



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 04:19 AM EDT

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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : 1.13
EDS : 2.35
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.35

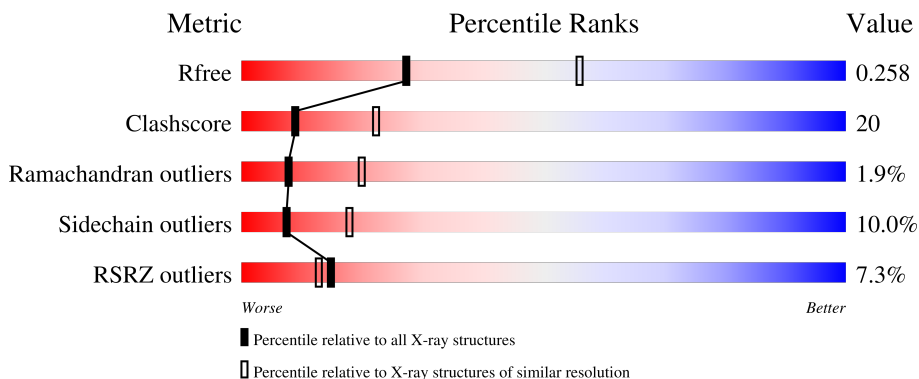
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	349	
1	C	349	
1	E	349	
1	G	349	
1	I	349	

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Mol	Chain	Length	Quality of chain
1	K	349	 66% 26% 5% .
1	M	349	 19% 62% 30% 5% .
1	O	349	 67% 25% . 5%
2	B	354	 4% 62% 30% 6% .
2	D	354	 5% 55% 36% 6% .
2	F	354	 11% 56% 36% 6% .
2	H	354	 10% 55% 36% 6% .
2	J	354	 6% 58% 34% 6% .
2	L	354	 10% 57% 34% 6% .
2	N	354	 19% 55% 35% 8% .
2	P	354	 15% 55% 31% 6% 8%

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

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

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

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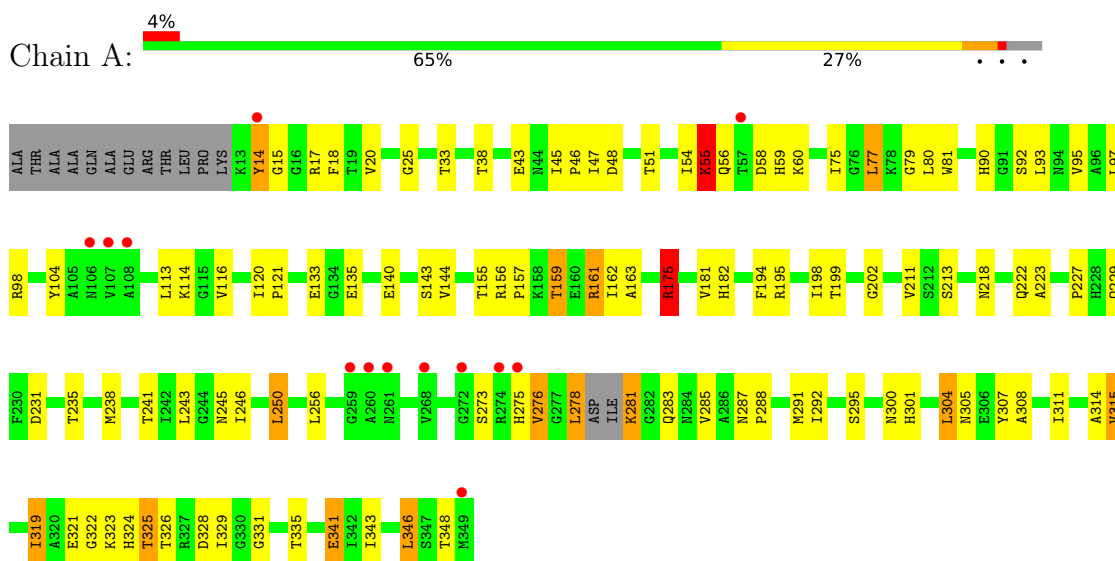
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	N	345	Total	C	N	O	S	0	0	0
			2598	1640	444	508	6			
2	P	326	Total	C	N	O	S	0	0	0
			2454	1549	418	481	6			

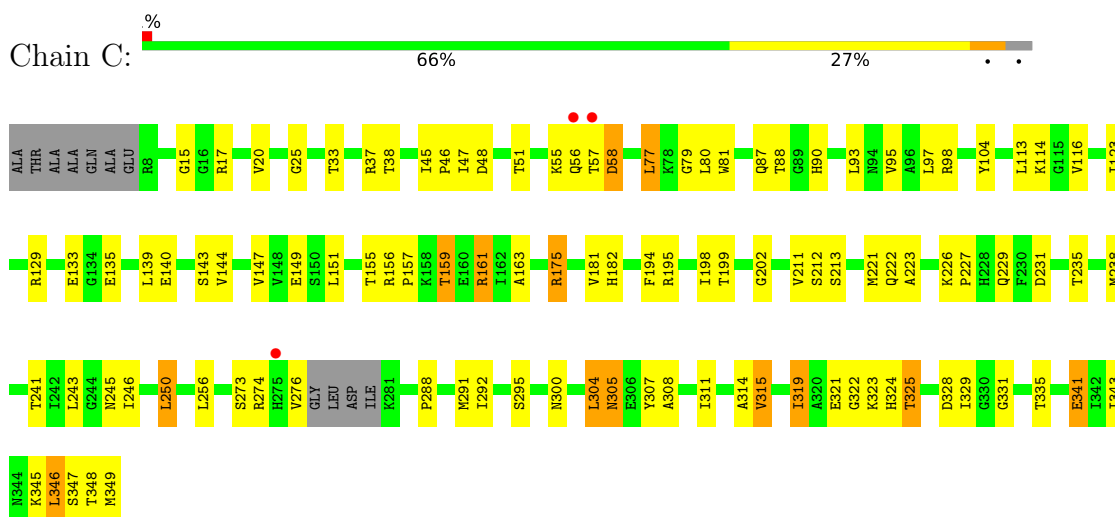
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

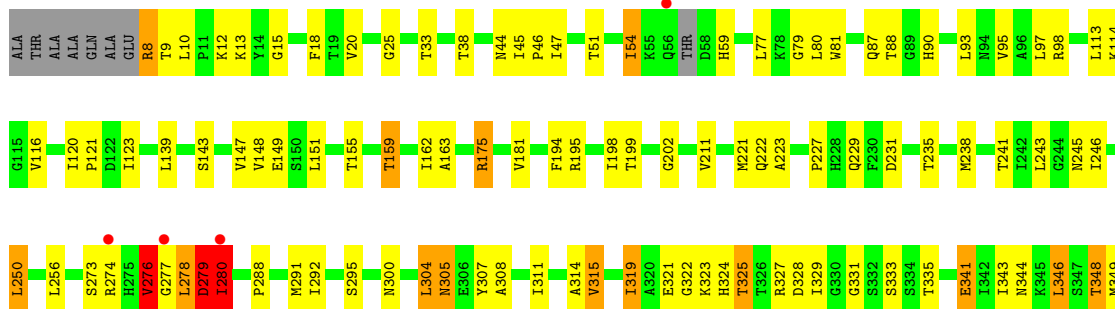


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

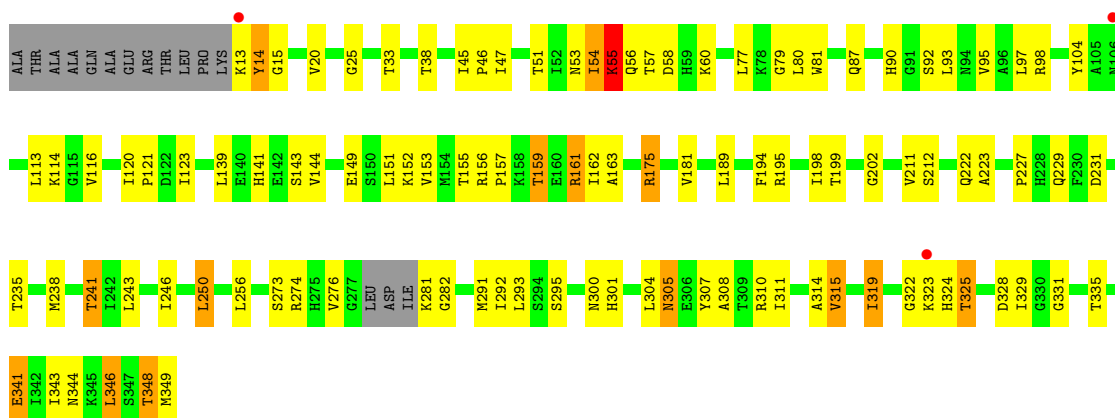


- Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

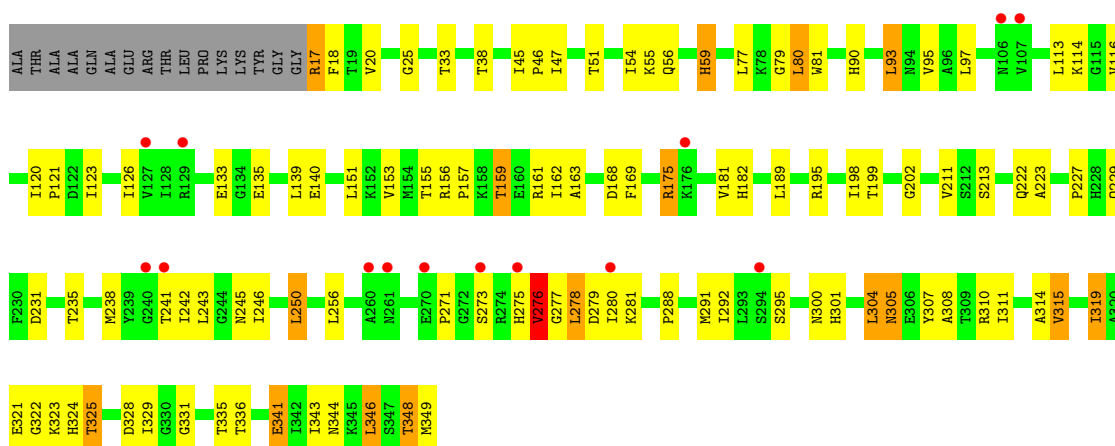




• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

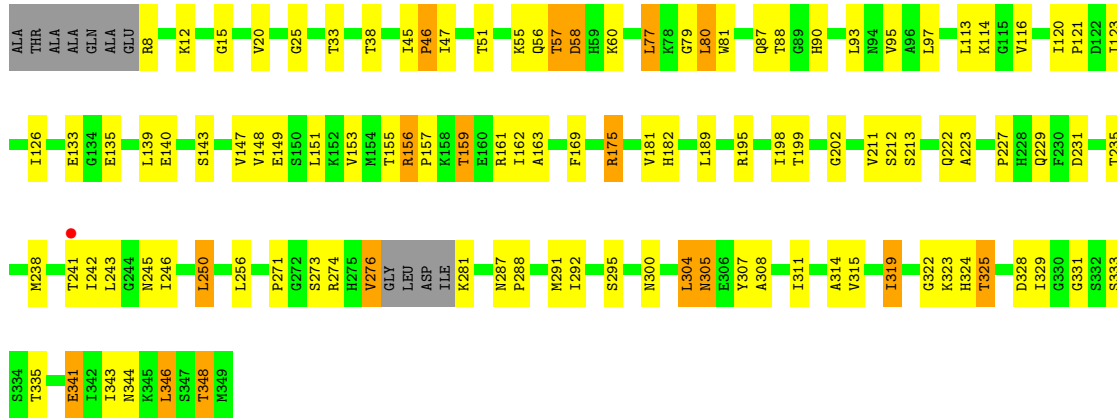


• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

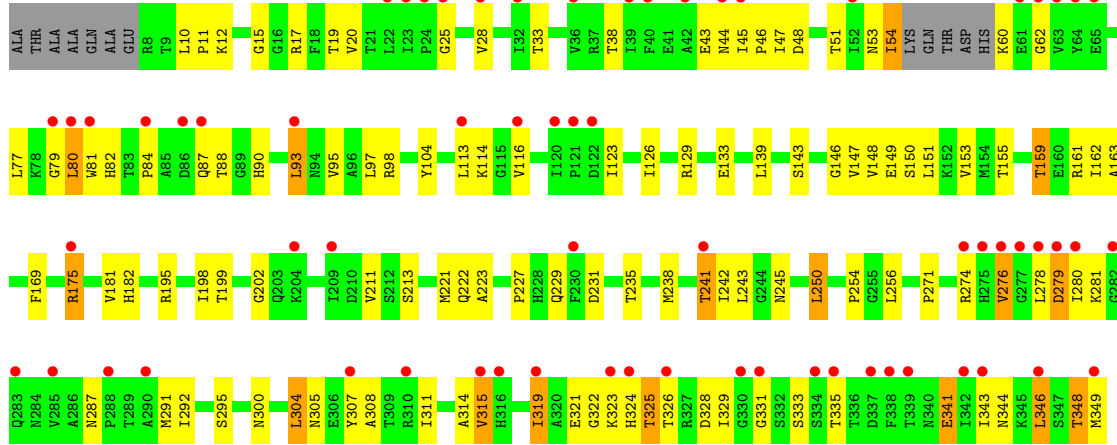


• Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1

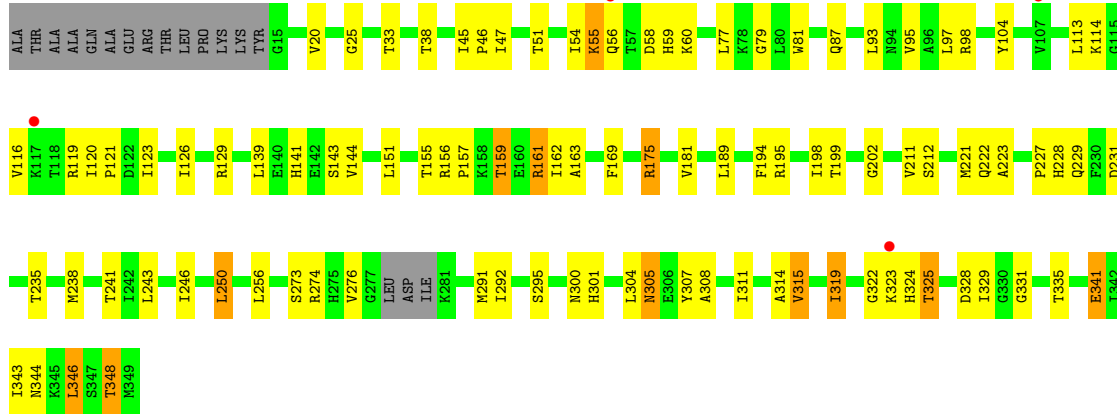




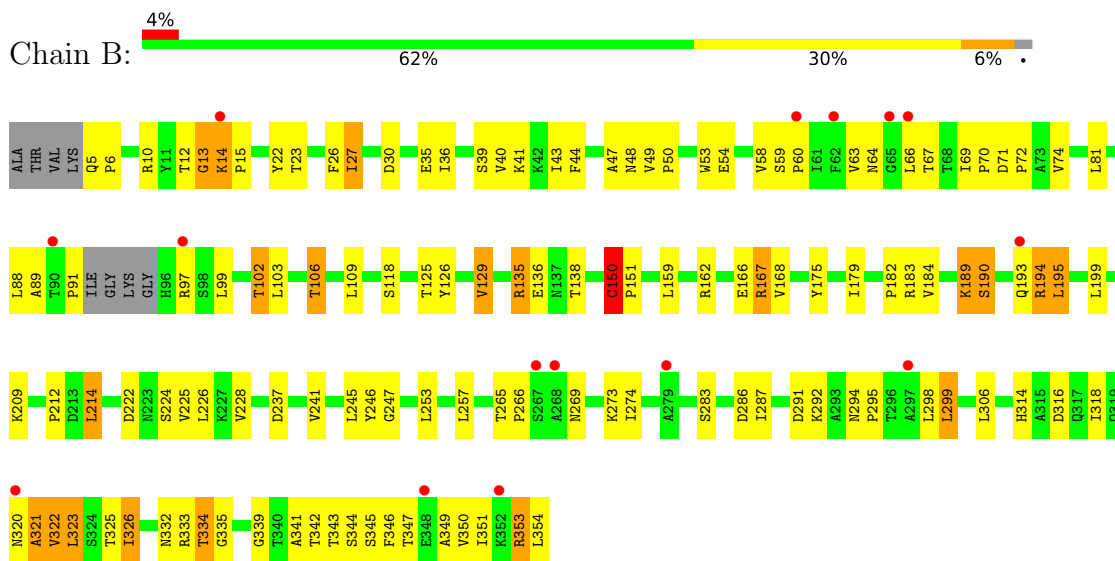
● Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



