
2:D:221:ILE:O	2:D:225:VAL:HG13	2.12	0.50
1:G:152:LYS:O	2:H:155:GLN:HA	2.12	0.50
2:L:66:LEU:HD21	2:L:97:ARG:NH2	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:62:PHE:HE1	2:L:96:HIS:HB3	1.76	0.50
1:E:155:THR:O	1:E:159:THR:CG2	2.60	0.50
1:G:223:ALA:O	1:G:227:PRO:HG3	2.11	0.50
2:P:135:ARG:HD3	2:P:247:GLY:CA	2.31	0.50
1:C:175:ARG:NH1	1:C:175:ARG:CG	2.61	0.50
2:D:135:ARG:CD	2:D:247:GLY:HA3	2.35	0.50
1:A:175:ARG:NH1	1:A:175:ARG:CG	2.65	0.50
2:P:58:VAL:HG12	2:P:69:ILE:HD11	1.94	0.50
1:C:90:HIS:HB3	2:D:193:GLN:HG3	1.93	0.50
2:H:348:GLU:O	2:H:352:LYS:HG2	2.10	0.50
2:J:332:ASN:HA	2:J:341:ALA:HB2	1.93	0.50
1:K:90:HIS:CB	2:L:193:GLN:HG3	2.42	0.50
2:H:44:PHE:CD2	2:H:49:VAL:HG21	2.47	0.50
2:P:67:THR:OG1	2:P:97:ARG:HB3	2.11	0.50
2:F:221:ILE:O	2:F:225:VAL:HG13	2.12	0.50
2:B:322:VAL:CG2	2:B:323:LEU:N	2.71	0.50
1:C:116:VAL:HG23	1:C:319:ILE:CD1	2.42	0.50
1:C:87:GLN:HB3	1:C:276:VAL:HG12	1.93	0.50
2:P:136:GLU:OE2	2:P:138:THR:HB	2.12	0.50
1:M:54:ILE:HD13	1:M:81:TRP:CZ2	2.38	0.50
1:M:146:GLY:O	2:N:162:ARG:N	2.42	0.50
2:P:287:ILE:HG13	2:P:292:LYS:HB2	1.94	0.50
2:J:291:ASP:C	2:J:343:THR:HG22	2.32	0.50
1:O:54:ILE:HG22	1:O:59:HIS:HB3	1.94	0.50
1:E:155:THR:HG22	2:F:153:VAL:HG13	1.94	0.50
2:N:182:PRO:HD2	2:N:237:ASP:O	2.12	0.50
2:J:63:VAL:O	2:J:64:ASN:HB2	2.11	0.50
2:B:44:PHE:CD2	2:B:49:VAL:HG21	2.47	0.50
2:J:44:PHE:CD2	2:J:49:VAL:HG21	2.47	0.49
2:N:228:VAL:HG12	2:N:257:LEU:CD1	2.42	0.49
2:N:228:VAL:HG22	2:N:235:TYR:CD1	2.46	0.49
1:O:156:ARG:HG2	1:O:157:PRO:HD3	1.94	0.49
2:L:62:PHE:CE1	2:L:96:HIS:HB3	2.47	0.49
1:E:202:GLY:HA3	1:E:211:VAL:HG21	1.94	0.49
2:B:71:ASP:N	2:B:72:PRO:CD	2.75	0.49
2:L:166:GLU:O	2:L:167:ARG:HB2	2.12	0.49
2:J:334:THR:HG22	2:J:335:GLY:H	1.77	0.49
2:F:88:LEU:HD13	2:F:99:LEU:HD23	1.94	0.49
1:O:151:LEU:CD2	2:P:157:ILE:HG12	2.42	0.49
1:K:116:VAL:HG23	1:K:319:ILE:CD1	2.42	0.49
2:N:12:THR:HB	2:N:81:LEU:HD12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:15:PRO:HG3	2:L:22:TYR:CZ	2.47	0.49
2:J:89:ALA:O	2:J:91:PRO:HD3	2.12	0.49
2:L:316:ASP:O	2:L:320:ASN:HB3	2.12	0.49
2:F:334:THR:HG22	2:F:335:GLY:H	1.77	0.49
1:O:325:THR:CG2	1:O:329:ILE:HG13	2.39	0.49
2:P:316:ASP:O	2:P:320:ASN:HB3	2.11	0.49
1:A:235:THR:HG21	1:A:243:LEU:HD12	1.94	0.49
1:G:311:ILE:O	1:G:315:VAL:HG13	2.13	0.49
2:D:100:ASN:O	2:D:104:ARG:HG3	2.12	0.49
1:K:314:ALA:HB2	1:K:346:LEU:HD13	1.95	0.49
2:F:40:VAL:HG22	2:F:299:LEU:CD1	2.42	0.49
2:L:126:TYR:HB2	2:L:257:LEU:O	2.12	0.49
1:K:155:THR:O	1:K:159:THR:CG2	2.60	0.49
1:G:139:LEU:HD23	1:G:151:LEU:HD12	1.94	0.49
1:E:221:MET:SD	2:F:261:SER:HA	2.53	0.49
2:N:157:ILE:HD13	1:O:151:LEU:HD11	1.93	0.49
1:O:38:THR:HG22	1:O:343:ILE:CD1	2.40	0.49
2:J:41:LYS:HG2	2:J:53:TRP:NE1	2.28	0.49
2:D:316:ASP:O	2:D:320:ASN:HB3	2.13	0.49
2:L:71:ASP:N	2:L:72:PRO:CD	2.74	0.49
2:D:342:THR:HG23	2:D:344:SER:N	2.28	0.49
1:K:155:THR:HG22	2:L:153:VAL:HG13	1.94	0.49
1:I:235:THR:HG21	1:I:243:LEU:HD12	1.95	0.49
2:F:44:PHE:O	2:F:49:VAL:HG22	2.12	0.49
2:P:100:ASN:O	2:P:104:ARG:HG3	2.12	0.49
2:J:88:LEU:HD13	2:J:99:LEU:HD23	1.94	0.49
2:N:70:PRO:O	2:N:74:VAL:HG23	2.13	0.49
1:M:54:ILE:CA	1:M:62:GLY:HA3	2.30	0.49
2:H:291:ASP:C	2:H:343:THR:HG22	2.32	0.49
2:L:39:SER:O	2:L:43:ILE:HG13	2.12	0.49
2:H:58:VAL:HG12	2:H:69:ILE:HD11	1.94	0.49
2:H:273:LYS:HE3	2:H:274:ILE:CD1	2.43	0.49
2:F:228:VAL:HG12	2:F:257:LEU:CD1	2.43	0.49
2:B:58:VAL:HG12	2:B:69:ILE:HD11	1.95	0.48
2:L:342:THR:HG22	2:L:345:SER:HB3	1.95	0.48
1:M:90:HIS:HB3	2:N:193:GLN:CG	2.43	0.48
2:L:58:VAL:HG12	2:L:69:ILE:HD11	1.94	0.48
2:L:224:SER:O	2:L:228:VAL:HG23	2.12	0.48
1:I:324:HIS:CG	1:I:341:GLU:HG3	2.48	0.48
2:N:16:ASN:HB2	2:N:21:LYS:O	2.13	0.48
2:P:221:ILE:O	2:P:225:VAL:HG13	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:39:SER:O	2:J:43:ILE:HG13	2.12	0.48
2:F:332:ASN:HA	2:F:341:ALA:HB2	1.95	0.48
2:F:326:ILE:HG21	2:F:350:VAL:HG22	1.95	0.48
1:K:135:GLU:OE2	2:L:189:LYS:HE2	2.13	0.48
2:D:97:ARG:HH21	2:D:102:THR:CG2	2.24	0.48
2:N:342:THR:HG23	2:N:344:SER:H	1.78	0.48
2:H:150:CYS:HB2	2:H:151:PRO:HD2	1.94	0.48
2:N:130:ASP:HB3	2:N:236:THR:HB	1.96	0.48
2:L:100:ASN:O	2:L:104:ARG:HG3	2.14	0.48
1:E:323:LYS:O	1:E:324:HIS:HB2	2.13	0.48
2:N:194:ARG:NH2	2:N:194:ARG:CB	2.75	0.48
2:P:326:ILE:HG12	2:P:350:VAL:CG2	2.43	0.48
2:D:351:ILE:HA	2:D:354:LEU:HB2	1.94	0.48
2:L:291:ASP:C	2:L:343:THR:HG22	2.33	0.48
1:M:38:THR:HG22	1:M:343:ILE:CD1	2.39	0.48
2:H:190:SER:O	2:H:194:ARG:HG2	2.13	0.48
2:L:245:LEU:HD23	2:L:246:TYR:CE1	2.48	0.48
1:A:135:GLU:OE2	2:B:189:LYS:HE2	2.14	0.48
2:L:70:PRO:O	2:L:74:VAL:HG23	2.13	0.48
1:K:195:ARG:O	1:K:199:THR:HG23	2.13	0.48
1:M:87:GLN:HA	1:M:274:ARG:HB3	1.95	0.48
1:A:113:LEU:CD1	1:A:256:LEU:HD22	2.41	0.48
2:B:136:GLU:OE2	2:B:138:THR:HB	2.13	0.48
2:J:118:SER:OG	2:J:129:VAL:HG13	2.14	0.48
2:P:270:ILE:N	2:P:270:ILE:HD12	2.28	0.48
2:L:162:ARG:HH11	2:L:162:ARG:HB2	1.78	0.48
2:P:194:ARG:CB	2:P:194:ARG:NH2	2.75	0.48
2:F:157:ILE:HD11	1:G:151:LEU:CD1	2.44	0.48
1:K:202:GLY:HA3	1:K:211:VAL:HG21	1.95	0.48
1:I:168:ASP:OD2	1:M:12:LYS:HE3	2.13	0.48
1:G:246:ILE:HD11	2:H:253:LEU:HD12	1.96	0.48
1:C:45:ILE:HG23	1:C:46:PRO:HD2	1.96	0.48
1:C:20:VAL:HG13	1:C:47:ILE:HG23	1.95	0.48
1:K:147:VAL:HG22	2:L:161:THR:HG22	1.94	0.48
1:O:175:ARG:NH1	1:O:175:ARG:CG	2.61	0.48
2:F:159:LEU:HD23	1:G:144:VAL:HG12	1.94	0.48
1:A:38:THR:HG22	1:A:343:ILE:CD1	2.39	0.48
2:L:66:LEU:CD2	2:L:97:ARG:NH2	2.76	0.48
2:H:41:LYS:HG2	2:H:53:TRP:NE1	2.28	0.48
2:L:221:ILE:O	2:L:225:VAL:HG13	2.13	0.48
2:H:162:ARG:NH1	2:H:162:ARG:HB2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:150:SER:O	2:N:157:ILE:HA	2.14	0.48
2:N:159:LEU:HD22	1:O:143:SER:HB3	1.94	0.48
2:F:58:VAL:HG12	2:F:69:ILE:HD11	1.96	0.48
1:C:45:ILE:HG12	1:C:307:TYR:CD2	2.48	0.48
1:O:119:ARG:NH2	2:P:230:THR:O	2.47	0.48
1:G:153:VAL:HA	2:H:154:VAL:O	2.13	0.48
1:I:18:PHE:CE1	1:M:44:ASN:ND2	2.81	0.48
1:M:54:ILE:HA	1:M:62:GLY:CA	2.31	0.48
1:O:139:LEU:HD23	1:O:151:LEU:HD12	1.94	0.48
2:L:342:THR:HG23	2:L:344:SER:N	2.28	0.48
2:J:12:THR:HB	2:J:81:LEU:HD12	1.95	0.48
2:H:44:PHE:O	2:H:49:VAL:HG22	2.14	0.48
1:E:321:GLU:O	1:E:323:LYS:N	2.46	0.48
1:K:120:ILE:HA	1:K:121:PRO:HD3	1.70	0.48
1:K:12:LYS:HB2	1:K:12:LYS:HE3	1.51	0.48
1:M:181:VAL:HG11	1:M:243:LEU:HD11	1.96	0.48
2:N:189:LYS:O	2:N:190:SER:C	2.52	0.48
1:G:281:LYS:CG	1:G:282:GLY:N	2.77	0.48
2:F:7:SER:HA	2:F:10:ARG:HG2	1.96	0.48
2:H:150:CYS:CB	2:H:151:PRO:CD	2.91	0.48
1:E:324:HIS:CG	1:E:341:GLU:HG3	2.49	0.48
2:L:162:ARG:HB2	2:L:162:ARG:NH1	2.29	0.48
1:M:323:LYS:O	1:M:324:HIS:HB2	2.14	0.48
2:L:113:VAL:HB	2:L:268:ALA:HB3	1.94	0.48
2:J:71:ASP:N	2:J:72:PRO:CD	2.76	0.48
2:L:88:LEU:HD13	2:L:99:LEU:HD23	1.96	0.48
2:F:162:ARG:HB2	2:F:162:ARG:NH1	2.29	0.48
2:D:182:PRO:HD2	2:D:237:ASP:O	2.14	0.48
1:M:146:GLY:O	2:N:161:THR:CA	2.62	0.47
2:N:245:LEU:HD23	2:N:246:TYR:CE1	2.49	0.47
2:B:135:ARG:HD3	2:B:247:GLY:CA	2.36	0.47
2:F:97:ARG:HH22	2:F:102:THR:CG2	2.27	0.47
2:P:342:THR:HG23	2:P:344:SER:N	2.29	0.47
1:C:139:LEU:HD23	1:C:151:LEU:HD12	1.96	0.47
2:D:71:ASP:N	2:D:72:PRO:HD2	2.29	0.47
2:L:12:THR:HB	2:L:81:LEU:CD1	2.43	0.47
1:O:120:ILE:HA	1:O:121:PRO:HD3	1.71	0.47
1:C:25:GLY:HA2	1:C:81:TRP:CZ2	2.49	0.47
2:N:348:GLU:O	2:N:352:LYS:HG2	2.13	0.47
1:C:123:ILE:HD13	1:C:250:LEU:HB3	1.95	0.47
2:J:166:GLU:O	2:J:167:ARG:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:54:ILE:N	1:M:54:ILE:HD12	2.29	0.47
2:D:190:SER:O	2:D:194:ARG:HG2	2.15	0.47
2:H:39:SER:OG	2:H:347:THR:HG22	2.15	0.47
2:D:67:THR:O	2:D:102:THR:HG21	2.13	0.47
1:A:45:ILE:HG12	1:A:307:TYR:CD2	2.48	0.47
2:P:245:LEU:HD23	2:P:246:TYR:CE1	2.49	0.47
2:N:40:VAL:HG22	2:N:299:LEU:CD1	2.44	0.47
2:N:66:LEU:HD21	2:N:97:ARG:NH2	2.29	0.47
2:N:39:SER:OG	2:N:347:THR:HG22	2.14	0.47
2:J:273:LYS:HE3	2:J:274:ILE:CD1	2.44	0.47
2:F:150:CYS:CB	2:F:151:PRO:CD	2.92	0.47
1:C:151:LEU:CD2	2:D:157:ILE:HG12	2.44	0.47
2:P:40:VAL:HG22	2:P:299:LEU:CD1	2.44	0.47
2:H:40:VAL:HG22	2:H:299:LEU:CD1	2.44	0.47
2:N:69:ILE:CG2	2:N:106:THR:HG21	2.45	0.47
2:F:326:ILE:HG12	2:F:350:VAL:CG2	2.44	0.47
2:F:190:SER:O	2:F:194:ARG:HG2	2.14	0.47
2:N:291:ASP:C	2:N:343:THR:HG22	2.35	0.47
1:A:116:VAL:HG23	1:A:319:ILE:CD1	2.44	0.47
2:P:71:ASP:N	2:P:72:PRO:CD	2.77	0.47
2:L:44:PHE:CD2	2:L:49:VAL:HG21	2.48	0.47
2:N:109:LEU:HD13	2:N:269:ASN:HB3	1.97	0.47
2:B:322:VAL:HG23	2:B:323:LEU:HG	1.97	0.47
2:B:287:ILE:HD11	2:B:292:LYS:CD	2.39	0.47
2:F:291:ASP:C	2:F:343:THR:HG22	2.34	0.47
2:P:39:SER:OG	2:P:347:THR:HG22	2.14	0.47
1:O:55:LYS:N	1:O:55:LYS:HD2	2.29	0.47
2:L:69:ILE:HG22	2:L:106:THR:HG21	1.97	0.47
2:F:150:CYS:SG	2:H:153:VAL:HG21	2.54	0.47
1:A:195:ARG:O	1:A:199:THR:HG23	2.13	0.47
2:H:194:ARG:NH2	2:H:194:ARG:CB	2.77	0.47
2:J:190:SER:O	2:J:194:ARG:HG2	2.15	0.47
2:H:70:PRO:O	2:H:74:VAL:HG23	2.14	0.47
1:O:54:ILE:HD12	1:O:54:ILE:N	2.29	0.47
1:A:155:THR:O	1:A:159:THR:HG23	2.13	0.47
2:D:12:THR:HB	2:D:81:LEU:HD12	1.97	0.47
2:H:162:ARG:HB2	2:H:162:ARG:HH11	1.80	0.47
2:H:109:LEU:HD13	2:H:269:ASN:HB3	1.97	0.47
2:J:316:ASP:O	2:J:320:ASN:HB3	2.15	0.47
2:B:162:ARG:HB2	2:B:162:ARG:NH1	2.30	0.47
2:H:118:SER:OG	2:H:129:VAL:HG13	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:189:LEU:HA	1:O:189:LEU:HD12	1.75	0.47
1:M:88:THR:CG2	2:N:189:LYS:HE3	2.45	0.47
1:C:88:THR:HB	2:D:189:LYS:HE3	1.96	0.47
2:P:97:ARG:NH2	2:P:102:THR:CG2	2.78	0.47
2:F:66:LEU:HD21	2:F:97:ARG:HH21	1.79	0.47
2:J:342:THR:HG23	2:J:344:SER:N	2.30	0.47
1:O:55:LYS:HD3	1:O:59:HIS:NE2	2.28	0.47
2:D:274:ILE:HG22	2:D:275:SER:N	2.29	0.47
2:L:67:THR:O	2:L:102:THR:HG21	2.15	0.47
1:C:113:LEU:CD1	1:C:256:LEU:HD22	2.44	0.47
1:K:139:LEU:HD23	1:K:151:LEU:HD12	1.97	0.47
1:C:155:THR:O	1:C:159:THR:HG23	2.14	0.47
1:A:292:ILE:O	1:A:295:SER:HB3	2.14	0.47
2:N:316:ASP:O	2:N:320:ASN:HB3	2.14	0.47