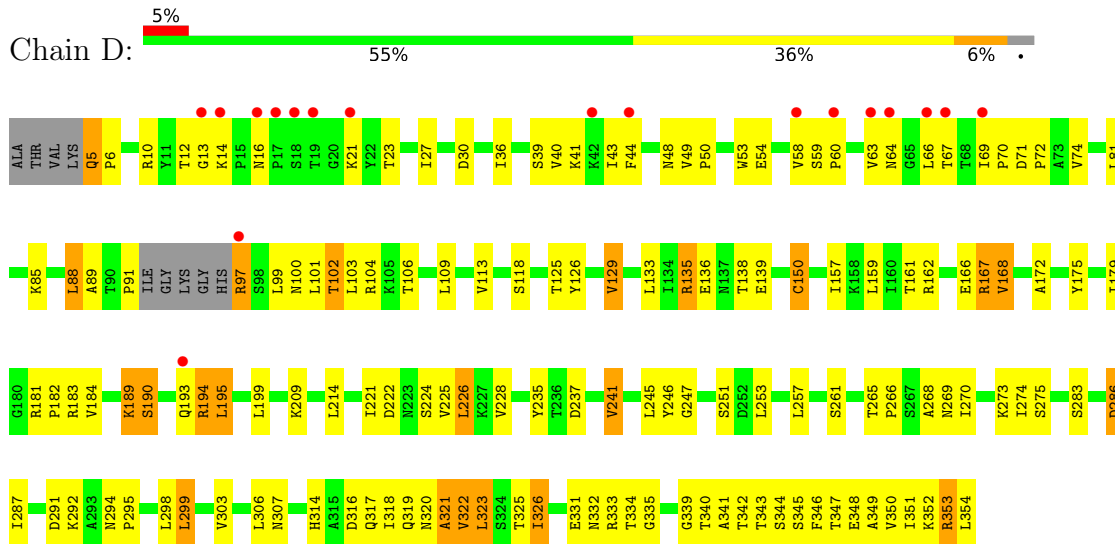
● Molecule 1: Isocitrate dehydrogenase [NAD] subunit 1



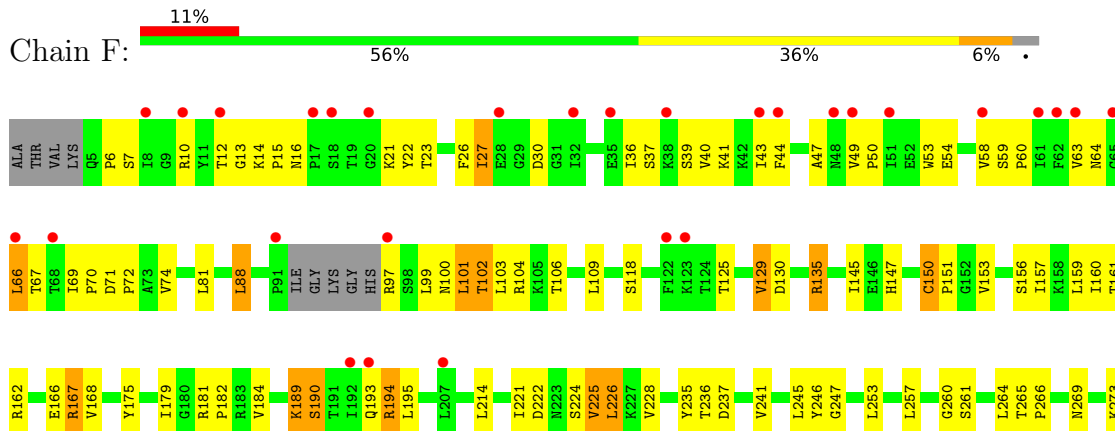
● Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

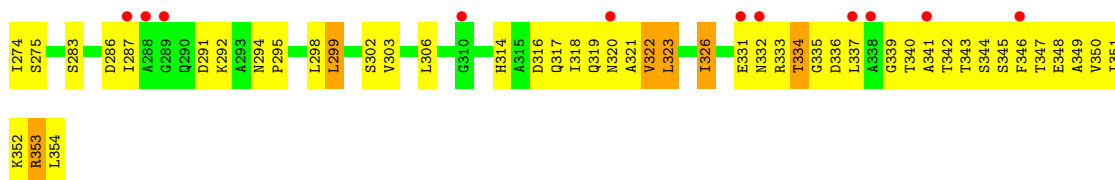


- Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

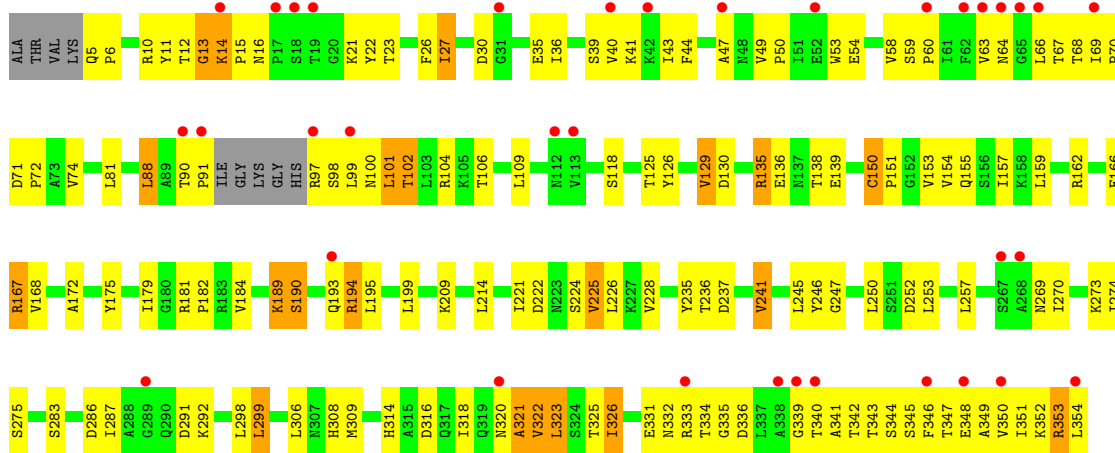


- Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

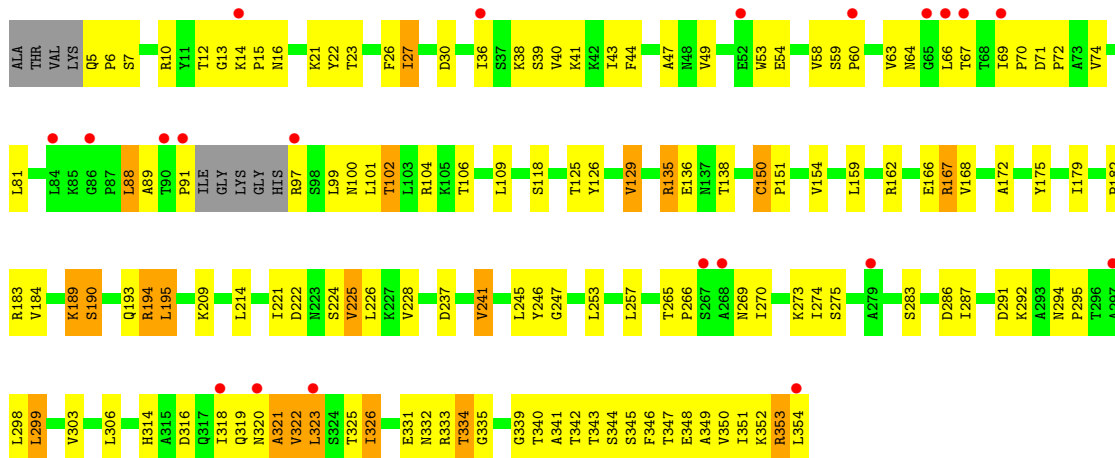




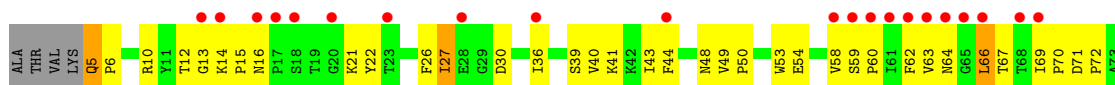
• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

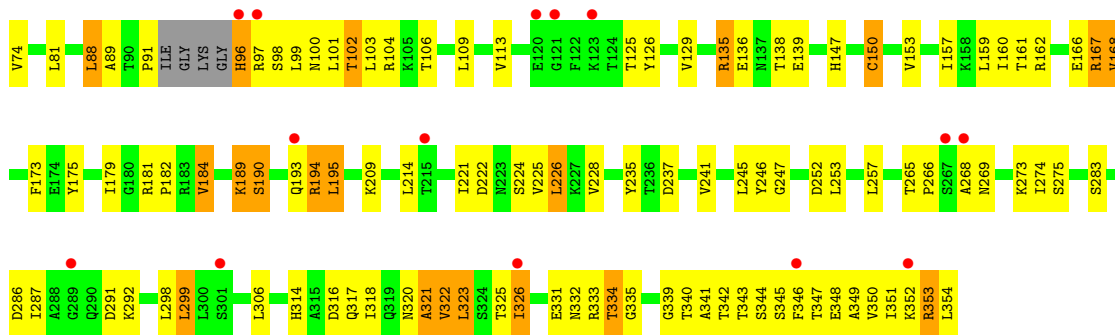


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

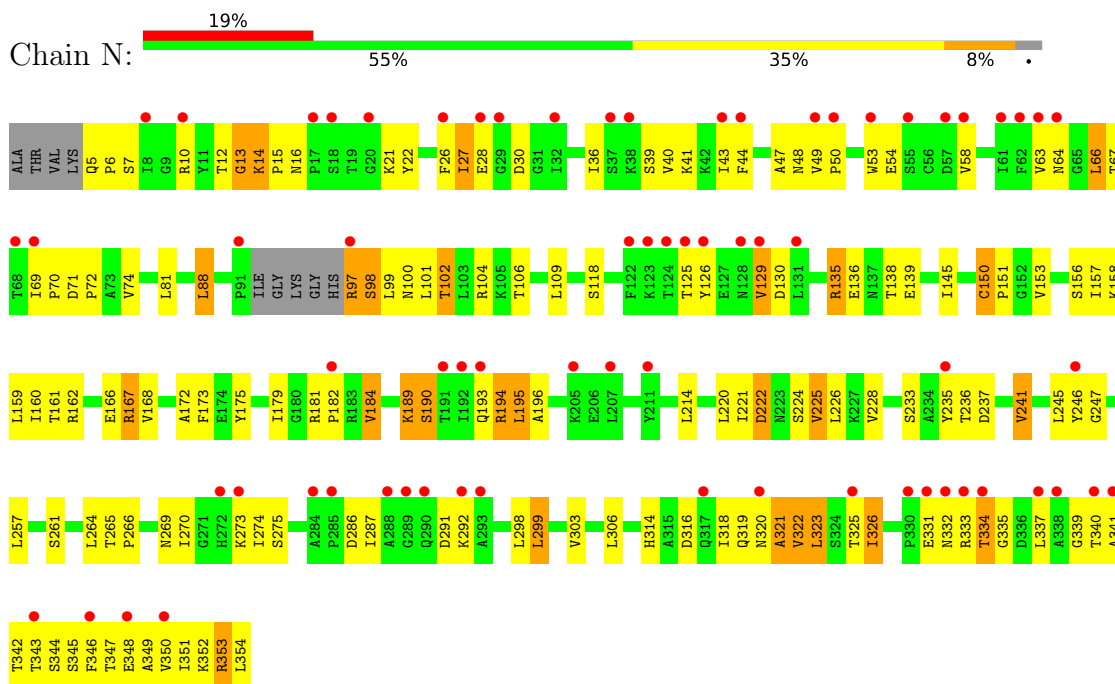


• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2

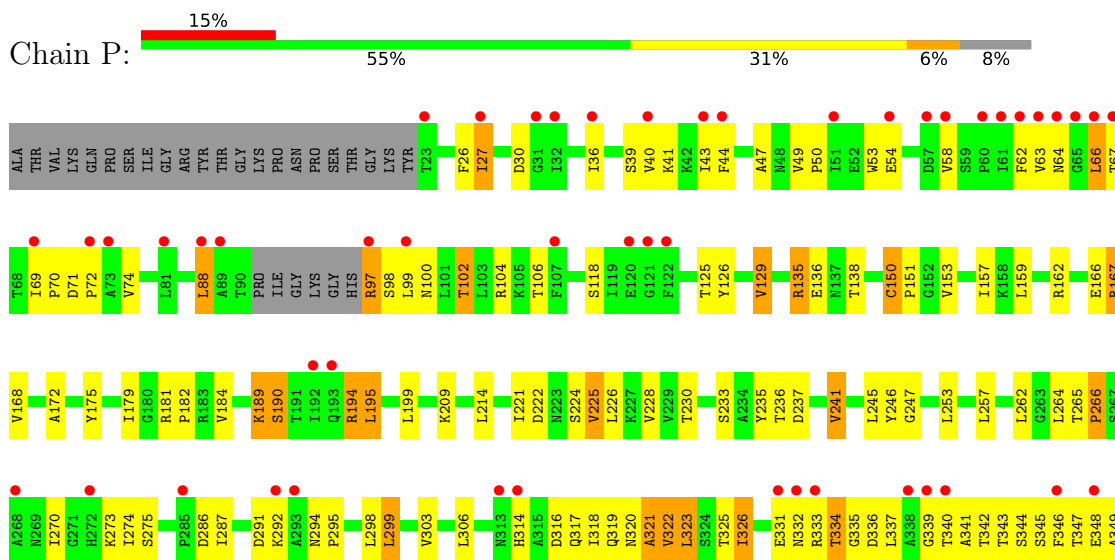




• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2



• Molecule 2: Isocitrate dehydrogenase [NAD] subunit 2



V350
I351
K352
R353
L354

4 Data and refinement statistics

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) 96.5 (35.74-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.68Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.239 , 0.264 0.231 , 0.258	Depositor DCC
R_{free} test set	9220 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	71.3	Xtrriage
Anisotropy	0.225	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 43.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.005 for k,h,-h-k-l	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	41336	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtrriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

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(°)	Ideal(°)
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

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:HG3	1:K:175:ARG:HH11	1.27	0.98
1:G:54:ILE:H	1:G:54:ILE:HD12	1.29	0.96
1:E:175:ARG:HH11	1:E:175:ARG:HG3	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:G:175:ARG:HH11	1:G:175:ARG:HG3	1.31	0.95
1:M:175:ARG:HH11	1:M:175:ARG:HG3	1.29	0.95
2:N:287:ILE:HD11	2:N:292:LYS:HD2	1.46	0.95
2:H:194:ARG:HH21	2:H:194:ARG:HG3	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
1:M:181:VAL:HB	1:M:235:THR:HG22	1.47	0.94
2:P:287:ILE:HD11	2:P:292:LYS:HD2	1.47	0.94
2:J:318:ILE:O	2:J:322:VAL:HG21	1.68	0.94
2:B:189:LYS:HD2	2:B:190:SER:H	1.29	0.94
2:L:189:LYS:HD2	2:L:190:SER:H	1.32	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:F:189:LYS:HD2	2:F:190:SER:H	1.32	0.92
2:N:97:ARG:HD2	2:N:101:LEU:HD12	1.50	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:HH11	1:I:175:ARG:HG3	1.35	0.92
2:J:135:ARG:HD3	2:J:247:GLY:HA3	1.51	0.92
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
2:N:318:ILE:O	2:N:322:VAL:HG21	1.70	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:HH21	2:P:194:ARG:HG3	1.36	0.91
2:H:194:ARG:HH21	2:H:194:ARG:CG	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:HH21	2:F:194:ARG:HG3	1.37	0.88
2:B:135:ARG:HD3	2:B:247:GLY:HA3	1.53	0.88
2:L:194:ARG:HG3	2:L:194:ARG:HH21	1.37	0.88
2:B:194:ARG:HH21	2:B:194:ARG:HG3	1.34	0.88
2:P:194:ARG:HH21	2:P:194:ARG:CG	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:B:159:LEU:HD22	1:C:143:SER:HB3	1.54	0.87
2:D:287:ILE:HD11	2:D:292:LYS:HD2	1.56	0.87
2:F:194:ARG:HH21	2:F:194:ARG:CG	1.87	0.87
1:K:175:ARG:HH11	1:K:175:ARG:CG	1.87	0.87
1:A:301:HIS:HE1	1:E:15:GLY:O	1.57	0.87
1:A:175:ARG:HH11	1:A:175:ARG:HG3	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:HH21	2:J:194:ARG:CG	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:HH21	2:B:194:ARG:CG	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:HH11	1:E:175:ARG:CG	1.91	0.83
1:G:175:ARG:HH11	1:G:175:ARG:CG	1.91	0.83
2:H:343:THR:O	2:H:347:THR:HG23	1.78	0.83
1:O:175:ARG:HH11	1:O:175:ARG:CG	1.92	0.83
2:B:287:ILE:HD11	2:B:292:LYS:HD2	1.61	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: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:B:102:THR:O	2:B:106:THR:HG23	1.79	0.82
2:J:67:THR:HG21	2:J:97:ARG:N	1.95	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:HH11	1:C:175:ARG:CG	1.93	0.81
2:L:318:ILE:O	2:L:322:VAL:HG21	1.79	0.81
1:M:175:ARG:HH11	1:M:175:ARG:CG	1.93	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: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:F:322:VAL:O	2:F:326:ILE: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:L:97:ARG:HG2	2:L:98:SER:H	1.48	0.78
1:M:151:LEU:CD2	2:N:157:ILE:HG12	2.14	0.78
2:N:97:ARG:HH12	2:N:102:THR:CG2	1.96	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: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
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
2:H:322:VAL:O	2:H:326:ILE:HG23	1.85	0.77
1:K:15:GLY:O	1:O:301:HIS:HE1	1.68	0.77
2:P:97:ARG:HG3	2:P:98:SER:H	1.49	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:HH11	1:A:175:ARG:CG	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:H:97:ARG:NH2	2:H:102:THR:HG23	2.00	0.75
2:N:322:VAL:O	2:N:326:ILE:HG23	1.84	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:HD23	2:H:323:LEU:H	1.52	0.73
1:M:17:ARG:NH1	1:M:48:ASP:OD1	2.20	0.73
1:M:325:THR:HG23	1:M:329:ILE:HG13	1.71	0.73
1:C:211:VAL:O	2:J:38:LYS:HE3	1.87	0.73
1:C:15:GLY:O	1:G:301:HIS:HE1	1.71	0.73
2:F:69:ILE:HD12	2:F:70:PRO:HD2	1.69	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:B:36:ILE:HG22	2:B:298:LEU:HD23	1.70	0.72
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
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:H:273:LYS:HG3	2:H:274:ILE:HD12	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
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:B:342:THR:CG2	2:B:345:SER:H	2.04	0.71
1:C:325:THR:HG23	1:C:329:ILE:HG13	1.71	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
2:N:159:LEU:CD2	1:O:144:VAL:HG12	2.20	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:H	2:J:323:LEU:HD23	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
1:O:325:THR:HG23	1:O:329:ILE:HG13	1.72	0.70
2:P:194:ARG:HH21	2:P:194:ARG:CB	2.05	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
2:D:322:VAL:HB	2:D:323:LEU:HD23	1.74	0.70
2:F:189:LYS:HD2	2:F:190:SER:N	2.05	0.70
1:M:147:VAL:HG22	2:N:161:THR:CG2	2.21	0.70
2:J:342:THR:CG2	2:J:345:SER:H	2.05	0.69
1:M:90:HIS:CB	2:N:193:GLN:HG3	2.22	0.69
1:O:55:LYS:HD3	1:O:59:HIS:CD2	2.27	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:79:GLY:HA2	1:A:291:MET:HE1	1.73	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
2:B:322:VAL:HG23	2:B:323:LEU:N	2.07	0.69
1:K:325:THR:HG23	1:K:329:ILE:HG13	1.74	0.69
2:N:287:ILE:HD11	2:N:292:LYS:CD	2.21	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
1:G:56:GLN:C	1:G:58:ASP:H	1.94	0.69
2:P:189:LYS:HD2	2:P:190:SER:N	2.08	0.69
2:B:189:LYS:HD2	2:B:190:SER:N	2.06	0.68
2:F:273:LYS:HG3	2:F:274:ILE:HD12	1.75	0.68
2:L:66:LEU:CD2	2:L:97:ARG:HH21	2.06	0.68
2:P:194:ARG:HG3	2:P:194:ARG:NH2	2.05	0.68
2:H:342:THR:CG2	2:H:345:SER:H	2.05	0.68
2:J:342:THR:HG22	2:J:345:SER:H	1.58	0.68
2:P:102:THR:O	2:P:106:THR:HG23	1.93	0.68
1:E:147:VAL:HG22	2:F:161:THR:HG22	1.74	0.68
2:H:102:THR:O	2:H:106:THR:HG23	1.93	0.68
2:N:194:ARG:HH21	2:N:194:ARG:CB	2.06	0.68
2:B:89:ALA:O	2:B:91:PRO:HD3	1.92	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
1:A:113:LEU:HD13	1:A:256:LEU:HD22	1.76	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
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:HH21	2:F:194:ARG:CB	2.06	0.67
1:M:90:HIS:HB3	2:N:193:GLN:HG3	1.76	0.67
2:D:273:LYS:HG3	2:D:274:ILE:HD12	1.75	0.67
1:G:175:ARG:HG3	1:G:175:ARG:NH1	2.09	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
2:D:349:ALA:O	2:D:353:ARG:HD3	1.94	0.67
1:E:90:HIS:CB	2:F:193:GLN:HG3	2.25	0.67
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
2:D:314:HIS:O	2:D:318:ILE:HG13	1.95	0.66
2:F:342:THR:CG2	2:F:345:SER:H	2.09	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: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
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:P:318:ILE:C	2:P:322:VAL:HG21	2.15	0.66
1:A:300:ASN:OD1	1:A:305:ASN:HB2	1.96	0.66
2:B:314:HIS:O	2:B:318:ILE:HG13	1.95	0.66
1:G:300:ASN:HA	1:G:305:ASN:HB3	1.78	0.66
2:H:69:ILE:HD12	2:H:70:PRO:HD2	1.77	0.66
1:M:149:GLU:HG3	2:N:159:LEU:CD1	2.25	0.66
2:P:273:LYS:HE3	2:P:274:ILE:HD11	1.78	0.66
2:J:273:LYS:HG3	2:J:274:ILE:HD12	1.76	0.66
1:C:315:VAL:O	1:C:319:ILE:HG23	1.96	0.66
2:P:97:ARG:CG	2:P:98:SER:H	2.07	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:L:349:ALA:O	2:L:353:ARG:HD3	1.96	0.65
2:N:189:LYS:HD2	2:N:190:SER:N	2.07	0.65
2:P:287:ILE:HD11	2:P:292:LYS:CD	2.24	0.65
2:D:291:ASP:O	2:D:343:THR:HG22	1.95	0.65
2:N:69:ILE:HD12	2:N:70:PRO:HD2	1.78	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
1:A:301:HIS:CE1	1:E:15:GLY:O	2.45	0.65
2:F:326:ILE:HD11	2:F:346:PHE:CE1	2.32	0.65
1:G:325:THR:HG22	1:G:331:GLY:HA3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:189:LYS:HD2	2:J:190:SER:N	2.06	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:69:ILE:HD12	2:P:70:PRO:HD2	1.79	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
1:A:305:ASN:HA	1:A:308:ALA:HB3	1.79	0.64
2:D:286:ASP:OD2	2:J:287:ILE:HG12	1.98	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
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:342:THR:HG22	2:F:345:SER:H	1.63	0.64
2:H:273:LYS:HE3	2:H:274:ILE:HD11	1.78	0.64
2:D:333:ARG:HB2	2:D:339:GLY:HA3	1.78	0.64
2:F:322:VAL:C	2:F:326:ILE:HG23	2.18	0.64
1:I:300:ASN:HA	1:I:305:ASN:HB3	1.78	0.64
2:J:194:ARG:HH21	2:J:194:ARG:CB	2.11	0.64
2:J:322:VAL:HB	2:J:323:LEU:HD23	1.78	0.64
1:M:223:ALA:O	1:M:227:PRO:HG3	1.98	0.64
2:N:342:THR:HG22	2:N:345:SER:H	1.61	0.64
2:H:322:VAL:HB	2:H:323:LEU:HD23	1.80	0.64
2:J:36:ILE:HG22	2:J:298:LEU:HD23	1.78	0.64
2:J:349:ALA:O	2:J:353:ARG:HD3	1.97	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:HG3	1:O:175:ARG:NH1	2.08	0.64
2:B:5:GLN:NE2	2:B:6:PRO:HD2	2.12	0.64
2:H:326:ILE:HG21	2:H:350:VAL:HA	1.80	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:B:224:SER:O	2:B:228:VAL:HG23	1.98	0.63
2:D:273:LYS:HE3	2:D:274:ILE:HD11	1.81	0.63
1:E:181:VAL:HB	1:E:235:THR:CG2	2.22	0.63
2:H:194:ARG:HH21	2:H:194:ARG:CB	2.10	0.63
1:M:222:GLN:HG3	1:M:229:GLN:OE1	1.98	0.63
2:N:318:ILE:C	2:N:322:VAL:HG21	2.19	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:B:342:THR:HG22	2:B:345:SER:H	1.61	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
2:F:159:LEU:HD22	1:G:143:SER:HB3	1.80	0.63
2:J:273:LYS:HE3	2:J:274:ILE:HD11	1.80	0.63
1:C:345:LYS:O	1:C:349:MET:HG3	1.99	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: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:C:246:ILE:HD11	2:D:253:LEU:HD12	1.81	0.63
1:I:135:GLU:OE2	2:J:189:LYS:HE2	1.99	0.63
1:I:305:ASN:HA	1:I:308:ALA:HB3	1.81	0.63
2:L:322:VAL:HB	2:L:323:LEU:HD23	1.79	0.63
1:O:123:ILE:HD13	1:O:250:LEU:HB3	1.81	0.63
2:P:326:ILE:HD11	2:P:346:PHE:CE1	2.34	0.63
2:F:245:LEU:HD23	2:F:246:TYR:CE1	2.34	0.63
1:E:325:THR:HG22	1:E:331:GLY:HA3	1.81	0.62
2:J:69:ILE:HD12	2:J:70:PRO:HD2	1.79	0.62
2:P:322:VAL:HB	2:P:323:LEU:HD23	1.81	0.62
2:B:349:ALA:O	2:B:353:ARG:HD3	1.99	0.62
2:D:36:ILE:HG22	2:D:298:LEU:HD23	1.80	0.62
2:J:322:VAL:HG23	2:J:323:LEU:N	2.13	0.62
2:J:333:ARG:HB2	2:J:339:GLY:HA3	1.81	0.62
2:N:194:ARG:HG3	2:N:194:ARG:NH2	2.03	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
2:L:351:ILE:HA	2:L:354:LEU:HB2	1.80	0.62
1:K:175:ARG:NH1	1:K:231:ASP:OD1	2.32	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
1:I:181:VAL:HB	1:I:235:THR:CG2	2.23	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:C:222:GLN:HG3	1:C:229:GLN:OE1	1.99	0.62
1:G:175:ARG:NH1	1:G:231:ASP:OD1	2.33	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
2:J:318:ILE:C	2:J:322:VAL:HG21	2.18	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
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
1:M:311:ILE:O	1:M:315:VAL:HG13	1.99	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
1:K:222:GLN:HG3	1:K:229:GLN:OE1	1.99	0.61
2:L:194:ARG:HG3	2:L:194:ARG:NH2	2.10	0.61
1:C:175:ARG:HG3	1:C:175:ARG:NH1	2.10	0.61
2:J:326:ILE:HG21	2:J:350:VAL:HA	1.80	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: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
1:M:305:ASN:HA	1:M:308:ALA:HB3	1.82	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:N:273:LYS:HE3	2:N:274:ILE:HD11	1.82	0.61
2:P:66:LEU:CD2	2:P:97:ARG:HH21	2.14	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:151:LEU:HD23	2:L:157:ILE:HG12	1.83	0.61
1:K:245:ASN:OD1	1:K:276:VAL:HG21	2.00	0.61
1:G:222:GLN:HG3	1:G:229:GLN:OE1	2.00	0.61
1:I:275:HIS:ND1	1:I:278:LEU:CD1	2.61	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
1:M:146:GLY:O	2:N:161:THR:HA	2.01	0.61
2:N:333:ARG:HB2	2:N:339:GLY:HA3	1.83	0.61
1:A:155:THR:O	1:A:159:THR:CG2	2.48	0.61
2:H:97:ARG:NH1	2:H:101:LEU:CD1	2.63	0.61
2:J:287:ILE:HD11	2:J:292:LYS:CD	2.30	0.61
1:K:55:LYS:HB3	1:K:57:THR:HG22	1.81	0.61
1:O:181:VAL:HB	1:O:235:THR:CG2	2.23	0.61
2:P:333:ARG:HB2	2:P:339:GLY:HA3	1.81	0.61
2:D:318:ILE:C	2:D:322:VAL:HG21	2.21	0.60
1:I:113:LEU:HD13	1:I:256:LEU:HD22	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:222:GLN:HG3	1:I:229:GLN:OE1	2.01	0.60
1:I:325:THR:HG22	1:I:331:GLY:HA3	1.82	0.60
2:J:97:ARG:HH21	2:J:102:THR:HG23	1.66	0.60
1:O:175:ARG:NH1	1:O:231:ASP:OD1	2.35	0.60
2:B:97:ARG:NH2	2:B:102:THR:HG23	2.16	0.60
2:J:97:ARG:HH21	2:J:102:THR:CG2	2.14	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
1:C:305:ASN:HA	1:C:308:ALA:HB3	1.83	0.60
2:F:273:LYS:HE3	2:F:274:ILE:HD11	1.84	0.60
2:L:322:VAL:C	2:L:326:ILE:HG23	2.22	0.60
2:L:322:VAL:HG23	2:L:323:LEU:N	2.16	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
1:C:300:ASN:OD1	1:C:305:ASN:HB2	2.02	0.59
2:D:322:VAL:HG23	2:D:323:LEU:N	2.16	0.59
1:A:144:VAL:HG12	2:D:159:LEU:HD21	1.83	0.59
1:A:305:ASN:HA	1:A:308:ALA:CB	2.31	0.59
2:B:40:VAL:HG22	2:B:299:LEU:HD13	1.84	0.59
2:B:175:TYR:O	2:B:179:ILE:HG12	2.02	0.59
2:P:97:ARG:CZ	2:P:102:THR:HG23	2.32	0.59
1:A:18:PHE:HZ	1:E:44:ASN:HD22	1.51	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: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: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:HH21	2:B:194:ARG:CB	2.15	0.59
1:E:175:ARG:NH1	1:E:231:ASP:OD1	2.36	0.59
2:F:6:PRO:O	2:F:10:ARG:HG2	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:36:ILE:HG22	2:H:298:LEU:HD23	1.85	0.59
1:M:123:ILE:HD13	1:M:250:LEU:HB3	1.82	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:F:333:ARG:HB2	2:F:339:GLY:HA3	1.84	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:P:97:ARG:HG3	2:P:98:SER:N	2.17	0.59
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
2:F:322:VAL:HG23	2:F:323:LEU:N	2.16	0.58
1:K:181:VAL:HB	1:K:235:THR:CG2	2.25	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
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:E:223:ALA:O	1:E:227:PRO:HG3	2.03	0.58
1:K:223:ALA:O	1:K:227:PRO:HG3	2.03	0.58
2:N:97:ARG:HG3	2:N:98:SER:N	2.16	0.58
1:A:175:ARG:NH1	1:A:231:ASP:OD1	2.37	0.58
1:E:245:ASN:OD1	1:E:276:VAL:HG21	2.03	0.58
1:E:305:ASN:HA	1:E:308:ALA:HB3	1.84	0.58
2:H:326:ILE:HD11	2:H:346:PHE:CE1	2.38	0.58
1:I:140:GLU:HB3	2:J:195:LEU:CD2	2.34	0.58
1:I:155:THR:O	1:I:159:THR:HG23	2.03	0.58
2:N:322:VAL:C	2:N:326:ILE:HG23	2.23	0.58
2:L:89:ALA:O	2:L:91:PRO:HD3	2.04	0.58
1:A:323:LYS:O	1:A:324:HIS:HB2	2.03	0.58
1:K:305:ASN:HA	1:K:308:ALA:CB	2.34	0.58
1:M:149:GLU:HG3	2:N:159:LEU:HD12	1.86	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
2:B:273:LYS:HE3	2:B:274:ILE:HD11	1.86	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:L:194:ARG:HH21	2:L:194:ARG:CB	2.16	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
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:O:305:ASN:HA	1:O:308:ALA:HB3	1.86	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
1:G:55:LYS:N	1:G:55:LYS:HD2	2.18	0.57
1:G:300:ASN:OD1	1:G:305:ASN:HB2	2.02	0.57
2:H:97:ARG:CG	2:H:98:SER:H	2.15	0.57
2:D:318:ILE:CA	2:D:322:VAL:HG11	2.33	0.57
2:J:326:ILE:HD11	2:J:346:PHE:CE1	2.38	0.57
1:M:175:ARG:NH1	1:M:231:ASP:OD1	2.37	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:B:273:LYS:HG3	2:B:274:ILE:HD12	1.85	0.57