2:P:265:THR:HA	2:P:266:PRO:HD3	1.67	0.47
2:B:316:ASP:O	2:B:320:ASN:HB3	2.15	0.47
2:P:150:CYS:HB2	2:P:151:PRO:CD	2.44	0.47
1:K:149:GLU:HG3	2:L:159:LEU:HD12	1.97	0.47
2:F:130:ASP:HB3	2:F:236:THR:HB	1.95	0.47
2:N:67:THR:O	2:N:102:THR:HG21	2.13	0.47
2:D:322:VAL:CG2	2:D:323:LEU:N	2.77	0.47
2:J:70:PRO:O	2:J:74:VAL:HG23	2.14	0.47
2:H:5:GLN:HA	2:H:6:PRO:HD3	1.82	0.47
1:M:123:ILE:CD1	1:M:250:LEU:HB3	2.45	0.47
2:J:58:VAL:HG12	2:J:69:ILE:HD11	1.96	0.47
2:N:224:SER:O	2:N:228:VAL:HG23	2.14	0.47
1:O:87:GLN:HA	1:O:274:ARG:HB3	1.97	0.47
2:F:100:ASN:O	2:F:104:ARG:HG3	2.15	0.47
1:A:54:ILE:N	1:A:54:ILE:HD12	2.30	0.47
2:J:209:LYS:HE2	2:J:209:LYS:HB3	1.75	0.47
2:D:44:PHE:O	2:D:49:VAL:HG22	2.15	0.47
2:F:67:THR:O	2:F:102:THR:HG21	2.15	0.47
2:N:126:TYR:HB2	2:N:257:LEU:O	2.15	0.47
2:F:182:PRO:HD2	2:F:237:ASP:O	2.15	0.47
1:K:20:VAL:HG13	1:K:47:ILE:HG23	1.97	0.47
1:O:223:ALA:O	1:O:227:PRO:HG3	2.16	0.47
2:F:71:ASP:N	2:F:72:PRO:CD	2.78	0.47
2:B:195:LEU:HD23	2:B:195:LEU:C	2.36	0.47
2:B:326:ILE:O	2:B:326:ILE:HD12	2.15	0.46
1:C:38:THR:HG22	1:C:343:ILE:CD1	2.43	0.46
2:H:274:ILE:HG22	2:H:275:SER:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:342:THR:HG23	2:H:344:SER:H	1.80	0.46
1:M:324:HIS:CG	1:M:341:GLU:HG3	2.50	0.46
1:O:324:HIS:CG	1:O:341:GLU:HG3	2.50	0.46
2:L:135:ARG:HD3	2:L:247:GLY:CA	2.34	0.46
2:N:44:PHE:O	2:N:49:VAL:HG22	2.14	0.46
2:B:159:LEU:HD21	1:C:144:VAL:HG12	1.97	0.46
1:O:325:THR:HG22	1:O:331:GLY:CA	2.43	0.46
2:F:166:GLU:O	2:F:167:ARG:HB2	2.15	0.46
2:H:221:ILE:O	2:H:225:VAL:HG13	2.15	0.46
2:J:182:PRO:HD2	2:J:237:ASP:O	2.15	0.46
1:O:246:ILE:HD11	2:P:253:LEU:HD12	1.97	0.46
2:D:162:ARG:NH1	2:D:162:ARG:HB2	2.30	0.46
1:O:311:ILE:O	1:O:315:VAL:HG13	2.15	0.46
1:O:20:VAL:HG13	1:O:47:ILE:HG23	1.98	0.46
2:L:16:ASN:HB2	2:L:21:LYS:O	2.15	0.46
2:D:194:ARG:CB	2:D:194:ARG:NH2	2.77	0.46
1:O:123:ILE:CD1	1:O:250:LEU:HB3	2.44	0.46
1:K:324:HIS:CG	1:K:341:GLU:HG3	2.50	0.46
1:E:149:GLU:OE1	1:G:149:GLU:OE1	2.34	0.46
2:B:287:ILE:HA	2:B:287:ILE:HD12	1.73	0.46
2:B:342:THR:HG23	2:B:344:SER:N	2.31	0.46
1:G:181:VAL:HG11	1:G:243:LEU:HD11	1.98	0.46
2:P:70:PRO:O	2:P:74:VAL:HG23	2.15	0.46
2:H:67:THR:O	2:H:102:THR:HG21	2.16	0.46
1:E:90:HIS:HB3	2:F:193:GLN:OE1	2.16	0.46
2:F:342:THR:HG23	2:F:344:SER:H	1.80	0.46
1:G:195:ARG:O	1:G:199:THR:HG23	2.16	0.46
2:J:40:VAL:HG22	2:J:299:LEU:CD1	2.46	0.46
2:H:181:ARG:HA	2:H:182:PRO:HD3	1.84	0.46
1:I:246:ILE:HD11	2:J:253:LEU:HD12	1.98	0.46
2:D:331:GLU:HA	2:D:340:THR:OG1	2.16	0.46
2:J:323:LEU:CD2	2:J:323:LEU:H	2.21	0.46
2:H:321:ALA:C	2:H:325:THR:HG22	2.35	0.46
1:C:147:VAL:HG22	2:D:161:THR:HG22	1.97	0.46
2:D:348:GLU:O	2:D:352:LYS:HG2	2.15	0.46
1:G:87:GLN:HA	1:G:274:ARG:HB3	1.98	0.46
1:M:93:LEU:HD23	1:M:93:LEU:HA	1.83	0.46
1:G:162:ILE:HA	1:G:162:ILE:HD12	1.73	0.46
2:F:189:LYS:O	2:F:190:SER:C	2.54	0.46
1:I:275:HIS:CG	1:I:278:LEU:HD12	2.49	0.46
2:D:58:VAL:HG12	2:D:69:ILE:HD11	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:273:LYS:HE3	2:N:274:ILE:CD1	2.45	0.46
2:D:183:ARG:HD2	2:D:237:ASP:OD2	2.16	0.46
1:I:139:LEU:HD23	1:I:151:LEU:HD12	1.98	0.46
1:E:120:ILE:HA	1:E:121:PRO:HD3	1.71	0.46
2:J:162:ARG:NH1	2:J:162:ARG:HB2	2.30	0.46
2:L:334:THR:HG22	2:L:335:GLY:H	1.80	0.46
2:F:326:ILE:O	2:F:326:ILE:HD12	2.16	0.46
2:F:194:ARG:CB	2:F:194:ARG:NH2	2.78	0.46
2:H:135:ARG:HD3	2:H:247:GLY:CA	2.38	0.46
2:H:5:GLN:CD	2:H:6:PRO:HD2	2.36	0.46
2:F:228:VAL:HG22	2:F:235:TYR:CD1	2.50	0.46
2:N:190:SER:O	2:N:194:ARG:HG2	2.16	0.46
2:N:326:ILE:HD12	2:N:326:ILE:O	2.16	0.46
1:A:324:HIS:CG	1:A:341:GLU:CG	2.99	0.46
2:D:162:ARG:HH11	2:D:162:ARG:HB2	1.80	0.46
2:F:265:THR:HA	2:F:266:PRO:HD3	1.74	0.46
2:J:221:ILE:O	2:J:225:VAL:HG13	2.16	0.46
2:B:97:ARG:HH21	2:B:102:THR:CG2	2.27	0.45
2:F:153:VAL:HG21	2:H:150:CYS:SG	2.56	0.45
2:D:41:LYS:HG2	2:D:53:TRP:NE1	2.30	0.45
1:I:120:ILE:HA	1:I:121:PRO:HD3	1.72	0.45
2:P:303:VAL:HG21	2:P:319:GLN:HB2	1.99	0.45
1:M:28:VAL:HG23	1:M:281:LYS:HE2	1.97	0.45
2:B:26:PHE:O	2:B:27:ILE:HB	2.15	0.45
1:I:45:ILE:HG23	1:I:46:PRO:HD2	1.97	0.45
2:H:135:ARG:CD	2:H:247:GLY:HA3	2.38	0.45
2:J:274:ILE:HG22	2:J:275:SER:N	2.30	0.45
1:G:155:THR:HG22	2:H:153:VAL:HG13	1.99	0.45
2:F:49:VAL:HA	2:F:50:PRO:HD3	1.72	0.45
2:B:71:ASP:N	2:B:72:PRO:HD2	2.32	0.45
2:J:71:ASP:N	2:J:72:PRO:HD2	2.31	0.45
2:L:60:PRO:HG3	2:L:99:LEU:HD13	1.98	0.45
2:N:166:GLU:O	2:N:167:ARG:HB2	2.16	0.45
2:H:63:VAL:O	2:H:64:ASN:HB2	2.16	0.45
1:K:126:ILE:HD13	1:K:169:PHE:HE1	1.81	0.45
1:A:281:LYS:HD3	1:A:281:LYS:HA	1.73	0.45
2:D:195:LEU:HD23	2:D:195:LEU:C	2.36	0.45
2:P:189:LYS:O	2:P:190:SER:C	2.54	0.45
2:D:287:ILE:HA	2:D:287:ILE:HD12	1.79	0.45
2:D:5:GLN:OE1	2:D:307:ASN:O	2.35	0.45
2:H:59:SER:HA	2:H:60:PRO:HD3	1.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:242:ILE:HD11	2:J:221:ILE:HD13	1.97	0.45
2:H:139:GLU:H	2:H:139:GLU:HG2	1.60	0.45
1:E:279:ASP:OD1	1:E:279:ASP:N	2.50	0.45
2:J:326:ILE:O	2:J:326:ILE:HD12	2.17	0.45
2:J:135:ARG:HD3	2:J:247:GLY:CA	2.35	0.45
2:N:322:VAL:HG23	2:N:323:LEU:HG	1.98	0.45
2:J:47:ALA:CB	2:J:354:LEU:HD11	2.40	0.45
2:L:273:LYS:HE3	2:L:274:ILE:CD1	2.45	0.45
2:D:273:LYS:HE3	2:D:274:ILE:CD1	2.45	0.45
2:N:5:GLN:HA	2:N:6:PRO:HD3	1.73	0.45
2:L:265:THR:HA	2:L:266:PRO:HD3	1.75	0.45
2:P:118:SER:OG	2:P:129:VAL:HG13	2.16	0.45
1:E:87:GLN:HA	1:E:274:ARG:HB3	1.98	0.45
2:F:318:ILE:HG22	2:F:318:ILE:O	2.16	0.45
2:D:44:PHE:CD2	2:D:49:VAL:HG21	2.51	0.45
2:P:67:THR:O	2:P:102:THR:HG21	2.16	0.45
1:M:149:GLU:HA	2:N:158:LYS:O	2.17	0.45
2:F:69:ILE:HG22	2:F:106:THR:HG21	1.98	0.45
1:E:13:LYS:HD2	1:E:18:PHE:CE1	2.52	0.45
2:H:43:ILE:HD13	2:H:350:VAL:HG11	1.97	0.45
2:B:70:PRO:O	2:B:74:VAL:HG23	2.17	0.45
1:C:325:THR:HG22	1:C:331:GLY:CA	2.46	0.45
1:G:56:GLN:C	1:G:58:ASP:N	2.65	0.45
2:D:97:ARG:NH2	2:D:102:THR:HG23	2.30	0.45
1:M:304:LEU:O	1:M:305:ASN:CG	2.54	0.45
2:D:60:PRO:HG3	2:D:99:LEU:HD13	1.98	0.45
2:H:90:THR:HG22	2:H:91:PRO:O	2.17	0.45
2:L:181:ARG:HA	2:L:182:PRO:HD3	1.79	0.45
2:H:331:GLU:HA	2:H:340:THR:OG1	2.16	0.45
2:F:145:ILE:HD12	1:G:141:HIS:ND1	2.32	0.45
1:O:60:LYS:HB2	1:O:60:LYS:HE3	1.82	0.45
1:A:25:GLY:HA2	1:A:81:TRP:CZ2	2.52	0.45
1:E:151:LEU:HA	2:F:156:SER:O	2.17	0.45
2:L:43:ILE:HD13	2:L:350:VAL:HG11	1.99	0.45
2:P:150:CYS:CB	2:P:151:PRO:CD	2.94	0.45
1:K:149:GLU:HG3	2:L:159:LEU:CD1	2.47	0.45
2:N:331:GLU:HA	2:N:340:THR:OG1	2.17	0.45
2:F:294:ASN:HA	2:F:295:PRO:HD3	1.73	0.45
1:E:54:ILE:HD13	1:E:81:TRP:HZ2	1.81	0.45
2:L:189:LYS:HB2	2:L:246:TYR:OH	2.17	0.45
1:C:155:THR:O	1:C:159:THR:HG22	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:45:ILE:HG23	1:E:46:PRO:HD2	1.99	0.45
2:F:181:ARG:HA	2:F:182:PRO:HD3	1.70	0.45
1:M:287:ASN:CB	1:M:326:THR:HG21	2.47	0.45
2:D:49:VAL:HG12	2:D:314:HIS:ND1	2.32	0.45
1:A:175:ARG:HG3	1:A:231:ASP:OD1	2.16	0.45
2:H:342:THR:HG22	2:H:345:SER:HB3	1.99	0.45
2:D:67:THR:HG21	2:D:97:ARG:N	2.32	0.45
1:K:45:ILE:HG12	1:K:307:TYR:CD2	2.52	0.45
2:H:49:VAL:HA	2:H:50:PRO:HD3	1.72	0.45
2:P:71:ASP:N	2:P:72:PRO:HD2	2.32	0.45
2:F:16:ASN:HB2	2:F:21:LYS:O	2.17	0.45
1:A:182:HIS:HE2	1:A:213:SER:HB3	1.81	0.45
2:B:166:GLU:HG2	2:B:166:GLU:O	2.16	0.45
2:H:26:PHE:O	2:H:27:ILE:HB	2.17	0.45
1:K:87:GLN:HA	1:K:274:ARG:HB3	1.98	0.45
2:N:195:LEU:HD23	2:N:195:LEU:C	2.37	0.45
2:P:190:SER:O	2:P:194:ARG:HG2	2.16	0.45
2:P:326:ILE:HD11	2:P:346:PHE:CD1	2.51	0.45
2:B:135:ARG:CD	2:B:247:GLY:HA3	2.37	0.45
2:P:291:ASP:C	2:P:343:THR:HG22	2.37	0.45
1:M:155:THR:O	1:M:159:THR:HG22	2.16	0.45
2:B:273:LYS:HE3	2:B:274:ILE:CD1	2.45	0.45
1:I:323:LYS:O	1:I:324:HIS:HB2	2.17	0.45
2:D:303:VAL:HG21	2:D:319:GLN:HB2	1.99	0.45
2:J:109:LEU:HD13	2:J:269:ASN:HB3	1.98	0.45
2:B:326:ILE:HG12	2:B:350:VAL:CG2	2.47	0.44
2:F:326:ILE:HD11	2:F:346:PHE:CD1	2.52	0.44
1:K:88:THR:HB	2:L:189:LYS:HE3	1.98	0.44
2:N:135:ARG:HD3	2:N:247:GLY:CA	2.32	0.44
2:N:135:ARG:CD	2:N:247:GLY:HA3	2.32	0.44
2:L:318:ILE:O	2:L:318:ILE:HG22	2.16	0.44
1:E:38:THR:HG22	1:E:343:ILE:CD1	2.43	0.44
1:G:281:LYS:HD3	1:G:282:GLY:N	2.32	0.44
2:D:69:ILE:HG22	2:D:106:THR:HG21	1.98	0.44
2:H:130:ASP:HB3	2:H:236:THR:HB	1.99	0.44
2:N:150:CYS:CB	2:N:151:PRO:CD	2.95	0.44
1:M:80:LEU:HD21	1:M:271:PRO:HG2	1.98	0.44
1:A:55:LYS:HD3	1:A:59:HIS:ND1	2.32	0.44
2:N:100:ASN:O	2:N:104:ARG:HG3	2.17	0.44
2:J:15:PRO:HG3	2:J:22:TYR:CZ	2.52	0.44
2:J:326:ILE:HG12	2:J:350:VAL:CG2	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:194:PHE:O	1:E:198:ILE:HG12	2.17	0.44
2:P:228:VAL:HG22	2:P:235:TYR:CD1	2.52	0.44
2:B:49:VAL:HA	2:B:50:PRO:HD3	1.73	0.44
2:N:150:CYS:SG	2:P:153:VAL:HG21	2.56	0.44
1:G:324:HIS:CG	1:G:341:GLU:HG3	2.52	0.44
2:N:265:THR:HA	2:N:266:PRO:HD3	1.67	0.44
2:N:15:PRO:HG3	2:N:22:TYR:CZ	2.52	0.44
1:A:140:GLU:OE2	2:B:194:ARG:HA	2.17	0.44
2:B:190:SER:O	2:B:194:ARG:HG2	2.18	0.44
2:J:194:ARG:CB	2:J:194:ARG:NH2	2.79	0.44
2:L:323:LEU:CD2	2:L:323:LEU:H	2.21	0.44
1:M:324:HIS:HA	1:M:333:SER:OG	2.17	0.44
2:D:265:THR:HA	2:D:266:PRO:HD3	1.69	0.44
2:L:173:PHE:CD2	2:L:184:VAL:HG11	2.52	0.44
2:D:209:LYS:HB3	2:D:209:LYS:HE2	1.73	0.44
1:A:275:HIS:CE1	1:A:278:LEU:CD1	3.01	0.44
2:L:287:ILE:HA	2:L:287:ILE:HD12	1.79	0.44
1:M:143:SER:HB3	2:P:159:LEU:CD2	2.45	0.44
1:G:202:GLY:HA3	1:G:211:VAL:HG21	1.99	0.44
2:H:228:VAL:HG12	2:H:257:LEU:CD1	2.46	0.44
2:B:12:THR:HB	2:B:81:LEU:HD12	1.99	0.44
2:P:316:ASP:O	2:P:320:ASN:CB	2.66	0.44
2:L:71:ASP:N	2:L:72:PRO:HD2	2.32	0.44
2:N:88:LEU:HD13	2:N:99:LEU:HD23	1.99	0.44
2:H:166:GLU:O	2:H:167:ARG:HB2	2.17	0.44
2:P:182:PRO:HD2	2:P:237:ASP:O	2.17	0.44
2:P:331:GLU:HA	2:P:340:THR:OG1	2.17	0.44
2:P:162:ARG:HB2	2:P:162:ARG:NH1	2.33	0.44
1:K:304:LEU:O	1:K:305:ASN:CG	2.56	0.44
2:D:316:ASP:O	2:D:320:ASN:CB	2.66	0.44
2:L:49:VAL:HA	2:L:50:PRO:HD3	1.69	0.44
2:F:331:GLU:HA	2:F:340:THR:OG1	2.17	0.44
2:J:294:ASN:HA	2:J:295:PRO:HD3	1.75	0.44
2:B:109:LEU:HD13	2:B:269:ASN:HB3	2.00	0.44
1:M:182:HIS:HE2	1:M:213:SER:HB3	1.81	0.44
1:E:162:ILE:HA	1:E:162:ILE:HD12	1.76	0.44
1:G:189:LEU:HA	1:G:189:LEU:HD12	1.73	0.44
2:F:103:LEU:HA	2:F:103:LEU:HD12	1.82	0.44
2:H:270:ILE:N	2:H:270:ILE:HD12	2.33	0.44
2:B:351:ILE:HA	2:B:354:LEU:HB2	1.98	0.44
2:J:69:ILE:HG22	2:J:106:THR:HG21	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:342:THR:HG23	2:H:344:SER:N	2.33	0.44
1:C:133:GLU:OE1	1:C:155:THR:HG23	2.17	0.44
1:E:155:THR:O	1:E:159:THR:HG23	2.17	0.44
1:M:45:ILE:HG23	1:M:46:PRO:HD2	2.00	0.44
1:O:323:LYS:O	1:O:324:HIS:HB2	2.18	0.44
2:L:41:LYS:HG2	2:L:53:TRP:NE1	2.33	0.44
1:A:120:ILE:HA	1:A:121:PRO:HD3	1.69	0.44
1:I:156:ARG:N	1:I:157:PRO:CD	2.81	0.44
2:N:71:ASP:N	2:N:72:PRO:CD	2.81	0.44
2:H:71:ASP:N	2:H:72:PRO:HD2	2.32	0.44
2:F:322:VAL:HG23	2:F:323:LEU:HG	2.00	0.44
1:C:149:GLU:HG3	2:D:159:LEU:HD12	1.99	0.44
1:A:43:GLU:OE2	1:A:346:LEU:HG	2.18	0.44
2:H:299:LEU:HD12	2:H:299:LEU:HA	1.86	0.44
1:G:90:HIS:HB3	2:H:193:GLN:OE1	2.18	0.44
1:G:310:ARG:HG2	1:G:349:MET:HE2	1.99	0.44
2:P:264:LEU:HD21	2:P:337:LEU:HD21	1.98	0.44
1:G:104:TYR:CZ	1:G:161:ARG:HD2	2.53	0.44
2:B:294:ASN:HA	2:B:295:PRO:HD3	1.74	0.44
2:D:199:LEU:HD23	2:D:199:LEU:C	2.38	0.44
2:D:103:LEU:HD12	2:D:103:LEU:HA	1.83	0.44
1:O:45:ILE:HG12	1:O:307:TYR:CD2	2.52	0.44
2:L:166:GLU:O	2:L:166:GLU:HG2	2.17	0.44
2:J:166:GLU:O	2:J:166:GLU:HG2	2.18	0.44
2:D:294:ASN:HA	2:D:295:PRO:HD3	1.75	0.44
2:F:316:ASP:O	2:F:320:ASN:HB3	2.17	0.44
2:J:348:GLU:O	2:J:352:LYS:HG2	2.17	0.44
2:P:199:LEU:C	2:P:199:LEU:HD23	2.38	0.44
2:L:190:SER:O	2:L:194:ARG:HG2	2.17	0.44
1:M:148:VAL:HG11	2:N:196:ALA:HB2	2.00	0.44
1:O:155:THR:O	1:O:159:THR:HG22	2.17	0.44
2:N:299:LEU:HA	2:N:299:LEU:HD12	1.80	0.44
2:B:26:PHE:O	2:B:27:ILE:CB	2.66	0.44
1:G:323:LYS:O	1:G:324:HIS:HB2	2.17	0.44
1:C:221:MET:SD	2:D:261:SER:HA	2.58	0.44
2:F:26:PHE:CE2	2:F:37:SER:HB3	2.53	0.44
2:P:209:LYS:HE2	2:P:209:LYS:HB3	1.78	0.44
1:K:60:LYS:HB2	1:K:60:LYS:HE3	1.83	0.44
2:F:326:ILE:HG12	2:F:350:VAL:HG23	2.00	0.43
2:H:69:ILE:HG22	2:H:106:THR:HG21	1.99	0.43
2:B:342:THR:HG23	2:B:345:SER:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:12:THR:HB	2:L:81:LEU:HD12	1.98	0.43
2:F:71:ASP:N	2:F:72:PRO:HD2	2.33	0.43
1:C:104:TYR:CZ	1:C:161:ARG:HD2	2.53	0.43
2:B:63:VAL:O	2:B:64:ASN:HB2	2.18	0.43
2:P:318:ILE:HG22	2:P:318:ILE:O	2.18	0.43
2:L:97:ARG:CG	2:L:98:SER:N	2.80	0.43
2:F:342:THR:HG23	2:F:344:SER:N	2.34	0.43
2:J:228:VAL:HG12	2:J:257:LEU:CD1	2.48	0.43
2:N:130:ASP:O	2:N:181:ARG:NH2	2.51	0.43
1:A:54:ILE:HG22	1:A:56:GLN:O	2.19	0.43
2:N:166:GLU:O	2:N:166:GLU:HG2	2.18	0.43
1:C:104:TYR:CE1	1:C:161:ARG:HD2	2.54	0.43
2:J:100:ASN:O	2:J:104:ARG:HG3	2.18	0.43
1:G:120:ILE:HA	1:G:121:PRO:HD3	1.72	0.43
2:H:16:ASN:HB2	2:H:21:LYS:O	2.18	0.43
2:N:173:PHE:CD2	2:N:184:VAL:HG11	2.53	0.43
2:N:175:TYR:O	2:N:179:ILE:HG12	2.18	0.43
2:B:199:LEU:C	2:B:199:LEU:HD23	2.39	0.43
1:E:325:THR:HG22	1:E:331:GLY:CA	2.48	0.43
2:H:68:THR:CG2	2:H:69:ILE:N	2.81	0.43
1:E:304:LEU:O	1:E:305:ASN:CG	2.57	0.43
1:C:194:PHE:O	1:C:198:ILE:HG12	2.19	0.43
2:J:162:ARG:HH11	2:J:162:ARG:HB2	1.83	0.43
2:N:321:ALA:C	2:N:325:THR:HG22	2.38	0.43
1:A:14:TYR:CG	1:A:15:GLY:N	2.84	0.43
1:K:344:ASN:O	1:K:348:THR:HG23	2.18	0.43
2:B:15:PRO:HG3	2:B:22:TYR:CZ	2.52	0.43
1:A:60:LYS:HE3	1:A:60:LYS:HB2	1.84	0.43
2:N:162:ARG:NH1	2:N:162:ARG:HB2	2.34	0.43
2:J:67:THR:O	2:J:102:THR:HG21	2.18	0.43
2:B:69:ILE:HG22	2:B:106:THR:HG21	2.00	0.43
2:F:97:ARG:HH12	2:F:101:LEU:HD13	1.83	0.43
1:I:38:THR:HG22	1:I:343:ILE:CD1	2.44	0.43
1:E:90:HIS:HB2	2:F:193:GLN:HG3	1.97	0.43
1:G:123:ILE:CD1	1:G:250:LEU:HB3	2.48	0.43
2:J:26:PHE:O	2:J:27:ILE:HB	2.18	0.43
2:N:326:ILE:HG12	2:N:350:VAL:HG23	2.00	0.43
1:I:280:ILE:HG13	1:I:280:ILE:H	1.62	0.43
1:A:194:PHE:O	1:A:198:ILE:HG12	2.18	0.43
2:H:60:PRO:HG3	2:H:99:LEU:HD13	2.01	0.43
2:L:316:ASP:O	2:L:320:ASN:CB	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:321:GLU:O	1:I:323:LYS:N	2.52	0.43
2:L:103:LEU:HD12	2:L:103:LEU:HA	1.82	0.43
2:D:326:ILE:O	2:D:326:ILE:HD12	2.19	0.43
1:O:155:THR:O	1:O:159:THR:HG23	2.18	0.43
2:B:162:ARG:HB2	2:B:162:ARG:HH11	1.84	0.43
2:L:321:ALA:C	2:L:325:THR:HG22	2.39	0.43
1:A:156:ARG:N	1:A:157:PRO:CD	2.81	0.43
2:P:321:ALA:C	2:P:325:THR:HG22	2.39	0.43
2:J:321:ALA:C	2:J:325:THR:HG22	2.39	0.43
1:A:17:ARG:NH1	1:A:48:ASP:OD1	2.52	0.43
2:H:318:ILE:HG22	2:H:318:ILE:O	2.18	0.43
1:G:113:LEU:CD1	1:G:256:LEU:HD22	2.47	0.43
2:D:59:SER:HA	2:D:60:PRO:HD3	1.80	0.43
1:O:202:GLY:HA3	1:O:211:VAL:HG21	2.01	0.43
1:M:245:ASN:CB	2:N:225:VAL:HG22	2.49	0.43
2:H:71:ASP:N	2:H:72:PRO:CD	2.81	0.43
2:H:136:GLU:OE2	2:H:138:THR:HB	2.18	0.43
2:H:13:GLY:O	2:H:14:LYS:HB3	2.19	0.43
1:A:162:ILE:HD12	1:A:162:ILE:HA	1.74	0.43
1:I:93:LEU:HD23	1:I:93:LEU:HA	1.86	0.43
2:N:287:ILE:CG1	2:N:292:LYS:HB2	2.48	0.43
2:P:287:ILE:HA	2:P:287:ILE:HD12	1.85	0.43
2:J:322:VAL:CG2	2:J:323:LEU:N	2.75	0.43
1:C:321:GLU:O	1:C:323:LYS:N	2.52	0.43
2:N:233:SER:HA	2:N:236:THR:HG23	2.00	0.43
2:N:228:VAL:HG22	2:N:235:TYR:CE1	2.53	0.43
2:P:181:ARG:HA	2:P:182:PRO:HD3	1.78	0.43
2:D:136:GLU:OE2	2:D:138:THR:HB	2.18	0.43
2:J:16:ASN:HB2	2:J:21:LYS:O	2.19	0.43
2:J:270:ILE:HD12	2:J:270:ILE:N	2.33	0.43
2:H:209:LYS:HB3	2:H:209:LYS:HE2	1.72	0.43
2:L:209:LYS:HE2	2:L:209:LYS:HB3	1.73	0.43
2:D:318:ILE:C	2:D:322:VAL:HG11	2.39	0.43
1:I:277:GLY:O	1:I:278:LEU:C	2.57	0.43
1:G:151:LEU:HB3	2:H:155:GLN:NE2	2.34	0.43
2:L:317:GLN:O	2:L:322:VAL:HG13	2.19	0.43
1:M:241:THR:HG22	1:M:242:ILE:N	2.33	0.43
2:D:321:ALA:C	2:D:325:THR:HG22	2.40	0.43
1:K:133:GLU:HG2	1:K:153:VAL:O	2.19	0.43
2:D:270:ILE:HD12	2:D:270:ILE:N	2.34	0.43
1:K:140:GLU:OE2	2:L:194:ARG:HA	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:49:VAL:HG12	2:N:314:HIS:ND1	2.33	0.43
2:D:323:LEU:CD2	2:D:323:LEU:H	2.22	0.43
2:N:157:ILE:CD1	1:O:151:LEU:CD1	2.97	0.43
1:A:325:THR:CG2	1:A:329:ILE:HG13	2.45	0.43
1:I:90:HIS:CG	2:J:193:GLN:HG3	2.54	0.43
2:D:175:TYR:O	2:D:179:ILE:HG12	2.19	0.43
2:D:109:LEU:HD13	2:D:269:ASN:HB3	2.00	0.43
2:B:265:THR:HA	2:B:266:PRO:HD3	1.69	0.43
2:P:348:GLU:O	2:P:352:LYS:HG2	2.19	0.43
1:M:60:LYS:HB2	1:M:60:LYS:HE3	1.84	0.43
1:E:181:VAL:HG11	1:E:243:LEU:HD11	2.00	0.42
2:D:322:VAL:HG23	2:D:323:LEU:HG	2.01	0.42
2:B:212:PRO:HG2	1:O:228:HIS:HD2	1.77	0.42
2:N:342:THR:HG23	2:N:344:SER:N	2.33	0.42
1:A:321:GLU:O	1:A:323:LYS:N	2.52	0.42
2:B:166:GLU:O	2:B:167:ARG:HB2	2.19	0.42
1:A:20:VAL:HG13	1:A:47:ILE:HG23	2.01	0.42
2:B:209:LYS:HE2	2:B:209:LYS:HB3	1.76	0.42
1:K:77:LEU:HA	1:K:77:LEU:HD23	1.84	0.42
2:N:326:ILE:HD11	2:N:346:PHE:CD1	2.54	0.42
1:K:116:VAL:HG23	1:K:319:ILE:HD13	2.01	0.42
1:K:55:LYS:HD3	1:K:55:LYS:HA	1.90	0.42
2:P:49:VAL:HA	2:P:50:PRO:HD3	1.69	0.42
2:J:126:TYR:HB2	2:J:257:LEU:O	2.19	0.42
2:F:299:LEU:HA	2:F:299:LEU:HD12	1.81	0.42
2:L:228:VAL:HG12	2:L:257:LEU:CD1	2.48	0.42
2:P:40:VAL:HG22	2:P:299:LEU:HD13	2.01	0.42
2:N:71:ASP:N	2:N:72:PRO:HD2	2.35	0.42
1:K:162:ILE:HD12	1:K:162:ILE:HA	1.81	0.42
2:D:139:GLU:H	2:D:139:GLU:HG2	1.65	0.42
2:L:331:GLU:HA	2:L:340:THR:OG1	2.19	0.42
2:J:195:LEU:HD23	2:J:195:LEU:C	2.40	0.42
1:I:45:ILE:HG12	1:I:307:TYR:CD2	2.54	0.42
2:B:342:THR:HG22	2:B:345:SER:CB	2.49	0.42
1:M:90:HIS:HB2	2:N:193:GLN:HG3	1.99	0.42
2:B:126:TYR:HB2	2:B:257:LEU:O	2.19	0.42
1:E:288:PRO:O	1:E:292:ILE:HG13	2.19	0.42
2:P:294:ASN:HA	2:P:295:PRO:HD3	1.75	0.42
2:F:264:LEU:HD21	2:F:337:LEU:HD21	2.00	0.42
1:I:126:ILE:HD13	1:I:169:PHE:HE1	1.84	0.42
1:A:75:ILE:HG23	1:A:75:ILE:HD12	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:181:VAL:HG11	1:I:243:LEU:HD11	2.01	0.42
2:J:342:THR:HG22	2:J:345:SER:HB3	2.00	0.42
1:E:116:VAL:HG23	1:E:319:ILE:HD13	2.00	0.42
1:K:155:THR:O	1:K:159:THR:HG23	2.19	0.42
2:L:182:PRO:HD2	2:L:237:ASP:O	2.19	0.42
1:G:344:ASN:O	1:G:348:THR:HG23	2.19	0.42
2:D:113:VAL:HB	2:D:268:ALA:HB3	2.02	0.42
1:O:344:ASN:O	1:O:348:THR:HG23	2.20	0.42
2:D:318:ILE:HG22	2:D:318:ILE:O	2.19	0.42
2:D:326:ILE:HG21	2:D:350:VAL:HG22	2.01	0.42
2:F:157:ILE:CD1	1:G:151:LEU:HD11	2.49	0.42
2:D:351:ILE:HG23	2:D:354:LEU:HD23	2.00	0.42
1:C:202:GLY:HA3	1:C:211:VAL:HG21	2.02	0.42
2:B:228:VAL:HG12	2:B:257:LEU:CD1	2.50	0.42
1:K:242:ILE:HD11	2:L:221:ILE:HD13	2.01	0.42
2:H:166:GLU:HG2	2:H:166:GLU:O	2.19	0.42
2:D:118:SER:OG	2:D:129:VAL:HG13	2.20	0.42
1:K:148:VAL:HB	2:L:160:ILE:HG22	2.00	0.42
2:D:16:ASN:HB2	2:D:21:LYS:O	2.20	0.42
1:O:104:TYR:CZ	1:O:161:ARG:HD2	2.55	0.42
2:H:189:LYS:O	2:H:190:SER:C	2.57	0.42
2:J:326:ILE:HD11	2:J:346:PHE:CD1	2.55	0.42
2:H:326:ILE:HD11	2:H:346:PHE:CD1	2.54	0.42
2:H:326:ILE:HG12	2:H:350:VAL:CG2	2.50	0.42
1:I:113:LEU:CD1	1:I:256:LEU:HD22	2.49	0.42
1:A:287:ASN:CB	1:A:326:THR:HG21	2.49	0.42
1:E:8:ARG:C	1:E:10:LEU:H	2.22	0.42
1:C:182:HIS:HE2	1:C:213:SER:HB3	1.84	0.42
1:C:77:LEU:HA	1:C:77:LEU:HD23	1.91	0.42
1:O:162:ILE:HA	1:O:162:ILE:HD12	1.73	0.42
2:B:326:ILE:HG12	2:B:350:VAL:HG23	2.02	0.42
1:I:304:LEU:O	1:I:305:ASN:CG	2.58	0.42
1:I:90:HIS:HB3	2:J:193:GLN:HG3	2.00	0.42
1:A:218:ASN:O	1:A:222:GLN:HB2	2.20	0.42
1:M:245:ASN:HB3	2:N:225:VAL:HG22	2.01	0.42
2:H:334:THR:HB	2:H:336:ASP:OD1	2.20	0.42
2:J:44:PHE:O	2:J:49:VAL:HG22	2.20	0.42
2:F:334:THR:HB	2:F:336:ASP:OD1	2.20	0.42
1:E:20:VAL:HG13	1:E:47:ILE:HG23	2.00	0.42
2:B:103:LEU:HD12	2:B:103:LEU:HA	1.81	0.42
2:F:287:ILE:CG1	2:F:292:LYS:HB2	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:175:ARG:HG3	1:C:231:ASP:OD1	2.20	0.42
2:D:326:ILE:HD11	2:D:346:PHE:CD1	2.55	0.42
2:L:326:ILE:HG12	2:L:350:VAL:CG2	2.50	0.42
2:H:5:GLN:CG	2:H:6:PRO:HD2	2.49	0.42
2:B:299:LEU:HD12	2:B:299:LEU:HA	1.95	0.42
1:C:288:PRO:O	1:C:292:ILE:HG13	2.20	0.42
1:K:90:HIS:HB3	2:L:193:GLN:HG3	2.01	0.42
2:B:321:ALA:C	2:B:325:THR:HG22	2.40	0.42