2:F:287:ILE:HG13	2:F:292:LYS:HB2	1.87	0.57
2:D:88:LEU:HD13	2:D:99:LEU:HD23	1.87	0.57
1:E:113:LEU:HD13	1:E:256:LEU:HD22	1.87	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: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:I:54:ILE:HG23	1:I:59:HIS:HB3	1.86	0.57
1:M:116:VAL:HG23	1:M:319:ILE:CD1	2.35	0.57
1:M:199:THR:HA	1:M:211:VAL:HG11	1.86	0.57
1:C:151:LEU:HD23	2:D:157:ILE:HG12	1.87	0.57
1:C:79:GLY:HA2	1:C:291:MET:CE	2.35	0.57
1:E:54:ILE:HD12	1:E:54:ILE:N	2.04	0.57
2:F:44:PHE:CD2	2:F:49:VAL:HG21	2.39	0.57
1:I:278:LEU:HD22	1:I:280:ILE:HG12	1.85	0.57
1:I:292:ILE:O	1:I:295:SER:HB3	2.05	0.57
1:I:310:ARG:HG2	1:I:349:MET:CE	2.35	0.57
2:L:351:ILE:HG23	2:L:354:LEU:HD23	1.86	0.57
2:N:326:ILE:HD11	2:N:346:PHE:CE1	2.39	0.57
2:B:67:THR:OG1	2:B:97:ARG:HB3	2.04	0.57
1:E:314:ALA:HB2	1:E:346:LEU:HD13	1.86	0.57
2:H:287:ILE:HD11	2:H:292:LYS:CD	2.28	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
2:B:333:ARG:HB2	2:B:339:GLY:HA3	1.86	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:N:12:THR:HB	2:N:81:LEU:CD1	2.35	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:6:PRO:O	2:B:10:ARG:HG2	2.05	0.56
2:B:47:ALA:HB2	2:B:354:LEU:HD21	1.87	0.56
1:E:123:ILE:HD13	1:E:250:LEU:HB3	1.86	0.56
1:E:163:ALA:HB2	1:E:198:ILE:HD13	1.86	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
1:O:79:GLY:HA2	1:O:291:MET:HE1	1.87	0.56
1:A:311:ILE:O	1:A:315:VAL:HG13	2.05	0.56
2:D:245:LEU:HD23	2:D:246:TYR:CE1	2.39	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:E:139:LEU:HD23	1:E:151:LEU:HD12	1.87	0.56
1:I:189:LEU:HB3	2:J:154:VAL:HG11	1.87	0.56
2:N:39:SER:O	2:N:43:ILE:HG13	2.05	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
1:K:325:THR:HG22	1:K:331:GLY:HA3	1.87	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:A:222:GLN:HG3	1:A:229:GLN:OE1	2.06	0.56
1:G:20:VAL:HG13	1:G:47:ILE:HG23	1.88	0.56
1:I:280:ILE:HD12	1:I:280:ILE:O	2.05	0.56
2:B:97:ARG:NH2	2:B:102:THR:CG2	2.69	0.56
1:G:123:ILE:HD13	1:G:250:LEU:HB3	1.86	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:A:223:ALA:O	1:A:227:PRO:HG3	2.05	0.56
2:B:40:VAL:HG22	2:B:299:LEU:CD1	2.36	0.56
1:C:155:THR:O	1:C:159:THR:CG2	2.54	0.56
1:E:199:THR:HA	1:E:211:VAL:HG11	1.86	0.56
2:H:318:ILE:CA	2:H:322:VAL:HG11	2.34	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
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
1:I:310:ARG:HG2	1:I:349:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:318:ILE:CA	2:J:322:VAL:HG11	2.35	0.56
1:M:10:LEU:HD22	1:M:11:PRO:HD2	1.88	0.56
1:M:300:ASN:OD1	1:M:305:ASN:HB2	2.06	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:L:318:ILE:CA	2:L:322:VAL:HG11	2.33	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
1:C:276:VAL:O	2:D:226:LEU:HD12	2.06	0.55
1:E:246:ILE:HD11	2:F:253:LEU:HD12	1.88	0.55
1:E:305:ASN:HA	1:E:308:ALA:CB	2.37	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
2:D:166:GLU:O	2:D:167:ARG:HB2	2.05	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
1:K:281:LYS:O	1:K:281:LYS:HD2	2.06	0.55
2:P:322:VAL:HG23	2:P:323:LEU:N	2.21	0.55
1:A:79:GLY:HA2	1:A:291:MET:CE	2.36	0.55
1:A:246:ILE:HD11	2:B:253:LEU:HD12	1.88	0.55
1:C:79:GLY:HA2	1:C:291:MET:HE1	1.87	0.55
1:C:223:ALA:O	1:C:227:PRO:HG3	2.07	0.55
1:G:58:ASP:HA	1:G:92:SER:HB2	1.88	0.55
1:G:116:VAL:HG23	1:G:319:ILE:CD1	2.37	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
2:N:5:GLN:HG3	2:N:6:PRO:HD2	1.89	0.55
1:K:79:GLY:HA2	1:K:291:MET:CE	2.37	0.55
2:L:332:ASN:HA	2:L:341:ALA:HB2	1.89	0.55
2:N:6:PRO:O	2:N:10:ARG:HG2	2.07	0.55
1:O:54:ILE:CG2	1:O:59:HIS:HB3	2.37	0.55
1:O:199:THR:HA	1:O:211:VAL:HG11	1.88	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
1:E:143:SER:HB3	2:H:159:LEU:CD2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:199:THR:HA	1:G:211:VAL:HG11	1.88	0.55
1:I:55:LYS:HD3	1:I:55:LYS:N	2.20	0.55
1:M:181:VAL:HB	1:M:235:THR:CG2	2.29	0.55
2:N:287:ILE:HG13	2:N:292:LYS:HB2	1.89	0.55
2:N:318:ILE:CA	2:N:322:VAL:HG11	2.33	0.55
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
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:K:276:VAL:O	2:L:226:LEU:HD12	2.07	0.54
1:M:113:LEU:CD1	1:M:256:LEU:HD22	2.37	0.54
1:O:235:THR:HG21	1:O:243:LEU:HD12	1.88	0.54
1:A:90:HIS:CB	2:B:193:GLN:HG3	2.37	0.54
2:H:67:THR:OG1	2:H:97:ARG:HB3	2.07	0.54
1:I:277:GLY:O	1:I:279:ASP:N	2.40	0.54
1:M:139:LEU:HD23	1:M:151:LEU:HD12	1.87	0.54
2:N:332:ASN:HA	2:N:341:ALA:HB2	1.89	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:P:322:VAL:C	2:P:326:ILE:HG23	2.28	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:J:245:LEU:HD23	2:J:246:TYR:CE1	2.43	0.54
2:P:97:ARG:CG	2:P:98:SER:N	2.71	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:D:224:SER:O	2:D:228:VAL:HG23	2.07	0.54
1:E:300:ASN:OD1	1:E:305:ASN:HB2	2.07	0.54
1:I:175:ARG:HG3	1:I:175:ARG:NH1	2.11	0.54
2:L:342:THR:HG23	2:L:344:SER:H	1.73	0.54
1:O:116:VAL:HG23	1:O:319:ILE:CD1	2.37	0.54
2:H:322:VAL:HG23	2:H:323:LEU:N	2.20	0.54
1:I:223:ALA:O	1:I:227:PRO:HG3	2.07	0.54
2:N:102:THR:O	2:N:106:THR:HG23	2.07	0.54
1:O:195:ARG:O	1:O:199:THR:HG23	2.08	0.54
2:D:63:VAL:O	2:D:64:ASN:HB2	2.08	0.54
2:F:97:ARG:HH22	2:F:102:THR:HG23	1.73	0.54
2:H:175:TYR:O	2:H:179:ILE:HG12	2.07	0.54
1:K:300:ASN:OD1	1:K:305:ASN:HB2	2.07	0.54
2:N:157:ILE:CD1	1:O:151:LEU:HD11	2.38	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)
2:L:5:GLN:HA	2:L:5:GLN:HE21	1.73	0.54
1:M:155:THR:O	1:M:159:THR:HG23	2.08	0.54
2:D:291:ASP:C	2:D:343:THR:HG22	2.28	0.54
1:G:235:THR:HG21	1:G:243:LEU:HD12	1.90	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
1:O:300:ASN:OD1	1:O:305:ASN:HB2	2.06	0.54
1:A:18:PHE:HZ	1:E:44:ASN:HD21	1.53	0.54
2:F:63:VAL:O	2:F:64:ASN:HB2	2.08	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:L:194:ARG:CG	2:L:194:ARG:NH2	2.61	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
2:H:150:CYS:HB2	2:H:151:PRO:CD	2.38	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:F:274:ILE:HG22	2:F:275:SER:N	2.24	0.53
2:F:348:GLU:O	2:F:352:LYS:HG2	2.09	0.53
1:G:79:GLY:HA2	1:G:291:MET:CE	2.37	0.53
1:G:181:VAL:HB	1:G:235:THR:CG2	2.27	0.53
1:I:140:GLU:HB3	2:J:195:LEU:HD21	1.91	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: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
1:E:325:THR:CG2	1:E:329:ILE:HG13	2.36	0.53
2:P:291:ASP:O	2:P:343:THR:HG22	2.08	0.53
2:F:118:SER:OG	2:F:129:VAL:HG13	2.08	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:L:66:LEU:HD21	2:L:97:ARG:HH21	1.74	0.53
2:L:326:ILE:O	2:L:326:ILE:HD12	2.08	0.53
2:P:88:LEU:HD13	2:P:99:LEU:HD23	1.89	0.53
1:A:245:ASN:OD1	1:A:276:VAL:HG21	2.09	0.53
2:D:342:THR:HG23	2:D:344:SER:H	1.74	0.53
1:I:116:VAL:HG23	1:I:319:ILE:CD1	2.39	0.53
2:P:44:PHE:CD2	2:P:49:VAL:HG21	2.44	0.53
1:C:314:ALA:HB2	1:C:346:LEU:HD13	1.90	0.53
1:E:195:ARG:O	1:E:199:THR:HG23	2.09	0.53
1:K:25:GLY:HA2	1:K:81:TRP:CZ2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:45:ILE:HG23	1:K:46:PRO:HD2	1.90	0.53
1:M:79:GLY:HA2	1:M:291:MET:CE	2.38	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
1:K:325:THR:CG2	1:K:329:ILE:HG13	2.39	0.53
1:M:25:GLY:HA2	1:M:81:TRP:CZ2	2.44	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
1:C:323:LYS:O	1:C:324:HIS:HB2	2.09	0.52
2:D:39:SER:O	2:D:43:ILE:HG13	2.09	0.52
2:L:326:ILE:HD11	2:L:346:PHE:CE1	2.44	0.52
2:H:88:LEU:HD13	2:H:99:LEU:HD23	1.91	0.52
1:I:175:ARG:CG	1:I:175:ARG:NH1	2.59	0.52
1:O:79:GLY:HA2	1:O:291:MET:CE	2.39	0.52
1:A:199:THR:HA	1:A:211:VAL:HG11	1.90	0.52
1:C:55:LYS:HB3	1:C:57:THR:HG22	1.90	0.52
2:D:5:GLN:HA	2:D:5:GLN:HE21	1.72	0.52
1:E:25:GLY:HA2	1:E:81:TRP:CZ2	2.44	0.52
1:I:20:VAL:HG13	1:I:47:ILE:HG23	1.90	0.52
1:M:54:ILE:H	1:M:54:ILE:HD12	1.74	0.52
1:O:56:GLN:C	1:O:58:ASP:H	2.12	0.52
2:F:12:THR:HB	2:F:81:LEU:CD1	2.40	0.52
1:G:54:ILE:CD1	1:G:54:ILE:N	2.72	0.52
2:H:12:THR:HB	2:H:81:LEU:HD12	1.92	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
1:M:314:ALA:HB2	1:M:346:LEU:HD13	1.89	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:245:LEU:HD23	2:H:246:TYR:CE1	2.44	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
2:B:342:THR:HG22	2:B:345:SER:HB3	1.90	0.52
2:D:12:THR:HB	2:D:81:LEU:CD1	2.40	0.52
1:I:195:ARG:O	1:I:199:THR:HG23	2.10	0.52
1:K:15:GLY:O	1:O:301:HIS:CE1	2.56	0.52
1:O:314:ALA:HB2	1:O:346:LEU:HD13	1.92	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
1:A:155:THR:O	1:A:159:THR:HG22	2.09	0.52
2:B:342:THR:HG23	2:B:344:SER:H	1.74	0.52
1:G:314:ALA:HB2	1:G:346:LEU:HD13	1.92	0.52
1:M:148:VAL:N	2:N:160:ILE:O	2.34	0.52
2:N:157:ILE:HD11	1:O:151:LEU:CD1	2.40	0.52
2:N:326:ILE:HG12	2:N:350:VAL:CG2	2.40	0.52
2:P:135:ARG:CD	2:P:247:GLY:HA3	2.29	0.52
1:C:347:SER:HA	1:G:14:TYR:CE1	2.45	0.52
1:E:235:THR:HG21	1:E:243:LEU:HD12	1.90	0.52
2:J:175:TYR:O	2:J:179:ILE:HG12	2.10	0.52
1:M:163:ALA:HB2	1:M:198:ILE:HD13	1.91	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:A:275:HIS:ND1	1:A:278:LEU:CD1	2.66	0.51
1:C:235:THR:HG21	1:C:243:LEU:HD12	1.92	0.51
2:F:70:PRO:O	2:F:74:VAL:HG23	2.11	0.51
2:H:97:ARG:CZ	2:H:102:THR:HG23	2.40	0.51
2:J:12:THR:HB	2:J:81:LEU:CD1	2.39	0.51
1:M:88:THR:CB	2:N:189:LYS:HE3	2.34	0.51
1:M:175:ARG:HG3	1:M:175:ARG:NH1	2.09	0.51
1:M:202:GLY:HA3	1:M:211:VAL:HG21	1.91	0.51
1:A:175:ARG:HG3	1:A:175:ARG:NH1	2.15	0.51
2:B:159:LEU:CD2	1:C:143:SER:HB3	2.35	0.51
2:D:332:ASN:HA	2:D:341:ALA:HB2	1.92	0.51
2:F:12:THR:HB	2:F:81:LEU:HD12	1.91	0.51
2:N:69:ILE:HG22	2:N:106:THR:HG21	1.93	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
1:E:311:ILE:O	1:E:315:VAL:HG13	2.10	0.51
2:H:67:THR:HG21	2:H:97:ARG:N	2.25	0.51
1:I:123:ILE:HD13	1:I:250:LEU:HB3	1.92	0.51
2:J:135:ARG:CD	2:J:247:GLY:HA3	2.34	0.51
2:P:166:GLU:O	2:P:167:ARG:HB2	2.10	0.51
2:P:273:LYS:HE3	2:P:274:ILE:CD1	2.40	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
1:M:20:VAL:HG13	1:M:47:ILE:HG23	1.93	0.51
2:P:224:SER:O	2:P:228:VAL:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:ALA:HB2	1:A:346:LEU:HD13	1.93	0.51
1:C:135:GLU:OE2	2:D:189:LYS:HE2	2.10	0.51
1:C:324:HIS:CG	1:C:341:GLU:HG3	2.46	0.51
2:J:342:THR:HG23	2:J:344:SER:H	1.75	0.51
2:L:348:GLU:O	2:L:352:LYS:HG2	2.10	0.51
1:A:143:SER:HB3	2:D:159:LEU:HD22	1.93	0.51
1:C:325:THR:CG2	1:C:329:ILE:HG13	2.38	0.51
2:J:47:ALA:HA	2:J:354:LEU:HD21	1.91	0.51
2:B:41:LYS:HG2	2:B:53:TRP:NE1	2.26	0.51
2:D:70:PRO:O	2:D:74:VAL:HG23	2.11	0.51
2:D:334:THR:HG22	2:D:335:GLY:H	1.75	0.51
1:K:311:ILE:O	1:K:315:VAL:HG13	2.10	0.51
1:M:45:ILE:HG12	1:M:307:TYR:CD2	2.45	0.51
2:N:334:THR:HG22	2:N:335:GLY:H	1.76	0.51
2:D:71:ASP:N	2:D:72:PRO:CD	2.74	0.51
1:E:54:ILE:HD13	1:E:81:TRP:CZ2	2.46	0.51
2:F:303:VAL:HG21	2:F:319:GLN:HB2	1.93	0.51
1:G:292:ILE:O	1:G:295:SER:HB3	2.11	0.51
1:I:311:ILE:O	1:I:315:VAL:HG13	2.11	0.51
2:P:41:LYS:HG2	2:P:53:TRP:NE1	2.26	0.51
2:P:44:PHE:O	2:P:49:VAL:HG22	2.11	0.51
2:P:97:ARG:NH2	2:P:102:THR:HG23	2.26	0.51
2:P:342:THR:HG23	2:P:344:SER:H	1.75	0.51
2:B:332:ASN:HA	2:B:341:ALA:HB2	1.92	0.50
1:E:45:ILE:HG12	1:E:307:TYR:CD2	2.47	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:P:274:ILE:HG22	2:P:275:SER:N	2.26	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:J:5:GLN:HG3	2:J:6:PRO:CD	2.38	0.50
2:F:166:GLU:HG2	2:F:166:GLU:O	2.11	0.50
2:N:58:VAL:HG12	2:N:69:ILE:HD11	1.92	0.50
2:D:221:ILE:O	2:D:225:VAL:HG13	2.12	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
1:M:175:ARG:CG	1:M:175:ARG:NH1	2.61	0.50
1:E:155:THR:O	1:E:159:THR:CG2	2.60	0.50
1:G:152:LYS:O	2:H:155:GLN:HA	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:223:ALA:O	1:G:227:PRO:HG3	2.11	0.50
2:L:62:PHE:HE1	2:L:96:HIS:HB3	1.76	0.50
2:L:66:LEU:HD21	2:L:97:ARG:NH2	2.26	0.50
1:A:175:ARG:CG	1:A:175:ARG:NH1	2.65	0.50
1:C:90:HIS:HB3	2:D:193:GLN:HG3	1.93	0.50
1:C:175:ARG:CG	1:C:175:ARG:NH1	2.61	0.50
2:D:135:ARG:CD	2:D:247:GLY:HA3	2.35	0.50
2:H:44:PHE:CD2	2:H:49:VAL:HG21	2.47	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:P:58:VAL:HG12	2:P:69:ILE:HD11	1.94	0.50
2:P:135:ARG:HD3	2:P:247:GLY:CA	2.31	0.50
2:F:221:ILE:O	2:F:225:VAL:HG13	2.12	0.50
2:P:67:THR:OG1	2:P:97:ARG:HB3	2.11	0.50
2:B:322:VAL:CG2	2:B:323:LEU:N	2.71	0.50
1:C:87:GLN:HB3	1:C:276:VAL:HG12	1.93	0.50
1:C:116:VAL:HG23	1:C:319:ILE:CD1	2.42	0.50
2:P:136:GLU:OE2	2:P:138:THR:HB	2.12	0.50
2:B:44:PHE:CD2	2:B:49:VAL:HG21	2.47	0.50
1:E:155:THR:HG22	2:F:153:VAL:HG13	1.94	0.50
2:J:63:VAL:O	2:J:64:ASN:HB2	2.11	0.50
2:J:291:ASP:C	2:J:343:THR:HG22	2.32	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:N:182:PRO:HD2	2:N:237:ASP:O	2.12	0.50
1:O:54:ILE:HG22	1:O:59:HIS:HB3	1.94	0.50
2:P:287:ILE:HG13	2:P:292:LYS:HB2	1.94	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:B:71:ASP:N	2:B:72:PRO:CD	2.75	0.49
1:E:202:GLY:HA3	1:E:211:VAL:HG21	1.94	0.49
2:F:88:LEU:HD13	2:F:99:LEU:HD23	1.94	0.49
2:J:334:THR:HG22	2:J:335:GLY:H	1.77	0.49
2:L:62:PHE:CE1	2:L:96:HIS:HB3	2.47	0.49
2:L:166:GLU:O	2:L:167:ARG:HB2	2.12	0.49
2:F:334:THR:HG22	2:F:335:GLY:H	1.77	0.49
2:J:89:ALA:O	2:J:91:PRO:HD3	2.12	0.49
1:K:116:VAL:HG23	1:K:319:ILE:CD1	2.42	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:L:316:ASP:O	2:L:320:ASN:HB3	2.12	0.49
2:N:12:THR:HB	2:N:81:LEU:HD12	1.94	0.49
1:O:151:LEU:CD2	2:P:157:ILE:HG12	2.42	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
2:D:100:ASN:O	2:D:104:ARG:HG3	2.12	0.49
2:F:40:VAL:HG22	2:F:299:LEU:CD1	2.42	0.49
1:G:311:ILE:O	1:G:315:VAL:HG13	2.13	0.49
1:K:155:THR:O	1:K:159:THR:CG2	2.60	0.49
1:K:314:ALA:HB2	1:K:346:LEU:HD13	1.95	0.49
2:L:126:TYR:HB2	2:L:257:LEU:O	2.12	0.49
1:E:221:MET:SD	2:F:261:SER:HA	2.53	0.49
1:G:139:LEU:HD23	1:G:151:LEU:HD12	1.94	0.49
2:D:316:ASP:O	2:D:320:ASN:HB3	2.13	0.49
2:J:41:LYS:HG2	2:J:53:TRP:NE1	2.28	0.49
2:L:71:ASP:N	2:L:72:PRO:CD	2.74	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: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
2:F:44:PHE:O	2:F:49:VAL:HG22	2.12	0.49
1:I:235:THR:HG21	1:I:243:LEU:HD12	1.95	0.49
2:J:88:LEU:HD13	2:J:99:LEU:HD23	1.94	0.49
2:P:100:ASN:O	2:P:104:ARG:HG3	2.12	0.49
2:F:228:VAL:HG12	2:F:257:LEU:CD1	2.43	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: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
1:M:54:ILE:CA	1:M:62:GLY:HA3	2.30	0.49
2:N:70:PRO:O	2:N:74:VAL:HG23	2.13	0.49
2:B:58:VAL:HG12	2:B:69:ILE:HD11	1.95	0.48
2:F:332:ASN:HA	2:F:341:ALA:HB2	1.95	0.48
1:I:324:HIS:CG	1:I:341:GLU:HG3	2.48	0.48
2:J:39:SER:O	2:J:43:ILE:HG13	2.12	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
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