1:M:276:VAL:HG11	2:N:222:ASP:HB3	2.02	0.42
2:L:40:VAL:HG22	2:L:299:LEU:CD1	2.50	0.42
1:E:277:GLY:HA3	2:F:226:LEU:HD12	2.01	0.42
2:N:303:VAL:HG21	2:N:319:GLN:HB2	2.01	0.42
2:P:323:LEU:H	2:P:323:LEU:CD2	2.22	0.42
2:B:287:ILE:HG13	2:B:292:LYS:HB2	2.02	0.42
1:I:202:GLY:HA3	1:I:211:VAL:HG21	2.01	0.42
1:E:123:ILE:CD1	1:E:250:LEU:HB3	2.50	0.42
2:D:228:VAL:HG12	2:D:257:LEU:CD1	2.49	0.42
1:G:194:PHE:O	1:G:198:ILE:HG12	2.20	0.42
2:L:44:PHE:O	2:L:49:VAL:HG22	2.20	0.42
2:J:303:VAL:HG21	2:J:319:GLN:HB2	2.01	0.42
2:H:172:ALA:HB2	2:H:241:VAL:CG1	2.49	0.42
1:K:80:LEU:HD21	1:K:271:PRO:HG2	2.02	0.42
2:J:331:GLU:HA	2:J:340:THR:OG1	2.20	0.42
2:L:136:GLU:OE2	2:L:138:THR:HB	2.20	0.42
2:N:139:GLU:H	2:N:139:GLU:HG2	1.70	0.42
2:F:194:ARG:NH2	2:F:194:ARG:CG	2.58	0.42
2:J:189:LYS:O	2:J:190:SER:C	2.58	0.42
2:P:194:ARG:CG	2:P:194:ARG:NH2	2.56	0.42
2:D:135:ARG:HD3	2:D:247:GLY:CA	2.36	0.42
2:J:47:ALA:HB2	2:J:354:LEU:HD21	2.02	0.42
1:I:288:PRO:O	1:I:292:ILE:HG13	2.20	0.42
2:F:260:GLY:O	2:F:261:SER:HB3	2.19	0.42
2:B:316:ASP:O	2:B:320:ASN:CB	2.68	0.42
1:O:45:ILE:HG23	1:O:46:PRO:HD2	2.01	0.42
2:L:136:GLU:HA	2:L:168:VAL:HG11	2.01	0.42
1:G:156:ARG:HG2	1:G:157:PRO:HD3	2.02	0.42
2:N:26:PHE:O	2:N:27:ILE:HB	2.19	0.42
2:P:26:PHE:O	2:P:27:ILE:HB	2.19	0.42
2:P:69:ILE:HG22	2:P:106:THR:HG21	2.02	0.41
2:F:66:LEU:CD2	2:F:97:ARG:HH21	2.32	0.41
1:C:15:GLY:O	1:G:301:HIS:CE1	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:123:ILE:CD1	1:K:250:LEU:HB3	2.49	0.41
2:J:59:SER:HA	2:J:60:PRO:HD3	1.79	0.41
2:P:162:ARG:HB2	2:P:162:ARG:HH11	1.84	0.41
2:H:11:TYR:CD1	2:H:309:MET:HA	2.55	0.41
1:K:287:ASN:HA	1:K:288:PRO:HD3	1.89	0.41
1:M:344:ASN:O	1:M:348:THR:HG23	2.19	0.41
2:P:233:SER:HA	2:P:236:THR:HG23	2.02	0.41
2:L:139:GLU:HG2	2:L:139:GLU:H	1.67	0.41
2:B:47:ALA:CA	2:B:354:LEU:HD21	2.50	0.41
2:H:189:LYS:HB2	2:H:246:TYR:OH	2.20	0.41
2:L:97:ARG:HH11	2:L:101:LEU:HD12	1.84	0.41
2:F:273:LYS:HE3	2:F:274:ILE:CD1	2.48	0.41
2:N:274:ILE:CG2	2:N:275:SER:N	2.83	0.41
2:H:5:GLN:NE2	2:H:308:HIS:HA	2.35	0.41
2:D:5:GLN:HA	2:D:6:PRO:HD3	1.95	0.41
2:H:40:VAL:HG22	2:H:299:LEU:HD13	2.02	0.41
1:I:182:HIS:HE2	1:I:213:SER:HB3	1.85	0.41
2:H:100:ASN:O	2:H:104:ARG:HG3	2.20	0.41
1:M:104:TYR:CE1	1:M:161:ARG:HD2	2.55	0.41
2:B:35:GLU:H	2:B:35:GLU:HG2	1.71	0.41
2:P:317:GLN:O	2:P:322:VAL:HG13	2.21	0.41
2:H:97:ARG:HH11	2:H:101:LEU:CD1	2.27	0.41
1:A:133:GLU:OE1	1:A:155:THR:HG23	2.20	0.41
2:F:299:LEU:O	2:F:302:SER:HB2	2.20	0.41
2:F:130:ASP:O	2:F:181:ARG:NH2	2.53	0.41
1:M:126:ILE:HD13	1:M:169:PHE:HE1	1.85	0.41
2:B:150:CYS:HB2	2:B:151:PRO:CD	2.51	0.41
2:N:13:GLY:O	2:N:14:LYS:HB3	2.21	0.41
1:A:283:GLN:O	1:A:285:VAL:HG13	2.19	0.41
2:B:214:LEU:HD12	2:B:214:LEU:HA	1.89	0.41
2:J:287:ILE:HG13	2:J:292:LYS:HB2	2.01	0.41
1:M:90:HIS:HB3	2:N:193:GLN:OE1	2.21	0.41
2:D:85:LYS:HE2	2:D:88:LEU:HD21	2.02	0.41
2:L:228:VAL:HG22	2:L:235:TYR:CD1	2.56	0.41
2:L:59:SER:HA	2:L:60:PRO:HD3	1.80	0.41
2:D:40:VAL:HG22	2:D:299:LEU:CD1	2.50	0.41
1:I:301:HIS:HE1	1:M:15:GLY:O	2.02	0.41
2:N:264:LEU:HD21	2:N:337:LEU:HD21	2.01	0.41
2:B:13:GLY:O	2:B:14:LYS:HB3	2.20	0.41
1:K:156:ARG:N	1:K:157:PRO:CD	2.83	0.41
2:J:265:THR:HA	2:J:266:PRO:HD3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:162:ILE:HA	1:I:162:ILE:HD12	1.79	0.41
1:O:181:VAL:HG11	1:O:243:LEU:HD11	2.02	0.41
2:J:322:VAL:HG23	2:J:323:LEU:HG	2.01	0.41
2:D:49:VAL:HA	2:D:50:PRO:HD3	1.72	0.41
1:M:149:GLU:HG3	2:N:159:LEU:HD13	2.01	0.41
1:O:116:VAL:HG23	1:O:319:ILE:HD13	2.00	0.41
1:G:325:THR:HG22	1:G:331:GLY:CA	2.47	0.41
1:C:87:GLN:HA	1:C:274:ARG:HB3	2.03	0.41
1:K:346:LEU:HD12	1:K:346:LEU:HA	1.90	0.41
1:I:156:ARG:HG2	1:I:157:PRO:HD3	2.03	0.41
2:L:109:LEU:HD13	2:L:269:ASN:HB3	2.03	0.41
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.92	0.41
2:J:318:ILE:O	2:J:318:ILE:HG22	2.21	0.41
2:L:62:PHE:CZ	2:L:67:THR:HG22	2.56	0.41
1:M:321:GLU:O	1:M:323:LYS:N	2.52	0.41
2:N:40:VAL:HG22	2:N:299:LEU:HD13	2.03	0.41
2:J:316:ASP:O	2:J:320:ASN:CB	2.69	0.41
2:N:136:GLU:OE2	2:N:138:THR:HB	2.21	0.41
2:D:172:ALA:HB2	2:D:241:VAL:CG1	2.50	0.41
2:J:150:CYS:HB2	2:J:151:PRO:CD	2.51	0.41
2:H:194:ARG:CG	2:H:194:ARG:NH2	2.55	0.41
2:H:287:ILE:HG13	2:H:292:LYS:HB2	2.03	0.41
2:N:318:ILE:HG22	2:N:318:ILE:O	2.21	0.41
2:D:326:ILE:HG12	2:D:350:VAL:CG2	2.50	0.41
2:F:69:ILE:CG2	2:F:106:THR:HG21	2.51	0.41
1:C:55:LYS:HD3	1:C:55:LYS:HA	1.82	0.41
2:N:181:ARG:HA	2:N:182:PRO:HD3	1.74	0.41
2:B:60:PRO:HG3	2:B:99:LEU:HD13	2.03	0.41
2:L:26:PHE:O	2:L:27:ILE:HB	2.20	0.41
2:F:109:LEU:HD13	2:F:269:ASN:HB3	2.02	0.41
1:M:254:PRO:HD2	1:M:278:LEU:HD23	2.02	0.41
2:J:136:GLU:OE2	2:J:138:THR:HB	2.20	0.41
2:P:175:TYR:O	2:P:179:ILE:HG12	2.21	0.41
1:K:189:LEU:HA	1:K:189:LEU:HD12	1.75	0.41
1:K:140:GLU:HB3	2:L:195:LEU:HD21	2.02	0.41
2:N:189:LYS:HB2	2:N:246:TYR:OH	2.21	0.41
2:J:40:VAL:HG22	2:J:299:LEU:HD13	2.02	0.41
1:O:45:ILE:HA	1:O:46:PRO:HD3	1.88	0.41
2:B:118:SER:OG	2:B:129:VAL:HG13	2.20	0.41
1:O:126:ILE:HD13	1:O:169:PHE:HE1	1.85	0.41
1:K:182:HIS:HE2	1:K:213:SER:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:ILE:HG23	1:G:46:PRO:HD2	2.03	0.41
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.92	0.41
2:P:195:LEU:C	2:P:195:LEU:HD23	2.41	0.41
2:F:287:ILE:HD12	2:F:287:ILE:HA	1.81	0.41
1:G:54:ILE:CD1	1:G:54:ILE:H	2.02	0.41
1:G:175:ARG:CG	1:G:175:ARG:NH1	2.59	0.41
2:H:287:ILE:HA	2:H:287:ILE:HD12	1.80	0.41
2:F:323:LEU:CD2	2:F:323:LEU:H	2.12	0.41
2:L:189:LYS:O	2:L:190:SER:C	2.59	0.41
1:C:140:GLU:OE2	2:D:194:ARG:HA	2.20	0.41
1:C:140:GLU:HB3	2:D:195:LEU:CD2	2.50	0.41
2:H:39:SER:HB2	2:H:347:THR:CG2	2.51	0.41
1:M:149:GLU:CG	2:N:159:LEU:CD1	2.98	0.41
1:I:319:ILE:HD12	1:I:319:ILE:O	2.21	0.41
1:I:155:THR:O	1:I:159:THR:HG22	2.21	0.41
1:O:194:PHE:O	1:O:198:ILE:HG12	2.21	0.41
2:N:7:SER:HA	2:N:10:ARG:HG2	2.03	0.41
1:M:43:GLU:OE2	1:M:346:LEU:HG	2.21	0.41
2:J:60:PRO:HG3	2:J:99:LEU:HD13	2.03	0.41
1:M:12:LYS:HB3	1:M:19:THR:HB	2.03	0.41
2:F:162:ARG:HB2	2:F:162:ARG:HH11	1.86	0.41
2:J:183:ARG:HD2	2:J:237:ASP:OD2	2.20	0.41
2:D:136:GLU:HA	2:D:168:VAL:HG11	2.03	0.41
1:G:45:ILE:HG12	1:G:307:TYR:CD2	2.56	0.41
1:I:80:LEU:HD21	1:I:271:PRO:HG2	2.02	0.41
1:C:156:ARG:N	1:C:157:PRO:CD	2.84	0.41
1:M:162:ILE:HA	1:M:162:ILE:HD12	1.73	0.41
2:H:250:LEU:HA	2:H:250:LEU:HD23	1.81	0.41
1:C:37:ARG:HH11	1:C:37:ARG:HD3	1.76	0.41
2:B:334:THR:HG22	2:B:335:GLY:H	1.84	0.41
1:O:221:MET:SD	2:P:262:LEU:HD22	2.61	0.41
2:B:322:VAL:CG2	2:B:323:LEU:H	2.34	0.41
1:E:279:ASP:HB2	1:E:280:ILE:H	1.67	0.41
2:F:317:GLN:O	2:F:322:VAL:HG13	2.21	0.41
2:H:228:VAL:HG22	2:H:235:TYR:CD1	2.56	0.41
2:H:182:PRO:HD2	2:H:237:ASP:O	2.21	0.41
2:B:59:SER:HA	2:B:60:PRO:HD3	1.80	0.41
1:M:133:GLU:HG2	1:M:153:VAL:O	2.21	0.41
2:N:172:ALA:HB2	2:N:241:VAL:CG1	2.50	0.41
2:D:133:LEU:HD23	2:D:251:SER:HB3	2.03	0.41
2:B:39:SER:HB2	2:B:347:THR:HG21	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:280:ILE:HG22	1:E:327:ARG:CZ	2.51	0.40
2:N:49:VAL:HA	2:N:50:PRO:HD3	1.70	0.40
2:F:39:SER:OG	2:F:347:THR:HG22	2.20	0.40
2:P:62:PHE:CZ	2:P:67:THR:HG22	2.56	0.40
2:H:69:ILE:CD1	2:H:70:PRO:HD2	2.50	0.40
1:E:346:LEU:HD12	1:E:346:LEU:HA	1.94	0.40
1:C:226:LYS:N	1:C:227:PRO:HD3	2.36	0.40
2:D:126:TYR:HB2	2:D:257:LEU:O	2.20	0.40
2:L:5:GLN:CA	2:L:5:GLN:HE21	2.33	0.40
1:I:344:ASN:O	1:I:348:THR:HG23	2.20	0.40
1:E:278:LEU:HA	1:E:278:LEU:HD22	1.74	0.40
2:H:199:LEU:C	2:H:199:LEU:HD23	2.42	0.40
1:A:181:VAL:HG11	1:A:243:LEU:HD11	2.04	0.40
2:B:39:SER:O	2:B:43:ILE:HG13	2.22	0.40
2:B:189:LYS:HB2	2:B:246:TYR:OH	2.21	0.40
1:A:304:LEU:O	1:A:305:ASN:CG	2.60	0.40
2:P:342:THR:HG22	2:P:345:SER:HB3	2.02	0.40
2:L:274:ILE:HG22	2:L:275:SER:N	2.36	0.40
2:B:5:GLN:CD	2:B:6:PRO:HD2	2.42	0.40
2:N:26:PHE:CD2	2:N:28:GLU:HG2	2.57	0.40
2:H:316:ASP:O	2:H:320:ASN:HB3	2.22	0.40
1:I:133:GLU:HG2	1:I:153:VAL:O	2.22	0.40
1:A:104:TYR:CE1	1:A:161:ARG:HD2	2.56	0.40
2:B:43:ILE:HD13	2:B:350:VAL:HG11	2.03	0.40
1:G:241:THR:HG21	2:H:189:LYS:NZ	2.36	0.40
2:L:287:ILE:HG13	2:L:292:LYS:HB2	2.02	0.40
2:J:159:LEU:CD2	1:K:143:SER:HB3	2.44	0.40
1:C:79:GLY:HA2	1:C:291:MET:HE3	2.04	0.40
2:D:228:VAL:HG22	2:D:235:TYR:CD1	2.57	0.40
1:A:202:GLY:HA3	1:A:211:VAL:HG21	2.03	0.40
2:D:181:ARG:HA	2:D:182:PRO:HD3	1.80	0.40
1:A:45:ILE:HG23	1:A:46:PRO:HD2	2.04	0.40
2:L:299:LEU:HA	2:L:299:LEU:HD12	1.84	0.40
2:F:59:SER:HA	2:F:60:PRO:HD3	1.77	0.40
2:J:172:ALA:HB2	2:J:241:VAL:CG1	2.51	0.40
1:G:293:LEU:HD23	1:G:293:LEU:HA	1.89	0.40
1:G:60:LYS:HB2	1:G:60:LYS:HE3	1.83	0.40
2:D:317:GLN:O	2:D:322:VAL:HG13	2.21	0.40
2:J:7:SER:HA	2:J:10:ARG:HG2	2.04	0.40
2:P:334:THR:HB	2:P:336:ASP:OD1	2.20	0.40
2:N:316:ASP:O	2:N:320:ASN:CB	2.70	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:104:TYR:CZ	1:M:161:ARG:HD2	2.57	0.40
2:F:15:PRO:HG3	2:F:22:TYR:CZ	2.57	0.40
2:P:172:ALA:HB2	2:P:241:VAL:CG1	2.52	0.40
1:C:304:LEU:O	1:C:305:ASN:CG	2.60	0.40
2:F:7:SER:HA	2:F:10:ARG:CG	2.50	0.40
2:N:270:ILE:CD1	2:N:270:ILE:N	2.83	0.40
2:F:224:SER:O	2:F:228:VAL:HG23	2.21	0.40
2:F:26:PHE:O	2:F:27:ILE:HB	2.22	0.40
1:E:344:ASN:O	1:E:348:THR:HG23	2.21	0.40
2:H:35:GLU:HG2	2:H:35:GLU:H	1.71	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	331/349 (95%)	311 (94%)	16 (5%)	4 (1%)	16 39
1	C	334/349 (96%)	315 (94%)	16 (5%)	3 (1%)	21 49
1	E	337/349 (97%)	320 (95%)	12 (4%)	5 (2%)	13 32
1	G	330/349 (95%)	309 (94%)	14 (4%)	7 (2%)	9 23
1	I	331/349 (95%)	310 (94%)	16 (5%)	5 (2%)	13 32
1	K	334/349 (96%)	315 (94%)	15 (4%)	4 (1%)	16 39
1	M	333/349 (95%)	315 (95%)	15 (4%)	3 (1%)	21 49
1	O	328/349 (94%)	309 (94%)	16 (5%)	3 (1%)	21 49
2	B	342/354 (97%)	310 (91%)	23 (7%)	9 (3%)	7 16
2	D	341/354 (96%)	307 (90%)	25 (7%)	9 (3%)	7 16
2	F	341/354 (96%)	307 (90%)	26 (8%)	8 (2%)	8 20
2	H	341/354 (96%)	304 (89%)	29 (8%)	8 (2%)	8 20

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	J	341/354 (96%)	309 (91%)	24 (7%)	8 (2%)	8 20
2	L	342/354 (97%)	306 (90%)	27 (8%)	9 (3%)	7 16
2	N	341/354 (96%)	301 (88%)	30 (9%)	10 (3%)	6 14
2	P	322/354 (91%)	289 (90%)	27 (8%)	6 (2%)	10 25
All	All	5369/5624 (96%)	4937 (92%)	331 (6%)	101 (2%)	10 25

All (101) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	304	LEU
1	C	58	ASP
1	C	304	LEU
1	E	276	VAL
1	E	304	LEU
2	F	54	GLU
1	G	14	TYR
1	G	15	GLY
1	G	304	LEU
1	I	278	LEU
1	I	304	LEU
1	K	304	LEU
1	M	304	LEU
2	N	54	GLU
1	O	304	LEU
2	P	54	GLU
2	P	321	ALA
1	A	14	TYR
1	A	322	GLY
2	B	13	GLY
2	B	54	GLU
2	B	167	ARG
2	B	321	ALA
2	B	322	VAL
2	D	13	GLY
2	D	54	GLU
2	D	167	ARG
2	D	321	ALA
2	D	322	VAL
1	E	279	ASP
1	E	322	GLY
2	F	13	GLY