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

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

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:189:LEU:HD12	1:O:189:LEU:HA	1.75	0.47
1:A:292:ILE:O	1:A:295:SER:HB3	2.14	0.47
2:B:316:ASP:O	2:B:320:ASN:HB3	2.15	0.47
1:C:88:THR:HB	2:D:189:LYS:HE3	1.96	0.47
1:C:113:LEU:CD1	1:C:256:LEU:HD22	2.44	0.47
1:C:155:THR:O	1:C:159:THR:HG23	2.14	0.47
2:D:274:ILE:HG22	2:D:275:SER:N	2.29	0.47
2:F:66:LEU:HD21	2:F:97:ARG:HH21	1.79	0.47
2:F:130:ASP:HB3	2:F:236:THR:HB	1.95	0.47
2:J:342:THR:HG23	2:J:344:SER:N	2.30	0.47
1:K:139:LEU:HD23	1:K:151:LEU:HD12	1.97	0.47
1:K:149:GLU:HG3	2:L:159:LEU:HD12	1.97	0.47
2:L:67:THR:O	2:L:102:THR:HG21	2.15	0.47
1:M:88:THR:CG2	2:N:189:LYS:HE3	2.45	0.47
2:N:316:ASP:O	2:N:320:ASN:HB3	2.14	0.47
1:O:55:LYS:HD3	1:O:59:HIS:NE2	2.28	0.47
2:P:97:ARG:NH2	2:P:102:THR:CG2	2.78	0.47
2:P:150:CYS:HB2	2:P:151:PRO:CD	2.44	0.47
2:P:265:THR:HA	2:P:266:PRO:HD3	1.67	0.47
2:D:322:VAL:CG2	2:D:323:LEU:N	2.77	0.47
2:H:5:GLN:HA	2:H:6:PRO:HD3	1.82	0.47
2:J:70:PRO:O	2:J:74:VAL:HG23	2.14	0.47
1:M:123:ILE:CD1	1:M:250:LEU:HB3	2.45	0.47
2:N:67:THR:O	2:N:102:THR:HG21	2.13	0.47
1:A:54:ILE:HD12	1:A:54:ILE:N	2.30	0.47
2:F:100:ASN:O	2:F:104:ARG:HG3	2.15	0.47
2:J:58:VAL:HG12	2:J:69:ILE:HD11	1.96	0.47
2:J:209:LYS:HE2	2:J:209:LYS:HB3	1.75	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:B:195:LEU:HD23	2:B:195:LEU:C	2.36	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:F:71:ASP:N	2:F:72:PRO:CD	2.78	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
2:N:126:TYR:HB2	2:N:257:LEU:O	2.15	0.47
1:O:223:ALA:O	1:O:227:PRO:HG3	2.16	0.47
2:B:326:ILE:HD12	2:B:326:ILE:O	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:B:159:LEU:HD21	1:C:144:VAL:HG12	1.97	0.46
2:D:162:ARG:NH1	2:D:162:ARG:HB2	2.30	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
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
1:O:246:ILE:HD11	2:P:253:LEU:HD12	1.97	0.46
1:O:325:THR:HG22	1:O:331:GLY:CA	2.43	0.46
2:L:16:ASN:HB2	2:L:21:LYS:O	2.15	0.46
1:O:20:VAL:HG13	1:O:47:ILE:HG23	1.98	0.46
1:O:311:ILE:O	1:O:315:VAL:HG13	2.15	0.46
2:D:194:ARG:CB	2:D:194:ARG:NH2	2.77	0.46
1:K:324:HIS:CG	1:K:341:GLU:HG3	2.50	0.46
1:O:123:ILE:CD1	1:O:250:LEU:HB3	2.44	0.46
2:B:287:ILE:HD12	2:B:287:ILE:HA	1.73	0.46
2:B:342:THR:HG23	2:B:344:SER:N	2.31	0.46
1:E:149:GLU:OE1	1:G:149:GLU:OE1	2.34	0.46
2:D:331:GLU:HA	2:D:340:THR:OG1	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:181:VAL:HG11	1:G:243:LEU:HD11	1.98	0.46
1:G:195:ARG:O	1:G:199:THR:HG23	2.16	0.46
2:H:67:THR:O	2:H:102:THR:HG21	2.16	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:J:40:VAL:HG22	2:J:299:LEU:CD1	2.46	0.46
2:P:70:PRO:O	2:P:74:VAL:HG23	2.15	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:G:162:ILE:HD12	1:G:162:ILE:HA	1.73	0.46
2:H:321:ALA:C	2:H:325:THR:HG22	2.35	0.46
2:J:323:LEU:H	2:J:323:LEU:CD2	2.21	0.46
1:M:93:LEU:HD23	1:M:93:LEU:HA	1.83	0.46
2:D:58:VAL:HG12	2:D:69:ILE:HD11	1.96	0.46
2:D:183:ARG:HD2	2:D:237:ASP:OD2	2.16	0.46
1:E:120:ILE:HA	1:E:121:PRO:HD3	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:189:LYS:O	2:F:190:SER:C	2.54	0.46
1:I:139:LEU:HD23	1:I:151:LEU:HD12	1.98	0.46
1:I:275:HIS:CG	1:I:278:LEU:HD12	2.49	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:N:273:LYS:HE3	2:N:274:ILE:CD1	2.45	0.46
2:F:194:ARG:NH2	2:F:194:ARG:CB	2.78	0.46
2:F:228:VAL:HG22	2:F:235:TYR:CD1	2.50	0.46
2:F:326:ILE:HD12	2:F:326:ILE:O	2.16	0.46
2:H:5:GLN:CD	2:H:6:PRO:HD2	2.36	0.46
2:H:135:ARG:HD3	2:H:247:GLY:CA	2.38	0.46
1:A:324:HIS:CG	1:A:341:GLU:CG	2.99	0.46
2:D:162:ARG:HB2	2:D:162:ARG:HH11	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: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
2:B:26:PHE:O	2:B:27:ILE:HB	2.15	0.45
2:B:97:ARG:HH21	2:B:102:THR:CG2	2.27	0.45
2:D:41:LYS:HG2	2:D:53:TRP:NE1	2.30	0.45
2:F:153:VAL:HG21	2:H:150:CYS:SG	2.56	0.45
1:I:120:ILE:HA	1:I:121:PRO:HD3	1.72	0.45
1:M:28:VAL:HG23	1:M:281:LYS:HE2	1.97	0.45
2:P:303:VAL:HG21	2:P:319:GLN:HB2	1.99	0.45
1:A:281:LYS:HD3	1:A:281:LYS:HA	1.73	0.45
2:B:71:ASP:N	2:B:72:PRO:HD2	2.32	0.45
2:F:49:VAL:HA	2:F:50:PRO:HD3	1.72	0.45
1:G:155:THR:HG22	2:H:153:VAL:HG13	1.99	0.45
2:H:63:VAL:O	2:H:64:ASN:HB2	2.16	0.45
2:H:135:ARG:CD	2:H:247:GLY:HA3	2.38	0.45
1:I:45:ILE:HG23	1:I:46:PRO:HD2	1.97	0.45
2:J:71:ASP:N	2:J:72:PRO:HD2	2.31	0.45
2:J:274:ILE:HG22	2:J:275:SER:N	2.30	0.45
1:K:126:ILE:HD13	1:K:169:PHE:HE1	1.81	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:D:5:GLN:OE1	2:D:307:ASN:O	2.35	0.45
2:D:195:LEU:C	2:D:195:LEU:HD23	2.36	0.45
2:D:287:ILE:HD12	2:D:287:ILE:HA	1.79	0.45
2:H:59:SER:HA	2:H:60:PRO:HD3	1.78	0.45
2:H:139:GLU:H	2:H:139:GLU:HG2	1.60	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:P:189:LYS:O	2:P:190:SER:C	2.54	0.45
2:D:273:LYS:HE3	2:D:274:ILE:CD1	2.45	0.45
1:E:87:GLN:HA	1:E:274:ARG:HB3	1.98	0.45
1:E:279:ASP:N	1:E:279:ASP:OD1	2.50	0.45
2:J:47:ALA:CB	2:J:354:LEU:HD11	2.40	0.45
2:J:135:ARG:HD3	2:J:247:GLY:CA	2.35	0.45
2:J:326:ILE:HD12	2:J:326:ILE:O	2.17	0.45
2:L:265:THR:HA	2:L:266:PRO:HD3	1.75	0.45
2:L:273:LYS:HE3	2:L:274:ILE:CD1	2.45	0.45
2:N:5:GLN:HA	2:N:6:PRO:HD3	1.73	0.45
2:N:322:VAL:HG23	2:N:323:LEU:HG	1.98	0.45
2:P:118:SER:OG	2:P:129:VAL:HG13	2.16	0.45
2:D:44:PHE:CD2	2:D:49:VAL:HG21	2.51	0.45
1:E:13:LYS:HD2	1:E:18:PHE:CE1	2.52	0.45
2:F:69:ILE:HG22	2:F:106:THR:HG21	1.98	0.45
2:F:318:ILE:O	2:F:318:ILE:HG22	2.16	0.45
1:M:149:GLU:HA	2:N:158:LYS:O	2.17	0.45
2:P:67:THR:O	2:P:102:THR:HG21	2.16	0.45
1:A:25:GLY:HA2	1:A:81:TRP:CZ2	2.52	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
2:D:60:PRO:HG3	2:D:99:LEU:HD13	1.98	0.45
2:D:97:ARG:NH2	2:D:102:THR:HG23	2.30	0.45
2:F:145:ILE:HD12	1:G:141:HIS:ND1	2.32	0.45
1:G:56:GLN:C	1:G:58:ASP:N	2.65	0.45
2:H:43:ILE:HD13	2:H:350:VAL:HG11	1.97	0.45
2:H:90:THR:HG22	2:H:91:PRO:O	2.17	0.45
2:H:331:GLU:HA	2:H:340:THR:OG1	2.16	0.45
2:L:181:ARG:HA	2:L:182:PRO:HD3	1.79	0.45
1:M:304:LEU:O	1:M:305:ASN:CG	2.54	0.45
1:O:60:LYS:HE3	1:O:60:LYS:HB2	1.82	0.45
1:E:151:LEU:HA	2:F:156:SER:O	2.17	0.45
2:F:294:ASN:HA	2:F:295:PRO:HD3	1.73	0.45
1:K:149:GLU:HG3	2:L:159:LEU:CD1	2.47	0.45
2:L:43:ILE:HD13	2:L:350:VAL:HG11	1.99	0.45
2:N:331:GLU:HA	2:N:340:THR:OG1	2.17	0.45
2:P:150:CYS:CB	2:P:151:PRO:CD	2.94	0.45
1:C:155:THR:O	1:C:159:THR:HG22	2.16	0.45
1:E:45:ILE:HG23	1:E:46:PRO:HD2	1.99	0.45
1:E:54:ILE:HD13	1:E:81:TRP:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:181:ARG:HA	2:F:182:PRO:HD3	1.70	0.45
2:L:189:LYS:HB2	2:L:246:TYR:OH	2.17	0.45
1:M:287:ASN:CB	1:M:326:THR:HG21	2.47	0.45
1:A:175:ARG:HG3	1:A:231:ASP:OD1	2.16	0.45
1:A:182:HIS:HE2	1:A:213:SER:HB3	1.81	0.45
2:B:166:GLU:O	2:B:166:GLU:HG2	2.16	0.45
2:D:49:VAL:HG12	2:D:314:HIS:ND1	2.32	0.45
2:D:67:THR:HG21	2:D:97:ARG:N	2.32	0.45
2:F:16:ASN:HB2	2:F:21:LYS:O	2.17	0.45
2:H:26:PHE:O	2:H:27:ILE:HB	2.17	0.45
2:H:49:VAL:HA	2:H:50:PRO:HD3	1.72	0.45
2:H:342:THR:HG22	2:H:345:SER:HB3	1.99	0.45
1:K:45:ILE:HG12	1:K:307:TYR:CD2	2.52	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:71:ASP:N	2:P:72:PRO:HD2	2.32	0.45
2:B:135:ARG:CD	2:B:247:GLY:HA3	2.37	0.45
2:B:273:LYS:HE3	2:B:274:ILE:CD1	2.45	0.45
2:D:303:VAL:HG21	2:D:319:GLN:HB2	1.99	0.45
1:I:323:LYS:O	1:I:324:HIS:HB2	2.17	0.45
2:J:109:LEU:HD13	2:J:269:ASN:HB3	1.98	0.45
1:M:155:THR:O	1:M:159:THR:HG22	2.16	0.45
2:P:190:SER:O	2:P:194:ARG:HG2	2.16	0.45
2:P:291:ASP:C	2:P:343:THR:HG22	2.37	0.45
2:P:326:ILE:HD11	2:P:346:PHE:CD1	2.51	0.45
1:A:55:LYS:HD3	1:A:59:HIS:ND1	2.32	0.44
2:B:326:ILE:HG12	2:B:350:VAL:CG2	2.47	0.44
2:D:69:ILE:HG22	2:D:106:THR:HG21	1.98	0.44
1:E:38:THR:HG22	1:E:343:ILE:CD1	2.43	0.44
2:F:326:ILE:HD11	2:F:346:PHE:CD1	2.52	0.44
1:G:281:LYS:HD3	1:G:282:GLY:N	2.32	0.44
2:H:130:ASP:HB3	2:H:236:THR:HB	1.99	0.44
2:J:15:PRO:HG3	2:J:22:TYR:CZ	2.52	0.44
1:K:88:THR:HB	2:L:189:LYS:HE3	1.98	0.44
2:L:318:ILE:O	2:L:318:ILE:HG22	2.16	0.44
1:M:80:LEU:HD21	1:M:271:PRO:HG2	1.98	0.44
2:N:100:ASN:O	2:N:104:ARG:HG3	2.17	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:N:150:CYS:CB	2:N:151:PRO:CD	2.95	0.44
2:B:49:VAL:HA	2:B:50:PRO:HD3	1.73	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
1:G:324:HIS:CG	1:G:341:GLU:HG3	2.52	0.44
2:J:326:ILE:HG12	2:J:350:VAL:CG2	2.48	0.44
2:N:15:PRO:HG3	2:N:22:TYR:CZ	2.52	0.44
2:N:150:CYS:SG	2:P:153:VAL:HG21	2.56	0.44
2:N:265:THR:HA	2:N:266:PRO:HD3	1.67	0.44
2:P:228:VAL:HG22	2:P:235:TYR:CD1	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:D:209:LYS:HE2	2:D:209:LYS:HB3	1.73	0.44
2:D:265:THR:HA	2:D:266:PRO:HD3	1.69	0.44
2:J:194:ARG:NH2	2:J:194:ARG:CB	2.79	0.44
2:L:173:PHE:CD2	2:L:184:VAL:HG11	2.52	0.44
2:L:323:LEU:H	2:L:323:LEU:CD2	2.21	0.44
1:M:324:HIS:HA	1:M:333:SER:OG	2.17	0.44
1:A:275:HIS:CE1	1:A:278:LEU:CD1	3.01	0.44
2:B:12:THR:HB	2:B:81:LEU:HD12	1.99	0.44
1:G:202:GLY:HA3	1:G:211:VAL:HG21	1.99	0.44
2:H:166:GLU:O	2:H:167:ARG:HB2	2.17	0.44
2:H:228:VAL:HG12	2:H:257:LEU:CD1	2.46	0.44
2:L:71:ASP:N	2:L:72:PRO:HD2	2.32	0.44
2:L:287:ILE:HD12	2:L:287:ILE:HA	1.79	0.44
1:M:143:SER:HB3	2:P:159:LEU:CD2	2.45	0.44
2:N:88:LEU:HD13	2:N:99:LEU:HD23	1.99	0.44
2:P:162:ARG:NH1	2:P:162:ARG:HB2	2.33	0.44
2:P:182:PRO:HD2	2:P:237:ASP:O	2.17	0.44
2:P:316:ASP:O	2:P:320:ASN:CB	2.66	0.44
2:P:331:GLU:HA	2:P:340:THR:OG1	2.17	0.44
2:B:109:LEU:HD13	2:B:269:ASN:HB3	2.00	0.44
2:D:316:ASP:O	2:D:320:ASN:CB	2.66	0.44
1:E:162:ILE:HD12	1:E:162:ILE:HA	1.76	0.44
2:F:103:LEU:HD12	2:F:103:LEU:HA	1.82	0.44
2:F:331:GLU:HA	2:F:340:THR:OG1	2.17	0.44
1:G:189:LEU:HA	1:G:189:LEU:HD12	1.73	0.44
2:H:270:ILE:HD12	2:H:270:ILE:N	2.33	0.44
2:J:294:ASN:HA	2:J:295:PRO:HD3	1.75	0.44
1:K:304:LEU:O	1:K:305:ASN:CG	2.56	0.44
2:L:49:VAL:HA	2:L:50:PRO:HD3	1.69	0.44
1:M:182:HIS:HE2	1:M:213:SER:HB3	1.81	0.44
1:A:120:ILE:HA	1:A:121:PRO:HD3	1.69	0.44
2:B:351:ILE:HA	2:B:354:LEU:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:H:71:ASP:N	2:H:72:PRO:HD2	2.32	0.44
2:H:342:THR:HG23	2:H:344:SER:N	2.33	0.44
1:I:156:ARG:N	1:I:157:PRO:CD	2.81	0.44
2:J:69:ILE:HG22	2:J:106:THR:HG21	2.00	0.44
2:L:41:LYS:HG2	2:L:53:TRP:NE1	2.33	0.44
1:M:45:ILE:HG23	1:M:46:PRO:HD2	2.00	0.44
2:N:71:ASP:N	2:N:72:PRO:CD	2.81	0.44
1:O:323:LYS:O	1:O:324:HIS:HB2	2.18	0.44
1:A:43:GLU:OE2	1:A:346:LEU:HG	2.18	0.44
2:B:294:ASN:HA	2:B:295:PRO:HD3	1.74	0.44
1:C:149:GLU:HG3	2:D:159:LEU:HD12	1.99	0.44
2:D:103:LEU:HD12	2:D:103:LEU:HA	1.83	0.44
2:D:199:LEU:HD23	2:D:199:LEU:C	2.38	0.44
2:F:322:VAL:HG23	2:F:323:LEU:HG	2.00	0.44
1:G:90:HIS:HB3	2:H:193:GLN:OE1	2.18	0.44
1:G:104:TYR:CZ	1:G:161:ARG:HD2	2.53	0.44
1:G:310:ARG:HG2	1:G:349:MET:HE2	1.99	0.44
2:H:299:LEU:HD12	2:H:299:LEU:HA	1.86	0.44
1:O:45:ILE:HG12	1:O:307:TYR:CD2	2.52	0.44
2:P:264:LEU:HD21	2:P:337:LEU:HD21	1.98	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:166:GLU:O	2:J:166:GLU:HG2	2.18	0.44
2:J:348:GLU:O	2:J:352:LYS:HG2	2.17	0.44
2:L:166:GLU:O	2:L:166:GLU:HG2	2.17	0.44
2:P:199:LEU:HD23	2:P:199:LEU:C	2.38	0.44
2:B:26:PHE:O	2:B:27:ILE:CB	2.66	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
1:G:323:LYS:O	1:G:324:HIS:HB2	2.17	0.44
1:K:60:LYS:HE3	1:K:60:LYS:HB2	1.83	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
2:N:299:LEU:HD12	2:N:299:LEU:HA	1.80	0.44
1:O:155:THR:O	1:O:159:THR:HG22	2.17	0.44
2:P:209:LYS:HE2	2:P:209:LYS:HB3	1.78	0.44
2:B:63:VAL:O	2:B:64:ASN:HB2	2.18	0.43
2:B:342:THR:HG23	2:B:345:SER:H	1.82	0.43
1:C:104:TYR:CZ	1:C:161:ARG:HD2	2.53	0.43