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Mol	Chain	Res	Type
2	F	167	ARG
2	F	321	ALA
2	F	322	VAL
1	G	57	THR
2	H	13	GLY
2	H	54	GLU
2	H	167	ARG
2	H	321	ALA
2	H	322	VAL
1	I	322	GLY
2	J	13	GLY
2	J	54	GLU
2	J	167	ARG
2	J	321	ALA
2	J	322	VAL
1	K	58	ASP
2	L	13	GLY
2	L	54	GLU
2	L	167	ARG
2	L	321	ALA
2	L	322	VAL
1	M	322	GLY
2	N	13	GLY
2	N	98	SER
2	N	167	ARG
2	N	321	ALA
2	N	322	VAL
2	P	167	ARG
2	P	322	VAL
2	B	190	SER
2	H	190	SER
1	I	59	HIS
2	J	190	SER
1	K	57	THR
1	K	322	GLY
2	L	190	SER
2	N	190	SER
2	P	190	SER
1	C	322	GLY
2	D	190	SER
2	F	190	SER
1	G	55	LYS

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Mol	Chain	Res	Type
1	G	322	GLY
2	L	48	ASN
2	B	27	ILE
2	D	27	ILE
2	D	48	ASN
2	F	27	ILE
1	I	276	VAL
2	J	27	ILE
1	A	55	LYS
2	B	14	LYS
2	B	48	ASN
2	D	14	LYS
1	G	276	VAL
2	H	14	LYS
2	H	27	ILE
2	L	27	ILE
1	M	280	ILE
2	N	27	ILE
2	N	48	ASN
1	O	322	GLY
2	P	27	ILE
2	J	14	LYS
2	L	14	LYS
2	N	14	LYS
2	F	14	LYS
1	E	280	ILE
1	O	276	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	279/289 (96%)	252 (90%)	27 (10%)	10 23
1	C	283/289 (98%)	254 (90%)	29 (10%)	9 21
1	E	285/289 (99%)	250 (88%)	35 (12%)	6 14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	G	278/289 (96%)	248 (89%)	30 (11%)	8 18
1	I	279/289 (96%)	251 (90%)	28 (10%)	9 22
1	K	283/289 (98%)	252 (89%)	31 (11%)	8 18
1	M	281/289 (97%)	254 (90%)	27 (10%)	10 24
1	O	276/289 (96%)	249 (90%)	27 (10%)	10 23
2	B	292/297 (98%)	264 (90%)	28 (10%)	10 24
2	D	291/297 (98%)	263 (90%)	28 (10%)	10 24
2	F	291/297 (98%)	262 (90%)	29 (10%)	9 22
2	H	291/297 (98%)	263 (90%)	28 (10%)	10 24
2	J	291/297 (98%)	263 (90%)	28 (10%)	10 24
2	L	292/297 (98%)	263 (90%)	29 (10%)	10 22
2	N	291/297 (98%)	265 (91%)	26 (9%)	12 27
2	P	275/297 (93%)	248 (90%)	27 (10%)	10 23
All	All	4558/4688 (97%)	4101 (90%)	457 (10%)	9 22

All (457) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	THR
1	A	51	THR
1	A	55	LYS
1	A	77	LEU
1	A	80	LEU
1	A	93	LEU
1	A	95	VAL
1	A	97	LEU
1	A	98	ARG
1	A	114	LYS
1	A	159	THR
1	A	161	ARG
1	A	175	ARG
1	A	238	MET
1	A	241	THR
1	A	250	LEU
1	A	273	SER
1	A	276	VAL
1	A	281	LYS

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Mol	Chain	Res	Type
1	A	315	VAL
1	A	319	ILE
1	A	325	THR
1	A	328	ASP
1	A	335	THR
1	A	341	GLU
1	A	346	LEU
1	A	348	THR
2	B	23	THR
2	B	30	ASP
2	B	66	LEU
2	B	88	LEU
2	B	102	THR
2	B	106	THR
2	B	125	THR
2	B	129	VAL
2	B	135	ARG
2	B	150	CYS
2	B	168	VAL
2	B	184	VAL
2	B	189	LYS
2	B	194	ARG
2	B	195	LEU
2	B	214	LEU
2	B	222	ASP
2	B	225	VAL
2	B	226	LEU
2	B	241	VAL
2	B	283	SER
2	B	286	ASP
2	B	299	LEU
2	B	306	LEU
2	B	323	LEU
2	B	326	ILE
2	B	334	THR
2	B	353	ARG
1	C	33	THR
1	C	51	THR
1	C	56	GLN
1	C	58	ASP
1	C	77	LEU
1	C	80	LEU

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Mol	Chain	Res	Type
1	C	93	LEU
1	C	95	VAL
1	C	97	LEU
1	C	98	ARG
1	C	114	LYS
1	C	129	ARG
1	C	159	THR
1	C	161	ARG
1	C	175	ARG
1	C	212	SER
1	C	238	MET
1	C	241	THR
1	C	250	LEU
1	C	273	SER
1	C	305	ASN
1	C	315	VAL
1	C	319	ILE
1	C	325	THR
1	C	328	ASP
1	C	335	THR
1	C	341	GLU
1	C	346	LEU
1	C	348	THR
2	D	5	GLN
2	D	23	THR
2	D	30	ASP
2	D	66	LEU
2	D	88	LEU
2	D	97	ARG
2	D	101	LEU
2	D	102	THR
2	D	125	THR
2	D	129	VAL
2	D	135	ARG
2	D	150	CYS
2	D	168	VAL
2	D	184	VAL
2	D	189	LYS
2	D	194	ARG
2	D	195	LEU
2	D	214	LEU
2	D	222	ASP

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Mol	Chain	Res	Type
2	D	226	LEU
2	D	241	VAL
2	D	283	SER
2	D	286	ASP
2	D	299	LEU
2	D	306	LEU
2	D	323	LEU
2	D	326	ILE
2	D	353	ARG
1	E	8	ARG
1	E	9	THR
1	E	12	LYS
1	E	33	THR
1	E	51	THR
1	E	54	ILE
1	E	59	HIS
1	E	77	LEU
1	E	80	LEU
1	E	93	LEU
1	E	95	VAL
1	E	97	LEU
1	E	98	ARG
1	E	114	LYS
1	E	159	THR
1	E	175	ARG
1	E	238	MET
1	E	241	THR
1	E	250	LEU
1	E	273	SER
1	E	276	VAL
1	E	278	LEU
1	E	279	ASP
1	E	280	ILE
1	E	305	ASN
1	E	315	VAL
1	E	319	ILE
1	E	325	THR
1	E	328	ASP
1	E	333	SER
1	E	335	THR
1	E	341	GLU
1	E	346	LEU

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Mol	Chain	Res	Type
1	E	348	THR
1	E	349	MET
2	F	23	THR
2	F	30	ASP
2	F	66	LEU
2	F	88	LEU
2	F	101	LEU
2	F	102	THR
2	F	125	THR
2	F	129	VAL
2	F	135	ARG
2	F	147	HIS
2	F	150	CYS
2	F	168	VAL
2	F	184	VAL
2	F	189	LYS
2	F	194	ARG
2	F	195	LEU
2	F	214	LEU
2	F	222	ASP
2	F	225	VAL
2	F	226	LEU
2	F	241	VAL
2	F	283	SER
2	F	286	ASP
2	F	299	LEU
2	F	306	LEU
2	F	323	LEU
2	F	326	ILE
2	F	334	THR
2	F	353	ARG
1	G	13	LYS
1	G	33	THR
1	G	51	THR
1	G	53	ASN
1	G	54	ILE
1	G	55	LYS
1	G	77	LEU
1	G	80	LEU
1	G	93	LEU
1	G	95	VAL
1	G	97	LEU

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Mol	Chain	Res	Type
1	G	98	ARG
1	G	114	LYS
1	G	159	THR
1	G	161	ARG
1	G	175	ARG
1	G	212	SER
1	G	238	MET
1	G	241	THR
1	G	250	LEU
1	G	273	SER
1	G	305	ASN
1	G	315	VAL
1	G	319	ILE
1	G	325	THR
1	G	328	ASP
1	G	335	THR
1	G	341	GLU
1	G	346	LEU
1	G	348	THR
2	H	23	THR
2	H	30	ASP
2	H	66	LEU
2	H	88	LEU
2	H	101	LEU
2	H	102	THR
2	H	125	THR
2	H	129	VAL
2	H	135	ARG
2	H	150	CYS
2	H	168	VAL
2	H	184	VAL
2	H	189	LYS
2	H	194	ARG
2	H	195	LEU
2	H	214	LEU
2	H	222	ASP
2	H	225	VAL
2	H	226	LEU
2	H	241	VAL
2	H	252	ASP
2	H	283	SER
2	H	286	ASP

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Mol	Chain	Res	Type
2	H	299	LEU
2	H	306	LEU
2	H	323	LEU
2	H	326	ILE
2	H	353	ARG
1	I	17	ARG
1	I	33	THR
1	I	51	THR
1	I	77	LEU
1	I	80	LEU
1	I	93	LEU
1	I	95	VAL
1	I	97	LEU
1	I	114	LYS
1	I	159	THR
1	I	161	ARG
1	I	175	ARG
1	I	238	MET
1	I	241	THR
1	I	250	LEU
1	I	273	SER
1	I	276	VAL
1	I	281	LYS
1	I	305	ASN
1	I	315	VAL
1	I	319	ILE
1	I	325	THR
1	I	328	ASP
1	I	335	THR
1	I	336	THR
1	I	341	GLU
1	I	346	LEU
1	I	348	THR
2	J	23	THR
2	J	30	ASP
2	J	66	LEU
2	J	88	LEU
2	J	101	LEU
2	J	102	THR
2	J	125	THR
2	J	129	VAL
2	J	135	ARG

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Mol	Chain	Res	Type
2	J	150	CYS
2	J	168	VAL
2	J	184	VAL
2	J	189	LYS
2	J	194	ARG
2	J	195	LEU
2	J	214	LEU
2	J	222	ASP
2	J	225	VAL
2	J	226	LEU
2	J	241	VAL
2	J	283	SER
2	J	286	ASP
2	J	299	LEU
2	J	306	LEU
2	J	323	LEU
2	J	326	ILE
2	J	334	THR
2	J	353	ARG
1	K	8	ARG
1	K	33	THR
1	K	46	PRO
1	K	51	THR
1	K	56	GLN
1	K	58	ASP
1	K	77	LEU
1	K	80	LEU
1	K	93	LEU
1	K	95	VAL
1	K	97	LEU
1	K	114	LYS
1	K	156	ARG
1	K	159	THR
1	K	161	ARG
1	K	175	ARG
1	K	212	SER
1	K	238	MET
1	K	241	THR
1	K	250	LEU
1	K	273	SER
1	K	276	VAL
1	K	305	ASN

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Mol	Chain	Res	Type
1	K	319	ILE
1	K	325	THR
1	K	328	ASP
1	K	333	SER
1	K	335	THR
1	K	341	GLU
1	K	346	LEU
1	K	348	THR
2	L	5	GLN
2	L	30	ASP
2	L	66	LEU
2	L	88	LEU
2	L	96	HIS
2	L	102	THR
2	L	125	THR
2	L	129	VAL
2	L	135	ARG
2	L	147	HIS
2	L	150	CYS
2	L	168	VAL
2	L	184	VAL
2	L	189	LYS
2	L	194	ARG
2	L	195	LEU
2	L	214	LEU
2	L	222	ASP
2	L	226	LEU
2	L	241	VAL
2	L	252	ASP
2	L	283	SER
2	L	286	ASP
2	L	299	LEU
2	L	306	LEU
2	L	323	LEU
2	L	326	ILE
2	L	334	THR
2	L	353	ARG
1	M	33	THR
1	M	51	THR
1	M	54	ILE
1	M	77	LEU
1	M	80	LEU

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Mol	Chain	Res	Type
1	M	93	LEU
1	M	95	VAL
1	M	97	LEU
1	M	98	ARG
1	M	114	LYS
1	M	129	ARG
1	M	159	THR
1	M	175	ARG
1	M	238	MET
1	M	241	THR
1	M	250	LEU
1	M	276	VAL
1	M	279	ASP
1	M	315	VAL
1	M	319	ILE
1	M	325	THR
1	M	328	ASP
1	M	335	THR
1	M	341	GLU
1	M	346	LEU
1	M	348	THR
1	M	349	MET
2	N	30	ASP
2	N	66	LEU
2	N	88	LEU
2	N	97	ARG
2	N	102	THR
2	N	125	THR
2	N	129	VAL
2	N	135	ARG
2	N	150	CYS
2	N	168	VAL
2	N	184	VAL
2	N	189	LYS
2	N	194	ARG
2	N	195	LEU
2	N	214	LEU
2	N	222	ASP
2	N	225	VAL
2	N	226	LEU
2	N	241	VAL
2	N	286	ASP

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Mol	Chain	Res	Type
2	N	299	LEU
2	N	306	LEU
2	N	323	LEU
2	N	326	ILE
2	N	334	THR
2	N	353	ARG
1	O	33	THR
1	O	51	THR
1	O	55	LYS
1	O	77	LEU
1	O	93	LEU
1	O	95	VAL
1	O	97	LEU
1	O	98	ARG
1	O	114	LYS
1	O	129	ARG
1	O	159	THR
1	O	161	ARG
1	O	175	ARG
1	O	212	SER
1	O	238	MET
1	O	241	THR
1	O	250	LEU
1	O	273	SER
1	O	305	ASN
1	O	315	VAL
1	O	319	ILE
1	O	325	THR
1	O	328	ASP
1	O	335	THR
1	O	341	GLU
1	O	346	LEU
1	O	348	THR
2	P	30	ASP
2	P	66	LEU
2	P	88	LEU
2	P	97	ARG
2	P	102	THR
2	P	125	THR
2	P	129	VAL
2	P	135	ARG
2	P	150	CYS

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Mol	Chain	Res	Type
2	P	168	VAL
2	P	184	VAL
2	P	189	LYS
2	P	194	ARG
2	P	195	LEU
2	P	214	LEU
2	P	222	ASP
2	P	225	VAL
2	P	226	LEU
2	P	241	VAL
2	P	266	PRO
2	P	286	ASP
2	P	299	LEU
2	P	306	LEU
2	P	323	LEU
2	P	326	ILE
2	P	334	THR
2	P	353	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	HIS
2	D	5	GLN
2	F	155	GLN
1	G	56	GLN
1	G	283	GLN
1	G	301	HIS
2	H	155	GLN
1	I	90	HIS
1	I	301	HIS
2	J	155	GLN
2	J	193	GLN
2	L	5	GLN
2	L	155	GLN
2	N	155	GLN
1	O	283	GLN
1	O	301	HIS
2	P	155	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	335/349 (95%)	0.01	15 (4%) 37 36	13, 38, 80, 100	0
1	C	338/349 (96%)	-0.04	3 (0%) 85 86	11, 38, 75, 93	0
1	E	341/349 (97%)	-0.11	4 (1%) 81 81	18, 42, 78, 117	0
1	G	334/349 (95%)	-0.03	3 (0%) 85 86	16, 41, 79, 96	0
1	I	333/349 (95%)	0.11	15 (4%) 37 36	17, 40, 78, 113	0
1	K	338/349 (96%)	-0.12	3 (0%) 85 86	13, 41, 78, 98	0
1	M	337/349 (96%)	0.96	67 (19%) 1 1	21, 48, 91, 121	0
1	O	332/349 (95%)	-0.15	4 (1%) 81 81	17, 43, 79, 97	0
2	B	346/354 (97%)	0.31	14 (4%) 42 41	21, 60, 102, 119	0
2	D	345/354 (97%)	0.26	19 (5%) 29 27	21, 66, 105, 123	0
2	F	345/354 (97%)	0.56	43 (12%) 5 4	24, 69, 107, 121	0
2	H	345/354 (97%)	0.51	36 (10%) 8 6	24, 69, 108, 127	0
2	J	345/354 (97%)	0.50	24 (6%) 19 17	24, 67, 105, 120	0
2	L	346/354 (97%)	0.46	36 (10%) 8 6	24, 69, 106, 121	0
2	N	345/354 (97%)	1.08	70 (20%) 1 1	28, 77, 111, 122	0
2	P	326/354 (92%)	0.77	57 (17%) 2 1	30, 74, 109, 119	0
All	All	5431/5624 (96%)	0.32	413 (7%) 17 15	11, 53, 103, 127	0

All (413) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	341	ALA	9.5
2	N	192	ILE	7.7
1	M	282	GLY	7.6
2	P	65	GLY	7.0
1	M	62	GLY	6.9