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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:316:ASP:O	2:L:320:ASN:CB	2.66	0.43
2:N:326:ILE:HG12	2:N:350:VAL:HG23	2.00	0.43
1:A:17:ARG:NH1	1:A:48:ASP:OD1	2.52	0.43
1:A:156:ARG:N	1:A:157:PRO:CD	2.81	0.43
2:B:162:ARG:HB2	2:B:162:ARG:HH11	1.84	0.43
2:D:326:ILE:O	2:D:326:ILE:HD12	2.19	0.43
2:J:321:ALA:C	2:J:325:THR:HG22	2.39	0.43
2:L:321:ALA:C	2:L:325:THR:HG22	2.39	0.43
1:O:155:THR:O	1:O:159:THR:HG23	2.18	0.43
2:P:321:ALA:C	2:P:325:THR:HG22	2.39	0.43
1:A:162:ILE:HD12	1:A:162:ILE:HA	1.74	0.43
2:D:59:SER:HA	2:D:60:PRO:HD3	1.80	0.43
1:G:113:LEU:CD1	1:G:256:LEU:HD22	2.47	0.43
2:H:13:GLY:O	2:H:14:LYS:HB3	2.19	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:318:ILE:O	2:H:318:ILE:HG22	2.18	0.43
1:I:93:LEU:HD23	1:I:93:LEU:HA	1.86	0.43
1:M:245:ASN:CB	2:N:225:VAL:HG22	2.49	0.43
1:O:202:GLY:HA3	1:O:211:VAL:HG21	2.01	0.43
1:C:321:GLU:O	1:C:323:LYS:N	2.52	0.43
2:D:136:GLU:OE2	2:D:138:THR:HB	2.18	0.43
2:H:209:LYS:HE2	2:H:209:LYS:HB3	1.72	0.43
2:J:16:ASN:HB2	2:J:21:LYS:O	2.19	0.43
2:J:270:ILE:N	2:J:270:ILE:HD12	2.33	0.43
2:J:322:VAL:CG2	2:J:323:LEU:N	2.75	0.43
2:L:209:LYS:HE2	2:L:209:LYS:HB3	1.73	0.43
2:N:228:VAL:HG22	2:N:235:TYR:CE1	2.53	0.43
2:N:233:SER:HA	2:N:236:THR:HG23	2.00	0.43
2:N:287:ILE:CG1	2:N:292:LYS:HB2	2.48	0.43
2:P:181:ARG:HA	2:P:182:PRO:HD3	1.78	0.43
2:P:287:ILE:HD12	2:P:287:ILE:HA	1.85	0.43
2:D:270:ILE:N	2:D:270:ILE:HD12	2.34	0.43
2:D:318:ILE:C	2:D:322:VAL:HG11	2.39	0.43
2:D:321:ALA:C	2:D:325:THR:HG22	2.40	0.43
1:G:151:LEU:HB3	2:H:155:GLN:NE2	2.34	0.43
1:I:277:GLY:O	1:I:278:LEU:C	2.57	0.43
1:K:133:GLU:HG2	1:K:153:VAL:O	2.19	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
1:A:325:THR:CG2	1:A:329:ILE:HG13	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:265:THR:HA	2:B:266:PRO:HD3	1.69	0.43
2:D:109:LEU:HD13	2:D:269:ASN:HB3	2.00	0.43
2:D:175:TYR:O	2:D:179:ILE:HG12	2.19	0.43
2:D:323:LEU:H	2:D:323:LEU:CD2	2.22	0.43
1:I:90:HIS:CG	2:J:193:GLN:HG3	2.54	0.43
1:K:140:GLU:OE2	2:L:194:ARG:HA	2.19	0.43
1:M:60:LYS:HE3	1:M:60:LYS:HB2	1.84	0.43
2:N:49:VAL:HG12	2:N:314:HIS:ND1	2.33	0.43
2:N:157:ILE:CD1	1:O:151:LEU:CD1	2.97	0.43
2:P:348:GLU:O	2:P:352:LYS:HG2	2.19	0.43
1:A:20:VAL:HG13	1:A:47:ILE:HG23	2.01	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
2:B:209:LYS:HE2	2:B:209:LYS:HB3	1.76	0.42
2:B:212:PRO:HG2	1:O:228:HIS:HD2	1.77	0.42
2:D:322:VAL:HG23	2:D:323:LEU:HG	2.01	0.42
1:E:181:VAL:HG11	1:E:243:LEU:HD11	2.00	0.42
1:K:77:LEU:HD23	1:K:77:LEU:HA	1.84	0.42
2:N:342:THR:HG23	2:N:344:SER:N	2.33	0.42
2:D:139:GLU:H	2:D:139:GLU:HG2	1.65	0.42
2:F:299:LEU:HD12	2:F:299:LEU:HA	1.81	0.42
2:J:126:TYR:HB2	2:J:257:LEU:O	2.19	0.42
1:K:55:LYS:HD3	1:K:55:LYS:HA	1.90	0.42
1:K:116:VAL:HG23	1:K:319:ILE:HD13	2.01	0.42
1:K:162:ILE:HD12	1:K:162:ILE:HA	1.81	0.42
2:L:228:VAL:HG12	2:L:257:LEU:CD1	2.48	0.42
2:L:331:GLU:HA	2:L:340:THR:OG1	2.19	0.42
2:N:71:ASP:N	2:N:72:PRO:HD2	2.35	0.42
2:N:326:ILE:HD11	2:N:346:PHE:CD1	2.54	0.42
2:P:40:VAL:HG22	2:P:299:LEU:HD13	2.01	0.42
2:P:49:VAL:HA	2:P:50:PRO:HD3	1.69	0.42
1:A:75:ILE:HD12	1:A:75:ILE:HG23	1.84	0.42
2:B:126:TYR:HB2	2:B:257:LEU:O	2.19	0.42
2:B:342:THR:HG22	2:B:345:SER:CB	2.49	0.42
1:E:288:PRO:O	1:E:292:ILE:HG13	2.19	0.42
2:F:264:LEU:HD21	2:F:337:LEU:HD21	2.00	0.42
1:I:45:ILE:HG12	1:I:307:TYR:CD2	2.54	0.42
1:I:126:ILE:HD13	1:I:169:PHE:HE1	1.84	0.42
2:J:195:LEU:HD23	2:J:195:LEU:C	2.40	0.42
1:M:90:HIS:HB2	2:N:193:GLN:HG3	1.99	0.42
2:P:294:ASN:HA	2:P:295:PRO:HD3	1.75	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:113:VAL:HB	2:D:268:ALA:HB3	2.02	0.42
1:E:116:VAL:HG23	1:E:319:ILE:HD13	2.00	0.42
1:G:344:ASN:O	1:G:348:THR:HG23	2.19	0.42
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: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:O:344:ASN:O	1:O:348:THR:HG23	2.20	0.42
2:B:228:VAL:HG12	2:B:257:LEU:CD1	2.50	0.42
1:C:202:GLY:HA3	1:C:211:VAL:HG21	2.02	0.42
2:D:16:ASN:HB2	2:D:21:LYS:O	2.20	0.42
2:D:118:SER:OG	2:D:129:VAL:HG13	2.20	0.42
2:D:318:ILE:O	2:D:318:ILE:HG22	2.19	0.42
2:D:326:ILE:HG21	2:D:350:VAL:HG22	2.01	0.42
2:D:351:ILE:HG23	2:D:354:LEU:HD23	2.00	0.42
2:F:157:ILE:CD1	1:G:151:LEU:HD11	2.49	0.42
2:H:166:GLU:O	2:H:166:GLU:HG2	2.19	0.42
1:K:148:VAL:HB	2:L:160:ILE:HG22	2.00	0.42
1:K:242:ILE:HD11	2:L:221:ILE:HD13	2.01	0.42
1:O:104:TYR:CZ	1:O:161:ARG:HD2	2.55	0.42
1:A:287:ASN:CB	1:A:326:THR:HG21	2.49	0.42
1:C:77:LEU:HD23	1:C:77:LEU:HA	1.91	0.42
1:C:182:HIS:HE2	1:C:213:SER:HB3	1.84	0.42
1:E:8:ARG:C	1:E:10:LEU:H	2.22	0.42
2:H:189:LYS:O	2:H:190:SER:C	2.57	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
2:J:326:ILE:HD11	2:J:346:PHE:CD1	2.55	0.42
1:O:162:ILE:HD12	1:O:162:ILE:HA	1.73	0.42
1:A:218:ASN:O	1:A:222:GLN:HB2	2.20	0.42
2:B:103:LEU:HD12	2:B:103:LEU:HA	1.81	0.42
2:B:326:ILE:HG12	2:B:350:VAL:HG23	2.02	0.42
1:E:20:VAL:HG13	1:E:47:ILE:HG23	2.00	0.42
2:F:334:THR:HB	2:F:336:ASP:OD1	2.20	0.42
2:H:334:THR:HB	2:H:336:ASP:OD1	2.20	0.42
1:I:90:HIS:HB3	2:J:193:GLN:HG3	2.00	0.42
1:I:304:LEU:O	1:I:305:ASN:CG	2.58	0.42
2:J:44:PHE:O	2:J:49:VAL:HG22	2.20	0.42
1:M:245:ASN:HB3	2:N:225:VAL:HG22	2.01	0.42
2:B:299:LEU:HD12	2:B:299:LEU:HA	1.95	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:321:ALA:C	2:B:325:THR:HG22	2.40	0.42
1:C:175:ARG:HG3	1:C:231:ASP:OD1	2.20	0.42
1:C:288:PRO:O	1:C:292:ILE:HG13	2.20	0.42
2:D:326:ILE:HD11	2:D:346:PHE:CD1	2.55	0.42
1:E:277:GLY:HA3	2:F:226:LEU:HD12	2.01	0.42
2:F:287:ILE:CG1	2:F:292:LYS:HB2	2.48	0.42
2:H:5:GLN:CG	2:H:6:PRO:HD2	2.49	0.42
1:K:90:HIS:HB3	2:L:193:GLN:HG3	2.01	0.42
2:L:40:VAL:HG22	2:L:299:LEU:CD1	2.50	0.42
2:L:326:ILE:HG12	2:L:350:VAL:CG2	2.50	0.42
1:M:276:VAL:HG11	2:N:222:ASP:HB3	2.02	0.42
2:N:303:VAL:HG21	2:N:319:GLN:HB2	2.01	0.42
2:B:287:ILE:HG13	2:B:292:LYS:HB2	2.02	0.42
2:D:228:VAL:HG12	2:D:257:LEU:CD1	2.49	0.42
1:E:123:ILE:CD1	1:E:250:LEU:HB3	2.50	0.42
1:G:194:PHE:O	1:G:198:ILE:HG12	2.20	0.42
2:H:172:ALA:HB2	2:H:241:VAL:CG1	2.49	0.42
1:I:202:GLY:HA3	1:I:211:VAL:HG21	2.01	0.42
2:J:303:VAL:HG21	2:J:319:GLN:HB2	2.01	0.42
2:J:331:GLU:HA	2:J:340:THR:OG1	2.20	0.42
1:K:80:LEU:HD21	1:K:271:PRO:HG2	2.02	0.42
2:L:44:PHE:O	2:L:49:VAL:HG22	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:P:323:LEU:H	2:P:323:LEU:CD2	2.22	0.42
2:B:316:ASP:O	2:B:320:ASN:CB	2.68	0.42
2:D:135:ARG:HD3	2:D:247:GLY:CA	2.36	0.42
2:F:194:ARG:CG	2:F:194:ARG:NH2	2.58	0.42
2:F:260:GLY:O	2:F:261:SER:HB3	2.19	0.42
1:G:156:ARG:HG2	1:G:157:PRO:HD3	2.02	0.42
1:I:288:PRO:O	1:I:292:ILE:HG13	2.20	0.42
2:J:47:ALA:HB2	2:J:354:LEU:HD21	2.02	0.42
2:J:189:LYS:O	2:J:190:SER:C	2.58	0.42
2:L:136:GLU:HA	2:L:168:VAL:HG11	2.01	0.42
2:N:26:PHE:O	2:N:27:ILE:HB	2.19	0.42
1:O:45:ILE:HG23	1:O:46:PRO:HD2	2.01	0.42
2:P:26:PHE:O	2:P:27:ILE:HB	2.19	0.42
2:P:194:ARG:CG	2:P:194:ARG:NH2	2.56	0.42
1:C:15:GLY:O	1:G:301:HIS:CE1	2.61	0.41
2:F:66:LEU:CD2	2:F:97:ARG:HH21	2.32	0.41
2:H:11:TYR:CD1	2:H:309:MET:HA	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:59:SER:HA	2:J:60:PRO:HD3	1.79	0.41
1:K:123:ILE:CD1	1:K:250:LEU:HB3	2.49	0.41
1:K:287:ASN:HA	1:K:288:PRO:HD3	1.89	0.41
2:L:139:GLU:H	2:L:139:GLU:HG2	1.67	0.41
1:M:344:ASN:O	1:M:348:THR:HG23	2.19	0.41
2:P:69:ILE:HG22	2:P:106:THR:HG21	2.02	0.41
2:P:162:ARG:HB2	2:P:162:ARG:HH11	1.84	0.41
2:P:233:SER:HA	2:P:236:THR:HG23	2.02	0.41
2:B:35:GLU:H	2:B:35:GLU:HG2	1.71	0.41
2:B:47:ALA:CA	2:B:354:LEU:HD21	2.50	0.41
2:D:5:GLN:HA	2:D:6:PRO:HD3	1.95	0.41
2:F:273:LYS:HE3	2:F:274:ILE:CD1	2.48	0.41