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Mol	Chain	Res	Type	RSRZ
1	M	275	HIS	6.7
2	F	193	GLN	6.5
2	N	126	TYR	6.4
1	M	278	LEU	6.3
1	M	61	GLU	6.2
2	H	350	VAL	6.1
2	P	64	ASN	6.0
1	M	277	GLY	5.8
2	J	66	LEU	5.8
2	H	340	THR	5.6
2	N	289	GLY	5.5
2	P	32	ILE	5.5
1	M	330	GLY	5.5
2	N	18	SER	5.4
2	N	333	ARG	5.4
2	N	20	GLY	5.3
2	H	91	PRO	5.3
2	L	44	PHE	5.3
1	M	93	LEU	5.3
2	L	193	GLN	5.2
2	N	193	GLN	5.1
1	M	338	PHE	5.0
2	L	346	PHE	5.0
2	F	289	GLY	5.0
2	F	338	ALA	4.9
2	H	64	ASN	4.9
2	P	31	GLY	4.8
2	N	331	GLU	4.7
1	M	324	HIS	4.7
1	M	63	VAL	4.7
2	J	14	LYS	4.7
1	M	25	GLY	4.7
1	M	280	ILE	4.7
2	N	43	ILE	4.6
2	H	348	GLU	4.6
2	P	354	LEU	4.6
2	H	18	SER	4.6
2	P	97	ARG	4.5
2	J	65	GLY	4.5
2	N	330	PRO	4.5
1	M	81	TRP	4.5
1	M	40	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
2	D	13	GLY	4.5
1	M	342	ILE	4.4
2	J	90	THR	4.4
2	N	293	ALA	4.4
2	P	353	ARG	4.4
2	P	51	ILE	4.4
2	P	44	PHE	4.4
1	M	65	GLU	4.4
2	H	47	ALA	4.4
2	P	121	GLY	4.4
2	P	66	LEU	4.3
2	L	66	LEU	4.3
2	N	62	PHE	4.3
2	H	338	ALA	4.2
2	H	66	LEU	4.1
2	D	58	VAL	4.1
2	D	14	LYS	4.1
1	M	23	ILE	4.1
1	M	113	LEU	4.1
2	N	348	GLU	4.0
2	L	17	PRO	4.0
2	N	332	ASN	4.0
2	F	310	GLY	4.0
2	L	58	VAL	4.0
2	N	44	PHE	4.0
2	D	97	ARG	4.0
2	J	67	THR	3.9
2	N	63	VAL	3.9
2	P	73	ALA	3.9
2	N	292	LYS	3.9
2	D	66	LEU	3.9
2	P	346	PHE	3.9
2	F	331	GLU	3.9
2	B	90	THR	3.9
2	P	23	THR	3.9
2	F	28	GLU	3.9
2	P	192	ILE	3.9
2	L	96	HIS	3.9
2	N	8	ILE	3.9
2	F	8	ILE	3.8
2	H	354	LEU	3.8
2	P	340	THR	3.8

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Mol	Chain	Res	Type	RSRZ
2	F	320	ASN	3.8
2	H	339	GLY	3.8
2	N	122	PHE	3.8
2	N	32	ILE	3.8
2	B	14	LYS	3.8
2	N	58	VAL	3.7
1	M	337	ASP	3.7
2	L	59	SER	3.7
2	F	62	PHE	3.7
2	P	348	GLU	3.7
1	M	335	THR	3.7
2	H	17	PRO	3.7
2	P	107	PHE	3.7
1	M	285	VAL	3.7
2	L	14	LYS	3.6
2	P	352	LYS	3.6
2	N	125	THR	3.6
2	P	62	PHE	3.6
2	D	17	PRO	3.6
2	L	36	ILE	3.6
2	L	63	VAL	3.6
1	M	24	PRO	3.5
2	H	99	LEU	3.5
2	P	122	PHE	3.5
1	M	274	ARG	3.5
1	M	310	ARG	3.5
2	F	192	ILE	3.5
2	P	293	ALA	3.5
1	M	120	ILE	3.5
2	P	63	VAL	3.5
2	F	38	LYS	3.5
1	I	106	ASN	3.4
2	B	66	LEU	3.4
2	N	124	THR	3.4
2	N	191	THR	3.4
2	P	67	THR	3.4
2	D	193	GLN	3.4
2	L	16	ASN	3.4
2	F	341	ALA	3.4
2	L	69	ILE	3.4
2	B	352	LYS	3.4
2	N	123	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	M	32	ILE	3.4
2	L	13	GLY	3.4
1	M	39	ILE	3.3
1	M	121	PRO	3.3
2	J	69	ILE	3.3
2	F	58	VAL	3.3
1	M	346	LEU	3.3
2	F	346	PHE	3.3
2	H	14	LYS	3.3
2	P	292	LYS	3.3
2	P	351	ILE	3.3
2	L	20	GLY	3.3
1	O	323	LYS	3.3
2	P	338	ALA	3.3
2	N	91	PRO	3.3
1	M	204	LYS	3.2
1	M	87	GLN	3.2
2	F	32	ILE	3.2
2	F	337	LEU	3.2
2	N	28	GLU	3.2
2	F	91	PRO	3.2
2	F	287	ILE	3.2
1	G	13	LYS	3.2
2	H	268	ALA	3.2
2	D	69	ILE	3.1
2	D	63	VAL	3.1
2	B	65	GLY	3.1
2	F	61	ILE	3.1
2	H	60	PRO	3.1
2	N	205	LYS	3.1
2	P	313	ASN	3.1
2	N	290	GLN	3.1
2	L	18	SER	3.1
2	P	81	LEU	3.1
2	F	12	THR	3.1
2	N	334	THR	3.1
1	A	57	THR	3.1
2	N	284	ALA	3.0
1	M	45	ILE	3.0
1	M	349	MET	3.0
2	N	337	LEU	3.0
2	F	35	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
2	N	97	ARG	3.0
2	L	352	LYS	3.0
2	P	58	VAL	3.0
2	P	350	VAL	3.0
2	F	65	GLY	3.0
2	F	122	PHE	3.0
2	F	123	LYS	3.0
2	F	18	SER	3.0
1	M	116	VAL	3.0
2	F	288	ALA	3.0
2	N	285	PRO	3.0
1	M	319	ILE	3.0
2	L	65	GLY	3.0
2	H	63	VAL	2.9
2	N	68	THR	2.9
1	M	316	HIS	2.9
2	L	64	ASN	2.9
2	N	288	ALA	2.9
2	P	69	ILE	2.9
1	C	275	HIS	2.9
2	H	193	GLN	2.9
2	P	60	PRO	2.9
1	M	343	ILE	2.9
1	M	315	VAL	2.9
2	H	40	VAL	2.9
2	H	65	GLY	2.9
1	M	288	PRO	2.8
1	M	279	ASP	2.8
2	J	97	ARG	2.8
2	N	207	LEU	2.8
2	P	40	VAL	2.8
2	P	99	LEU	2.8
1	M	79	GLY	2.8
1	K	241	THR	2.8
2	F	44	PHE	2.8
2	F	20	GLY	2.8
1	M	283	GLN	2.8
2	F	48	ASN	2.8
2	L	61	ILE	2.8
2	P	72	PRO	2.8
2	D	18	SER	2.8
2	P	36	ILE	2.8

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Mol	Chain	Res	Type	RSRZ
2	J	267	SER	2.8
2	N	61	ILE	2.8
2	F	17	PRO	2.8
2	H	90	THR	2.8
1	E	274	ARG	2.7
2	J	52	GLU	2.7
2	J	323	LEU	2.7
1	O	117	LYS	2.7
2	P	43	ILE	2.7
2	F	63	VAL	2.7
2	L	121	GLY	2.7
1	A	14	TYR	2.7
2	P	61	ILE	2.7
1	I	260	ALA	2.7
2	P	331	GLU	2.7
1	C	56	GLN	2.7
1	I	107	VAL	2.7
1	I	129	ARG	2.7
1	M	339	THR	2.7
1	I	261	ASN	2.7
2	J	60	PRO	2.7
1	M	22	LEU	2.7
2	N	55	SER	2.7
2	N	338	ALA	2.7
1	M	175	ARG	2.6
2	P	57	ASP	2.6
2	N	129	VAL	2.6
1	M	290	ALA	2.6
2	J	91	PRO	2.6
2	P	339	GLY	2.6
1	O	56	GLN	2.6
2	F	207	LEU	2.6
2	F	10	ARG	2.6
2	J	279	ALA	2.6
1	M	326	THR	2.6
2	N	340	THR	2.6
2	H	69	ILE	2.6
1	C	57	THR	2.6
1	I	176	LYS	2.6
1	M	52	ILE	2.6
1	M	209	ILE	2.6
2	N	182	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	279	ALA	2.6
2	H	42	LYS	2.6
2	L	123	LYS	2.6
2	P	120	GLU	2.6
1	M	64	TYR	2.6
1	G	323	LYS	2.6
2	L	62	PHE	2.6
2	N	272	HIS	2.5
2	B	193	GLN	2.5
1	E	277	GLY	2.5
2	B	268	ALA	2.5
2	B	97	ARG	2.5
2	L	215	THR	2.5
2	P	314	HIS	2.5
1	M	230	PHE	2.5
2	L	289	GLY	2.5
1	A	260	ALA	2.5
2	H	320	ASN	2.5
2	B	62	PHE	2.5
2	D	21	LYS	2.5
2	J	320	ASN	2.5
2	P	333	ARG	2.5
2	H	113	VAL	2.5
2	H	333	ARG	2.5
1	E	56	GLN	2.5
2	L	120	GLU	2.5
1	M	86	ASP	2.5
2	J	268	ALA	2.5
2	J	297	ALA	2.5
1	M	44	ASN	2.5
2	N	128	ASN	2.5
2	N	69	ILE	2.4
2	H	97	ARG	2.4
2	H	289	GLY	2.4
1	M	122	ASP	2.4
1	A	106	ASN	2.4
2	F	332	ASN	2.4
2	F	49	VAL	2.4
2	N	273	LYS	2.4
2	N	211	TYR	2.4
2	N	320	ASN	2.4
2	H	62	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	L	97	ARG	2.4
2	N	10	ARG	2.4
2	L	326	ILE	2.4
2	F	68	THR	2.4
2	N	37	SER	2.4
2	H	112	ASN	2.4
1	A	274	ARG	2.4
2	P	54	GLU	2.4
1	A	268	VAL	2.4
1	M	42	ALA	2.4
2	P	268	ALA	2.4
2	B	348	GLU	2.4
1	M	80	LEU	2.4
2	D	44	PHE	2.4
1	M	323	LYS	2.4
1	M	36	VAL	2.4
2	D	42	LYS	2.4
1	M	334	SER	2.4
1	M	241	THR	2.4
2	N	38	LYS	2.3
2	N	53	TRP	2.3
1	I	241	THR	2.3
1	M	331	GLY	2.3
1	A	342	ILE	2.3
1	I	270	GLU	2.3
2	H	346	PHE	2.3
2	H	267	SER	2.3
1	I	240	GLY	2.3
1	M	84	PRO	2.3
2	J	84	LEU	2.3
2	D	67	THR	2.3
1	A	349	MET	2.3
2	D	16	ASN	2.3
2	N	246	TYR	2.3
2	J	86	GLY	2.3
2	N	29	GLY	2.3
2	F	66	LEU	2.3
1	E	280	ILE	2.3
1	I	273	SER	2.3
1	I	127	VAL	2.3
1	M	276	VAL	2.3
2	D	60	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
2	N	350	VAL	2.2
1	I	280	ILE	2.2
2	N	325	THR	2.2
1	G	106	ASN	2.2
1	A	272	GLY	2.2
1	I	294	SER	2.2
2	F	97	ARG	2.2
2	L	267	SER	2.2
1	A	261	ASN	2.2
2	H	52	GLU	2.2
1	I	272	GLY	2.2
2	F	51	ILE	2.2
2	P	88	LEU	2.2
2	N	26	PHE	2.2
2	N	50	PRO	2.2
2	L	28	GLU	2.2
1	A	108	ALA	2.2
2	N	317	GLN	2.2
2	N	346	PHE	2.2
2	F	352	LYS	2.2
2	P	193	GLN	2.1
2	B	60	PRO	2.1
2	N	17	PRO	2.1
2	N	235	TYR	2.1
2	H	19	THR	2.1
2	J	354	LEU	2.1
2	L	23	THR	2.1
2	B	267	SER	2.1
1	M	317	GLU	2.1
2	J	352	LYS	2.1
2	L	68	THR	2.1
2	F	43	ILE	2.1
2	F	56	CYS	2.1
2	L	60	PRO	2.1
2	J	36	ILE	2.1
1	I	275	HIS	2.1
2	L	268	ALA	2.1
2	P	89	ALA	2.1
1	A	259	GLY	2.1
2	N	213	ASP	2.1
2	N	131	LEU	2.1
2	P	52	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	P	251	SER	2.1
2	D	64	ASN	2.1
2	N	49	VAL	2.1
1	K	87	GLN	2.1
2	J	318	ILE	2.1
1	A	275	HIS	2.1
2	N	57	ASP	2.1
1	M	307	TYR	2.1
2	L	301	SER	2.1
1	M	28	VAL	2.1
1	O	107	VAL	2.1
2	N	64	ASN	2.1
2	P	332	ASN	2.1
2	P	27	ILE	2.1
2	N	343	THR	2.0
2	F	26	PHE	2.0
1	K	240	GLY	2.0
2	P	68	THR	2.0
2	H	10	ARG	2.0
2	P	110	PHE	2.0
1	A	273	SER	2.0
2	H	22	TYR	2.0
2	J	301	SER	2.0
2	D	19	THR	2.0
2	J	71	ASP	2.0
2	P	55	SER	2.0
2	B	297	ALA	2.0
2	D	269	ASN	2.0
2	L	216	LEU	2.0
1	A	270	GLU	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.