2:H:5:GLN:NE2	2:H:308:HIS:HA	2.35	0.41
2:H:40:VAL:HG22	2:H:299:LEU:HD13	2.02	0.41
2:H:100:ASN:O	2:H:104:ARG:HG3	2.20	0.41
2:H:189:LYS:HB2	2:H:246:TYR:OH	2.20	0.41
1:I:182:HIS:HE2	1:I:213:SER:HB3	1.85	0.41
2:L:97:ARG:HH11	2:L:101:LEU:HD12	1.84	0.41
1:M:104:TYR:CE1	1:M:161:ARG:HD2	2.55	0.41
2:N:274:ILE:CG2	2:N:275:SER:N	2.83	0.41
1:A:133:GLU:OE1	1:A:155:THR:HG23	2.20	0.41
1:A:283:GLN:O	1:A:285:VAL:HG13	2.19	0.41
2:B:150:CYS:HB2	2:B:151:PRO:CD	2.51	0.41
2:B:214:LEU:HD12	2:B:214:LEU:HA	1.89	0.41
2:F:130:ASP:O	2:F:181:ARG:NH2	2.53	0.41
2:F:299:LEU:O	2:F:302:SER:HB2	2.20	0.41
2:H:97:ARG:HH11	2:H:101:LEU:CD1	2.27	0.41
1:M:126:ILE:HD13	1:M:169:PHE:HE1	1.85	0.41
2:N:13:GLY:O	2:N:14:LYS:HB3	2.21	0.41
2:P:317:GLN:O	2:P:322:VAL:HG13	2.21	0.41
2:B:13:GLY:O	2:B:14:LYS:HB3	2.20	0.41
2:D:40:VAL:HG22	2:D:299:LEU:CD1	2.50	0.41
2:D:85:LYS:HE2	2:D:88:LEU:HD21	2.02	0.41
1:I:162:ILE:HD12	1:I:162:ILE:HA	1.79	0.41
1:I:301:HIS:HE1	1:M:15:GLY:O	2.02	0.41
2:J:265:THR:HA	2:J:266:PRO:HD3	1.70	0.41
2:J:287:ILE:HG13	2:J:292:LYS:HB2	2.01	0.41
1:K:156:ARG:N	1:K:157:PRO:CD	2.83	0.41
2:L:59:SER:HA	2:L:60:PRO:HD3	1.80	0.41
2:L:228:VAL:HG22	2:L:235:TYR:CD1	2.56	0.41
1:M:90:HIS:HB3	2:N:193:GLN:OE1	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:264:LEU:HD21	2:N:337:LEU:HD21	2.01	0.41
1:A:250:LEU:HD12	1:A:250:LEU:HA	1.92	0.41
1:C:87:GLN:HA	1:C:274:ARG:HB3	2.03	0.41
2:D:49:VAL:HA	2:D:50:PRO:HD3	1.72	0.41
1:G:325:THR:HG22	1:G:331:GLY:CA	2.47	0.41
1:I:156:ARG:HG2	1:I:157:PRO:HD3	2.03	0.41
2:J:322:VAL:HG23	2:J:323:LEU:HG	2.01	0.41
1:K:346:LEU:HD12	1:K:346:LEU:HA	1.90	0.41
2:L:109:LEU:HD13	2:L:269:ASN:HB3	2.03	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:O:181:VAL:HG11	1:O:243:LEU:HD11	2.02	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:J:316:ASP:O	2:J:320:ASN:CB	2.69	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:N:136:GLU:OE2	2:N:138:THR:HB	2.21	0.41
2:B:60:PRO:HG3	2:B:99:LEU:HD13	2.03	0.41
1:C:55:LYS:HD3	1:C:55:LYS:HA	1.82	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
2:F:109:LEU:HD13	2:F:269:ASN:HB3	2.02	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:J:136:GLU:OE2	2:J:138:THR:HB	2.20	0.41
1:K:189:LEU:HA	1:K:189:LEU:HD12	1.75	0.41
2:L:26:PHE:O	2:L:27:ILE:HB	2.20	0.41
1:M:254:PRO:HD2	1:M:278:LEU:HD23	2.02	0.41
2:N:181:ARG:HA	2:N:182:PRO:HD3	1.74	0.41
2:N:318:ILE:O	2:N:318:ILE:HG22	2.21	0.41
2:P:175:TYR:O	2:P:179:ILE:HG12	2.21	0.41
1:A:77:LEU:HD23	1:A:77:LEU:HA	1.92	0.41
2:B:118:SER:OG	2:B:129:VAL:HG13	2.20	0.41
1:G:45:ILE:HG23	1:G:46:PRO:HD2	2.03	0.41
2:J:40:VAL:HG22	2:J:299:LEU:HD13	2.02	0.41
1:K:140:GLU:HB3	2:L:195:LEU:HD21	2.02	0.41
1:K:182:HIS:HE2	1:K:213:SER:HB3	1.86	0.41
2:N:189:LYS:HB2	2:N:246:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:45:ILE:HA	1:O:46:PRO:HD3	1.88	0.41
1:O:126:ILE:HD13	1:O:169:PHE:HE1	1.85	0.41
2:P:195:LEU:C	2:P:195:LEU:HD23	2.41	0.41
2:B:334:THR:HG22	2:B:335:GLY:H	1.84	0.41
1:C:37:ARG:HH11	1:C:37:ARG:HD3	1.76	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
1:C:156:ARG:N	1:C:157:PRO:CD	2.84	0.41
2:D:136:GLU:HA	2:D:168:VAL:HG11	2.03	0.41
2:F:162:ARG:HB2	2:F:162:ARG:HH11	1.86	0.41
2:F:287:ILE:HA	2:F:287:ILE:HD12	1.81	0.41
2:F:323:LEU:H	2:F:323:LEU:CD2	2.12	0.41
1:G:45:ILE:HG12	1:G:307:TYR:CD2	2.56	0.41
1:G:54:ILE:H	1:G:54:ILE:CD1	2.02	0.41
1:G:175:ARG:CG	1:G:175:ARG:NH1	2.59	0.41
2:H:39:SER:HB2	2:H:347:THR:CG2	2.51	0.41
2:H:250:LEU:HD23	2:H:250:LEU:HA	1.81	0.41
2:H:287:ILE:HA	2:H:287:ILE:HD12	1.80	0.41
1:I:80:LEU:HD21	1:I:271:PRO:HG2	2.02	0.41
1:I:155:THR:O	1:I:159:THR:HG22	2.21	0.41
1:I:319:ILE:O	1:I:319:ILE:HD12	2.21	0.41
2:J:60:PRO:HG3	2:J:99:LEU:HD13	2.03	0.41
2:J:183:ARG:HD2	2:J:237:ASP:OD2	2.20	0.41
2:L:189:LYS:O	2:L:190:SER:C	2.59	0.41
1:M:12:LYS:HB3	1:M:19:THR:HB	2.03	0.41
1:M:43:GLU:OE2	1:M:346:LEU:HG	2.21	0.41
1:M:149:GLU:CG	2:N:159:LEU:CD1	2.98	0.41
1:M:162:ILE:HD12	1:M:162:ILE:HA	1.73	0.41
2:N:7:SER:HA	2:N:10:ARG:HG2	2.03	0.41
1:O:194:PHE:O	1:O:198:ILE:HG12	2.21	0.41
1:O:221:MET:SD	2:P:262:LEU:HD22	2.61	0.41
2:B:59:SER:HA	2:B:60:PRO:HD3	1.80	0.41
2:B:322:VAL:CG2	2:B:323:LEU:H	2.34	0.41
2:D:133:LEU:HD23	2:D:251:SER:HB3	2.03	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:182:PRO:HD2	2:H:237:ASP:O	2.21	0.41
2:H:228:VAL:HG22	2:H:235:TYR:CD1	2.56	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: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: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
1:E:278:LEU:HD22	1:E:278:LEU:HA	1.74	0.40
1:E:280:ILE:HG22	1:E:327:ARG:CZ	2.51	0.40
1:E:346:LEU:HD12	1:E:346:LEU:HA	1.94	0.40
2:F:39:SER:OG	2:F:347:THR:HG22	2.20	0.40
2:H:69:ILE:CD1	2:H:70:PRO:HD2	2.50	0.40
2:H:199:LEU:C	2:H:199:LEU:HD23	2.42	0.40
1:I:344:ASN:O	1:I:348:THR:HG23	2.20	0.40
2:L:5:GLN:HE21	2:L:5:GLN:CA	2.33	0.40
2:N:49:VAL:HA	2:N:50:PRO:HD3	1.70	0.40
2:P:62:PHE:CZ	2:P:67:THR:HG22	2.56	0.40
1:A:104:TYR:CE1	1:A:161:ARG:HD2	2.56	0.40
1:A:181:VAL:HG11	1:A:243:LEU:HD11	2.04	0.40
1:A:304:LEU:O	1:A:305:ASN:CG	2.60	0.40
2:B:5:GLN:CD	2:B:6:PRO:HD2	2.42	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
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
2:L:274:ILE:HG22	2:L:275:SER:N	2.36	0.40
2:N:26:PHE:CD2	2:N:28:GLU:HG2	2.57	0.40
2:P:342:THR:HG22	2:P:345:SER:HB3	2.02	0.40
1:A:45:ILE:HG23	1:A:46:PRO:HD2	2.04	0.40
1:A:202:GLY:HA3	1:A:211:VAL:HG21	2.03	0.40
2:B:43:ILE:HD13	2:B:350:VAL:HG11	2.03	0.40
1:C:79:GLY:HA2	1:C:291:MET:HE3	2.04	0.40
2:D:181:ARG:HA	2:D:182:PRO:HD3	1.80	0.40
2:D:228:VAL:HG22	2:D:235:TYR:CD1	2.57	0.40
2:F:59:SER:HA	2:F:60:PRO:HD3	1.77	0.40
1:G:60:LYS:HE3	1:G:60:LYS:HB2	1.83	0.40
1:G:241:THR:HG21	2:H:189:LYS:NZ	2.36	0.40
1:G:293:LEU:HD23	1:G:293:LEU:HA	1.89	0.40
2:J:159:LEU:CD2	1:K:143:SER:HB3	2.44	0.40
2:J:172:ALA:HB2	2:J:241:VAL:CG1	2.51	0.40
2:L:287:ILE:HG13	2:L:292:LYS:HB2	2.02	0.40
2:L:299:LEU:HD12	2:L:299:LEU:HA	1.84	0.40
2:D:317:GLN:O	2:D:322:VAL:HG13	2.21	0.40
2:F:15:PRO:HG3	2:F:22:TYR:CZ	2.57	0.40
2:J:7:SER:HA	2:J:10:ARG:HG2	2.04	0.40
1:M:104:TYR:CZ	1:M:161:ARG:HD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:316:ASP:O	2:N:320:ASN:CB	2.70	0.40
2:P:172:ALA:HB2	2:P:241:VAL:CG1	2.52	0.40
2:P:334:THR:HB	2:P:336:ASP:OD1	2.20	0.40
1:C:304:LEU:O	1:C:305:ASN:CG	2.60	0.40
1:E:344:ASN:O	1:E:348:THR:HG23	2.21	0.40
2:F:7:SER:HA	2:F:10:ARG:CG	2.50	0.40
2:F:26:PHE:O	2:F:27:ILE:HB	2.22	0.40
2:F:224:SER:O	2:F:228:VAL:HG23	2.21	0.40
2:H:35:GLU:H	2:H:35:GLU:HG2	1.71	0.40
2:N:270:ILE:N	2:N:270:ILE:CD1	2.83	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%)	13	32
1	C	334/349 (96%)	315 (94%)	16 (5%)	3 (1%)	17	40
1	E	337/349 (97%)	320 (95%)	12 (4%)	5 (2%)	10	26
1	G	330/349 (95%)	309 (94%)	14 (4%)	7 (2%)	7	18
1	I	331/349 (95%)	310 (94%)	16 (5%)	5 (2%)	10	26
1	K	334/349 (96%)	315 (94%)	15 (4%)	4 (1%)	13	32
1	M	333/349 (95%)	315 (95%)	15 (4%)	3 (1%)	17	40
1	O	328/349 (94%)	309 (94%)	16 (5%)	3 (1%)	17	40
2	B	342/354 (97%)	310 (91%)	23 (7%)	9 (3%)	5	13
2	D	341/354 (96%)	307 (90%)	25 (7%)	9 (3%)	5	13
2	F	341/354 (96%)	307 (90%)	26 (8%)	8 (2%)	6	16
2	H	341/354 (96%)	304 (89%)	29 (8%)	8 (2%)	6	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	J	341/354 (96%)	309 (91%)	24 (7%)	8 (2%)	6	16
2	L	342/354 (97%)	306 (90%)	27 (8%)	9 (3%)	5	13
2	N	341/354 (96%)	301 (88%)	30 (9%)	10 (3%)	4	10
2	P	322/354 (91%)	289 (90%)	27 (8%)	6 (2%)	8	20
All	All	5369/5624 (96%)	4937 (92%)	331 (6%)	101 (2%)	8	20

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%)	8 19
1	C	283/289 (98%)	254 (90%)	29 (10%)	7 17
1	E	285/289 (99%)	250 (88%)	35 (12%)	4 11

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	G	278/289 (96%)	248 (89%)	30 (11%)	6	15
1	I	279/289 (96%)	251 (90%)	28 (10%)	7	18
1	K	283/289 (98%)	252 (89%)	31 (11%)	6	14
1	M	281/289 (97%)	254 (90%)	27 (10%)	8	19
1	O	276/289 (96%)	249 (90%)	27 (10%)	8	18
2	B	292/297 (98%)	264 (90%)	28 (10%)	8	19
2	D	291/297 (98%)	263 (90%)	28 (10%)	8	19
2	F	291/297 (98%)	262 (90%)	29 (10%)	7	18
2	H	291/297 (98%)	263 (90%)	28 (10%)	8	19
2	J	291/297 (98%)	263 (90%)	28 (10%)	8	19
2	L	292/297 (98%)	263 (90%)	29 (10%)	8	18
2	N	291/297 (98%)	265 (91%)	26 (9%)	9	22
2	P	275/297 (93%)	248 (90%)	27 (10%)	8	18
All	All	4558/4688 (97%)	4101 (90%)	457 (10%)	7	18

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

Sometimes 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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	335/349 (95%)	-0.04	13 (3%) 39 38	13, 38, 80, 100	0
1	C	338/349 (96%)	-0.08	3 (0%) 84 85	11, 38, 75, 93	0
1	E	341/349 (97%)	-0.15	4 (1%) 79 80	18, 42, 78, 117	0
1	G	334/349 (95%)	-0.08	3 (0%) 84 85	16, 41, 79, 96	0
1	I	333/349 (95%)	0.05	14 (4%) 36 35	17, 40, 78, 113	0
1	K	338/349 (96%)	-0.17	1 (0%) 94 95	13, 41, 78, 98	0
1	M	337/349 (96%)	0.90	66 (19%) 1 0	21, 48, 91, 121	0
1	O	332/349 (95%)	-0.20	4 (1%) 79 80	17, 43, 79, 97	0
2	B	346/354 (97%)	0.27	15 (4%) 35 33	21, 60, 102, 119	0
2	D	345/354 (97%)	0.22	18 (5%) 27 25	21, 66, 105, 123	0
2	F	345/354 (97%)	0.51	40 (11%) 4 3	24, 69, 107, 121	0
2	H	345/354 (97%)	0.47	35 (10%) 7 5	24, 69, 108, 127	0
2	J	345/354 (97%)	0.46	21 (6%) 21 20	24, 67, 105, 120	0
2	L	346/354 (97%)	0.42	35 (10%) 7 5	24, 69, 106, 121	0
2	N	345/354 (97%)	1.05	69 (20%) 1 0	28, 77, 111, 122	0
2	P	326/354 (92%)	0.72	54 (16%) 1 1	30, 74, 109, 119	0
All	All	5431/5624 (96%)	0.27	395 (7%) 15 13	11, 53, 103, 127	0

All (395) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	N	341	ALA	9.6
2	N	192	ILE	7.9
2	P	65	GLY	7.0
1	M	62	GLY	6.9
1	M	275	HIS	6.7

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Mol	Chain	Res	Type	RSRZ
1	M	282	GLY	6.6
2	F	193	GLN	6.5
2	N	126	TYR	6.2
1	M	61	GLU	6.2
1	M	277	GLY	6.1
2	P	64	ASN	6.0
2	J	66	LEU	5.8
2	H	350	VAL	5.8
1	M	278	LEU	5.8
2	H	340	THR	5.4
2	N	289	GLY	5.4
2	N	20	GLY	5.3
1	M	330	GLY	5.3
2	P	32	ILE	5.3
2	L	44	PHE	5.3
2	N	18	SER	5.2
1	M	25	GLY	5.2
1	M	93	LEU	5.2
2	N	333	ARG	5.2
2	H	91	PRO	5.1
2	L	193	GLN	5.1
1	M	338	PHE	4.9
2	L	346	PHE	4.9
2	F	289	GLY	4.9
1	M	280	ILE	4.9
2	N	193	GLN	4.8
2	F	338	ALA	4.8
2	P	31	GLY	4.8
2	H	64	ASN	4.7
1	M	63	VAL	4.7
2	H	18	SER	4.7
1	M	324	HIS	4.6
2	N	331	GLU	4.6
2	N	43	ILE	4.5
2	P	44	PHE	4.5
2	J	65	GLY	4.5
2	H	348	GLU	4.5
2	J	90	THR	4.4
2	N	330	PRO	4.4
2	P	97	ARG	4.4
1	M	81	TRP	4.4
2	P	353	ARG	4.4

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Mol	Chain	Res	Type	RSRZ
2	H	47	ALA	4.4
2	J	14	LYS	4.4
1	M	40	PHE	4.3
2	N	62	PHE	4.3
1	M	342	ILE	4.3
2	D	13	GLY	4.3
2	P	121	GLY	4.3
2	L	66	LEU	4.3
2	P	354	LEU	4.2
1	M	65	GLU	4.2
2	P	51	ILE	4.2
2	P	66	LEU	4.1
2	N	8	ILE	4.1
2	F	8	ILE	4.1
2	N	293	ALA	4.1
2	N	332	ASN	4.0
2	D	14	LYS	4.0
2	D	97	ARG	4.0
2	H	338	ALA	4.0
1	M	113	LEU	4.0
2	H	66	LEU	4.0
2	H	354	LEU	4.0
2	N	58	VAL	3.9
2	N	44	PHE	3.9
2	D	66	LEU	3.9
1	M	23	ILE	3.9
2	F	320	ASN	3.9
2	D	58	VAL	3.9
2	L	17	PRO	3.9
2	N	348	GLU	3.9
2	N	63	VAL	3.9
2	J	67	THR	3.9
2	L	58	VAL	3.8
2	N	292	LYS	3.8
2	F	62	PHE	3.8
2	L	96	HIS	3.8
2	P	73	ALA	3.8
2	P	192	ILE	3.8
2	P	23	THR	3.8
2	P	346	PHE	3.8
2	F	28	GLU	3.8
2	N	32	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
2	P	107	PHE	3.7
2	H	339	GLY	3.7
2	L	14	LYS	3.7
2	N	125	THR	3.7
2	F	310	GLY	3.7
2	N	122	PHE	3.7
2	B	14	LYS	3.7
2	F	331	GLU	3.7
2	P	340	THR	3.7
2	B	90	THR	3.6
2	L	59	SER	3.6
1	M	337	ASP	3.6
2	H	17	PRO	3.6
2	P	352	LYS	3.6
2	F	192	ILE	3.6
2	L	36	ILE	3.6
2	F	341	ALA	3.6
1	M	274	ARG	3.6
2	L	63	VAL	3.6
2	P	348	GLU	3.6
2	D	17	PRO	3.5
1	M	120	ILE	3.5
1	M	285	VAL	3.5
1	M	335	THR	3.5
2	P	62	PHE	3.5
2	B	66	LEU	3.5
2	P	63	VAL	3.5
1	M	310	ARG	3.5
2	P	122	PHE	3.4
2	D	193	GLN	3.4
2	L	69	ILE	3.4
2	L	16	ASN	3.4
1	O	323	LYS	3.4
2	N	124	THR	3.4
2	N	91	PRO	3.4
1	M	87	GLN	3.4
1	M	24	PRO	3.3
2	F	38	LYS	3.3
2	P	338	ALA	3.3
1	I	106	ASN	3.3
1	M	39	ILE	3.3
1	M	346	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
2	H	99	LEU	3.3
2	F	32	ILE	3.3
2	F	287	ILE	3.3
2	J	69	ILE	3.2
2	P	293	ALA	3.2
2	F	91	PRO	3.2
1	M	32	ILE	3.2
2	P	67	THR	3.2
2	B	352	LYS	3.2
2	F	337	LEU	3.2
1	A	57	THR	3.2
2	H	268	ALA	3.2
2	N	123	LYS	3.2
1	M	121	PRO	3.2
2	N	28	GLU	3.2
2	L	18	SER	3.2
2	N	191	THR	3.2
2	F	58	VAL	3.1
2	P	313	ASN	3.1
2	D	63	VAL	3.1
2	N	337	LEU	3.1
2	H	14	LYS	3.1
2	L	13	GLY	3.1
2	L	20	GLY	3.1
2	B	65	GLY	3.1
2	L	352	LYS	3.1
2	P	292	LYS	3.1
2	L	65	GLY	3.1
1	M	204	LYS	3.1
2	F	346	PHE	3.0
2	P	58	VAL	3.0
2	P	81	LEU	3.0
2	N	97	ARG	3.0
2	N	290	GLN	3.0
2	N	284	ALA	3.0
2	H	60	PRO	3.0
2	P	351	ILE	3.0
2	F	18	SER	3.0
2	H	63	VAL	3.0
2	N	288	ALA	3.0
2	N	205	LYS	3.0
2	J	97	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
2	F	61	ILE	2.9
1	M	116	VAL	2.9
2	P	350	VAL	2.9
1	G	13	LYS	2.9
2	P	60	PRO	2.9
2	D	69	ILE	2.9
1	M	349	MET	2.9
2	N	207	LEU	2.9
2	F	122	PHE	2.9
2	H	65	GLY	2.9
2	N	68	THR	2.9
2	P	40	VAL	2.9
1	M	316	HIS	2.9
2	L	64	ASN	2.9
2	F	65	GLY	2.9
2	P	69	ILE	2.9
2	F	123	LYS	2.9
2	F	17	PRO	2.9
2	N	285	PRO	2.9
2	P	72	PRO	2.9
2	N	334	THR	2.8
2	F	288	ALA	2.8
2	D	18	SER	2.8
1	M	45	ILE	2.8
1	M	343	ILE	2.8
2	F	35	GLU	2.8
2	P	99	LEU	2.8
2	F	12	THR	2.8
2	F	48	ASN	2.8
2	H	193	GLN	2.8
1	M	315	VAL	2.8
1	C	275	HIS	2.8
2	F	63	VAL	2.8
2	H	40	VAL	2.8
2	P	43	ILE	2.8
2	P	61	ILE	2.8
1	M	283	GLN	2.8
2	L	121	GLY	2.8
1	M	288	PRO	2.7
2	H	90	THR	2.7
2	H	69	ILE	2.7
2	J	267	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	M	79	GLY	2.7
1	M	22	LEU	2.7
1	M	319	ILE	2.7
2	P	36	ILE	2.7
2	F	44	PHE	2.7
2	F	20	GLY	2.7
2	L	61	ILE	2.7
2	B	193	GLN	2.7
1	M	52	ILE	2.7
2	N	340	THR	2.7
2	J	60	PRO	2.7
1	K	241	THR	2.7
1	E	277	GLY	2.6
2	N	338	ALA	2.6
1	I	107	VAL	2.6
1	E	274	ARG	2.6
2	P	339	GLY	2.6
1	I	260	ALA	2.6
2	H	113	VAL	2.6
2	P	331	GLU	2.6
2	J	323	LEU	2.6
1	C	56	GLN	2.6
2	N	61	ILE	2.6
2	J	279	ALA	2.6
1	I	129	ARG	2.6
1	M	80	LEU	2.6
2	H	42	LYS	2.6
2	L	289	GLY	2.6
2	F	207	LEU	2.6
1	M	209	ILE	2.6
1	I	261	ASN	2.6
1	M	339	THR	2.6
1	A	14	TYR	2.6
1	M	64	TYR	2.6
1	M	175	ARG	2.6
1	M	326	THR	2.5
1	M	290	ALA	2.5
1	M	230	PHE	2.5
1	O	117	LYS	2.5
2	B	62	PHE	2.5
1	C	57	THR	2.5
2	F	49	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	N	129	VAL	2.5
2	L	215	THR	2.5
2	N	182	PRO	2.5
2	P	57	ASP	2.5
2	F	10	ARG	2.5
1	G	323	LYS	2.5
1	M	279	ASP	2.5
2	H	333	ARG	2.5
2	N	69	ILE	2.5
2	N	272	HIS	2.5
2	J	52	GLU	2.5
2	F	332	ASN	2.5
2	N	128	ASN	2.5
1	O	56	GLN	2.5
1	M	36	VAL	2.5
2	L	62	PHE	2.5
2	N	320	ASN	2.5
2	J	91	PRO	2.5
2	H	97	ARG	2.5
2	N	37	SER	2.4
2	H	62	PHE	2.4
2	B	268	ALA	2.4
2	B	97	ARG	2.4
2	L	123	LYS	2.4
1	M	84	PRO	2.4
1	A	260	ALA	2.4
2	F	68	THR	2.4
2	J	84	LEU	2.4
2	J	297	ALA	2.4
2	L	326	ILE	2.4
2	N	55	SER	2.4
2	N	10	ARG	2.4
1	M	323	LYS	2.4
2	P	54	GLU	2.4
2	P	314	HIS	2.4
1	A	274	ARG	2.4
1	I	176	LYS	2.4
2	D	21	LYS	2.4
2	B	279	ALA	2.4
2	J	268	ALA	2.4
1	M	86	ASP	2.4
1	M	276	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	67	THR	2.4
2	L	120	GLU	2.4
1	M	334	SER	2.3
1	M	44	ASN	2.3
2	L	97	ARG	2.3
1	E	56	GLN	2.3
2	H	320	ASN	2.3
2	P	120	GLU	2.3
1	M	122	ASP	2.3
1	A	106	ASN	2.3
1	M	42	ALA	2.3
1	A	349	MET	2.3
2	H	267	SER	2.3
1	I	241	THR	2.3
1	A	268	VAL	2.3
2	D	44	PHE	2.3
2	J	320	ASN	2.3
2	N	38	LYS	2.3
2	N	211	TYR	2.3
1	I	240	GLY	2.3
2	H	289	GLY	2.3
1	I	273	SER	2.3
2	P	268	ALA	2.3
2	P	333	ARG	2.3
2	N	273	LYS	2.2
2	N	350	VAL	2.2
2	D	16	ASN	2.2
2	J	86	GLY	2.2
2	B	348	GLU	2.2
2	F	66	LEU	2.2
2	N	325	THR	2.2
1	M	331	GLY	2.2
2	H	112	ASN	2.2
2	N	17	PRO	2.2
2	N	26	PHE	2.2
1	E	280	ILE	2.2
2	D	60	PRO	2.2
2	N	246	TYR	2.2
2	L	267	SER	2.2
2	P	27	ILE	2.2
1	M	241	THR	2.2
2	H	346	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
1	I	127	VAL	2.1
1	I	280	ILE	2.1
2	F	43	ILE	2.1
1	I	294	SER	2.1
2	D	64	ASN	2.1
1	M	28	VAL	2.1
2	N	235	TYR	2.1
2	L	68	THR	2.1
2	N	53	TRP	2.1
2	P	332	ASN	2.1
2	N	49	VAL	2.1
1	A	272	GLY	2.1
2	F	97	ARG	2.1
2	P	89	ALA	2.1
2	L	23	THR	2.1
1	I	275	HIS	2.1
2	N	50	PRO	2.1
2	B	297	ALA	2.1
2	B	267	SER	2.1
2	N	29	GLY	2.1
1	A	275	HIS	2.1
1	M	307	TYR	2.1
2	F	51	ILE	2.1
2	N	317	GLN	2.1
2	B	320	ASN	2.1
2	N	346	PHE	2.1
1	A	259	GLY	2.1
2	H	52	GLU	2.1
2	L	28	GLU	2.1
2	B	60	PRO	2.1
1	A	108	ALA	2.1
1	A	261	ASN	2.1
2	H	19	THR	2.1
2	N	64	ASN	2.1
2	N	343	THR	2.1
2	P	88	LEU	2.1
2	J	318	ILE	2.1
2	P	193	GLN	2.1
2	N	131	LEU	2.0
2	L	60	PRO	2.0
2	D	19	THR	2.0
2	L	301	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	N	57	ASP	2.0
2	P	272	HIS	2.0
2	J	36	ILE	2.0
1	I	270	GLU	2.0
1	G	106	ASN	2.0
1	A	107	VAL	2.0
2	P	285	PRO	2.0
2	D	42	LYS	2.0
2	H	31	GLY	2.0
2	L	268	ALA	2.0
2	J	354	LEU	2.0
1	O	107	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.